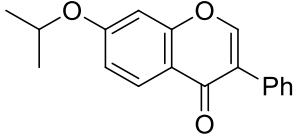
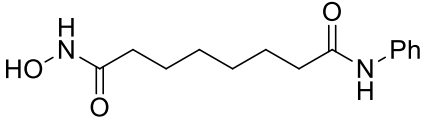
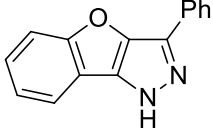
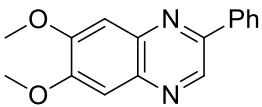
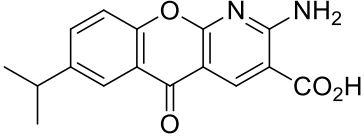
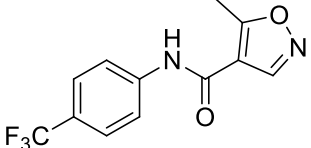
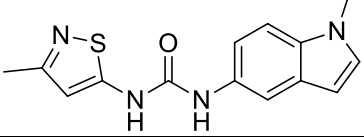
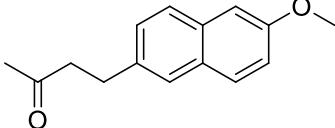
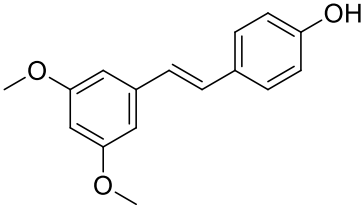
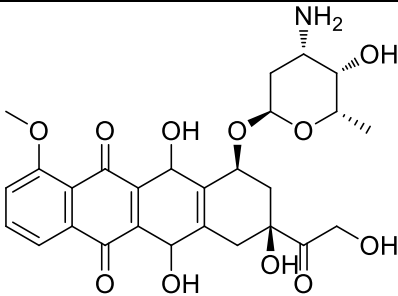
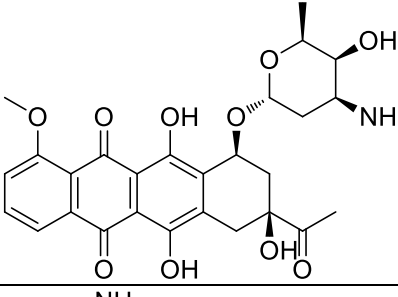
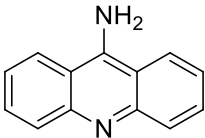
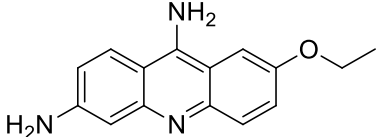
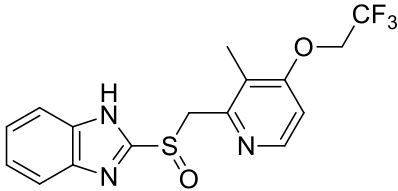
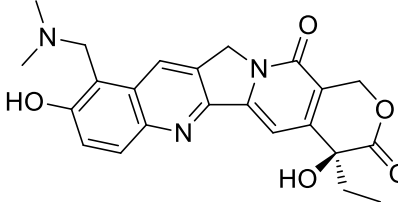
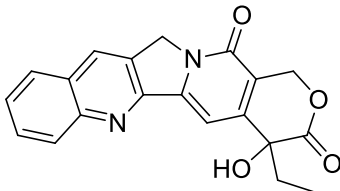
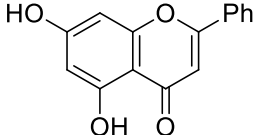


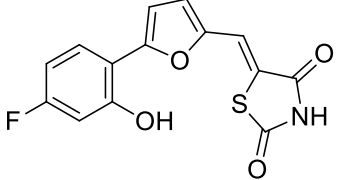
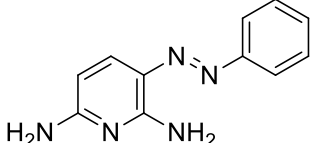
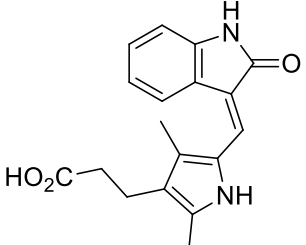
Supplementary Table 1. Complete Screening Data

Please see attached spreadsheet.

Supplementary Table 2. Sources of *Hepcidin* modulators identified in the screen that were characterized further in quantitative realtime RT-PCR and/or Western blot experiments.
Ph represents a Phenyl group.

Regulator Name	Structure	Functional Category	Vendor	Item #
Ipriflavone		Isoflavone	LKT Laboratories	I6068-1g
Vorinostat		Anti-neoplastic	Selleck Chemicals	S1047
GTP 14564		Kinase Inhibitor	R&D Systems	2086
AG-1296		Kinase Inhibitor	Cayman Chemical	10010592
Amlexanox		Anti-inflammatory	LKT laboratories	A4944-500mg
Leflunomide		Anti-inflammatory	Selleck Chemicals	S1247
SB 204741		Serotonin 5-HT2B receptor antagonist	Sigma-Aldrich	S0693-10MG
Nabumetone		Anti-inflammatory	Sigma-Aldrich	N6142-5G
Pterostilbene		Anti-oxidant	LKT laboratories	P7718-50mg

Regulator Name	Structure	Functional Category	Vendor	Item #
Doxorubicin		Anti-neoplastic	Selleck Chemicals	S1208
Daunorubicin		Anti-neoplastic	Selleck Chemicals	S3035
9-Aminoacridine		Anti-microbial	Sigma-Aldrich	92817-1G
Ethacridine Lactate		Anti-microbial	LKT Laboratories	E7228-25g
Lansoprazole		Proton pump inhibitor	Selleck Chemicals	S1354
Topotecan hydrochloride		Anti-neoplastic	Selleck Chemicals	S1231
Camptothecin		Anti-neoplastic	Selleck Chemicals	S1288
Chrysin		Anti-inflammatory, flavone	Selleck Chemicals	S2281

Regulator Name	Structure	Functional Category	Vendor	Item #
AS-252424		Kinase Inhibitor	Selleck Chemicals	S2671
Phenazopyridine hydrochloride		Analgesic	Sigma-Aldrich	34076-100MG
SU-6668		Kinase inhibitor	Selleck Chemicals	S1470

Supplementary Table 3. Primers and probes used in realtime quantitative RT-PCR assays

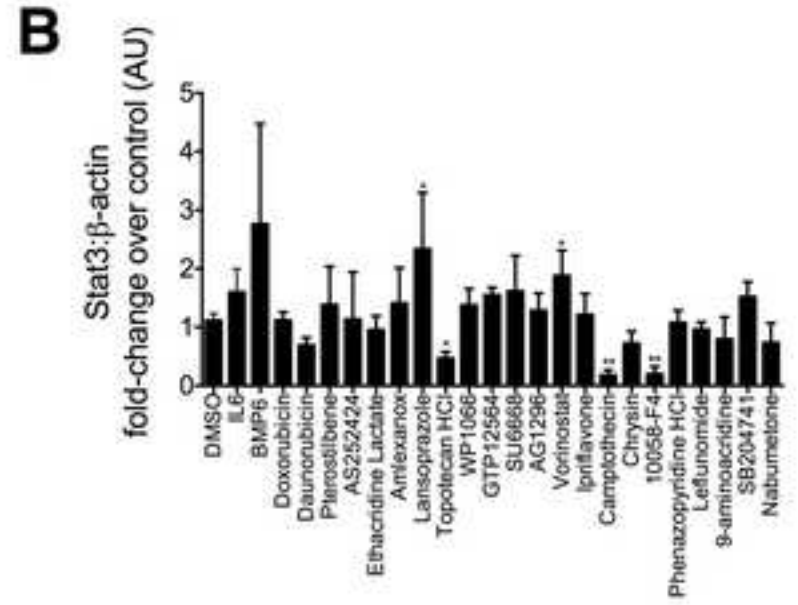
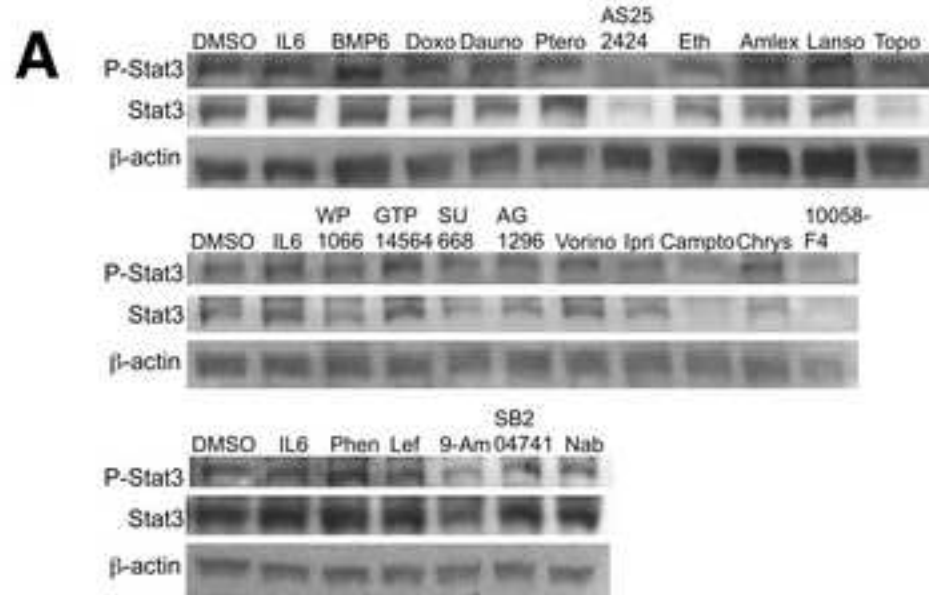
Primer Name	Species	Sequence	Citation or Manufacturer
Hepcidin	Human	5'-CCTGACCAGTGGCTCTGTTT-3'	[1]
		5'-CACATCCCACACTTTGATCG-3'	
G3PD	Human	5'-TGGTATCGTGGAAGGACTC- 3'	[1]
		5'-AGTAGAGGCAGGGATGATG-3'	
ID1	Human	5'-GTAAACGTGCTGCTCTACGACATGA-3'	[2]
		5'-AGCTCCAACCTGAAGGTCCCTGA-3'	
ID3	Human	5'-TCAGCTTAGCCAGGTGGAAATC-3'	[2]
		5'-GGCTGTCTGGATGGGAAGGT-3'	
SOCS3	Human	Taqman Assay Hs02330328_s1	Life Technologies
VEGFA	Human	Taqman Assay Hs00900055_m1	Life Technologies
IL-6 Receptor	Human	Taqman Assay Hs01075667_m1	Life Technologies
18S	Eukaryotic	Taqman Assay 4310893E	Life Technologies

REFERENCES

1. Nemeth, E., et al., *IL-6 mediates hypoferrremia of inflammation by inducing the synthesis of the iron regulatory hormone hepcidin*. J Clin Invest, 2004. 113(9): p. 1271-6.
2. Feng, X., et al., *Olf1/EBF associated zinc finger protein interfered with antinuclear antibody production in patients with systemic lupus erythematosus*. Arthritis Res Ther, 2010. 12(2): p. R59.

Supplementary Figure 1. Effect of treatment with Hepcidin stimulating agents for 24

hours on P-Stat3 and Stat3 protein levels. **A.** Following 16 hours of serum starvation in α -MEM/1%FBS, HepG2 cells were treated for 24 hours in α -MEM/1%FBS with the chemicals at the same concentrations as given in Figure 2. Protein was extracted from the cells, separated by SDS-PAGE, and blotted for incubation with antibodies against P-Stat3. Following immunoblotting, the membranes were stripped and re-probed with antibody against Stat3. The blots were then stripped again and probed for β -actin as a loading control. Each chemical was evaluated in three biological replicates. **B.** Protein levels were measured as fold-change over DMSO-treated control by densitometry analysis using Image Studio Lite Version 3.1.4 (LiCor Biosciences, Lincoln, NE). The global P-value generated using the Kruskal-Wallis test was <0.05 . Unpaired Student's t-tests were performed compared to DMSO alone. * denotes $0.009 \leq P < 0.05$, **denotes $0.0009 \leq P < 0.009$.



Primary Screen Data

Plate	Well	Type (X=experimental; N=negative control; P=positive control; E=empty)	CrosstalkCorr _Luminescen ce_A	Luminescence _A	z score Corrium_A	CrosstalkCorr _Luminescen ce_B	Luminescence _B	z score Corrium_B	Viability_A	z score Viability_A	Viability_B	z score Viability_B	Library Well Type	Reagent Vendi Vendor	Reagent ID	Compound Names (where available)	Screening	Screening
																	(HEPCIDIN STIMULATOR)	(HEPCIDIN REPRESSOR):
													Weak(W)=z score>3,<4;	Weak(W)=z score<-1,>- 2				
													Medium(M)=z-1.5;Medium(score≥4,<5	Medium(M)=z-score<- 1.5,>-2;				
													Strong(S)=z- score≥2					
1577 A01	X		1394	1400	0.08897685	1833	1840	0.36441631	1515909	-2.1184486	2016836	-2.24574297	experimental	ChemBridge	5100670			
1577 A02	X		990	1000	-0.51027577	1067	1080	-0.69873206	1781337	-1.26672044	2367279	-1.29969266	experimental	ChemBridge	5108100			
1577 A03	X		1190	1200	-0.21361606	1150	1160	-0.58353452	1708839	-1.49935825	2489407	-0.96999786	experimental	ChemBridge	5100219			
1577 A04	X		2150	2160	1.21035058	2028	2040	0.63506113	1882739	-0.941333	2442359	-1.09700789	experimental	ChemBridge	5108485			
1577 A05	X		906	920	-0.63487285	1426	1440	-0.20046801	1706025	-1.50838805	2390859	-1.23603647	experimental	ChemBridge	5100461			
1577 A06	X		1628	1640	0.43606872	1704	1720	0.18537435	1829724	-1.11145208	2260261	-1.58859674	experimental	ChemBridge	5109412			
1577 A07	X		985	1000	-0.51769227	1944	1960	0.51847567	1960387	-0.69216943	2617814	-0.62335238	experimental	ChemBridge	5100819			
1577 A08	X		2190	2200	1.26968252	2347	2360	1.0778083	2075985	-0.32122864	2486957	-0.97661184	experimental	ChemBridge	5110193			
1577 A09	X		1226	1240	-0.16021731	1506	1520	-0.08943423	1804012	-1.19395896	2388224	-1.24314987	experimental	ChemBridge	5101225			
1577 A10	X		1190	1200	-0.21361606	1108	1120	-0.64182726	2055314	-0.38755952	2656851	-0.51796872	experimental	ChemBridge	5116267			
1577 A11	X		1149	1160	-0.2744313	1149	1160	-0.58492245	1903662	-0.87419348	2486323	-0.97832338	experimental	ChemBridge	5101885			
1577 A12	X		1471	1480	0.20319084	1630	1640	0.08266811	1991492	-0.59235703	2383045	-1.25713101	experimental	ChemBridge	5116944			
1577 A13	X		987	1000	-0.51472567	1025	1040	-0.75702479	2146567	-0.09473906	2647536	-0.54311534	experimental	ChemBridge	5102245			
1577 A14	X		2071	2080	1.09316999	2309	2320	1.02506726	2012676	-0.52437999	2827214	-0.05805949	experimental	ChemBridge	5117544			
1577 A15	X		1188	1200	-0.21658256	1205	1200	-0.59495725	2077707	-0.31570289	2725417	-0.33286904	experimental	ChemBridge	5102391			
1577 A16	X		989	1000	-0.51175907	1269	1280	-0.41837179	2337561	0.51813899	3394762	1.47408402	experimental	ChemBridge	5118906			
1577 A17	X		1349	1360	0.02222842	1106	1120	-0.6446031	2154352	-0.06975788	2849688	0.00261096	experimental	ChemBridge	5103568			
1577 A18	X		1591	1600	0.38118667	1510	1520	-0.08388255	2056441	-0.3839431	2498498	-0.94545594	experimental	ChemBridge	5119052			
1577 A19	X		907	920	-0.63338956	1184	1200	-0.53634517	1954839	-0.70997233	2784287	-0.17394453	experimental	ChemBridge	5103898			
1577 A20	X		822	840	-0.75946993	1738	1760	0.23256371	1938048	-0.76385273	4081819	3.32885211	experimental	ChemBridge	5105989			
1577 A21	X		1832	1840	0.73866163	3507	3520	2.68773801	1478983	-2.23693992	1816816	-2.78571377	experimental	ChemBridge	5104182			
1577 A22	X		840	840	0.75205349	1284	1280	-0.58462947	2084602	-0.87959164	2423	-0.06474664	experimental	ChemBridge	5106696			
1577 A23	X		991	1000	-0.50879247	827	840	-1.03183338	1802423	-1.19905787	2087152	-2.05591902	empty					
1577 A24	P		1071	1080	-0.39012859	1752	1760	0.25199462	1649344	-1.69027091	2067410	-2.10921421	empty					
1577 B01	X		950	960	-0.56960772	1227	1240	-0.47666452	1981530	-0.62432395	2411002	-1.18165874	experimental	ChemBridge	5105849			
1577 B02	X		990	1000	-0.51027577	1588	1600	0.02437538	2115829	-0.19337379	2787117	-0.16630471	experimental	ChemBridge	5135339			
1577 B03	X		306	320	-1.524852	265	280	-1.81184564	2235527	0.19072343	2781048	-0.18268848	experimental	ChemBridge	5105276			
1577 B04	X		1225	1240	-0.16170061	1386	1400	-0.25984609	2091175	-0.27248566	2694236	-0.41704477	experimental	ChemBridge	5136288			
1577 B05	X		1104	1120	-0.34117974	1145	1160	-0.42670586	15094714	0.8105553	2887592	0.10431512	experimental	ChemBridge	5100310			
1577 B06	X		2306	2320	1.44174515	2145	2160	0.79744803	2084002	-0.78537465	2725080	-1.13285566	experimental	ChemBridge	5194288			
1577 B07	X		1384	1400	0.07414387	1303	1320	-0.37118243	2491169	0.10110443	2990914	0.38386242	experimental	ChemBridge	5176992			
1577 B08	X		1182	1200	-0.22548245	942	960	-0.87222233	2171497	-0.01474153	2752303	-0.26028802	experimental	ChemBridge	5195236			
1577 B09	X		1267	1280	-0.09402007	1225	1240	-0.47944036	2347619	0.55041387	2895244	0.12607914	experimental	ChemBridge	5181147			
1577 B10	X		1106	1120	-0.33821314	1428	1440	-0.19769216	2391434	0.69101112	3140201	0.78687521	experimental	ChemBridge	5209100			
1577 B11	X		1066	1080	-0.39754508	864	880	-0.98048026	2594704	1.34328143	3088610	0.64760079	experimental	ChemBridge	5182760			
1577 B12	X		1107	1120	-0.33672984	1164	1160	-0.59047414	2258983	0.26599106	2885189	-0.70338154	experimental	ChemBridge	5120550			
1577 B13	X		1067	1080	-0.39606178	1106	1120	-0.6446031	2259886	0.26920957	2823307	-1.08067409	experimental	ChemBridge	5186096			
1577 B14	X		1064	1080	-0.40051168	1622	1640	0.07156474	2312832	0.43878635	2739671	-0.29438917	experimental	ChemBridge	5211456			
1577 B15	X		1185	1200	-0.27017681	1621	1640	0.07017681	2490732	1.00964715	3022024	0.46784647	experimental	ChemBridge	5190278			
1577 B16	X		1067	1080	-0.39606178	1303	1320	-0.37118243	2242810	0.21409375	3042926	0.52427318	experimental	ChemBridge	5190737			
1577 B17	X		1307	1320	-0.04007012	2066	2080	0.68780218	2097408	-0.25248468	3045015	0.52991261	experimental	ChemBridge	5132935			
1577 B18	X		822	840	-0.75946993	1220	1240	-0.48637997	2268646	0.2699852	3011512	0.43946845	experimental	ChemBridge	5190950			
1577 B19	X		2182	2200	1.25781613	2142	2160	0.79328426	5520153	10.73077134	5648520	7.58829307	experimental	ChemBridge	5133814			
1577 B20	X		3347	3360	2.98585897	2783	2800	1.68294237	2052755	-0.39577106	2839980	-0.02359666	experimental	ChemBridge	5191765			
1577 B21	X		1138	1160	-0.29074758	1373	1400	-0.27407288	2104618	-0.22934861	2638055	-0.56749528	experimental	ChemBridge	5134609			
1577 B22	X		1588	1600	0.37673678	1585	1600	0.02021162	1947072	-0.73489574	2480015	-0.99535235	experimental	ChemBridge	5192966			
1577 B23	N		1341	1360	0.01036203	1183	1200	-0.53773309	1972739	-0.65253327	2645351	-0.54901393	empty					
1577 B24	P		1900	2200	0.83952593	1531	1760	-0.05473618	1888075	-0.92421038	2282717	-1.52797488	empty					
1577 C01	X		911	920	-0.62745636	1189	1200	-0.52940556	1723768	-1.45145279	2501070	-0.93851261	experimental	ChemBridge	5101672			
1577 C02	X		1306	1320	-0.04155342	1384	1400	-0.25876074	2055074	-0.38832965	2723251	-0.33871634	experimental	ChemBridge	5108110			
1577 C03	X		1225	1240	-0.16170061	1145	1160	-0.98048026	2297594	0.38989335	2835993	-0.03435984	experimental	ChemBridge	5100310			
1577 C04	X		1667	1680	0.49391736	1387	1400	-0.25459697	2421667	0.78802545	2995888	0.39729015	experimental	ChemBridge	5108495			
1577 C05	X		1026	1040	-0.45687702	1105	1120	-0.64599102	2102459	-0.23627659	2692257	-0.42238724	experimental	ChemBridge	5100462			
1577 C06	X		784	800	-0.81583528	1065	1080	-0.70150791	1970748	-0.65892212	2654196	-0.52513611	experimental	ChemBridge	5109431			
1577 C07	X		865	880	-0.6956881	939	960	-0.8763861	2214494	0.12323093	3044299	0.52797971	experimental	ChemBridge	5100832			
1577 C08	X		1469	1480	0.20022425	1348	1360	-0.30872594	2483036	0.98495156	2947177	0.26579071	experimental	ChemBridge	5110209			
1577 C09	X		986	1000	-0.51620897	1227	1240	-0.47666452	1988701	-0.60131303	2947070	0.26550185	experimental	ChemBridge	5101309			
1577 C10	X		1186	1200	-0.21964925	1105	1120	-0.75980164	2211140	0.11246303	2727371	-0.32705414	experimental	ChemBridge	5116331			
1577 C11	X		1369	1360	0.02222842	1868	1880	0.41299359	1988856	-0.60081562	2639307	-0.47759374	experimental	ChemBridge	5109107			
1577 C12	X		826	840	-0.75353674	1386	1400	-0.25598489	2039819	-0.43728121	3184067	0.90529517	experimental	ChemBridge	5117019	BETAMIPRON		
1577 C13	X		1348	1360	0.02074512	1026	1040	-0.75563687	2319587	0.46046238	2639154	-0.56574325	experimental	ChemBridge	5102267			
1577 C14	X		984	1000	-0.51917556	1221	1240	-0.48499205	2067597	-0.34814477	3289984	1.191227	experimental	ChemBridge	5117604			
1577 C15	X		1869	1880	0.79354368	2426	2440	1.18745416	2102978	-0.23461118	2898437	0.13421299	experimental	ChemBridge	5102412			
1577 C16	X		906	920	-0.63487285	822	840	-1.03877299	2195559	0.06247068	2903026	0.14660138	experimental	ChemBridge	5118936			
1577 C17	X		1027	1040	-0.45539373	1024	1040	-0.75841272	1966585	-0.67228075	2779010	-0.18819023	experimental	ChemBridge	5103812			
1577 C18	X		1049	1060	-0.45391043	1238	1240	-0.47526767	2181427	-0.01711217	2818374	-0.15365316	experimental	ChemBridge	5190834			
1577 C19	X		1066	1080	-0.39754508	825	840											

1577 D07	X	1629	1640	0.43755202	3349	3360	2.46850631	2161204	-0.04777059	2959030	0.29778888	experimental	ChemBridge	5177011
1577 D08	X	825	840	-0.75502004	1060	1080	-0.70844752	2328250	0.48826095	3073539	0.60691554	experimental	ChemBridge	5195246
1577 D09	X	869	880	-0.6897549	986	1000	-0.81115376	2567158	1.25488946	3157175	0.83415573	experimental	ChemBridge	5181421
1577 D10	X	1189	1200	-0.21509936	1269	1280	-0.41837179	2326199	0.48167953	2867556	0.29380969	experimental	ChemBridge	5209256
1577 D11	X	840	840	-0.7205344	904	920	-0.92496338	2241684	0.77255378	3178511	0.89031257	experimental	ChemBridge	5185003
1577 D12	X	1029	1040	-0.45242713	828	840	-1.03044546	2528844	1.13194421	2890504	0.11158237	experimental	ChemBridge	5210667
1577 D13	X	1223	1240	-0.1646672	983	1000	-0.81531753	2605669	1.37846686	2867079	0.04955943	experimental	ChemBridge	5186249
1577 D14	X	1108	1120	-0.33524654	1346	1360	-0.31150178	2305809	0.41625035	3112628	0.71243958	experimental	ChemBridge	5211581
1577 D15	X	706	720	-0.93153257	1061	1080	-0.7070596	2303904	0.41013742	2709693	-0.3753173	experimental	ChemBridge	5190474
1577 D16	X	903	920	-0.63932275	1304	1320	-0.36979451	2326367	0.48221862	2842897	-0.01572191	experimental	ChemBridge	5190759
1577 D17	X	1066	1080	-0.39754508	1226	1240	-0.47805244	2613066	1.40220299	3106421	0.69568327	experimental	ChemBridge	5133046
1577 D18	X	1146	1160	-0.2788912	1144	1160	-0.59186206	2254357	0.25114675	2856490	0.02205337	experimental	ChemBridge	5190983
1577 D19	X	1259	1280	-0.11126846	1137	1160	-0.60157751	2377131	0.6451145	2860924	0.03294349	experimental	ChemBridge	5133918
1577 D20	X	1748	1760	0.61406455	2426	2440	1.18745416	1980229	-0.62849871	2641969	-0.55814393	experimental	ChemBridge	5191816
1577 D21	X	827	840	-0.75205344	1581	1600	0.01465993	2116661	-0.190704	2531021	-0.85765737	experimental	ChemBridge	5134611
1577 D22	X	307	320	-1.5233687	304	320	-1.75771667	1149463	-3.29433199	1362626	-4.01183783	experimental	ChemBridge	5193093
1577 D23	N	1338	1600	0.00591213	1527	1880	-0.06028787	1931013	-0.78642724	2294361	-1.49654092	empty		
1577 D24	P	86135	86680	125.785182	116736	117280	159.840837	2055074	-0.38632965	2735220	-0.30640502	empty		
1577 E01	X	1073	1080	-0.38716199	1229	1240	-0.47388867	1826087	-1.1231228	2399273	-1.21322217	experimental	ChemBridge	5101720
1577 E02	X	628	640	-1.04722986	1064	1080	-0.70289583	2113864	-0.19967925	2955656	0.28868048	experimental	ChemBridge	5108143
1577 E03	X	708	720	-0.92856597	1024	1040	-0.75841272	2043476	-0.42554631	3093490	0.66077494	experimental	ChemBridge	5100324
1577 E04	X	829	840	-0.74908684	986	1000	-0.81115376	2189242	0.04220015	3131179	0.76251957	experimental	ChemBridge	5108055
1577 E05	X	1188	1200	-0.21658266	1427	1440	-0.19908009	2113114	-0.20208592	3268589	1.1334694	experimental	ChemBridge	5100475
1577 E06	X	1188	1200	-0.21658266	1025	1040	-0.75702479	2576964	1.28635593	3399253	1.48620785	experimental	ChemBridge	5109439
1577 E07	X	866	880	-0.6942048	861	880	-0.98464403	2269611	0.3000951	2956076	0.28981431	experimental	ChemBridge	5100963
1577 E08	X	1150	1160	-0.2729488	1144	1170	-0.43321519	2143240	0.82227388	2923251	0.75032644	experimental	ChemBridge	5110248
1577 E09	X	909	920	-0.63042296	1307	1320	-0.36563074	2239667	0.2040802	2838457	-0.02738806	experimental	ChemBridge	5101371
1577 E10	X	748	760	-0.86923403	985	1000	-0.81254168	1994078	-0.58405885	2704557	-0.38918236	experimental	ChemBridge	5116355
1577 E11	X	869	880	-0.6897549	1509	1520	-0.08527047	1978922	-0.63269273	3090300	0.65216327	experimental	ChemBridge	5102092
1577 E12	X	986	1000	-0.51620897	862	880	-0.98325611	2157105	-0.06092382	2856174	0.02012047	experimental	ChemBridge	5117202
1577 E13	X	2468	2480	1.68203952	2787	2800	1.68849406	2151677	-0.07834165	2777259	-0.19291721	experimental	ChemBridge	5102323
1577 E14	X	1105	1120	-0.33969644	1420	1440	-0.20879554	2455180	0.89556484	3125770	0.74791752	experimental	ChemBridge	5117742
1577 E15	X	983	1000	-0.52065886	1582	1600	0.01604785	2311659	0.43502233	2803733	-0.12444842	experimental	ChemBridge	5102419
1577 E16	X	2959	3000	0.17481276	1827	2000	2.45187149	2396401	0.70949785	2969488	0.90435293	experimental	ChemBridge	5119003
1577 E17	X	1539	1560	0.30405515	1260	1280	-0.43086309	2184751	0.02778904	2979663	0.3534894	experimental	ChemBridge	5103831
1577 E18	X	1460	1480	0.18687456	1779	1800	0.28946852	2310822	0.43233649	3614329	2.06682358	experimental	ChemBridge	5119134
1577 E19	X	3226	3240	2.80637985	3583	3600	2.7932801	2503958	1.05208787	2803514	-0.12203963	experimental	ChemBridge	5104026
1577 E20	X	1536	1560	0.29960525	2690	1720	0.16594344	2454110	0.89213133	3209768	0.97467717	experimental	ChemBridge	5106406
1577 E21	X	1667	1680	0.49391736	1303	2320	1.01673973	1944486	-0.74319392	3172608	0.87436063	experimental	ChemBridge	5104261
1577 E22	X	1266	1280	-0.10088537	1102	1120	-0.65015479	2282031	0.33994946	2763517	-0.23001489	experimental	ChemBridge	5106991
1577 E23	X	1800	1800	0.30100858	1527	1580	0.57674578	2144969	-0.09985866	2830205	-0.79048252	empty		
1577 E24	P	85061	85600	124.192119	109314	109920	149.539678	2221029	0.144200	2846811	-0.00515574	empty		
1577 F01	X	873	880	-0.68382171	1310	1320	-0.36146698	1965232	-0.67662238	2751524	-0.262391	experimental	ChemBridge	5107341
1577 F02	X	669	680	-0.98641462	1305	1320	-0.36840659	1998209	-0.57080295	2799423	-0.13308363	experimental	ChemBridge	5135549
1577 F03	X	950	960	-0.56960772	1266	1280	-0.42253555	2338867	0.5223297	2934564	0.23174086	experimental	ChemBridge	5105502
1577 F04	X	789	800	-0.80841879	1027	1040	-0.75424895	2136442	-0.12722903	2992645	0.3885354	experimental	ChemBridge	5136871
1577 F05	X	1149	1160	-0.2744313	945	960	-0.86805857	2267206	0.29237773	3349643	1.35228419	experimental	ChemBridge	5107707
1577 F06	X	907	920	-0.63338956	1827	1840	-0.35608978	2312010	0.43614865	3236514	0.20226144	experimental	ChemBridge	5134764
1577 F07	X	870	880	-0.68827216	1065	1080	-0.70150791	1984736	-0.61403627	2306744	-1.46311197	experimental	ChemBridge	5107002
1577 F08	X	784	800	-0.81583528	1223	1240	-0.48221621	2387321	0.67781305	3219327	1.0004825	experimental	ChemBridge	5197007
1577 F09	X	1067	1080	-0.39606178	1185	1200	-0.53495725	2328167	0.48799462	3304180	1.2295503	experimental	ChemBridge	5181551
1577 F10	X	1070	1080	-0.39161189	1069	1080	-0.69595622	2348716	0.55393401	2882671	0.09165134	experimental	ChemBridge	5210096
1577 F11	X	1029	1040	-0.45242713	906	920	-0.92218753	2463713	0.92294626	3166015	0.85656227	experimental	ChemBridge	5185231
1577 F12	X	589	600	-1.1050785	1108	1120	-0.64182726	2454435	0.89317422	2898917	0.13550879	experimental	ChemBridge	5210670
1577 F13	X	823	840	-0.75798664	1058	1080	-0.71122336	2590486	1.32974635	3423347	1.55125163	experimental	ChemBridge	5186661
1577 F14	X	669	680	-0.98641462	1226	1240	-0.47805244	2225986	0.16010745	3183681	0.90425313	experimental	ChemBridge	5211664
1577 F15	X	1060	1080	-0.40644487	1213	1240	-0.49609543	2422061	0.78928975	3586258	1.99104356	experimental	ChemBridge	5190510
1577 F16	X	1019	1040	-0.46726011	1180	1200	-0.54189686	2516298	1.09168552	2798630	-0.1352244	experimental	ChemBridge	5190772
1577 F17	X	1586	1600	0.37377018	1463	1480	-0.14911489	2303752	0.40964967	2563765	-0.76926219	experimental	ChemBridge	5133575
1577 F18	X	986	1000	-0.51620897	1142	1160	-0.5946379	2887237	2.28198644	3013077	0.4436933	experimental	ChemBridge	5191043
1577 F19	X	660	680	-0.9997643	1296	1320	-0.38089789	2174825	-0.00462336	2886303	0.10145623	experimental	ChemBridge	5134027
1577 F20	X	1468	1480	0.19874095	1863	1880	0.40605398	2285295	0.35042326	2464874	-1.03622675	experimental	ChemBridge	5191835
1577 F21	X	905	920	-0.63635615	1496	1520	-0.10331346	2179949	0.01237997	2823135	0.20008731	experimental	ChemBridge	5135063
1577 F22	X	1024	1040	-0.45984362	1262	1280	-0.42808724	2275360	0.31854298	2482980	-0.98734809	experimental	ChemBridge	5193130
1577 F23	N	1941	2240	0.90034117	2042	2320	0.65449204	2191975	0.05097003	2716592	-0.35669287	empty		
1577 F24	P	97239	97840	142.255729	89083	89760	121.460625	1990943	-0.59411871	2408718	-1.18782459	empty		
1577 G01	X	750	760	-0.86626743	1029	1040	-0.75147311	1875725	-0.96384012	2553175	-0.79785079	experimental	ChemBridge	5101739
1577 G02	X	1347	1360	0.01926182	1425	1440	-0.20185593	1903647	-0.87424161	2931070	0.22230851	experimental	ChemBridge	5108151
1577 G03	X	1186	1200	-0.21954925	1303	1320	-0.37118243	2067760	-0.34762173	3014008	0.44620661	experimental	ChemBridge	5100336
1577 G04	X	908	920	-0.63190626	1276	1280	-0.42114783	2145314	0.89598483	3434928	1.55551967	experimental	ChemBridge	5108661
1577 G05	X	906	920	-0.63487285	864	880	-0.9804802	2104374	-0.23013185	2795167	-0.30307305	experimental	ChemBridge	5100517
1577 G06	X	1140	1160	-0.28778099	1381	1400	-0.2629245	2223921	0.1534811	2776272	-0.19558169	experimental	ChemBridge	5109527
1577 G07	X	943	960	-0.57999081	1061	1080	-0.7070596	2260424	0.27061506	2932043	0.22493521	experimental	ChemBridge	5101006
1577 G08	X	2267	2280	1.38389651	2466	2480	1.24297104	2116602	-0.19089332	2998297	0.40379344	experimental	ChemBridge	5110269
1577 G09	X	1545	1560	0.31295494	1663	1680	0.12846955	2140719	-0.11350462	2729488	-0.32187903	experimental	ChemBridge	510

1577 H01	X	1070	1080	-0.39161189	988	1000	-0.80837791	2045936	-0.41765245	3035905	0.5053194	experimental	ChemBridge	5107345
1577 H02	X	1905	1920	0.84694242	1422	1440	-0.2060197	2164242	-0.038022	2630914	-0.58798783	experimental	ChemBridge	5135609
1577 H03	X	1421	1440	0.12902591	1942	1960	0.51569983	2120244	-0.17920656	2876337	0.07455218	experimental	ChemBridge	5105531
1577 H04	X	1065	1080	-0.39902838	1261	1280	-0.42947515	2372768	0.6311414	2839112	-0.02583984	experimental	ChemBridge	5136684
1498	X	1498	1520	2433999	2023	2040	0.62812152	2334068	0.506893025	3358971	1.3774767	experimental	ChemBridge	5107840
1577 H06	X	4105	4120	4.11019929	2581	2600	1.40258209	2323687	0.47361881	3127030	0.75131899	experimental	ChemBridge	5194880
1577 H07	X	1419	1440	0.12605932	1742	1760	0.2381154	2476571	0.96420612	2811763	-0.09977076	experimental	ChemBridge	5180197
1577 H08	X	1182	1200	-0.22548245	981	1000	-0.81809337	2054268	-0.39091601	2776644	-0.19457745	experimental	ChemBridge	5202053
1577 H09	X	1060	1080	-0.40644487	1498	1520	-0.10053761	2527314	1.12703461	2814011	-0.09370209	experimental	ChemBridge	5181553
1577 H10	X	2949	2960	2.39550614	3347	3360	2.46573047	2372136	0.62908612	3208368	0.97089776	experimental	ChemBridge	5210416
1577 H11	X	1021	1040	-0.46429352	1060	1080	-0.70844752	2368518	0.61747637	2966050	0.30216221	experimental	ChemBridge	5185233
1577 H12	X	1028	1040	-0.45391043	825	840	-1.03746922	2634507	1.47100471	2717833	0.02046331	experimental	ChemBridge	5210672
1577 H13	X	944	960	-0.57850751	1383	1400	-0.26014866	2198888	0.07315306	2952410	0.27991763	experimental	ChemBridge	5187115
1577 H14	X	707	720	-0.93004927	1186	1200	-0.53356933	2365045	0.60633191	3197503	0.94156678	experimental	ChemBridge	5211741
1577 H15	X	1617	1640	0.41975243	1167	1200	-0.55993985	2415624	0.76863415	3214812	0.98829388	experimental	ChemBridge	5190624
1577 H16	X	1059	1080	-0.40792817	1742	1760	0.2381154	2301855	0.40356241	3012820	0.44299995	experimental	ChemBridge	5190804
1577 H17	X	2461	2480	1.67165643	1890	1920	0.44352788	2206643	0.09803797	2761518	-0.23541136	experimental	ChemBridge	5133580
1577 H18	X	3103	3120	2.62393412	4063	4080	3.45948274	2113683	-0.20026006	2500383	-0.94036723	experimental	ChemBridge	5191309
1577 H19	X	783	800	-0.81731858	1056	1080	-0.71399921	2237367	0.19662778	2717833	-0.35334268	experimental	ChemBridge	5134037
1577 H20	X	827	840	-0.75205344	1144	1160	-0.59186206	2140731	-0.11346611	2975010	0.34092823	experimental	ChemBridge	5192437
1577 H21	X	1611	1640	0.41085264	1885	1920	0.43658827	2226818	0.16277724	2660695	-0.50759152	experimental	ChemBridge	5132526
1577 H22	X	4501	4520	4.69758553	3899	3920	3.2318635	2139874	-0.11621613	2737359	-0.30063061	W experimental	ChemBridge	5193138
1577 H23	N	1910	2240	0.85435892	1965	2400	0.54762204	2207611	0.10114417	2603336	-0.66243695	empty		
1577 H24	P	104038	104760	152.340676	141192	141800	193.783861	2257084	0.25989782	2842603	-0.01651559	empty		
1577 I01	X	706	720	-0.93153257	1503	1520	-0.093598	2069680	-0.34345017	2585210	-0.71136961	experimental	ChemBridge	5101879
1577 I02	X	1160	1160	-0.28778099	1779	1790	0.28945852	1869437	-0.984306	2433113	-1.12115937	experimental	ChemBridge	5138141
1577 I03	X	2225	2240	3.215197	2022	2040	0.6267336	2388359	0.08114388	3192194	0.8737413	experimental	ChemBridge	5100356
1577 I04	X	1424	1440	0.13347581	1424	1440	-0.20324385	2800378	2.00326582	3369168	1.40499086	experimental	ChemBridge	5108683
1577 I05	X	1345	1360	0.01629522	1061	1080	-0.7070596	2551110	1.20339326	3002424	0.41493463	experimental	ChemBridge	5100552
1577 I06	X	1055	1080	-0.41386137	1459	1480	-0.15466658	2524887	1.11924665	3431871	1.57426288	experimental	ChemBridge	5109754
1577 I07	X	1106	1120	-0.33821314	1505	1520	-0.09082216	2442477	0.85480236	3345155	1.34016575	experimental	ChemBridge	5101009
1577 I08	X	1307	1320	-0.04007012	826	840	-1.0332211	2697584	1.67341161	3357674	1.37396185	experimental	ChemBridge	5110420
1577 I09	X	1147	1160	-0.2773979	1547	1560	-0.03252943	2488423	1.00223783	3203422	0.47701966	experimental	ChemBridge	5101647
1577 I10	X	855	880	-0.71052178	1013	1040	-0.8916798	2795463	0.987651	2795463	1.07981929	experimental	ChemBridge	5116167
1577 I11	X	1428	1440	0.139409	1784	1800	0.29640813	2402464	0.72640521	1951046	-2.42334861	experimental	ChemBridge	5102143
1577 I12	X	1026	1040	-0.45687702	1465	1480	-0.14633904	2153608	-0.07214529	3094243	0.66280773	experimental	ChemBridge	5117238
1577 I13	X	1588	1600	0.37673678	1503	1520	-0.093598	2292463	0.37342456	2869457	0.05597904	experimental	ChemBridge	5102355
1577 I14	X	1144	1160	-0.28184779	1098	1120	-0.65570648	2443742	0.8588616	3081294	0.62785082	experimental	ChemBridge	5118551
1577 I15	X	1863	1880	0.78464388	3104	3120	2.12846538	2390142	0.68686532	3233558	1.03890028	experimental	ChemBridge	5102527
1577 I16	X	1660	1680	0.48353427	1411	1440	-0.22128684	2234149	0.18630159	3152300	0.81953748	experimental	ChemBridge	5119129
1577 I17	X	1480	1480	0.06821067	1312	1320	0.15315313	2297371	1.35183953	3433154	-0.50129126	experimental	ChemBridge	5103843
1577 I18	X	1459	1480	0.18539126	1131	1160	-0.60990505	2629535	4.5505013	3432336	1.57551819	experimental	ChemBridge	5119195
1577 I19	X	867	880	-0.6927215	1426	1440	-0.20046801	2384466	0.66865168	2844727	-0.01078167	experimental	ChemBridge	5104092
1577 I20	X	1141	1160	-0.28629769	1457	1480	-0.15744242	2170020	-0.01948106	2472406	-1.01589349	experimental	ChemBridge	5106496
1577 I21	X	3542	3560	3.2751022	4180	4200	3.62186963	1859302	-1.01653966	2502143	-0.93561596	experimental	ChemBridge	5104603
1577 I22	X	1361	1400	0.0400028	1723	1760	0.21174487	1963672	-0.68162824	2281095	-1.5323536	experimental	ChemBridge	5107328
1577 I23	N	1934	2320	0.88995808	1772	2040	2.97575306	2100533	-0.24245691	2630203	-0.58990723	empty		
1577 I24	P	126729	127360	185.992604	85373	86080	116.311434	2278411	0.32833329	2929656	1.70219199	empty		
1577 J01	X	2548	2560	8.00703441	2945	2960	9.0778576	2057796	-0.370950176	2701304	-0.79764411	experimental	ChemBridge	5107372
1577 J02	X	1985	2000	0.96560631	2301	2320	0.10196388	1954450	-0.71122058	2512550	-0.90752139	experimental	ChemBridge	5135615
1577 J03	X	1063	1080	-0.40199498	1100	1120	-0.65293063	2413356	0.7613564	3153910	0.82388381	experimental	ChemBridge	5105734
1577 J04	X	783	800	-0.81731858	1261	1280	-0.42947516	2796471	1.9907287	3277821	1.15839196	experimental	ChemBridge	5136983
1577 J05	X	1226	1240	-0.16021731	1744	1760	0.24089124	2476953	0.96543191	3048049	0.53810315	experimental	ChemBridge	5108050
1577 J06	X	1987	2000	0.96857291	1904	1920	0.46295879	2178990	0.09030265	2767161	-0.2201776	experimental	ChemBridge	5195052
1577 J07	X	946	960	-0.57554091	1102	1120	-0.65015479	2317927	0.45513563	2947106	0.26559904	experimental	ChemBridge	5180306
1577 J08	X	908	920	-0.63190626	822	840	-1.03877299	2122906	-0.17066451	2374540	-1.27982102	experimental	ChemBridge	5202180
1577 J09	X	1062	1080	-0.40347828	1061	1080	-0.7070596	2860143	2.19504489	2953277	0.28225817	experimental	ChemBridge	5181956
1577 J10	X	3107	3120	2.62986731	2744	2760	1.6288134	2420056	0.78285593	3312766	1.25272893	experimental	ChemBridge	5120498
1577 J11	X	1100	1120	-0.34711293	1779	1800	0.28946852	2480514	0.97685875	3363109	1.38863408	experimental	ChemBridge	5185406
1577 J12	X	908	920	-0.63190626	1021	1040	-0.76257648	2482547	0.98338242	3229500	1.02794537	experimental	ChemBridge	5210947
1577 J13	X	986	1000	-0.51620897	1743	1760	0.23950332	2257847	0.26234576	3491850	1.73618123	experimental	ChemBridge	5187361
1577 J14	X	1184	1200	-0.22251585	1616	1640	0.0632372	2519042	1.10049071	3334289	1.31083207	experimental	ChemBridge	5211742
1577 J15	X	1381	1400	0.06969397	1854	1880	0.39356268	2377302	0.64566322	3166195	0.8570482	experimental	ChemBridge	5190641
1577 J16	X	2424	2440	1.61677439	2780	2800	1.6787786	2016330	-0.51265473	3428019	1.56386408	experimental	ChemBridge	5190682
1577 J17	X	1381	1400	0.06969397	1615	1640	0.06184928	2213565	0.12024988	2950728	0.27537693	experimental	ChemBridge	5133753
1577 J18	X	1786	1800	0.67042989	2104	2120	0.74054322	2165051	-0.03542601	2903401	0.14761372	experimental	ChemBridge	5191454
1577 J19	X	865	880	-0.6956881	1063	1080	-0.70428375	2092737	-0.26747338	2860638	0.03217141	experimental	ChemBridge	5134150
1577 J20	X	1225	1240	-0.16170061	982	1000	-0.81670545	2235090	0.18932115	2695392	-0.41392405	experimental	ChemBridge	5192544
1577 J21	X	1973	2000	0.94780673	1772	1800	0.27975306	2176931	0.00269555	2730970	-0.31787825	experimental	ChemBridge	5135290
1577 J22	X	3240	3260	2.79748005	2576	2600	1.39562248	2168813	0.02335418	3622746	-0.5965191	experimental	ChemBridge	5193139
1577 J23	N	1976	2320	0.95225662	2126	2440	0.7710775	2285573	0.48387955	2936669	0.01335801	empty		
1577 J24	P	110346	111000	161.697323	99466	100280	135.871421	2248916	0.2336872	2727173	-0.32812857	empty		
1577 K01	X	1307	1320	-0.04007012	1185	1200	-0.53495725	2202074	-0.49807355	2707359	-0.38161813	experimental	ChemBridge	5101886
1577 K02	X	425	440	-1.34833947	502	520	-1.48290809	1800817	-1.20421135	2456256	-1.05949177	experimental	ChemBridge	5108194
1577 K03	X	907	920	-0.63338956	1266	1280	-0.42253555	2202562	0.08494251	29587				

1577 K19	X	1184	1200	-0.22251585	1138	1160	-0.60018959	2326570	0.48287003	3143659	0.79621037	experimental	ChemBridge	5104126
1577 K20	X	1106	1120	-0.33821314	1784	1800	0.29640813	2667331	1.57633318	2981495	0.35843503	experimental	ChemBridge	5106567
1577 K21	X	1418	1440	0.12457602	1689	1720	0.16455552	2505024	1.05550855	2699435	-0.40300963	experimental	ChemBridge	5104902
1577 K22	X	1250	1280	-0.11423505	2093	2120	0.72527608	2448678	0.87470066	2830351	-0.22036275	experimental	ChemBridge	5107330
1577 K23	N	1824	2120	0.02679524	2943	3520	1.90500991	2014091	-0.5198394	emty				
1577 K24	P	95536	96240	139.729672	192047	192560	264.366643	2365846	0.60890223	3283586	1.17395507	empty		
1577 L01	X	1470	1480	0.20170754	1709	1720	0.19231396	1735432	-1.41402435	2312822	-1.4467039	experimental	ChemBridge	5107442
1577 L02	X	789	800	-0.80841879	1507	1520	-0.08804631	1940282	-0.75668409	2707701	-0.38069487	experimental	ChemBridge	5135916
1577 L03	X	789	800	-0.80841879	903	920	-0.9263513	2085453	-0.29084691	2298663	-1.48492731	experimental	ChemBridge	5105867
1577 L04	X	1065	1080	-0.39902838	1504	1520	-0.09221008	2084160	-0.294996	2953791	0.28364576	experimental	ChemBridge	5137141
1577 L05	X	669	680	-0.98641462	1026	1040	-0.75656887	2334489	0.50828119	2944286	0.25798621	experimental	ChemBridge	5108057
1577 L06	X	1109	1120	-0.33736324	946	960	-0.86667065	2129303	-0.15013726	3019115	0.43823474	experimental	ChemBridge	5195108
1577 L07	X	907	920	-0.63389556	1185	1200	-0.53495725	2386271	0.67444372	2757181	-0.24711945	experimental	ChemBridge	5180456
1577 L08	X	1229	1240	-0.15576741	1622	1640	0.07156474	2303435	0.40863245	3231003	1.03200284	experimental	ChemBridge	5205154
1577 L09	X	783	800	-0.81731858	1057	1080	-0.71261129	2248575	0.23259297	3001280	0.4118463	experimental	ChemBridge	5181966
1577 L10	X	1301	1320	-0.04896992	1939	1960	0.51153606	2253649	0.24887486	3034442	0.50136991	experimental	ChemBridge	5210529
1577 L11	X	3507	3520	3.22318675	3583	3600	2.7932801	2193913	0.05718885	3007578	0.42884828	experimental	ChemBridge	5185407
1577 L12	X	782	800	-0.81880188	1300	1320	-0.3753462	2163532	-0.04030031	2915746	0.18094009	experimental	ChemBridge	5211063
1577 L13	X	908	920	-0.63190626	904	920	-0.92496338	2422610	0.79426031	3349715	1.35247586	experimental	ChemBridge	5189175
1577 L14	X	787	800	-0.81138538	1179	1200	-0.54328478	2383086	0.66422342	3110697	0.70722669	experimental	ChemBridge	5211778
1577 L15	X	1148	1160	-0.2759146	1784	1800	0.29640813	2422695	0.79132418	2801149	-0.12842414	experimental	ChemBridge	5190648
1577 L16	X	1147	1160	-0.2773979	1181	1200	-0.54050894	2218465	0.13597342	2858235	0.02568431	experimental	ChemBridge	5190888
1577 L17	X	983	1000	-0.52065886	1020	1040	-0.76396441	2513113	1.08146522	2851911	0.00861214	experimental	ChemBridge	5193757
1577 L18	X	1583	1600	0.36932028	1778	1800	0.28808059	2160923	-0.04867229	2792166	-0.15267451	experimental	ChemBridge	5191582
1577 L19	X	2225	2240	1.32159797	2943	2960	1.90500991	2228572	0.16840563	2876461	0.07488693	experimental	ChemBridge	5134249
1577 L20	X	908	960	-0.2874073	1164	1180	-0.10765071	2086275	-0.28881092	2838195	-0.40320368	experimental	ChemBridge	5192683
1577 L21	X	3104	3120	2.62541747	4940	4960	4.67669047	2220716	0.09589662	2813318	-0.09557291	experimental	ChemBridge	5135308
1577 L22	X	1017	1040	-0.47022671	1410	1440	-0.22267476	2135946	-0.12882063	2964189	0.31171603	experimental	ChemBridge	5193159
1577 L23	N	2007	2400	0.99823888	1926	2160	0.49349307	2036225	-0.44881394	2733853	-0.31009535	empty		
1577 L24	P	129554	130080	190.188523	72476	73360	98.4114016	1712555	-0.01134653	2623918	-0.60687412	empty		
1577 M01	X	1266	1280	-0.10088537	977	1000	-0.82364506	1757048	-1.28690113	2463183	-1.04079175	experimental	ChemBridge	5103518
1577 M02	X	1028	1040	-0.45391043	1465	1480	-0.14633904	2090276	-0.27537045	2640277	-0.56271162	experimental	ChemBridge	5108251
1577 M03	X	1148	1160	-0.2759146	1466	1480	-0.14495112	2096002	-0.25699637	2671603	-0.47614445	experimental	ChemBridge	5100429
1577 M04	X	1464	1480	-0.19429105	1261	1280	-0.19429105	2299832	0.07947024	2832912	0.00949494	experimental	ChemBridge	5105974
1577 M05	X	1026	1040	-0.45687702	983	1000	-0.81531753	2024417	-0.48670447	2757137	-0.24723823	experimental	ChemBridge	5100597
1577 M06	X	788	800	-0.80990209	1349	1360	-0.30733801	2100859	-0.24141081	2831938	-0.04530665	experimental	ChemBridge	5110005
1577 M07	X	1189	1200	-0.21509936	745	760	-1.145643	2206349	0.09709456	2659331	-0.41246897	experimental	ChemBridge	5101117
1577 M08	X	1223	1240	-0.1646672	1021	1040	-0.76257648	2369521	0.62069488	3003637	0.41820922	experimental	ChemBridge	5110579
1577 M09	X	2549	2560	1.80218671	2867	2880	1.79952783	2038030	-0.4430219	2849864	0.00308609	experimental	ChemBridge	5101816
1577 M10	X	984	1000	-0.51917556	1260	1280	-0.43086309	2026182	-0.48104078	2914739	0.1782216	experimental	ChemBridge	5116891
1577 M11	X	850	860	-0.30134569	1197	1200	-0.69467885	1961037	-0.69008365	2802021	0.44403943	experimental	ChemBridge	5102151
1577 M12	X	901	920	-0.6428935	1057	1080	-0.71261129	2498837	-0.72932306	2867789	0.05147613	experimental	ChemBridge	5117427
1577 M13	X	1426	1440	0.13644241	1102	1120	-0.65015479	2222747	0.14971387	2740082	-0.29327964	experimental	ChemBridge	5102369
1577 M14	X	627	640	-1.04871316	1145	1160	-0.59047414	1997590	-0.57278925	3200599	0.94992469	experimental	ChemBridge	5118682
1577 M15	X	1267	1280	-0.0940207	1502	1520	-0.09498592	2169185	-0.02216048	3179913	0.89408109	experimental	ChemBridge	5102990
1577 M16	X	1464	1480	0.19280775	1741	1760	0.23672747	2310403	0.43099197	2723470	-0.33812513	experimental	ChemBridge	5119047
1577 M17	X	2066	2080	1.0857535	2742	2760	1.62603756	2260868	0.27203981	2558647	-0.78307866	experimental	ChemBridge	5103859
1577 M18	X	1464	1480	0.18835786	1939	1960	0.51152606	2433748	0.628792	2833147	-0.04320368	experimental	ChemBridge	5119227
1577 M19	X	1400	1400	0.07414387	1379	1360	-0.146239	-0.09589045		1384719	0.40080077	experimental	ChemBridge	5104894
1577 M20	X	984	1000	-0.51917556	1422	1440	-0.2060197	2286784	0.35520129	3286863	1.1828016	experimental	ChemBridge	5106594
1577 M21	X	2143	2160	1.1996749	1936	1960	0.5073723	2118615	-0.18443383	2596916	-0.67976828	experimental	ChemBridge	5105095
1577 M22	X	981	1000	-0.52362546	1259	1280	-0.43225101	2339685	0.52495456	2870207	0.05800373	experimental	ChemBridge	5105769
1577 M23	N	2103	2360	1.14063554	2223	2560	0.90570596	1829478	-1.11224147	2784234	-0.17408761	empty		
1577 M24	P	82366	83040	120.194629	110073	110640	150.593111	2070973	-0.33731153	2776870	-0.19396734	empty		
1577 N01	X	2429	2440	1.62419088	4669	4680	4.30056357	1768115	-1.30914833	2864436	0.04242443	experimental	ChemBridge	5107549
1577 N02	X	1024	1040	-0.45984362	1174	1200	-0.55022439	1872507	-0.97416632	2632019	-0.58500479	experimental	ChemBridge	5136037
1577 N03	X	744	760	-0.87516722	1182	1200	-0.53912102	2232920	0.18235786	3114770	0.71822209	experimental	ChemBridge	5105919
1577 N04	X	1865	1880	0.78761048	2543	2560	1.34984105	1871509	-0.97736879	2668486	-0.48655906	experimental	ChemBridge	5137235
1577 N05	X	1864	1880	0.78612718	2183	2200	0.85018907	2742662	1.81067177	3130182	0.75982808	experimental	ChemBridge	5108063
1577 N06	X	866	880	-0.6942048	1141	1160	-0.59602582	1823458	-1.13155896	2808221	-0.10933269	experimental	ChemBridge	5195154
1577 N07	X	948	960	-0.57257431	1666	1680	0.13263331	2269684	0.30032934	2928111	0.21432044	experimental	ChemBridge	5180510
1577 N08	X	708	720	-0.92856597	1345	1360	-0.3128897	2123418	-0.16902156	2863355	0.03950618	experimental	ChemBridge	5209028
1577 N09	X	906	920	-0.63487285	1061	1080	-0.7070596	2121145	-0.17631535	3350351	1.84065783	experimental	ChemBridge	5182258
1577 N10	X	788	800	-0.80990209	1302	1320	-0.37257036	2185508	0.03021817	2871650	0.06189923	experimental	ChemBridge	5210645
1577 N11	X	1382	1400	0.07117727	2017	2040	0.61979399	2056282	-0.38445332	2375912	-1.27638715	experimental	ChemBridge	5185661
1577 N12	X	3498	3520	3.20983706	4695	4720	4.33664954	1849088	-1.04931522	2304108	-1.47022808	experimental	ChemBridge	5211302
1577 N13	X	2339	2360	1.49069401	3016	3040	2.00632823	2285380	0.35069602	2701084	-0.39855802	experimental	ChemBridge	5190249
1577 N14	X	783	800	-0.81731858	1218	1240	-0.48915588	1995712	-0.57881553	2472278	-1.01623903	experimental	ChemBridge	5211789
1577 N15	X	1344	1360	0.01481192	1583	1600	0.01743577	2275191	0.31800068	2875787	0.07306741	experimental	ChemBridge	5190650
1577 N16	X	1137	1160	-0.29223088	1018	1040	-0.7674025	2098635	-0.2464737	2703147	-0.31645367	experimental	ChemBridge	5190907
1577 N17	X	902	920	-0.64080605	1459	1480	-0.1546688	1169643	-0.02069081	3082553	0.06124959	experimental	ChemBridge	5133767
1577 N18	X	1547	1560	0.31592153	1613	1640	-0.14911489	2032291	-0.4614377	2830292	-0.04975017	experimental	ChemBridge	5191662
1577 N19	X	944	960	-0.57850751	1022	1040	-0.76118856	2005377	-0.54780165	2860623	0.03213092	experimental	ChemBridge	5134275
1577 N20	X	1028	1040	-0.45391043	1345	1360	-0.3128897	1988140	-0.60311322	2801276	-0.12800813	experimental	ChemBridge	5192890
1577 N21	X	623	640	-1.05464635	703	720	-1.20393573	1260830	-2.936698	1587109	-3.40582711	experimental	ChemBridge	5135304

1577 O13	X		1410	1440	0.11270963	1011	1040	-0.7764557	1909145	-0.85659916	2488167	-0.97334534	experimental	ChemBridge	5102373
1577 O14	X		1378	1400	0.06524407	1858	1880	0.39911437	2105269	-0.22725963	2827961	-0.0560429	experimental	ChemBridge	5118843
1577 O15	X		2258	2280	1.37054682	1938	1960	0.51014814	2073933	-0.32781327	2823947	-0.06687903	experimental	ChemBridge	5103022
1577 O16	X		4142	4160	4.16508134	2701	2720	1.36913275	2132695	-0.13925272	2703418	-0.39257719	experimental	ChemBridge	5110448
1577 O17	X		2058	1480	0.18390796	2059	2110	0.67808672	2111120	-0.20844670	2759911	-0.23974959	experimental	ChemBridge	5103884
1577 O18	X		1061	1080	-0.40496157	1255	1280	-0.4378027	2092470	-0.26833016	2831903	-0.04540114	experimental	ChemBridge	5119299
1577 O19	X		1666	1680	0.49243406	2024	2040	0.62950945	1640108	-1.71990818	2414681	-1.17172697	experimental	ChemBridge	5104162
1577 O20	X		1500	1520	0.2462065	1980	2000	0.56844087	2250645	0.23923537	3048040	1.51090094	experimental	ChemBridge	5106649
1577 O21	X		1340	1360	0.00887873	1058	1080	-0.71122336	1830964	-1.10747306	2414740	-1.1715677	experimental	ChemBridge	5105175
1577 O22	X		940	960	-0.5844407	1342	1360	-0.31705347	1957015	-0.70298979	2779583	-0.18664337	experimental	ChemBridge	5105809
1577 O23	N		2394	2640	1.43877856	2123	2480	0.76691374	1948795	-0.72936683	2450027	-1.07630748	empty		
1577 O24	P		1100318	110040	160.152492	115897	116560	158.672206	1831567	-1.1055381	2670495	-0.48221543	empty		
1577 P01	X		1311	1320	-0.03413693	1630	1640	0.08266811	1682100	-1.58516065	2512674	-0.90718664	experimental	ChemBridge	5107573
1577 P02	X		1749	1760	0.61554785	1947	1960	0.52263944	1818234	-1.14832218	2494201	-0.95705605	experimental	ChemBridge	5136276
1577 P03	X		1067	1080	-0.39606178	1147	1160	-0.58769829	1958698	-0.69758924	2642073	-0.55786317	experimental	ChemBridge	5105953
1577 P04	X		1351	1360	0.02519501	1549	1560	-0.02975358	1960572	-0.69157578	2547028	-0.81444513	experimental	ChemBridge	5137278
1577 P05	X		1108	1120	-0.33524654	1389	1400	-0.25182113	1929176	-0.79232196	2399767	-1.21198857	experimental	ChemBridge	5108099
1577 P06	X		950	960	-0.58960772	1388	1400	-0.25320905	1842846	-1.06934508	2473766	-1.01222205	experimental	ChemBridge	5195235
1577 P07	X		1264	1280	-0.10385196	1584	1600	0.01882369	1994083	-0.58404281	2699418	-0.40203552	experimental	ChemBridge	5180519
1577 P08	X		3310	3320	2.93097693	2708	2720	1.57884821	2074344	-0.32649442	2521959	-0.882121	experimental	ChemBridge	5209067
1577 P09	X		945	960	-0.57702421	1143	1160	-0.59324998	1857098	-1.02361204	2549082	-0.80890018	experimental	ChemBridge	5182716
1577 P10	X		951	960	-0.56812442	1946	1960	0.52125152	1743059	-1.38955018	2580834	-0.91971271	experimental	ChemBridge	5210648
1577 P11	X		1632	1640	0.44200191	1747	1760	0.24505501	1852904	-1.03707011	2328864	-1.40339718	experimental	ChemBridge	5185936
1577 P12	X		896	920	-0.64970584	1460	1480	-0.15327858	1914118	-0.80466137	2468346	-1.0268538	experimental	ChemBridge	5211309
1577 P13	X		3504	3520	3.21873685	2743	2760	1.62742548	2085261	-0.29146301	2575277	-0.73818458	experimental	ChemBridge	5190260
1577 P14	X		3143	3160	3.68324666	2382	2400	3.51443077	1892052	-0.91144886	2393940	-0.22878022	experimental	ChemBridge	5214820
1577 P15	X		781	800	-0.82028518	1541	1560	-0.04085666	2001392	-0.56058906	2419391	-0.90919193	experimental	ChemBridge	5190576
1577 P16	X		1222	1240	-0.16615005	1343	1360	-0.31566555	1992886	-0.58788385	2346656	-1.35536618	experimental	ChemBridge	5190925
1577 P17	X		1387	1400	0.07859376	1741	1760	0.23672747	2230489	0.17455706	2514031	-0.9035233	experimental	ChemBridge	5133772
1577 P18	X		1789	1800	0.67487979	3028	3040	2.0229833	1992850	-0.5879937	2353355	-1.33728166	experimental	ChemBridge	5191712
1577 P19	X		1182	1200	-0.22548245	1098	1120	-0.65570648	1800530	-1.2051323	3127892	0.75364603	experimental	ChemBridge	5134306
1577 P20	X		2821	2840	2.20564392	2541	2560	1.3470652	1973107	-0.6513524	2467053	-1.03034436	experimental	ChemBridge	5192933
1577 P21	X		3903	3920	3.81057298	3546	3560	2.74192698	1809262	-1.1771123	2708334	-0.37898603	experimental	ChemBridge	5135308
1577 P22	X		17398	17400	0.53989962	2588	2600	0.01048739	1990147	-0.59667785	2097472	-1.34070742	experimental	ChemBridge	5154475
1577 P23	N		2404	2840	1.58710841	2517	2840	1.31375507	1861389	-1.00984271	2339902	-1.3843975	empty		
1577 P24	P		145833	146160	214.33514	107414	107760	146.902626	1679307	-1.59412307	2007908	-2.27203152	empty		
1578 A01	X		6990	7000	5.95980529	4034	4040	3.09805005	2989813	0.87593958	2185381	-1.00279979	experimental	ChemBridge	5193621
1578 A02	X		1890	1920	0.07349691	1019	1040	-0.80666	2641761	0.06096735	2128856	-1.12332348	experimental	ChemBridge	5119314
1578 A03	X		1910	1920	0.09658047	1352	1360	-0.37539351	2311375	-0.71263951	2161651	-1.05339735	experimental	ChemBridge	5110918
1578 A04	X		1223	1240	-0.69639899	1306	1320	-0.43496786	2537063	-0.18418556	2015883	-1.36420669	experimental	ChemBridge	5119773
1578 A05	X		1609	1620	-0.37852777	1946	1960	-0.34389244	2040358	-1.34737241	2494542	-0.94054212	experimental	ChemBridge	5113646
1578 A06	X		1505	1520	0.08083657	1228	1240	-0.53598524	1554125	-2.48575882	1381771	-2.71627249	experimental	ChemBridge	5122776
1578 A07	X		2465	2480	0.73714932	1191	1200	-0.58390374	2348061	-0.62673835	1841365	-1.73631732	experimental	ChemBridge	5115013
1578 A08	X		1864	1880	0.04348828	908	920	-0.95041549	2721788	0.24835252	2106377	-1.17048604	experimental	ChemBridge	5128689
1578 A09	X		1937	1960	0.12774328	1626	1640	-0.02053761	2280260	-0.78549604	1844308	-1.7300422	experimental	ChemBridge	5115670
1578 A10	X		1986	2000	0.18429801	1668	1680	0.03385636	2347863	-0.62720197	2125352	-1.13079478	experimental	ChemBridge	5130634
1578 A11	X		1417	1440	-0.47429294	1257	1280	-0.49842745	2353281	-0.61451559	2205314	-0.96029826	experimental	ChemBridge	5116050
1578 A12	X		2760	2780	2.0545460	4027	4040	3.08898439	2181302	-1.01770086	2231448	-1.00112834	experimental	ChemBridge	5154775
1578 A13	X		2480	2490	0.63904448	1062	1080	-0.75097093	1920486	-1.92082678	2312488	-0.90448956	experimental	ChemBridge	5211822
1578 A14	X		2258	2280	0.49823445	1150	1160	-0.63700261	3514975	2.10561919	2197851	-0.97621102	experimental	ChemBridge	5155825
1578 A15	X		3057	3080	1.42042277	1387	1400	-0.33006521	3452333	1.95894142	2677537	0.0465847	experimental	ChemBridge	5212413
1578 A16	X		3100	3120	1.47005243	2031	2040	0.50397568	3771316	2.70584788	2446816	-0.50932963	experimental	ChemBridge	5156745
1578 A17	X		2458	2480	0.72907008	1226	1240	-0.53857543	2842751	0.53159033	2428713	-0.48396262	experimental	ChemBridge	5213176
1578 A18	X		2263	2280	0.50400534	1629	1640	-0.01665233	2512604	-0.24145695	2760105	0.22263778	experimental	ChemBridge	5160525
1578 A19	X		1740	1760	-0.09962981	1384	1400	-0.33395049	2277518	-0.79191661	2500730	-0.33040658	experimental	ChemBridge	5213788
1578 A20	X		3137	3160	1.51275702	2580	2600	1.21498259	1716063	-2.10657705	2097472	-1.19024105	experimental	ChemBridge	5162465
1578 A21	X		4378	4400	2.94509205	3983	4000	3.03200023	2065483	-1.28840161	2253718	-0.85709032	experimental	ChemBridge	5214530
1578 A22	X		2218	2240	0.45206733	1732	1760	0.11674241	2334208	-0.65917548	2031320	-1.33129162	experimental	ChemBridge	5137326
1578 A23	N		1736	1760	-0.10424652	3376	3960	2.24587784	2035302	-1.35907116	2034724	-1.32403354	empty		
1578 A24	P		2514	2960	0.79370405	197439	197800	253.57581	2007156	-1.4249757	1719691	-1.99575297	empty		
1578 B01	X		1360	1400	-0.53821749	1124	1160	-0.67067507	2235093	-0.89125567	2245356	-0.87491994	experimental	ChemBridge	5140335
1578 B02	X		1386	1400	-0.50820886	1708	1720	0.08566014	2479576	-0.31879277	2224835	-0.91867521	experimental	ChemBridge	5261006
1578 B03	X		258	280	-1.81012177	264	280	-1.78445638	2092215	-1.22580798	2029970	-1.33417011	experimental	ChemBridge	5140994
1578 B04	X		2505	2520	0.78331645	1425	1440	-0.28085161	2026081	-1.38066235	1876637	-1.66110969	experimental	ChemBridge	5261526
1578 B05	X		2262	2280	0.50285117	2424	2440	1.01294784	2675334	0.13957935	2467100	-0.40211312	experimental	ChemBridge	5142859
1578 B06	X		1141	1160	-0.7909825	1063	1080	-0.74967584	2418036	-0.46289018	2596997	-0.13857722	experimental	ChemBridge	5262476
1578 B07	X		1608	1640	-0.25198132	1102	1120	-0.69916715	2861301	0.57502561	2728198	0.15460506	experimental	ChemBridge	5144179
1578 B08	X		1134	1160	-0.79906175	1185	1200	-0.5916743	2633007	0.04046965	2562451	-0.19880388	experimental	ChemBridge	5163227
1578 B09	X		4103	4120	2.62769307	2144	2160	0.65032136	2343283	-0.63792615	2046736	-1.29842133	experimental	ChemBridge	5214970
1578 B10	X		4059	4080	-0.28690427	1257	1280	-0.49396947	2184038	-1.01770086	2453700	-0.43060486	experimental	ChemBridge	5169061
1578 B11	X		3259	3280	0.65356675	2263	2280	0.80443765	2252484	-0.75887324	2312488	-0.89914654	experimental	ChemBridge	5215962
1578 B12	X		2893	2920	1.23113756	2213	2240	0.73968289	2550891	-0.15180866	2544742	-0.23656335	experimental	ChemBridge	5169134
1578 B13	X		1774	1800	-0.06038775	1144	1160	-0.64477318	2688307	0.16995595	25157				

1578 C07	X		6184	6200	5.02953773	2588	2600	1.22534334	3195894	1.35848326	2519987	-0.28934644	experimental	ChemBridge	5115325
1578 C08	X		1292	1320	-0.6167016	981	1000	-0.85587359	3259310	1.50697337	2687834	0.06854016	experimental	ChemBridge	5129945
1578 C09	X		1220	1240	-0.69980243	1345	1360	-0.38445918	2150053	-1.09037899	1959586	-1.48424423	experimental	ChemBridge	5115800
1578 C10	X		1364	1320	-0.60285147	1705	1720	0.08177498	2616298	0.00134512	2733141	0.1651446	experimental	ChemBridge	5130650
1578 C11	X		1020	1200	-0.74712373	1020	1040	-0.8053649	16051368	0.00013682	2678812	-0.14472762	experimental	ChemBridge	5116052
1578 C12	X		1499	1520	-0.37778673	1984	2000	0.44310624	2171901	-1.03922127	1977289	-1.44649756	experimental	ChemBridge	5154484
1578 C13	X		1461	1480	-0.4216455	1101	1120	-0.70046225	2642746	0.06327375	2559458	-0.20518561	experimental	ChemBridge	5211833
1578 C14	X		1540	1560	-0.33046543	2107	2120	0.60240287	2625006	0.02173511	2810455	0.32999502	experimental	ChemBridge	5155836
1578 C15	X		1778	1800	-0.05577104	824	840	-1.05920343	2767376	0.35509793	2787026	0.28003925	experimental	ChemBridge	5212148
1578 C16	X		2101	2120	0.31702849	868	880	-1.00221927	2412329	-0.47625326	2555697	-0.21320489	experimental	ChemBridge	5156796
1578 C17	X		2219	2240	0.45322151	1706	1720	0.08306995	2419311	-0.45990474	2601227	-0.11612495	experimental	ChemBridge	5213200
1578 C18	X		1574	1600	-0.28660666	1303	1320	-0.43885315	2290473	-0.76158205	2656193	0.00147974	experimental	ChemBridge	5160943
1578 C19	X		2058	2080	0.26739883	1423	1440	-0.2834418	2109237	-1.18595056	2311760	-0.73333205	experimental	ChemBridge	5213858
1578 C20	X		3018	3040	1.37540982	1502	1520	-0.18112933	2431791	-0.43068251	2589184	-0.14180326	experimental	ChemBridge	5162501
1578 C21	X		1855	1880	0.03310067	1823	1840	0.23459602	2418498	-0.46180884	2834170	0.3805606	experimental	ChemBridge	5214537
1578 C22	X		2693	2720	1.00030193	1497	1520	-0.18760481	2845796	0.53872027	2598520	-0.12189687	experimental	ChemBridge	5137337
1578 C23	N		2725	3160	1.03723563	2406	2800	0.98963614	2333205	-0.66152403	2223254	-0.92204625	empty		
1578 C24	P	140402	141320	159.941016	129037	129760	164.988753	2351567	-0.61852896	2341717	-0.66945716		experimental	ChemBridge	5140350
1578 D01	X		2573	2600	0.86180056	3250	3280	2.08269593	2525537	-0.20883245	2356817	-0.63726065	experimental	ChemBridge	5261020
1578 D02	X		1220	1240	-0.69980243	900	920	-0.96077625	2599379	-0.03827113	2786688	0.27931856	experimental	ChemBridge	5261020
1578 D03	X		1858	1880	0.03656321	938	960	-0.91156266	3154838	1.26234964	3177856	1.1133745	experimental	ChemBridge	5141013
1578 D04	X		823	840	-1.15801114	1065	1080	-0.74708565	2678479	1.04694344	2920329	0.56427048	experimental	ChemBridge	5261675
1578 D05	X		1388	1400	-0.50590005	986	1000	-0.84939812	3024759	0.95776649	2924704	0.57359894	experimental	ChemBridge	5144030
1578 D06	X		1381	1400	-0.51397975	1347	1360	-0.38186899	2528899	-0.20330177	2855130	0.42525191	experimental	ChemBridge	5262496
1578 D07	X		1570	1600	-0.29584009	1061	1080	-0.75226603	2895544	0.65520643	2807189	0.32303119	experimental	ChemBridge	5144180
1578 D08	X		1147	1160	-0.78405743	1390	1420	-0.32617996	26992491	0.17957288	2659291	-0.41493268	experimental	ChemBridge	5136059
1578 D09	X		188	200	-0.89096724	346	360	-1.897825863	2913831	0.68902585	3092895	0.93221902	experimental	ChemBridge	5215082
1578 D10	X		1632	1660	-0.22428105	1590	1600	-0.06716101	3195888	1.64811577	3223388	1.21045871	experimental	ChemBridge	5169066
1578 D11	X		1104	1120	-0.83368709	1066	1080	-0.74579055	2568107	-0.11149528	2940884	0.60809824	experimental	ChemBridge	5215423
1578 D12	X		1662	1680	-0.1896557	1220	1240	-0.54634599	2450890	-0.38596174	2283451	-0.79369305	experimental	ChemBridge	5169137
1578 D13	X		1543	1560	-0.3270029	1306	1320	-0.43496786	2431887	-0.43045773	2261080	-0.84139293	experimental	ChemBridge	5215572
1578 D14	X		1543	1560	-0.3270029	1544	1560	-0.12673536	2753869	0.32347096	3106431	0.96108074	experimental	ChemBridge	5172686
1578 D15	X		1461	1480	-0.4216455	1066	1080	-0.74579055	2569772	-0.10759664	2495954	-0.34059006	experimental	ChemBridge	5217526
1578 D16	X		1190	1200	-0.4596955	1067	1100	-0.80406981	2744452	0.49512109	2578621	0.41493268	experimental	ChemBridge	5173171
1578 D17	X		1461	1480	-0.4216455	1303	1320	-0.43885315	2427015	-0.44186563	2502457	-0.32672424	experimental	ChemBridge	5218494
1578 D18	X		1663	1680	-0.18850152	1744	1760	0.13228355	2551923	-0.14939051	2619491	-0.0771821	experimental	ChemBridge	5267053
1578 D19	X		1497	1520	-0.38009509	1506	1520	-0.17594895	2414088	-0.47213452	2404502	-0.53558578	experimental	ChemBridge	5260219
1578 D20	X		1937	1960	0.12774328	1180	1200	-0.59814978	2645203	0.06902688	2883257	0.48522484	experimental	ChemBridge	5267982
1578 D21	X		776	800	-1.21225751	1421	1440	-0.28603199	2304538	-0.72864851	2734492	0.16802525	experimental	ChemBridge	5260741
1578 D22	X		2573	2600	0.86180056	1580	1600	-0.08011196	2770124	0.36153244	2451115	-0.43619664	experimental	ChemBridge	5268500
1578 D23	N		3240	3240	1.06262755	2334	2340	0.06267952	26444242	0.06677656	2747562	0.49492029	empty		
1578 D24	P	160709	161560	183.378911	125535	126240	160.453332	2503344	-0.26313942	2278659	-0.80391064		empty		
1578 E01	X		2584	2600	0.87449652	2743	2760	1.426083	2816197	0.46941349	2860043	0.43572751	experimental	ChemBridge	5193909
1578 E02	X		1174	1200	-0.75289462	1251	1280	-0.50619806	2970676	0.83112983	3099401	0.94609124	experimental	ChemBridge	5119355
1578 E03	X		3903	3920	2.39685745	4705	4720	3.96705849	2736072	0.28179886	2977932	0.6870927	experimental	ChemBridge	5111125
1578 E04	X		1100	1120	-0.8383038	1854	1880	0.27474395	2718951	0.24170962	3324969	1.42705167	experimental	ChemBridge	5119806
1578 E05	X		942	960	-1.02066394	1225	1240	-0.53987052	2360017	-0.59874308	2833794	0.37975888	experimental	ChemBridge	5114474
1578 E06	X		2364	2400	-0.84366609	1225	1240	-0.53987052	2827176	0.49512109	2429486	-0.41493268	experimental	ChemBridge	5123420
1578 E07	X		1501	1520	-0.37547838	1026	1040	-0.79759434	2576736	0.05130857	2793997	0.29485991	experimental	ChemBridge	5115327
1578 E08	X		1188	1200	-0.73673613	1028	1040	-0.79500415	2883567	0.62716199	2739323	0.16681202	experimental	ChemBridge	5129946
1578 E09	X		231	240	-1.84128458	432	440	-1.5668805	1593651	-2.39320773	1262111	-2.97141385	experimental	ChemBridge	5115803
1578 E10	X		186	200	-1.8932226	386	400	-1.62645484	1133113	-3.47156866	927534	-3.68480537	experimental	ChemBridge	5130983
1578 E11	X		1106	1120	-0.83137873	1026	1040	-0.79759434	2277876	-0.79107823	2965874	0.6613824	experimental	ChemBridge	5116053
1578 E12	X		2024	2040	0.22815678	1578	2600	1.22275315	3416532	1.87511251	3193682	1.147119	experimental	ChemBridge	5154843
1578 E13	X		1263	1280	-0.65017277	1023	1040	-0.80147962	2677204	0.143958	2790667	-0.11509291	experimental	ChemBridge	5211878
1578 E14	X		1180	1200	-0.74596955	1021	1040	-0.80406981	2650584	0.08162662	2868461	0.49367653	experimental	ChemBridge	5156306
1578 E15	X		1818	1840	-0.00960392	1342	1360	-0.38834446	2576546	-0.09173516	2543126	-0.24000902	experimental	ChemBridge	5212505
1578 E16	X		1743	1760	-0.09616727	1343	1360	-0.38704937	2762747	0.34425902	2900124	0.52118899	experimental	ChemBridge	5156984
1578 E17	X		1261	1280	-0.65248113	1465	1480	-0.22904783	2340097	-0.64538625	2372360	-0.60411957	experimental	ChemBridge	5213269
1578 E18	X		1381	1400	-0.51397975	1186	1200	-0.59037921	2616374	0.00152307	2526702	-0.27502859	experimental	ChemBridge	5161253
1578 E19	X		2179	2200	0.40705438	581	600	-1.37391141	2388865	-0.53119479	2087142	-1.21226688	experimental	ChemBridge	5213911
1578 E20	X		2498	2520	0.7752372	2367	2400	0.96502934	2817029	0.47136164	3407601	1.60324121	experimental	ChemBridge	5162600
1578 E21	X		1777	1800	-0.05692522	1374	1800	0.18148714	2792600	0.41416054	3424021	1.63825225	experimental	ChemBridge	5213420
1578 E22	X		2607	2640	0.90104262	1297	1320	-0.44662371	2908874	0.68641895	3520228	1.84388667	experimental	ChemBridge	5214545
1578 E23	N		2463	2920	0.73484097	2379	2720	0.95466858	2221997	-0.92192027	2535708	-0.25582582	empty		
1578 E24	P	148355	149280	169.120194	110102	110920	140.466138	2563664	-0.12189867	2579169	-0.16315744		empty		
1578 F01	X		1864	1880	0.04348828	1303	1320	-0.43885315	2620599	0.01141602	2573544	-0.17515117	experimental	ChemBridge	5140718
1578 F02	X		1101	1120	-0.83714962	1546	1560	-0.12414517	1735923	-2.06007437	1749206	-1.93282052	experimental	ChemBridge	5261122
1578 F03	X		1536	1560	-0.33508214	1012	1040	-0.81572566	2924445	0.72287882	2861812	0.43949994	experimental	ChemBridge	5141040
1578 F04	X		1304	1320	-0.60285147	1486	1480	-0.29028508	2672867	0.13280781	2479256	0.26070023	experimental	ChemBridge	5261713
1578 F05	X		1304	1320	-0.60285147	943	960	-0.90509718	1655197	1.2805949	2901884	0.52481169	experimental	ChemBridge	5144033
1578 F06	X		1781	1800	-0.05230851	1544	1560	-0.12673536	2534653	-0.18982864	2680213	0.05229052	experimental	ChemBridge	5262623
1578 F07	X		1183	1200	-0.74250702	1543	1560	-0.12803046	2821474	0.48176972	32				

1578 G01	X	1746	1760	-0.09270474	1388	1400	-0.32877011	3041635	0.99728206	3228041	1.22037992	experimental	ChemBridge	5194054
1578 G02	X	1863	1880	0.0423341	1063	1080	-0.74967584	3144528	1.23820852	3198185	1.15672039	experimental	ChemBridge	5119483
1578 G03	X	1903	1920	0.08850122	1427	1440	-0.27826142	2977566	0.84726294	3010366	0.75616381	experimental	ChemBridge	5111923
1578 G04	X	1344	1360	-0.55668434	1023	1040	-0.80147962	2805562	0.44451138	2668341	0.02697681	experimental	ChemBridge	5121924
1578 G05	X	1304	1320	-0.60285147	1226	1240	-0.53857543	2604810	-0.02555433	2240452	-0.66634345	experimental	ChemBridge	5114507
1578 G06	X	1580	1600	-0.28429831	1658	1680	0.02090542	2786788	0.40055616	3232821	1.23057193	experimental	ChemBridge	5127036
1578 G07	X	1504	1520	-0.37201584	1902	1920	0.33690848	2100811	-1.20568024	2396328	-0.55301454	experimental	ChemBridge	5115427
1578 G08	X	899	920	-1.0702936	1376	1400	-0.34431125	2510312	-0.24682368	2807351	0.32337661	experimental	ChemBridge	5129951
1578 G09	X	1307	1320	-0.59938893	1665	1680	0.02997108	2282154	-0.78106119	2407588	-0.52900575	experimental	ChemBridge	5115805
1578 G10	X	943	960	-1.01950977	1263	1280	-0.49065693	2416996	-0.46532537	3049616	0.83993871	experimental	ChemBridge	5130991
1578 G11	X	622	640	-1.39000994	945	960	-0.90249699	1897962	-1.68065611	2969499	0.6691117	experimental	ChemBridge	5161335
1578 G12	X	2185	2200	0.41397945	903	920	-0.95689095	2875698	0.00873653	2240452	-0.8853337	experimental	ChemBridge	5155676
1578 G13	X	1459	1480	-0.42395386	2066	2080	0.54930399	2073442	-1.26976542	1213208	-1.11404406	experimental	ChemBridge	5211912
1578 G14	X	1738	1760	-0.10193817	1097	1120	-0.70564262	2559250	-0.13223416	2813020	0.33546416	experimental	ChemBridge	5156343
1578 G15	X	2097	2120	0.31241178	1261	1280	-0.49324712	3075344	1.0762125	2642651	-0.0277999	experimental	ChemBridge	5212757
1578 G16	X	1741	1760	-0.09847563	1223	1240	-0.54246071	2585666	-0.07038045	3119775	0.98953308	experimental	ChemBridge	5157043
1578 G17	X	1459	1480	-0.42395386	1224	1240	-0.54116562	2600229	-0.03628084	2606805	-0.10423143	experimental	ChemBridge	5213303
1578 G18	X	1423	1440	-0.46550427	1226	1240	-0.53857543	2578429	-0.08732607	2841120	0.39537952	experimental	ChemBridge	5161800
1578 G19	X	1649	1680	-0.20466002	1492	1520	-0.19408028	2543467	-0.16919044	2622213	-0.07137819	experimental	ChemBridge	5214057
1578 G20	X	4701	4720	0.31789159	3826	3840	2.82867039	2589653	-0.0610448	2409641	-0.5246283	experimental	ChemBridge	5162729
1578 G21	X	1730	1760	-0.11117159	1138	1160	-0.65254375	2287989	-0.7673984	2389481	-0.56761384	experimental	ChemBridge	5214569
1578 G22	X	1727	1760	-0.11463412	1137	1160	-0.65383884	3043676	1.00206211	2582562	-0.15592282	experimental	ChemBridge	5138038
1578 G23	N	2468	2840	0.74061186	2392	2800	0.97150481	2289830	-0.76308765	2327041	-0.70074961	empty		
1578 G24	P	120350	136.797436		133310	134120	0.522692	2516389	-0.23259424	2554230	-0.21633286	empty		
1578 H01	X	1140	1160	-0.79213668	1700	1720	0.07529939	2739137	0.28897563	2940491	0.60726028	experimental	ChemBridge	5140739
1578 H02	X	1064	1120	-0.83599545	1144	1280	-0.17858114	2281188	-0.7833231	2623396	-0.0709868	experimental	ChemBridge	5261126
1578 H03	X	1062	1080	-0.87985421	1304	1320	-0.43755805	2563645	-0.29194316	3045022	-0.07694329	experimental	ChemBridge	5141496
1578 H04	X	1062	1080	-0.88216257	1181	1200	-0.59685468	2527940	-0.20554729	2794421	0.29542382	experimental	ChemBridge	5261933
1578 H05	X	1181	1200	-0.74481537	1061	1080	-0.75226603	2847940	0.5437405	3102629	0.95297404	experimental	ChemBridge	5144040
1578 H06	X	2300	2320	0.54670993	2703	2720	1.37427922	2475067	-0.32935071	2896124	0.51266011	experimental	ChemBridge	5262721
1578 H07	X	1680	1720	-0.16888005	1612	1640	-0.03866893	2722254	0.24944367	2858426	0.43227971	experimental	ChemBridge	5144227
1578 H08	X	3343	3360	1.75051771	3303	3320	2.15133594	2749685	0.31367403	3204436	1.17004889	experimental	ChemBridge	5169012
1578 H09	X	1016	1040	-0.93525476	1617	1640	-0.03219346	2888535	0.63879468	2894268	0.50870271	experimental	ChemBridge	5215116
1578 H10	X	2104	2120	0.20406112	1261	1280	-0.49324712	2097913	-0.21468921	2712469	0.88650851	experimental	ChemBridge	5169083
1578 H11	X	1704	1720	-0.14118022	2065	2080	0.5480089	2955871	0.79646356	3184045	1.12657081	experimental	ChemBridge	5215587
1578 H12	X	1660	1680	-0.19196406	1423	1440	-0.2834418	2744152	0.30071837	2752994	0.20747557	experimental	ChemBridge	5169180
1578 H13	X	2019	2040	0.22238588	1857	1880	0.27862923	2715399	0.23339252	2900946	0.52294167	experimental	ChemBridge	5215587
1578 H14	X	1939	1960	0.13005164	1903	1920	0.33820358	2357322	-0.60505349	2538964	-0.24888331	experimental	ChemBridge	5172848
1578 H15	X	1460	1480	-0.42279968	1423	1440	-0.2834418	2515947	-0.23362919	2662827	0.01521976	experimental	ChemBridge	5217961
1578 H16	X	1461	1480	-0.4216455	1422	1440	-0.2847369	2749141	0.31240024	3034177	0.80701937	experimental	ChemBridge	5173336
1578 H17	X	2264	2280	0.18515952	1824	1840	-0.50515925	2538429	-0.18098704	2816236	-0.23280292	experimental	ChemBridge	5218281
1578 H18	X	1291	1320	-0.61785578	1206	1240	-0.56447732	2578884	-0.08626067	2619603	-0.07694329	experimental	ChemBridge	5215836
1578 H19	X	2661	2680	0.96336823	3104	3120	1.89361213	2292241	-0.75744223	2885698	0.49042959	experimental	ChemBridge	5260356
1578 H20	X	1527	1560	-0.34546975	1329	1360	-0.40518069	2497924	-0.27583048	2584632	-0.15150913	experimental	ChemBridge	5268238
1578 H21	X	1817	1840	-0.01075809	1582	1600	-0.07752177	2930451	0.73694202	2573048	-0.17620875	experimental	ChemBridge	5260769
1578 H22	X	2736	2760	1.04993159	2101	2120	0.5946323	2607875	-0.01837754	2479114	-0.37649664	experimental	ChemBridge	5268610
1578 H23	N	2662	2960	0.96452241	12744	12760	0.95725877	2676884	0.14320871	2411344	-0.52099713	empty		
1578 H24	P	93665	94.991893		122744	123480	156.8387723	2465658	-0.35118211	2552221	-0.42744175	empty		
1578 I01	X	3967	3960	4.47676129	4026	4040	0.8868993	3198467	0.6684953	2802257	0.31251509	experimental	ChemBridge	5194136
1578 I02	X	2016	2040	0.21892335	1417	1440	-0.29121237	2655319	0.09271374	3123097	0.99661631	experimental	ChemBridge	5119533
1578 I03	X	1540	1560	-0.33046543	1180	1200	-0.59814978	3099651	1.13312793	2892267	0.50443614	experimental	ChemBridge	5191940
1578 I04	X	2583	2600	0.87334234	3026	3040	1.79259475	3096492	1.12573106	2606606	-0.10580714	experimental	ChemBridge	5212966
1578 I05	X	1777	1800	-0.05692522	1219	1240	-0.54764109	3049461	1.01560683	2902103	0.52540865	experimental	ChemBridge	5114509
1578 I06	X	2484	2520	0.75907871	1621	1640	-0.02701308	3794640	2.7604616	3171322	1.09944258	experimental	ChemBridge	5127824
1578 I07	X	6577	6600	5.48312972	1583	1600	-0.07622667	4211432	3.71034887	2569754	-0.18323228	experimental	ChemBridge	5115555
1578 I08	X	2154	2200	0.37819993	1089	1120	-0.71600338	3808997	2.79314225	3071457	0.88650851	experimental	ChemBridge	5129953
1578 I09	X	1342	1360	-0.5589927	1584	1600	-0.07493158	2923997	0.72182982	2778322	0.26148042	experimental	ChemBridge	5115838
1578 I10	X	1741	1760	-0.09847563	1423	1440	-0.2834418	2873034	0.60249871	3055431	0.85233756	experimental	ChemBridge	5131173
1578 I11	X	1102	1120	-0.83599545	1381	1400	-0.33783577	2606763	-0.02098132	2902338	0.52590972	experimental	ChemBridge	5116156
1578 I12	X	1102	1120	-0.83599545	1101	1120	-0.70046225	2599492	-0.03800654	2900940	0.52292888	experimental	ChemBridge	5155727
1578 I13	X	2181	2200	0.40936274	2622	2640	1.26937656	2418104	-0.46273096	2590482	-0.13903564	experimental	ChemBridge	5211915
1578 I14	X	2101	2120	0.31702849	1380	1400	-0.33913087	2534578	-0.19000425	2430490	-0.48017366	experimental	ChemBridge	5156401
1578 I15	X	1177	1200	-0.74943209	1102	1120	-0.6916715	2877880	0.61361159	2538005	-0.25092811	experimental	ChemBridge	5212807
1578 I16	X	1064	1080	-0.87985421	1583	1600	-0.07622667	3066025	1.05493184	2910192	0.54265617	experimental	ChemBridge	5157217
1578 I17	X	1333	1360	-0.5693803	1409	1440	-0.30157313	2546822	-0.16133463	2568272	-0.18639223	experimental	ChemBridge	5213504
1578 I18	X	3582	3600	2.02636628	5383	5400	4.84513259	2902163	0.67070498	3634608	2.0872699	experimental	ChemBridge	5161820
1578 I19	X	1970	2000	0.16583116	1446	1480	-0.25365463	2902909	0.67245175	2623544	-0.06854021	experimental	ChemBridge	5214059
1578 I20	X	2301	2320	0.54786411	2143	2160	0.64902627	2761009	0.34018945	3037453	0.81400452	experimental	ChemBridge	5162793
1578 I21	X	1699	1720	-0.14695111	1622	1640	-0.02571799	2748323	0.31048487	2584404	-0.15199527	experimental	ChemBridge	5214578
1578 I22	X	1560	1560	-0.33623652	1056	1060	-0.73817415	2824899	0.48978944	2642271	-0.24183207	experimental	ChemBridge	5138617
1578 I23	X	2521	2840	0.8017833	2200	2560	0.72284666	2387803	-0.53368149	2551426	-0.22231116	experimental	ChemBridge	5138617
1578 I24	P	101456	102320	114.990395	116504	117280	148.757333	2418414	-0.46200508	2429717	-0.48182187	empty		
1578 J01	X	1372	1400	-0.52436735	1609	1640	-0.04255422	4873706	5.2871209	5083797	5.17725857	experimental	ChemBridge	5140778
1578 J02	X	1582	1600	-0.28198995	1303	1320	-0.43885315	2636314	0.04821307	2755246	0.21227733	experimental	ChemBridge	5261175
1578 J03	X	1064	1080	-0.87985421	1103	1120								

1578 J19	X	1702	1720	-0.14348858	1104	1120	-0.69657696	2882312	0.62422338	2912718	0.54804216	experimental	ChemBridge	5260358
1578 J20	X	1339	1360	-0.56245523	1261	1280	-0.49324712	2922834	0.71910663	2974825	0.6804679	experimental	ChemBridge	5268261
1578 J21	X	1543	1560	-0.32700229	1501	1520	-0.18242443	2652651	0.08646655	2616550	-0.08345295	experimental	ChemBridge	5260784
1578 J22	X	1413	1440	-0.47704605	2098	2120	-0.59074702	2442354	-0.40594899	2733754	0.16645167	experimental	ChemBridge	5268728
1578 J23	N	2673	3280	0.97721837	2807	3240	1.50896905	3629390	0.05541556	2762615	0.15122916	empty		
1578 J24	P	200303	201280	229.077439	141159	141840	180.687889	2424284	-0.44826034	2672464	0.03576795	empty		
1578 K01	X	4227	4240	2.77081116	5226	5240	4.64180275	3003536	0.90807232	3238126	1.24188335	experimental	ChemBridge	5194204
1578 K02	X	1537	1560	-0.33392797	1652	1680	0.01313485	2874593	0.60614915	3035719	0.81030725	experimental	ChemBridge	5119550
1578 K03	X	1065	1080	-0.87870004	1824	1840	0.23589111	2762127	0.34280727	3066972	0.8769455	experimental	ChemBridge	5112086
1578 K04	X	1419	1440	-0.47012098	1616	1640	-0.03348855	2891508	0.64575603	2846589	0.40704063	experimental	ChemBridge	5112204
1578 K05	X	1703	1720	0.1423344	1862	1880	0.2851047	2620876	0.01206462	2669892	0.03028389	experimental	ChemBridge	5114577
1578 K06	X	1661	1680	-0.19080988	1182	1200	-0.59555959	2599533	0.11962419	320461	1.17061393	experimental	ChemBridge	5128194
1578 K07	X	1656	1680	-0.19658077	1263	1280	-0.49065693	3048601	1.01359312	2526164	-0.27617572	experimental	ChemBridge	5115631
1578 K08	X	3572	3600	2.01482449	1656	1680	0.01831523	3144971	1.23924582	3190918	1.14122555	experimental	ChemBridge	5130345
1578 K09	X	1697	1720	-0.14925947	1742	1760	0.12969336	2487596	-0.30001375	2890040	0.49968769	experimental	ChemBridge	5115839
1578 K10	X	1382	1400	-0.51282557	1462	1480	-0.23293311	2544007	-0.16792602	2793282	0.29337842	experimental	ChemBridge	5131432
1578 K11	X	1461	1480	-0.4216455	1542	1560	-0.12932555	2341289	-0.64259515	2794737	0.2964808	experimental	ChemBridge	5116157
1578 K12	X	1264	1280	-0.64901859	1624	1640	-0.0231278	2475746	-0.32776081	2824575	0.36010196	experimental	ChemBridge	51155739
1578 K13	X	1540	1560	-0.33046543	1216	1240	-0.55152637	2718727	0.24118512	2446691	-0.44562958	experimental	ChemBridge	5212001
1578 K14	X	2781	2800	1.10186961	3102	3120	1.89102194	2122369	-1.15520166	2404493	-0.53560497	experimental	ChemBridge	5156699
1578 K15	X	1655	1680	-0.19773495	1536	1560	-0.13709612	2371432	-0.57201458	2944964	0.6167977	experimental	ChemBridge	5123024
1578 K16	X	1421	1440	-0.46781263	1782	1800	0.18149714	2770953	0.36347357	3610633	2.03614995	experimental	ChemBridge	5158408
1578 K17	X	2220	2240	0.45437569	1501	1520	-0.18242443	2753844	0.32341243	3226298	1.21666347	experimental	ChemBridge	5123591
1578 K18	X	1821	1840	-0.00614138	1584	1600	-0.07493158	1813004	-1.87958734	3152969	1.06030996	experimental	ChemBridge	5161922
1578 K19	X	1340	1360	-0.56130105	1181	1200	-0.59685468	2279006	-0.78843231	2921764	0.56733021	experimental	ChemBridge	5124085
1578 K20	X	1704	1720	-0.14118007	1584	1600	-0.07493158	2805171	0.44495985	276354	1.29653029	experimental	ChemBridge	5162345
1578 K21	X	1179	1200	-0.74712373	1502	1520	-0.18112933	2166943	-1.0508305	2421011	-0.39374041	experimental	ChemBridge	5124753
1578 K22	X	2736	2760	1.04993159	1856	1880	0.27733414	2877596	0.61318075	2719554	0.12849817	experimental	ChemBridge	5140095
1578 K23	N	3381	4080	1.79437647	2604	2960	1.24606486	2702087	0.20222215	2676312	0.04397273	empty		
1578 K24	P	230838	231920	264.320268	114057	114800	145.588237	3820622	2.82129908	2704452	0.10397338	empty		
1578 L01	X	1333	1360	-0.5693803	1370	1400	-0.35208181	2860770	0.57378226	2571906	-0.17864375	experimental	ChemBridge	5140811
1578 L02	X	1102	1120	-0.83599545	1262	1280	-0.49195202	2315483	-0.70302053	2489774	-0.35376718	experimental	ChemBridge	5261280
1578 L03	X	1215	1240	-0.7057332	1055	1080	-0.76003659	2705238	0.20960209	2791833	0.29028883	experimental	ChemBridge	5141877
1578 L04	X	3206	3280	1.56931174	3061	3200	1.83791232	2862529	-0.04049558	2814812	-0.38097198	experimental	ChemBridge	5212405
1578 L05	X	1056	1080	-0.88908764	1976	2000	0.43274548	2800824	0.43341724	3408866	1.60593847	experimental	ChemBridge	5144111
1578 L06	X	1622	1640	-0.23582283	2021	2040	0.49102474	2576385	-0.09211214	2493009	-0.34686945	experimental	ChemBridge	5262889
1578 L07	X	1699	1720	-0.14695111	1623	1640	-0.02442289	2372144	-0.57034742	2444715	-0.44984285	experimental	ChemBridge	5144439
1578 L08	X	1695	1720	-0.15156782	1140	1160	-0.64995356	2797388	0.42537176	2944418	0.61563351	experimental	ChemBridge	5169045
1578 L09	X	1623	1640	-0.23466865	1863	1880	0.2863998	2598238	-0.04094281	3038853	0.81634996	experimental	ChemBridge	5125242
1578 L10	X	1180	1200	-0.74596955	1380	1400	-0.33913087	1998641	-1.44491378	2216569	-0.93630014	experimental	ChemBridge	5169104
1578 L11	X	2186	2200	-0.46344411	1423	1440	-0.41513233	2821476	0.4401784	3413283	0.25682276	experimental	ChemBridge	5215542
1578 L12	X	1361	1360	-0.56014688	1622	1640	-0.02571799	2547048	-0.16080544	2626292	-0.06266595	experimental	ChemBridge	5170706
1578 L13	X	1460	1480	-0.42279968	1702	1720	0.07788958	2686778	0.16633757	2806741	0.32207596	experimental	ChemBridge	5216193
1578 L14	X	1935	1960	0.12543492	2012	2040	0.47936888	2687874	0.16894207	2997600	0.72902919	experimental	ChemBridge	5173069
1578 L15	X	1102	1120	-0.83599545	1462	1480	-0.23293311	2670008	0.12710839	2906349	0.53446205	experimental	ChemBridge	5218328
1578 L16	X	1144	1160	-0.64606827	1143	1160	-0.64606827	2439784	-0.41196671	2408196	-0.52770936	experimental	ChemBridge	5173350
1578 L17	X	1218	1240	-0.70211078	1223	1240	-0.54246071	2447079	-0.39488529	2470679	-0.39448191	experimental	ChemBridge	5218903
1578 L18	X	1563	1600	-0.28083577	2144	2200	-0.59555958	2598429	-0.04049558	3165088	-0.12740226	experimental	ChemBridge	5267444
1578 L19	X	1542	1560	-0.32815708	2144	2160	0.65032136	2552326	-0.14844668	3083861	-0.91295656	experimental	ChemBridge	5260566
1578 L20	X	1424	1440	-0.46435009	1542	1560	-0.12932555	2438855	-0.41414198	2812177	0.3336667	experimental	ChemBridge	5268298
1578 L21	X	1302	1320	-0.60515982	1260	1280	-0.49454221	2408574	-0.48504568	3881398	2.61348029	experimental	ChemBridge	5269799
1578 L22	X	1613	1640	-0.24621043	1498	1520	-0.18630971	2405459	-0.49233953	2580800	-0.15967979	experimental	ChemBridge	5268909
1578 L23	N	2806	3320	1.13072406	2577	2920	1.2110973	2732756	0.27403436	2563351	-0.19688488	empty		
1578 L24	P	167203	168200	190.874143	111188	111840	141.872611	2879447	0.61751491	2593680	-0.13221861	empty		
1578 M01	X	3987	4000	2.49380841	3866	3880	2.88047417	2853252	0.55617698	2823648	0.35812539	experimental	ChemBridge	5194213
1578 M02	X	1926	1960	0.11504732	1971	2000	0.42627001	2958497	0.80026124	2814712	0.33097188	experimental	ChemBridge	5119600
1578 M03	X	3302	3320	1.7031964	2541	2560	1.1644739	2476875	-0.32511723	2230600	-0.90753437	experimental	ChemBridge	5113007
1578 M04	X	1170	1200	-0.75751133	1973	2000	0.42886602	3229023	1.43605562	2895966	0.51232322	experimental	ChemBridge	5122191
1578 M05	X	1625	1640	-0.23236029	1418	1440	-0.28991727	2711654	0.22462351	2518137	-0.29329104	experimental	ChemBridge	5114807
1578 M06	X	1621	1640	-0.236977	1623	1640	-0.02442289	3239217	1.45992512	3305732	1.38603417	experimental	ChemBridge	5128282
1578 M07	X	2060	2080	0.26970719	1221	1240	-0.5450509	1888617	-1.70253766	1664081	-2.11432568	experimental	ChemBridge	5115663
1578 M08	X	1660	1680	-0.19196406	1624	1640	-0.0231278	2677979	0.14577268	2546286	-0.23327121	experimental	ChemBridge	5130381
1578 M09	X	1098	1120	-0.84061216	1371	1400	-0.34301615	2367750	-0.58063607	2413283	-0.51686276	experimental	ChemBridge	5115581
1578 M10	X	1667	1680	-0.18508481	2024	2040	0.49491002	2717670	0.23871012	2780911	0.26700073	experimental	ChemBridge	5131445
1578 M11	X	898	920	-1.07144778	1380	1400	-0.33913087	2185112	-1.0082874	2338301	-0.6764082	experimental	ChemBridge	5116230
1578 M12	X	1505	1520	-0.37086167	1424	1440	-0.28214671	3706606	2.55432784	2760993	0.22453119	experimental	ChemBridge	5155786
1578 M13	X	1976	2000	0.17275623	1377	1400	-0.34301615	2226738	-0.9108191	2131795	-1.11705689	experimental	ChemBridge	5212095
1578 M14	X	3219	3240	1.60739962	3179	3200	1.99074422	4538651	4.50258146	4342048	3.59568708	experimental	ChemBridge	5156701
1578 M15	X	1419	1440	-0.47012098	1579	1600	-0.08140705	2624000	0.01937954	2755213	0.25485135	experimental	ChemBridge	5213048
1578 M16	X	1621	1640	-0.236977	1383	1400	-0.35245358	3024895	0.95080194	2635088	0.12878389	experimental	ChemBridge	5160007
1578 M17	X	2464	2480	0.7359145	1825	1840	0.23718624	2479919	-0.31798693	2364288	-0.62133084	experimental	ChemBridge	5213768
1578 M18	X	1380	1400	-0.51513393	1222	1240	-0.54375581	2563957	-0.12121261	2411643	-0.52035996	experimental	ChemBridge	5161930
1578 M19	X	1736	1760	-0.10424652	1422	1440	-0.2847369	2349235	-0.6239894	1997412	-1.40359091	experimental	ChemBridge	5214159
1578 M20	X	1021	1040	-0.92948387	1061	1080	-0.75226603	3292548	1.58480096	4196063	3.28441506	experimental	ChemBridge	5162985
1578 M21	X	1784	1800	-0.04884597	2145									

1578 N13	X	2021	2040	0.22469424	1461	1480	-0.23422821	2788553	0.40468439	2854113	0.42308345	experimental	ChemBridge	5216447
1578 N14	X	1774	1800	-0.06038775	2099	2120	0.59204211	1882139	-1.71770605	2013108	-1.3701236	experimental	ChemBridge	5173151
1578 N15	X	1341	1360	-0.56014688	1298	1320	-0.44532862	2605841	-0.0231402	2756101	0.21410037	experimental	ChemBridge	5218347
1578 N16	X	1500	1520	-0.37663256	1182	1200	-0.59555892	2571322	-1.13018515	2807010	0.3226492	experimental	ChemBridge	5173622
1578 N17	X	1421	1440	-0.74943209	1421	1440	-0.28603199	2701847	0.20166011	2840133	-0.24839075	experimental	ChemBridge	5218908
1578 N18	X	1215	1240	-0.70557332	1623	1640	-0.02442289	2126012	-1.14667148	2695256	0.0843655	experimental	ChemBridge	5267649
1578 N19	X	4380	4400	2.94740041	1662	1680	0.02608579	2682592	0.15657413	2942801	-0.34731295	experimental	ChemBridge	5260598
1578 N20	X	1376	1400	-0.51975064	1343	1360	-0.38704937	2364310	-0.58869092	2765125	0.23334152	experimental	ChemBridge	5268370
1578 N21	X	1133	1160	-0.80021592	1500	1520	-0.18371952	2689566	0.17290392	2713552	0.12337658	experimental	ChemBridge	5260895
1578 N22	X	2137	2160	0.3585789	1576	1600	-0.08529234	2256264	-0.84168326	2509503	-0.31170063	experimental	ChemBridge	5268958
1578 N23	N	2691	3040	0.99799358	3447	3840	2.33782956	3516462	2.10910104	3095060	0.93683528	empty		
1578 N24	P	111606	112280	126.705303	128803	129400	164.692177	2415586	-0.46862699	243371	-0.47296463	empty		
1578 O01	X	548	560	-1.47541012	1066	1080	-0.74579055	1506598	-2.59704444	1696789	-2.04458505	experimental	ChemBridge	5194243
1578 O02	X	1694	1720	-0.152722	1731	1760	0.11544732	2828584	0.49841796	2653489	-0.00469091	experimental	ChemBridge	5119651
1578 O03	X	3496	3520	1.92710696	4815	4840	4.10951889	2631625	0.03723366	2903752	0.52892468	experimental	ChemBridge	5113156
1578 O04	X	1976	2000	0.17275623	1370	1400	-0.35208181	2729050	0.26535667	2617095	-0.08229089	experimental	ChemBridge	5122606
1578 O05	X	1539	1560	-0.33161961	1458	1480	-0.23811349	2285393	-0.77347699	2020000	-0.96736444	experimental	ChemBridge	5114990
1578 O06	X	2504	2520	0.78216227	3104	3120	1.89361213	2525506	-0.21124656	2639529	-0.03445669	experimental	ChemBridge	5128636
1578 O07	X	1097	1120	-0.84176634	1654	1680	0.01572504	2181271	-1.01728119	2554459	-0.21584458	experimental	ChemBridge	5115667
1578 O08	X	1584	1600	-0.27968159	1461	1480	-0.23422821	2452181	-0.38293883	2555756	-0.20924109	experimental	ChemBridge	5130458
1578 O09	X	1339	1360	-0.56245523	1378	1400	-0.34172106	2246575	-0.86437029	2279229	-0.80269528	experimental	ChemBridge	5116029
1578 O10	X	1342	1360	-0.5589927	1341	1360	-0.38963955	2217292	-0.93293714	2470734	-0.39436463	experimental	ChemBridge	5131913
1578 O11	X	1780	1800	-0.05346268	1654	1680	-0.33783577	2353702	-0.61352981	2430352	-0.48046791	experimental	ChemBridge	5116245
1578 O12	X	1423	1440	-0.46550427	1363	1400	-0.33524558	2655472	0.09307199	2418581	-0.50556626	experimental	ChemBridge	5155807
1578 O13	X	1735	1760	-0.1054007	1898	1920	0.33172811	2470314	-0.34047997	2414840	-0.5135429	experimental	ChemBridge	5212113
1578 O14	X	2180	2200	-0.48028045	2676	2720	-0.34431125	1934702	-1.59460851	1867917	-0.15129473	experimental	ChemBridge	5172482
1578 O15	X	1977	1800	-0.05692522	2663	2680	1.32247542	3335200	0.65683162	223667	-0.89343827	experimental	ChemBridge	5213089
1578 O16	X	2813	2840	1.13880331	1890	1920	0.32136735	2949365	0.78122961	3168210	1.09280711	experimental	ChemBridge	5160120
1578 O17	X	2579	2600	0.86872563	1981	2000	0.43922095	2778466	0.38106544	2418266	-0.50623791	experimental	ChemBridge	5213777
1578 O18	X	1578	1600	-0.28660666	1500	1520	-0.18371952	2141127	-1.11127934	2052536	-1.28605446	experimental	ChemBridge	5162110
1578 O19	X	2534	2560	0.81678761	1822	1840	0.23330092	2577046	-0.09056439	2561237	-0.2013924	experimental	ChemBridge	5214348
1578 O20	X	1692	1720	-0.15503036	1582	1600	-0.07752177	2530260	-0.20011495	2379022	-0.58991472	experimental	ChemBridge	5163090
1578 O21	X	4060	4080	2.57806341	1743	1760	0.13098845	2136340	-1.12248822	2067303	-1.25456797	experimental	ChemBridge	5214918
1578 O22	X	1809	1840	-0.01991921	1458	1480	-0.01991921	2535783	-0.18127293	2472759	-0.40125499	experimental	ChemBridge	5140012
1578 O23	N	2267	2640	0.50862206	2225	2520	0.75522402	2561629	-0.12666368	2410781	-0.52219757	empty		
1578 O24	P	120092	120800	136.499658	92211	93040	117.295602	2849519	0.54743777	2420822	-0.50078796	empty		
1578 P01	X	1354	1360	-0.54514256	1632	1640	-0.01276704	2000756	-1.43996146	2148341	-1.08177719	experimental	ChemBridge	5140985
1578 P02	X	1463	1480	-0.41933715	1659	1680	0.02220051	2360723	-0.59708996	2267153	-0.82844396	experimental	ChemBridge	5261469
1578 P03	X	2703	2720	1.01184371	3736	3760	2.71211188	1652411	-2.25561976	1636025	-2.17414722	experimental	ChemBridge	5142417
1578 P04	X	1023	1040	-0.92717552	1822	1840	0.23330092	2331533	-0.66543906	2473708	-0.38802341	experimental	ChemBridge	5262448
1578 P05	X	1300	1320	-0.58023475	1187	1200	-0.58023475	2158745	-1.07003637	1867397	-0.38647873	experimental	ChemBridge	5141748
1578 P06	X	1463	1480	-0.41933715	1219	1240	-0.54764109	2292010	0.75798313	2116867	-1.14888666	experimental	ChemBridge	5262929
1578 P07	X	1989	2000	0.18776054	2866	2880	1.58537963	2366266	-0.5841109	2424926	-0.49203733	experimental	ChemBridge	5144826
1578 P08	X	1025	1040	-0.92486716	1821	1840	0.23200583	2430827	-0.43293974	2693038	0.07963623	experimental	ChemBridge	5169047
1578 P09	X	1708	1720	-0.13656351	2344	2360	0.90934027	1463882	-2.697065	1332640	-0.82103056	experimental	ChemBridge	5215319
1578 P10	X	1866	1880	0.04579663	2104	2120	0.59851758	2422490	-0.45246103	2341167	-0.67062988	experimental	ChemBridge	5169130
1578 P11	X	1705	1720	-0.10024006	1786	1800	0.18667752	2331061	-0.66654426	2679202	0.05013485	experimental	ChemBridge	5215549
1578 P12	X	1482	1490	-0.48282557	1271	1240	-0.4950509	2413859	-0.84292439	2480787	-0.37293583	experimental	ChemBridge	5172482
1578 P13	X	2947	2960	-0.29342157	3306	3320	2.15522123	2948979	-0.2919689	2671150	-0.18025571	experimental	ChemBridge	5216449
1578 P14	X	1461	1480	-0.4216455	1623	1640	-0.02442289	1740781	-2.04869925	1693542	-2.05150837	experimental	ChemBridge	5173156
1578 P15	X	1461	1480	-0.4216455	1174	1200	-0.60592034	2657278	0.09730079	2389039	-0.56855628	experimental	ChemBridge	5218437
1578 P16	X	3383	3400	1.79668483	4506	4520	3.70933468	1930682	-1.60404143	1949254	-1.50627432	experimental	ChemBridge	5173677
1578 P17	X	1659	1680	-0.19311824	1617	1640	-0.03219346	2536819	-0.18475689	2535023	-0.25728639	experimental	ChemBridge	5219425
1578 P18	X	1227	1240	-0.69172318	1306	1320	-0.43496786	2229218	-0.90501212	2161019	-1.05474492	experimental	ChemBridge	5267872
1578 P19	X	1344	1360	-0.55668434	1547	1560	-0.12285008	2431656	-0.43099862	2526849	-0.27471515	experimental	ChemBridge	5260655
1578 P20	X	1785	1800	-0.04769179	1347	1360	-0.38186899	2342279	-0.64027704	2472056	-0.39154584	experimental	ChemBridge	5258457
1578 P21	X	2058	2080	0.26739883	1226	1240	-0.53857543	2740625	0.29245982	2155040	-1.06749345	experimental	ChemBridge	5260896
1578 P22	X	1859	1880	0.03771739	1622	1640	-0.02571799	2188092	-1.00130965	2364578	-0.6207125	experimental	ChemBridge	5269023
1578 P23	N	2851	3240	1.18266207	3021	3480	1.78611928	2425291	-0.44590242	2302750	-0.75254335	empty		
1578 P24	P	129321	129680	147.151568	154081	154360	197.423101	2166172	-1.05263587	2211847	-0.94636848	empty		
1579 A01	X	1277	1280	2.73060623	2238	2240	6.36814899	1729487	-2.04993187	1897906	-1.89843574	experimental	ChemBridge	5269250
1579 A02	X	393	400	-0.48647896	391	400	-0.55393133	1716657	-2.07683976	1769518	-2.16504838	experimental	ChemBridge	5265704
1579 A03	X	877	880	1.27491158	597	600	0.21810362	2413859	-0.61462344	2167591	-1.3384034	experimental	ChemBridge	5270350
1579 A04	X	235	240	-1.06147835	436	440	-0.38528292	2036397	-1.40626072	2235733	-1.19689859	experimental	ChemBridge	5214568
1579 A05	X	595	600	0.24864684	395	400	-0.53894036	2778133	0.14935514	2412640	-0.82953058	experimental	ChemBridge	5219626
1579 A06	X	996	1000	1.70798074	1077	1080	2.01702	2489134	-0.45675192	2484038	-0.68126431	experimental	ChemBridge	5147705
1579 A07	X	553	560	0.0957989	474	480	-0.2428687	2489735	-0.45549147	2287858	-1.08865495	experimental	ChemBridge	5219754
1579 A08	X	1312	1320	0.28579952	634	640	0.35677009	2930509	0.46892777	3026650	0.44553276	experimental	ChemBridge	5150529
1579 A09	X	1874	1880	4.90323051	1155	1160	2.30934391	2457984	-0.52208168	2072544	-1.53577957	experimental	ChemBridge	5219830
1579 A10	X	312	320	-0.78125713	274	280	-0.99241719	2284129	-0.88670143	2365309	-0.51729563	experimental	ChemBridge	5151206
1579 A11	X	397	400	0.47192202	397	400	-0.53144887	1697138	-0.02811272	2621118	-0.38200604	experimental	ChemBridge	5202214
1579 A12	X	516	520	-0.03885285	315	320	-0.83875975	2383899	-0.67745745	2708167	-0.21583432	experimental	ChemBridge	5152534
1579 A13	X	354	360	-0.62840919	476	480	-0.23537322	2355908	-0.73616195	2692114	-0.24917024	experimental	ChemBridge	5222116
1579 A14	X	393	400	-0.48647896	315	320	-0.83875975	2402188	-0.6391006	2611082	-0.41744264	experimental	ChemBridge	5173872
1579 A15	X	396	400	-0.47556125	396	400	-0.53519261	2224603	-1.0115431					

1579 B07	X		194	200	-1.21068706	235	240	-1.13857915	2704722	-0.00460707	3070665	0.53693504	W	experimental	ChemBridge	5228174
1579 B08	X		473	480	-0.19534003	514	520	-0.092959	3092872	0.80944576	2910233	0.20377929		experimental	ChemBridge	5236198
1579 B09	X		471	480	-0.2026185	793	800	0.95266114	3008069	0.63159153	3264861	0.94020567		experimental	ChemBridge	5229219
1579 B10	X		516	520	-0.03865295	355	360	-0.68885005	2855522	0.31166027	2833687	0.25248425		experimental	ChemBridge	5237897
1579 B11	X		355	360	-0.62476995	475	480	-0.23912096	2610673	-0.18185261	2944193	0.07430119		experimental	ChemBridge	5248474
1579 B12	X		554	560	0.094943814	675	680	0.51042753	2412977	-0.61647322	2478852	-0.69203365		experimental	ChemBridge	5238420
1579 B13	X		992	1000	1.69342379	713	720	0.65284174	2901163	0.40738147	3421559	1.26560733		experimental	ChemBridge	5249345
1579 B14	X		1513	1520	3.58946608	874	880	1.25622828	2413567	-0.61523584	2380535	-0.89620036		experimental	ChemBridge	5240462
1579 B15	X		472	480	-0.19897927	474	480	-0.2428687	2946283	0.50201	2726647	-0.17745844		experimental	ChemBridge	5251390
1579 B16	X		474	480	-0.19170079	273	280	-0.99616494	2696649	-0.02153828	2665253	-0.30495024		experimental	ChemBridge	5240581
1579 B17	X		594	600	0.2450076	475	480	-0.23912096	3163854	0.95831372	5200085	-0.64794085		experimental	ChemBridge	5254762
1579 B18	X		431	440	-0.34818797	271	280	-1.00366042	2814721	0.22608982	2741717	-0.14574851		experimental	ChemBridge	5240775
1579 B19	X		587	600	0.21953295	1110	1120	2.1406955	4405861	3.56312971	4618570	3.75134021		experimental	ChemBridge	5255970
1579 B20	X		1392	1400	3.14911845	992	1000	1.69846189	3036598	0.69142436	2805599	-0.01350541		experimental	ChemBridge	5271431
1579 B21	X		348	360	-0.65024461	351	360	-0.70384102	2575382	-0.27586714	2617317	-0.40449493		experimental	ChemBridge	5230972
1579 B22	X		1553	1560	3.73503555	1195	1200	2.45925361	2768187	0.12849576	2732914	-0.16444429		experimental	ChemBridge	5272779
1579 B23	N		623	640	0.35054547	432	440	-0.40027389	2746565	0.08314872	2437878	-0.77712093		empty		
1579 B24	P		1262	2040	2.67601769	395	400	-0.53894036	2380423	-0.68474754	2186973	-1.29815441		experimental	ChemBridge	5269399
1579 C01	X		597	600	0.2592531	397	400	-0.53144487	2231921	-0.99619537	2463021	-0.72490856		experimental	ChemBridge	5265746
1579 C02	X		275	280	-0.91590889	474	480	-0.2428687	2707999	0.00226566	3365156	1.14856299		experimental	ChemBridge	5257407
1579 C03	X		316	320	-0.76670018	516	520	-0.08546352	2500759	-0.43237123	3104688	0.60758776		experimental	ChemBridge	5260746
1579 C04	X		276	280	-0.91226965	355	360	-0.68885005	2742907	0.07547693	2380575	-0.89611729		experimental	ChemBridge	5145962
1579 C05	X		396	400	-0.47556125	356	360	-0.68510231	2744056	0.07788669	2761950	-0.10414765		experimental	ChemBridge	5219646
1579 C06	X		275	280	-0.91590889	316	320	-0.83501201	3217787	1.07142544	3313651	1.04152379		experimental	ChemBridge	5147906
1579 C07	X		557	560	0.11035585	436	440	-0.38526292	3290923	1.2248109	2998444	0.38695971		experimental	ChemBridge	5219756
1579 C08	X		474	480	-0.1710079	354	360	-0.69259728	3177115	-0.98613554	3666369	0.48357113		experimental	ChemBridge	5234149
1579 C09	X		395	400	-0.47920049	475	480	-0.23912096	2323578	1.10954333	3035823	0.46458156		experimental	ChemBridge	5219940
1579 C10	X		355	360	-0.62476995	275	280	-0.98866945	2224801	-1.01112788	2852766	0.08444236		experimental	ChemBridge	5151224
1579 C11	X		395	400	-0.47920049	435	440	-0.38903066	2442888	-0.55374197	2816432	0.00899058		experimental	ChemBridge	5220215
1579 C12	X		274	280	-0.91954812	353	360	-0.69634554	2474037	-0.48841431	3537592	1.50656338		experimental	ChemBridge	5152539
1579 C13	X		394	400	-0.48283973	394	400	-0.5426881	2712581	0.01187532	3313354	1.04090704		experimental	ChemBridge	5222308
1579 C14	X		392	400	-0.4901182	554	560	0.05695069	3559840	1.78880072	3209073	0.82435538		experimental	ChemBridge	5173909
1579 C15	X		393	400	-0.48647896	472	480	-0.25036419	3602027	1.87727798	3801027	2.05361687		experimental	ChemBridge	5263084
1579 C16	N		674	680	0.53613254	954	960	0.73004783	1152327	0.8646625	1152327	0.8646625		experimental	ChemBridge	5174463
1579 C17	X		632	640	0.3832986	593	600	0.20311265	2692616	-0.02999655	2827919	0.03284467		experimental	ChemBridge	5263844
1579 C18	X		673	680	0.5325073	593	600	0.20311265	2036727	-1.40556862	2805803	-1.50974088		experimental	ChemBridge	5175091
1579 C19	X		1153	1160	2.27934089	873	880	1.25248054	2635417	-0.14995792	1987204	-1.71299803		experimental	ChemBridge	5264570
1579 C20	X		549	560	0.08124196	352	360	-0.70009328	3360550	1.37083707	2770851	-0.08566368		experimental	ChemBridge	5175698
1579 C21	X		511	520	-0.05704904	274	280	-0.99241719	2638743	-0.14298242	2688578	-0.25651316		experimental	ChemBridge	5265368
1579 C22	X		592	600	0.23772913	433	440	-0.39652614	2867372	0.33651284	2740882	-0.14789781		experimental	ChemBridge	5176658
1579 C23	N		593	600	-0.48647896	396	400	-0.53613254	2531723	0.36743157	3666369	0.48357113		empty		
1579 C24	X		591	600	0.23408989	396	400	-0.53519261	2717096	-1.06932257	2678762	-0.31635294		empty		
1579 D01	X		235	240	-1.06147835	396	400	-0.53519261	2261770	-0.93359415	2371122	-0.91574755		experimental	ChemBridge	5224601
1579 D02	X		515	520	-0.04249209	555	560	0.06069844	2797603	0.19018886	2956280	0.29940125		experimental	ChemBridge	5232534
1579 D03	X		394	400	-0.48283973	393	400	-0.54643584	2868935	0.33979086	2920656	0.22542386		experimental	ChemBridge	5226242
1579 D04	X		315	320	-0.77033942	355	360	-0.68885005	2720020	0.02747686	2898278	0.17895334		experimental	ChemBridge	5233964
1579 D05	X		516	520	-0.03865295	516	520	-0.08546352	2947824	0.50524188	2913284	0.21011504		experimental	ChemBridge	5226796
1579 D06	X		275	280	-0.786018	354	360	-0.98866945	2594706	0.23339662	3021930	0.43371113		experimental	ChemBridge	5234149
1579 D07	X		195	200	-1.20704782	396	400	-0.53519261	2841095	0.28140305	2818030	-0.41197906		experimental	ChemBridge	5228174
1579 D08	X		556	560	0.10671661	475	480	-0.23912096	3103469	0.83167047	3031663	0.45594284		experimental	ChemBridge	5236221
1579 D09	X		354	360	-0.62840919	395	400	-0.53894036	3069604	0.76064664	3077524	0.55117855		experimental	ChemBridge	5229359
1579 D10	X		555	560	0.10307737	475	480	-0.23912096	3046670	0.712548	3123506	0.64666553		experimental	ChemBridge	5238120
1579 D11	X		554	560	0.09943814	633	640	0.35302235	2900761	0.40653837	2861616	0.10282042		experimental	ChemBridge	5248554
1579 D12	X		716	720	0.68899448	555	560	0.05695069	33279439	3352485	1.12216712			experimental	ChemBridge	5238436
1579 D13	X		353	360	-0.63204843	494	500	-0.05695069	3391296	1.43531954	2864365	0.10852904		experimental	ChemBridge	5245691
1579 D14	X		514	520	-0.04613133	352	360	-0.70009328	2729640	0.04765254	3432523	1.28837536		experimental	ChemBridge	5240463
1579 D15	X		875	880	1.2676331	915	920	1.40988572	3462052	1.58371351	3313057	1.04029028		experimental	ChemBridge	5251526
1579 D16	X		392	400	-0.4901182	632	640	0.34927461	2910512	0.42698879	3142582	0.68627907		experimental	ChemBridge	5240604
1579 D17	X		795	800	0.97649417	514	520	-0.092959	2404600	-0.634042	2497628	-0.65304309		experimental	ChemBridge	5254941
1579 D18	X		313	320	-0.77761789	594	600	0.20686039	2720797	0.02910644	3000371	0.39096135		experimental	ChemBridge	5240801
1579 D19	X		512	520	-0.0534098	392	400	-0.55018358	2554583	-0.31948812	2819512	0.01538656		experimental	ChemBridge	5256075
1579 D20	X		791	800	0.96193722	674	680	0.50667979	2628882	-0.16366354	2669740	-0.29563246		experimental	ChemBridge	5271443
1579 D21	X		1674	1680	4.17538318	955	960	1.55979542	2609602	-0.20409878	2774165	-0.07878178		experimental	ChemBridge	5231049
1579 D22	X		391	400	-0.49375744	354	360	-0.69259728	2820371	0.23793936	2618458	-0.40212551		experimental	ChemBridge	5272969
1579 D23	N		474	480	-0.19170079	553	560	0.05320295	2498051	-0.43805062	2775804	-0.07536782		empty		
1579 D24	P		513	520	-0.04977056	516	520	-0.08546352	2458504	-0.5209911	2553048	-0.537957		empty		
1579 E01	X		517	520	-0.03521362	316	320	-0.83501201	2286783	-0.8811353	2498786	-0.65063837		experimental	ChemBridge	5269447
1579 E02	X		633	640	0.38693783	513	520	-0.09670675	3064777	0.75052315	2952458	0.29146442		experimental	ChemBridge	5265763
1579 E03	X		875	880	1.2676331	1075	1080	2.00952451	2449214	-0.43561151	2964300	0.31611801		experimental	ChemBridge	5270430
1579 E04	X		475	480	-0.18806156	354	360	-0.69259728	3042314	0.70341232	3145113	0.70378703		experimental	ChemBridge	5145143
1579 E05	X		395	400	-0.47920049	395	400	-0.53894036	3064511	0.74996527	2785017	-0.0562463		experimental	ChemBridge	5219672
1579 E06	X		356	360	-0.62113072	516	520	-0.08546352	3688453	2.05853607	3238768	0.88602051		experimental	ChemBridge	5148699
1579 E07	X		277	280	-0.90863041	236	240	-1.13483141	3135022	0.89784542						

1579 F01	X	277	280	-0.90863041	356	360	-0.68510231	2729212	0.04675491	2568980	-0.50487235	experimental	ChemBridge	5224761
1579 F02	X	355	360	-0.62476995	516	520	-0.08546352	2826588	0.25097804	2831366	0.04000277	experimental	ChemBridge	5232548
1579 F03	X	315	320	-0.77033942	353	360	-0.69634554	3510438	1.68519171	3115985	0.6310473	experimental	ChemBridge	5226263
1579 F04	X	276	280	-0.91226695	355	360	-0.68855005	2858948	0.31884549	2822644	0.02189052	experimental	ChemBridge	5234050
1579 F05	X	355	360	-0.62476995	436	440	-0.3528292	2348671	-0.75133985	2714041	-0.20362627	experimental	ChemBridge	5226860
1579 F06	X	277	280	-0.90863041	396	400	-0.53519261	2978302	0.56916228	3481143	1.38934045	experimental	ChemBridge	5234207
1579 F07	X	34	40	-1.79296492	35	40	-1.88812764	1009459	-3.56002033	1031243	-3.69816248	experimental	ChemBridge	5228304
1579 F08	X	435	440	-0.33363102	276	280	-0.98492171	2893659	0.39164361	3239717	0.88799122	experimental	ChemBridge	5237126
1579 F09	X	672	680	0.52886806	435	440	-0.38903066	3238644	1.11516806	3039809	0.47285896	experimental	ChemBridge	5229704
1579 F10	X	795	800	0.97649417	556	560	0.06444618	2748945	0.08814021	2864084	0.10794551	experimental	ChemBridge	5238177
1579 F11	X	355	360	-0.62476995	354	360	-0.6925978	3320656	1.08716884	3503209	0.50068562	experimental	ChemBridge	5248611
1579 F12	X	515	520	-0.04249209	875	880	1.25997602	3418773	1.49294605	2845455	0.27712954	experimental	ChemBridge	5238482
1579 F13	X	873	880	1.26035463	793	800	0.95266114	3094586	0.81304407	2876507	0.13374332	experimental	ChemBridge	5250120
1579 F14	X	594	600	0.2450076	632	640	0.34927461	3539873	1.74692466	2779953	-0.06676232	experimental	ChemBridge	5240468
1579 F15	X	475	480	-0.18806156	675	680	0.51042753	2836948	0.27270569	3677811	1.79774448	experimental	ChemBridge	5252736
1579 F16	X	434	440	-0.33727026	514	520	-0.092959	2802527	0.20051579	3019665	0.43102759	experimental	ChemBridge	5240637
1579 F17	X	513	520	-0.04977056	514	520	-0.092959	2006424	-1.469122	2406264	-0.84277109	experimental	ChemBridge	5255506
1579 F18	X	675	680	0.53978577	594	600	0.20686039	2449155	-0.54059842	2585560	-0.47044204	experimental	ChemBridge	5240810
1579 F19	X	233	240	-1.06875683	514	520	-0.092959	2691333	-0.03268733	3327516	1.07031608	experimental	ChemBridge	5256107
1579 F20	X	553	560	0.0957989	392	400	-0.55018358	2601523	-0.22104257	2907661	0.19843823	experimental	ChemBridge	5271547
1579 F21	X	1154	1160	2.28298013	1354	1360	3.05514466	3038453	0.69531478	3855556	0.09023612	experimental	ChemBridge	5231058
1579 F22	X	631	640	0.37965936	514	520	-0.092959	2574536	-0.27764142	2648962	-0.3387804	experimental	ChemBridge	5273140
1579 F23	N	544	1040	0.06304577	474	480	-0.2428687	3097913	0.82001807	2912272	0.20801351	empty		
1579 F24	P	169228	613.944041		356	360	-0.68510231	2439514	-0.56081814	2408325	-0.83849118	empty		
1579 G01	X	236	240	-1.05783912	395	400	-0.53894036	2302707	-0.84773847	2566254	-0.5105332	experimental	ChemBridge	5269569
1579 G02	X	356	360	-0.62112695	435	440	-1.28446885	1926257	-1.6330588	1862562	-1.71461212	experimental	ChemBridge	5234825
1579 G03	X	276	280	-0.91226695	396	400	-0.53519261	2325203	-0.8219363	3167621	0.73829001	experimental	ChemBridge	5270838
1579 G04	X	275	280	-0.91590889	395	400	-0.53894036	2374769	-0.69660547	3216397	0.83956452	experimental	ChemBridge	5146013
1579 G05	X	716	720	0.68899448	356	360	-0.68510231	2621219	-0.17973487	2831074	0.0393964	experimental	ChemBridge	5219673
1579 G06	X	433	440	-0.3409095	274	280	-0.99241719	3111058	0.8475866	3222602	0.85244993	experimental	ChemBridge	5148700
1579 G07	X	956	960	1.56241127	877	880	1.26747151	3725823	2.13691081	2936211	0.25772563	experimental	ChemBridge	5219807
1579 G08	X	633	640	0.38693783	474	480	-0.2428687	2651564	-0.11609341	3105361	0.60898533	experimental	ChemBridge	5150868
1579 G09	X	672	680	0.52886806	634	640	0.35677009	2509957	-0.4130806	2753846	-0.12097655	experimental	ChemBridge	5220010
1579 G10	X	434	440	-0.3454873	675	680	-0.92507483	48425074	0.2680488	3296268	0.31804873	experimental	ChemBridge	5151174
1579 G11	X	195	200	-1.20704782	114	120	-1.59205599	1383172	-2.77624569	1357594	-3.02045659	experimental	ChemBridge	5220597
1579 G12	X	275	280	-0.91590889	395	400	-0.53894036	2551086	-0.32682225	2996922	0.3837991	experimental	ChemBridge	5152636
1579 G13	X	633	640	0.38693783	431	440	-0.40402163	2646626	-0.1264497	3250462	0.91030447	experimental	ChemBridge	5222726
1579 G14	X	274	280	-0.91954812	475	480	-0.23912096	2673759	-0.06954464	3373506	1.16581968	experimental	ChemBridge	5174382
1579 G15	X	355	360	-0.62476995	353	360	-0.69634554	3400992	1.4556546	2960344	0.30784062	experimental	ChemBridge	5263105
1579 G16	X	594	600	0.2450076	714	720	0.65658949	2791437	0.17725133	4041265	2.55249908	experimental	ChemBridge	5147689
1579 G17	X	640	640	0.39057707	714	714	0.65658949	2945799	0.5009893	3462083	1.28472161	experimental	ChemBridge	5264008
1579 G18	X	634	640	0.39057707	354	360	-0.6925978	2519668	-0.39271408	2658431	-0.31911992	experimental	ChemBridge	5157175
1579 G19	X	514	520	-0.04613133	514	520	-0.092959	2947074	0.50366894	2867013	0.11402792	experimental	ChemBridge	5264723
1579 G20	X	394	400	-0.48283973	354	360	-0.6925978	2894343	0.39307813	3125421	0.65064225	experimental	ChemBridge	5175910
1579 G21	X	432	440	-0.34454873	672	680	0.4991843	2880253	0.36352769	2985871	0.36085041	experimental	ChemBridge	5265459
1579 G22	X	632	640	-1.15357012	231	240	-1.15357012	2693923	-0.02725542	2467017	-0.7166104	experimental	ChemBridge	5259588
1579 G23	N	640	640	0.37238089	476	480	-0.23537322	2685023	-0.04592107	2610552	-0.41854324	empty		
1579 G24	P	1147	1640	2.25705447	1236	1240	2.25705447	2393303	-0.65773478	2723269	-0.20780446	empty		
1579 H01	X	827	880	1.27491158	1236	1240	2.25705447	2072725	0.275007133	2257216	1.82288664	experimental	ChemBridge	5225099
1579 H02	X	354	360	-0.62840919	514	520	-0.092959	2748900	0.08804583	2751588	-0.12566555	experimental	ChemBridge	5233087
1579 H03	X	356	360	-0.62113072	275	280	-0.98866945	2655588	-0.10765402	2970247	0.32840535	experimental	ChemBridge	5226315
1579 H04	X	476	480	-0.18442232	476	480	-0.23537322	2530851	-0.36926038	3096545	0.59067787	experimental	ChemBridge	5234058
1579 H05	X	354	360	-0.62840919	274	280	-0.99241719	1585604	-2.35169244	1704069	-2.30096086	experimental	ChemBridge	5227184
1579 H06	X	395	400	-0.47920049	596	600	0.21435588	2959964	0.53070266	3371196	1.16102269	experimental	ChemBridge	5234414
1579 H07	X	273	280	-0.92318736	312	320	-0.85000298	2924823	0.45700273	2887135	0.1558136	experimental	ChemBridge	5228398
1579 H08	X	434	440	-0.33727026	434	440	-0.3927784	2823699	0.24491905	3632968	1.70462276	experimental	ChemBridge	5237184
1579 H09	X	873	880	1.26035463	753	760	0.80275144	2687122	-0.04151891	2732294	-0.16573179	experimental	ChemBridge	5229753
1579 H10	X	953	960	1.55149356	833	840	1.10257084	2177389	-1.11056334	2079649	-1.52102521	experimental	ChemBridge	5238197
1579 H11	X	515	520	-0.04249209	915	920	-0.04988572	2996386	0.6078092	3458761	1.34286162	experimental	ChemBridge	5248627
1579 H12	X	393	400	-0.48647896	350	360	-0.70758877	2796614	0.18811467	3073276	0.54235708	experimental	ChemBridge	5238490
1579 H13	X	955	960	1.55877203	1355	1360	3.0588924	2911125	0.42827441	2505365	-0.63697631	experimental	ChemBridge	5250809
1579 H14	X	313	320	-0.77761789	392	400	-0.55018358	2915198	0.43681656	3472374	1.3711306	experimental	ChemBridge	5240469
1579 H15	X	395	400	-0.47920049	435	440	-0.38903066	3077055	0.77627335	3463904	1.35354166	experimental	ChemBridge	5225258
1579 H16	X	635	640	0.39421631	514	520	-0.092959	2617103	-0.18836721	3241184	0.89103762	experimental	ChemBridge	5240660
1579 H17	X	234	240	-1.06511759	314	320	-0.84250749	2334376	-0.78132023	2116946	-1.44357364	experimental	ChemBridge	5255544
1579 H18	X	351	360	-0.6393269	353	360	-0.69634554	2894423	0.39324592	3144204	0.68964734	experimental	ChemBridge	5240812
1579 H19	X	715	720	0.68535524	835	840	1.11006632	2830624	0.2594426	3092572	0.58242748	experimental	ChemBridge	5256116
1579 H20	X	513	520	-0.04977056	434	440	-0.3927784	2824433	0.24645844	3000828	0.39191037	experimental	ChemBridge	5271705
1579 H21	X	633	640	0.38693783	631	640	0.34552686	2407582	-0.62778796	2709372	-0.21333199	experimental	ChemBridge	5231125
1579 H22	X	952	960	1.54785432	1555	1560	3.80844989	2201231	-1.0675038	2923269	0.86572809	experimental	ChemBridge	5273335
1579 H23	X	553	560	0.0957989	311	320	-0.85375072	2111776	0.84909243	2685780	-0.2623253	experimental	ChemBridge	5273335
1579 H24	P	432	440	-0.34454873	597	600	0.21810362	2473028	-0.49053045	2570961	-0.50075857	empty		
1579 I01	X	512	520	-0.0534098	393	400	-0.54643584	2429221	-0.58240527	2816668	0.00948066	experimental	ChemBridge	5269773
1579 I02	X	435	440	-0.33363102	395	400	-0.53894036	2691739	-0.03183585	2781833	-0.06285828	experimental	ChemBridge	5266089
1579 I03	X	395	400	-0.47920049	395	400	-0.53894036	2518249	-0.3956901	3307446	1.02863839	experimental	ChemBridge	5270526
1579 I04	X	395	400	-0.47920049	514	520	-0.092959	2929382	0.46656415	3412338	1.24645885	experimental	ChemBridge	5146515
1579 I05	X	595	600	0.24864684	596									

1579 I19	X	349	360	-0.64660537	473	480	-0.24661644	2749959	0.09026684	2853826	0.08664358	experimental	ChemBridge	5265083
1579 I20	X	754	760	0.82728547	393	400	-0.54643584	2866605	0.33490424	2784988	-0.05630655	experimental	ChemBridge	5175983
1579 I21	X	391	400	-0.49375744	392	400	-0.55018358	2404119	-0.63505078	2237004	-1.19417615	experimental	ChemBridge	5265619
1579 I22	X	873	880	1.26035463	672	680	-0.4991843	2293692	-0.6666543	2580003	-0.48198188	experimental	ChemBridge	5259601
1579 I23	N	353	360	-0.63204843	554	560	0.05695069	2552920	-0.36492111	2604027	-0.44019197	empty		
1579 I24	P	396	400	-0.47556125	435	440	-0.38903066	2424427	-0.59245955	2466877	-0.17295348	empty		
1579 J01	X	1596	1600	3.89152273	917	920	1.4173812	2352814	-0.74265089	2204258	-1.26222601	experimental	ChemBridge	5225597
1579 J02	X	352	360	-0.63568766	394	400	-0.5426881	2810061	0.21631657	3045460	0.48459392	experimental	ChemBridge	5233731
1579 J03	X	434	440	-0.33277026	434	440	-0.3927784	3188148	1.00926464	2988884	0.36710726	experimental	ChemBridge	5226712
1579 J04	X	231	240	-1.0760353	470	480	-0.25785967	2852220	0.3047351	3312785	1.03972544	experimental	ChemBridge	5234059
1579 J05	X	354	360	-0.62840919	353	360	-0.69634554	3125948	0.87881485	3079063	0.55437446	experimental	ChemBridge	5232766
1579 J06	X	875	880	1.26035371	834	840	1.10631858	3378543	1.40857313	3744916	0.62612572	experimental	ChemBridge	5234833
1579 J07	X	514	520	-0.04613133	591	600	0.19561717	3510735	1.68581459	2862171	0.10397294	experimental	ChemBridge	5228552
1579 J08	X	356	360	-0.62113072	555	560	0.06069844	3053932	0.72777832	2970473	0.32887467	experimental	ChemBridge	5237501
1579 J09	X	315	320	-0.77033942	274	280	-0.99241719	3424095	1.50410768	3099961	0.59777116	experimental	ChemBridge	5229970
1579 J10	X	516	520	-0.03885285	674	680	0.50667979	2874722	0.35192773	3043637	0.48080824	experimental	ChemBridge	5238266
1579 J11	X	394	400	-0.48283973	573	600	0.20311265	2576943	-0.27259331	3003055	0.39653499	experimental	ChemBridge	5248694
1579 J12	X	353	360	-0.63204843	292	280	-0.99991268	2822461	0.24232264	2854890	0.0888531	experimental	ChemBridge	5238755
1579 J13	X	992	1000	1.69342379	794	800	0.95640888	3102095	0.82878883	2744916	-0.13952073	experimental	ChemBridge	5250822
1579 J14	X	473	480	-0.19534003	394	400	-0.5426881	2838400	0.27575092	3138250	0.67728317	experimental	ChemBridge	5240489
1579 J15	X	315	320	-0.77033942	516	520	-0.08546352	3162861	0.95623114	3375194	1.169325	experimental	ChemBridge	5253429
1579 J16	X	595	600	0.24864684	314	320	-0.84250749	2760354	0.11206789	2905769	0.19450927	experimental	ChemBridge	5240668
1579 J17	X	354	360	-0.62840919	515	520	-0.08921126	3412926	1.48068335	3110771	0.62021982	experimental	ChemBridge	5256483
1579 J18	X	471	480	-0.2026185	473	480	-0.24661644	2689463	-0.03660922	2774325	-0.07844952	experimental	ChemBridge	5240815
1579 J19	X	594	600	0.2450076	353	360	-0.69634554	3014388	0.64484413	3061254	0.517392	experimental	ChemBridge	5256200
1579 J20	X	800	810	0.9692157	574	600	0.20057677	1865142	-1.7613032	2175961	-1.4759826	experimental	ChemBridge	5272235
1579 J21	X	834	840	1.18705444	994	1000	0.70591877	2894253	-0.39289344	2964604	0.31668701	experimental	ChemBridge	5231142
1579 J22	X	672	680	0.52886806	392	400	-0.55018358	2732128	0.05287053	3128728	0.65750963	experimental	ChemBridge	5273636
1579 J23	N	433	440	-0.3409095	554	560	0.05695069	2887582	0.37889854	2742331	-0.1448879	empty		
1579 J24	P	596	600	0.25228608	475	480	-0.23912096	2554870	-0.31888621	2524248	-0.59776356	empty		
1579 K01	X	473	480	-0.19534003	354	360	-0.6925978	1464685	-2.60529145	1751768	-2.20190833	experimental	ChemBridge	5269914
1579 K02	X	313	320	-0.77761789	474	480	-0.2428687	2559245	-0.30971068	2980738	0.35019114	experimental	ChemBridge	5266651
1579 K03	X	991	1000	1.68978455	790	800	0.94141791	2814297	0.22520058	2804333	-0.01613441	experimental	ChemBridge	5270556
1579 K04	X	1874	1900	3.20323081	1494	1880	1.90323081	2787909	0.1698805	2897580	0.1594535	experimental	ChemBridge	5146371
1579 K05	X	472	480	-0.19897927	350	360	-0.70758877	3230087	1.09722178	2812381	0.0005782	experimental	ChemBridge	5219711
1579 K06	X	234	240	-1.06511759	633	640	0.35302235	3142469	0.91346374	3644886	1.72937188	experimental	ChemBridge	5149499
1579 K07	X	316	320	-0.76670018	554	560	0.05695069	3325274	1.296854	3432556	1.28844388	experimental	ChemBridge	5219813
1579 K08	X	276	280	-0.91226965	394	400	-0.5426881	3805938	2.30493308	3539478	1.51047988	experimental	ChemBridge	5151048
1579 K09	X	356	360	-0.62113072	434	440	-0.3927784	2780444	0.15420192	3006755	0.40421847	experimental	ChemBridge	5220072
1579 K10	X	314	320	-0.77397866	592	600	0.1936491	2724737	0.03736966	2901280	0.18518734	experimental	ChemBridge	5152010
1579 K11	X	840	850	0.9577677	594	600	0.20057677	2744923	0.07970502	3234822	1.03427626	experimental	ChemBridge	5220779
1579 K12	X	311	320	-0.78489637	472	480	-0.25036419	2789962	0.17416367	3479419	1.38576037	experimental	ChemBridge	5153845
1579 K13	X	1474	1480	3.44753585	1074	1080	2.00577677	3016816	0.64993629	3277473	0.96639596	experimental	ChemBridge	5223930
1579 K14	X	312	320	-0.78125713	353	360	-0.69634554	3327149	1.30078637	3616142	1.66968161	experimental	ChemBridge	5174592
1579 K15	X	276	280	-0.91226965	355	360	-0.68885005	3329073	1.30482151	3766740	1.98185523	experimental	ChemBridge	5263294
1579 K16	X	395	400	-0.47920049	435	440	-0.38903066	3369873	1.39038986	3047945	0.48975431	experimental	ChemBridge	5174705
1579 K17	X	555	560	0.10307737	554	560	0.05695069	3234751	1.10700342	3157886	0.71805961	experimental	ChemBridge	5264050
1579 K18	X	13	20	0.67807677	594	600	0.20057677	2260855	-0.93551314	3079709	-1.27793647	experimental	ChemBridge	5175195
1579 K19	X	594	600	0.2450076	395	400	-0.53894036	0.1811404	0.9348177	3398844	0.21843699	experimental	ChemBridge	5264899
1579 K20	X	354	360	-0.62840919	193	200	-1.29598433	3113588	0.85289268	2614134	-0.4111048	experimental	ChemBridge	5175989
1579 K21	X	354	360	-0.62840919	314	320	-0.84250749	3108622	0.84247767	3065495	0.52619893	experimental	ChemBridge	5265623
1579 K22	X	552	560	0.09215966	353	360	-0.69634554	3107025	0.83912834	2935863	0.25700297	experimental	ChemBridge	5259647
1579 K23	N	714	720	0.681716	594	600	0.20686039	3046764	0.71274514	2820901	0.01827098	empty		
1579 K24	P	671	680	0.52522883	553	560	0.05320295	3309843	1.26449113	2925824	0.23615582	empty		
1579 L01	X	435	440	-0.33363102	715	720	0.66033723	2314169	-0.82369964	2667886	-0.29948251	experimental	ChemBridge	5225809
1579 L02	X	475	480	-0.18806156	673	680	0.50293205	2741073	0.07163055	2887680	0.1594535	experimental	ChemBridge	5233771
1579 L03	X	473	480	-0.19534003	633	640	0.35302235	3179510	0.99114848	3426573	1.27601949	experimental	ChemBridge	5226730
1579 L04	X	352	360	-0.63568766	390	400	-0.55767907	2374105	-0.69799805	2347481	-0.96484084	experimental	ChemBridge	5234071
1579 L05	X	393	400	-0.48647896	514	520	-0.092959	3393702	1.44036555	3651579	1.74327068	experimental	ChemBridge	5227793
1579 L06	X	435	440	-0.33363102	552	560	0.04945521	2826975	0.25178968	3351158	1.11941145	experimental	ChemBridge	5235017
1579 L07	X	235	240	-1.06147835	354	360	-0.6925978	3088639	0.80056805	3517154	1.46412149	experimental	ChemBridge	5228759
1579 L08	X	476	480	-0.18442232	434	440	-0.3927784	2892342	0.38888151	3161409	0.72537553	experimental	ChemBridge	5237681
1579 L09	X	395	400	-0.47920049	435	440	-0.38903066	3368993	2.01772333	3234822	0.87782618	experimental	ChemBridge	5220145
1579 L10	X	316	320	-0.76670018	433	440	-0.39652614	279520	-0.89636772	2094607	-1.48996318	experimental	ChemBridge	5238286
1579 L11	X	354	360	-0.62840919	433	440	-0.39652614	3685601	2.05255468	3325537	1.06620646	experimental	ChemBridge	5248791
1579 L12	X	436	440	-0.32999179	434	440	-0.3927784	2932861	0.47386053	3001397	0.39309196	experimental	ChemBridge	5240331
1579 L13	X	392	400	-0.4901182	593	600	0.20311265	3024309	0.66565109	3293957	1.0006269	experimental	ChemBridge	5251174
1579 L14	X	396	400	-0.47556125	434	440	-0.3927784	2800067	0.19535652	2729474	-0.17158785	experimental	ChemBridge	5240494
1579 L15	X	316	320	-0.76670018	355	360	-0.68885005	3546147	1.76008289	3180822	0.72415656	experimental	ChemBridge	5235382
1579 L16	X	436	440	-0.32999179	435	440	-0.08921126	2981388	0.57563444	3187216	0.01269526	experimental	ChemBridge	5232766
1579 L17	X	234	240	-1.06511759	354	360	-0.6925978	3298365	1.24041874	3029497	0.45144489	experimental	ChemBridge	5255697
1579 L18	X	795	800	0.97649417	595	600	0.21060813	1784130	-1.93533121	2042222	-1.59874674	experimental	ChemBridge	5240819
1579 L19	X	314	320	-0.77397866	394	400	-0.5426881	2431761	-0.57707822	3226863	0.8609246	experimental	ChemBridge	5256221
1579 L20	X	356	360	-0.62113072	555	560	0.06069844	2996925	0.60821962	3101239	0.60042551	experimental	ChemBridge	5272272
1579 L21	X	353	360	-0.63204843	472	480	-0.25036419	2588746	-0.24783931	2868593	0.11730897	experimental	ChemBridge	5232123
1579 L22	X	995	1000	1.7043415	954	960	1.55604768	2650440	-0.11845073	2839735	0.05738197	experimental	ChemBridge	5273734
1579 L23	N	426	440	-0.36638415	587									

1579 M13	X	395	400	-0.47920049	473	480	-0.24661644	2750269	0.09091699	2629156	-0.37990987	experimental	ChemBridge	5224020
1579 M14	X	275	280	-0.91590889	714	720	0.65658949	2256463	-0.94472433	3073984	0.54382733	experimental	ChemBridge	5174602
1579 M15	X	395	400	-0.47920049	594	560	0.05695069	2713740	0.01430605	2787541	-0.05100495	experimental	ChemBridge	5263301
1579 M16	X	555	560	0.10307737	554	560	0.05695069	2430744	-0.57921114	2867000	-0.91887005	experimental	ChemBridge	5175081
1579 M17	X	315	320	-0.77033942	594	400	-0.54268881	2639071	-0.14292452	3154521	0.71107118	experimental	ChemBridge	5264057
1579 M18	X	515	520	-0.04249209	514	520	-0.092959	2930015	0.46789172	2919769	0.2235819	experimental	ChemBridge	5175211
1579 M19	X	435	440	-0.33363102	594	600	0.20686039	2272433	-0.91123103	2000637	-1.68510284	experimental	ChemBridge	5265200
1579 M20	X	474	480	-0.19170079	473	480	-0.24661644	2779459	0.15213611	2724524	-0.1818671	experimental	ChemBridge	5176442
1579 M21	X	715	720	0.68535524	834	840	1.10631858	2592042	-0.24092673	2873454	0.12740341	experimental	ChemBridge	5265679
1579 M22	X	430	440	-0.35182721	629	640	0.33803138	2641287	-0.13764699	2677888	-0.27871219	experimental	ChemBridge	5259946
1579 M23	N	713	1320	0.67807677	819	1360	1.0463547	2499390	-0.43524239	2646685	-0.34350886	empty		
1579 M24	P	208265	208280	756.008922	185267	185280	692.313703	2285561	-0.88160089	2549451	-0.54436336	empty		
1579 N01	X	355	360	-0.62476995	515	520	-0.08921126	1949966	-1.5875293	2260462	-1.14554594	experimental	ChemBridge	5226161
1579 N02	X	436	440	-0.32999179	234	240	-1.14232689	1226819	-0.10415913	1307633	-3.12420643	experimental	ChemBridge	5233894
1579 N03	X	435	440	-0.33363102	314	320	-0.84250749	2408470	-0.62592559	2511845	-0.62351984	experimental	ChemBridge	5226757
1579 N04	X	436	440	-0.32999179	356	360	-0.68510231	2666203	-0.08539157	2572057	-0.4984826	experimental	ChemBridge	5234076
1579 N05	X	272	280	-0.9268266	435	440	-0.38903066	2316763	-0.81625933	2416688	-0.82112444	experimental	ChemBridge	5227857
1579 N06	X	594	600	0.2450076	313	320	-0.84625524	2737661	0.06447469	2854250	0.08752406	experimental	ChemBridge	5235222
1579 N07	X	394	400	-0.48283973	514	520	-0.092959	2462478	-0.51265658	2614425	-0.41050051	experimental	ChemBridge	5228446
1579 N08	X	634	640	0.39057707	914	920	1.40613798	2815734	0.22821435	3016986	0.42546434	experimental	ChemBridge	5237740
1579 N09	X	355	360	-0.62476995	313	320	-0.84625524	2580810	-0.26448319	2465174	-0.72043761	experimental	ChemBridge	5230305
1579 N10	X	356	360	-0.62113072	676	680	0.51417527	2443166	-0.55315893	2540535	-0.56394171	experimental	ChemBridge	5238311
1579 N11	X	394	400	-0.48283973	273	280	-0.99616494	2576542	-0.27343431	2458929	-0.73340608	experimental	ChemBridge	5248817
1579 N12	X	635	640	0.39421631	915	920	1.40988572	2723779	0.03536048	2926745	0.23806838	experimental	ChemBridge	5240447
1579 N13	X	755	760	0.8309247	553	560	0.05320295	2245417	-0.9678907	2578834	-0.48440937	experimental	ChemBridge	5251234
1579 N14	X	355	440	-0.62476995	594	594	0.20686039	3020516	0.65769617	2838325	0.54247034	experimental	ChemBridge	5254263
1579 N15	X	355	440	-0.62476995	394	400	-0.54268881	2481014	0.47377817	2828488	-0.58893794	experimental	ChemBridge	5235980
1579 N16	X	474	480	-0.19170079	594	600	0.20686039	2533012	-0.336472819	2616375	-0.4064511	experimental	ChemBridge	5240765
1579 N17	X	476	480	-0.18442232	514	520	-0.092959	2417579	-0.60682161	2508515	-0.63043497	experimental	ChemBridge	5255887
1579 N18	X	474	480	-0.19170079	434	440	-0.3927784	2734722	0.05831083	2702085	-0.2284643	experimental	ChemBridge	5240849
1579 N19	X	395	400	-0.47920049	555	560	0.06069844	2574934	-0.27680671	2676229	-0.28132665	experimental	ChemBridge	5256271
1579 N20	X	475	480	-0.18806156	354	360	-0.6925978	2549980	-0.32914183	2427336	-0.79901262	experimental	ChemBridge	5272415
1579 N21	X	393	400	-0.48647896	512	520	-0.10045449	2426069	-0.58901585	2553940	-0.53610466	experimental	ChemBridge	5231235
1579 N22	X	440	440	-0.33363102	511	520	-0.33363102	2114958	0.1991513	22045936	0.70459316	experimental	ChemBridge	5273969
1579 N23	N	508	520	-0.06796675	629	640	0.33803138	2387832	-0.66920891	2196986	-1.27736125	empty		
1579 N24	P	1314	1920	2.86525799	1180	1720	2.40330747	2632392	-0.15630214	2421275	-0.811599	empty		
1579 O01	X	596	600	0.25228608	955	960	1.55979542	2066812	-1.34247245	2196279	-1.27882942	experimental	ChemBridge	5270187
1579 O02	X	274	280	-0.91954812	512	520	-0.10045449	2131415	-1.20698293	2412986	-0.82881207	experimental	ChemBridge	5266833
1579 O03	X	435	440	-0.33363102	914	920	1.40613798	2310522	-0.83134836	2944696	0.27534572	experimental	ChemBridge	5271005
1579 O04	X	635	640	0.39421631	434	440	-0.3927784	2613604	-0.19570553	2994114	0.37796796	experimental	ChemBridge	5147629
1579 O05	X	440	440	-0.33363102	313	320	-0.84625524	2664189	-0.08961546	2613292	-0.213292	experimental	ChemBridge	5219753
1579 O06	X	434	440	-0.33727026	395	400	-0.53894036	2760597	0.11257753	2847729	0.07398245	experimental	ChemBridge	5150050
1579 O07	X	394	400	-0.48283973	274	280	-0.99241719	2320676	-0.81005274	2392702	-0.87093416	experimental	ChemBridge	5219826
1579 O08	X	875	880	1.2676331	794	800	0.95640888	2840170	0.27946308	2977946	0.34439323	experimental	ChemBridge	5151120
1579 O09	X	314	320	-0.77397866	394	400	-0.54268881	2418553	-0.60477888	2737503	-0.15491469	experimental	ChemBridge	5220184
1579 O10	X	315	320	-0.77033942	474	480	-0.2428687	2389842	-0.66499341	2768286	-0.09099002	experimental	ChemBridge	5152412
1579 O11	X	595	600	0.24864684	474	480	-0.2428687	2007550	-1.46676048	2396897	-0.86222276	experimental	ChemBridge	5220849
1579 O12	X	394	440	-0.33727026	354	360	-0.6925978	2411359	-0.6196659	2565428	-0.57247037	experimental	ChemBridge	5154263
1579 O13	X	313	320	-0.77033942	432	440	-0.372604	2326004	-0.7014660	2825571	-0.40965304	experimental	ChemBridge	5242228
1579 O14	X	316	320	-0.76670018	435	440	-0.38903066	2764613	0.12100014	2714789	-0.20208296	experimental	ChemBridge	5174617
1579 O15	X	355	360	-0.62476995	394	400	-0.54268881	2455312	-0.52768557	2748347	-0.13239586	experimental	ChemBridge	5263722
1579 O16	X	674	680	0.53614654	753	760	0.80275144	2864727	0.33096558	2654626	-0.32701844	experimental	ChemBridge	5175082
1579 O17	X	393	400	-0.48647896	472	480	-0.25036419	2658622	-0.10129092	2506102	-0.63544584	experimental	ChemBridge	5264100
1579 O18	X	475	480	-0.18806156	474	480	-0.2428687	2797274	0.18949886	2673972	-0.28684422	experimental	ChemBridge	5175471
1579 O19	X	394	400	-0.48283973	474	480	-0.2428687	2637272	-0.1460675	2564315	-0.51455976	experimental	ChemBridge	5265231
1579 O20	X	512	520	-0.0534098	513	520	-0.09570675	2744611	0.07905067	3631757	1.70210798	experimental	ChemBridge	5176475
1579 O21	X	875	880	1.2676331	952	960	1.54855219	2330040	-0.79041397	2404719	-0.84597946	experimental	ChemBridge	5265688
1579 O22	X	474	480	-0.19170079	1154	1160	2.30559617	2152876	-1.16197356	2479403	-0.69088943	experimental	ChemBridge	5259966
1579 O23	N	393	400	-0.48647896	352	360	-0.70009328	2180028	-1.10502866	2255007	-1.15687388	empty		
1579 O24	P	632	640	0.3832986	552	560	0.04945521	2280202	-0.89493739	2364272	-0.92997237	empty		
1579 P01	X	677	680	0.54706425	796	800	0.96390437	1746000	-2.01529976	1814689	-2.07124554	experimental	ChemBridge	5226197
1579 P02	X	556	560	0.10671661	474	480	-0.2428687	1962966	-1.56026488	2272251	-1.12106471	experimental	ChemBridge	5233908
1579 P03	X	435	440	-0.33363102	795	800	0.96015663	2186115	-1.09226262	2508619	-0.4630219	experimental	ChemBridge	5226758
1579 P04	X	554	560	0.09943814	353	360	-0.69634554	2186189	-1.09210742	2441084	-0.7704633	experimental	ChemBridge	5234077
1579 P05	X	996	1000	1.70798074	1236	1240	2.61291105	1976071	-1.53278024	2131748	-1.41283556	experimental	ChemBridge	5227932
1579 P06	X	474	480	-0.19170079	674	680	0.50667979	2146675	-1.17497869	2567798	-0.50732691	experimental	ChemBridge	5235788
1579 P07	X	516	520	-0.03885285	356	360	-0.68510231	2514464	-0.40362824	2567792	-0.50733937	experimental	ChemBridge	5229212
1579 P08	X	474	480	-0.19170079	475	520	-0.08921126	2265780	-0.92518412	2717790	-0.19585104	experimental	ChemBridge	5237886
1579 P09	X	676	680	0.54342501	516	480	-0.23537322	2382980	-0.67938484	2745631	-0.13803595	experimental	ChemBridge	5230789
1579 P10	X	435	440	-0.33363102	395	400	-0.53894036	2322652	-0.80059055	25651506	-1.01787098	experimental	ChemBridge	5238318
1579 P11	X	715	720	0.68535524	916	920	1.41363346	2175366	-1.13480612	2482713	-0.68801383	experimental	ChemBridge	5248991
1579 P12	X	434	440	-0.33727026	353	360	-0.69634554	1986265	-1.51140074	2022918	-1.63883375	experimental	ChemBridge	5240449
1579 P13	X	756	760	0.83456394	1276	1280	2.76282075	2369551	-0.70754899	2310340	-1.04196846	experimental	ChemBridge	5251243
1579 P14	X	476	480	-0.18442232	434	440	-0.3927784	2344898	-0.75925283	2396532	-0.86298072	experimental	ChemBridge	5240576
1579 P15	X	395	400	-0.47920049	395	400	-0.53894036	2471616	-0.49349179	2137007	-1.40191464	experimental	ChemBridge	5254323
1579 P16	X	835	840	1.12206364	914	920	1.40613798	2377685	-0.69048985	2462051	-0.72692288	experimental	ChemBridge	5240774
1579 P17	X	755	760	0										

1580 A07	X		434	440	-0.54907612	354	360	-0.92575781	2053931	-1.76352072	1666749	-2.24043595	experimental	ChemBridge	5242396
1580 A08	X		676	680	0.32645295	716	720	0.42141393	2552564	-0.85585291	2575687	-0.46942019	experimental	ChemBridge	5313216
1580 A09	X		555	560	-0.11131158	595	600	-0.02888381	2570714	-0.82281424	2845409	0.05611831	experimental	ChemBridge	5243212
1580 A10	X		516	520	-0.25240924	516	520	-0.32287985	2065001	-1.74154095	282353	-1.54721037	experimental	ChemBridge	5314659
1580 A11	X		355	360	-0.83488933	395	400	-0.77317759	2979310	-0.07904110	2253589	-0.01909019	experimental	ChemBridge	5244547
1580 A12	X		517	520	-0.24879135	476	480	-0.47173861	3372586	0.63684326	3327312	0.99507983	experimental	ChemBridge	5316327
1580 A13	X		356	360	-0.83127144	397	400	-0.76573465	2704794	-0.57874676	2457267	-0.70015506	experimental	ChemBridge	5244803
1580 A14	X		592	600	0.02255503	394	400	-0.77689606	2661322	-0.65787938	2762895	-0.10465569	experimental	ChemBridge	5258524
1580 A15	X		1750	1760	4.21206544	1194	1200	2.20027606	2067858	-1.73816923	1920493	-1.74602971	experimental	ChemBridge	5245939
1580 A16	X		1713	1720	4.07820356	674	680	0.26511223	3018138	-0.00836281	2937826	0.23618775	experimental	ChemBridge	5257462
1580 A17	X		351	360	-0.84936088	515	520	-0.32660132	2885197	-0.25035695	2586152	-0.44902972	experimental	ChemBridge	5301378
1580 A18	X		717	720	0.47478639	796	800	0.71913144	2823080	-0.35250742	2873553	0.10591082	experimental	ChemBridge	5256929
1580 A19	X		274	280	-1.12793831	395	400	-0.77317759	2892630	-0.23682657	2671279	-0.28228763	experimental	ChemBridge	5302168
1580 A20	X		516	520	-0.25240924	435	440	-0.62431883	3111887	0.16228965	2858205	0.08105061	experimental	ChemBridge	5256297
1580 A21	X		596	600	0.03702186	517	520	-0.31915838	2506883	-0.9390066	2496811	-0.62310575	experimental	ChemBridge	5302789
1580 A22	X		513	520	-0.26326291	395	400	-0.77317759	2207437	-1.48409185	2270152	-1.06473836	experimental	ChemBridge	5308761
1580 A23	N		1035	1040	1.625275	595	600	-0.02888381	2247563	-1.41105	2216219	-1.16982384	empty		
1580 A24	P		794	800	0.75336382	956	960	1.31456646	2105948	-1.66883354	1974419	-1.64095786	experimental	ChemBridge	5307887
1580 B01	X		595	600	0.03340397	472	480	-0.48662448	2145089	-1.59758469	2153707	-1.29162504	experimental	ChemBridge	5339928
1580 B02	X		634	640	0.17450163	1195	1200	2.20399753	2238094	-1.42828654	2194542	-1.21206029	experimental	ChemBridge	5306695
1580 B03	X		554	560	-0.11492947	352	360	-0.93320075	2940317	-0.15002134	2598141	-0.42566981	experimental	ChemBridge	5309581
1580 B04	X		515	520	-0.25602713	476	480	-0.47173861	2641877	-0.69327536	2870061	0.10415137	experimental	ChemBridge	5309581
1580 B05	X		275	280	-1.12432042	275	280	-1.21975385	3176061	0.27910638	2524991	-0.56819856	experimental	ChemBridge	5284096
1580 B06	X		472	480	-0.41159635	353	360	-0.92947928	2973723	-0.08921198	2716994	-0.19409127	experimental	ChemBridge	5310520
1580 B07	X		875	880	1.04641281	956	960	1.31456646	2553477	-0.85419097	2177447	-1.24536896	experimental	ChemBridge	5282818
1580 B08	X		280	280	1.13155623	313	320	-0.78338041	2666736	0.64802427	2173953	-1.05723232	experimental	ChemBridge	5281197
1580 B09	X		475	480	-0.40078608	354	360	-0.92575781	2840218	-0.33223278	2697058	-0.23294232	experimental	ChemBridge	5281197
1580 B10	X		314	320	-0.98322276	474	480	-0.47918154	3198672	0.32026546	2979970	0.31830302	experimental	ChemBridge	5286205
1580 B11	X		676	680	0.32645295	633	640	0.11253201	3188900	0.30247737	3006209	0.36942827	experimental	ChemBridge	5279533
1580 B12	X		314	320	-0.98322276	714	720	0.41397099	3272871	0.45533082	1875398	-1.83389484	experimental	ChemBridge	5259044
1580 B13	X		395	400	-0.69017378	234	240	-1.37233408	3876020	1.55235039	2680139	-0.26590121	experimental	ChemBridge	5326103
1580 B14	X		512	520	-0.26688008	314	320	-1.07461657	3246258	0.40688684	2645749	-0.33290824	experimental	ChemBridge	5340250
1580 B15	X		1272	1280	2.48271463	1153	1160	2.04769583	3969912	-1.72416316	2882419	0.12823026	experimental	ChemBridge	5325634
1580 B16	X		393	400	-0.7540997	484	480	-0.78062053	3132729	0.2002286	3093838	0.54016857	experimental	ChemBridge	5258615
1580 B17	X		516	520	-0.25240924	394	400	-0.77689606	3345637	0.58778767	2997855	0.35315096	experimental	ChemBridge	5320771
1580 B18	X		392	400	-0.70102744	434	440	-0.6280403	2976490	-0.08417518	2740990	-0.14733638	experimental	ChemBridge	5343522
1580 B19	X		835	840	0.90169726	474	480	-0.47918154	3429147	0.73980195	3275289	0.89371587	experimental	ChemBridge	5319676
1580 B20	X		594	600	0.02978608	835	840	0.86426873	2902308	-0.21920959	2756979	-0.11618269	experimental	ChemBridge	5331294
1580 B21	X		393	400	-0.69740956	312	320	-1.08205951	2914768	-0.1965285	2721878	-0.18457506	experimental	ChemBridge	5340205
1580 B22	X		795	800	0.75698171	756	760	0.57027268	2890152	-0.24133731	2613044	-0.39663213	experimental	ChemBridge	5335157
1580 B23	N		360	360	-0.85297877	433	433	0.71540997	2820441	-0.36823317	3572553	-0.82585899	empty		
1580 B24	P		1035	1040	1.625275	635	640	0.11997495	2373018	-1.18268272	2295075	-1.01617726	empty		
1580 C01	X		235	240	-1.26903597	316	320	-1.06717363	1436291	-2.88781844	1467102	-2.62943717	experimental	ChemBridge	5274216
1580 C02	X		435	440	-0.54545823	392	400	-0.78434199	2224783	-1.45251672	1898584	-1.78871819	experimental	ChemBridge	5303988
1580 C03	X		435	440	-0.54545823	515	520	-0.32660132	3141637	0.21644395	3460384	1.25436331	experimental	ChemBridge	5275858
1580 C04	X		315	320	-0.97960488	475	480	-0.47546008	2799748	-0.40590082	2551109	-0.51730908	experimental	ChemBridge	5305384
1580 C05	X		274	280	-1.12793831	394	400	-0.77689606	2885081	-0.25056811	2982823	0.32386194	experimental	ChemBridge	5277208
1580 C06	X		1115	1120	1.9047061	795	800	0.7540997	2636259	-0.70350187	2511141	-1.19140872	experimental	ChemBridge	5316333
1580 C07	X		473	480	-0.26688008	473	480	-0.48290301	2936333	-0.19369791	2958888	0.27722559	experimental	ChemBridge	5242388
1580 C08	X		395	400	-0.69017378	475	480	-0.47546008	2906324	-0.21189922	2786234	-0.05918093	experimental	ChemBridge	5313263
1580 C09	X		435	440	-0.54545823	555	560	-0.17774256	3383600	0.65689218	3253578	0.81959148	experimental	ChemBridge	5243223
1580 C10	X		435	440	-0.54545823	554	560	-0.18146403	3099345	0.1394593	2948410	0.25688101	experimental	ChemBridge	5314983
1580 C11	X		433	440	-0.55269401	712	720	0.40652805	3281246	0.47057593	3334493	1.00907161	experimental	ChemBridge	5244584
1580 C12	X		355	360	-0.83488933	594	600	-0.03260528	3244706	0.40406172	2846494	0.05910917	experimental	ChemBridge	5316383
1580 C13	X		474	480	-0.40436057	472	480	-0.48662448	2730504	-0.53194653	2778396	-0.07445284	experimental	ChemBridge	5244983
1580 C14	X		473	480	-0.40797846	393	400	-0.78062053	3132729	0.2002286	3093838	0.54016857	experimental	ChemBridge	5258615
1580 C15	X		272	280	-1.13517409	433	440	-0.63176177	3390521	0.66949057	3170429	0.68940192	experimental	ChemBridge	5246062
1580 C16	X		436	440	-0.54184034	475	480	-0.47546008	3018034	-0.00855212	2991216	0.34021524	experimental	ChemBridge	5257527
1580 C17	X		434	440	-0.54907612	515	520	-0.32660132	3088559	0.11982541	2968719	0.29638107	experimental	ChemBridge	5301508
1580 C18	X		515	520	-0.25602713	353	360	-0.92947928	2982449	-0.07332794	2847174	0.05955731	experimental	ChemBridge	5256974
1580 C19	X		474	480	-0.40436057	435	440	-0.62431883	3044900	0.04035239	2898057	0.15870004	experimental	ChemBridge	5302173
1580 C20	X		474	480	-0.40436057	473	480	-0.48290301	3051857	0.0530163	2531510	-0.55549665	experimental	ChemBridge	5256304
1580 C21	X		435	440	-0.54545823	515	520	-0.32660132	3286622	0.48036193	2975668	0.30992081	experimental	ChemBridge	5302841
1580 C22	X		474	480	-0.40436057	354	360	-0.92575781	2763692	-0.47153401	2830629	0.02732029	experimental	ChemBridge	5308775
1580 C23	N		515	520	-0.25602713	395	400	-0.77317759	2892072	-0.23784231	2822071	0.0106455	empty		
1580 C24	P		434	440	-0.54907612	276	280	-1.21603239	2523917	-0.9079994	2577485	-0.46591689	empty		
1580 D01	X		636	640	0.1817374	636	640	0.12369642	2302731	-1.31062701	2191575	-1.21784132	experimental	ChemBridge	5349825
1580 D02	X		355	360	-0.83488933	635	640	0.11997495	3071468	0.08871445	3060534	0.47527755	experimental	ChemBridge	5339932
1580 D03	X		355	360	-0.83488933	435	440	-0.62431883	2873368	-0.27188943	2626245	-0.37091071	experimental	ChemBridge	5306915
1580 D04	X		316	320	-0.54184034	354	360	-0.92203631	3466487	-0.80777247	3197526	-1.16651331	experimental	ChemBridge	5309694
1580 D05	X		316	320	-0.97588699	554	560	-0.18146403	3137358	0.20845483	2709024	-0.20862037	experimental	ChemBridge	5284384
1580 D06	X		353	360	-0.8421251	633	640	0.11253201	3341050	0.57943789	3320150	0.98112506	experimental	ChemBridge	5310891
1580 D07	X		476	480	-0.39712479	275	280	-1.21975385	3220161	0.35938215	2859668	0.07669194	experimental	ChemBridge	5283495
1580 D08	X		313	320	-0.98684065	393	400	-0.78062053	3464408	0.80398798	3453229	1.24042219	experimental	ChemBridge	5317886
1580 D09	X		355	360	-0.834										

1580 H19	X		633	640	0.17088374	952	960	1.29968059	2471849	-1.00277942	2562770	-0.49458826	experimental	ChemBridge	5320091
1580 H20	X		874	880	1.04279492	1193	1200	2.19655459	2946630	-0.13852971	2976154	0.31086776	experimental	ChemBridge	5332338
1580 H21	X		391	400	-0.70464533	430	440	-0.64292618	3184209	0.29393828	3411208	1.15854658	experimental	ChemBridge	5340218
1580 H22	X		994	1000	1.47694157	894	1000	1.45598228	31011730	0.14380074	2745932	-0.13770716	experimental	ChemBridge	5336225
1580 H23	N		513	520	-0.26326291	393	400	-0.78062053	3037649	0.02271533	2814434	-0.00441404	empty		
1580 H24	P		396	400	-0.68655589	436	440	-0.62059736	2460049	-1.02425911	2466106	-0.68293275	empty		
1580 I01	X		356	360	-0.83127144	677	680	0.27627664	2711362	-0.56679095	2528721	-0.56093086	experimental	ChemBridge	5274942
1580 I02	X		435	440	-0.54545823	434	440	-0.6280403	3212674	0.34575347	2650882	-0.32290687	experimental	ChemBridge	5304264
1580 I03	X		515	520	-0.25602713	435	440	-0.62431883	3139521	0.21259216	3037865	0.43110825	experimental	ChemBridge	5276083
1580 I04	X		553	560	-0.11854736	434	440	-0.6280403	3615473	1.07897347	3292043	0.92636012	experimental	ChemBridge	5306021
1580 I05	X		554	560	-0.11492947	434	440	-0.6280403	3117821	0.17309139	2878128	0.11986998	experimental	ChemBridge	5278212
1580 I06	X		875	880	1.04641261	873	880	1.00568454	3699062	1.23113156	3761847	1.85382276	experimental	ChemBridge	5312613
1580 I07	X		273	280	1.1315562	393	400	-0.78062053	3114747	0.16749575	3048419	0.45167214	experimental	ChemBridge	5242864
1580 I08	X		556	560	-0.10769369	555	560	-0.1774256	3838299	1.48458639	3452725	1.23944017	experimental	ChemBridge	5313915
1580 I09	X		395	400	-0.69017378	434	440	-0.6280403	3355785	0.6062602	2989574	0.33701589	experimental	ChemBridge	5243599
1580 I10	X		392	400	-0.70102744	632	640	0.10881054	2711925	-0.56576612	2433241	-0.74696684	experimental	ChemBridge	5315243
1580 I11	X		474	480	-0.40436057	432	440	-0.63548324	3147430	0.22698901	3080756	0.5279674	experimental	ChemBridge	5244651
1580 I12	X		1071	1080	1.755519	1513	1520	3.38742464	2779088	-0.44350848	2558612	-0.50268989	experimental	ChemBridge	5316794
1580 I13	X		1393	1400	2.92047917	912	920	1.15082183	3327148	0.55413191	2511863	-0.59377775	experimental	ChemBridge	5245438
1580 I14	X		392	400	-0.70102744	433	440	-0.63176177	3410746	0.706330638	3134578	0.61954822	experimental	ChemBridge	5258729
1580 I15	X		435	440	-0.54545823	553	560	-0.1851855	3598191	1.04751483	2995441	0.34844742	experimental	ChemBridge	5246601
1580 I16	X		314	320	-0.98322276	394	400	-0.77689906	3533297	0.92938748	3042245	0.43964244	experimental	ChemBridge	5258043
1580 I17	X		394	400	-0.69379167	554	560	-0.18146403	3296252	0.49789154	3133264	0.61698796	experimental	ChemBridge	5320122
1580 I18	X		515	520	-0.25602713	674	680	0.26511223	3025421	0.00489453	2563681	-0.49281322	experimental	ChemBridge	5257213
1580 I19	X		594	600	0.02978608	392	400	-0.78434199	2251638	-1.40363223	2171107	-1.25777221	experimental	ChemBridge	5302449
1580 I20	X		393	400	0.02616819	752	760	0.55530681	3108684	0.15645919	3612109	0.36143965	experimental	ChemBridge	5256357
1580 I21	X		394	400	-0.69379167	514	520	-0.32032279	3150393	0.23238227	28513026	0.06760829	experimental	ChemBridge	5301365
1580 I22	X		592	600	0.0225503	749	760	0.5442224	5024174	3.6432493	5150770	4.54798757	experimental	ChemBridge	5309245
1580 I23	N		354	360	-0.83850722	433	440	-0.63176177	2774053	-0.45267375	2600343	-0.42137933	empty		
1580 I24	P		516	520	-0.25240924	675	680	0.2688337	2568697	-0.82648581	2632449	-0.35882255	empty		
1580 J01	X		516	520	-0.25240924	395	400	-0.77317759	2746501	-0.502827	2541945	-0.53516463	experimental	ChemBridge	5308438
1580 J02	X		395	400	-0.69017378	315	320	-1.0708951	3278409	0.46541171	2865499	0.09526257	experimental	ChemBridge	5340140
1580 J03	X		473	480	-0.40797846	234	240	-1.37233408	2945027	-0.14144767	2821417	0.00937121	experimental	ChemBridge	5307139
1580 J04	X		593	600	0.02616819	435	440	-0.25964502	3177715	0.2811575	2761847	0.35184356	experimental	ChemBridge	5295246
1580 J05	X		313	320	-0.98684065	352	360	-0.9320075	3320860	0.54268579	3154699	0.65875288	experimental	ChemBridge	5285136
1580 J06	X		714	720	0.46393272	1114	1120	1.90255855	3429248	0.7399858	3723072	1.76619645	experimental	ChemBridge	5311281
1580 J07	X		475	480	-0.40074268	353	360	-0.92947928	3478921	0.83040618	2830310	0.02669873	experimental	ChemBridge	5283883
1580 J08	X		435	440	-0.54545823	434	440	-0.6280403	3818143	1.44789671	3396220	1.12934328	experimental	ChemBridge	5319266
1580 J09	X		433	440	-0.55269401	353	360	-0.92947928	3952283	1.69207287	3145287	0.64041412	experimental	ChemBridge	5282070
1580 J10	X		1155	1160	2.05942165	1035	1040	1.6085265	3758021	1.33845535	3585890	1.49890486	experimental	ChemBridge	5286753
1580 J11	X		593	600	0.02616819	392	400	-0.70102744	35212581	0.90251229	32088101	0.59478344	experimental	ChemBridge	5279836
1580 J12	X		593	600	0.02616819	435	440	-0.48662448	3291824	0.4898312	2997184	0.35184356	experimental	ChemBridge	5295246
1580 J13	X		431	440	-0.55992978	433	440	-0.63176177	3462678	0.80083884	3024361	0.40479645	experimental	ChemBridge	5328734
1580 J14	X		555	560	-0.11131158	473	480	-0.48290301	3140719	0.2147729	2887315	0.13776985	experimental	ChemBridge	5340566
1580 J15	X		553	560	-0.11854736	953	960	1.30340206	2758886	-0.48028243	2708294	-0.21104274	experimental	ChemBridge	5325862
1580 J16	X		754	760	0.60864827	634	640	0.11625348	2456661	-1.03042633	2142084	-1.31427182	experimental	ChemBridge	5341593
1580 J17	X		515	520	-0.25602713	434	440	-0.6280403	3636020	1.11637907	3462206	1.25791338	experimental	ChemBridge	5321443
1580 J18	X		195	200	-1.41375152	554	560	-0.18146403	2860545	-0.29252129	3617292	0.16772914	experimental	ChemBridge	5330391
1580 J19	X		475	480	-0.40074268	354	360	-0.92947928	32877029	2.63252527	2638726	-0.34659217	experimental	ChemBridge	5320163
1580 J20	X		554	560	-0.11492947	554	560	-0.18146403	3126676	0.18921025	2843524	0.05244549	experimental	ChemBridge	5333336
1580 J21	X		391	400	-0.70464533	268	280	-1.24580414	2941416	-0.14802081	2930687	0.2222778	experimental	ChemBridge	5340221
1580 J22	X		1154	1160	2.05580376	1755	1760	4.28802011	2748500	-0.49918819	3017340	0.39111641	experimental	ChemBridge	5337160
1580 J23	N		552	560	-0.12216525	430	440	-0.64292618	2675164	-0.63268262	3141546	0.63312498	empty		
1580 J24	P		515	520	-0.25602713	795	800	0.71540997	2781855	-0.43847167	2968882	0.29669866	empty		
1580 K01	X		596	600	0.03702186	756	760	0.57027268	2856176	-0.30318424	2682870	-0.26059001	experimental	ChemBridge	5274996
1580 K02	X		434	440	-0.54907612	513	520	-0.33404426	3249159	0.41216757	2917263	0.19612188	experimental	ChemBridge	5304275
1580 K03	X		832	840	0.89084359	714	720	0.41397099	2960821	-0.11269765	2614203	-0.39437388	experimental	ChemBridge	5276323
1580 K04	X		713	720	0.46031484	752	760	0.55538681	2636023	-0.70393146	2406513	-0.79904644	experimental	ChemBridge	5306444
1580 K05	X		635	640	0.17811952	875	880	1.01312748	3212152	0.34480327	3276595	0.89626054	experimental	ChemBridge	5278376
1580 K06	X		513	520	-0.26326291	312	320	-1.08205951	3530488	0.92427422	3068740	0.49126649	experimental	ChemBridge	5312990
1580 K07	X		395	400	-0.69017378	474	480	-0.47918154	3334208	0.56698332	3495177	1.32215556	experimental	ChemBridge	5243157
1580 K08	X		314	320	-0.98322276	632	640	0.10881054	3955238	1.6974519	3647287	1.61853354	experimental	ChemBridge	5313916
1580 K09	X		355	360	-0.83488933	475	480	-0.47546008	3518534	0.90251421	3231703	0.80879094	experimental	ChemBridge	5243608
1580 K10	X		472	480	-0.41159635	232	240	-1.37977702	3636558	1.11735476	3742357	1.80377221	experimental	ChemBridge	5315464
1580 K11	X		595	600	0.03340397	675	680	0.2688337	3629908	1.10524968	3291919	0.92611851	experimental	ChemBridge	5244667
1580 K12	X		393	400	-0.69740956	513	520	-0.33404426	3659321	1.15879053	3623008	0.57122724	experimental	ChemBridge	5316930
1580 K13	X		555	560	-0.11131158	474	480	-0.47918154	3566930	0.99061005	3390882	1.11894248	experimental	ChemBridge	5245612
1580 K14	X		474	480	-0.40436057	554	560	-0.18146403	3521502	0.9079169	3561795	1.45195707	experimental	ChemBridge	5258922
1580 K15	X		553	560	-0.11854736	633	640	0.11253201	3363710	0.62068617	3561509	1.45139982	experimental	ChemBridge	5248293
1580 K16	X		280	280	0.31559929	273	280	-1.22719679	4011463	1.79780896	1078252	0.50960526	experimental	ChemBridge	5258151
1580 K17	X		432	440	-0.55631919	393	400	-0.78062053	3390592	0.66961981	3227566	0.80073023	experimental	ChemBridge	5302073
1580 K18	X		316	320	-0.97598699	434	440	-0.6280403	3843192	1.49349318	3501144	1.33378193	experimental	ChemBridge	5257243
1580 K19	X		313	320	-0.98684065	473	480	-0.48290301	3238290	0.3923826	3485783	1.30385187	experimental	ChemBridge	5302483
1580 K20	X		473	480	-0.40797846	552	560	-0.18890697	4430638	2.56282839	3543231	1.41578614	experimental	ChemBridge	5256383
1580 K21	X		1074	1080	1.76637266	1									

1581 D01	X		912	920	-0.56956786	594	600	-0.90892926	2514905	-1.14558639	2348992	-1.41874639	experimental	ChemBridge	5420788
1581 D02	X		990	1000	-0.33266718	593	600	-0.91300574	3057054	-0.12554239	3222414	0.22915508	experimental	ChemBridge	5466967
1581 D03	X		907	920	-0.5847538	589	600	-0.92931169	3305113	0.34117634	3287933	0.35277099	experimental	ChemBridge	5421190
1581 D04	X		909	920	-0.57867942	753	600	-0.92076794	3899301	1.45913082	3772036	1.26613708	experimental	ChemBridge	5490085
1581 D05	X		989	1000	-0.33570436	592	600	-0.91708223	3585011	0.86783272	3550365	0.68856406	experimental	ChemBridge	5421546
1581 D06	X		1228	1240	0.39018363	632	640	-0.75402278	3061884	-0.11645483	2844985	-0.48294721	experimental	ChemBridge	5492700
1581 D07	X		1269	1280	0.51470834	831	840	0.05719799	3549078	0.80019229	3865942	1.44331127	experimental	ChemBridge	5422161
1581 D08	X		988	1000	-0.33874155	831	840	0.05719799	3675293	1.03766363	3389668	0.5447163	experimental	ChemBridge	5510924
1581 D09	X		987	1000	-0.34177874	709	720	-0.44013333	3774079	1.22352779	3233089	0.2492958	experimental	ChemBridge	5423411
1581 D10	X		1670	1680	1.73262083	1631	1640	3.31838703	3269218	0.27364052	3558541	0.86333211	experimental	ChemBridge	5511114
1581 D11	X		748	760	-1.06766673	990	1000	0.70535932	4214434	2.05204813	3258260	0.29678639	experimental	ChemBridge	5424337
1581 D12	X		950	960	-0.45415471	671	680	-0.59503981	3855693	1.37708312	3393364	1.66235552	experimental	ChemBridge	5511490
1581 D13	X		870	880	-0.69712977	512	520	-1.24320113	2617381	-0.95277956	2936598	-0.31009926	experimental	ChemBridge	5425267
1581 D14	X		828	840	-0.82469167	753	760	-0.26076794	3634384	0.96069405	3366535	0.50107084	experimental	ChemBridge	5352866
1581 D15	X		1110	1120	0.03179541	751	760	-0.26892091	3863975	1.39266556	3539929	0.82821651	experimental	ChemBridge	5460975
1581 D16	X		829	840	-0.82165448	791	800	-0.10586146	2880435	-0.457848	3294706	0.36554973	experimental	ChemBridge	5353999
1581 D17	X		950	960	-0.45415471	590	600	-0.92523252	3656361	1.0020434	3835601	1.38606634	experimental	ChemBridge	5462629
1581 D18	X		789	800	-0.94314201	712	720	-0.42790387	3501355	0.71040228	3136507	0.06707275	experimental	ChemBridge	5354186
1581 D19	X		708	720	-1.18915426	673	680	-0.58686864	3709383	1.10180338	3380332	0.52710189	experimental	ChemBridge	5465177
1581 D20	X		949	960	-0.45719189	551	560	-1.08421817	3582679	0.86341199	3270348	0.31959304	experimental	ChemBridge	5354801
1581 D21	X		948	960	-0.46022908	672	680	-0.59063333	3221680	0.18419859	2898922	-0.38118327	experimental	ChemBridge	5466114
1581 D22	X		1188	1200	0.2686961	672	680	-0.59063333	3209087	0.16050508	3057420	-0.08214216	empty	ChemBridge	5355791
1581 D23	N		1027	1040	-0.22029121	709	720	-0.44013333	3429820	0.57581041	3122892	0.04138508	empty		
1581 D24	P		1107	1120	0.02268385	474	480	-1.39810761	2964223	-0.30020232	2736555	-0.6875241	empty		
1581 E01	X		911	920	-0.57260505	754	760	-0.25669145	2639734	-0.91072278	2645705	-0.85893247	experimental	ChemBridge	5339434
1581 E02	X		857	860	-0.70762416	659	660	-0.60319227	3288252	0.30945266	3393484	0.48689269	experimental	ChemBridge	5428268
1581 E03	X		1469	1480	1.12145999	1512	1520	2.8338266	2285643	-0.35397576	3220774	0.22660806	experimental	ChemBridge	5322150
1581 E04	X		947	960	-0.46326627	710	720	-0.43605685	3163201	0.07417136	3885992	1.48113998	experimental	ChemBridge	5406722
1581 E05	X		789	800	-0.94314201	712	720	-0.42790387	3531079	0.76632748	3424961	0.61130425	experimental	ChemBridge	5324012
1581 E06	X		909	920	-0.57867942	712	720	-0.42790387	3423181	0.56331925	2876568	-0.42335898	experimental	ChemBridge	5411311
1581 E07	X		868	880	-0.70320414	671	680	-0.59503981	3494167	0.69687819	3170013	0.13028914	experimental	ChemBridge	5325325
1581 E08	X		988	1000	-0.33874155	712	720	-0.42790387	3586293	0.87021167	3601397	0.94418932	experimental	ChemBridge	5429930
1581 E09	X		1068	1080	-0.09576649	592	600	-0.91708223	2784482	-0.63838191	1654745	-2.78595906	experimental	ChemBridge	5425850
1581 E10	X		1006	1020	-0.34815933	673	680	-0.58233502	3495926	-0.5884576	3393952	0.29593392	experimental	ChemBridge	5430539
1581 E11	X		948	960	-0.46022908	510	520	-1.25135411	3749179	1.17667887	4115492	1.91414188	experimental	ChemBridge	5426756
1581 E12	X		987	1000	-0.34177874	792	800	-0.10178497	3408744	0.53615628	3800592	1.32001422	experimental	ChemBridge	5431283
1581 E13	X		1068	1080	-0.09576649	512	520	-1.24320113	2967764	-0.29353999	3342035	0.45484623	experimental	ChemBridge	5427607
1581 E14	X		1308	1320	0.63315868	591	600	-0.92115872	4027610	1.700542	3566030	0.86727347	experimental	ChemBridge	5431860
1581 E15	X		947	960	-0.46326627	992	1000	0.71351229	3642977	0.97686164	3123082	0.04174355	experimental	ChemBridge	5428236
1581 E16	X		1029	1040	-0.21421684	871	880	0.22025745	2185921	-1.76456412	2261224	-1.5843399	experimental	ChemBridge	5452138
1581 E17	X		947	960	-0.46022908	551	560	-0.46022908	3169468	0.08596261	3258364	0.22323068	experimental	ChemBridge	5428268
1581 E18	X		1149	1160	0.15024575	913	920	-0.39146987	3387258	0.49573072	3258815	0.95217336	experimental	ChemBridge	5451720
1581 E19	X		1228	1240	0.39018363	471	480	-1.41033707	3515058	0.73618424	3055850	-0.08510431	experimental	ChemBridge	5404196
1581 E20	X		1107	1120	0.02268385	912	920	0.38739338	3521479	0.74826524	3726109	1.17948576	experimental	ChemBridge	5417152
1581 E21	X		1109	1120	0.02875822	791	800	-0.10586146	3396688	0.51347313	3049103	-0.097834	experimental	ChemBridge	5404694
1581 E22	X		987	1000	-0.34177874	712	720	-0.42790387	3129779	0.01128844	2923658	-0.3345134	experimental	ChemBridge	5419706
1581 E23	N		1261	1280	0.49041084	672	680	-0.59063333	3311119	0.35247653	3175171	0.14002083	empty		
1581 E24	P		1765	1780	0.02115371	712	720	-0.42790387	2811076	-0.5884576	3165453	0.73017067	empty		
1581 F01	X		1351	1360	0.76373778	673	680	-0.58686864	2489526	-0.490181276	2686231	-0.50104442	experimental	ChemBridge	5420812
1581 F02	X		1107	1120	0.02268385	831	840	0.05719799	3121827	-0.00367311	3059274	-0.07779516	experimental	ChemBridge	5467378
1581 F03	X		1146	1160	0.14113419	869	880	0.21210447	3386249	0.49383233	3802086	1.32283297	experimental	ChemBridge	5421199
1581 F04	X		1147	1160	0.14417138	511	520	-1.24727762	3325065	0.37871569	3305668	0.38623194	experimental	ChemBridge	5490688
1581 F05	X		828	840	-0.82469167	633	640	-0.74994629	3471510	0.65424943	3807050	1.33219864	experimental	ChemBridge	5421562
1581 F06	X		908	920	-0.58171661	632	640	-0.75402278	2576642	-1.02942929	2953646	-0.27793449	experimental	ChemBridge	5493232
1581 F07	X		989	1000	-0.33570436	752	760	-0.26484442	3227103	0.19440187	4054016	1.79815397	experimental	ChemBridge	5424317
1581 F08	X		1028	1040	-0.21725402	752	760	-0.26484442	3364963	0.45378309	3928552	1.5582313	experimental	ChemBridge	5510934
1581 F09	X		1068	1080	-0.09576649	712	720	-0.42790387	3933931	1.52428657	4449226	2.543804	experimental	ChemBridge	5423531
1581 F10	X		948	960	-0.46022908	552	560	-1.08014168	3845018	1.3569983	3820413	1.35741086	experimental	ChemBridge	5511229
1581 F11	X		1307	1320	0.6301215	952	960	0.55045284	4042833	1.72918381	3428020	0.61707572	experimental	ChemBridge	5424487
1581 F12	X		1387	1400	0.87309656	950	960	0.54229986	3882022	1.42662068	3680169	1.09280991	experimental	ChemBridge	5511518
1581 F13	X		907	920	-0.5847538	831	840	0.05719799	3678041	1.04283395	3685085	1.10208502	experimental	ChemBridge	5425281
1581 F14	X		1107	1120	0.02268385	872	880	0.22433393	3657175	1.00357493	3743929	1.21310708	experimental	ChemBridge	5353414
1581 F15	X		1147	1160	0.14417138	671	680	-0.59503981	3021737	-0.19199072	2643486	-0.8631191	experimental	ChemBridge	5461285
1581 F16	X		1068	1080	-0.09576649	631	640	-0.75809926	3587277	0.87206305	3858939	1.43009858	experimental	ChemBridge	5354009
1581 F17	X		1029	1040	-0.21421684	752	760	-0.26484442	3882997	1.42845513	3890630	1.48989058	experimental	ChemBridge	5462997
1581 F18	X		907	920	-0.5847538	591	600	-0.92115872	3466209	0.64427569	3184349	0.15733714	experimental	ChemBridge	5354200
1581 F19	X		1107	1120	0.02268385	672	680	-0.59063333	3749908	1.17805047	3535190	0.81927535	experimental	ChemBridge	5465194
1581 F20	X		1227	1240	0.38714644	952	960	0.55045284	3770293	1.2164045	3098357	-0.00490556	experimental	ChemBridge	5356343
1581 F21	X		867	880	-0.70624133	711	720	-0.43198036	3202996	0.14904497	2808895	-0.55092379	experimental	ChemBridge	5468348
1581 F22	X		904	920	-0.59386537	669	680	-0.60319227	2904790	-0.41202448	3265633	0.73613833	experimental	ChemBridge	5355808
1581 F23	N		1443	1460	1.04317921	632	640	-0.75402278	3490721	1.6903946	3366521	-0.50104442	empty		
1581 F24	P		203061	203080	613.394998	671	680	-0.59503981	3193139	0.13049919	2719370	-0.71994735	empty		
1581 G01	X		909	920	-0.57867942	914	920	0.39554636	2887649	-0.44427498	2854216	-0.46553091	experimental	ChemBridge	5339462
1581 G02	X		1188	1200	0.2686961	750	760	-0.2729974	2517286	-1.14110658	2823681	-0.52314186	experimental	ChemBridge	5405

1581 G19	X	1027	1040	-0.22029121	672	680	-0.59096333	2926508	-0.37116244	2739063	-0.68279221	experimental	ChemBridge	5404210
1581 G20	X	1267	1280	0.50863397	511	520	-1.24727762	3329582	0.38721434	3100461	-0.00093591	experimental	ChemBridge	5417796
1581 G21	X	1024	1040	-0.22940278	708	720	-0.44420982	3423047	0.56306713	3089573	-0.0214785	experimental	ChemBridge	5404743
1581 G22	X	1660	1680	1.72654665	1631	1640	3.31838703	3304988	0.34094304	2783777	-0.68144509	experimental	ChemBridge	5419872
1581 G23	N	1060	1080	-0.120064	705	720	-0.45643928	3285748	0.30473767	3119864	0.03567209	empty		
1581 G24	P	1446	2040	1.05229066	1186	1600	1.50435063	2999750	-0.23335888	2624524	-0.89889506	empty		
1581 H01	X	1107	1120	0.02268385	711	720	-0.43198036	2791940	-0.62434981	2800362	-0.56713825	experimental	ChemBridge	5420834
1581 H02	X	1106	1120	0.01964666	671	680	-0.59503981	2826029	-0.56021195	2959588	-0.26621419	experimental	ChemBridge	5467386
1581 H03	X	1306	1320	0.6301215	710	720	-0.43605685	3167152	0.0816051	3779760	1.2807101	experimental	ChemBridge	5421235
1581 H04	X	1385	1400	0.86702218	830	840	0.05312151	3185164	0.11549437	3243875	0.26964594	experimental	ChemBridge	5490854
1581 H05	X	1102	1120	0.00749791	792	800	-0.10178497	3404213	0.52763128	3745423	1.21592584	experimental	ChemBridge	5412697
1581 H06	X	1306	1320	0.62708471	711	720	-0.43198036	3781735	1.23793242	3373053	0.51495331	experimental	ChemBridge	5493249
1581 H07	X	1185	1200	0.25958453	910	920	0.37924041	3188593	0.1407608	3295533	0.36711005	experimental	ChemBridge	5422355
1581 H08	X	1587	1600	1.4805342	1112	1120	1.20269064	4269373	2.15541491	4175484	2.0273299	experimental	ChemBridge	5510936
1581 H09	X	1025	1040	-0.22636559	630	640	-0.76217575	3124592	0.00152919	2987930	-0.21325023	experimental	ChemBridge	5423562
1581 H10	X	1229	1240	0.39322081	792	800	-0.10178497	2912564	-0.39739784	3236187	0.25514085	experimental	ChemBridge	5511232
1581 H11	X	787	800	-0.94921639	870	880	0.22025745	3707190	1.09767729	3414598	0.59175219	experimental	ChemBridge	5424584
1581 H12	X	1068	1080	-0.09576649	831	840	0.05312151	3440928	0.59670992	3928359	1.56107458	experimental	ChemBridge	5511528
1581 H13	X	1108	1120	0.02572104	751	760	-0.26892091	3061022	1.38710935	3450710	0.65888537	experimental	ChemBridge	5425369
1581 H14	X	1108	1120	0.02572104	791	800	-0.10586146	3562938	0.82626964	3741937	1.20934874	experimental	ChemBridge	5353428
1581 H15	X	987	1000	-0.34177874	791	800	-0.10586146	1927261	-2.25122845	1893801	-2.27756367	experimental	ChemBridge	5461568
1581 H16	X	1029	1040	-0.21421684	711	720	-0.43198036	2877267	-0.46380853	3096573	-0.00827147	experimental	ChemBridge	5354205
1581 H17	X	867	880	-0.70624133	831	840	0.05719799	3792610	1.25839355	3056422	-0.0840251	experimental	ChemBridge	5463110
1581 H18	X	987	1000	-0.34177874	751	760	-0.26892091	3736536	1.15289128	3381462	0.52923388	experimental	ChemBridge	5354336
1581 H19	X	907	920	-0.5847538	952	960	0.55045284	3728197	1.1372016	3801696	1.32209715	experimental	ChemBridge	5465378
1581 H20	X	1226	1240	0.38410925	830	840	0.05312151	3201596	0.14641089	3261766	0.22449814	experimental	ChemBridge	5355027
1581 H21	X	1587	1600	1.4805342	1310	1320	2.00983493	2071568	-1.9797322	1793402	-2.46698933	experimental	ChemBridge	5466418
1581 H22	X	1024	1040	-0.22940278	904	920	0.35478149	2761353	-0.68189873	2937731	-0.30796161	experimental	ChemBridge	5355880
1581 H23	N	1147	1160	0.14417138	1023	1440	0.83988336	3337633	0.40236216	3026945	-0.13963991	empty		
1581 H24	P	1147	1160	0.14417138	141427	141440	573.194865	2645069	-0.90068507	2919877	-0.34164708	empty		
1581 I01	X	2309	2320	3.67338412	1393	1400	2.34818329	2579121	-1.02476509	2565725	-1.00983222	experimental	ChemBridge	5339508
1581 I02	X	1024	1040	-0.22940278	749	760	-0.27707388	2924980	-0.37403735	3178192	0.14572061	experimental	ChemBridge	5406174
1581 I03	X	946	960	-0.46630346	871	880	0.22025745	3008426	-0.21703513	3273146	0.32487208	experimental	ChemBridge	5322281
1581 I04	X	1072	1080	-0.09576649	830	840	0.05312151	4748892	1.70744381	3234286	0.23249814	experimental	ChemBridge	5410408
1581 I05	X	2347	2360	3.78879727	671	680	-0.59503981	3482627	0.67516587	3039327	-0.12646684	experimental	ChemBridge	5324067
1581 I06	X	1102	1120	0.00749791	631	640	-0.75809926	3647055	0.98453432	3369374	0.50642723	experimental	ChemBridge	5411728
1581 I07	X	1266	1280	0.50559678	911	920	0.3833169	3678076	1.0428998	3253192	0.2872245	experimental	ChemBridge	5325563
1581 I08	X	1346	1360	0.74857184	789	800	-0.11401443	3123042	-0.00138711	3019900	-0.15293184	experimental	ChemBridge	5429985
1581 I09	X	1107	1120	0.02268385	911	920	0.3833169	2255215	-1.63418865	2501479	-1.13104634	experimental	ChemBridge	5426004
1581 I10	X	1107	1120	0.02268385	751	760	-0.26892091	3896359	1.4535955	3958875	1.61864968	experimental	ChemBridge	5430586
1581 I11	X	969	980	-0.79191889	750	760	-0.27520974	2988576	0.25438257	3254826	0.23249814	experimental	ChemBridge	5427373
1581 I12	X	987	1000	-0.34177874	710	720	-0.43605685	2864697	-0.48754587	302515542	0.2515542	experimental	ChemBridge	5433447
1581 I13	X	1068	1080	-0.09576649	711	720	-0.43198036	2943746	-0.33872944	2983656	-0.22131406	experimental	ChemBridge	5427733
1581 I14	X	1027	1040	-0.22029121	990	1000	0.70535932	3789616	1.25276039	3154331	0.10070162	experimental	ChemBridge	5431976
1581 I15	X	1108	1120	0.02572104	831	840	0.05719799	3453107	0.6196245	3646312	1.02893128	experimental	ChemBridge	5428340
1581 I16	X	1067	1080	-0.09880368	591	600	-0.92115872	3717644	1.11734631	3695323	1.12140124	experimental	ChemBridge	5452219
1581 I17	X	1427	1440	0.99458409	632	640	-0.75402278	3064503	-0.11512723	2927051	-0.32811176	experimental	ChemBridge	5429292
1581 I18	X	1505	1520	2.12148477	750	760	-0.27520974	2636161	-0.91744532	3147454	-0.62749815	experimental	ChemBridge	5454028
1581 I19	X	1067	1080	0.26565891	631	640	-0.75809926	3118128	-0.02486801	3064373	0.06902338	experimental	ChemBridge	5404210
1581 I20	X	1105	1120	0.01660947	590	600	-0.9252352	3149045	0.04753709	3128939	0.05279406	experimental	ChemBridge	5418134
1581 I21	X	1265	1280	0.50255959	907	920	0.36701095	3616170	0.92642473	3076707	-0.04575302	experimental	ChemBridge	5404831
1581 I22	X	1067	1080	-0.09880368	1109	1120	1.19046119	1874728	-2.35006838	1703378	-2.63683827	experimental	ChemBridge	5420319
1581 I23	N	1027	1040	-0.22029121	786	800	-0.12624389	3165940	0.07932474	3135607	0.0653747	empty		
1581 I24	P	1271	1280	0.52078272	1026	1440	0.85211282	2808126	-0.59389613	3075329	-0.04835292	empty		
1581 J01	X	1545	1560	1.3529723	949	960	0.53822338	2116830	-1.89455764	2462770	-1.20407933	experimental	ChemBridge	5420837
1581 J02	X	1144	1160	0.13505981	830	840	0.05312151	3095418	-0.05361119	3066213	-0.06555224	experimental	ChemBridge	5467706
1581 J03	X	1263	1280	0.49648521	828	840	0.04496854	3430618	0.57731184	3501533	0.75577406	experimental	ChemBridge	5421287
1581 J04	X	1386	1400	0.87005937	950	960	0.54229986	3437829	0.59087921	3402116	0.56820217	experimental	ChemBridge	5490920
1581 J05	X	1022	1040	-0.23547715	791	800	-0.10586146	3328570	0.38531028	3137558	0.06905569	experimental	ChemBridge	5421744
1581 J06	X	1107	1120	0.02268385	791	800	-0.10586146	3590761	0.87861813	3817038	1.35104319	experimental	ChemBridge	5493421
1581 J07	X	987	1000	-0.34177874	870	880	0.21618096	3742218	1.16358187	4111996	1.90754591	experimental	ChemBridge	5422614
1581 J08	X	908	920	-0.58171661	949	960	0.53822338	4359816	2.32558186	4151485	1.98205054	experimental	ChemBridge	5510398
1581 J09	X	867	880	-0.70624133	911	920	0.3833169	3424569	0.56593075	3371596	0.51061952	experimental	ChemBridge	5423756
1581 J10	X	1147	1160	0.14417138	710	720	-0.43605685	3484758	0.67917531	3743513	1.21338221	experimental	ChemBridge	5511264
1581 J11	X	946	960	-0.46630346	631	640	-0.75809926	3461489	0.63539509	3619270	0.97791064	experimental	ChemBridge	5424603
1581 J12	X	1308	1320	0.63315868	1192	1200	1.52880955	3645270	0.98117588	3325933	0.42446629	experimental	ChemBridge	5511543
1581 J13	X	947	960	-0.46326627	589	600	-0.92931169	3827675	1.32436774	3581889	0.90738322	experimental	ChemBridge	5425461
1581 J14	X	1108	1120	0.02572104	990	1000	0.70535932	3718268	1.11852035	3902674	1.51261422	experimental	ChemBridge	5353502
1581 J15	X	1068	1080	-0.09576649	749	760	-0.27707388	3497031	0.70226675	3483042	0.72088675	experimental	ChemBridge	5461629
1581 J16	X	1048	1060	-0.21725402	833	840	0.06535097	3227738	0.19159661	3696224	0.744552	experimental	ChemBridge	5354028
1581 J17	X	986	1000	-0.34841593	550	560	-0.08829465	3913767	0.8654327	3344852	0.46016132	experimental	ChemBridge	5463417
1581 J18	X	1586	1600	1.47749702	1272	1280	1.85492845	3088508	-0.06636223	3461551	0.68033928	experimental	ChemBridge	5354349
1581 J19	X	1065	1080	-0.10487806	709	720	-0.44013333	3272788	0.28035741	3298711	0.37310604	experimental	ChemBridge	5465506
1581 J20	X	1346	1360	0.74857184	909	920	0.37516393	2772761	-0.66043477	2595356	-0.95392686	experimental	ChemBridge	5355113
1581 J21	X	1067	1080	0.86702218	1468	1480	2.65391977	3058540	-0.12274651	2858216	-0.45798403	experimental	ChemBridge	5466647
1581 J22	X	1227	1240	0.38714644	1									

1581 K13	X	1068	1080	-0.09576649	751	760	-0.26892091	3421547	0.56024491	3491856	0.73751629	experimental	ChemBridge	5427748
1581 K14	X	988	1000	-0.33874155	1030	1040	0.86841877	3857467	1.38042087	3585936	0.91501877	experimental	ChemBridge	5432005
1581 K15	X	948	960	-0.46022908	990	1000	0.70535932	3266297	0.26814471	3628482	0.99529109	experimental	ChemBridge	5428361
1581 K16	X	1048	1040	-0.21725402	630	640	-0.76217575	4131107	1.89765982	4242598	2.15139512	experimental	ChemBridge	5452308
1581 K17	X	908	920	-0.58171661	792	800	-0.10172657	4253669	1.12568811	3772472	1.72696724	experimental	ChemBridge	5429302
1581 K18	X	1147	1160	0.14417138	629	640	-0.76625224	3602882	0.90142358	3494272	0.7420746	experimental	ChemBridge	5415575
1581 K19	X	987	1000	-0.34177874	871	880	0.22025745	3369939	0.46314534	3744530	1.214241	experimental	ChemBridge	5404356
1581 K20	X	1266	1280	0.50559678	829	840	0.04904502	4087340	1.81292296	3916480	1.53866225	experimental	ChemBridge	5418585
1581 K21	X	1226	1240	0.38410925	1029	1040	0.86434228	3871649	1.40710406	3624739	0.9882291	experimental	ChemBridge	5404845
1581 K22	X	1026	1040	-0.2233284	709	720	-0.44013333	3561668	0.82388015	3008765	-0.17394045	experimental	ChemBridge	5420394
1581 K23	N	1107	1120	0.02268385	670	680	-0.5991163	3382714	0.48718129	2922769	-0.33619069	empty		
1581 K24	P	1190	1200	0.27477047	992	1000	0.71351229	3583079	0.86416458	4151733	1.98251844	experimental		
1581 L01	X	1507	1520	1.23755915	670	680	-0.5991163	2893773	-0.43275278	2967060	-0.25262604	experimental	ChemBridge	5420840
1581 L02	X	1299	1320	0.60582399	826	840	0.03681556	3027231	-0.18165385	3060506	-0.07631975	experimental	ChemBridge	5467830
1581 L03	X	1061	1080	-0.11702681	867	880	0.2039515	3467773	0.64721833	3573456	0.89147252	experimental	ChemBridge	5421293
1581 L04	X	1866	1880	2.32790973	1191	1200	1.52473306	2698475	-0.8002026	3164064	0.11906505	experimental	ChemBridge	5491180
1581 L05	X	944	960	-0.47237784	828	840	0.04496854	3046682	-0.14505713	3314587	0.40305958	experimental	ChemBridge	5421949
1581 L06	X	908	920	-0.58171661	771	780	0.22025745	3248303	0.23428931	3615507	0.97081092	experimental	ChemBridge	5509643
1581 L07	X	988	1000	-0.33874155	830	840	0.05312151	3777422	1.22391759	4151733	1.98251844	experimental	ChemBridge	5422924
1581 L08	X	829	840	-0.82165448	830	840	0.05312151	3599135	0.89437367	3588394	0.91965632	experimental	ChemBridge	5510982
1581 L09	X	868	880	-0.70320414	751	760	-0.26892091	3694931	1.07461129	3728442	1.18388748	experimental	ChemBridge	5423282
1581 L10	X	1067	1080	-0.09880368	750	760	-0.2729974	3698163	1.08069314	3496691	0.74714799	experimental	ChemBridge	5511358
1581 L11	X	947	960	-0.46326627	792	800	-0.10178497	3949038	1.55271013	3638160	1.01355075	experimental	ChemBridge	5424817
1581 L12	X	1067	1080	-0.09880368	630	640	-0.76217575	3419002	0.55545653	3673319	1.07988589	experimental	ChemBridge	5512386
1581 L13	X	948	960	-0.46022908	790	800	-0.10995394	2930148	-0.36431384	3821287	1.35905986	experimental	ChemBridge	5425204
1581 L14	X	988	1000	-0.33874155	830	840	0.05312151	3777422	-1.30821235	3727476	5.1227983	experimental	ChemBridge	5353576
1581 L15	X	1107	1120	0.02268385	950	960	0.54229986	3904058	-0.46801105	3352123	0.77778591	experimental	ChemBridge	5467651
1581 L16	X	1267	1280	0.50863397	950	960	0.54229986	3373591	0.47001652	3646133	1.02859356	experimental	ChemBridge	5354034
1581 L17	X	1067	1080	-0.09880368	830	840	0.05312151	3696234	1.07706376	4050339	1.80008408	experimental	ChemBridge	5463541
1581 L18	X	1027	1040	-0.22029121	871	880	0.22025745	3518785	0.74319653	3167258	0.12509123	experimental	ChemBridge	5354514
1581 L19	X	945	960	-0.46934065	789	800	-0.11401443	3827667	1.32435269	4168480	2.01411532	experimental	ChemBridge	5465567
1581 L20	X	1348	1360	0.75464621	831	840	0.05719799	3324194	0.37707692	3384646	0.5352412	experimental	ChemBridge	5355121
1581 L21	X	1106	1120	0.01964666	749	760	-0.2707388	3253312	0.24371365	3222586	0.22947959	experimental	ChemBridge	5466664
1581 L22	X	1267	1280	0.50863397	951	960	0.54229986	3307013	0.33207012	4194337	1.90859808	experimental	ChemBridge	5355919
1581 L23	N	1025	1040	-0.22636559	706	720	-0.45236279	3197820	0.13930641	2917461	-0.3462054	empty		
1581 L24	P	1307	1320	0.6301215	988	1480	0.69720634	2797867	-0.61319826	2821196	-0.52783035	empty		
1581 M01	X	1503	1520	1.22541039	989	1000	0.70128283	2693712	-0.8091641	2467198	-1.19572494	experimental	ChemBridge	5339894
1581 M02	X	2824	2840	5.23753606	2509	2520	6.897542	2386295	-1.38756389	2645778	-0.85879474	experimental	ChemBridge	5406375
1581 M03	X	1101	1120	0.00446072	866	880	0.19987501	2887885	-0.44383095	3102295	0.00252434	experimental	ChemBridge	5322588
1581 M04	X	1263	1280	0.49648521	628	640	-0.77032872	3131764	0.10502319	2922386	-0.33691331	experimental	ChemBridge	5410648
1581 M05	X	1560	1560	0.00000000	1311	1320	1.35904668	3013914	1.71164149	2745598	-0.85862412	experimental	ChemBridge	5421358
1581 M06	X	1024	1040	-0.22940278	708	720	-0.44420982	2431468	-1.30257167	2352054	-1.41296699	experimental	ChemBridge	5412294
1581 M07	X	1186	1200	0.26262172	792	800	-0.10178497	3043958	-0.15018229	3681004	1.09438532	experimental	ChemBridge	5325594
1581 M08	X	1147	1160	0.14417138	671	680	-0.59503981	3435865	0.58718398	2983244	-0.22209139	experimental	ChemBridge	5430280
1581 M09	X	1068	1080	-0.09576649	792	800	-0.10178497	3289517	0.31183274	2996776	-0.19656032	experimental	ChemBridge	5426222
1581 M10	X	1027	1040	-0.22029121	630	640	-0.76217575	2784486	-0.63837329	2948533	-0.28758128	experimental	ChemBridge	5430741
1581 M11	X	987	1000	-0.34177874	751	760	-0.26892091	3217982	0.13774087	2863820	-0.44741086	experimental	ChemBridge	5427358
1581 M12	X	1249	1240	-0.39018363	1111	1120	1.19861416	2776510	-0.95330105	3374447	-0.36053104	experimental	ChemBridge	5411421
1581 M13	X	908	920	-0.58171661	710	720	-0.47611416	2739411	-0.35247112	3354181	0.00778659	experimental	ChemBridge	5427651
1581 M14	X	1104	1120	0.01357228	706	720	-0.45236279	2797259	-0.61434221	2885984	-0.40559363	experimental	ChemBridge	5432098
1581 M15	X	1266	1280	0.50559678	588	600	-0.93338818	3325270	0.37910139	3218766	0.22227233	experimental	ChemBridge	5428821
1581 M16	X	1345	1360	0.74553465	910	920	0.37924041	2886583	-0.44628064	2512054	-1.11109429	experimental	ChemBridge	5425446
1581 M17	X	1106	1120	0.01964666	950	960	0.54229986	3370221	0.46367592	3271420	0.32161556	experimental	ChemBridge	5429416
1581 M18	X	1305	1320	0.62404712	869	880	0.21210447	3717975	1.11796908	3078893	-0.04162865	experimental	ChemBridge	5415800
1581 M19	X	1868	1880	2.3339841	1351	1360	2.17697087	2819446	-0.57259775	2374440	-1.37073317	experimental	ChemBridge	5404557
1581 M20	X	864	880	-0.7153529	589	600	-0.92931169	1185354	-3.64711369	1194537	-3.59687801	experimental	ChemBridge	5419273
1581 M21	X	1106	1120	0.01964666	831	840	0.05719799	3195956	0.13579933	2948270	-0.28807748	experimental	ChemBridge	5404935
1581 M22	X	1426	1440	0.9915469	867	880	0.2039515	1649581	-2.77367858	1516497	-2.98843012	experimental	ChemBridge	5420480
1581 M23	N	1421	1440	0.97636096	1303	1800	1.98129953	3364448	0.45281412	2824616	-0.52137778	empty		
1581 M24	P	1849	2280	2.27627752	167771	168240	680.58582	2964190	-0.30026441	2805856	-0.55677262	empty		
1581 N01	X	1428	1440	0.99762127	711	720	-0.43198036	2113849	-1.90016634	2120706	-1.84945781	experimental	ChemBridge	5420861
1581 N02	X	1418	1440	0.96724939	904	920	0.35478149	3165464	0.07842916	3042021	-0.11119574	experimental	ChemBridge	5467870
1581 N03	X	1502	1520	1.2223732	866	880	0.19987501	3085983	-0.06923149	2873853	-0.42848142	experimental	ChemBridge	5421358
1581 N04	X	1145	1160	0.138097	871	880	0.22025745	2944111	-0.3380427	2922178	-0.33730574	experimental	ChemBridge	5491227
1581 N05	X	1220	1240	0.36588612	787	800	-0.1221674	3049693	-0.13939199	2891767	-0.39468274	experimental	ChemBridge	5422032
1581 N06	X	1905	1920	2.44636007	1272	1280	1.85492845	3277128	0.28852305	3510429	0.72755831	experimental	ChemBridge	5509739
1581 N07	X	1664	1680	1.7143977	670	680	-0.5991163	2804659	-0.60041923	2919907	-0.34159048	experimental	ChemBridge	5423129
1581 N08	X	1265	1280	0.50529599	671	680	-0.59503981	3208469	0.15934232	2858736	-0.45700294	experimental	ChemBridge	5511097
1581 N09	X	986	1000	-0.34481593	830	840	0.05312151	3054112	-0.13107771	2985054	-0.21867643	experimental	ChemBridge	5423875
1581 N10	X	1308	1320	0.63018363	991	1000	0.74961358	3227439	0.19503105	3104887	-0.10601481	experimental	ChemBridge	5411362
1581 N11	X	1106	1120	0.01964666	710	720	-0.43605685	2897508	-0.42572547	3104887	0.00738264	experimental	ChemBridge	5424902
1581 N12	X	1147	1160	0.14417138	711	720	-0.43198036	3173645	0.09382157	3291732	0.35993863	experimental	ChemBridge	5512436
1581 N13	X	904	920	-0.59386537	627	640	-0.77440521	2629053	-0.9308189	2903000	-0.37348923	experimental	ChemBridge	5425527
1581 N14	X	2187	2200	3.30284715	2149	2160	5.43000693	3081187	-0.08013657	3126394	0.04799236	experimental	ChemBridge	5353712
1581 N15	X	1383	1400	0.8609478	1467	1480	2.64984328	2881157	-0.45648957	2789576	-0.58748839	experimental	ChemBridge	5461960
1581 N16	X	1345	1360	0.74553465	949	960								

1581 007	X	1224	1240	0.37803487	751	760	-0.26892091	3496494	0.7012564	3336417	0.44424665	experimental	ChemBridge	5325628
1581 008	X	1346	1360	0.74857184	1031	1040	0.87249525	3164648	0.07689387	3022219	-0.14855654	experimental	ChemBridge	5430292
1581 009	X	1147	1160	0.14417138	831	840	0.05719799	2851345	-0.51258033	2858186	-0.45804064	experimental	ChemBridge	5426433
1581 010	X	1084	1080	-0.10791525	789	800	-0.11401443	2730528	-0.73089541	2739855	-0.68299408	experimental	ChemBridge	5430747
1581 011	X	1267	1280	0.50863897	831	840	0.05719799	2277305	-0.65363883	2873975	-0.42825124	experimental	ChemBridge	5427383
1581 012	X	1027	1040	-0.22029121	712	720	-0.42790387	2327388	-1.4983964	2418593	-1.28742889	experimental	ChemBridge	5431481
1581 013	X	1108	1120	0.02572104	631	640	-0.75809926	1906146	-2.29095956	1961051	-2.15068185	experimental	ChemBridge	5427902
1581 014	X	1144	1160	0.13505981	866	880	0.19987501	3073594	-0.09442267	2932547	-0.31774236	experimental	ChemBridge	5432156
1581 015	X	1185	1200	0.25958453	869	880	0.21210447	2967853	-0.29337254	3155369	0.10266003	experimental	ChemBridge	5428832
1581 016	X	1345	1360	0.74553465	770	680	-0.5991163	3339225	0.40535748	2775860	-0.61336662	experimental	ChemBridge	5452643
1581 017	X	1306	1320	0.62708431	651	760	-0.26892091	3015179	-0.20432948	2821009	-0.52818317	experimental	ChemBridge	5429505
1581 018	X	1306	1320	0.62708431	790	800	-0.10993794	3480475	0.67111692	3044459	-0.10714307	experimental	ChemBridge	5416101
1581 019	X	1187	1200	0.26565891	1070	1080	0.10314782	3311259	0.35273994	2983436	-0.22172914	experimental	ChemBridge	5404583
1581 020	X	1067	1080	-0.09880368	869	880	0.21210447	3013765	-0.2069899	2890449	-0.39716944	experimental	ChemBridge	5419144
1581 021	X	866	880	-0.70927852	570	760	-0.2729974	1167675	-3.68037642	1073596	-3.82505964	experimental	ChemBridge	5404961
1581 022	X	1068	1080	-0.09576649	828	840	0.04496854	3086706	-0.06975266	3208217	0.20236933	experimental	ChemBridge	5420769
1581 023	N	1181	1200	0.24743578	1114	1600	1.21084362	2744932	-0.71279456	2576100	-0.98948396	empty		
1581 024	P	1809	2240	2.15479	163450	163920	662.971323	2947046	-0.33252055	2491630	-1.14962863	empty		
1581 P01	X	1071	1080	-0.08665493	1074	1080	1.04778416	1963955	-2.18218932	1811575	-2.43270099	experimental	ChemBridge	5420876
1581 P02	X	1747	1760	1.96648432	1030	1040	0.86841877	2516330	-1.14290258	2642640	-0.86471527	experimental	ChemBridge	5467883
1581 P03	X	1303	1320	0.61797274	948	960	0.53414689	2434572	-1.29673155	2737044	-0.68660149	experimental	ChemBridge	5421384
1581 P04	X	1389	1400	0.87917093	912	920	0.38739338	2053101	-2.01446266	2079508	-1.92718684	experimental	ChemBridge	5491247
1581 P05	X	1062	1080	-0.11398962	711	720	-0.43198036	2062553	-1.99667888	1909862	-2.24726109	experimental	ChemBridge	5422033
1581 P06	X	2670	2680	4.76980907	1114	1120	1.21084362	2379481	-1.40038431	2371394	-1.37648012	experimental	ChemBridge	5510868
1581 P07	X	1185	1200	0.25958453	712	720	-0.42790387	2753742	-0.69621869	2852974	-0.46787421	experimental	ChemBridge	5432310
1581 P08	X	1149	1160	0.15024599	753	760	-0.26707843	2556952	-1.06647569	2803725	-3.56670321	experimental	ChemBridge	5411098
1581 P09	X	1109	1120	0.02875822	592	600	-0.91708223	2246692	-1.31532002	1142341	-1.16989489	experimental	ChemBridge	5423883
1581 P10	X	1590	1600	1.48964577	1193	1200	1.53288603	2231051	-1.6796528	2281148	-1.54674892	experimental	ChemBridge	5511452
1581 P11	X	1309	1320	0.63619587	912	920	0.38739338	2534161	-1.10935656	2576647	-0.98922548	experimental	ChemBridge	5425008
1581 P12	X	1030	1040	-0.21117965	592	600	-0.91708223	2714378	-0.77028138	2471631	-1.18736111	experimental	ChemBridge	5512451
1581 P13	X	1151	1160	0.15632013	1034	1040	0.88472471	2798835	-0.61137699	2379217	-1.36172032	experimental	ChemBridge	5425594
1581 P14	X	1110	1120	0.03179541	992	1000	0.71351229	2688633	-0.81872015	2891600	-0.39499782	experimental	ChemBridge	5353888
1581 P15	X	1269	1280	0.51470834	752	760	-0.26484442	2760463	-0.68357325	2482088	-1.1676317	experimental	ChemBridge	5462282
1581 P16	N	1409	1480	0.87917093	953	960	0.59459997	3260756	-1.10878835	2376890	-1.28363029	empty		
1581 P17	X	1109	1120	0.02875822	832	840	0.06127448	2473445	-1.22359267	2673768	-0.80598549	experimental	ChemBridge	5464752
1581 P18	X	1190	1200	0.27477047	953	960	0.55452932	2797960	-0.61302329	2641958	-0.86600201	experimental	ChemBridge	5354654
1581 P19	X	990	1000	-0.33266718	871	880	0.22025745	2698478	-0.80019696	2776270	-0.61259307	experimental	ChemBridge	5465854
1581 P20	X	1150	1160	0.15328294	912	1200	1.52880955	2784569	-0.63821822	2642982	-0.86407001	experimental	ChemBridge	5355315
1581 P21	X	1271	1280	0.52078272	1192	920	0.38739338	3022735	-0.1901113	2625394	-0.89725361	experimental	ChemBridge	5466739
1581 P22	X	1109	1120	0.02875822	832	840	0.06127448	2686784	-1.04421398	2338393	-1.43874371	experimental	ChemBridge	5366324
1581 P23	N	1067	1120	1.22145989	1027	1030	1.12214599	2534463	-1.10878835	2461023	-1.28363029	empty		
1581 P24	P	1549	1560	3.65121005	1442	1920	2.54793112	2360756	-1.43561508	2085500	-0.91588162	empty		
1582 A01	X	1916	1920	2.81323968	1156	1160	1.46484243	2726651	-0.9916281	1793991	-2.32010836	experimental	ChemBridge	5528697
1582 A02	X	710	720	-0.41465706	673	680	-0.18893074	1464743	-3.31896945	1623703	-2.68128023	experimental	ChemBridge	5403253
1582 A03	X	752	760	-0.30224275	514	520	-0.73334055	2340310	-1.70415816	2089633	-1.69306725	experimental	ChemBridge	5531789
1582 A04	X	1390	1400	2.2194458	793	800	0.22194458	1927870	-2.4648227	1808551	-2.28922737	experimental	ChemBridge	5683077
1582 A05	X	1990	2000	3.01130299	1392	1400	2.27289723	2274566	-1.82541005	1736486	-2.44207343	experimental	ChemBridge	5535419
1582 A06	X	1600	1.93801394	1313	1320	2.00246139	3033230	-0.42620338	2455603	-1.00170206	2167066	experimental	ChemBridge	5686075
1582 A07	X	832	840	-0.08812024	532	560	-0.60329003	3151916	-0.20731037	2675555	-0.31570619	experimental	ChemBridge	5375404
1582 A08	X	594	600	-0.72513469	636	640	-0.3156173	2721152	-1.00176992	2758565	-0.27429773	experimental	ChemBridge	5688908
1582 A09	X	635	640	-0.61539691	435	440	-1.00383347	2994039	-0.49848347	2714990	-1.51202956	experimental	ChemBridge	5539066
1582 A10	X	715	720	-0.40124744	514	520	-0.73334055	2284111	-1.80780617	2299254	-1.24847216	experimental	ChemBridge	5512466
1582 A11	X	795	800	-0.1871519	1276	1280	1.87571775	2122316	-2.10620526	2023324	-1.83370515	experimental	ChemBridge	5691482
1582 A12	X	354	360	-1.3675022	473	480	-0.87372295	2533026	-1.34873137	2500991	-0.82059861	experimental	ChemBridge	5513865
1582 A13	X	636	640	-0.61272038	596	600	-0.45257254	3133859	-0.24061296	1866286	-2.16677447	experimental	ChemBridge	5693826
1582 A14	X	474	480	-1.04631844	555	560	-0.59295814	2665619	-1.10418963	2536299	-0.74571122	experimental	ChemBridge	5523004
1582 A15	X	554	560	-0.83219594	555	560	-0.59295814	2875459	-0.71718098	2414194	-1.00469047	experimental	ChemBridge	5705215
1582 A16	X	874	880	0.02429407	555	560	-0.59295814	2775381	-0.90175519	2775052	-0.23932967	experimental	ChemBridge	5524802
1582 A17	X	792	800	-0.19518149	591	560	-0.60665399	3106152	-0.29171308	2443232	-0.94310241	experimental	ChemBridge	5705556
1582 A18	X	593	600	-0.72781122	595	600	-0.4559997	3180957	-0.15374995	2775292	-0.23882064	experimental	ChemBridge	5526224
1582 A19	X	953	960	0.23574004	713	720	-0.0519723	2410989	-1.57380463	1885994	-2.12497484	experimental	ChemBridge	5713146
1582 A20	X	1272	1280	1.08955353	1034	1040	1.04711918	2629049	-1.17163581	2112818	-1.64389309	experimental	ChemBridge	5367662
1582 A21	X	1351	1360	1.3009995	951	960	0.76293042	2824300	-0.81153371	2107128	-1.65596128	experimental	ChemBridge	5402708
1582 A22	X	911	920	0.12332573	1033	1040	1.04369522	3079058	-0.34168263	2424258	-0.98334526	experimental	ChemBridge	5373477
1582 A23	N	1067	1080	0.54086461	712	720	-0.05539627	2554790	-1.30859194	2151579	-1.56168305	empty		
1582 A24	P	1243	1760	1.01193412	994	1000	0.91016074	2053449	-2.23321691	1817092	-2.27111235	empty		
1582 B01	X	628	640	-0.63413263	592	600	-0.46627159	2405029	-1.58479668	2071904	-1.73066953	experimental	ChemBridge	5374569
1582 B02	X	792	800	-0.19518149	633	640	-0.32588919	3066629	-0.36460548	2392064	-1.05162704	experimental	ChemBridge	5547145
1582 B03	X	672	680	-0.51636525	594	600	-0.45942367	3451055	0.34439274	2639984	-0.52880178	experimental	ChemBridge	5380460
1582 B04	X	591	600	-0.73316428	433	440	-1.01068139	3814007	0.10137858	2675266	0.7518187	experimental	ChemBridge	5549121
1582 B05	X	468	480	-0.08812024	471	480	-0.80057087	2144058	-0.09270163	2301453	-1.24381456	experimental	ChemBridge	5398225
1582 B06	X	791	800	-0.19785803	431	440	-1.01752931	3295661	0.05779904	2612000	-0.58515437	experimental	ChemBridge	5452876
1582 B07	X	551	560	-0.84022554	874	880	0.49928542	3397726	0.24603787	2810244	-0.16468929	experimental	ChemBridge	5344384
1582 B08	X	672	680	-0.51636525	473	480	-0.87372295	3414618	0.27719185	3038595	0.31963115	experimental	ChemBridge	5454280
1582 B09	X	553	560	-0.83487247	434	440	-1.00725743	3476872	0.39200712	2798671	-0.18923502	experimental	ChemBridge	5345090
1582 B10	X	394	400	-1.26044095	515									

1582 C01	X		1314	1320	1.20196784	874	880	0.49928542	3345562	0.14983163	2550081	-0.71648131	experimental	ChemBridge	5529092
1582 C02	X		788	800	-0.20588762	591	600	-0.46969555	3294055	0.05483709	3108071	0.46698608	experimental	ChemBridge	5403625
1582 C03	X		712	720	-0.409304	592	600	-0.46627159	2966627	-0.54903952	3575973	1.45938157	experimental	ChemBridge	5531873
1582 C04	X		633	640	-0.62074987	514	520	-0.73334055	3483694	0.40458896	3697827	1.71782748	experimental	ChemBridge	5683201
1582 C05	X		634	640	-0.18807344	594	760	0.0884101	3977139	1.3146513	3204517	0.67154296	experimental	ChemBridge	5535556
1582 C06	X		632	640	-0.6234265	474	480	-0.87029899	3487399	0.4114221	2921824	0.07196601	experimental	ChemBridge	5686906
1582 C07	X		632	640	-0.6234265	553	560	-0.59980607	4087351	1.51791568	3263556	0.79676157	experimental	ChemBridge	5537935
1582 C08	X		872	880	0.01894101	433	440	-0.11068139	4102122	1.54515788	3179164	0.61777059	experimental	ChemBridge	5689208
1582 C09	X		832	840	-0.08812024	515	720	-0.04512438	3207635	-0.10454762	3163660	0.58488742	experimental	ChemBridge	5539122
1582 C10	X		433	440	-1.15605623	393	400	-1.14763983	3714549	0.83035564	3263636	0.79693125	experimental	ChemBridge	5512542
1582 C11	X		832	840	-0.08812024	554	560	-0.59638211	2905550	-0.66168405	2449623	-0.92594743	experimental	ChemBridge	5691491
1582 C12	X		712	720	-0.409304	634	640	-0.32246522	3037476	-0.41837246	2967184	0.03159378	experimental	ChemBridge	5713892
1582 C13	X		553	560	-0.83487247	473	480	-0.87372295	3104918	-0.29398895	3618305	1.54916551	experimental	ChemBridge	5695351
1582 C14	X		551	560	-0.84022554	552	560	-0.60323003	2825047	-0.81015601	3829402	1.99689112	experimental	ChemBridge	5523448
1582 C15	X		792	800	-0.19518149	914	920	0.63624386	2373423	-1.64308774	2006453	-1.86948765	experimental	ChemBridge	5705264
1582 C16	X		991	1000	0.33744823	831	840	0.3520551	2867010	-0.7327635	3506540	1.31211783	experimental	ChemBridge	5524841
1582 C17	X		948	960	0.22235739	1228	1240	1.71136762	2570839	-1.27899272	2722136	-0.35156172	experimental	ChemBridge	5710089
1582 C18	X		790	800	-0.20053456	591	600	-0.46969555	2913601	-0.64683556	2896768	0.01882355	experimental	ChemBridge	5526290
1582 C19	X		1072	1080	0.55424727	593	600	-0.46284763	2590849	-1.2420882	2267184	-1.31649094	experimental	ChemBridge	5713892
1582 C20	X		910	920	0.1206492	633	640	-0.32588919	3671157	0.75032763	3939707	0.107280499	experimental	ChemBridge	5367697
1582 C21	X		830	840	-0.09347331	472	480	-0.87714691	3905921	1.18330369	3151320	0.55871493	experimental	ChemBridge	5402719
1582 C22	X		711	720	-0.41198053	551	560	-0.60665399	3398964	0.24832112	2761592	-0.26787762	experimental	ChemBridge	5373525
1582 C23	N		940	960	0.20094514	941	1400	0.72869081	3245124	-0.03540653	2671343	-0.4592941	empty		
1582 C24	P		1628	2640	2.04239866	156665	156680	533.921596	3077811	-0.34398248	2607223	-0.59528614	empty		
1582 D01	X		790	800	-0.20053456	833	840	0.35890302	2936898	-0.60386882	2379907	-1.07744114	experimental	ChemBridge	5375330
1582 D02	X		1320	1340	0.18224671	950	1320	1.19121026	3073454	-0.3536429	3274853	0.82072191	experimental	ChemBridge	5547572
1582 D03	X		670	680	-0.52171831	1073	1080	1.18065366	3632884	0.67974040	3696189	1.64323144	experimental	ChemBridge	5380482
1582 D04	X		513	520	-0.94193372	393	400	-1.14763983	2863974	-0.73836281	3829432	-0.21519329	experimental	ChemBridge	5550024
1582 D05	X		474	480	-1.04631844	474	480	-0.87029899	4222733	1.76760117	3197243	0.65611519	experimental	ChemBridge	5398248
1582 D06	X		553	560	-0.83487247	474	480	-0.87029899	3720979	0.84221451	3325971	0.9291405	experimental	ChemBridge	5452929
1582 D07	X		672	680	-0.51636525	514	520	-0.73334055	3359351	0.17526273	3416613	1.12138741	experimental	ChemBridge	5344542
1582 D08	X		751	760	-0.30491928	554	560	-0.59638211	3628847	0.67229514	3456975	1.20699308	experimental	ChemBridge	5455095
1582 D09	X		792	800	-0.19518149	393	400	-1.14763983	4532940	2.33971703	3523166	1.3473807	experimental	ChemBridge	5345100
1582 D10	X		910	920	-0.10516751	633	640	-0.18934053	3161064	-0.4536429	3425126	1.71544351	experimental	ChemBridge	5456285
1582 D11	X		910	920	0.1206492	712	720	-0.05539627	3938869	1.2403812	3813162	1.96244694	experimental	ChemBridge	5346138
1582 D12	X		792	800	-0.19518149	513	520	-0.73676451	3815861	1.01720572	3376610	1.03654315	experimental	ChemBridge	5457211
1582 D13	X		631	640	-0.62610303	594	600	-0.45942367	2935407	-0.60661868	3228121	-1.3993415	experimental	ChemBridge	5347263
1582 D14	X		1073	1080	0.5569238	714	720	-0.04854834	3235242	-0.05363194	2941781	0.11429375	experimental	ChemBridge	5458055
1582 D15	X		471	480	-1.05434804	392	400	-1.15106379	4142680	1.61995915	3087266	0.42285977	experimental	ChemBridge	5348398
1582 D16	X		511	520	-0.94728679	553	560	-0.59980607	3180103	-0.15532499	2698888	-0.4008695	experimental	ChemBridge	5468046
1582 D17	X		872	880	0.01894101	671	680	-0.19577862	3765233	0.92597663	3071687	0.38981757	experimental	ChemBridge	5505846
1582 D18	X		990	1000	0.33477717	911	920	0.62597198	3101785	-0.29397615	2796295	-0.19427439	experimental	ChemBridge	5468907
1582 D19	X		549	560	-0.8455786	511	520	-0.74361243	3551985	0.53053829	3322123	0.92116998	experimental	ChemBridge	5542117
1582 D20	X		1069	1080	0.54621767	792	800	0.21852062	3884303	1.14343354	2919994	0.06808467	experimental	ChemBridge	5470201
1582 D21	X		670	680	-0.52171831	673	680	-0.18893074	3615373	0.647445	3056387	0.35736704	experimental	ChemBridge	5543531
1582 D22	X		748	760	-0.31294887	552	560	-0.60323003	3717735	0.83623159	2794454	-0.19817905	experimental	ChemBridge	5471796
1582 D23	N		1214	1720	0.93431471	663	680	-0.22317036	3701265	0.80585592	2985835	0.20772997	empty		
1582 D24	P		170449	171120	453.897098	1653	2520	3.16655105	2964131	-0.5536429	3377238	-0.66206416	empty		
1582 E01	X		800	800	-0.19250496	594	600	-0.59638211	3235676	-0.05283151	2396762	0.64166283	experimental	ChemBridge	5530148
1582 E02	X		1029	1040	0.43915642	792	800	0.21852062	3662721	0.73476908	3349583	0.97922031	experimental	ChemBridge	5403662
1582 E03	X		750	760	-0.30759581	472	480	-0.87714691	3376107	0.20616588	3352420	0.98523743	experimental	ChemBridge	5532003
1582 E04	X		552	560	-0.837549	434	440	-1.00725743	3913268	1.19685379	3534427	1.37126469	experimental	ChemBridge	5683290
1582 E05	X		513	520	-0.94193372	554	560	-0.59638211	3895584	1.16423913	3374487	1.03204038	experimental	ChemBridge	5535826
1582 E06	X		753	760	-0.29956621	554	560	-0.59638211	3124516	-0.25784429	3680510	1.68109904	experimental	ChemBridge	5687035
1582 E07	X		871	880	0.01626448	593	600	-0.46284763	3724256	0.8482583	3319509	0.91543494	experimental	ChemBridge	5538091
1582 E08	X		912	920	0.12602226	673	680	-0.18893074	4917905	0.04970933	4045124	2.45442612	experimental	ChemBridge	5689744
1582 E09	X		711	720	-0.41198053	553	560	-0.59980607	4088913	1.52079648	3742439	1.81244718	experimental	ChemBridge	5539968
1582 E10	X		591	600	-0.46969555	591	600	-0.46969555	3663660	0.73650088	3167729	0.59351756	experimental	ChemBridge	5512990
1582 E11	X		1432	1440	1.51779853	993	1000	0.90673678	3129934	-0.24785185	2699647	-0.3992597	experimental	ChemBridge	5691498
1582 E12	X		590	600	-0.73584081	593	600	-0.46284763	3699300	0.80223186	2819915	-0.14417761	experimental	ChemBridge	5521390
1582 E13	X		632	640	-0.6234265	434	440	-1.00725743	3690142	0.78534173	3110816	0.47280808	experimental	ChemBridge	5696551
1582 E14	X		631	640	-0.62610303	394	400	-1.14421587	3638503	0.69010374	3710577	1.74486956	experimental	ChemBridge	5523973
1582 E15	X		632	640	-0.6234265	434	440	-1.00725743	3653891	0.71848388	3071687	0.38981757	experimental	ChemBridge	5505269
1582 E16	X		712	720	-0.409304	553	560	-0.59980607	3660028	0.72980237	3721958	1.76908086	experimental	ChemBridge	5524906
1582 E17	X		430	440	-1.16408582	391	400	-1.15448775	1950099	-2.42382567	1908640	-2.07694387	experimental	ChemBridge	5710104
1582 E18	X		1232	1240	0.98249227	1352	1360	2.13593879	2965988	-0.55021803	3348312	0.97652458	experimental	ChemBridge	5526577
1582 E19	X		707	720	-0.42268665	670	680	-0.19920263	2085194	-2.17466949	2416311	-1.00020043	experimental	ChemBridge	5714516
1582 E20	X		1669	1680	2.15213645	831	840	0.3520551	3661515	0.73254854	3390100	1.06515473	experimental	ChemBridge	5367705
1582 E21	X		707	720	-0.42268665	510	520	-0.74703639	4138438	1.61213561	2981057	0.19759608	experimental	ChemBridge	5402722
1582 E22	X		988	1000	0.32941864	790	800	0.21852062	4162746	1.65896694	3029226	1.04313933	experimental	ChemBridge	5373557
1582 E23	N		1329	2000	1.24211581	1102	1520	1.27994853	3640592	0.50283151	2699042	-0.40054288	empty		
1582 E24	P		226164	227240	603.020028	142224	142240	484.476175	3532978	0.49548361	2821818	-0.14014145	empty		
1582 F01	X		632	640	-0.6234265	553	560	-0.59980607	2844417	-0.77443185	2521905	-0.77624112	experimental	ChemBridge	5375477
1582 F02	X		989	1000	0.33209517	753	760	0.08498614	3672868	0.75348323	2838099	-0.10561031	experimental	ChemBridge	5548259
1582 F03	X														

1582 F19	X		1110	1120	0.65595546	832	840	0.35547906	4015764	1.38588752	3062964	0.37131651	experimental	ChemBridge	5542382
1582 F20	X		1227	1240	0.96910962	990	1000	0.8964649	3411406	0.27126795	3378593	1.04074899	experimental	ChemBridge	5470342
1582 F21	X		1150	1160	0.76301671	1031	1040	1.0368473	4069585	1.48514978	2879462	-0.01788156	experimental	ChemBridge	5543568
1582 F22	X		543	560	-0.86163779	950	960	0.75950646	3103451	-0.29669454	3754887	-0.28200857	experimental	ChemBridge	5472319
1582 F23	N		1295	1295	1.15111374	507	520	-0.75730827	3741919	0.88083423	2714268	-0.36824933	empty		
1582 F24	P	197811	198480	527.132337	1105	1520	1.29022041	3221217	-0.07949829		2562020	-0.69115932	empty		
1582 G01	X		793	800	-0.19250496	995	1000	0.9135847	3503916	0.44188446	2843375	-0.09442019	experimental	ChemBridge	5530285
1582 G02	X		870	880	0.01358795	590	600	-0.47311951	3488265	0.41301927	2700687	-0.39705392	experimental	ChemBridge	5403706
1582 G03	X		750	760	-0.30759581	834	840	0.36232698	3323554	0.10924219	2789322	-0.20906375	experimental	ChemBridge	5532536
1582 G04	X		629	640	-0.63145609	430	440	-1.02095327	3014706	-0.46036725	3348778	0.97751294	experimental	ChemBridge	5683587
1582 G05	X		710	720	-0.41465706	672	680	-0.19235471	3219132	-0.08334367	3205723	0.67410083	experimental	ChemBridge	5536284
1582 G06	X		1667	1680	2.14678338	1151	1160	1.44772262	3586154	0.59355629	3254523	0.77845143	experimental	ChemBridge	5687596
1582 G07	X		827	840	-0.1015029	629	640	-0.33958503	3599365	0.61792139	3196033	0.65354885	experimental	ChemBridge	5538279
1582 G08	X		710	720	-0.41465706	432	440	-1.01410535	3624077	0.66349782	3316504	0.90906149	experimental	ChemBridge	5690603
1582 G09	X		1151	1160	0.76569324	913	920	0.6328199	3256911	-0.01366772	3410753	1.10895865	experimental	ChemBridge	5540145
1582 G10	X		510	520	-0.94996332	709	720	-0.06566815	3290259	0.04783611	3734266	1.79511268	experimental	ChemBridge	5513714
1582 G11	X		1113	1120	0.66398505	793	800	0.22194458	3094655	-0.31291703	2758283	-0.27489594	experimental	ChemBridge	5691534
1582 G12	X		551	560	-0.84022554	512	520	-0.74018847	2956396	-0.56790859	3489980	1.27699495	experimental	ChemBridge	5521408
1582 G13	X		632	640	-0.62342655	754	760	0.0884101	3122884	-0.25900989	3165905	0.58964895	experimental	ChemBridge	5698605
1582 G14	X		712	720	-0.409304	432	440	-1.01410535	1278977	-3.66157833	1097703	-3.79689852	experimental	ChemBridge	5524195
1582 G15	X		672	680	-0.51636525	674	680	-0.18550678	3409204	0.26720679	3094283	0.43774246	experimental	ChemBridge	5705272
1582 G16	X		551	560	-0.84022554	511	520	-0.74361243	3128696	-0.2501351	3511554	1.32275226	experimental	ChemBridge	5525122
1582 G17	X		593	600	-0.72781122	794	800	0.22536854	3543016	0.51399673	3101755	0.45359018	experimental	ChemBridge	5710481
1582 G18	X		552	560	-0.837549	553	560	-0.59980607	3270206	0.01085229	3571081	1.44900589	experimental	ChemBridge	5527239
1582 G19	X		791	800	-0.19785803	472	480	-0.87174691	3748652	0.89325193	3564367	1.43476585	experimental	ChemBridge	5715330
1582 G20	X		589	600	-0.73851735	500	520	-0.87372295	3715427	0.83157493	3101720	0.40899662	experimental	ChemBridge	5537938
1582 G21	X		906	920	-0.10994803	629	640	-0.33958503	2897849	-0.54678578	2626239	-0.55476332	experimental	ChemBridge	5402738
1582 G22	X		1831	1840	2.58573452	1192	1200	1.58810502	3590942	0.45133836	2479248	-0.86671137	experimental	ChemBridge	5373646
1582 G23	N		828	920	-0.09882637	592	600	-0.46627159	3233257	-0.05729288	2713657	-0.36954523	empty		
1582 G24	P	1339	1920	1.26888112	592	600	-0.46627159	3061875	-0.3733733		2862621	-0.05360044	empty		
1582 H01	X		988	1000	0.32941864	631	640	-0.33273711	3074218	-0.35060906	2560539	-0.69430044	experimental	ChemBridge	5376208
1582 H02	X		948	960	0.22235739	752	760	0.08156218	3459471	0.35991439	3041744	0.32631001	experimental	ChemBridge	5548504
1582 H03	X		947	960	0.21968086	669	680	-0.20262659	3599928	0.61895973	2748032	-0.29663767	experimental	ChemBridge	5384938
1582 H04	X		1300	1300	0.9995	1212	1300	0.0058229	3005829	0.0058229	3187701	1.9643237	experimental	ChemBridge	5551121
1582 H05	X		465	480	-1.07040723	428	440	-1.02780119	3193275	-0.13103182	2490142	-0.84360877	experimental	ChemBridge	5401524
1582 H06	X		2308	2320	3.86243994	1439	1360	2.1256669	3801697	0.991083	3494344	1.28644165	experimental	ChemBridge	5453377
1582 H07	X		1386	1400	1.39467809	1340	1440	2.40300774	3716562	0.83406823	3183818	0.62764148	experimental	ChemBridge	5344582
1582 H08	X		829	840	-0.09614984	511	520	-0.74361243	3325426	0.11269473	2941823	0.11438283	experimental	ChemBridge	5455338
1582 H09	X		949	960	0.22503392	591	600	-0.46969555	3683289	0.77270272	3228520	0.72245206	experimental	ChemBridge	5345123
1582 H10	X		872	880	0.01894101	1033	1040	1.04369522	3293547	0.05390018	2704639	-0.38867193	experimental	ChemBridge	5456382
1582 H11	X		720	720	-0.41465706	473	480	-0.87372295	3476199	0.71866544	4196159	1.13122368	experimental	ChemBridge	5346318
1582 H12	X		672	680	-0.51636525	631	640	-0.32589919	3617915	0.65213322	3595970	1.50179415	experimental	ChemBridge	5401524
1582 H13	X		753	760	-0.29956621	553	560	-0.59980607	3305515	0.0759728	3136598	0.52749034	experimental	ChemBridge	5347538
1582 H14	X		509	520	-0.95263985	554	560	-0.59638211	3226424	-0.069895	2995276	0.22775383	experimental	ChemBridge	5459498
1582 H15	X		832	840	-0.08812024	473	480	-0.87372295	3818863	1.02274232	3741765	1.81101766	experimental	ChemBridge	5348429
1582 H16	X		632	640	-0.62342655	594	600	-0.45942367	3555533	0.53708188	3225586	0.7162292	experimental	ChemBridge	5468147
1582 H17	X		632	640	-0.62342655	553	560	-0.59980607	3273336	0.01662496	3208216	0.67938835	experimental	ChemBridge	5541090
1582 H18	X		720	720	-0.409304	473	480	-0.87372295	3293239	0.0513034	3011745	0.08340003	experimental	ChemBridge	5469117
1582 H19	X		710	720	-0.41465706	593	600	-0.46284763	1.54534	1.64182152	3157837	0.57253714	experimental	ChemBridge	5425296
1582 H20	X		791	800	-0.19785803	632	640	-0.32931315	3152640	-0.20597509	2951900	0.13575562	experimental	ChemBridge	5470712
1582 H21	X		1111	1120	0.65863199	793	800	0.22194458	3852056	1.08396028	3161462	0.58022558	experimental	ChemBridge	5544981
1582 H22	X		714	800	-0.40395093	711	720	-0.05882023	3214934	-0.09108605	2606815	-0.59615148	experimental	ChemBridge	5472654
1582 H23	N	26149	26160	67.6736224	393	400	-1.14763983	3578422	0.57929614		2862167	-0.05456335	empty		
1582 H24	P	1236	1320	0.9931984	552	560	-0.60323003	3200919	-0.11693397	2779671	-0.22953302		empty		
1582 I01	X		2311	2320	3.87046954	1254	1240	1.73191139	3642171	0.69686864	2576584	-0.66026984	experimental	ChemBridge	5530417
1582 I02	X		1184	1200	0.85401877	790	800	0.21167269	3268204	0.00716	2788578	-0.21424735	experimental	ChemBridge	5403785
1582 I03	X		1429	1440	1.50976894	832	840	0.35547906	2886427	-0.69695266	3046308	0.33599001	experimental	ChemBridge	5532332
1582 I04	X		867	880	0.00555835	590	600	-0.47311951	3825318	1.0346473	3202015	0.66623635	experimental	ChemBridge	5683618
1582 I05	X		753	760	-0.29956621	634	640	-0.32246522	3608717	0.63516931	2982771	0.20123138	experimental	ChemBridge	5536352
1582 I06	X		666	680	-0.53242444	590	600	-0.47311951	3374866	0.2038771	2882732	-0.01094606	experimental	ChemBridge	5687930
1582 I07	X		870	880	0.01358795	791	800	0.21509665	3492486	0.42080407	3236202	0.73874518	experimental	ChemBridge	5538389
1582 I08	X		671	680	-0.51904178	552	560	-0.60323003	3478555	0.39511108	3269608	0.80959755	experimental	ChemBridge	5691373
1582 I09	X		832	840	-0.08812024	473	480	-0.87372295	3476199	0.39628221	3174063	0.60695164	experimental	ChemBridge	5540232
1582 I10	X		471	480	-1.05434804	552	560	-0.60323003	3185384	-0.14558522	3281349	0.83449959	experimental	ChemBridge	5517937
1582 I11	X		632	640	-0.62342655	593	600	-0.46284763	2873709	-0.72040851	2958812	0.15041561	experimental	ChemBridge	5691552
1582 I12	X		673	680	-0.51368872	673	680	-0.18893074	3537339	0.50352662	2892202	0.00913931	experimental	ChemBridge	5521481
1582 I13	X		549	560	-0.8455786	592	600	-0.46627159	3203640	-0.11191562	3119172	0.49053072	experimental	ChemBridge	5701409
1582 I14	X		1385	1400	1.39200156	753	760	0.08498614	2838256	-0.78579461	2584630	-0.6432047	experimental	ChemBridge	5524395
1582 I15	X		789	800	-0.20321109	673	680	-0.18893074	3789914	0.96935158	3235069	0.73634215	experimental	ChemBridge	5705296
1582 I16	X		880	880	0.01526448	593	600	-0.46284763	3919281	1.20794359	3011745	0.27540903	experimental	ChemBridge	5525212
1582 I17	X		831	840	-0.09079677	552	560	-0.60323003	3586160	0.59356736	2941270	0.13209995	experimental	ChemBridge	5710568
1582 I18	X		830	840	-0.09347331	633	640	-0.32589919	3671907	0.75171085	2990190	0.21696669	experimental	ChemBridge	5527376
1582 I19	X		1151	1160	0.76569324	672	680	-0.19235471	4045486	1.44070391	3353028	0.98652697	experimental	ChemBridge	5716268
1582 I20	X		670	680	-0.52171831	753	760	0.08498614	3927864	1.22377324	2867937	-0.04232548	experimental	ChemBridge	5373044
1582 I21	X	</													

1582 J13	X		784	800	-0.21659374	674	680	-0.18550678	3714463	0.83019703	2487461	-0.84929503	experimental	ChemBridge	5347572
1582 J14	X	3347	3360	6.64335595	591	600	-0.46969555	3297380	0.06069639		3173800	0.60639383	experimental	ChemBridge	5459563
1582 J15	X	744	760	-0.3236655	593	600	-0.46284763	3914565	1.19924585		2881112	-0.014382	experimental	ChemBridge	5348610
1582 J16	X	670	680	-0.52171831	473	480	-0.87372295	3792630	0.9743607		3427306	1.14406669	experimental	ChemBridge	5468155
1582 J17	X	791	800	-0.19785803	833	840	-0.35890302	3536325	0.50165655		2697897	-0.04241032	experimental	ChemBridge	5541175
1582 J18	X	590	600	-0.73584081	632	640	-0.32931315	3642970	0.69834224		3090443	0.42959802	experimental	ChemBridge	5469146
1582 J19	X	991	1000	0.33744823	673	680	-0.18893074	3371766	0.19815976		2963725	0.16083582	experimental	ChemBridge	5542543
1582 J20	X	750	760	-0.30759581	550	560	-0.61007795	3505178	0.44421197		2761998	-0.26701652	experimental	ChemBridge	5470864
1582 J21	X	831	840	-0.09079677	1432	1440	2.40985567	2532624	-1.34947278		2647102	-0.51070488	experimental	ChemBridge	5545481
1582 J22	X	711	720	-0.41198053	827	840	0.33835925	3522228	0.47565735		3063780	0.3728945	experimental	ChemBridge	5472848
1582 J23	N	711	720	-0.41198053	1131	1640	1.3792434	3218642	-0.08424737		2920705	0.06959267	empty		
1582 J24	P	553	560	-0.83487447	17431	17280	567.903765	3075142	-0.34890493		3371174	0.26080879	empty		
1582 K01	X	1312	1320	1.19661478	994	1000	0.91016074	2930439	-0.61578118		2646726	-0.51150236	experimental	ChemBridge	5531136
1582 K02	X	787	800	-0.20856415	790	800	0.21167269	4125639	1.58853037		3524612	1.35044759	experimental	ChemBridge	5403790
1582 K03	X	1031	1040	0.44450948	793	800	0.22194458	2418708	-1.55956845		2244652	-1.36428012	experimental	ChemBridge	5534332
1582 K04	X	868	880	0.00823488	592	600	-0.46627159	3428148	0.30214528		3384964	1.05426154	experimental	ChemBridge	5684463
1582 K05	X	1351	1360	1.3009995	673	680	-0.18893074	3703793	0.81051831		3169615	0.59751766	experimental	ChemBridge	5537260
1582 K06	X	1109	1120	0.65327892	992	1000	0.90331282	3781957	0.95467645		3497745	1.29344641	experimental	ChemBridge	5688362
1582 K07	X	830	840	-0.09347331	752	760	0.08156218	3852305	1.08442136		3371174	1.02501368	experimental	ChemBridge	5538527
1582 K08	X	871	880	0.01626448	591	600	-0.46969555	3554269	0.53475068		3761724	1.85334965	experimental	ChemBridge	5691375
1582 K09	X	871	880	0.01626448	673	680	-0.18893074	3597811	0.61505534		3379342	1.04233758	experimental	ChemBridge	5540414
1582 K10	X	671	680	-0.51904178	552	560	-0.60323003	3243267	-0.0388314		3785439	1.90364792	experimental	ChemBridge	5513749
1582 K11	X	592	600	-0.73048775	593	600	-0.46284763	2802611	-0.85153481		3367721	1.01769005	experimental	ChemBridge	5691553
1582 K12	X	520	520	-0.94461026	474	480	-0.87029899	3865614	0.59422024		3277975	0.82734351	experimental	ChemBridge	5521620
1582 K13	X	829	840	-0.09614984	432	440	-1.01410535	3840142	1.06198725		3210579	0.68440015	experimental	ChemBridge	5703585
1582 K14	X	503	520	-0.70783225	1063	1080	1.04369522	3622799	0.6611408		3651781	1.76737562	experimental	ChemBridge	5524610
1582 K15	X	589	600	-0.38857037	512	520	-0.74018847	3818182	-0.40170703		2990606	0.67844746	experimental	ChemBridge	5705352
1582 K16	X	871	880	0.01626448	433	440	-1.01068139	3569442	0.56273429		3367463	1.01714285	experimental	ChemBridge	5525229
1582 K17	X	911	920	0.12332573	672	680	-0.19235471	3001944	-0.48390246		2778559	-0.23337617	experimental	ChemBridge	5711169
1582 K18	X	792	800	-0.19518149	673	680	-0.18893074	3956440	1.27647606		3238390	0.74338581	experimental	ChemBridge	5527466
1582 K19	X	670	680	-0.52171831	633	640	-0.32588919	3266876	0.00471076		3528405	1.35849235	experimental	ChemBridge	5718334
1582 K20	X	951	960	-0.23038698	513	520	-0.73676451	3765647	0.92459586		2988829	0.2134438	experimental	ChemBridge	5373315
1582 K21	X	909	920	0.11797267	629	640	-0.33958503	3486859	0.41042618		2802802	-0.18047338	experimental	ChemBridge	5402808
1582 K22	X	829	840	-0.0824897	789	800	-0.6824897	3174443	0.61030263		3092920	0.82892803	experimental	ChemBridge	5475410
1582 K23	N	1230	1240	0.97713921	1232	1600	1.72506346	3515102	0.46251484		3084980	0.41801129	empty		
1582 K24	P	909	920	0.11797267	123487	124000	420.321417	3258029	-0.01160579		2634900	-0.53658468	empty		
1582 L01	X	1028	1040	0.43647989	711	720	-0.05882023	2866787	-0.73317478		2300456	-1.24592278	experimental	ChemBridge	5378055
1582 L02	X	1390	1400	1.40538422	1112	1120	1.31418814	2836752	-0.78856844		2572159	-0.66889149	experimental	ChemBridge	5549455
1582 L03	X	628	640	-0.63413263	391	400	-1.15448775	3851708	1.08331847		2919310	0.06663395	experimental	ChemBridge	5391110
1582 L04	X	911	920	0.12332573	714	720	-0.04854834	3782659	0.95597115		2849788	-0.08081855	experimental	ChemBridge	5551608
1582 L05	X	509	520	-0.67332003	552	560	-0.60323003	3613989	0.64489248		3211675	0.60280703	experimental	ChemBridge	5402660
1582 L06	X	590	600	-0.73584081	512	560	-0.60323003	3529231	0.4885730		3211675	0.68672471	experimental	ChemBridge	5453984
1582 L07	X	748	760	-0.31294887	630	640	-0.33616107	4107784	1.55560033		3652015	1.62066264	experimental	ChemBridge	5344688
1582 L08	X	710	720	-0.41465706	713	720	-0.0519723	1643022	-2.99016886		1652999	-2.61914496	experimental	ChemBridge	5455898
1582 L09	X	871	880	0.01626448	512	520	-0.74018847	3727267	0.93757976		3329127	0.93583421	experimental	ChemBridge	5345258
1582 L10	X	791	800	-0.19785803	913	920	0.6328199	2356757	-1.6738249		2226699	-1.40235749	experimental	ChemBridge	5456609
1582 L11	X	912	920	0.12602026	753	760	0.08498614	3796661	0.9319989		3296951	0.86759061	experimental	ChemBridge	5346749
1582 L12	X	829	840	-0.7316428	513	520	-0.74018847	3018518	-0.45338677		2045358	-0.42087003	experimental	ChemBridge	5457520
1582 L13	X	831	840	-0.09079677	673	680	-0.18893074	4137081	1.60632889		3197378	0.65640152	experimental	ChemBridge	5347619
1582 L14	X	1069	1080	0.54621767	951	960	0.76293042	2966166	-0.54988975		2576000	-0.66150847	experimental	ChemBridge	5459675
1582 L15	X	591	600	-0.73316428	832	840	0.35547906	3825495	1.03497374		3109176	0.46932973	experimental	ChemBridge	5348682
1582 L16	X	791	800	-0.19785803	713	720	-0.0519723	3254994	-0.01720325		1346965	0.54947821	experimental	ChemBridge	5468341
1582 L17	X	751	760	-0.30491928	671	680	-0.19577867	4133622	1.60325345		3263548	0.79674461	experimental	ChemBridge	5541245
1582 L18	X	671	680	-0.51904178	592	600	-0.46627159	3282882	0.03423068		2925917	0.08064704	experimental	ChemBridge	5469336
1582 L19	X	711	720	-0.41198053	633	640	-0.32588919	3728662	0.8563843		2984844	0.20562811	experimental	ChemBridge	5542614
1582 L20	X	591	600	-0.73316428	592	600	-0.46627159	3589311	0.59378976		3092800	0.43459709	experimental	ChemBridge	5471413
1582 L21	X	908	920	0.11529614	951	960	0.76293042	3931246	1.23001068		3577283	1.46216001	experimental	ChemBridge	5545932
1582 L22	X	869	880	0.01091142	630	640	-0.33616107	3367502	0.19029564		3228942	0.7233471	experimental	ChemBridge	5473010
1582 L23	N	743	760	-0.32633153	781	800	0.18085704	4616710	2.49421434		2891890	0.00847757	empty		
1582 L24	P	1465	2000	1.60612406	1793	2640	3.64590559	3227879	-0.06721154		2552954	-0.71038783	empty		
1582 M01	X	1392	1400	1.41073728	913	920	0.6328199	3635281	0.68416139		3000573	0.23898849	experimental	ChemBridge	5531412
1582 M02	X	828	840	-0.09882637	830	840	0.34863113	3129779	-0.24813772		2725367	-0.34470894	experimental	ChemBridge	5404081
1582 M03	X	711	720	-0.41198053	512	520	-0.74018847	2567985	-1.28425636		2777787	-1.23852888	experimental	ChemBridge	5534523
1582 M04	X	911	920	0.12332573	632	640	-0.32931315	2543294	1.32979406		2715795	-0.35852686	experimental	ChemBridge	5685868
1582 M05	X	751	760	-0.30491928	633	640	-0.32588919	2818640	-0.82197246		2869967	-0.03801996	experimental	ChemBridge	5537273
1582 M06	X	708	720	-0.42001012	631	640	-0.33273711	2847703	-0.76837147		2587421	-0.63728514	experimental	ChemBridge	5688578
1582 M07	X	1830	1840	2.58305799	1352	1360	2.13593879	3714937	0.83107123		3484879	1.26617599	experimental	ChemBridge	5538561
1582 M08	X	909	920	0.11797267	750	760	0.07471425	3237344	-0.04975521		2809102	-0.16711142	experimental	ChemBridge	5691429
1582 M09	X	711	720	-0.41198053	553	560	-0.59980607	2913635	-0.64677285		30704956	0.39675091	experimental	ChemBridge	5540425
1582 M10	X	829	840	-0.19785803	592	600	-0.46627159	3468890	0.37725889		2762785	0.66276511	experimental	ChemBridge	5513753
1582 M11	X	670	680	-0.52171831	432	440	-1.01410535	3217289	-0.08674272		2830055	-0.122671	experimental	ChemBridge	5691559
1582 M12	X	872	880	0.01894101	674	680	-0.18550678	3072114	-0.35448948		2832102	-0.11832963	experimental	ChemBridge	5522446
1582 M13	X	750	760	-0.30759581	552	560	-0.60323003	3225660	-0.07130405		2569131	-0.67607726	experimental	ChemBridge	5703669
1582 M14	X	991	1000	0.33744823	551	560	-0.60665399	2722668	-0.99897396		2335072	-1.17250407	experimental	ChemBridge	5524582
1582 M15	X	591													

1582 N07	X	1067	1080	0.54086461	830	840	0.34863113	3272903	0.01582638	2707034	-0.38359227	experimental	ChemBridge	5344703
1582 N08	X	667	680	-0.52974791	669	680	-0.20262659	3328291	0.11797866	2771805	-0.24621639	experimental	ChemBridge	5456002
1582 N09	X	630	600	-0.62877956	591	600	-0.46969555	2880792	-0.70734531	2486927	-0.85042761	experimental	ChemBridge	5345322
1582 N10	X	792	800	-0.19518149	712	800	-0.05359627	3245020	-0.03159834	2683378	-0.42116066	experimental	ChemBridge	5456110
1582 N11	X	911	840	-0.19788503	793	800	0.22194468	3087789	-0.3255708	2688828	0.02544091	experimental	ChemBridge	5347042
1582 N12	X	631	640	-0.62610303	590	600	-0.47311951	3110346	-0.28397807	2919483	0.06700087	experimental	ChemBridge	5457649
1582 N13	X	711	720	-0.41198053	692	1000	0.90331282	2818777	-0.8217198	2924002	0.07658543	experimental	ChemBridge	5347942
1582 N14	X	830	840	-0.09347331	791	800	0.21509665	3382242	0.21748068	2971605	0.17754889	experimental	ChemBridge	5460361
1582 N15	X	871	880	0.01626448	811	920	0.62597198	3264935	0.001113097	2463786	-0.89950846	experimental	ChemBridge	5348721
1582 N16	X	831	840	-0.09079677	811	920	0.62597198	2869368	-0.72841464	2604972	-0.60006039	experimental	ChemBridge	5464896
1582 N17	X	548	560	-0.84825513	666	680	-0.21289847	3031614	-0.42918377	2533549	-0.75154481	experimental	ChemBridge	5541701
1582 N18	X	1391	1400	1.40806075	1512	1520	2.68377255	2830677	-0.79977258	2524302	-0.77393565	experimental	ChemBridge	5459507
1582 N19	X	668	680	-0.52707137	789	800	0.20824873	3220401	-0.08100324	2480241	-0.86460827	experimental	ChemBridge	5542762
1582 N20	X	1071	1080	0.55157074	791	760	0.07813821	3152742	-0.20578698	2768427	-0.25338095	experimental	ChemBridge	5471423
1582 N21	X	866	880	0.00288182	668	680	-0.20605055	2779980	-0.89327324	2313214	-1.21886373	experimental	ChemBridge	5546256
1582 N22	X	946	960	0.21700432	910	920	0.62254802	3126141	-0.25484729	2606566	-0.5966796	experimental	ChemBridge	5473158
1582 N23	N	1482	2080	1.6516251	944	960	0.73896269	3197789	-0.12270664	2830110	-0.12255455	empty		
1582 N24	P	201733	202280	537.629693	1628	2120	3.08095203	3213651	-0.09345229	2626222	-0.55499026	empty		
1582 O01	X	1264	1280	1.06814127	985	1000	0.87934509	3458818	0.35871006	2674456	-0.45268849	experimental	ChemBridge	5531672
1582 O02	X	788	800	-0.20588762	909	920	0.61912405	2209079	-1.94618795	2055262	-1.76596633	experimental	ChemBridge	5683061
1582 O03	X	867	880	0.00555835	707	720	-0.07251607	2766869	-0.9174539	2945270	0.12169374	experimental	ChemBridge	5534717
1582 O04	X	1466	1480	1.68008006	1467	1480	2.5296943	2511426	-1.38856832	2689796	-0.42015315	experimental	ChemBridge	5686208
1582 O05	X	903	920	0.10191348	828	840	0.34178321	2795808	-0.8640816	2904339	0.03488124	experimental	ChemBridge	5537370
1582 O06	X	2349	2360	3.97217772	1191	1200	1.58468106	3029915	-0.43231724	2638728	-0.52846569	experimental	ChemBridge	5688649
1582 O07	X	942	960	0.20629882	787	800	0.20140081	3977431	1.31518984	2817135	-0.15007385	experimental	ChemBridge	5539300
1582 O08	X	1948	1960	2.89889806	1708	1960	3.35486891	3149390	-0.21196808	2641315	-1.00612603	experimental	ChemBridge	5541479
1582 O09	X	1309	1320	1.18885118	1148	1160	1.43745074	3026444	-0.43871882	2630322	-0.54628377	experimental	ChemBridge	5540481
1582 O10	X	589	600	-0.73851735	870	880	0.48558958	2993789	-0.49894455	2731658	-0.33136606	experimental	ChemBridge	5513831
1582 O11	X	952	960	0.23306351	670	680	-0.19920263	3021848	-0.44719524	2754207	-0.28354082	experimental	ChemBridge	5692598
1582 O12	X	749	760	-0.31027234	950	960	0.75950646	3051425	-0.39264627	3142981	0.54102835	experimental	ChemBridge	5522990
1582 O13	X	991	1000	0.33744823	910	920	0.62254802	2528143	-1.35737731	2396731	-1.04172858	experimental	ChemBridge	5705187
1582 O14	X	750	760	-0.30759581	750	760	0.07471425	2943648	-0.59141797	2907690	0.04198854	experimental	ChemBridge	5524754
1582 O15	X	710	720	-0.41465706	669	680	-0.20262659	2844895	-0.77355028	2793167	-0.200990871	experimental	ChemBridge	5705403
1582 O16	X	990	1000	0.72929079	749	760	-0.20053459	2122340	-0.82067019	2694265	-0.247806778	experimental	ChemBridge	5526221
1582 O17	X	1031	1040	0.44450948	1352	1360	2.13593879	1964299	-2.39763656	1762667	-2.38654491	experimental	ChemBridge	5711914
1582 O18	X	868	880	0.00823488	627	640	-0.34643295	2830717	-0.79969881	2600434	-0.60986825	experimental	ChemBridge	5528440
1582 O19	X	750	760	-0.30759581	791	800	0.21509665	3247967	-0.03016317	2663409	-0.47611859	experimental	ChemBridge	5719821
1582 O20	X	987	1000	0.32674211	749	760	0.07129029	3462767	0.36599322	2775852	-0.23763291	experimental	ChemBridge	5373446
1582 O21	X	1149	1160	0.76034018	1191	1200	1.58468106	3046089	-0.40248748	2770612	-0.24874668	experimental	ChemBridge	5402894
1582 O22	X	986	1000	0.32465558	909	920	0.61912405	3059562	-0.37763918	2941636	-0.11398622	experimental	ChemBridge	5374458
1582 O23	X	1400	1362	25.5972	749	760	0.08159218	3055342	-0.38357802	2647333	-0.71806778	empty		
1582 O24	P	2473	3800	4.3040676	947	960	0.74923457	2646685	-1.13910867	2293035	-1.06166233	empty		
1582 P01	X	3673	3680	7.51590515	3474	3480	9.40158406	2149382	-2.05628734	1878872	-2.14008023	experimental	ChemBridge	5380201
1582 P02	X	1143	1160	0.74428099	1144	1160	1.42375489	2529564	-1.35511634	2280231	-1.28881894	experimental	ChemBridge	5549815
1582 P03	X	1508	1520	1.72121491	1189	1200	1.57783314	2912666	-0.64855998	2175717	-1.51048763	experimental	ChemBridge	5397643
1582 P04	X	2148	2160	3.43419494	1950	1960	4.18346747	2762937	-0.92470577	2531057	-0.75683021	experimental	ChemBridge	5553381
1582 P05	X	1268	1280	1.10788474	790	800	0.21672689	2417965	-2.05890072	2060208	-1.75547613	experimental	ChemBridge	5402425
1582 P06	X	947	960	0.21968006	752	760	0.08159218	2512796	-1.38984163	2641315	-1.24712132	experimental	ChemBridge	9451213
1582 P07	X	951	960	0.23038698	831	840	0.35205051	2932767	-0.61146559	2652082	-0.50014256	experimental	ChemBridge	5344828
1582 P08	X	1229	1240	0.97446268	1430	1440	2.400300774	2921191	-0.6328373	2640692	-0.52430015	experimental	ChemBridge	5456108
1582 P09	X	751	760	-0.30491928	830	840	0.34863113	2763607	-0.92347002	2813360	-0.6501402	experimental	ChemBridge	5345446
1582 P10	X	634	640	-0.61807344	793	800	0.22194458	2368587	-1.65200679	2330210	-1.18281611	experimental	ChemBridge	5457054
1582 P11	X	752	760	-0.30224275	752	760	0.08156218	3274326	0.01845082	2833012	-0.11639957	experimental	ChemBridge	5347092
1582 P12	X	1313	1320	1.19929131	1183	1160	1.45457054	3013178	-0.46318535	2561233	-0.6928285	experimental	ChemBridge	5457747
1582 P13	X	791	800	-0.19785803	831	840	0.35205051	2553966	-1.31011165	2219567	-1.41748409	experimental	ChemBridge	5348282
1582 P14	X	832	840	-0.08812024	912	920	0.62939594	2748405	-0.95150712	2494267	-0.83485986	experimental	ChemBridge	5460896
1582 P15	X	1153	1160	0.7710463	1273	1280	1.86544586	2792152	-0.87082438	2422354	-0.98738354	experimental	ChemBridge	5348814
1582 P16	X	792	800	-0.19518149	832	840	0.3547906	1530102	-3.19842761	1534615	-2.87023119	experimental	ChemBridge	5468663
1582 P17	X	712	720	-0.409304	831	840	0.35205051	2729412	-0.98653598	2507080	-0.67257982	experimental	ChemBridge	5541959
1582 P18	X	832	840	-0.08812024	953	960	0.76977834	2660291	-1.11401608	2593570	-0.62424343	experimental	ChemBridge	5469631
1582 P19	X	991	1000	0.33744823	872	880	0.4924375	2995913	-0.49502725	2546738	-0.72357163	experimental	ChemBridge	5542838
1582 P20	X	1472	1480	1.62485978	1153	1160	1.45457054	2363882	-1.66068424	2116098	-1.63693638	experimental	ChemBridge	5471463
1582 P21	X	829	840	-0.09614984	871	880	0.48901354	2642599	-1.1466455	2486607	-0.85110632	experimental	ChemBridge	5546969
1582 P22	X	1148	1160	0.7576365	792	800	0.21852062	2368677	-1.65184008	2103073	-1.66456172	experimental	ChemBridge	5473309
1582 P23	N	1495	2240	1.68642	911	920	0.62597198	2767905	-0.9155432	2129478	-1.60855811	empty		
1582 P24	P	254623	254640	679.191432	1635	1640	3.10491975	2279431	-1.81643751	1989307	-1.90585341	empty		
1920 A01	N	528	560	-0.18368998	518	520	-0.09640999	1789261	-1.98490782	1429244	-2.71555851	empty		
1920 A02	E	156	160	-2.32291181	195	200	-0.25667727	782608	-4.9575342	79344	-7.21121393	empty		
1920 A03	X	596	600	0.01852502	837	840	0.06187254	2318045	-0.42341914	1739071	-1.68372249	experimental	NINDS	1500101
1920 A04	X	750	760	0.86463115	674	680	-0.11824207	2217362	-0.72073404	1712573	-1.61877378	experimental	NINDS	1500201
1920 A05	X	596	600	0.01852502	595	600	-0.05820386	2447267	-0.04182913	1816174	-0.24684161	experimental	NINDS	1500102
1920 A06	X	435	440	-0.83290655	515	520	-0.09789854	2332644	-0.38030858	1485452	-2.52836553	experimental	NINDS	1500202
1920 A07	X	516	520	-0.40719077	474	480	-0.11824207	2512146	0.14975727	1880458	-1.21285263	experimental	NINDS	1500103
1920 A08	X	555	560	-0.19965432	795	800	0.04103284	2105073	-1.05232124	1495883	-2.49362653	experimental	NINDS	1500205
1920 A09	X	716	720	0.6570987	674	680	-0.01900537	3165479	0.207903669	1824162	-1.40033868	experimental	NINDS	1500104
1920 A10	X	435	440	-0.838228	835	840	0.06088018	2716649	0.75365058	1833713	-1.36853039			

1920 B01	N	476	480	-0.62004866	557	560	-0.07705884	2250340	-0.62335066	2018971	-0.75155422	empty							
1920 B02	E	197	200	-2.10473247	237	240	-0.23583756	81547	-7.02775346	91240	-7.17159595	empty							
1920 B03	X	355	360	-1.26394379	274	280	-0.21747877	2159217	-0.89243508	2079508	-0.54994411	experimental	NINDS	1500310					Furosemide
1920 B04	X	440	440	-0.83822828	475	480	-0.11774588	1780821	-2.00983097	1653669	-1.96807545	experimental	NINDS	1500334					Furozaron
1920 B05	X	275	280	-1.68965958	714	720	0.00084187	201112	-3.0911535	20112	-3.0911535	experimental	NINDS	1500311					Fusidic acid
1920 B06	X	315	320	-1.47680168	513	520	-0.09889091	2360554	-0.2978909	2464028	0.73064662	experimental	NINDS	1500435					Nitromide
1920 B07	X	395	400	-1.05108589	594	600	-0.05870005	2290011	-0.50620298	2481621	0.78923768	experimental	NINDS	1500313					Gemfibrozil
1920 B08	X	395	400	-1.05108589	473	480	-0.11873825	2700677	0.70648558	2005835	-0.79530185	experimental	NINDS	1500436					Norepinephrine
1920 B09	X	474	480	-0.63069155	474	480	-0.11824207	2430933	-0.09006311	2149330	-0.31741158	experimental	NINDS	1500314					Gentamicin sulfate
1920 B10	X	354	360	-1.26926524	472	480	-0.11923443	2611069	0.44187493	2230682	-0.04647999	experimental	NINDS	1500437					Norethindrone
1920 B11	X	475	480	-0.62537011	513	520	-0.09889091	1365117	-3.23739666	1245045	-3.32900782	experimental	NINDS	1500315					Gentian violet
1920 B12	X	394	400	-1.06172879	392	400	-0.15892911	1950753	-1.50802514	215157	-0.30866272	experimental	NINDS	1500438					Norethindrone acetate
1920 B13	X	595	600	0.01320358	713	720	0.00034579	2440027	-0.06320871	1973120	-0.90425464	experimental	NINDS	1500316					Glucosamine hydrochloride
1920 B14	X	394	400	-1.05640734	994	1000	0.13977336	2745391	0.83852514	1951439	-0.97646021	experimental	NINDS	1500439					Nitroglydrol
1920 B15	X	515	520	-0.41251221	433	440	-0.13858559	2786157	0.95890633	2333532	0.29604773	experimental	NINDS	1500321					Guaiifenesin
1920 B16	X	474	480	-0.63069155	554	560	-0.07854739	2385768	-0.22343446	2422916	0.59372879	experimental	NINDS	1500440					Nitrofurantoin
1920 B17	X	395	400	-1.05108589	551	560	-0.08003594	1974753	-1.43715362	1872819	-1.23829326	experimental	NINDS	1500322					Guanabenz acetate
1920 B18	X	433	440	-0.8488709	553	560	-0.07904357	2413068	-0.1428181	2306312	0.20539528	experimental	NINDS	1500441					Norgestrel
1920 B19	X	513	520	-0.42315511	794	800	0.04053665	2182182	-0.82461989	2267525	0.07622053	experimental	NINDS	1500323					Guanethidine sulfate
1920 B20	X	393	400	-1.06172879	592	600	-0.05969241	2133534	-0.96827647	2086572	-0.52641843	experimental	NINDS	1500442					Nortriptyline
1920 B21	X	514	520	-0.41783366	512	520	-0.09938709	1954393	-1.49727629	2134517	-0.36674423	experimental	NINDS	1500324					Halazone
1920 B22	X	672	680	0.42295502	787	800	0.03706337	2041858	-1.23899388	1930675	-1.04561185	experimental	NINDS	1500443					Noscapine hydrochloride
1920 B23	E	507	960	-0.45508379	726	1520	0.00679618	90023	-7.002724	90185	-7.17510948	empty							
1920 B24	P	151712	153040	804.174363	268418	270040	132.831151	1978689	-1.42553069	1765534	-1.59559113	empty							
1920 C01	N	477	480	-0.61472721	436	440	-0.13709704	3086965	-1.8471864	1976170	-0.89409704	empty							
1920 C02	E	156	200	-2.01602842	156	190	-0.17774588	1033300	-6.96283809	858368	-7.18742147	empty							
1920 C03	X	436	440	-0.83299655	477	480	-0.11675352	2940799	-0.1455611	22874567	44.256467	experimental	NINDS	1500112					Amiloride hydrochloride
1920 C04	X	395	400	-1.05108589	394	400	-0.15793675	2571412	0.3247686	2066227	-0.59417464	experimental	NINDS	1500213					Cyclophosphamide hydrate
1920 C05	X	435	440	-0.838228	473	480	-0.11873825	2920234	1.35483306	2491262	0.8213457	experimental	NINDS	1500113					Potassium p-aminobenzoate
1920 C06	X	555	560	-0.19965432	474	480	-0.11824207	2449655	-0.03477741	2205111	-0.13164067	experimental	NINDS	1500215					Cycloperine
1920 C07	X	395	400	-1.05108589	474	480	-0.11824207	3009375	1.61806467	2312564	0.2262167	experimental	NINDS	1500114					6-aminocaproic acid
1920 C08	X	315	320	-1.47680168	475	480	-0.11774588	2731654	0.79796005	2389149	0.48127246	experimental	NINDS	1500216					Cyproterone acetate
1920 C09	X	594	600	0.00788213	393	400	-0.15843293	2715931	0.75153034	2152256	-0.30766694	experimental	NINDS	1500115					Aminoglutethimide
1920 C10	X	634	640	0.22074002	595	600	-0.02069897	20206893	-0.9617508	2675525	0.07622053	experimental	NINDS	1500217					Cyramine
1920 C11	X	394	400	-1.05640734	393	400	-0.02019313	2839950	1.117756	2148107	-0.32148462	experimental	NINDS	1500116					Aminosalicylate sodium
1920 C12	X	595	600	0.01320358	674	680	-0.01900537	2525894	0.19035484	2155920	-0.2954645	experimental	NINDS	1500220					Danzol
1920 C13	X	313	320	-1.48744458	473	480	-0.11873825	2274883	-0.55087567	2183097	-0.20495526	experimental	NINDS	1500117					Amtriptyline hydrochloride
1920 C14	X	635	640	0.22606147	554	560	-0.07854739	2691956	0.68073264	2135565	-0.36325401	experimental	NINDS	1500222					Dapsone
1920 C15	X	433	440	-0.8488709	250	360	-0.22938717	1986542	-1.40234093	1683066	-1.87023941	experimental	NINDS	1500119					Amodiaquine dihydrochloride
1920 C16	X	633	640	0.21541857	433	440	-0.13858559	2781844	0.94617013	2265997	0.07113174	experimental	NINDS	1500224					Deferoxamine mesylate
1920 C17	X	713	720	0.00345782	713	720	0.00345782	2814588	1.0415781	2814588	1.0415781	experimental	NINDS	1500225					Amoxicillin
1920 C18	X	914	920	-0.074528	673	680	-0.01950155	2983994	1.5311508	2165650	-0.29303333	experimental	NINDS	1500225					Sodium hydrochloride
1920 C19	X	751	760	0.84334936	512	520	-0.09938709	2788527	0.96590489	2296458	0.17257789	experimental	NINDS	1500122					Amphotericin B
1920 C20	X	954	960	1.92260317	552	560	-0.07953975	2310941	-0.44439711	2821868	-0.05485252	experimental	NINDS	1500226					Methoclopramide hydrochloride
1920 C21	X	512	520	-0.42847655	872	880	0.07923897	2801252	1.00348157	2216028	-0.09528311	experimental	NINDS	1500123					Ampicillin sodium
1920 C22	X	671	680	0.41763357	1109	1120	0.19683446	1957615	-1.48776179	1859743	-1.28184107	experimental	NINDS	1500227					Desipramine hydrochloride
1920 C23	E	632	1280	0.21009713	803	1400	0.04500231	91740	-6.99765373	93236	-7.16494854	empty							
1920 C24	P	20054	221000	1167.852272	201990	203960	99.424108	2039650	-1.96976558	2109355	-0.41716924	empty							
1920 D01	N	236	240	-0.89719602	637	640	-0.03736416	2208303	-0.74453211	2073712	-0.56924668	empty							
1920 D02	E	237	240	-1.89187458	196	200	-0.25618108	83676	-7.02146656	90804	-7.17304798	empty							
1920 D03	X	396	400	-1.04576445	354	360	-0.17774588	2319861	-0.41805653	2010004	-0.78141757	experimental	NINDS	1500325					Haloperidol
1920 D04	X	274	280	-1.69498102	554	560	-0.07854739	2473796	0.03651048	2316847	0.24048064	experimental	NINDS	1500444					Novobocin sodium
1920 D05	X	596	600	0.01852502	754	760	0.02068931	2478342	0.04993473	2131142	-0.37798472	experimental	NINDS	1500327					Hetacillin potassium
1920 D06	X	434	440	-0.84354945	474	480	-0.11824207	2708381	0.72923534	2357549	0.37603303	experimental	NINDS	1500445					Nylidrin hydrochloride
1920 D07	X	395	400	-1.05108589	395	400	-0.15744056	1689454	-2.27963592	1606133	-2.12645413	experimental	NINDS	1500328					Hexachlorophene
1920 D08	X	435	440	-0.838228	394	400	-0.15793675	2798775	0.99618704	2367548	0.40933331	experimental	NINDS	1500446					Wystiantin
1920 D09	X	634	640	0.22074002	635	640	-0.03835652	2563029	0.30001376	2561674	1.05584313	experimental	NINDS	1500330					Hexylresorcinol
1920 D10	X	594	600	0.00788213	593	600	-0.05919623	2784067	0.9527346	2150139	-0.31471732	experimental	NINDS	1500447					Orphenadrine citrate
1920 D11	X	274	280	-1.69498102	473	480	-0.11873825	2771479	0.91556249	2755425	1.10163894	experimental	NINDS	1500331					Histamine dihydrochloride
1920 D12	X	635	640	0.22606147	473	480	-0.11873825	2853226	1.15695976	2684942	1.46637017	experimental	NINDS	1500448					Oxacillin sodium
1920 D13	X	514	520	-0.41783366	595	600	-0.05820386	2509406	0.14166611	2300522	0.18611248	experimental	NINDS	1500332					Homatropine bromide
1920 D14	X	634	640	0.22074002	289	400	-0.21003602	2299843	-0.47716928	2381914	0.45717229	experimental	NINDS	1500450					Oxidopamine hydrochloride
1920 D15	X	592	600	0.00276977	36514	36520	17.7642115	2992799	1.56911607	2470737	0.75299002	experimental	NINDS	1500333					Homatropine methylbromide
1920 D16	X	1033	1040	0.24399751	530	640	-0.09045579	2846710	1.13771814	2382565	0.45934936	experimental	NINDS	1500451					Oxybenzone
1920 D17	X	713	720	0.04113436	632	640	-0.03984507	2559861	0.29065872	1945088	-0.99761134	experimental	NINDS	1500334					Hydralazine hydrochloride
1920 D18	X	511	520	-0.433798	752	760	0.01969695	2424759	-0.10829481	2257934	0.04427903	experimental	NINDS	1500453					Oxymetazoline hydrochloride
1920 D19	X	674	680	0.43359792	752</														

1920 E19	X	512	520	-0.42847655	711	720	-0.00064658	2627722	0.49105091	2408107	0.54440946	experimental	NINDS	1500134	Bacitracin
1920 E20	X	593	600	0.00256068	792	800	0.03954429	2321976	-0.41181097	2571694	1.08921336	experimental	NINDS	1500239	Dicumarol
1920 E21	X	714	720	0.64645581	752	760	0.01969695	2817290	1.05084146	2410009	0.55074381	experimental	NINDS	1500135	Baclofen
1920 E22	X	640	640	0.20477568	591	600	-0.06018886	2670079	0.61613003	2949785	0.01713991	experimental	NINDS	1500240	Dicyclomine hydrochloride
1920 E23	X	531	1040	-0.32736906	620	1120	-0.04529928	93137	-6.9912842	93137	-7.1712398	empty			
1920 E24	P	171844	172920	911.305741	168941	170040	83.4723045	2529149	0.1999668	2313334	0.22878108	empty			
1920 F01	N	437	440	-0.82758511	557	560	-0.07705884	2725051	0.77846152	2646392	1.33798472	experimental	NINDS	1500339	Hydrocortisone hemisuccinate
1920 F02	E	156	160	-2.32291181	235	240	-0.23682993	83864	-7.02091114	88834	-7.17960888	empty			
1920 F03	X	755	760	0.86463515	754	760	0.02068931	2166358	-0.87134785	2057638	-0.62277912	experimental	NINDS	1500339	Hydrocortisone hemisuccinate
1920 F04	X	433	440	-0.8488709	513	520	-0.09889091	2635064	0.51273169	2582742	1.12600719	experimental	NINDS	1500457	Oxytetracycline
1920 F05	X	634	640	0.22074002	354	360	-0.17784009	2303561	-0.4661901	2117403	-0.42374005	experimental	NINDS	1500341	Hydroflumethiazide
1920 F06	X	634	640	0.22074002	474	480	-0.11824207	2258245	-0.80000735	195849	-0.96114055	experimental	NINDS	1500459	Paspaverine hydrochloride
1920 F07	X	475	480	-0.62537011	634	640	-0.03885271	1785466	-1.99611438	1652016	-1.97364714	experimental	NINDS	1500343	Hydroxyprogesterone caproate
1920 F08	X	434	440	-0.84354945	555	560	-0.0780512	3011168	1.62335936	2311007	0.22103133	experimental	NINDS	1500460	Parachlorophenol
1920 F09	X	433	440	-0.8488709	514	520	-0.09839473	2563243	0.3006457	2380346	0.45195528	experimental	NINDS	1500344	Hydroxyurea
1920 F10	X	593	600	0.00256068	433	440	-0.13858559	2718957	0.76046606	2465728	0.73630824	experimental	NINDS	1500464	Penicillamine
1920 F11	X	594	600	0.00788213	314	320	-0.09839473	2666366	0.60516588	2115924	-0.42866565	experimental	NINDS	1500345	Hydroxyzine pamoate
1920 F12	X	595	600	0.01320358	594	600	-0.15793675	2537535	0.22473049	2435849	0.63880036	experimental	NINDS	1500465	Benzyd penicillin potassium
1920 F13	X	354	360	-1.26926524	354	360	-0.17778409	2400413	-0.18018806	2217028	-0.09195275	experimental	NINDS	1500346	Hycoscyamine
1920 F14	X	515	520	-0.41251221	674	680	-0.01900537	2582084	0.3562888	2405122	0.53446833	experimental	NINDS	1500467	Penicillin v potassium
1920 F15	X	434	440	-0.84354945	393	400	-0.15843293	2436875	-0.0725165	2332593	0.29292052	experimental	NINDS	1500347	Ibuprofen
1920 F16	X	434	440	-0.84354945	594	600	-0.05870005	2630674	0.49976811	2708671	1.54539633	experimental	NINDS	1500472	Phenacetamide
1920 F17	X	512	520	-0.42847655	430	440	-0.14007414	2142972	-0.94040624	2024077	-0.73454939	experimental	NINDS	1500348	Imipramine hydrochloride
1920 F18	X	1313	1320	0.83400277	1392	1400	0.33725459	2354174	-0.31673092	2498273	0.84619352	experimental	NINDS	1500473	Phenazopyridine hydrochloride
1920 F19	X	710	720	0.62517002	750	760	0.01870458	2299134	-0.47926295	2308551	0.21285196	experimental	NINDS	1500349	Indapamide
1920 F20	X	673	680	0.42827647	551	560	-0.00033594	3526075	1.62249414	1609127	2.11743399	experimental	NINDS	1500474	Phenindolol
1920 F21	X	472	480	-0.61333445	792	800	0.03954429	2363736	-0.09048452	2264640	-0.22880017	experimental	NINDS	1500350	Indomethacin
1920 F22	X	711	720	0.63049147	631	640	-0.04034126	2267069	-0.57395026	2421661	0.58954918	experimental	NINDS	1500478	Pheniramine maleate
1920 F23	E	538	1120	-0.29011892	541	1040	-0.08499777	83869	-7.00760822	91168	-7.17183753	empty			
1920 F24	P	197215	198200	1046.31618	168729	169640	83.3671136	2210456	-0.74112732	2013741	-0.76897201	empty			
1920 G01	N	397	400	-1.040443	397	400	-0.1564482	3053523	1.74843284	1967589	-0.92267487	empty			
1920 G02	E	156	160	-2.32291181	156	160	-0.27602842	108397	-6.94846594	87835	-7.18293583	empty			
1920 G03	X	633	640	0.21541857	593	600	-0.05919623	3158791	2.05928716	2347502	0.34257288	experimental	NINDS	1500136	Beclomethasone dipropionate
1920 G04	X	440	440	0.84354945	594	600	-0.05870005	2630674	0.49976811	2708671	1.54539633	experimental	NINDS	1500241	Difenestrol
1920 G05	X	674	680	0.43359792	674	680	-0.01900537	3165284	2.07846086	2706508	1.53819276	experimental	NINDS	1500137	Benserazide hydrochloride
1920 G06	X	593	600	0.00256068	634	640	-0.03885271	2745866	0.83992781	2492259	0.82466607	experimental	NINDS	1500242	Diethylcarbamazine citrate
1920 G07	X	474	480	-0.63069155	554	560	-0.07854739	2663701	0.59729619	2331717	0.29000312	experimental	NINDS	1500138	Benzethonium chloride
1920 G08	X	594	600	0.00788213	154	160	-0.27702079	2796131	0.98835936	2421868	-2.74012326	experimental	NINDS	1500244	Diethylstilbestrol
1920 G09	X	633	640	0.21541857	713	720	0.00034579	2712166	0.74041237	1197651	-0.15648517	experimental	NINDS	1500139	Benzocaine
1920 G10	X	834	840	1.28502949	873	880	0.07973515	2526278	0.19148879	2523600	0.92904294	experimental	NINDS	1500245	Diffusal
1920 G11	X	463	460	-0.03478289	474	480	-0.11824207	2258245	-0.80000735	195849	-0.96114055	experimental	NINDS	1500141	Benzisazide
1920 G12	X	474	480	-0.63069155	474	480	-0.11824207	1929200	1.857165891	1951669	-0.97569423	experimental	NINDS	1500246	Digoxin
1920 G13	X	555	560	-0.19965432	554	560	-0.07854739	2449725	-0.0345707	1928278	-0.15439703	experimental	NINDS	1500142	Benzotropine
1920 G14	X	473	480	-0.636013	513	520	-0.09889091	1869479	-1.74802566	1784144	-1.53361131	experimental	NINDS	1500247	Digoxin
1920 G15	X	594	600	0.00788213	673	680	-0.01901555	2910471	1.32600311	2432998	0.62730549	experimental	NINDS	1500144	Betamethasone
1920 G16	X	433	440	-0.8488709	833	840	0.05988781	2360329	-0.29855532	2313767	0.23022312	experimental	NINDS	1500248	Dihydroergotamine mesylate
1920 G17	X	714	720	0.64645581	752	760	0.01969695	3184332	2.13470922	2550536	1.01874956	experimental	NINDS	1500145	Betamethasone valerate
1920 G18	X	588	590	0.02404656	868	880	0.07725423	2926261	1.37853663	2670242	1.41741389	experimental	NINDS	1500249	Bithionol
1920 G19	X	1032	1040	-0.33867607	791	800	0.03904829	2827409	1.08522626	2827409	1.08522626	experimental	NINDS	1500250	Benzocaine chloride
1920 G20	X	751	760	0.84334936	832	840	0.05939163	2344970	-0.34391015	2314184	0.23161188	experimental	NINDS	1500251	Dimenhydrinate
1920 G21	X	631	640	0.20477568	756	760	0.01920076	2848541	1.14312505	2273608	0.09647912	experimental	NINDS	1500147	Bisacodyl
1920 G22	X	790	800	1.05088581	790	800	0.03855192	2494431	0.09744523	2232531	-0.04032215	experimental	NINDS	1500253	Dimethadione
1920 G23	E	709	1200	0.61984857	535	960	-0.08797487	89213	-7.00511591	91176	-7.17180909	empty			
1920 G24	P	165139	166240	875.625436	142691	143720	70.4474875	2319803	-0.4182278	2221213	-0.07801518	empty			
1920 H01	N	597	600	0.02384647	357	360	-0.17629554	2676813	0.63601566	2257841	0.39039331	empty			
1920 H02	E	234	240	-1.90783892	156	160	-0.27602842	82577	-7.02471189	88521	-7.1806512	empty			
1920 H03	X	914	920	1.71074528	835	840	0.06088018	2472234	0.03189793	2101426	-0.47694924	experimental	NINDS	1500351	Indoprofen
1920 H04	X	353	360	-1.27458668	393	400	-0.15843293	2525945	0.19050545	2293629	0.1631563	experimental	NINDS	1500480	Phenolphthalein
1920 H05	X	514	520	-0.41783366	394	400	-0.15793675	2340485	-0.35715426	2107159	-0.45785627	experimental	NINDS	1500353	Iodoquinol
1920 H06	X	514	520	-0.41783366	513	520	-0.09889091	2773113	0.92038766	2680170	1.45047769	experimental	NINDS	1500482	Phenylbutazone
1920 H07	X	394	400	-1.05640734	394	400	-0.07854739	2303312	-0.4669254	2387980	0.47737927	experimental	NINDS	1500354	Ipratropium bromide
1920 H08	X	514	520	-0.41783366	555	560	-0.15744056	2664992	0.60110848	2608124	1.21053844	experimental	NINDS	1500483	Phenylephrine hydrochloride
1920 H09	X	554	560	-0.20497577	714	720	0.00084197	2560724	0.29320714	2348971	0.34745518	experimental	NINDS	1500355	Isoniazid
1920 H10	X	473	480	-0.636013	592	600	-0.05969241	2959286	0.39526805	2417689	0.57632099	experimental	NINDS	1500485	Phenytion sodium
1920 H11	X	395	400	-1.05108589	554	560	-0.07854739	2423586	-0.11175865	2409703	0.54972472	experimental	NINDS	1500356	Isopropamide iodide
1920 H12	X	475	480	-0.62537011	473	480	-0.11873825	2468959	0.02222692	2403804	0.53007891	experimental	NINDS	1500486	Phyostigmine salicylate
1920 H13	X	553	560	-2.1029721	555	560	-0.0780512	2344150	-0.34633159	2292805	0.16041208	experimental	NINDS	1500357	Isoproterenol hydrochloride
1920 H14	X	794	800	1.0721716	373	380	-0.17828027	2761086	0.88487216	2496844	0.83993578	experimental	NINDS	1500487	Pilocarpine nitrate
1920 H15	X	633	640	0.21541857	674	680	-0.01900537	2431677	-0.08786609	2309405	0.21259609	experimental	NINDS	1500358	Isonorbide dinitrate
1920 H16	X	434	440	0.00788213	472	480	-0.11824207	2713452	0.74420991	2635940	1.12899967	experimental	NINDS	1500488	Indinavir
1920 H17	X	431	440	-0.85951379	511	520	-0.09888328	2680696	0.64782079	2533396	0.29206463	experimental	NINDS	1500359	Isosuxrine hydrochloride
1920 H18	X	993	1000	2.13113962	1153	1160	0.21866653	2566596	0.31054704	2410718	0.55310503	experimental	NINDS	1500489	Piperacillin sodium
1920 H19	X	669	680	0.40699068	471	48									

1920 I13	X	434	440	-0.84354945	433	440	-0.13858559	2502125	0.12016546	2352078	0.35781262	experimental	NINDS	1500157	Capreomycin sulfate
1920 I14	X	514	520	-0.41783366	714	720	0.00084197	2868259	1.20135191	2224496	-0.06708161	experimental	NINDS	1500261	Disopyramide phosphate
1920 I15	X	433	440	-0.8488709	472	480	-0.11923443	2702430	0.71166216	2428260	0.61252535	experimental	NINDS	1500158	Carbachol
1920 I16	X	673	680	-0.42827647	593	600	0.00345799	2454655	-0.02001251	3022662	0.19330666	experimental	NINDS	1500262	Disulfiram
1920 I17	X	673	680	-0.42827647	493	600	-0.05919623	2707833	0.72761711	2500258	2.43500258	experimental	NINDS	1500159	Carbamazepine
1920 I18	X	711	720	0.63049147	512	520	-0.09938709	2555052	0.27645784	2551173	1.03419245	experimental	NINDS	1500263	Dopamine hydrochloride
1920 I19	X	872	880	1.48724449	594	600	-0.05870005	3149056	2.03053989	2558918	1.04666465	experimental	NINDS	1500160	Carbenicillin disodium
1920 I20	X	671	680	0.41763357	712	720	-0.00015039	2807706	1.0225401	2376279	0.4384107	experimental	NINDS	1500266	Doxycycline hydrochloride
1920 I21	X	591	600	-0.00808221	952	960	0.11893365	2488740	0.08063982	2360999	0.38752227	experimental	NINDS	1500161	Carbinoxamine maleate
1920 I22	X	790	800	1.05088581	788	800	0.03755955	2221083	-0.709746	2086249	-0.52749414	experimental	NINDS	1500264	Doxepin hydrochloride
1920 I23	E	795	1360	1.07749304	650	1120	-0.03091377	88374	-7.00759346	93205	-7.17504287	empty			
1920 I24	P	190571	191640	101746049	158358	159440	78.2211945	2528098	0.19686321	2329207	0.633272976	empty			
1920 J01	N	557	560	-0.18901142	397	400	-0.1564482	2212725	-0.72099095	2309001	0.21435062	empty			
1920 J02	E	236	240	-1.89719602	196	200	-0.25618108	84633	-7.01864056	90352	-7.1745531	empty			
1920 J03	X	314	320	-1.48212313	635	640	-0.03835652	2232291	-0.676649	2127571	-0.38987693	experimental	NINDS	1500363	Lactulose
1920 J04	X	554	560	-0.20497577	394	400	-0.15793675	2286468	-0.51666539	2351081	0.35449224	experimental	NINDS	1500492	Polymyxin b sulfate
1920 J05	X	473	480	-0.636013	515	520	-0.09789854	2502773	0.12207899	2207214	-0.12463692	experimental	NINDS	1500364	Leucovorin calcium
1920 J06	X	674	680	0.43359792	474	480	-0.11824207	2761067	0.88481606	2543656	0.99583667	experimental	NINDS	1500494	Praziquantel
1920 J07	X	674	680	0.43359792	393	400	-0.15843293	2742117	0.82885708	2330280	0.28521739	experimental	NINDS	1500365	Levonordesrin
1920 J08	X	673	680	0.42827647	994	1000	0.13977336	2638851	0.52391463	2749948	1.68286367	experimental	NINDS	1500476	Phenelzine sulfate
1920 J09	X	513	520	-0.42315511	473	480	-0.11873825	2683524	0.65583311	2426203	0.60467569	experimental	NINDS	1500368	Lincomycin hydrochloride
1920 J10	X	674	680	0.43359792	594	600	-0.05870005	2903280	1.30476823	2702987	1.52646655	experimental	NINDS	1500495	Prazosin hydrochloride
1920 J11	X	432	440	-0.85419234	713	720	0.00034579	2589520	0.37824116	2263081	0.0614204	experimental	NINDS	1500372	Mafenide hydrochloride
1920 J12	X	1114	1120	2.77503475	992	1000	0.13878899	2841877	1.12344639	2534214	0.9643914	experimental	NINDS	1500496	Propolisolone
1920 J13	X	393	400	-1.06172879	472	480	-0.11923443	2077467	-1.13384121	2351421	0.35562457	experimental	NINDS	1500373	Maprotiline hydrochloride
1920 J14	X	434	440	-0.84354945	515	520	-0.09540685	2639860	0.52689019	2128908	1.66241525	experimental	NINDS	1500497	Propolisolone acetate
1920 J15	X	674	680	0.43359792	753	760	0.02019311	2515028	-2.7961244	1515205	-4.29277277	experimental	NINDS	1500375	Mechlorethamine
1920 J16	X	673	680	0.42827647	792	800	0.03954429	2662113	0.59260685	2835105	1.9664673	experimental	NINDS	1500499	Prednisone
1920 J17	X	552	560	-0.21561866	513	520	-0.09889091	2325975	-0.400002	2352375	0.35880173	experimental	NINDS	1500376	Mecizline hydrochloride
1920 J18	X	671	680	0.41763357	513	520	-0.09889091	2426907	-0.10195181	2677747	1.44240822	experimental	NINDS	1500500	Primaquine diphosphate
1920 J19	X	832	840	1.2743866	613	520	-0.09889091	2355834	-0.31182897	2335074	0.30118314	experimental	NINDS	1500379	Metroxprogesterone acetate
1920 J20	X	711	720	0.63049147	571	680	-0.02049392	2641120	0.53061494	2537800	0.97633407	experimental	NINDS	1500501	Primidone
1920 J21	X	712	720	0.63581291	751	760	0.01920076	2407426	-0.15947881	2345678	0.3364983	experimental	NINDS	1500380	Medrysone
1920 J22	E	720	600	0.13430366	871	880	-0.01340366	2422167	0.11594837	2119317	0.10487873	experimental	NINDS	1500502	Probenecid
1920 J23	E	728	1280	0.72095607	447	1000	-0.13163902	87980	-7.00875693	92525	-7.16731643	empty			
1920 J24	P	186258	187320	988.009083	187151	188080	92.5078062	2188954	-0.80462231	2151993	-0.30854283	empty			
1920 K01	N	476	480	-0.62004866	477	480	-0.11675352	3256129	2.34672434	2065016	-0.99820771	empty			
1920 K02	E	196	200	-2.11005392	236	240	-0.23633374	107048	-6.95244951	89251	-7.17822004	empty			
1920 K03	X	514	520	-0.41783366	556	560	-0.0780512	2746387	0.84146631	2994109	2.496600815	experimental	NINDS	1500162	Carisoprodol
1920 K04	X	434	440	-0.84354945	395	400	-0.15744056	2505249	0.12939057	2377622	0.44288338	experimental	NINDS	1500267	Doxylamine succinate
1920 K05	X	475	480	-0.65537811	435	440	-0.17748135	2831585	1.09105432	2014608	2.85120335	experimental	NINDS	1500163	Doxylamine
1920 K06	X	473	480	-0.636013	434	440	-0.13808941	2538353	1.13304009	2364719	0.39991172	experimental	NINDS	1500268	Doxylamine hydrochloride
1920 K07	X	434	440	-0.84354945	514	520	-0.09839473	2907592	1.31750148	2741367	1.65428584	experimental	NINDS	1500164	Cefazolin sodium
1920 K08	X	513	520	-0.42315511	633	640	-0.03934889	2795723	0.98715454	2413258	0.56246335	experimental	NINDS	1500269	Daphylline
1920 K09	X	594	600	0.00788213	554	560	-0.07854739	3315294	2.52143742	2877931	2.10909337	experimental	NINDS	1500165	Cefotaxime sodium
1920 K10	X	473	480	-0.636013	394	400	-0.15793675	2762726	0.88971505	2613055	1.226966045	experimental	NINDS	1500270	Trisodium ethylenediamine tetracetate
1920 K11	X	433	440	-0.8488709	514	520	-0.09839473	2683200	0.65487635	2751649	1.68852862	experimental	NINDS	1500166	Cephalothin sodium
1920 K12	X	640	650	0.21541857	514	520	0.00345799	1763526	-2.06090277	1766786	-1.61186661	experimental	NINDS	1500272	Emetine
1920 K13	X	354	360	-0.26926524	354	360	-0.07854739	2668499	0.41160927152	2668499	0.41160927152	experimental	NINDS	1500167	Chlaphirin sodium
1920 K14	X	515	520	-0.41251221	473	480	-0.11873825	2718593	0.75939118	2522992	0.92701808	experimental	NINDS	1500273	Ephedrine (1r,2s) hydrochloride
1920 K15	X	473	480	-0.636013	553	560	-0.07904357	2618980	0.46523596	2835829	1.96887848	experimental	NINDS	1500180	Chlorothiazide
1920 K16	X	511	520	-0.433798	713	720	0.00034579	2670224	0.61655848	2437965	0.6438474	experimental	NINDS	1500274	Adrenaline bitartrate
1920 K17	X	872	880	1.48724449	633	640	-0.03934889	2599688	0.40826707	2633940	1.29651506	experimental	NINDS	1500181	Chlorotrianisene
1920 K18	X	1112	1120	2.76439185	793	800	0.04004047	2300331	-0.47572823	2622011	1.25678717	experimental	NINDS	1500275	Equilin
1920 K19	X	470	480	-0.65197734	672	680	-0.01999773	2372218	-0.26344734	2888570	2.14452509	experimental	NINDS	1500182	Chloroxylenol
1920 K20	X	751	760	0.84334936	952	960	0.11893365	2823400	1.06888417	2488917	0.8135336	experimental	NINDS	1500276	Ergocalciferol
1920 K21	X	791	800	1.05620726	751	760	0.01920076	3053085	1.74713943	2790951	1.8194185	experimental	NINDS	1500183	Chlorpheniramine (s) maleate
1920 K22	X	750	760	0.83802791	710	720	-0.00114276	2413994	-0.14008364	2432635	0.62609657	experimental	NINDS	1500277	Ergonovine maleate
1920 K23	E	926	1440	1.77460265	608	1080	-0.05175348	84458	-7.01915733	87006	-7.1856697	empty			
1920 K24	P	172868	174000	916.754903	159363	160360	78.7198589	2689460	0.673362	2305607	0.20304737	empty			
1920 L01	N	636	640	0.23138292	436	440	-0.13709704	2361269	-0.29577952	2274894	0.10076197	empty			
1920 L02	E	234	240	-1.90783892	276	280	-0.2164864	80325	-7.031362	87088	-7.18542361	empty			
1920 L03	X	1035	1040	2.35464041	475	480	-0.11774588	2138045	-0.95495557	2014608	-0.76608459	experimental	NINDS	1500381	Megestrol acetate
1920 L04	X	513	520	-0.42315511	514	520	-0.09839473	2522231	0.17953808	2698948	1.51301522	experimental	NINDS	1500382	Procainamide hydrochloride
1920 L05	X	354	360	-1.26926524	514	520	-0.09839473	2405479	-0.16522827	2174254	-0.23440565	experimental	NINDS	1500383	Mepenzolate bromide
1920 L06	X	755	760	0.86463515	594	600	-0.05870005	2390556	-0.44996348	2578846	1.11303211	experimental	NINDS	1500504	Meclozine hydrochloride
1920 L07	X	393	400	-1.06172879	754	760	0.02068931	2250674	-0.62236437	2137087	-0.3581852	experimental	NINDS	1500387	Procainopurine
1920 L08	X	714	720	0.64645581	433	440	-0.13858559	2207763	-0.7490797	1914193	-1.10050287	experimental	NINDS	1500505	Prochlorperazine edisylate
1920 L09	X	673	680	0.42827647	434	440	-0.13808941	2615734	0.45565059	2436693	0.69961118	experimental	NINDS	1500390	Metaproterenol
1920 L10	X	753	760	-0.21029721	475	480	-0.11774588	2845049	1.13576622	1367876	0.41042567	experimental	NINDS	1500277	Crocylic acid hydrochloride
1920 L11	X	514	520	-0.64645581	354	360	-0.07854739	2467248	0.01717437	2367005	0.40759293	experimental	NINDS	1500393	Methacholine chloride
1920 L12	X	549	560	-0.231583	474	480	-0.11824207	2913629	1.33532862	2376628	0.439573	experimental	NINDS	1500508	Progesterone
1920 L13	X	475	480	-0.62537011	435	440	-0.13759322								

1920 M07	X		394	400	-1.05640734	474	480	-0.11824207	2646785	0.54734357	2434452	0.63214784	experimental	NINDS	1500186	Chlortetracycline hydrochloride
1920 M08	X		594	600	0.00788213	513	520	-0.09888091	2533090	0.21160449	2370098	0.41782574	experimental	NINDS	1500283	Estradiol cypionate
1920 M09	X		474	480	-0.63069155	514	520	-0.09839473	2533334	0.21232502	2409468	0.54894208	experimental	NINDS	1500187	Chlorthalidone
1920 M10	X		454	440	-0.84354945	474	480	-0.11824207	2462511	0.0031861	2320705	0.25332917	experimental	NINDS	1500284	Estradiol valerate
1920 M11	X		550	560	-0.28626156	475	480	-0.11774588	2287558	-0.51344661	2435466	0.63754349	experimental	NINDS	1500168	Ephedrine
1920 M12	X		1874	1880	6.81933473	395	400	-0.15744056	2366490	-0.28036201	2123383	-0.40382448	experimental	NINDS	1500285	Estril
1920 M13	X		309	320	-1.50873037	233	240	-0.23782229	1112690	-3.98280859	192470	-3.17106541	experimental	NINDS	1500169	Cetylpyridinium chloride
1920 M14	X		474	480	-0.63069155	513	640	-0.03934889	2429583	-0.09404963	2470316	0.517581794	experimental	NINDS	1500286	Estrone
1920 M15	X		594	600	0.00788213	634	880	0.08023133	2584079	0.362174	2618953	1.24660293	experimental	NINDS	1500171	Chlorambucil
1920 M16	X		392	400	-1.06705024	552	560	-0.07953975	2302429	-0.46953288	2204348	-0.13418174	experimental	NINDS	1500287	Ethacrynic acid
1920 M17	X		673	680	0.42827647	834	840	0.06038399	2573891	0.33208904	2518594	0.91237114	experimental	NINDS	1500173	Chloramphenicol hemisuccinate
1920 M18	X		712	720	0.63581291	632	640	-0.03984507	2774022	0.92307192	2315644	0.24083699	experimental	NINDS	1500288	Ethambutol hydrochloride
1920 M19	X		912	920	1.70010238	753	760	0.02019313	2592991	0.38849096	2662360	1.40781575	experimental	NINDS	1500174	Chloramphenicol
1920 M20	X		791	800	1.05620726	672	680	-0.01999773	2196760	-0.78157134	2238904	-0.01909775	experimental	NINDS	1500291	Ethinyl estradiol
1920 M21	X		551	560	-0.22094011	752	760	0.01969695	2367299	-0.27797305	2495880	0.83672531	experimental	NINDS	1500177	Chlorhexidine
1920 M22	X		910	920	1.68945949	709	720	-0.00163894	2238732	-0.65762886	2187543	-0.19014847	experimental	NINDS	1500292	Ethionamide
1920 M23	E		1018	1640	2.2641758	789	1360	0.03805574	85773	-7.01527416	90905	-7.17271162	empty			
1920 M24	P	210038	211200	1114.5531	193479	194880	95.6476554	2394443	-0.19781736	2514156	0.897591	empty				
1920 N01	N		436	440	-0.83290655	276	280	-0.2164864	2227251	-0.69153202	21755647	-0.22876645	empty			
1920 N02	E		155	160	-2.32823326	197	200	-0.2556849	79950	-7.03246937	81129	-7.20526923	empty			
1920 N03	X		594	600	0.00788213	435	440	-0.13759322	1947682	-1.51709374	1974450	-0.89982526	experimental	NINDS	1500399	Methoxamine hydrochloride
1920 N04	X		594	600	0.00788213	554	560	-0.07854739	2393731	-0.19991988	2909539	-0.51320689	experimental	NINDS	1500516	Pseudoephedrine hydrochloride
1920 N05	X		553	560	-0.21029721	354	360	-0.17784009	2062239	-1.17880919	2060795	-0.61226517	experimental	NINDS	1500400	Methoxsalen
1920 N06	X		632	640	0.21009713	635	640	-0.03835652	2403036	-0.1724424	2459310	0.71493397	experimental	NINDS	1500517	Pyrantel pamoate
1920 N07	X		474	480	-0.63069155	392	400	-0.15892911	2220274	-0.71213497	2037951	-0.68834395	experimental	NINDS	1500401	Methscopolamine bromide
1920 N08	X		453	440	-0.84887609	834	840	-0.06038399	2265950	0.37725464	2584800	0.90332023	experimental	NINDS	1500518	Razafinamide
1920 N09	X		514	520	-0.41783366	674	680	-0.01900537	2157585	-0.89754534	1973399	-0.90332547	experimental	NINDS	1500402	Methopropate
1920 N10	X		473	480	-0.636013	472	480	-0.11923443	2338980	-0.3615985	2126894	-0.39213158	experimental	NINDS	1500519	Pyriminidine maleate
1920 N11	X		554	560	-0.20497577	634	640	-0.03885271	2218062	-0.71866696	2146333	-0.32739268	experimental	NINDS	1500404	Methylergonovine maleate
1920 N12	X		548	560	-0.23690445	633	640	-0.03934889	2254539	-0.6109511	2455613	0.70262163	experimental	NINDS	1500520	Pyrimethamine
1920 N13	X		1074	1080	2.56217686	794	800	0.04053665	2209243	-0.74470929	2154820	-0.2991279	experimental	NINDS	1500406	Methylprednisolone
1920 N14	X		832	840	1.2743866	752	760	0.01969695	1550365	-2.69036298	1535176	-2.36276662	experimental	NINDS	1500521	Pyrvinium pamoate
1920 N15	X		392	400	-1.06705024	472	480	-0.11923443	2376421	-0.25103597	2149949	-0.31535009	experimental	NINDS	1500410	Metoclopramide hydrochloride
1920 N16	X		354	360	-0.83290655	473	480	-0.11873825	2384425	-0.70214134	2105781	-1.66494218	experimental	NINDS	1500522	Quinacrine hydrochloride
1920 N17	X		633	640	0.21541857	552	560	-0.07904357	2177602	-0.83814454	2077463	-0.5567547	experimental	NINDS	1500411	Metoprolol tartrate
1920 N18	X		552	560	-0.21561866	593	600	-0.05919623	2436592	-0.07335219	2423219	-0.00472724	experimental	NINDS	1500523	Quinidine gluconate
1920 N19	X		632	640	0.21009713	633	640	-0.03934889	2176671	-0.84089376	2042909	-0.67183202	experimental	NINDS	1500412	Metronidazole
1920 N20	X		592	600	-0.00276077	512	520	-0.09938709	2216972	-0.72188571	2140158	-0.34795766	experimental	NINDS	1500524	Quinine sulfate
1920 N21	X		552	560	-0.21561866	553	560	-0.07904357	1895142	-1.67224332	1984116	-0.86763398	experimental	NINDS	1500413	Miconazole nitrate
1920 N22	X		789	800	1.04556436	792	800	0.03954429	2453705	-0.02281784	2156656	-0.29301335	experimental	NINDS	1500525	Racephedrine hydrochloride
1920 N23	E		1360	98.98170699	193479	83694	77.0214134	83694	77.0214134	77.0214134	77.0214134	77.0214134	empty			
1920 N24	P	196378	197560	1041.86213	188177	189320	93.0168904	2101991	-1.06142332	2154512	-0.30015365	empty				
1920 O01	N		476	480	-0.62004866	517	520	-0.09609618	2765410	0.89764085	1934272	-1.03363254	empty			
1920 O02	E		275	280	-1.68965958	156	160	-0.27602842	253206	-6.52084783	82516	-7.20065002	empty			
1920 O03	X		794	800	1.0721716	595	600	-0.05820386	2868255	1.2013401	2181477	-0.21035044	experimental	NINDS	1500178	Chlorocresol
1920 O04	X		512	520	-0.42847655	473	480	-0.11873825	2331384	-0.38402933	1760487	-1.61239947	experimental	NINDS	1500293	Ethopropazine hydrochloride
1920 O05	X		631	640	0.20477568	475	480	-0.11774588	2488127	0.07882964	1867812	-1.25496881	experimental	NINDS	1500179	Chloroquine diphosphate
1920 O06	X		1193	1200	3.49542900	675	680	-0.11873825	2311136	-0.44382128	1992375	-0.83947971	experimental	NINDS	1500295	Eucaliptol hydrochloride
1920 O07	X		600	600	0.00808291	674	680	-0.01900537	2157585	-0.02612376	1958159	-0.34391127	experimental	NINDS	1500180	Chlorzoxazone
1920 O08	X		754	760	0.8593137	353	360	-0.17828027	2278321	-0.54072332	2049317	-0.65049106	experimental	NINDS	1500296	Eugenol
1920 O09	X		632	640	0.21009713	392	400	-0.15892911	2298040	-0.48249351	2230349	-0.04728927	experimental	NINDS	1500189	Clopirox olamine
1920 O10	X		874	880	1.49788739	955	960	-0.1204222	2094487	-1.08358149	2050850	-0.64538562	experimental	NINDS	1500299	Fludrocortisone acetate
1920 O11	X		432	440	-0.85419234	392	400	-0.15892911	2043276	-1.23480656	2135522	-0.36339722	experimental	NINDS	1500190	Cinoxacin
1920 O12	X		754	760	0.8593137	714	720	0.00084197	2416286	-1.13331541	2063995	-0.60160801	experimental	NINDS	1500300	Flumethazone pivalate
1920 O13	X		471	480	-0.6466559	511	520	-0.09988328	1970886	-1.44857279	2016070	-0.76121256	experimental	NINDS	1500191	Clemastine
1920 O14	X		631	640	0.20477568	672	680	-0.01999773	2245486	-0.63768443	2105785	-0.46243219	experimental	NINDS	1500303	Fluocinonide
1920 O15	X		992	1000	2.12581817	793	800	0.04004047	2395445	-0.19485847	2327640	0.27642523	experimental	NINDS	1500192	Clidinium bromide
1920 O16	X		672	680	0.42295502	673	680	-0.01950155	2317645	-0.42460033	2269527	0.08288792	experimental	NINDS	1500304	Fluorometholone
1920 O17	X		711	720	0.63049147	592	600	-0.05969241	2431673	-0.0878779	2165048	-0.26506496	experimental	NINDS	1500195	Clofibric acid
1920 O18	X		793	800	1.06685015	712	720	-0.00015039	2109490	-1.03927792	2138818	-0.35242035	experimental	NINDS	1500305	Fluorouracil
1920 O19	X		672	680	0.42295502	632	640	-0.03984507	2570817	0.32301157	2294908	0.16741583	experimental	NINDS	1500196	Flumiphene citrate
1920 O20	X		752	760	0.84867081	873	880	0.07973515	2192043	-0.79550055	2250088	0.01814901	experimental	NINDS	1500308	Flurbiprofen
1920 O21	X		711	720	0.63049147	472	480	-0.11873825	1866909	-1.75561481	1958732	-0.95217189	experimental	NINDS	1500200	Citrimizole
1920 O22	X		790	800	1.05088581	474	480	-0.1202268	1253152	-3.56802708	1066020	-3.92522585	experimental	NINDS	1500309	Furazolidone
1920 O23	E		702	1280	0.58259844	534	1120	-0.08847106	90547	-7.00117663	84930	-7.19261053	empty			
1920 O24	P	194275	195640	1030.67113	197932	199280	97.8571605	2144756	-0.93513812	2233078	-0.03850044	empty				
1920 P01	N		758	760	0.88059949	718	720	0.00282671	1837244	-1.84321497	1781799	-1.54142279	empty			
1920 P02	E		235	240	-1.90251747	195	200	-0.25667727	72875	-7.05336117	76193	-7.2217079	empty			
1920 P03	X		595	600	0.01320358	796	800	0.04152902	1943050	-1.53077195	1933381	-1.03659989	experimental	NINDS	1500415	Minoxidil
1920 P04	X		555	560	0.86463515	715	720	0.00138116	2192546	-0.79401528	1912568	-0.43840275	experimental	NINDS	1500526	Reserpine
1920 P05	X		674	680	0.43358922	435	440	-0.13759322	1908356	-1.63026966	1958159	-0.9				

1921 A01	N	718	720	-0.05645334	798	800	0.10907872	1471446	-1.11502386	1557210	-0.97868565	empty				
1921 A02	E	156	160	-0.44929377	156	160	-0.56646486	80772	-2.48326179	82861	-2.37406749	empty				
1921 A03	X	556	560	-0.16969204	556	560	-0.14556544	1964730	-0.62969812	2065605	-0.49752064	experimental	NINDS	1500539	Spironolactone	
1921 A04	X	635	635	-0.17091904	635	640	-0.16643778	1795251	-0.79644288	1903533	-0.65091195	experimental	NINDS	1500563	Yohimbine hydrochloride	
1921 A05	X	475	480	-0.26311339	595	600	-0.10527774	2039342	-0.55628982	2193737	-0.52838811	experimental	NINDS	1500545	Streptococin sulfate	
1921 A06	X	596	600	-0.14173187	675	680	-0.02034786	1768087	-0.82316864	2003683	-0.55612606	experimental	NINDS	1500665	Acetabutoil hydrochloride	
1921 A07	X	355	355	360	-0.31019191	394	400	-0.3160297	2148532	-0.44886144	2255783	-0.31752871	experimental	NINDS	1500543	Streptozosin
1921 A08	X	795	800	-0.002623	914	920	0.23113955	1932380	-0.66152621	1985020	-0.57378945	experimental	NINDS	1500666	Acemetacin	
1921 A09	X	673	680	-0.08790853	954	960	0.27322949	2189373	-0.40867934	2554810	-0.03451778	experimental	NINDS	1500544	Sulfabenzamide	
1921 A10	X	834	840	0.02463117	514	520	-0.18975987	2019073	-0.57623185	2061396	-0.50150421	experimental	NINDS	1500667	Adenosine phosphate	
1921 A11	X	515	520	-0.19835122	475	480	-0.23079757	2138312	-0.458991656	2323537	-0.25340366	experimental	NINDS	1500545	Sulfacetamide	
1921 A12	X	395	400	-0.28223174	596	600	-0.10347549	1953511	-0.63581679	192434	-0.62947416	experimental	NINDS	1500668	Ketolifen fumarate	
1921 A13	X	395	400	-0.28223174	275	280	-0.44124728	2150963	-0.44646966	2258198	-0.31524306	experimental	NINDS	1500546	Sulfadiazine	
1921 A14	X	676	680	-0.08581152	556	560	-0.14556544	2026215	-0.56920508	2105731	-0.45954382	experimental	NINDS	1500669	Benfluorex hydrochloride	
1921 A15	X	434	440	-0.25497057	396	400	-0.3139252	2224176	-0.37443783	2333198	-0.24426011	experimental	NINDS	1500547	Sulfamerazine	
1921 A16	X	755	760	-0.03059018	435	440	-0.27288751	2078944	-0.51732676	2193397	-0.37657327	experimental	NINDS	1500673	Sulfamethizole	
1921 A17	X	752	760	-0.03268719	554	560	-0.14766993	2095533	-0.50100054	2473326	-0.11163746	experimental	NINDS	1500548	Sulfamethazine	
1921 A18	X	1154	1160	0.24831255	1234	1240	0.56785909	2197698	-0.40048865	2060832	-0.502038	experimental	NINDS	1500674	Mycophenolic acid	
1921 A19	X	671	680	-0.08930654	631	640	-0.06664679	2214806	-0.38365666	2292027	-0.28322596	experimental	NINDS	1500549	Sulfamethizole	
1921 A20	X	1034	1040	0.16443203	875	880	0.19010186	2133636	-0.46351712	2185620	-0.38393373	experimental	NINDS	1500675	Oleandomycin phosphate	
1921 A21	X	953	960	0.10781268	594	600	-0.10557999	2139900	-0.45735418	2212801	-0.35820856	experimental	NINDS	1500550	Sulfamethoxazole	
1921 A22	X	628	640	-0.11936373	391	400	-0.31918645	1372990	-1.21189144	1489965	-1.04232896	experimental	NINDS	1500676	Ouabain	
1921 A23	E	1087	2080	0.20147926	1021	1760	0.34373015	83985	-2.48010062	81918	-2.37495998	empty				
1921 A24	P	340307	341040	237.317729	252760	253480	265.235731	2309515	-0.29047562	1933308	-0.62273172	empty				
1921 B01	N	595	600	-0.14243087	396	400	-0.3139252	2066411	-0.52965757	2083561	-0.48052638	empty				
1921 B02	E	595	600	-0.4220128	156	160	-0.56646486	80772	-2.48326179	82861	-2.37406749	empty				
1921 B03	X	594	600	-0.14312987	476	480	-0.22974532	2263721	-0.33553082	2038294	-0.33368885	experimental	NINDS	1501002	Droperidol	
1921 B04	X	634	640	-0.1151697	434	440	-0.27393976	2679404	-0.07344587	2505515	-0.08117253	experimental	NINDS	1501203	Retinol	
1921 B05	X	434	440	-0.25497057	434	440	-0.27393976	2313560	-0.28649588	2208204	-0.36255934	experimental	NINDS	1501003	Famotidine	
1921 B06	X	435	440	-0.25427156	634	640	-0.06349005	2574042	-0.0302163	2494735	-0.09137514	experimental	NINDS	1501204	Lapachol	
1921 B07	X	315	320	-0.33815208	473	480	-0.23290207	2389616	-0.21166691	2522336	-0.06525247	experimental	NINDS	1501004	Dropropizine	
1921 B08	X	553	560	-0.17178905	753	760	0.06172753	1857178	-0.73551496	2220770	-0.35066639	experimental	NINDS	1501205	Lanatoside c	
1921 B09	X	793	800	-0.00402801	592	600	-0.10768449	2386900	-0.21433909	2433425	-0.14940134	experimental	NINDS	1501005	Etodolac	
1921 B10	X	673	680	-0.04927184	474	480	-0.22974532	2241874	-0.17985479	2262922	-0.09139066	experimental	NINDS	1501206	Terbutaline maleate	
1921 B11	X	473	480	-0.2277094	594	600	-0.10557999	2514219	-0.08907416	2651272	-0.05720352	experimental	NINDS	1501007	Fentorol hydrobromide	
1921 B12	X	634	640	-0.1151697	593	600	-0.10663224	2568141	-0.0360221	2373886	-0.20575139	experimental	NINDS	1501215	Ketoprofen	
1921 B13	X	754	760	-0.03128918	714	720	0.02068984	2184572	-0.41340289	2321099	-0.25571108	experimental	NINDS	1501008	Fenfenbut	
1921 B14	X	472	480	-0.2284084	673	680	-0.02245235	2725981	-0.11927143	2603745	0.0117962	experimental	NINDS	1501217	Lisinopril	
1921 B15	X	674	680	-0.08720953	474	480	-0.23184982	1884048	-0.70907846	1980542	-0.57802761	experimental	NINDS	1501009	1,9-tyrhydrastine	
1921 B16	X	472	480	-0.2284084	594	600	-0.10557999	2535749	-0.06789151	2611078	0.01873644	experimental	NINDS	1502001	Acetyl-l-leucine	
1921 B17	X	840	840	-0.11018637	631	640	-0.06172753	2344893	-0.25173282	2377706	-0.36572759	experimental	NINDS	1501010	Tetrolidate	
1921 B18	X	749	760	-0.0347842	831	840	0.14380292	2321495	-0.2786889	2339126	-0.23864962	experimental	NINDS	1502003	Buformin	
1921 B19	X	952	960	0.10711368	832	840	0.14485517	2627245	0.02212837	2430429	-0.15223687	experimental	NINDS	1501011	Fenoprofen	
1921 B20	X	510	520	-0.20184624	431	440	-0.27709651	2386851	-0.2143873	2506001	-0.08071256	experimental	NINDS	1502004	Bumetanide	
1921 B21	X	870	880	0.04979532	753	760	0.06172753	2212139	-0.38628063	2201087	-0.36929515	experimental	NINDS	1501015	Flufenamic acid	
1921 B22	P	1149	1160	0.24481753	630	640	-0.06769904	2504962	-0.09818181	2384320	-0.19587624	experimental	NINDS	1502005	Carbenoxolone sodium	
1921 B23	E	580	1320	0.25191594	795	1520	0.10592197	91746	-2.47246483	89489	-2.36779449	empty				
1921 B24	E	249608	251120	173.918735	245508	246760	257.604829	2032833	3.56269385	1673310	3.73626452	empty				
1921 C01	N	637	640	-0.11307269	397	400	-0.21827956	2090022	-0.50125295	1981310	-0.62700074	empty				
1921 C02	E	196	200	-0.4213336	197	200	-0.52332267	88101	-2.47605103	89862	-2.36744147	empty				
1921 C03	X	553	560	-0.17178905	354	360	-0.35811964	2743213	0.13622543	2861350	0.2556037	experimental	NINDS	1500551	Sulfapyridine	
1921 C04	X	513	520	-0.19974923	555	560	-0.14661768	2233843	-0.36492679	2325340	-0.25169723	experimental	NINDS	1500677	Albuterol (+/-)	
1921 C05	X	474	480	-0.22701039	394	400	-0.3160297	2104257	-0.49242215	2780979	0.17953743	experimental	NINDS	1500552	Sulfasalazine	
1921 C06	X	515	520	-0.19835122	594	600	-0.10557999	2232962	-0.36579357	2405279	-0.17603982	experimental	NINDS	1500678	Gamga-aminobutyric acid	
1921 C07	X	434	440	-0.25497057	754	760	0.06277978	2671997	0.06615837	2225975	-0.34574017	experimental	NINDS	1500553	Sulfathiazole	
1921 C08	X	633	640	-0.11586871	432	440	-0.27604426	2442477	-0.15965873	2368242	-0.21109309	experimental	NINDS	1500679	Aminopterin	
1921 C09	X	512	520	-0.20044823	554	560	-0.14766993	2420490	-0.18129101	2536450	-0.05189443	experimental	NINDS	1500554	Sulfipyraxone	
1921 C10	X	553	560	-0.17178905	394	400	-0.3160297	2351364	-0.24930178	2439962	-0.14321446	experimental	NINDS	1500680	Arecoline hydrobromide	
1921 C11	X	434	440	-0.25497057	554	560	-0.14766993	2564292	-0.039809	2627176	0.03397222	experimental	NINDS	1500556	Sulindac	
1921 C12	X	474	480	-0.22701039	513	520	-0.19081212	2283174	-0.31639166	2461477	-0.12285182	experimental	NINDS	1500682	Captopril	
1921 C13	X	433	440	-0.25566957	553	560	-0.14872218	2133131	-0.46401398	2270228	-0.30385739	experimental	NINDS	1500557	Tamoxifen citrate	
1921 C14	X	673	680	-0.08790853	591	600	-0.10873674	2349422	-0.25121245	2606307	0.01422098	experimental	NINDS	1500684	Cimetidine	
1921 C15	X	553	560	-0.17178905	554	560	-0.14766993	2647002	0.04156662	2877706	0.36572759	experimental	NINDS	1500518	Terbutaline hemisulfate	
1921 C16	X	344	400	-0.31788096	472	480	-0.2395431	2160660	-0.43692911	2251462	-0.32161827	experimental	NINDS	1500685	Clozapine	
1921 C17	X	17753	17760	11.8510854	674	680	-0.02140011	2675360	0.06946712	2384801	-0.195421	experimental	NINDS	1500564	Tracracine hydrochloride	
1921 C18	X	663	720	-0.09489858	472	480	-0.2395431	2488475	-0.11440283	2458109	-0.12603943	experimental	NINDS	1500687	1,9-tyrhydrastine	
1921 C19	X	672	680	-0.08860754	753	760	0.06172753	2619879	0.0148812	2497665	-0.08860208	experimental	NINDS	1500566	Tetracycline hydrochloride	
1921 C20	X	713	720	-0.05994836	632	640	-0.0645423	2295339	-0.30442292	2420664	-0.16147884	experimental	NINDS	1500688	Kyrenic acid	
1921 C21	X	754	760	-0.03338619	592	600	-0.10768449	2524638	-0.07882325	2439493	-0.14365835	experimental	NINDS	1500567	Sulfathiazole	
1921 C22	X	909	920	0.07702949	571	580	0.05963303	2200424	-0.39780663	2322770	-0.29908545	experimental	NINDS	1500568	Tetrahydrozoline hydrochloride	
1921 C23	E	830	1360	0.02183515	676	1200	-0.01929561	92063	-0.07215295	89113	-0.36815035	empty				
1921 C24	P	178635	179840	124.3083	176150	177360	184.622968	2480313	-0.12243315	2254215	-0.31909791	empty				
1921 D01	N	396	400	-0.28153273	477	480	-0.22869307	2361556	-0.23927421							

1921 D19	X		433	440	-0.25566957	592	600	-0.10768449	2272334	-0.32705677	2308230	-0.26789801	experimental	NINDS	1501108	Mefexamide
1921 D20	X		549	560	-0.17458507	710	720	0.01648084	2572691	-0.03154555	2789378	0.18748657	experimental	NINDS	1502020	Folic acid
1921 D21	X		631	640	-0.11726671	550	560	-0.15187893	2498469	-0.10457006	2352168	-0.22630616	experimental	NINDS	1501109	Prubocul
1921 D22	X		670	680	-0.09000555	829	840	-0.14169842	2420702	-0.18108243	2341332	-0.23656177	experimental	NINDS	1502021	Phthalylsulfathiazole
1921 E	X		637	1120	-0.11307269	938	1440	0.25639351	92283	-0.47193649	empty	empty	empty	empty	empty	empty
1921 D24	P	162600	163640	113.099766	168928	170080	177.023629	2160100	-0.43748007	2064110	-0.49893557	empty	empty	empty	empty	empty
1921 E01	N		677	680	-0.08511251	397	400	-0.31287296	2203667	-0.39461595	2159164	-0.40897273	experimental	NINDS	1500568	Theophylline
1921 E02	E		196	200	-0.42133336	236	240	-0.48228497	90973	-2.47322536	94958	-2.36261842	experimental	NINDS	1500690	Melatonin
1921 E03	X		512	520	-0.20044823	513	520	-0.19081212	2648885	0.04341924	2668778	0.07334599	experimental	NINDS	1500691	Phentolamine hydrochloride
1921 E04	X		433	440	-0.25566957	512	520	-0.19186437	2474393	-0.12825764	2622176	0.02924003	experimental	NINDS	1500575	Acetyltryptophan
1921 E05	X		874	880	0.05259134	1233	1240	0.56680684	2676003	0.07009974	2871778	0.26547317	experimental	NINDS	1500702	Acetyltryptophan
1921 E06	X		502	520	-0.20743827	582	600	-0.11820697	2533413	-0.07018982	22840	-0.28997314	experimental	NINDS	1500576	Thiothixene
1921 E07	X		4594	4600	2.65288745	4034	4040	3.51415506	2363925	-0.23694343	1871463	-0.68126426	experimental	NINDS	1500572	Thimerosal
1921 E08	X		542	560	-0.1794781	464	480	-0.2423723	2525152	-0.07831754	2504422	-0.08220699	experimental	NINDS	1500695	Acetyl tyrosine ethyl ester
1921 E09	X		353	360	-0.31158992	514	520	-0.18975987	2522079	-0.08134097	2363701	-0.21539087	experimental	NINDS	1500573	Thioguanine
1921 E10	X		513	520	-0.19974923	475	480	-0.23079757	2336268	-0.26415423	2766121	0.16547523	experimental	NINDS	1500699	Acetyltryptophanamide
1921 E11	X		634	640	-0.1151697	234	240	-0.48438947	2711859	0.10537727	2191703	-0.37817654	experimental	NINDS	1500575	Thioridazine hydrochloride
1921 E12	X		472	480	-0.2284084	595	600	-0.10452774	2237938	-0.36089785	2587376	-0.00369606	experimental	NINDS	1500702	Acetyltryptophan
1921 E13	X		593	600	-0.14382888	394	400	-0.3160297	2209973	-0.38841169	2318633	-0.2580405	experimental	NINDS	1500576	Thiothixene
1921 E14	X		512	520	-0.20044823	473	480	-0.23290207	2433858	-0.16813868	2611068	0.01872698	experimental	NINDS	1500703	Acetylglutamic acid
1921 E15	X		594	600	-0.14312987	394	400	-0.3160297	2769658	0.16224378	2925888	0.316685	experimental	NINDS	1500578	Timolol maleate
1921 E16	X		553	560	-0.17178905	473	480	-0.23290207	2405440	-0.1960982	2529274	-0.05868608	experimental	NINDS	1500704	N-acetylproline
1921 E17	X		634	640	-0.1151697	754	760	0.06277978	2696706	0.09046874	2655745	0.06101105	experimental	NINDS	1500580	Tolazoline hydrochloride
1921 E18	X		673	680	-0.08790853	513	520	-0.19081212	2799666	0.19176766	2702918	0.10565743	experimental	NINDS	1500707	Citroten
1921 E19	X		549	560	-0.17458507	550	560	-0.15187893	2509618	-0.09360093	2553902	-0.03537717	experimental	NINDS	1500582	Tolmetin sodium
1921 E20	X		594	600	-0.17748985	431	440	-0.27499201	2399361	0.204791	2318122	-0.25643215	experimental	NINDS	1500583	Thrynsol
1921 E21	X		1069	1080	-0.8898718	1269	1280	0.60468779	2723027	0.18365009	2411571	-0.0088577	experimental	NINDS	1500583	Togifattate
1921 E22	X		749	760	-0.0347842	868	880	0.18273612	2358672	-0.24211168	2169035	-0.39963043	experimental	NINDS	1500715	Acetylglucosamine
1921 E23	E		595	1120	-0.14243087	796	1440	0.10697422	93006	-2.47122516	92413	-2.3650271	empty	empty	empty	empty
1921 E24	P	177288	178280	123.366741	218092	219120	228.756377	2578918	-0.02541896	2417581	-0.16439672	2480362	-0.10497832	empty	empty	empty
1921 F01	N		516	520	-0.19765221	437	440	-0.27078301	2530362	-0.0731916	2480362	-0.10497832	empty	empty	empty	empty
1921 F02	E		154	160	-0.45069178	195	200	-0.52542717	91079	-2.47312107	89755	-2.36754274	experimental	NINDS	1501110	Mebendazole
1921 F03	X		1074	1080	0.11923922	954	960	0.27322949	2379370	-0.22174761	2368206	-0.21112716	experimental	NINDS	1501111	Ripecemic acid
1921 F04	X		515	520	-0.20044823	236	240	-0.48228497	90973	-2.47322536	94958	-2.36261842	experimental	NINDS	1501111	Protoporpyrin ix
1921 F05	X		753	760	-0.03198819	712	720	0.01858534	1982331	-0.61238108	2295810	-0.27964558	experimental	NINDS	1502025	Succinylsulfathiazole
1921 F06	X		314	320	-0.33885109	433	440	-0.27499201	2812919	0.20480684	2652254	0.05770703	experimental	NINDS	1501113	Peruvoside
1921 F07	X		503	520	-0.20673927	423	440	-0.28551449	2000557	-0.59444913	1631497	-0.90837752	experimental	NINDS	1502026	Tranexamic acid
1921 F08	X		514	520	-0.19905022	475	480	-0.23079757	3471692	0.8529517	2938177	0.32901616	experimental	NINDS	1501114	Pimethixene maleate
1921 F09	X		474	480	-0.22701039	474	480	-0.23184982	2224243	-0.37437191	2136133	-0.43077017	experimental	NINDS	1502028	Cephalexin
1921 F10	X		634	640	-0.1151697	435	440	-0.27288751	3365769	0.74873758	2757279	0.15710682	experimental	NINDS	1502030	Triamcinolone hydrochloride
1921 F11	X		594	600	-0.14382888	394	400	-0.3160297	2605399	0.00606481	2605399	0.00606481	experimental	NINDS	1502030	Meibhydrolin naphthalenesulfonate
1921 F12	X		833	840	0.02393216	474	480	-0.23184982	2658293	0.05267596	2911367	0.30929415	experimental	NINDS	1501116	Cefoxitin sodium
1921 F13	X		792	800	-0.00472702	554	560	-0.14766993	2422739	-0.17907829	2426948	-0.15553143	experimental	NINDS	1501117	Mebeverine hydrochloride
1921 F14	X		632	640	-0.11656771	514	520	-0.18975987	2607637	0.00283671	2848300	0.24325267	experimental	NINDS	1502031	Cefuroxime sodium
1921 F15	X		593	600	-0.14382888	394	400	-0.3160297	2832080	0.22365871	2815473	0.2121839	experimental	NINDS	1501118	Mecloxycline sulfosalicylate
1921 F16	X		514	520	-0.19905022	394	400	-0.3160297	2832080	0.22365871	2815473	0.2121839	experimental	NINDS	1502033	Metampicillin sodium
1921 F17	X		474	480	-0.22701039	514	520	-0.18975987	2319189	-0.28095769	2278874	-0.29567448	experimental	NINDS	1501119	Trimethoprim
1921 F18	X		594	600	-0.14312987	394	400	-0.3160297	2832080	0.22365871	2815473	0.2121839	experimental	NINDS	1502037	Lomefloxacin hydrochloride
1921 F19	X		592	600	-0.15297888	793	800	0.10381747	2254908	-0.14420163	2211712	-0.35923924	experimental	NINDS	1501120	Miniprine hydrochloride
1921 F20	X		749	760	-0.0347842	868	880	0.18273612	2358672	-0.24211168	2169035	-0.39963043	experimental	NINDS	1502037	Fosfomicin
1921 F21	X		590	600	-0.14592589	549	560	0.27112499	2285163	-0.31443474	2457578	-0.12654199	experimental	NINDS	1502039	Fosfomicin
1921 F22	X		870	880	0.04979532	589	600	-0.11084123	2399133	-0.20230345	2435592	-0.1473504	experimental	NINDS	1502039	Fosfomicin
1921 F23	E		595	1120	-0.14243087	580	1120	-0.12031147	93878	-2.47036723	91772	-2.36563377	empty	empty	empty	empty
1921 F24	P	176798	177800	123.024229	182418	183480	191.218462	2162495	-0.43512371	2064326	-0.49873114	2354664	-0.16675941	empty	empty	empty
1921 G01	N		436	440	-0.25357256	357	360	-0.3549629	2103238	-0.499342471	2354664	-0.16675941	empty	empty	empty	empty
1921 G02	E		155	160	-0.44989278	236	240	-0.48228497	88971	-2.47519506	90909	-2.36722284	experimental	NINDS	1500584	Tranlycypromine sulfate
1921 G03	X		833	840	0.02393216	634	640	-0.06349005	2414624	-0.18706237	3107778	0.48883284	experimental	NINDS	1500750	Neohesperidin dihydrochalcone
1921 G04	X		473	480	-0.2277094	433	440	-0.27499201	2447766	-0.15445506	2764675	0.16410668	experimental	NINDS	1500585	Riactin
1921 G05	X		594	600	-0.14312987	632	640	-0.0645423	2912693	0.30297117	2647858	0.05354648	experimental	NINDS	1500753	Physostigmine
1921 G06	X		314	320	-0.33885109	792	800	0.10276523	2633808	0.02858548	2425777	-0.15663971	experimental	NINDS	1500586	Xanthurenic acid
1921 G07	X		595	600	-0.14243087	954	960	0.27322949	3357702	0.74080073	2483542	-0.10196864	experimental	NINDS	1500754	Nalidixic acid
1921 G08	X		554	560	-0.17109005	472	480	-0.23954321	2888456	0.27912519	2852839	0.24754856	experimental	NINDS	1500588	Triamcinolone diacetate
1921 G09	X		594	600	-0.14312987	433	440	-0.27499201	2733101	0.12627657	2703778	0.10647137	experimental	NINDS	1500760	Lobeline hydrochloride
1921 G10	X		433	440	-0.25566957	434	440	-0.27393976	2485964	-0.11687331	2638232	0.04443606	experimental	NINDS	1500590	Hecogenin
1921 G11	X		633	640	-0.11586871	554	560	-0.14766993	2940656	0.33048303	2872853	0.26649059	experimental	NINDS	1500591	Trifluoperazine hydrochloride
1921 G12	X		592	600	-0.14452788	513	520	-0.19081212	2441158	-0.16095645	2385065	-0.19517114	experimental	NINDS	1500591	Calciferol
1921 G13	X		592	600	-0.14452788	554	560	-0.14766993	2765922	0.15856806	2319824	-0.25691779	experimental	NINDS	1500592	Triphenylenediy hydrochloride
1921 G14	X		632	640	-0.08790853	314	320	-0.40020959	2589264	-0.15523988	2378886	-0.20101919	experimental	NINDS	1500594	Kinetin
1921 G15	X		593	600	-0.14382888	394	400	-0.3160297	2147368	-0.45000667	2151005	-0.36659473	experimental	NINDS	1500594	Trimethobenzamide hydrochloride
1921 G16	X		553	560	-0.17178905	593	600	-0.10653224	3839593	1.21491727	2354462	0.72224749	experimental	NINDS	1500763	Cefazolin sodium
1921 G17																

1921 H13	X	753	760	-0.03198819	514	520	-0.18975987	2902888	0.29332435	2597116	0.00552226	experimental	NINDS	1501129	Carbetapentane citrate	
1921 H14	X	512	560	-0.20044823	474	480	-0.23184982	2844336	0.23571699	2883429	0.27650013	experimental	NINDS	1502045	Promidic acid	
1921 H15	X	14312	14320	9.44581154	513	520	-0.19081212	2698549	0.092282	2536896	-0.04957944	experimental	NINDS	1501130	Aminopyridine	
1921 H16	X	717	800	-0.05175234	731	760	0.03857806	2869649	0.2606216	2603676	0.0117309	experimental	NINDS	1502045	Nevirovirine	
1921 H17	X	792	800	-0.00472702	351	360	-0.36127639	2517555	-0.08379182	2338107	1.5898017	experimental	NINDS	1501137	Nevirovirine	
1921 H18	X	752	760	-0.03268719	992	1000	0.31321494	2536480	-0.0671723	2706914	0.1094394	experimental	NINDS	1502047	Lithyronine sodium	
1921 H19	X	511	520	-0.20114723	1032	1040	0.35530488	2387755	-0.21349789	2349138	-0.22917387	experimental	NINDS	1501134	Pinmozide	
1921 H20	X	593	600	-0.14382888	431	440	-0.27709651	2683285	0.07726426	2717613	0.11956535	experimental	NINDS	1502050	Cephaloridine	
1921 H21	X	592	600	-0.14452788	712	720	0.01858534	2224096	-0.37451654	1989187	-0.56984564	experimental	NINDS	1501135	Nicardipine hydrochloride	
1921 H22	X	869	880	0.04909632	829	840	0.14169842	2583541	-0.02087055	2519341	-0.06808706	experimental	NINDS	1502082	Indole-2-carboxylic acid	
1921 H23	E	799	1320	0.00016601	911	1440	0.2279828	87284	-2.47685484	90458	-2.29566218	empty				
1921 H24	P	175461	176520	122.089661	178309	179200	186.894773	207070	-0.29288118	2761252	0.16086702	empty				
1921 I01	N	515	520	-0.19835122	477	480	-0.22869307	2176344	-0.42149814	2411625	-0.17003372	empty				
1921 I02	E	276	280	-0.36541325	195	200	-0.52542717	88514	-2.47564469	90709	-2.36663984	empty				
1921 I03	X	513	520	-0.19974923	715	720	0.02174209	2740042	0.13310559	2688528	0.09203817	experimental	NINDS	1500595	Trimethoprim	
1921 I04	X	674	680	-0.08720953	594	600	-0.10557999	2521942	-0.08147576	2603639	0.01169588	experimental	NINDS	1500772	Idopamidol	
1921 I05	X	673	680	-0.08790853	633	680	-0.0645423	2704285	0.09792546	2776049	0.17487148	experimental	NINDS	1500596	Trioxsalen	
1921 I06	X	873	880	0.05189233	14712	14720	14.7500652	2661193	0.05552867	2278987	-0.29566218	experimental	NINDS	1500774	Thyroxine	
1921 I07	X	552	560	-0.17248806	393	440	-0.31708195	3288723	0.67293459	2761252	0.16086702	experimental	NINDS	1500598	Triprolidine hydrochloride	
1921 I08	X	592	600	-0.14452788	474	480	-0.23184982	2798024	0.19015215	2662713	0.06760584	experimental	NINDS	1500779	Sufprofen methyl ester	
1921 I09	X	594	600	-0.14312987	554	560	-0.14766993	2589655	-0.01485519	2826103	0.22224455	experimental	NINDS	1500599	Tropicamide	
1921 I10	X	433	440	-0.25566957	594	600	-0.10557999	2701709	0.09539102	2755637	-0.01480631	experimental	NINDS	1500801	Allantoin	
1921 I11	X	593	600	-0.14382888	474	480	-0.23184982	3076892	0.4645211	2894307	0.28653996	experimental	NINDS	1500600	Triptophan	
1921 I12	X	594	600	-0.14312987	594	600	-0.10557999	2581980	-0.02240636	2497088	-0.08914817	experimental	NINDS	1500804	Alliazide	
1921 I13	X	472	480	-0.2284084	433	440	-0.27499201	3103552	0.49075099	3008043	0.39443972	experimental	NINDS	1500601	Tuaminoheptane sulfate	
1921 I14	X	717	800	-0.04042804	754	800	-0.06277978	2517555	-0.046398	2306503	0.0665482	experimental	NINDS	1500807	Adimolone	
1921 I15	X	793	800	-0.05715234	650	680	-0.04665407	2250726	-0.34831616	2320662	-0.34129853	experimental	NINDS	1500603	Tyrotrichin	
1921 I16	X	12991	13000	8.52242682	8672	8680	8.39448388	2802779	0.19483043	2732517	0.13367109	S	experimental	NINDS	1500810	Aminacrine
1921 I17	X	716	760	-0.05785135	610	640	-0.08874401	2705332	0.09895557	2466966	-0.11791236	experimental	NINDS	1500604	Urea	
1921 I18	X	632	640	-0.11656771	673	680	-0.02245235	2616536	0.01159214	2667455	0.07209385	experimental	NINDS	1500811	Berberine chloride	
1921 I19	X	952	960	0.10711368	430	440	-0.27814875	2908087	0.29843948	2664946	0.06971924	experimental	NINDS	1500605	Ursodiol	
1921 I20	X	632	640	-0.11656771	673	680	-0.02140011	2831571	0.22315793	2474520	-0.11050742	experimental	NINDS	1500812	Bekanamycin sulfate	
1921 I21	X	671	680	-0.08930654	831	840	0.14380292	2681399	0.07540869	3125281	0.50539837	experimental	NINDS	1500606	Valproate sodium	
1921 I22	X	909	920	0.07705649	829	909	0.07705649	2545677	0.0570412	2057042	-0.1904661	experimental	NINDS	1500813	Budesonide	
1921 I23	E	497	1080	-0.21093329	1007	1480	0.32899867	92703	-2.47152327	87285	-2.36988044	empty				
1921 I24	P	196765	197800	136.981249	158791	159800	166.356986	2585885	-0.01856436	2466257	-0.11832784	empty				
1921 J01	N	636	640	-0.11377169	357	360	-0.3549629	2440847	-0.16126243	2360805	-0.21813176	empty				
1921 J02	E	195	200	-0.4220326	237	240	-0.48123273	85895	-2.47822144	91143	-2.36622908	empty				
1921 J03	X	595	600	-0.14243087	435	440	-0.27288751	2330559	-0.26977113	2399714	-0.18130675	experimental	NINDS	1501137	Nefopam	
1921 J04	X	554	560	-0.17190905	354	360	-0.35811964	2482608	-0.12017517	2369087	-0.21029335	experimental	NINDS	1502084	Pfadiflen hydrochloride	
1921 J05	X	493	600	-0.08362974	593	600	-0.08362974	2598505	-0.0064796	24646809	0.05255367	experimental	NINDS	1501138	Cyclosporine hydrochloride	
1921 J06	X	673	680	-0.08790853	592	640	-0.10768449	2756511	0.14930889	2708820	0.11124331	experimental	NINDS	1502085	Cyclocresatin	
1921 J07	X	791	800	-0.00542602	632	640	-0.06349005	2597495	-0.00714167	2318168	-0.25848509	experimental	NINDS	1501139	Pramoxine hydrochloride	
1921 J08	X	1153	1160	0.24761355	434	440	-0.27604426	2790416	0.18266689	2941172	0.33115038	experimental	NINDS	1502094	Rosmarinic acid	
1921 J09	X	511	520	-0.20114723	594	600	-0.10557999	2885140	0.27586269	2710119	0.11247274	experimental	NINDS	1501140	Mephesisin	
1921 J10	X	674	680	-0.08720953	673	680	-0.02245235	2997864	0.38676808	2905857	0.29772687	experimental	NINDS	1502101	Perillic acid (-)	
1921 J11	X	793	800	-0.00402801	514	520	-0.18975987	2751010	0.14389664	2527580	-0.06028935	experimental	NINDS	1501142	Sulfachloropyridazine	
1921 J12	X	512	520	-0.20044823	514	520	-0.18975987	3117643	0.50461466	2527586	2.62927596	experimental	NINDS	1502102	Quinolonic acid	
1921 J13	X	514	520	-0.19905022	514	520	-0.18975987	6579267	0.05208412	2686803	0.09490556	experimental	NINDS	1501143	Sulfaphenazole	
1921 J14	X	633	640	-0.11586871	474	480	-0.23184982	2975308	0.36457598	2723897	0.12551278	experimental	NINDS	1502103	Anthraquinone	
1921 J15	X	630	640	-0.11796572	431	440	-0.27709651	2632401	0.02720118	2849607	0.24448966	experimental	NINDS	1501144	Sulfadimethoxine	
1921 J16	X	756	800	-0.02989117	531	560	-0.17187165	3252680	0.63747308	3153446	0.53205483	experimental	NINDS	1502106	Carboplatin	
1921 J17	X	632	640	-0.11656771	554	560	-0.14766993	2454387	-0.14794088	2388854	-0.19158508	experimental	NINDS	1505364	Cefprozil	
1921 J18	X	352	360	-0.31228892	432	440	-0.27604426	2781262	0.17366057	2603615	0.01167317	experimental	NINDS	1502107	Cisplatin	
1921 J19	X	992	1000	0.13507385	994	1000	0.31531943	2540867	-0.06285608	2696074	0.09918	experimental	NINDS	1501146	Sulfaguanidine	
1921 J20	X	631	640	-0.11726671	511	520	-0.19291662	2995222	0.38416871	3221688	0.59664175	experimental	NINDS	1502109	Zidovudine [a:1]	
1921 J21	X	790	800	-0.00612503	792	800	0.10276523	2485815	-0.11701991	2407012	-0.17439964	experimental	NINDS	1501147	Sulfamonomethoxine	
1921 J22	X	1148	1160	0.24411853	709	720	0.01542859	2076093	-0.52013177	1966769	-0.59106292	experimental	NINDS	1502111	Azactidine	
1921 J23	E	829	1360	0.02113614	664	1160	-0.03192259	90577	-2.47361497	91576	-2.36581927	empty				
1921 J24	P	178787	179840	124.414549	166799	167880	174.783392	2435189	-0.16682915	2356321	-0.22237559	empty				
1921 K01	N	516	520	-0.19765221	477	480	-0.22869307	2135578	-0.46160645	2537573	-0.05083158	empty				
1921 K02	E	155	160	-0.44999278	196	200	-0.52437492	90311	-2.47387668	90190	-2.36713104	empty				
1921 K03	X	596	600	-0.14173187	493	440	-0.27183526	2899855	0.29034028	2646809	0.05255367	experimental	NINDS	1500607	Vancomycin hydrochloride	
1921 K04	X	512	520	-0.20044823	473	480	-0.23290207	2388682	-0.21258584	2561990	-0.02772237	experimental	NINDS	1500822	Brucine	
1921 K05	X	594	600	-0.14312987	713	720	0.01963759	3462167	0.84358037	2626361	0.03320087	experimental	NINDS	1500609	Vidarabine	
1921 K06	X	393	400	-0.28362974	553	560	-0.14872218	2490349	-0.11255904	2394957	-0.18580897	experimental	NINDS	1500828	Canrenoic acid, potassium salt	
1921 K07	X	673	680	-0.08790853	471	480	-0.23500656	3138892	0.52552084	2966842	0.35544548	experimental	NINDS	1500613	Warfarin	
1921 K08	X	552	560	-0.17248806	995	1000	0.31637168	2729459	0.12269332	2573827	-0.01651937	experimental	NINDS	1500833	Canavanine	
1921 K09	X	634	640	-0.1151697	552	560	-0.14977443	3245279	0.63019148	2868612	0.26276067	experimental	NINDS	1500614	Xylometazoline hydrochloride	
1921 K10	X	472	480	-0.2284084	684	680	-0.02146111	2601043	-0.00365091	2726589	0.12615524	experimental	NINDS	1500836	Cephalosporin c sodium	
1921 K11	X	513	520	-0.19974923	474	480	-0.23184982	3103857	0.49105107	2688110	0.27439998	experimental	NINDS	1500615	Zomepirate sodium	
1921 K12	X	914	920	0.08055151	554	560	-0.14766993	2504638	-0.09850059	2569660	-0.02046318	experimental	NINDS	1500837	Chenodiol	
1921 K13	X	513	520	-0.19974923	554	560	-0.14766993	2744998	0.1379816							

1921 L07	X		674	680	-0.08720953	915	920	0.2321918	2681302	0.07531325	2493684	-0.09236985	experimental	NINDS	1501151	Ranitidine
1921 L08	X		433	440	-0.25566957	351	360	-0.36127639	2894432	0.28500477	3115154	0.49581378	experimental	NINDS	1502128	Cycloleucine
1921 L09	X		593	600	-0.14382888	515	520	-0.18870763	2523779	-0.07966839	2419766	-0.16232875	experimental	NINDS	1501152	Spiperone
1921 L10	X		915	920	0.08125052	514	520	-0.18975987	2973059	0.26236327	2876411	0.26580802	experimental	NINDS	1502155	N (g)-nitro-l-arginine
1921 L11	X		272	280	-0.36820927	274	280	-0.44229953	1048907	0.1035074594	10363071	0.47165855	experimental	NINDS	1501153	Sullectidil
1921 L12	X		593	600	-0.14382888	472	480	-0.23395431	3009048	0.39777165	2637384	0.04363348	experimental	NINDS	1502195	Piracetam
1921 L13	X		353	360	-0.31158992	633	640	-0.0645423	2517206	-0.08613535	2406665	-0.17472805	experimental	NINDS	1501154	Rindazole
1921 L14	X		513	520	-0.19974923	794	800	0.10486972	3122704	0.50959401	2778029	0.17674543	experimental	NINDS	1502196	Ethosuximide
1921 L15	X		592	600	-0.14452788	511	520	-0.19291662	2669206	0.0634124	2417159	-0.16479612	experimental	NINDS	1501155	Sulfamer
1921 L16	X		552	560	-0.17248806	394	400	-0.3160297	2846644	0.23798775	3000226	0.38685212	experimental	NINDS	1502197	Piperidolate hydrochloride
1921 L17	X		552	560	-0.17248806	633	640	-0.0645423	2394855	-0.20651243	2453385	-0.13051041	experimental	NINDS	1501156	Sulfamethoxypyridazine
1921 L18	X		672	680	-0.08860754	633	640	-0.0645423	2788121	0.18040892	2767526	0.16586934	experimental	NINDS	1502198	Amisindione
1921 L19	X		791	800	-0.00542602	630	640	-0.06769904	2488053	-0.11481802	2349897	-0.22845552	experimental	NINDS	1501161	Suprofen
1921 L20	X		871	880	0.05049433	1072	1080	0.39739482	2736743	0.12985981	2708625	0.111105876	experimental	NINDS	1502202	Cyclosporine
1921 L21	X		751	760	-0.03338619	671	680	-0.02455685	2781412	0.17380815	2674391	0.07865835	experimental	NINDS	1501170	Acetaminosalol
1921 L22	X		708	720	-0.06344338	709	720	0.01542859	2686005	0.07994038	2945568	0.33531093	experimental	NINDS	1502203	Troleanolysin
1921 L23	E		926	1480	0.08893956	729	1280	0.03647357	90504	-2.47368679	90937	-2.36642405	empty			
1921 L24	P	187167	188080	130.272205	185790	186960	194.724554	2196484	-0.40168307	2302809	-0.27302145	1987121	-0.57180099	empty		
1921 M01	N		836	840	0.02602917	557	560	-0.14451319	2123355	-0.47363226	1987121	-0.57180099	empty			
1921 M02	E		194	200	-0.42273161	195	200	-0.52542717	84407	-2.47968543	87786	-2.36940628	empty			
1921 M03	X		755	760	-0.03059018	916	920	0.23244005	2152837	-0.4446259	2020202	-0.54049183	experimental	NINDS	1500626	Dichlorophene
1921 M04	X		789	800	-0.00682403	508	520	-0.19607337	5151678	2.50583409	5186777	2.45647921	experimental	NINDS	1500665	Harmalol hydrochloride
1921 M05	X		630	640	-0.11796572	709	720	0.01542859	2725412	0.11871161	2975166	0.36332364	experimental	NINDS	1500629	Flopropione
1921 M06	X		1394	1400	0.41607359	1914	1920	1.28338811	2323236	-0.27697599	2405761	-0.17558364	experimental	NINDS	1500867	Harmine
1921 M07	X		470	480	-0.22980641	589	600	-0.11084123	2684748	0.07870366	2780562	0.17922794	experimental	NINDS	1500632	Hexestrol
1921 M08	X		654	660	-0.11519562	594	600	-0.10557999	2551680	-0.05221753	2605411	0.03330828	experimental	NINDS	1500635	Hormosin
1921 M09	X		272	280	-0.36820927	234	240	-0.48438947	122225	-1.4586107	1109809	-4.0212733	experimental	NINDS	1500633	Hecatinine
1921 M10	X		473	480	-0.2277094	475	480	-0.23079757	2530761	-0.07279904	2458719	-0.1254621	experimental	NINDS	1500872	Palmitine chloride
1921 M11	X		633	640	-0.11586871	513	520	-0.19081212	2533604	-0.0700019	2793196	0.19110008	experimental	NINDS	1500634	Ipromiazid sulfate
1921 M12	X		992	1000	0.13507385	1234	1240	0.56785909	2326531	-0.27373414	2419608	-0.16247829	experimental	NINDS	1500873	Piperine
1921 M13	X		791	800	-0.00542602	551	560	-0.15082668	2816643	0.20847076	2537817	-0.05006065	experimental	NINDS	1500636	Mecysteine hydrochloride
1921 M14	X		831	840	0.02253415	593	600	-0.10663224	8390912	5.69280877	8764854	5.84291191	experimental	NINDS	1500899	Esculetin
1921 M15	X		632	640	-0.11656771	594	600	-0.10557999	2332313	-0.26804543	2624831	0.03175282	experimental	NINDS	1500637	Merbromin
1921 M16	X		431	440	-0.16899333	469	480	-0.23711106	6486322	8.8198202	6749727	3.36718499	experimental	NINDS	1500638	Esculetin
1921 M17	X		471	480	-0.22910741	753	760	0.06172753	2550666	-0.05321517	2798737	-0.1963443	experimental	NINDS	1500639	Octopamine hydrochloride
1921 M18	X		913	920	0.07985251	752	760	0.06067528	2464530	-0.13796151	2156710	-0.11429529	experimental	NINDS	1500903	Etoposide
1921 M19	X		632	640	-0.11656771	1073	1080	0.39844707	2462051	-0.14040052	2365902	-0.21330776	experimental	NINDS	1500641	Pentamidine isethionate
1921 M20	X		672	680	-0.08860754	550	560	-0.15187893	2456919	-0.14544972	2407537	-0.17390276	experimental	NINDS	1500906	Lithocacin acid
1921 M21	X		751	760	-0.03338619	712	720	0.01858534	2604285	-0.00046122	2661690	0.06663763	experimental	NINDS	1500642	Phenacetic acid
1921 M22	X		790	800	-0.00612503	870	880	0.18484061	2501703	-0.10138824	2327006	-0.25012046	experimental	NINDS	1500909	Protoveratrine a
1921 M23	E		148285	149440	0.10393519	203115	204200	212.996585	2474161	-0.12844589	2578496	-0.01210044	empty			
1921 N01	N		515	520	-0.19835122	436	440	-0.27183526	2194017	-0.40411026	2229687	-0.34222699	empty			
1921 N02	E		195	200	-0.42203226	156	160	-0.56646486	85284	-2.47882258	82817	-2.37410914	empty			
1921 N03	X		713	720	-0.05994836	472	480	-0.23395431	2368868	-0.23208018	2280078	-0.29453497	experimental	NINDS	1501171	Saccharin
1921 N04	X		1232	1240	0.30283489	1433	1440	0.77725655	2522911	-0.08052239	2603619	0.01167695	experimental	NINDS	1502223	Resveratrol
1921 N05	X		552	560	-0.17248806	671	680	-0.02455685	2426194	-0.17567903	2241074	-0.33144988	experimental	NINDS	1501172	Acetobenzene
1921 N06	X		440	450	-0.25707588	469	480	-0.23711106	2727431	0.12069800	2603212	0.01195426	experimental	NINDS	1502230	Ascorbic acid
1921 N07	X		673	680	-0.08790853	433	440	-0.27499201	338081	-0.26237048	2737316	-0.17332119	experimental	NINDS	1501173	Acetaminosalol
1921 N08	X		872	880	0.05119333	834	840	0.14695966	3818480	1.19414489	4004925	1.33792803	experimental	NINDS	1502232	Campothecin
1921 N09	X		874	880	0.05259134	554	560	-0.14766993	2261265	-0.33794719	2461315	-0.12300515	experimental	NINDS	1501174	Todalazine hydrochloride
1921 N10	X		553	560	-0.17178905	354	360	-0.35811964	2888491	0.27915962	2756192	0.15607804	experimental	NINDS	1502234	Abiscic acid (cis,trans; +/-)
1921 N11	X		633	640	-0.11586871	515	520	-0.18870763	2361390	-0.23943753	2341271	-0.23661951	experimental	NINDS	1501175	Flurandrenolide
1921 N12	X		631	640	-0.11726671	432	440	-0.27604426	2742309	0.13533601	2549170	-0.03985572	experimental	NINDS	1502236	Abrine (I)
1921 N13	X		791	800	-0.00542602	754	760	0.06277978	2425803	-0.17606372	2533930	-0.05427946	experimental	NINDS	1501176	Hythromycin estolate
1921 N14	X		1112	1120	0.21895437	593	600	-0.10663224	2715869	0.10932257	2769017	0.16821612	experimental	NINDS	1502237	Harmol hydrochloride
1921 N15	X		511	520	-0.20114723	513	520	-0.19081212	2504309	-0.09882428	2449621	-0.13441353	experimental	NINDS	1501179	Estradiol propionate
1921 N16	X		591	600	-0.14522689	553	560	-0.14872218	16644799	13.8135339	17413759	14.0285755	experimental	NINDS	1502242	Scopoletin
1921 N17	X		913	920	0.07985251	553	560	-0.14872218	2481246	-0.1215152	3202613	-0.27320696	experimental	NINDS	1501180	Estradiol diacetate
1921 N18	X		630	640	-0.11796572	392	400	-0.3181342	2598524	-0.00612927	2868585	0.26245119	experimental	NINDS	1502244	Amygdalin
1921 N19	X		473	480	-0.2277094	552	560	-0.14977443	2362927	-0.23792533	2369136	-0.21024697	experimental	NINDS	1501181	Estrone acetate
1921 N20	X		432	440	-0.25636858	553	560	-0.14872218	2774732	0.16723592	2596669	0.00509992	experimental	NINDS	1502245	Ellagic acid
1921 N21	X		751	760	-0.00542602	712	720	0.01858534	2420467	-0.18131364	2091819	-0.47271068	experimental	NINDS	1501182	Estradiol acetate
1921 N22	X		989	1000	0.13297684	748	760	0.05646629	2678945	0.07299428	2366874	-0.21238782	experimental	NINDS	1501184	Thiathione
1921 N23	E		783	1400	-0.01101806	770	1320	0.07961576	85503	-2.47860711	85055	-2.371991	empty			
1921 N24	P	208595	209680	145.25047	184985	186320	193.919584	2212170	-0.38625013	2164352	-0.4040626	1775680	-0.77191706	empty		
1921 O01	N		596	600	-0.14173187	636	640	-0.06138555	2012878	-0.58232691	2369136	-0.21024697	experimental	NINDS	1500644	Phenylmercuric acetate
1921 O02	E		236	240	-0.39337342	236	240	-0.48228497	82081	-2.4819739	83124	-2.37381858	empty			
1921 O03	X		275	280	-0.36611226	195	200	-0.52542717	1138719	-1.44238289	1211596	-1.30578833	experimental	NINDS	1500938	Protoveratrine b
1921 O04	X		592	600	-0.14452788	832	840	-0.14485517	2287353	-0.31228008	2073776	-0.30049423	experimental	NINDS	1500645	Pregnenolone
1921 O05	X		553	560	-0.17178905	550	560	-0.15187893	2540782	-0.06293971	2737516	-0.13840234	experimental	NINDS	1500938	Ginkgolide a
1921 O06	X		553	560	-0.17178905	872	880	0.18694511	2236801	-0.362						

1921 P01	N		557	560	-0.16899303	717	720	0.02384658	1845835	-0.74667496	1832957	-0.71770785	empty			
1921 P02	E		277	280	-0.36471425	316	320	-0.39810509	75844	-2.48811028	79643	-2.37711313	empty			
1921 P03	X		316	320	-0.33745308	277	280	-0.43914278	974814	-1.60364358	997283	-1.50862257	experimental	NINDS	1501185	
1921 P04	X		594	680	-0.08651552	594	680	-0.10557999	270996	-0.32837319	2052052	-0.51042773	experimental	NINDS	1502252	
1921 P05	X		834	840	0.02463117	993	1000	0.04863719	2044633	-0.55108127	20921837	-0.47221338	experimental	NINDS	1501187	
1921 P06	X		834	840	0.02463117	1113	1120	0.44053701	2362896	-0.23795583	2390373	-0.19014744	experimental	NINDS	1502254	
1921 P07	X		595	600	-0.14243087	393	400	-0.31708195	2287969	-0.31167401	2193340	-0.37662722	experimental	NINDS	300340	
1921 P08	X		555	560	-0.17039104	676	680	-0.01929561	2362821	-0.23802962	2456224	-0.12782347	experimental	NINDS	1502255	
1921 P09	X		675	680	-0.08651052	595	600	-0.10452774	2159451	-0.43811886	2119033	-0.44695428	experimental	NINDS	1501194	
1921 P10	X		795	800	-0.00263	395	400	-0.31497745	2008527	-0.58660771	2130250	-0.43633807	experimental	NINDS	1502258	
1921 P11	X		634	640	-0.1151697	676	680	-0.01929561	2206147	-0.39217596	2133925	-0.43285991	experimental	NINDS	1501195	
1921 P12	X		594	600	-0.14312987	555	560	-0.14661768	2455601	-0.14575259	2455459	-0.12596372	experimental	NINDS	1502259	
1921 P13	X		635	640	-0.1144707	635	640	-0.0624378	2129599	-0.46748899	2079113	-0.48473614	experimental	NINDS	1501198	
1921 P14	X		435	440	-0.25427156	635	640	-0.0624378	2114722	-0.48212598	2204486	-0.36607821	experimental	NINDS	1502260	
1921 P15	X		594	600	-0.14312987	554	560	-0.14766993	2113989	-0.48284715	2059875	-0.50294374	experimental	NINDS	1501199	
1921 P16	X		754	760	-0.03128918	754	760	0.06277978	2347708	-0.25289888	2376824	-0.20297075	experimental	NINDS	1503002	
1921 P17	X		713	720	-0.05994836	752	760	0.06067528	2089490	-0.50695091	2242529	-0.33007282	experimental	NINDS	1501200	
1921 P18	X		1153	1160	0.24761355	1274	1280	0.60994903	1866147	-0.72669066	1936759	-0.61946556	experimental	NINDS	1503006	
1921 P19	X		633	640	-0.11586871	632	640	-0.06559454	2200138	-0.39808802	2231014	-0.34097106	experimental	NINDS	1501201	
1921 P20	X		633	640	-0.11586871	794	800	0.10486972	2392600	-0.20873105	2437482	-0.14556163	experimental	NINDS	1503007	
1921 P21	X		993	1000	0.1357285	714	720	0.02068984	2228281	-0.37039905	1971758	-0.58634113	experimental	NINDS	1501202	
1921 P22	X		950	960	0.10571567	669	680	-0.02666135	2266452	-0.33284388	2101818	-0.46324724	experimental	NINDS	1503009	
1921 P23	E		919	1800	0.08404653	855	1640	0.16905688	81351	-2.48269213	79734	-2.37702701	empty			
1921 P24	P	301467	281	210	0.1684	267975	268720	281	245692	1883794	-0.70932836	1889828	-0.6638829	empty		
1922 A01	N		557	560	-0.19847568	717	720	0.11312098	1385635	-2.41961886	1240735	-2.68703507	empty			
1922 A02	E		240	240	-0.69241628	717	720	0.11312098	787876	-5.6253794	229827	-5.77096495	empty			
1922 A03	X		635	640	-0.07845261	636	640	-0.04838743	1922300	-1.10407106	1564692	-0.82650549	experimental	NINDS	1503014	
1922 A04	X		714	720	0.04310921	514	520	-0.29163448	1534014	-2.05589165	1887070	-0.9683746	experimental	NINDS	1503029	
1922 A05	X		634	640	-0.07999137	835	840	0.34839755	1996423	-0.92237047	2036085	-0.57213088	experimental	NINDS	1503017	
1922 A06	X		555	560	-0.20155319	354	360	-0.61065356	1830037	-1.33023894	1633708	-1.642086	experimental	NINDS	1503298	
1922 A07	X		475	480	-0.32465377	475	480	-0.36939538	2142120	-0.56521774	1765755	-1.29096164	experimental	NINDS	1503036	
1922 A08	X		675	680	-0.01690232	835	840	0.34839755	1767760	-1.48290098	1731460	-1.38215501	experimental	NINDS	1503297	
1922 A09	X		555	560	-0.20155319	554	560	-0.21787971	1849816	-1.28175391	1925325	-0.86665126	experimental	NINDS	1503038	
1922 A10	X		635	640	-0.07845261	595	600	-0.07999137	803645	-0.39489386	1971816	-0.72468917	experimental	NINDS	1503041	
1922 A11	X		635	640	-0.07845261	595	600	-0.13013107	1891470	-1.17964584	1978186	-0.72608931	experimental	NINDS	1503041	
1922 A12	X		595	600	-0.1400029	635	640	-0.0503763	1808763	-1.38238873	1766448	-1.29390525	experimental	NINDS	1503322	
1922 A13	X		516	520	-0.26156472	514	520	-0.29163448	2065594	-0.7528089	1940055	-0.82748292	experimental	NINDS	1503043	
1922 A14	X		435	440	-0.38620406	515	520	-0.28964061	1721552	-1.59617245	1760012	-1.30623278	experimental	NINDS	1503324	
1922 A15	X		475	480	-0.32465377	635	640	-0.0503763	1847440	-1.28757829	1801674	-1.19544993	experimental	NINDS	1503044	
1922 A16	X		475	480	-0.32465377	595	600	-0.13013107	2049301	-0.79274857	2197763	-0.14221514	experimental	NINDS	1503330	
1922 A17	X		554	560	-0.20303074	554	560	-0.20303074	2118737	-0.637896	1872987	-1.70026592	experimental	NINDS	1503345	
1922 A18	X		1033	1040	0.53397276	994	1000	0.66542276	1740432	-1.54989117	1608195	-1.70992726	experimental	NINDS	1503341	
1922 A19	X		751	760	0.10004322	632	640	-0.05635791	2188373	-0.45183596	2302687	0.13678682	experimental	NINDS	1503051	
1922 A20	X		995	1000	0.47549998	874	880	0.42615845	1863308	-1.24868045	1961606	-0.77017696	experimental	NINDS	1503339	
1922 A21	X		632	640	-0.08306889	712	720	0.10315163	2165493	-0.50792259	1847052	-1.07478592	experimental	NINDS	1503053	
1922 A22	P	1071	1080	0.59244553	1232	1240	1.13996364	1991141	-0.93531844	2057479	-0.51524239	1908758	empty			
1922 A23	E		766	1480	0.12312458	502	1160	0.31556091	80399	-5.61919467	81027	-5.77079858	empty			
1922 A24	P	243911	245200	374	264248	224212	224760	445	732929	1980162	0.96223169	1818445	-1.15085439	empty		
1922 B0	N		676	680	-0.01536587	756	760	0.19088188	2011906	-0.88441639	2190015	-0.7015733	empty			
1922 B02	E		194	200	-0.75704455	115	120	-1.08718831	89112	-5.59783616	86502	-5.75624009	empty			
1922 B03	X		794	800	0.16620978	554	560	-0.21187971	2233132	-0.34211648	2299119	0.1272992	experimental	NINDS	1504027	
1922 B04	X		632	640	-0.08306889	713	720	-0.37338312	2677947	0.74827584	2405249	0.40950801	experimental	NINDS	1505281	
1922 B05	X		633	640	-0.08153013	473	480	-0.1051455	2175505	-0.48337979	2166209	-0.22659858	experimental	NINDS	1504030	
1922 B06	X		674	680	-0.01844108	593	600	-0.13411881	2695136	0.79041191	2514697	0.70053968	experimental	NINDS	1505294	
1922 B07	X		473	480	-0.32773128	674	680	0.0273846	2382941	0.02511615	2339763	0.23537509	experimental	NINDS	1504074	
1922 B08	X		713	720	0.04157045	592	600	-0.13611268	2397897	0.06177838	2797292	1.45198413	experimental	NINDS	1505296	
1922 B09	X		553	560	-0.20463071	474	480	-0.37138925	2029632	-0.84096395	2529806	0.74071581	experimental	NINDS	1504078	
1922 B10	X		834	840	0.22776007	634	640	-0.05237017	2790573	1.02436034	2698187	1.1884554	experimental	NINDS	1505299	
1922 B11	X		432	440	-0.39082033	513	520	-0.29362835	2307752	-0.15919757	2047187	-0.5426097	experimental	NINDS	1504085	
1922 B12	X		635	640	-0.07845261	593	600	-0.13411881	2521116	0.36382991	2221596	-0.07884114	experimental	NINDS	1505304	
1922 B13	X		274	280	-0.63394397	794	800	0.26664891	2227271	-0.35648378	2220629	-0.08236975	experimental	NINDS	1504088	
1922 B14	X		834	840	0.22776007	512	520	-0.29562222	2513599	0.34540319	1984336	-0.70973593	experimental	NINDS	1505305	
1922 B15	X		633	640	-0.08153013	594	600	-0.13212494	2126454	-0.60362041	1822769	-1.13056551	experimental	NINDS	1504094	
1922 B16	X		512	520	-0.26771975	590	600	-0.14010042	2339858	-0.08049488	2234953	-0.04332373	experimental	NINDS	1505306	
1922 B17	X		592	600	-0.14461917	552	560	-0.21586745	2404388	0.07769002	2180357	-0.1884992	experimental	NINDS	1504098	
1922 B18	X		1030	1040	0.52935649	911	920	0.49993161	2034448	-0.8291583	1801703	-1.19537281	experimental	NINDS	1505309	
1922 B19	X		912	920	0.34778314	992	1000	0.66143502	2169455	-0.49821039	2050280	-0.53438515	experimental	NINDS	1504099	
1922 B20	X		471	480	-0.3308088	590	600	-0.14010042	2376044	0.00820927	2261255	0.02661556	experimental	NINDS	1505310	
1922 B21	X		552	560	-0.20616946	512	520	-0.29562222	1389376	-2.41044841	1316319	-2.4860507	experimental	NINDS	1503223	
1922 B22	X		870	880	0.28315533	674	680	0.25867343	2277155	-0.23420119	2187257	-0.17015115	experimental	NINDS	1505312	
1922 B23	X		546	1160	-0.15402021	686	1240	0.05131103	85050	-5.6042268	2017775	-5.73690055	empty			
1922 B24	P	207734	208920	218	596628	187018	188080	371	572956	1992924	-0.9309477	1633546	-1.64251677	empty		
1922 C01	N		556	560	-0.20001443	556	560	-0.20789197	1923070	-1.10218353	1789400	-1.22808755	empty			
1922 C02	E		275	280	-0.63240521	155	160	-1.00743354	88622	-5.59903731	86616	-5.75593695	empty			
1922 C03	X		674	680	-0.01844108	755	760	0.18888801	2288561	-0.20624122	2108523	-0.379511				

1922 C19	X	471	480	-0.3308088	631	640	-0.05835178	2133071	-0.58739991	2435449	0.48981241	experimental	NINDS	1503080	Ambroxol hydrochloride
1922 C20	X	671	680	-0.02305735	953	960	0.58367412	2240420	-0.32425112	2208632	-0.11331354	experimental	NINDS	1503432	Mepartricin
1922 C21	X	792	800	0.16313227	592	600	-0.13611268	2441671	0.16908329	2230540	-0.05505828	experimental	NINDS	1503083	Amprilose
1922 C22	X	510	520	-0.27079727	550	560	-0.21985519	1212856	-0.59844319	1973587	-0.73831845	experimental	NINDS	1503500	Resorcinol monoacetate
1922 C23	E	478	480	-0.20037275	744	1160	0.16699545	87888	-5.00836676	878802	-5.74486602	empty			
1922 C24	P	163193	164120	250.058843	139826	140800	277.478279	2305557	-0.16457826	1966016	-0.75845039	empty			
1922 D01	N	396	400	-0.44621559	556	560	-0.20789197	2189437	-0.44922774	2145876	-0.28018715	empty			
1922 D02	E	236	240	-0.69241674	156	160	-1.00543967	92312	-5.58999187	90131	-5.74659026	empty			
1922 D03	X	554	560	-0.44915015	435	440	-0.44915015	2374180	0.00363997	2263765	0.03328986	experimental	NINDS	1504105	Tannic acid
1922 D04	X	394	400	-0.4492931	394	400	-0.53089879	2616217	0.59695469	2491752	0.63952694	experimental	NINDS	1505314	Saralfoxacin hydrochloride
1922 D05	X	354	360	-0.51084339	675	680	0.02937847	2275448	-0.23838562	2312247	0.16220768	experimental	NINDS	1504116	Formestane
1922 D06	X	519	520	-0.26156472	513	520	-0.29362835	2534378	0.39633956	2599805	0.92700873	experimental	NINDS	1505316	Protibionamide
1922 D07	X	314	320	-0.57239368	594	600	-0.13212494	2348392	-0.05957516	2562404	0.8273967	experimental	NINDS	1504136	Alaproclate
1922 D08	X	673	680	-0.01997984	833	840	0.34440981	2210752	-0.39697745	2502576	0.66830889	experimental	NINDS	1505317	Carmofur
1922 D09	X	874	880	0.28931036	554	560	-0.21187971	2671010	0.7312709	2263836	0.03347866	experimental	NINDS	1504137	Ancitabine hydrochloride
1922 D10	X	673	680	-0.01997984	474	480	-0.37138925	2769904	0.97369361	2621031	0.98329095	experimental	NINDS	1505319	Clopidol
1922 D11	X	514	520	-0.26464224	554	560	-0.21187971	2617878	0.60102636	2837533	1.55898842	experimental	NINDS	1504142	Acetriazoic acid
1922 D12	X	554	560	-0.20309195	394	400	-0.53089879	2532130	0.39082895	2684015	1.15077083	experimental	NINDS	1505323	Carbimazole
1922 D13	X	634	640	-0.07999137	594	600	-0.13212494	2388392	0.0384784	2383490	0.35164896	experimental	NINDS	1504144	Dithromycin
1922 D14	X	592	600	-0.14461917	913	920	0.50391935	2011834	-0.88459288	1711301	-1.43575952	experimental	NINDS	1505327	Chlormadinone acetate
1922 D15	X	874	880	0.28931036	633	640	-0.05436404	2551101	0.4373333	2675490	1.12810212	experimental	NINDS	1504145	Gliclazide
1922 D16	X	631	640	-0.08460764	470	480	-0.37936473	2740315	0.90116095	2587476	0.89406531	experimental	NINDS	1505329	Miltefosine
1922 D17	X	713	720	0.04157045	633	640	-0.05436404	2057446	-0.77278241	2419398	0.44713142	experimental	NINDS	1504148	Mepivacaine hydrochloride
1922 D18	X	552	560	-0.20616946	632	640	-0.05635791	2471441	0.24205965	2090341	-0.42789565	experimental	NINDS	1505330	Oxiconazole nitrate
1922 D19	X	832	840	0.22468256	633	640	-0.05436404	2113880	-0.63444355	2328225	0.20469456	experimental	NINDS	1504150	Meloxicam
1922 D20	X	1200	1200	0.77779864	432	440	-0.51512176	2801975	1.05231051	2583201	0.28440383	experimental	NINDS	1505332	Azaperone
1922 D21	X	890	840	0.22160504	593	600	-0.1341186	2248413	-0.30465757	2350003	0.84953613	experimental	NINDS	1505334	Nimustine
1922 D22	X	792	800	0.16313227	751	760	0.18091253	2453178	0.19729084	2054852	-0.52222781	experimental	NINDS	1505334	Securinine
1922 D23	E	232	560	-0.69857177	566	1000	-0.18795328	90165	-5.5925249	91710	-5.74239157	empty			
1922 D24	P	109472	110400	167.395267	146265	147120	290.316803	2071101	-0.73930938	2204076	-0.12542833	empty			
1922 E01	N	477	480	-0.32157625	636	640	-0.04838243	1967747	-0.99266506	1825220	-1.13283909	empty			
1922 E02	E	196	200	-0.75396703	196	200	-0.9256849	91697	-5.59149945	89991	-5.74696254	empty			
1922 E03	X	635	640	-0.07845261	514	520	-0.29163448	2481198	0.26597736	2301195	0.13281946	experimental	NINDS	1503085	Pyrrithylidone
1922 E04	X	473	480	-0.26464224	832	840	0.34440981	2209858	-0.70464224	2502576	0.66830889	experimental	NINDS	1503600	Triflurometholone
1922 E05	X	555	560	-0.20155319	354	360	-0.10653556	3040044	1.63589831	2129571	-0.32354355	experimental	NINDS	1503086	Tigrid hydrochloride
1922 E06	X	354	360	-0.51084339	475	480	-0.36939538	2433412	0.14883768	1979426	-0.72279204	experimental	NINDS	1503602	Salinomycin, sodium
1922 E07	X	395	400	-0.44775435	435	440	-0.44915015	2643750	0.6644474	2245546	-0.01515603	experimental	NINDS	1503092	Gluconalactone
1922 E08	X	594	600	-0.14154166	434	440	-0.45114402	2422096	0.12109833	2069600	-0.48444751	experimental	NINDS	1503603	Acyclovir
1922 E09	X	473	480	-0.32773128	354	360	-0.10653556	2205359	-0.41019752	2300296	0.13042894	experimental	NINDS	1503094	Toloxone
1922 E10	X	474	480	-0.32619253	595	600	-0.13013107	2209017	-0.40123052	2138607	-0.29951604	experimental	NINDS	1503604	Retinyl palmitate
1922 E11	X	474	480	-0.32619253	595	600	-0.13013107	2209017	-0.40123052	2138607	-0.29951604	experimental	NINDS	1503604	Retinyl palmitate
1922 E12	X	552	560	-0.20616946	613	520	-0.28964061	2063080	-0.75897157	1910113	-0.90710128	experimental	NINDS	1503607	Thalidomide
1922 E13	X	752	760	0.10158198	513	520	-0.29362835	2170945	-0.49455789	2414667	0.43455129	experimental	NINDS	1503101	Azlocillin sodium
1922 E14	X	593	600	-0.14308042	553	560	-0.21387358	1634989	-1.8083677	1522393	-1.93808218	experimental	NINDS	1503610	Benzalkonium chloride
1922 E15	X	472	480	-0.32927004	434	440	-0.45114402	2142463	-0.56437693	2343165	0.24442131	experimental	NINDS	1503104	Bendroflumethiazide
1922 E16	X	513	520	-0.26618099	433	440	-0.45313789	2079119	-0.71965454	2527110	0.73354691	experimental	NINDS	1503611	Pentoxifylline
1922 E17	X	633	640	-0.08153013	753	760	0.18490027	2225528	-0.36132027	2500292	0.66223554	experimental	NINDS	1503106	Bepiridil hydrochloride
1922 E18	X	473	480	-0.32773128	832	840	0.34440981	2158770	-0.52195161	2304236	0.14090574	experimental	NINDS	1503616	Fluoroxacin
1922 E19	X	632	640	-0.08306889	551	560	-0.21786132	2798694	0.04426767	2749317	0.2244065	experimental	NINDS	1503107	Bromhexine hydrochloride
1922 E20	X	751	760	0.10004322	673	680	0.02539073	2549729	0.43397007	2433675	0.48509552	experimental	NINDS	1503428	Choline chloride
1922 E21	X	591	600	-0.14615793	711	720	0.10115776	2664150	0.71445472	2463133	0.56342656	experimental	NINDS	1503108	Bromopride
1922 E22	X	991	1000	0.46934496	951	960	0.57968638	2192545	-0.44160897	2147167	-0.27675427	experimental	NINDS	1503620	Safrole
1922 E23	E	502	960	-0.28310732	547	1000	-0.2258368	91002	-5.59320313	90342	-5.7460292	empty			
1922 E24	P	154984	155800	237.427185	152790	153600	303.3268	2589809	0.53221973	2196985	-0.14428391	empty			
1922 F01	N	516	520	-0.26156472	556	560	-0.20789197	2455457	0.20287744	2296225	0.11963038	empty			
1922 F02	E	155	160	-0.81705608	195	200	-0.92767877	88330	-5.59975311	90254	-5.7462632	empty			
1922 F03	X	473	480	-0.32773128	715	720	0.10913324	2270382	-0.25080411	2190207	-0.1623072	experimental	NINDS	1504152	Nilutamide
1922 F04	X	634	640	-0.07999137	474	480	-0.37138925	1847579	-1.28723756	1668391	-1.54986091	experimental	NINDS	1505340	Azelastine hydrochloride
1922 F05	X	513	520	-0.26618099	434	440	-0.45114402	2353761	-0.04641392	2432959	0.48319129	experimental	NINDS	1504171	Venlafaxine
1922 F06	X	514	520	-0.26464224	555	560	-0.20988584	3181663	1.98305448	2772647	1.38645096	experimental	NINDS	1505347	Riboflavin
1922 F07	X	594	600	-0.14154166	355	360	-0.60865969	2416430	0.10720904	2130616	-0.3207648	experimental	NINDS	1504173	Fluoxetine
1922 F08	X	514	520	-0.26464224	475	480	-0.36939538	2692278	0.78340598	2589560	0.89960684	experimental	NINDS	1505354	Fipronil
1922 F09	X	474	480	-0.32619253	554	560	-0.21187971	2607033	0.57444159	2304236	0.14090574	experimental	NINDS	1504174	Bupropion
1922 F10	X	512	520	-0.26771925	510	520	-0.29960996	2868658	1.26038751	2722103	1.2520501	experimental	NINDS	1505360	Cefditoren pivoxil
1922 F11	X	673	680	-0.01997984	754	760	0.18689414	2661986	0.70915002	2185927	-0.17368809	experimental	NINDS	1504183	Trifluridine
1922 F12	X	872	880	0.28623285	733	440	-0.45313789	2818976	1.09398572	2719155	1.24421112	experimental	NINDS	1505361	Mofetilol
1922 F13	X	792	800	0.16313227	414	720	0.10713937	2526704	0.37752799	2526945	0.73310816	experimental	NINDS	1504184	Aminolevulinic acid hydrochloride
1922 F14	X	433	440	-0.38928157	514	520	-0.29163448	2999808	1.53726624	2653541	1.02134247	experimental	NINDS	1505365	Ceftriaxone sodium trihydrate
1922 F15	X	594	600	-0.14154166	434	440	-0.45114402	2287023	-0.21001138	2519563	0.71347879	experimental	NINDS	1504188	Prenperone
1922 F16	X	632	640	-0.08306889	674	680	0.02723846	2721717	0.85557085	2522373	0.72095082	experimental	NINDS	1505366	Ranitidine
1922 F17	X	632	640	-0.08153013	512	520	-0.29222232	2647708	0.67414985	2431748	0.47997114	experimental	NINDS	1504190	Axobenzon
1922 F18	X	593	600	-0.14308042	711	720	0.10115776	2812342	1.0772354	2614361	0.96555484	experimental	NINDS	270029	Prasterone acetate
1922 F19	X	553	560	-0.20463071	1072	1080	0.82094456	1993199	-0.93027358	1896896					

1922 G13	X	593	600	-0.14308042	593	600	-0.13411881	2575392	0.49687878	2367238	0.30843349	experimental	NINDS	1503134	Menthyl(-)
1922 G14	X	434	440	-0.38774281	354	360	-0.61065356	2211722	-0.39459965	2251661	0.00110428	experimental	NINDS	1503678	Celecoxib
1922 G15	X	553	560	-0.20463071	353	360	-0.61264743	2205949	-0.40875123	2205946	-0.12045584	experimental	NINDS	1503118	Trifluopromazine hydrochloride
1922 G16	X	513	520	-0.26618099	634	640	-0.05237017	2549922	0.43444318	2489765	0.63866631	experimental	NINDS	1503710	Clotapdogrel sulfate
1922 G17	X	553	560	-0.20463071	633	640	-0.05436404	2230700	-0.34807814	2460598	0.5566644	experimental	NINDS	1503135	Thonzylamine hydrochloride
1922 G18	X	673	680	-0.01997984	673	680	0.02539073	2536257	0.40094563	2367656	0.30954499	experimental	NINDS	1503720	Selametinol
1922 G19	X	512	520	-0.26771975	791	800	0.2606673	2987023	1.50592587	2650847	1.06257426	experimental	NINDS	1503136	Thiamphenicol
1922 G20	X	872	880	0.28623285	832	840	0.34241594	2418469	0.11220732	2470293	0.58246561	experimental	NINDS	1503722	Atorvastatin calcium
1922 G21	X	551	560	-0.20770822	750	760	0.17891866	1265148	-2.71497334	1406199	-2.24705203	experimental	NINDS	1503200	Cetrimonium bromide
1922 G22	X	1070	1080	0.59090678	830	840	0.3384282	2227474	-0.35598616	2336639	0.22706811	experimental	NINDS	1503801	Naproxol
1922 G23	E	542	1240	-0.22155703	638	1120	-0.0443947	89396	-5.59713998	91390	-5.74324427	empty			
1922 G24	P	237156	238000	363.869944	16305	163960	324.092948	2669811	0.72833175	236125	0.29430576	empty			
1922 H01	N	397	400	-0.44467683	396	400	-0.52691105	2253494	-0.29220232	2198357	-0.14063365	empty			
1922 H02	E	165	200	-0.80166851	373	400	-0.57277005	89239	-5.59752484	90671	-5.74515436	empty			
1922 H03	X	11154	11160	-16.1077345	8394	8400	15.4200552	2318864	-0.13195829	2310449	0.15742664	experimental	NINDS	1504218	Acrisorcin
1922 H04	X	482	520	-0.31388247	651	680	-0.01847439	2707166	0.81990151	2473704	0.59153576	experimental	NINDS	1505371	Cetirizine hydrochloride
1922 H05	X	793	800	0.16467103	594	600	-0.13212494	2141166	-0.56755632	2126597	-0.33145167	experimental	NINDS	1504226	Mercaptamine hydrochloride
1922 H06	X	673	680	-0.01997984	434	440	-0.45114402	2682042	0.75831407	2584481	0.88610135	experimental	NINDS	1505801	Topiramate
1922 H07	X	473	480	-0.32773128	475	480	-0.36939538	2815095	1.08447207	2767941	1.3739373	experimental	NINDS	1504229	Metaxalone
1922 H08	X	627	640	-0.09076267	473	480	-0.37338312	2636894	0.64746102	2555957	0.81025357	experimental	NINDS	1505802	Gemifloxacin mesylate
1922 H09	X	433	440	-0.38928157	471	480	-0.37737086	2615335	0.59479261	2615762	0.96928022	experimental	NINDS	1504231	Clarithromycin
1922 H10	X	592	600	-0.14461917	1070	1080	0.81695682	2862480	1.20062877	2549814	0.79391881	experimental	NINDS	1505803	Pravastatin sodium
1922 H11	X	554	560	-0.20309195	673	680	0.02539073	2749512	0.92370591	2619132	0.97824134	experimental	NINDS	1504235	Rofecoxib
1922 H12	X	633	640	-0.08153013	473	480	-0.37338312	2699225	0.80215137	2419253	0.44674585	experimental	NINDS	1505805	Gabapentin
1922 H13	X	553	560	-0.20463071	674	680	0.0273846	2568254	0.47938112	2597086	0.91961913	experimental	NINDS	1504236	Simvastatin
1922 H14	X	553	560	-0.20463071	594	600	-0.05237017	2797842	1.04217912	2259920	1.50417245	experimental	NINDS	1505811	Levodopa hydrochloride
1922 H15	X	873	880	-0.32777716	1074	1080	0.8249323	2208669	-0.39828573	2053723	-0.52669241	experimental	NINDS	1505812	Hydroquinone
1922 H16	X	673	680	-0.01997984	552	560	-0.21586745	2605163	0.56985759	2626785	0.99859133	experimental	NINDS	1505816	Pregabalin
1922 H17	X	472	480	-0.32927004	513	520	-0.29362835	2377468	0.01169997	2296538	0.12043609	experimental	NINDS	1504243	Oxcarbazepine
1922 H18	X	633	640	-0.08153013	393	400	-0.53289266	2582843	0.5151437	2721627	1.25078438	experimental	NINDS	1505817	Ramelteon
1922 H19	X	712	720	0.04003169	673	680	0.02539073	2417462	0.10973882	2542345	0.77405809	experimental	NINDS	1504244	Betamipron
1922 H20	X	911	920	0.34624438	511	520	-0.29761609	2449289	0.18775759	2533149	0.74960513	experimental	NINDS	1505818	Pantoprazole
1922 H21	X	591	600	-0.14615793	952	960	0.58168025	2191734	-0.44359701	2099339	-0.40393304	experimental	NINDS	1504257	Carvedilol tartrate
1922 H22	E	840	840	0.22160504	791	800	0.22160504	2873608	0.44359701	2323252	1.44359701	experimental	NINDS	1504250	Topotecan hydrochloride
1922 H23	E	684	1040	-0.00305351	580	760	-0.55881296	91143	-5.59285749	91312	-5.74344988	empty			
1922 H24	P	118669	119800	181.547217	127266	128160	252.435281	2263850	-0.26681625	2057405	-0.51543916	empty			
1922 I01	N	316	320	-0.56931617	556	560	-0.20789197	2042350	-0.80978782	1918420	-0.88501225	empty			
1922 I02	E	236	240	-0.69241674	195	200	-0.92767877	90294	-5.59493868	88281	-5.75150957	empty			
1922 I03	X	484	520	-0.31080495	572	600	-0.17599007	2366372	-0.01550008	1977494	-0.72792924	experimental	NINDS	1503203	Chlorprothixene hydrochloride
1922 I04	X	514	520	-0.26464224	553	560	-0.21387358	2542015	0.41506044	2192914	-0.15510905	experimental	NINDS	1503802	Azadirachtin
1922 I05	X	514	520	-0.14308042	594	600	-0.13212494	2187971	0.8067103	2734420	0.02803287	experimental	NINDS	1503204	Cinacalcin
1922 I06	X	473	480	-0.32773128	634	640	-0.05237017	2792389	1.02881197	2356856	0.28082685	experimental	NINDS	1503804	Cetuximab
1922 I07	X	547	560	-0.21386325	473	480	-0.37338312	2670524	0.73007955	2461275	0.55848597	experimental	NINDS	1503205	Citilone
1922 I08	X	2913	2920	3.42683633	874	880	0.42615845	2246855	-0.30847676	2167694	-0.22217121	experimental	NINDS	1503806	Homidium bromide
1922 I09	X	507	520	-0.27541354	673	680	0.02539073	2517503	0.35497322	2281912	0.08154443	experimental	NINDS	1503206	Clofocet
1922 I10	X	634	640	-0.07999137	712	720	0.10315163	2512383	0.34242236	2477896	0.60268265	experimental	NINDS	1503816	Amcinonide
1922 I11	X	433	440	-0.38928157	513	520	-0.29362835	2669485	0.72753261	2239257	-0.03187902	experimental	NINDS	1503207	Cyclobenzaprine hydrochloride
1922 I12	X	514	520	-0.26464224	594	600	-0.13212494	2378878	0.01515636	2237951	0.32948266	experimental	NINDS	1503818	Bupivacaine hydrochloride
1922 I13	X	473	480	-0.32773128	393	400	-0.53289266	2465879	0.2284253	223857	-0.03370315	experimental	NINDS	1504212	Butobutamine hydrochloride
1922 I14	X	674	680	-0.01844108	513	520	-0.29362835	2552876	0.44168443	2511487	0.69200401	experimental	NINDS	1503821	Cystamine dinitrochloride
1922 I15	X	513	520	-0.26618099	632	640	-0.05635791	2542474	0.41618556	2312702	0.16341756	experimental	NINDS	1503214	Exudine
1922 I16	X	392	400	-0.45237062	593	600	-0.13411881	2706335	0.81786445	2208572	-0.11347308	experimental	NINDS	1503822	Ramifenazone
1922 I17	X	714	720	0.04310921	714	720	0.10713937	2483186	0.27085062	2474965	0.59488886	experimental	NINDS	1503215	Enoxacin
1922 I18	X	673	680	-0.01997984	594	600	-0.13212494	2304875	-0.16625007	2211193	-0.10650362	experimental	NINDS	1503325	Thiodiglycin
1922 I19	X	631	640	-0.08460764	592	600	-0.13611268	2688607	0.77440711	2545839	0.78334894	experimental	NINDS	1503228	Paromomycin sulfate
1922 I20	X	911	920	0.34624438	672	680	0.02339686	2727898	0.87072267	2374971	0.3289962	experimental	NINDS	1503705	Anethole
1922 I21	X	791	800	0.16159351	791	800	0.2606673	2512810	0.34346909	2581248	0.87750452	experimental	NINDS	1503218	Heptaminol hydrochloride
1922 I22	X	829	840	0.22006629	710	720	0.09916389	2401965	0.07175042	2232343	-0.04787077	experimental	NINDS	1503902	Sodium beta-nicotinamide adenine dinucleotide phosphat
1922 I23	E	593	1040	-0.14308042	616	1040	-0.08825982	87348	-5.60216032	86146	-5.75718675	empty			
1922 I24	P	150685	151480	230.812068	143207	144000	284.219551	2430011	0.14050067	2347759	0.25663712	empty			
1922 J01	N	837	840	0.23237634	637	640	-0.04638856	2281203	-0.22427817	2142780	-0.28841968	empty			
1922 J02	E	275	280	-0.62420521	195	200	-0.92767877	88899	-5.59835829	89036	-5.74950196	empty			
1922 J03	X	554	560	-0.20309195	434	440	-0.28964061	2349243	-0.05748907	2251318	0.00019222	experimental	NINDS	1504258	Nateglinide
1922 J04	X	554	560	-0.20309195	434	440	-0.45114402	6274771	9.56531051	5757211	9.32267979	experimental	NINDS	1505821	Irinotecan hydrochloride
1922 J05	X	473	480	-0.32773128	434	440	-0.45114402	2307049	-0.16092086	2193482	-0.15359869	experimental	NINDS	1504259	Irbesartan
1922 J06	X	634	640	-0.07999137	514	520	-0.29163448	2898537	1.28901669	2722791	1.25387956	experimental	NINDS	1505822	Osetamivir tartrate
1922 J07	X	553	560	-0.20463071	394	400	-0.53089879	2517235	0.35431626	2531984	0.7465073	experimental	NINDS	1504260	Levofloxacin
1922 J08	X	586	600	-0.15385172	474	480	-0.37138925	2849476	1.16875156	2740331	1.30051993	experimental	NINDS	1505823	Tegaserod
1922 J09	X	633	640	-0.08153013	352	360	-0.6146413	2645773	0.66940646	2444494	0.51386385	experimental	NINDS	1504261	Candesartan cilexetil
1922 J10	X	632	640	-0.08306889	594	600	-0.13212494	2312468	-0.14763706	237951	0.04415489	experimental	NINDS	1505308	Chlorophyllide cu complex na salt
1922 J11	X	795	800	0.16774854	434	440	-0.45114402	2649142	0.67765053	2618059	0.97538814	experimental	NINDS	1504262	Rosiglitazone
1922 J12	X	472	480	-0.32927004	634	640	-0.05237017	1610840	-1.86756508	1650235	-1.59813928	experimental	NINDS	1505322	Cepharanthine
1922 J13	X	555	560	-0.20155319	634	640	-0.05237017								

1922 K07	X	634	640	-0.07999137	554	560	-0.21187971	2767680	0.96824184	2396210	0.38547253	experimental	NINDS	1503222	Fipexide hydrochloride
1922 K08	X	593	600	-0.14308042	553	560	-0.21387358	2307881	-0.15888135	2147103	-0.27692445	experimental	NINDS	1503908	Paclitaxel
1922 K09	X	513	520	-0.26618099	834	840	0.34640368	2872213	1.22448765	2485727	0.62350595	experimental	NINDS	1503226	Meclofenoxate hydrochloride
1922 K10	X	634	640	-0.07999137	553	560	-0.21387358	2301852	-0.17266507	2433786	0.48273127	experimental	NINDS	1503914	Subcitaine
1922 K11	X	313	320	-0.57393244	353	360	-0.61264743	2151573	-0.54204523	2440919	-0.84355521	experimental	NINDS	1503227	Perhexiline maleate
1922 K12	X	716	720	0.04618672	555	560	-0.20988584	2453151	0.19722466	2374677	0.32845375	experimental	NINDS	1503918	Clobetasol propionate
1922 K13	X	353	360	-0.51238215	314	320	-0.69040833	2712798	0.83370745	2094772	-0.41607709	experimental	NINDS	1503229	Methapyriene hydrochloride
1922 K14	X	514	520	-0.26464224	354	360	-0.61065356	2409973	0.09138075	2161955	-0.2374317	experimental	NINDS	1503920	Cloperastine hydrochloride
1922 K15	X	553	560	-0.20463071	554	560	-0.21187971	2629268	0.62894711	2135274	-0.30837878	experimental	NINDS	1503230	Nifedipine
1922 K16	X	592	600	-0.14461917	713	720	0.10514555	2699152	0.80025648	2430985	0.47794225	experimental	NINDS	1503921	Cyproterone
1922 K17	X	952	960	0.40933342	753	760	0.18490027	2748233	0.92057065	2456827	0.54665836	experimental	NINDS	1503231	Nimesulide
1922 K18	X	752	760	0.10158198	674	680	0.0273846	2843742	1.15469538	2452253	0.48131398	experimental	NINDS	1503922	Tryptamine
1922 K19	X	592	600	-0.14461917	672	680	0.02339686	3145189	1.89364434	2853754	1.60212146	experimental	NINDS	1503234	Beta-propiolactone
1922 K20	X	512	520	-0.26771975	712	720	0.10315163	2621523	0.60996149	2528215	0.7364852	experimental	NINDS	1503923	Iopanic acid
1922 K21	X	872	880	0.28623285	711	720	0.10115776	3015458	1.57562969	2661450	1.09076855	experimental	NINDS	1503237	Halcinonide
1922 K22	X	870	880	0.28315533	990	1000	0.65744728	2375093	0.00587804	2633708	1.01700018	experimental	NINDS	1503925	Ketorolac tromethamine
1922 K23	E	463	880	-0.34311885	572	1040	-0.17599007	89782	-5.59619376	87383	-5.75389473	empty			
1922 K24	P	140167	141080	214.627419	157974	158760	313.663018	2316507	-0.1377361	2739890	1.29934727	empty			
1922 L01	N	557	560	-0.19847568	596	600	-0.1281372	2380631	0.01945356	2271471	0.05378078	empty			
1922 L02	E	315	320	-0.57085492	235	240	-0.847924	85934	-5.60562651	84591	-5.7613216	empty			
1922 L03	X	713	720	0.04157045	595	600	-0.13013107	2968767	1.46117423	2688987	1.16399181	experimental	NINDS	1504303	Moxifloxacin hydrochloride
1922 L04	X	591	600	-0.14615793	469	480	-0.3813586	2790784	1.02487757	2680844	1.14233887	experimental	NINDS	2300259	Nicotine ditartrate
1922 L05	X	633	640	-0.08153013	715	720	0.10913324	2459158	0.21194985	2486591	0.6258034	experimental	NINDS	1504401	Pliglitazone hydrochloride
1922 L06	X	631	640	-0.08460764	639	280	-0.78013245	2700632	0.80388447	2385706	0.35754149	experimental	NINDS	2300228	Kaonic acid
1922 L07	X	593	600	-0.14308042	424	440	-0.45114402	2488247	0.28325865	2245684	-0.01478907	experimental	NINDS	1503200	Benazepril hydrochloride
1922 L08	X	553	560	-0.20463071	634	640	-0.05237017	2783963	1.00815699	2402969	0.33412666	experimental	NINDS	1503229	Hydruroid
1922 L09	X	553	560	-0.20463071	512	520	-0.29562222	2650289	-0.62467671	2368449	0.30233886	experimental	NINDS	1505229	Famciclovir
1922 L10	X	593	600	-0.14308042	593	600	-0.13411881	2844459	1.15645319	2077444	1.21307056	experimental	NINDS	2300720	Pinacidil
1922 L11	X	395	400	-0.44775435	715	720	0.10913324	2629389	0.62924373	2447548	0.5219847	experimental	NINDS	1505203	Ezetimibe
1922 L12	X	234	240	-0.69549426	314	320	-0.69040833	1237902	-2.78176252	1245877	-2.67336205	experimental	NINDS	2300094	Astemizole
1922 L13	X	515	520	-0.26310348	475	480	-0.36939538	2503779	0.32133104	2465039	0.56849477	experimental	NINDS	1505204	Almotriptan
1922 L14	X	673	680	-0.01997984	555	560	-0.20988584	2765400	0.96265278	2564472	0.83289569	experimental	NINDS	2300242	Loxapine succinate
1922 L15	X	793	800	0.16467103	474	480	-0.37138925	3102488	1.78896972	2428585	0.47156045	experimental	NINDS	1505205	Olimesartan medoxomil
1922 L16	X	608	600	-0.19909961	667	680	-0.33638349	27436283	-0.0055517	214387	1.59132712	experimental	NINDS	2300324	Perphenazine
1922 L17	X	632	640	-0.08306889	673	680	0.02539073	2702038	0.8073105	2254065	0.00749673	experimental	NINDS	1505207	Ceftibuten
1922 L18	X	712	720	0.04003169	392	400	-0.53488653	2442897	0.17208863	2423112	0.45700727	experimental	NINDS	2300214	Diltiazem hydrochloride
1922 L19	X	753	760	0.10312074	673	680	0.02539073	2731675	0.87998138	2336976	0.22796422	experimental	NINDS	1505208	Cefdinir
1922 L20	X	513	520	-0.26618099	631	640	-0.05835178	2906827	1.30933829	2640092	1.03397579	experimental	NINDS	2300309	Valsartan hydrochloride
1922 L21	X	632	640	-0.08306889	632	680	0.02339686	2621033	0.60876034	2339621	0.2349975	experimental	NINDS	1505209	Valsartan
1922 L22	X	670	680	-0.02459611	790	800	0.25867343	2523038	0.36854138	2722583	1.25332647	experimental	NINDS	2300206	Diazoxide
1922 L23	E	1088	1080	-0.19909961	667	680	-0.33638349	27436283	-0.0055517	214387	1.59132712	empty			
1922 L24	P	159473	160440	244.334666	124869	125760	247.655976	2336685	-0.08827298	2091983	-0.42349328	empty			
1922 M01	N	436	440	-0.3846653	715	720	0.10913324	2044142	-0.80539502	1928350	-0.85860753	empty			
1922 M02	E	235	240	-0.69395555	355	360	-0.60865969	88094	-5.60033162	83412	-5.76445666	empty			
1922 M03	X	791	800	0.16159351	391	400	-0.5368804	1470104	-2.21255672	1283911	-2.57222637	experimental	NINDS	1503239	Hycanthone
1922 M04	X	1392	1400	1.0863866	1875	1880	2.42202157	2127066	-0.6021202	2172118	-0.21040741	experimental	NINDS	1503926	Lansoprazole
1922 M05	X	668	680	-0.02767363	304	320	-0.71034702	2891998	1.27298739	2361272	0.29256938	experimental	NINDS	1503240	Pyridostigmine bromide
1922 M06	X	1440	1480	-0.21102593	2113	2120	-2.90055019	2323475	-0.12065517	2126118	-2.48896416	experimental	NINDS	1503242	Eflornithine
1922 M07	X	551	560	-0.20770892	510	520	-0.29560996	2605285	-0.17267258	2407811	-0.63171793	experimental	NINDS	1503242	Isosorbide
1922 M08	X	633	640	-0.08153013	393	400	-0.53289266	2407756	0.08594613	2147314	-0.27636338	experimental	NINDS	1503931	Morantel citrate
1922 M09	X	752	760	0.10158198	674	680	0.0273846	1910635	-1.13266593	1865965	-1.02449462	experimental	NINDS	1503244	Lasolacil sodium
1922 M10	X	753	760	0.10312074	514	520	-0.29163448	2362719	-0.02445482	2309520	0.15495635	experimental	NINDS	1503932	Oxyphenyclimine hydrochloride
1922 M11	X	474	480	-0.32619253	433	440	-0.45313789	2236376	-0.33416434	2170852	-0.21377381	experimental	NINDS	1503245	Levamisole hydrochloride
1922 M12	X	515	520	-0.26310348	434	440	-0.45114402	2226224	-0.35905033	2330285	0.21017228	experimental	NINDS	1503933	Pentolinium tartrate
1922 M13	X	554	560	-0.20309195	394	400	-0.53089879	2243144	-0.31757368	2203826	-0.1260931	experimental	NINDS	1503243	Latetolol hydrochloride
1922 M14	X	593	600	-0.14308042	554	560	-0.21187971	1349513	-2.50816613	1114287	-3.0232712	experimental	NINDS	1503934	Perphenazine
1922 M15	X	513	520	-0.26618099	554	560	-0.21187971	2451284	0.19264801	2214123	-0.09871249	experimental	NINDS	1503250	Mephentermine sulfate
1922 M16	X	633	640	-0.08153013	673	680	0.02539073	2078227	-0.72184114	2039225	-0.56378135	experimental	NINDS	1503935	Propafenone hydrochloride
1922 M17	X	552	560	-0.20616946	712	720	0.10315163	2728671	0.87261756	2315711	0.17141875	experimental	NINDS	1503251	Metaraminol bitartrate
1922 M18	X	591	600	-0.14615793	711	720	0.10115776	2056885	-0.77415761	2248862	-0.0063385	experimental	NINDS	1503936	Metizoline
1922 M19	X	713	720	0.04157045	551	560	-0.21786132	2613189	0.58953204	2501817	0.66629065	experimental	NINDS	1503252	Methazolamide
1922 M20	X	513	520	-0.26618099	1032	1040	0.74118979	2415497	0.10492194	2439601	0.50085294	experimental	NINDS	1503939	Ribostamycin sulfate
1922 M21	X	632	640	-0.08306889	751	760	0.18091253	1837803	-1.31120185	1890529	-0.95917683	experimental	NINDS	1503253	Methylbenzethonium chloride
1922 M22	X	790	800	0.16005476	950	960	0.57769251	2458492	0.21031726	2337592	0.22960222	experimental	NINDS	1503254	Thioctic acid
1922 M23	E	597	1160	-0.13692539	642	1080	-0.03641922	90787	-5.59373017	85689	-5.75840192	empty			
1922 M24	P	190867	191760	292.64241	147138	148080	292.057451	2542082	0.41522468	2395685	0.38407651	empty			
1922 N01	N	676	680	-0.01536357	676	680	0.03137234	2643300	0.6633443	2106220	-0.38563587	empty			
1922 N02	E	235	240	-0.69395555	355	280	-0.76816923	85586	-5.60647958	83079	-5.76534214	empty			
1922 N03	X	592	600	-0.14461917	475	440	-0.44915015	2034399	-0.82927842	2191036	-0.16010282	experimental	NINDS	1505210	Sibutramine hydrochloride
1922 N04	X	551	560	-0.03849794	349	360	-0.62065291	2356440	-0.03984678	2135063	0.35583127	experimental	NINDS	2300212	Terfenadine
1922 N05	X	553	560	-0.20463071	674	680	0.0273846	3384412	0.02872207	2284385	0.08811224	experimental	NINDS	1505212	Torsimone
1922 N06	X	631	640	-0.08460764	629	640	-0.06233952	2618700	0.60304136	2377045	0.33451115	experimental	NINDS	1600654	Chaulmosulfone
1922 N07	X	473	480	-0.32773128	434	440	-0.45114402	2161282	-0.518						

1922 001	N		675	680	-0.01690232	475	480	-0.36939538	1928184	-1.08964738	1736231	-1.36946851	empty			
1922 002	E		194	200	-0.75704455	195	200	-0.92767877	81006	-5.61770671	83598	-5.76396207	empty			
1922 003	X		834	840	0.22776007	634	640	-0.05237017	2144629	-0.55906733	1993863	-0.68440281	experimental	NINDS	1503257	Midodrine hydrochloride
1922 004	X		640	640	-0.08306889	673	680	0.02539073	2213019	-0.39143026	2030843	-0.58822367	experimental	NINDS	1503947	Caecydolic acid
1922 005	X		512	520	0.26771975	752	760	0.18200664	0944233	-0.68260503	3339819	-0.3339819	experimental	NINDS	1503260	Nadolol
1922 006	X		713	720	0.04157045	553	560	-0.21387358	2381778	0.02226524	2128241	-0.32780813	experimental	NINDS	1503954	Tulobuterol
1922 007	X		513	520	-0.26618099	433	440	-0.45313789	2148451	-0.54969831	1915784	-0.8920216	experimental	NINDS	1503262	Naltrexone hydrochloride
1922 008	X		592	600	-0.14461917	592	600	-0.13611268	2260997	-0.27380992	2285309	0.09057722	experimental	NINDS	1503973	2-thiouacil
1922 009	X		833	840	0.22622132	834	840	0.34640368	2195422	-0.43455647	1993753	-0.68469531	experimental	NINDS	1503266	Nocodazole
1922 010	X		552	560	-0.20616946	553	560	-0.21387358	2121682	-0.6153182	1994590	-0.68246966	experimental	NINDS	1503975	Fluconazole
1922 011	X		434	440	-0.38774281	513	520	-0.29362835	2205470	-0.40992542	1998214	-0.67283313	experimental	NINDS	1503267	Nomifensine maleate
1922 012	X		593	600	-0.14308042	550	560	-0.21985519	2033257	-0.83207785	1912916	-0.90495007	experimental	NINDS	1503978	Hydroxychloroquine sulfate
1922 013	X		553	560	-0.20463071	633	640	-0.05436404	2105672	-0.65456414	1917006	-0.8887722	experimental	NINDS	1503269	Pergolide mesylate
1922 014	X		633	640	-0.08153013	632	640	-0.05635791	2011477	-0.88546801	1966866	-0.75619016	experimental	NINDS	1503982	Agmatine sulfate
1922 015	X		593	600	-0.14308042	573	760	0.18490027	2378933	0.01529119	2169514	-0.21733167	experimental	NINDS	1503270	Prilocaine hydrochloride
1922 016	X		593	600	-0.14308042	792	800	0.26266117	2179083	-0.47460889	1958054	-0.77962203	experimental	NINDS	1503985	Brompheniramine maleate
1922 017	X		831	840	0.2231438	1033	1040	0.74318366	2620231	0.606679436	2353121	0.27089517	experimental	NINDS	1503273	Hydrocortisone butyrate
1922 018	X		1068	1080	0.58782926	425	440	-0.46908885	2204022	-0.41347496	1964886	-0.76145515	experimental	NINDS	1503991	Clebopride maleate
1922 019	X		791	800	0.16159351	873	880	0.42416458	2263680	-0.26723298	2209147	-0.11194411	experimental	NINDS	1503276	Roxithromycin
1922 020	X		703	720	0.02618288	667	680	0.01342751	1685028	-1.68570515	1487506	-2.03084971	experimental	NINDS	1503994	Convallatoxin
1922 021	X		3548	3560	0.440394716	2389	2400	3.44687036	1829634	-1.33122683	1736664	-1.36831712	experimental	NINDS	1503278	Minoxalanthrone hydrochloride
1922 022	X		1740	1760	1.62187411	1424	1440	1.52278654	2090476	-0.69181469	2124734	-0.33640555	experimental	NINDS	1504002	Baicalein
1922 023	E		505	1120	-0.27849105	607	1200	-0.10620464	85699	-5.60620258	83544	-5.76410566	empty			
1922 024	P	207570	208640	318.344272	199500	200880	396.460432	2290594	-0.20125764	2137183	-0.30330258	empty				
1922 P01	N		797	800	0.17082606	718	720	0.11511484	1871537	-1.22850838	1682900	-1.51128023	empty			
1922 P02	E		275	280	-0.63240521	275	280	-0.63240521	77624	-5.62599714	78954	-5.77870704	empty			
1922 P03	X		634	640	-0.07999137	675	680	0.022937847	2012422	-0.8833149	1927775	-0.93499365	experimental	NINDS	1505249	Apramycin
1922 P04	X		794	800	0.16620978	794	800	0.26664891	2359466	-0.03242903	2125576	-0.3341666	experimental	NINDS	107108	Salpha-androstan-3,17-dione
1922 P05	X		874	880	0.28931036	674	680	0.0273846	1976984	-0.97002204	2035737	-0.57305624	experimental	NINDS	1505256	Silibinin
1922 P06	X		593	600	-0.14308042	514	520	-0.29163448	2242543	-0.31904693	2368234	0.31108194	experimental	NINDS	107113	Androsterone acetate
1922 P07	X		715	720	0.04464796	795	800	0.26864278	2025243	-0.85172288	2015836	-0.62597471	experimental	NINDS	1505261	Telmisartan
1922 P08	X		555	560	-0.20155319	834	840	0.34640368	2266448	-0.26044767	1981316	-0.71776637	experimental	NINDS	200208	Asarylaldehyde
1922 P09	X		553	560	-0.20463071	514	520	-0.29163448	2135740	-0.58085728	1815647	-1.15829452	experimental	NINDS	1505262	Sertraline hydrochloride
1922 P10	X		895	900	-0.29084912	873	880	-0.29084912	1560184	-0.9174282	555	-0.9174282	experimental	NINDS	200022	Aklavine hydrochloride
1922 P11	X		473	480	-0.32773128	713	720	0.1051455	2081899	-0.71283982	2010465	-0.64025667	experimental	NINDS	1505263	Afluzocin
1922 P12	X		955	960	0.4139497	1314	1320	1.30346092	2225355	-0.36118054	2039443	-0.56320167	experimental	NINDS	200499	Acacetin
1922 P13	X		634	640	-0.07999137	752	760	0.1829064	2074890	-0.73002126	2121404	-0.34526203	experimental	NINDS	1505264	Trindolapril
1922 P14	X		675	680	-0.01690232	954	960	0.58566799	2118969	-0.62196869	2080873	-0.45303573	experimental	NINDS	200701	Benzylhydrazine hydrochloride
1922 P15	X		515	520	-0.26310348	594	600	-0.13212494	2008065	-0.89383198	2025587	-0.60004596	experimental	NINDS	1505265	Telithromycin
1922 P16	X		395	400	-0.44775435	354	360	-0.61065356	1509391	-2.116265096	1093919	-3.07743147	experimental	NINDS	200413	2,6-dimethoxyquinone
1922 P17	X		640	640	-0.08157813	551	560	-0.08157813	2056974	-0.7739164	1579552	-0.64043371	experimental	NINDS	1505267	Oxapropin
1922 P18	X		1273	1280	0.90327449	1675	1680	2.02324772	2311564	-0.14985307	2285234	0.09037778	experimental	NINDS	200789	Daidzein
1922 P19	X		672	680	-0.0215186	591	600	-0.13810655	1830221	-1.3297879	1831014	-1.11743234	experimental	NINDS	1505270	Propranolol hydrochloride (+/-)
1922 P20	X		754	760	0.1046595	593	600	-0.13411881	2263634	-0.26734574	1786300	-1.23633072	experimental	NINDS	200258	2',4'-dihydroxycalcone 4'-glucoside
1922 P21	X		824	840	0.2123725	988	1000	0.65345954	2159106	-0.5235793	2128968	-0.32514698	experimental	NINDS	1505271	Crotamiton
1922 P22	X		1269	1280	0.89711946	1149	1160	0.97447249	1920787	-1.10777994	1807245	-1.18063616	experimental	NINDS	200846	Apigenin
1922 P23	E		632	1280	-0.08306889	511	1320	-0.29761609	80894	-5.61798126	78852	-5.7765821	empty			
1922 P24	E	220952	221560	338.932921	27695	277080	549.973995	1882337	-1.20203392	167531	-1.05489861	empty				
1923 A01	N		637	640	-0.15664951	598	600	-0.4869651	1978823	-0.43734719	1436879	-0.93629796	empty			
1923 A02	E		237	240	-0.88071431	117	120	-0.01962081	76790	-4.49559884	77139	-3.8457789	empty			
1923 A03	X		316	320	-0.73771109	316	320	-1.38525172	1777851	-1.73811764	1665460	-1.61530199	experimental	NINDS	201315	7,8-dihydroxyflavone
1923 A04	E		595	600	-0.23267439	596	600	-0.49267208	1970670	-1.42555109	2060890	-1.06000021	empty			
1923 A05	X		874	880	0.27236231	675	680	-0.24083711	1692007	-1.87727386	1697635	-1.57011869	experimental	NINDS	201138	Deguelin(-)
1923 A06	E		713	720	-0.01907464	474	480	-0.88158178	2101500	-1.21347095	2337246	-0.67191388	empty			
1923 A07	X		834	840	0.19995561	835	840	0.26920839	2264330	-0.94951765	1863953	-1.33655856	experimental	NINDS	201606	Rutlantinone
1923 A08	E		635	640	-0.16026769	795	800	-0.14169702	2341932	-0.82372201	2412956	-0.56559943	empty			
1923 A09	X		396	400	-0.5928977	435	440	-1.00590537	1577729	-2.06252262	1881895	-1.31136263	experimental	NINDS	201580	Pomiferin
1923 A10	E		435	440	-0.52230117	715	720	-0.11332574	2197407	-1.05800224	2050466	-1.07463862	empty			
1923 A11	X		636	640	-0.15845753	675	680	-0.24083711	2503456	-0.56188578	2152327	-0.93159536	experimental	NINDS	201716	Norstictic acid
1923 A12	E		516	520	-0.37567761	516	520	-0.74769483	2236680	-0.99433929	2620814	-0.27369974	experimental	NINDS	201664	Celastrol
1923 A13	X		195	200	-0.95674134	234	240	-1.64665004	1040299	-2.93371602	998004	-2.5526095	experimental	NINDS	201664	Celastrol
1923 A14	E		475	480	-0.44989448	1190	1200	1.40087186	2519583	-0.53574333	2216974	-0.84081167	empty			
1923 A15	X		916	920	0.34838934	2752	2760	6.38019111	2242328	-0.98518368	2359663	-0.64043371	experimental	NINDS	201602	Pachyrrhizin
1923 A16	E		433	440	-0.52592151	788	800	0.11938253	2445800	-0.65534824	2150622	-0.93398969	empty			
1923 A17	X		914	920	0.34476901	713	720	-0.1197013	2560843	-0.46885939	2575790	-0.33692688	experimental	NINDS	201605	Bisanthrolantianone
1923 A18	E		673	680	-0.09148133	834	840	0.26602061	2536365	-0.50853911	2497992	-0.4461785	empty			
1923 A19	X		914	920	0.34476901	754	760	0.01099786	2104991	-1.20781191	1933534	-1.23883763	experimental	NINDS	201604	Pyrrromycin
1923 A20	X		713	720	-0.01907464	593	600	-0.50223543	2546873	-0.49150526	2392983	-0.59364249	experimental	NINDS	210031	Phenylacetohydroxamic acid
1923 A21	E		994	1000	0.4895824	1034	1040	0.90357749	2521624	-0.5324348	2315763	-0.70208242	empty			
1923 A22	E		871	880	-0.36993181	870	880	0.38107807	2601203	-0.40343437	2213691	-0.84541356	empty			
1923 A23	E		783	1560	0.10763708	732	1520	-0.591334	83134	-4.48531498	1487718	-3.85654002	empty			
1923 A24	P	266150	266600	480.466325	268837	269560	854.601806	2185148	-1.07787452	1852627	-1.35246364	empty				

1923 B19	E		592	600	-0.23810489	632	640	-0.37791184	2777074	-0.11834114	2422376	-0.55236594		empty	
1923 B20	E		633	640	-0.16388803	592	600	-0.50542322	3114663	0.42890279	2633732	-0.25555901		empty	
1923 B21	E		591	600	-0.23991506	711	720	-0.12607687	2541484	-0.50024102	2455707	-0.50555926		empty	
1923 B22	E		710	720	-0.02450514	748	760	-0.00812885	2856603	0.01057823	3162244	0.40251215		empty	
1923 B23	E		585	1040	-0.25077606	911	1640	0.51488001	85618	-4.48128833	90623	-3.82684333		empty	
1923 B24	P	152583	153760	274.891046	246775	248160	784.272906	2360128	-0.79422564	2080745	-1.03211786			empty	
1923 C01	N		676	680	-0.08605083	396	400	-1.13022896	2218560	-1.02371247	2065598	-1.05338877		empty	
1923 C02	E		235	240	-0.88433465	236	240	-1.64027447	89111	-4.47562605	91863	-3.825102		empty	
1923 C03	X		515	520	-0.37748778	554	560	-0.62655903	3099243	0.40390642	2912865	0.13642706		experimental	
1923 C04	E		705	720	-0.03355598	634	640	-0.37153627	2762953	-0.14123179	3003173	0.26324646		empty	
1923 C05	X		3673	3680	5.33902082	553	560	-0.62974681	2867789	0.02871114	2834782	0.02677522		experimental	
1923 C06	E		461	480	-0.47523682	472	480	-0.88795735	3222856	0.60428755	336342	0.76884871		empty	
1923 C07	X		1594	1600	1.57568283	1073	1080	1.02790108	2873613	0.03815206	2862987	0.06638346		experimental	
1923 C08	E		341	360	-0.69245691	792	800	0.13213366	2999671	0.24249662	2999886	0.25863053		empty	
1923 C09	X		3874	3880	5.70286446	593	600	-0.50223543	3415898	0.91721559	3345235	0.74360363		experimental	
1923 C10	E		585	600	-0.25077606	593	600	-0.50223543	3179829	0.53453923	3318877	0.70658913		empty	
1923 C11	X		474	480	-0.45170464	594	600	-0.49904765	3103195	0.41031275	3492486	0.950388		experimental	
1923 C12	E		473	480	-0.45351481	673	680	-0.24721268	2625141	-0.36463001	3230062	0.58186635		empty	
1923 C13	X		634	640	-0.16207786	712	720	-0.12288909	3028780	0.28968336	2851314	0.04999108		experimental	
1923 C14	E		353	360	-0.6707349	793	800	0.13532145	3170993	0.52021575	3124698	0.43390384		empty	
1923 C15	X		635	640	-0.16026769	632	640	-0.37791184	3122379	0.44141071	3660962	1.18697861		experimental	
1923 C16	E		554	560	-0.30689125	592	600	-0.50542322	2715124	-0.21876433	2726167	-0.12575267		empty	
1923 C17	X		552	560	-0.31051159	632	640	-0.37791184	2446434	-0.6543205	3477598	0.9294808		experimental	
1923 C18	E		714	720	-0.01726447	872	880	0.38715642	2927747	0.12590522	2897076	0.11425459		empty	
1923 C19	X		593	600	-0.23629472	791	800	0.12894588	3195810	0.56044501	2769290	-0.06519511		experimental	
1923 C20	E		592	600	-0.23810489	671	680	-0.44657299	2828738	-0.0229705	3129262	-0.37113145		empty	
1923 C21	X		592	600	-0.23810489	671	680	-0.25388625	2390715	-0.74464309	2088654	-0.02101127		experimental	
1923 C22	E		831	840	0.19452511	830	840	0.25326947	2879852	0.0482657	2697211	-0.16641554		empty	
1923 C23	E		629	1040	-0.17112887	630	1240	-0.38428741	85066	-4.48218314	86147	-3.83312898		empty	
1923 C24	P	138025	138920	248.538629	205802	207040	653.659816	2542095	-0.49925057	2542095	-0.49925057	2470271	-0.48510706		empty
1923 D01	N		475	480	-0.44989448	476	480	-0.87520621	2997695	0.23929345	2221964	-0.83380422		empty	
1923 D02	E		316	320	-0.73771109	275	280	-1.51595088	88467	-4.47667	93930	-3.82219932		empty	
1923 D03	E		395	400	-0.59470787	594	600	-0.49904765	2735326	-0.18601616	2554769	-0.36644664		empty	
1923 D04	E		334	360	-0.66892473	412	420	-0.66892473	3201248	0.5692812	2999663	3.257512		empty	
1923 D05	E		426	440	-0.53859268	515	520	-0.75088262	2892532	0.06882044	3085081	0.37826974		empty	
1923 D06	E		675	680	-0.087861	634	640	-0.37153627	3294117	0.7198042	3188877	0.52403032		empty	
1923 D07	E		471	480	-0.45713515	511	520	-0.76363376	3197747	0.56358495	2872229	0.07936198		empty	
1923 D08	E		475	480	-0.44989448	592	600	-0.50542322	2813266	-0.05967261	3358893	0.76278354		empty	
1923 D09	E		545	560	-0.32318276	672	680	-0.25040047	3004838	0.25087251	3100366	0.39973445		empty	
1923 D10	E		433	440	-0.52592151	711	720	-0.12607687	3846957	1.61597776	2777717	-0.05336108		empty	
1923 D11	E		520	530	-0.37929795	553	560	-0.62974681	3388932	0.87350273	3147362	0.06260307		empty	
1923 D12	E		594	600	-0.23448456	591	600	-0.508611	3724484	1.41744662	2894978	0.11130837		empty	
1923 D13	E		473	480	-0.45351481	953	960	0.64536695	3015741	0.26854667	2882746	0.09413099		empty	
1923 D14	E		634	640	-0.16207786	550	560	-0.63931016	3076936	0.36774597	2766107	-0.06966499		empty	
1923 D15	E		474	480	-0.45170464	553	560	-0.62974681	2891260	0.06675848	3448828	0.88907913		empty	
1923 D16	E		394	400	-0.59651803	593	600	-0.50223543	3473402	1.01043164	3057232	0.33916143		empty	
1923 D17	E		513	520	-0.37929795	552	560	-0.63293459	3206921	0.57845634	2646584	-0.23751097		empty	
1923 D18	E		433	440	-0.52592151	712	720	-0.12288909	3453213	0.97794555	3123262	0.44405349		empty	
1923 D19	E		582	590	-0.05151159	592	600	-0.12288909	27905809	-0.09647337	3016975	0.28262858		empty	
1923 D20	E		752	760	0.05152189	631	640	-0.38109963	3262460	0.66848706	3450250	0.89107605		empty	
1923 D21	E		752	760	0.05152189	631	760	0.0014345	2838760	-0.01834591	2740196	-0.10605177		empty	
1923 D22	E		830	840	0.19271495	869	880	0.37759306	3132103	0.45717366	2673628	-0.19953312		empty	
1923 D23	E		745	1200	0.03885072	754	1280	0.01099786	87904	-4.47758264	93223	-3.82319216		empty	
1923 D24	P	153713	154400	276.936535	177060	178120	562.036516	2590085	-0.42145705	2599734	-0.30330235			empty	
1923 E01	N		837	840	0.20538612	636	640	-0.3651607	2315677	-0.86628231	1993919	-1.15404749		empty	
1923 E02	E		234	240	-0.88614482	314	320	-1.39162728	87516	-4.4782116	96663	-3.8136137		empty	
1923 E03	X		554	560	-0.30689125	714	720	-0.11651352	3147396	0.48196417	2949692	0.18814316		experimental	
1923 E04	E		555	560	-0.30508109	594	600	-0.49904765	2831808	-0.02961536	2853062	0.05244579		empty	
1923 E05	X		195	200	-0.95674134	153	160	-1.90486057	1267167	-2.56595481	1227297	-2.23061367		experimental	
1923 E06	E		475	480	-0.44989448	594	600	-0.49904765	2838571	-0.01865229	2827865	0.01706168		empty	
1923 E07	X		395	400	-0.59470787	634	640	-0.37153627	2225323	-1.0127494	2266010	-0.77195049		experimental	
1923 E08	E		434	440	-0.52411134	633	640	-0.37472406	2980457	0.21135003	2807408	-0.01166605		empty	
1923 E09	X		434	440	-0.52411134	712	720	-0.12607687	3450626	0.97351093	3802227	1.38535684		experimental	
1923 E10	E		594	600	-0.23448456	1152	1160	1.27973605	3062740	0.34473374	3140198	0.45567047		empty	
1923 E11	X		554	560	-0.30689125	551	560	-0.63612238	2747944	-0.16556192	3754274	1.31801651		experimental	
1923 E12	E		632	640	-0.1656982	912	920	0.51466779	2666806	-0.29708955	2783976	-0.04457158		empty	
1923 E13	X		433	440	-0.52592151	619	680	-0.25996382	2757006	-0.15087209	3306763	0.68957746		experimental	
1923 E14	E		713	720	-0.01907464	1232	1240	1.5347588	2667926	-0.29527398	3065474	0.35073566		empty	
1923 E15	X		513	520	-0.37929795	751	760	0.0014345	2812915	-0.06024159	3230544	0.58254323		experimental	
1923 E16	E		713	720	-0.01907464	712	720	-0.12288909	2734064	-0.1880619	820249	0.00665393		empty	
1923 E17	X		793	800	-0.151573875	873	880	0.13979232	3018385	0.27283269	2902608	0.12202317		experimental	
1923 E18	E		752	760	0.05152189	711	720	-0.12607687	2811174	-0.06306381	2779731	-0.05053282		empty	
1923 E19	X		992	1000	0.48596206	711	720	-0.12607687	3394439	0.88242977	3113976	0.41884695		experimental	
1923 E20	E		831	840	0.19452511	831	840	0.25645726	3373379	0.84829076	2738715	-0.10813153		empty	
1923 E21	X		591	600	-0.23991506	1031	1040	0.89401414	3185108	0.54309668	3527176	0.99910312		experimental	
1923 E22	E		792	800	0.12392858	829	840	0.25008169	3240099	0.63223907	2800165	-0.02183739		empty	
1923 E23	E		910	800	-0.38653862	813	1280	0.19907714	86961	-4.47911128	90238	-3.82738399		empty	
1923 E24	N	96302	97160	173.013015	156927	157920	487.856833	2924407	0.121049097	2924407	0.121049097	3792982	0.29992353		empty
1923 F01	N		429	440	-0.5316218	476	480	-0.87520621	2595656	-0.14242626	2371720	-0.62350209		empty	
1923 F02	E		235	240	-0.88433465	275	280	-1.51595088	88431	-4.47672836	91164	-3.82680361		empty	
1923 F03	E		794	800	0.12754892	633	640	-0.37472406	2746672	-0.16762388	2392090	-0.594			

1923 F13	E	552	560	-0.31051159	672	680	-0.25040047	3273526	0.68642544	2700763	-0.16142747			empty
1923 F14	E	714	720	-0.01726447	710	720	-0.12926466	3722923	1.41491418	3007324	0.2690757			empty
1923 F15	E	473	480	-0.45351481	592	600	-0.50542322	3069564	0.35579569	2764260	-0.07225873			empty
1923 F16	E	634	640	-0.16207786	552	560	-0.63293459	3378537	0.85665206	3407504	0.8310479			empty
1923 F17	E	593	600	-0.23629472	512	520	-0.76044597	2997880	0.21955206	2539875	-0.38736226			empty
1923 F18	E	473	480	-0.45351481	713	720	-0.1197013	3336062	0.78779855	2918595	0.14447369			empty
1923 F19	E	512	520	-0.38291828	671	680	-0.25358825	2749615	-0.16285317	2543047	-0.38290783			empty
1923 F20	E	592	600	-0.23810489	631	640	-0.38109963	3077839	0.36920976	3137072	0.45128063			empty
1923 F21	E	714	720	-0.01726447	712	720	-0.12288909	2445868	-0.65523801	2740449	-0.10569648			empty
1923 F22	E	631	640	-0.16750836	510	520	-0.76682154	3080161	0.37297381	2934905	0.1673778			empty
1923 F23	E	423	840	-0.54402318	717	1200	-0.10695017	88333	-4.47688722	90099	-3.82757919			empty
1923 F24	P	140595	141280	253.190739	162490	163520	515.590497	2409572	-0.71407513	239160	-0.59521951			empty
1923 G01	N	2756	2760	3.67909733	396	400	-1.13022896	2589760	-0.42198389	2059254	-1.06229764			empty
1923 G02	E	269	280	-0.82278896	235	240	-1.64346225	90526	-4.47333229	94980	-3.82072481			empty
1923 G03	X	594	600	-0.23448456	795	800	0.14169702	3105074	0.41335868	2834923	0.02697322			experimental
1923 G04	E	393	400	-0.5983282	512	520	-0.76044597	3033377	0.29713526	2762139	-0.07523724	NINDS	300034	Testosterone propionate
1923 G05	X	635	640	-0.16026769	554	560	-0.62655903	2944145	0.15248697	2552911	-0.36905583			experimental
1923 G06	E	553	560	-0.30870142	593	600	-0.50223543	3091781	0.39181025	3256794	0.61940606			empty
1923 G07	X	634	640	-0.16207786	673	680	-0.24721268	3066247	0.35041871	3232122	0.58475921	NINDS	300038	Juglone
1923 G08	E	473	480	-0.45351481	793	800	0.13532145	3114738	0.42902437	3309531	0.69346456			empty
1923 G09	X	554	560	-0.30689125	672	680	-0.25040047	3013193	0.26441627	3509947	0.97490846			experimental
1923 G10	E	513	520	-0.38110812	672	680	-0.25040047	3575422	1.17580974	3787363	1.36448335			empty
1923 G11	X	595	600	-0.23267439	832	840	0.25964504	3436820	0.9511309	3340258	0.73661444	NINDS	300061	Eupatoriochromene
1923 G12	E	272	280	-0.81735846	552	560	-0.63293459	3321994	0.76499382	3195790	0.53373823			empty
1923 G13	X	393	400	-0.5983282	632	640	-0.37791184	2948523	0.15958387	3201001	0.51405603	NINDS	300546	Bergapten
1923 G14	E	393	400	-0.5983282	792	800	-0.12113366	3091781	0.16392662	3236090	-0.08971869			empty
1923 G15	X	594	600	-0.23448456	631	640	-0.38109963	2984878	0.21851663	3077009	0.36692454			experimental
1923 G16	E	514	520	-0.37929795	913	920	0.51785558	2909188	0.09582041	2852967	0.05231239			empty
1923 G17	X	393	400	-0.5983282	593	600	-0.50223543	2529489	-0.51968535	2182886	-0.8886814	NINDS	300565	Metergolone
1923 G18	E	554	560	-0.30689125	633	640	-0.37472406	2967854	0.19092011	2966571	0.21184632			empty
1923 G19	X	554	560	-0.30689125	953	960	0.64536695	3319324	0.76066565	3055643	0.33693			experimental
1923 G20	E	513	520	-0.38110812	872	880	0.38715642	3525874	1.09549065	3269989	0.63793578			empty
1923 G21	X	312	320	-0.74495176	392	400	-1.1429801	1055973	-2.90847	872643	-2.58822391	NINDS	310035	Sanguinarine sulfate
1923 G22	E	831	840	-0.19452511	717	840	-0.16074687	3104768	0.29272748	2033595	-0.10970927			empty
1923 G23	E	751	1160	0.04971172	822	1400	0.2277672	85987	-4.48069017	91893	-3.82505988			empty
1923 G24	P	137850	138640	248.22185	195783	196720	621.721404	2948706	0.15988052	2760587	-0.07741672			empty
1923 H01	N	550	560	-0.31413192	597	600	-0.4894843	2845892	-0.00678468	2348924	-0.65551448			empty
1923 H02	E	275	280	-0.81192795	235	240	-1.64346225	85290	-4.48182003	90846	-3.82653018			empty
1923 H03	E	554	560	-0.30689125	393	400	-1.13979232	2735942	-0.1850176	2537163	-0.39117072			empty
1923 H04	E	514	520	-0.37929795	674	680	-0.2440249	3403719	0.89747299	2861952	0.06493001			empty
1923 H05	E	440	440	-0.5241113	553	560	-0.62655903	3007277	0.25482622	2458641	-0.50446812			empty
1923 H06	E	433	440	-0.52592151	673	560	-0.62674681	3425673	0.93954536	2825964	0.01439211			empty
1923 H07	E	714	720	-0.01726447	673	680	-0.24721268	3343949	0.80058366	2649405	-0.23354944			empty
1923 H08	E	513	520	-0.38110812	672	680	-0.25040047	3481353	1.0233205	2459347	-0.50044762			empty
1923 H09	E	633	640	-0.16388803	552	560	-0.63293459	3170115	0.51879249	2481122	-0.46986902			empty
1923 H10	E	593	600	-0.23629472	552	560	-0.63293459	3481465	1.02350206	3100026	0.39925698			empty
1923 H11	E	553	560	-0.30870142	792	800	-0.13213366	3312841	0.75015648	2827898	0.01710802			empty
1923 H12	E	1114	1120	-0.45332498	513	520	-0.76044597	3104563	-4.1253033	2495961	-0.09273481			empty
1923 H13	E	632	640	-0.1656982	632	720	-0.1197013	3494002	1.04205249	2835076	0.02718808			empty
1923 H14	E	632	640	-0.1656982	632	640	-0.37791184	3673072	1.33410391	2862258	0.06535972			empty
1923 H15	E	793	800	0.12573875	752	760	0.00462229	3273717	0.68673506	2585022	-0.32396239			empty
1923 H16	E	432	440	-0.52773167	712	720	-0.12288909	3460062	0.98880702	2964771	0.20931858			empty
1923 H17	E	755	760	0.05695239	474	480	-0.88158178	3025441	0.28427072	1897795	-1.28903429			empty
1923 H18	E	512	520	-0.38291828	233	240	-1.64983782	3650246	1.29710214	1450087	-1.91774999			empty
1923 H19	E	592	600	-0.23810489	272	280	-1.52551423	3119901	0.43739378	1833670	-1.37908493			empty
1923 H20	E	832	840	-0.19633528	673	680	-0.24721268	3249777	0.64792746	2033595	-1.09833054			empty
1923 H21	E	832	840	-0.19633528	431	440	-0.101865651	3310240	0.74594016	2252448	-0.79099559			empty
1923 H22	E	871	880	0.26693181	831	840	0.25645726	3018746	0.27341788	2632732	-0.25696331			empty
1923 H23	E	613	1000	-0.20009138	650	1120	-0.32053172	90259	-4.4737651	94999	-3.82069812			empty
1923 H24	P	129550	130400	233.197461	157680	158840	500.257254	2748900	-0.16401221	2638713	-0.2485642			empty
1923 I01	N	516	520	-0.37567761	556	560	-0.62018346	2712271	-0.22338914	2134098	-0.95719432			empty
1923 I02	E	275	280	-0.81192795	315	320	-1.3884395	87103	-4.47888109	92815	-3.82376511			empty
1923 I03	X	714	720	-0.01726447	555	560	-0.62337124	3239116	0.63064559	2806684	-0.01268277	NINDS	310039	Alpha-tochopherol
1923 I04	E	633	640	-0.16388803	473	480	-0.88476956	3366474	0.8370975	2687417	-0.18016924			empty
1923 I05	X	633	640	-0.16388803	753	760	0.00781007	3561812	1.15374744	3301272	0.68186645	NINDS	310040	Alpha-tochopheryl acetate
1923 I06	E	634	640	-0.16207786	593	600	-0.50223543	3070146	0.35673913	3190668	0.52570284			empty
1923 I07	X	513	520	-0.38110812	632	640	-0.37791184	2985486	0.21950222	3468951	0.91733783			experimental
1923 I08	E	634	640	-0.16207786	753	760	0.00781007	3330221	0.77833008	33210643	0.55459628			empty
1923 I09	X	673	680	-0.09148133	713	720	-0.1197013	2555336	-0.47786643	2362488	-0.63646657	NINDS	330001	Dactinomycin
1923 I10	E	593	600	-0.23629472	751	760	-0.0014345	3260694	0.66562431	2495961	0.51094787			empty
1923 I11	E	633	640	-0.16207786	952	960	0.6417917	3541495	-0.51205676	2380989	-0.10037576			experimental
1923 I12	E	714	720	-0.01726447	632	640	-0.37791184	3167058	0.51383698	3172657	0.50125259			empty
1923 I13	X	512	520	-0.38291828	713	720	-0.1197013	3425974	0.93354915	3585272	1.08068725			experimental
1923 I14	E	593	600	-0.23629472	432	440	-1.01546872	3244415	0.63923546	3081577	0.37334908			empty
1923 I15	X	632	640	-0.1656982	673	680	-0.24721268	3360783	0.82787219	3124238	0.43325786	NINDS	1503142	Tenoxicam
1923 I16	E	674	680	-0.08967117	552	560	-0.63293459	2815406	-0.05620359	3009486	0.27211179			empty
1923 I17	X	432	440	-0.52773167	673	680	-0.24721268	3710711	1.39511809	2831555	0.02224354	NINDS	1501157	Suxibuzone
1923 I18	E	753	760	0.0533206	913	920	0.51785558	2920488	0.00375756	2818391	0.00375756			experimental
1923 I19	E	752	760	0.05152189	673	920	0.51466779	3550062	1.13470027	2980660	0.23163148			experimental
1923 I20	E	711	720	-0.02269497	870	880	0.38078085	3432162	0.94358012	2848570	0.04613768			empty
1923 I21	X	712	720	-0.02088481	1152</									

1923 N01	N	596	600	-0.23086422	556	560	-0.62018346	2901161	0.08280836	1954206	-1.2098164				empty
1923 N02	E	195	200	-0.95674134	475	480	-0.87839399	79633	-4.49099023	113679	-3.79446583				empty
1923 N03	E	594	600	-0.23448456	393	400	-1.13979232	2564918	-0.46225367	2174023	-0.9011277				empty
1923 N04	E	591	600	-0.23629472	591	600	-0.508611	2875052	0.04048473	2476262	-0.47388531				empty
1923 N05	E	551	560	-0.31232176	712	720	-0.12288909	2931205	0.13151076	2345853	-0.65982708				empty
1923 N06	E	554	560	-0.30689125	592	600	-0.50542322	2964436	0.18537941	2566242	-0.35033512				empty
1923 N07	E	553	560	-0.30870142	632	640	-0.37791184	2759333	-0.14709994	2528463	-0.40338812				empty
1923 N08	E	394	400	-0.59651803	553	560	-0.62974681	3155924	0.49578836	2392349	-0.59453281				empty
1923 N09	E	394	400	-0.59651803	512	720	-0.12288909	3008785	0.25727074	2165782	-0.91270053				empty
1923 N10	E	594	600	-0.23448456	713	720	-0.1197013	2997730	0.23935019	2535431	-0.39360296				empty
1923 N11	E	554	560	-0.30689125	673	680	-0.24721268	3062203	0.34386324	2144458	-0.94250536				empty
1923 N12	E	474	480	-0.45170464	473	480	-0.88476596	3068566	0.3541779	2322241	-0.68500896				empty
1923 N13	E	473	480	-0.45351481	513	520	-0.75725819	2761749	-0.14318352	2198496	-0.8667603				empty
1923 N14	E	594	600	-0.23448456	672	680	-0.25040047	3337680	0.79042139	2566333	-0.35020733				empty
1923 N15	E	632	640	-0.1656982	671	680	-0.25358825	2607662	-0.3929641	2252680	-0.79066979				empty
1923 N16	E	633	640	-0.16388803	511	520	-0.76363376	3253170	0.65342763	1613053	-1.68889707				empty
1923 N17	E	632	640	-0.1656982	472	480	-0.88795735	3084958	0.38074992	1533928	-1.80001219				empty
1923 N18	E	712	720	-0.02088481	472	480	-0.88795735	3393358	0.88067743	1913972	-1.26531695				empty
1923 N19	E	789	800	0.11849808	630	640	-0.38428741	2778818	-0.11551406	1985966	-1.16521588				empty
1923 N20	E	992	1000	0.48596206	592	600	-0.50542322	3083244	0.37797146	2333736	-0.67684296				empty
1923 N21	E	750	760	0.04790155	790	800	0.12575809	2688036	-0.26267495	2292541	-0.73469304				empty
1923 N22	E	789	800	0.11849808	828	840	0.2468939	2930632	0.13058191	2618469	-0.27699282				empty
1923 N23	E	742	1240	0.03342022	749	1240	-0.00494107	83357	-4.48495349	87279	-3.83153931				empty
1923 N24	P	167807	168840	302.449034	164864	166000	523.158297	2478015	-0.60312656	2469419	-0.48630352				empty
1923 O01	N	555	560	-0.30508109	594	600	-0.49904765	2252739	-0.96830708	2077729	-1.03653323				empty
1923 O02	E	675	680	-0.81191785	474	480	-0.88159178	2564764	81696	-4.48764603	86232	-3.33300621			empty
1923 O03	E	713	720	-0.01907495	793	800	0.35860245	2786842	-0.10250686	2719734	-0.57428853				experimental
1923 O04	E	671	680	-0.09510167	991	1000	0.76650276	2624404	-0.36582472	2503381	-0.43861073		1503042	Artemisinin	
1923 O05	X	1152	1160	0.77558884	911	920	0.51148001	2529640	-0.51944058	2269611	-0.76689361				experimental
1923 O06	E	551	560	-0.31232176	671	680	-0.25358825	2579055	-0.43933708	2561200	-0.35741559		NINDS	1504410	Picropodophyllotoxin
1923 O07	X	793	800	0.12573875	793	800	0.13532145	2877141	0.04387107	3056499	0.33813208				experimental
1923 O08	E	553	560	-0.30870142	472	480	-0.88795735	2867266	0.02786334	2893000	0.10853067		NINDS	1503114	Dibekacin
1923 O09	X	594	600	-0.23448456	673	680	-0.24721268	2498633	-0.56970404	2780562	-0.04936585		NINDS	1501133	Nicergoline
1923 O10	E	474	480	-0.38110812	632	640	-0.38110812	2771745	0.11015137	2899662	-0.88995412				experimental
1923 O11	X	554	560	-0.30689125	672	680	-0.25040047	2618070	-0.37609236	2876637	-0.08555213		NINDS	1505346	Ketanserin tartrate
1923 O12	E	553	560	-0.30870142	833	840	0.26283282	2676048	-0.28210793	2743776	-0.10102438				empty
1923 O13	X	594	600	-0.23448456	672	680	-0.25040047	2511543	-0.54877646	2769396	-0.06504625		NINDS	1503977	Lovastatin
1923 O14	E	512	520	-0.38291828	992	1000	0.76969055	2740544	-0.17755759	2721329	-0.13254667				empty
1923 O15	X	873	880	0.27055214	870	880	0.38078085	2728358	-0.19731153	2808703	-0.00984749		NINDS	1502060	Snap (s-nitroso-n-acetylpenicillamine)
1923 O16	E	551	560	-0.31232176	871	880	0.38396683	2925945	-0.12298411	2654570	-0.22629624				empty
1923 O17	E	840	840	0.19452521	829	840	0.19452521	3095764	0.39826683	2397621	-0.16993211		NINDS	1502113	Azaserine
1923 O18	E	549	560	-0.31594209	879	880	0.25008169	2982848	0.21522593	2798384	-0.02433844				experimental
1923 O19	X	1873	1880	2.08071953	1752	1760	3.1924067	2819832	-0.04902888	2438594	-0.52959102		NINDS	1500672	Quercetin
1923 O20	E	588	600	-0.24534556	588	600	-0.51817436	2727935	-0.19799723	2834956	0.02701956				empty
1923 O21	X	671	680	-0.09510167	911	920	0.51148001	3006205	0.25308847	2818724	0.00422499		NINDS	1505035	Enoxaparin sodium (1% wt/vol in 10%aqueous dmso)
1923 O22	E	910	920	0.33752834	948	960	0.62942803	2634266	-0.34983806	2674242	-0.19867088				empty
1923 O23	E	730	1280	0.01169821	794	1520	0.13850923	82306	-4.4866572	84354	-3.83564688				empty
1923 O24	P	185138	186400	333.821047	245646	246840	780.673898	2642707	-0.33615489	2496260	-0.47192221				empty
1923 P01	N	798	800	0.0478959	917	920	0.05060672	2151221	-1.13287141	1732307	-1.52142885				empty
1923 P02	E	275	280	-0.81192795	354	360	-1.26411591	77252	-4.49484992	110343	-3.79915057				empty
1923 P03	E	715	720	-0.0154543	595	600	-0.49585986	2249518	-0.97352843	1717034	-1.5428767				empty
1923 P04	E	633	640	-0.16388803	714	720	-0.11651352	2661811	-0.30518662	1966871	-1.19203096				empty
1923 P05	E	953	960	0.41536553	633	640	-0.37472406	2421429	-0.69485451	1834002	-1.3786187				empty
1923 P06	E	633	640	-0.16388803	634	640	-0.37153627	2735146	-0.18630794	2040748	-1.08828559				empty
1923 P07	E	834	840	0.19995561	594	600	-0.49904765	2567925	-0.45737921	1950103	-1.21557824				empty
1923 P08	E	754	760	0.05514222	635	640	-0.36834849	2771356	-0.12761023	2112190	-0.98795969				empty
1923 P09	E	555	560	-0.30508109	554	560	-0.62655903	2677822	-0.27923221	2012376	-1.12812835				empty
1923 P10	E	515	520	-0.37748778	755	760	0.01418564	2685732	-0.26640982	2061017	-1.05982186				empty
1923 P11	E	595	600	-0.23267439	594	600	-0.49904765	2564860	-0.46234769	1864207	-1.33620187				empty
1923 P12	E	635	640	-0.16026769	674	680	-0.2440249	2805263	-0.07264576	2011416	-1.12947648				empty
1923 P13	E	554	560	-0.30689125	554	560	-0.62655903	2499073	-0.56899078	1795947	-1.43205929				empty
1923 P14	E	715	720	-0.0154543	593	600	-0.50223543	2730979	-0.1930628	1900638	-1.28504186				empty
1923 P15	E	673	680	-0.09148133	833	800	0.13532145	2605857	-0.39589007	2337048	-0.67219193				empty
1923 P16	E	673	680	-0.09148133	833	840	0.26283282	2791158	-0.09551047	2508472	-0.43146145				empty
1923 P17	E	1194	1200	0.85161587	833	840	0.26283282	2695194	-0.25107157	2260467	-0.77973452				empty
1923 P18	E	473	480	-0.45351481	833	840	0.26283282	2699799	-0.2436067	2615310	-0.281429				empty
1923 P19	E	551	560	-0.31232176	710	720	-0.12926466	2503712	-0.5614708	2485571	-0.46362129				empty
1923 P20	E	675	680	-0.087861	874	880	0.39353199	2802273	-0.07749266	2657654	-0.22196538				empty
1923 P21	E	674	680	-0.08967117	672	680	-0.25040047	2462262	-0.62866274	2486108	-0.46286718				empty
1923 P22	E	711	720	-0.02269497	950	960	0.63508769	2604458	-0.33981577	2477502	-0.47495258				empty
1923 P23	E	745	1520	0.05885072	1124	1840	1.19047809	78495	-4.49283497	79905	-1.84189261				empty
1923 P24	P	265296	265840	478.920442	244120	244840	775.809339	2222722	-1.01696572	2172201	-0.90368633				empty
1989 A01	N	477	480	-0.27800167	718	720	0.48933909	1377379	-1.60269181	1223427	-1.42684034				empty
1989 A02	E	117	120	-0.74557931	76	80	-1.80528901	77730	-3.98393991	76348	-3.32822057				empty
1989 A03	X	516	520	-0.22734742	517	520	-0.22907251	1587224	-1.21820086	1439840	-1.06811753		BIOMOL	SL115	C16-ceramide
1989 A04	X	752	760	0.0791757	872	880	1.0397639	1465437	-1.44134983	1448856	-1.05317274		BIOMOL	L120	C-PAF
1989 A05	X	475	480	-0.28059932	353	360	-0.81523919	1547583	-1.29083995	1433353	-1.07887028		BIOMOL	SL145	C8 CERAMINE
1989 A06	X	996	1000	0.39608944	595	600	-0.28059932	22898152	-0.28059932	1585861	-0.6824589				

1989 A19	X	714	720	0.02982028	635	640	0.19268157	1865844	-0.70771451	1719951	-0.60380991	experimental	BIOMOL	H112	12(R)-HETE	
1989 A20	X	554	560	-0.177992	475	480	-0.37918837	1775372	-0.87347948	1687273	-0.65797645	experimental	BIOMOL	FA-002	docosahexenoic	
1989 A21	X	955	960	0.34283754	593	600	0.04256571	2003863	-0.45483278	1558348	-0.87168052	experimental	BIOMOL	H012	12(S)-HETE	
1989 A22	X	589	600	-0.13253307	1150	1160	2.03338791	1703226	-1.0056711	1605510	-0.79350552	experimental	BIOMOL	FA-012	docosapentaenoic acid	
1989 A23	E	1082	2040	0.50778854	1281	2080	6.50160642	80329	0.97777786	488977	-3.32568613	empty				
1989 A24	P	328524	329080	425.798232	272308	272920	971.202808	1719142	-0.97650543	1559083	-0.87046219	empty				
1989 B01	N	932	960	0.31296453	476	480	-0.37561418	1796448	-0.83486353	1813309	-0.44906114	empty				
1989 B02	E	115	120	-0.74817697	118	120	-1.65517315	80397	-3.97905337	82266	-3.31841099	empty				
1989 B03	X	456	480	-0.30527703	190	200	-1.39783168	1191332	-1.94357159	1078808	-1.66655853	experimental	BIOMOL	AC-104	BEPRIDIL HYDROCHLORIDE	
1989 B04	X	1804	1840	1.44554149	2032	2040	5.18582091	1548983	-1.28827484	1688663	-0.65534089	experimental	BIOMOL	GR-313	Lycorine	
1989 B05	X	293	320	-0.5169858	866	880	1.01831878	1579338	-1.23265768	1563526	-0.86039054	experimental	BIOMOL	CA-415	CYCLOFLAZONIC ACID	
1989 B06	X	3542	3560	3.70290246	1833	1840	4.47455769	4787140	6.64475416	488940	6.63544801	W	experimental	BIOMOL	GR-316	10-hydroxycycamptothecin
1989 B07	X	385	400	-0.39749373	429	440	-0.54360097	1727929	-0.96040568	1650239	-0.71936343	experimental	BIOMOL	AC-100	dantrolene	
1989 B08	X	74	80	-0.80142887	155	160	-1.52292823	1007575	-2.28025558	947971	-1.8834319	experimental	BIOMOL	GR-308	beta-lapachone	
1989 B09	X	516	520	-0.22734742	316	320	-0.94748411	2035144	-0.39751898	1760154	-0.53717004	experimental	BIOMOL	KC-115	DIAZOXIDE	
1989 B10	X	75	80	-0.80013004	156	160	-1.51935404	1251955	-1.83249667	1213758	-1.44286752	experimental	BIOMOL	T-113	Parthenolide	
1989 B11	X	115	120	-0.74817697	115	120	-1.66589571	1013418	-2.26954989	1013123	-1.77543696	experimental	BIOMOL	CA-204	dichlorobenzamil	
1989 B12	X	675	680	-0.02083396	514	520	-0.23979507	1107346	-2.09745275	1062547	-1.69351251	experimental	BIOMOL	PI-102	MG-132	
1989 B13	X	432	440	-0.33648887	432	440	-0.53287841	1848788	-0.73896492	1760981	-0.53575992	experimental	BIOMOL	CA-205	dilitazem	
1989 B14	X	593	600	-0.12733776	554	560	-0.09682759	1554086	-1.278925	1497803	-0.97203896	experimental	BIOMOL	EI-301	Helanalin	
1989 B15	X	513	520	-0.2312439	793	800	0.75740312	2025271	-0.41560853	1849115	-0.38970968	experimental	BIOMOL	KC-158	E-4031	
1989 B16	X	435	440	-0.33255239	554	560	-0.09682759	1893646	-0.65677502	1845766	-0.39526093	experimental	BIOMOL	GR-211	Bezafibrate	
1989 B17	X	475	480	-0.28059932	553	560	-0.10040177	2146285	-0.19388378	1724086	-0.59695579	experimental	BIOMOL	CM-102	FIPRONIL	
1989 B18	X	392	400	-0.38840194	753	760	0.61443564	1938067	-0.57538579	2049487	-0.05757618	experimental	BIOMOL	IM-100	cycloheximide-N-ethylethanoate	
1989 B19	X	514	520	-0.22994508	313	320	-0.95820667	2009117	-0.44520628	1882980	-0.33557558	experimental	BIOMOL	AC-130	FLUCELAZINE	
1989 B20	X	440	450	-0.33514505	514	520	-0.23979507	1107346	-2.09745275	1062547	-1.69351251	experimental	BIOMOL	A-165	ascomycin (FK-520)	
1989 B21	X	712	720	0.02722263	833	840	0.90037061	2036132	-0.39570876	20217482	-0.39570876	experimental	BIOMOL	AC-123	FLUFENAMIC ACID	
1989 B22	X	671	680	-0.02602927	707	720	0.45002304	2005762	-0.45135339	1600382	-0.80200561	experimental	BIOMOL	FR-100	U-74389G	
1989 B23	E	759	1320	0.08826749	1222	1840	2.29072938	85989	-3.96880757	84027	-3.31549198	empty				
1989 B24	P	188473	190000	243.896241	207998	209280	741.346837	1849975	-0.73679007	1769419	-0.52181252	empty				
1989 C01	N	9236	9240	11.0984222	437	440	-0.51000748	1837319	-0.7599787	1741339	-0.56835749	empty				
1989 C02	E	36	80	-0.85078428	76	80	-1.80528901	86538	-3.96780168	84200	-3.31520522	empty				
1989 C03	X	5725	5760	6.53824136	636	640	0.19625575	2513985	0.47982499	2035510	-0.08074424	experimental	BIOMOL	HP012	12(S)-HPETE	
1989 C04	X	1100	1104	-0.00138803	749	760	0.13394482	2260136	-0.19541551	2043562	-0.06437896	experimental	BIOMOL	FA-010	12-CYCLOSTRIENEOIC ACID (22:3 n-3)	
1989 C05	X	3392	3440	3.50807844	513	520	-0.24336926	2040032	-0.38856307	2035760	-0.08032984	experimental	BIOMOL	G234	12-METHOXYDODECANOIC ACID	
1989 C06	X	4856	4880	5.40956087	508	520	-0.26124019	2204116	-0.08792443	1781819	-0.50125844	experimental	BIOMOL	FA024	EICOSA-5,8-DIENOIC ACID (20:2 n-12)	
1989 C07	X	581	600	-0.14292368	1113	1120	1.90114299	2314083	-0.11355975	1970145	-0.18909228	experimental	BIOMOL	H0013	13(S)-HODE	
1989 C08	X	835	840	0.18697833	353	360	-0.81523919	2145030	-0.19618322	1961913	-0.20273747	experimental	BIOMOL	FA007	eicosadienoic	
1989 C09	X	633	640	-0.07538469	555	560	-0.09325234	2358112	0.19423074	1800594	-0.47013733	experimental	BIOMOL	HP013	13(S)-HPODE	
1989 C10	X	635	640	-0.02787073	395	400	-0.66512333	1785375	-0.85515174	1864151	-0.36478624	experimental	BIOMOL	FA001	eicosapentaenoic	
1989 C11	X	406	420	-0.32394508	714	720	0.47504235	2101664	-0.27563944	2043562	-0.06726479	experimental	BIOMOL	PG046	13,14-DIHYDRO-PGE1	
1989 C12	X	313	320	-0.49100926	512	520	-0.24694344	8833751	-0.76551607	1998004	-0.14291316	experimental	BIOMOL	FA008	EICOSATRIENEOIC ACID (20:3 n-3)	
1989 C13	X	955	960	0.34283754	1194	1200	2.19065214	1886011	-0.67076405	1783868	-0.49786209	experimental	BIOMOL	GR102	13-cis-retinoic	
1989 C14	X	432	440	-0.33648887	552	560	-0.10397596	2110416	-0.25960382	1835001	-0.41310482	experimental	BIOMOL	L110	ENANTIO-PAF C16	
1989 C15	X	675	680	-0.02083396	553	560	-0.10040177	2451192	0.36477415	1998244	-0.14251578	experimental	BIOMOL	K0013	13-KETOCTADECADIENEOIC ACID	
1989 C16	X	313	320	-0.49100926	714	720	-0.95463249	2216918	-0.0644683	1896781	-0.31069926	experimental	BIOMOL	G222	farnesylthioacetic acid	
1989 C17	X	554	560	-0.177992	554	560	-0.09682759	2359397	0.19658515	2061449	-0.03774815	experimental	BIOMOL	EI14	14,15-EPOXYEICOSATRIENEOIC ACID	
1989 C18	X	440	450	-0.07405896	435	440	-0.07405896	2145444	-0.19541551	2181668	0.65157171	experimental	BIOMOL	RA105	FLUPROSTENOL	
1989 C19	X	553	560	-0.19290893	435	440	-0.52155858	2297624	-0.73153777	2010184	-0.20879258	experimental	BIOMOL	H015	gamma-HETE	
1989 C20	X	713	720	0.02852146	474	480	-0.38276255	2187016	-0.11925546	1974014	-0.18267904	experimental	BIOMOL	FA006	gamma-linolenic	
1989 C21	X	792	800	-0.13112877	552	560	-0.10397596	2352366	0.18370278	2233525	0.24748234	experimental	BIOMOL	HP015	15(S)-HPETE	
1989 C22	X	550	560	-0.18318731	751	760	0.60728727	2352903	0.18468668	2032912	-0.08505064	experimental	BIOMOL	LE009	9,10-EODE-leukotoxin A	
1989 C23	E	541	1120	-0.19487675	821	1320	0.85748036	86129	-3.96855106	81918	-3.31898783	empty				
1989 C24	P	195927	197040	253.577696	166786	168040	594.074739	2205853	-0.08474186	2050118	-0.05653024	empty				
1989 D01	N	292	320	-0.51828462	396	400	-0.66154915	2772884	0.95418596	2243081	0.26332221	empty				
1989 D02	E	117	120	-0.74557931	117	120	-1.65874734	80286	-3.97925674	84590	-3.31455876	empty				
1989 D03	X	336	360	-0.46113624	395	400	-0.66512333	1482659	-1.40979527	1437028	-1.07277865	experimental	BIOMOL	CA-225	Flunarizine dihydrochloride	
1989 D04	X	1645	1680	1.23902803	474	480	-0.38276255	2197279	-0.10045134	1507243	-0.95639137	experimental	BIOMOL	EI-207	EBELEN	
1989 D05	X	343	360	-0.45204446	274	280	-1.09759997	1458722	-1.45365321	1256927	-1.37131126	experimental	BIOMOL	AC-116	FLUSPIRILINE	
1989 D06	X	502	520	-0.245531	593	600	0.04256571	2930021	1.24209614	2144500	0.09991589	experimental	BIOMOL	CM-266	TRIM	
1989 D07	X	555	560	-0.17669318	1032	1040	1.61163384	2496048	0.44696039	2051669	-0.05395933	experimental	BIOMOL	CA-245	FPL-64176	
1989 D08	X	273	280	-0.54296233	552	560	-0.10397596	2656841	0.74156919	2228881	0.23978451	experimental	BIOMOL	PD-195	zardaverine	
1989 D09	X	514	520	-0.22994508	714	720	0.47504235	2101664	-0.27563944	2043562	-0.06726479	experimental	BIOMOL	CA-422	gingerol	
1989 D10	X	554	560	-0.177992	474	480	-0.38276255	2636394	0.7041057	2579463	0.82090376	experimental	BIOMOL	PD-190	zaprinst	
1989 D11	X	394	400	-0.38580429	514	520	-0.23979507	2519883	0.49063145	1964722	-0.19808132	experimental	BIOMOL	AC-120	GLIPIZIDE	
1989 D12	X	435	440	-0.33255239	514	520	-0.23979507	2376399	0.22773662	2321894	0.39396141	experimental	BIOMOL	PD-185	vinpocetine	
1989 D13	X	352	360	-0.44035502	513	520	-0.24336926	2322626	0.12921244	2271864	0.31103246	experimental	BIOMOL	KC-120	GLYBURIDE	
1989 D14	X	355	360	-0.43645854	554	560	-0.811665	2108443	-0.2632188	1894853	-0.31389508	experimental	BIOMOL	PD-180	Trequin	
1989 D15	X	353	360	-0.43905619	395	400	0.04971408	2258305	0.01136196	2279121	0.32306155	experimental	BIOMOL	NA-135	GRAVINSANTOXIN III	
1989 D16	X	715	720	0.03111911	554	560	-0.09682759	2514061	1.21285385	2181668	0.65157171	experimental	BIOMOL	PD-179	siguzodan	
1989 D17	X	472	480	-0.284958	354	360	-0.811665	2297624	-0.73153777	207083017	-0.01364688	experimental	BIOMOL	CM-101	IAA-94	
1989 D18	X	593	600	-0.12733776	474	480	-0.38276255	2361682	0.20077178	2434115	0.57997719	experimental	BIOMOL	PD-175	Rolipram	
1989 D19	X	673	680	-0.02343161												

1989 E13	X	993	1000	0.39219296	394	400	-0.66869752	2749235	0.91085569	1992042	-0.15279611	experimental	BIOMOL	L-134	1-acyl-PAF
1989 E14	X	673	680	-0.02343161	475	480	-0.37918837	2484272	0.42538412	2155180	0.11761889	experimental	BIOMOL	FA023	linoleamide
1989 E15	X	513	520	-0.23124399	393	400	-0.67227171	2417570	0.30317111	2139493	0.09161636	experimental	BIOMOL	DG-140	1-HEXADECYL-2-ARACHIDONOYL-GLYCEROL
1989 E16	X	715	640	-0.07668351	715	720	0.47861653	2376192	0.23102188	2203448	0.19367717	experimental	BIOMOL	FA014	linoleic acid
1989 E17	X	754	750	0.08177336	355	360	-0.80809702	2567819	0.57846609	21010668	-0.12192195	experimental	BIOMOL	L-106	1-hexadecyl-2-methylglycero-3-PC
1989 E18	X	709	720	0.02332615	553	560	-0.10040177	2397801	0.26694988	2427853	0.56595739	experimental	BIOMOL	FA005	linolenic acid(18:3,n-3)
1989 E19	X	792	800	0.13112877	634	640	0.18910738	2507015	0.46705439	2466781	0.63412384	experimental	BIOMOL	EI-150	1-HEXADECYL-2-O-ACETYL-GLYCEROL
1989 E20	X	952	960	0.33894106	592	600	0.03899152	2594687	0.62768913	2500483	0.68998775	experimental	BIOMOL	LXA004	lipoxin A4
1989 E21	X	551	560	-0.18188848	591	600	0.03541733	2461677	0.38398502	2292873	0.34585665	experimental	BIOMOL	EI-149	1-HEXADECYL-2-O-METHYL-GLYCEROL
1989 E22	X	750	760	0.07657805	1031	1040	1.60805965	2527405	0.50441344	2239906	0.25805938	experimental	BIOMOL	LP101	L-NASPA
1989 E23	E	535	1080	-0.20266971	839	1360	0.92181573	89825	-3.96177916	82953	-3.17727223	empty			
1989 E24	P	184257	185320	238.420387	174714	175920	622.376446	2307238	0.10101818	2147665	0.10436665	empty			
1989 F01	N	477	480	-0.27800167	396	400	-0.66154915	2379888	0.23412925	1929534	-0.2564084	empty			
1989 F02	E	160	160	-0.69362624	77	80	-1.80171482	78085	-3.98328947	82905	-3.31735179	empty			
1989 F03	X	435	440	-0.33255239	475	480	-0.37918837	1819828	-0.79202613	1491727	-0.98211044	experimental	BIOMOL	AC-110	LOPERAMIDE
1989 F04	X	675	680	-0.02083396	594	600	0.0461399	2293543	0.07592587	1879903	-0.33867597	experimental	BIOMOL	EI-145	A-3
1989 F05	X	312	320	-0.49230809	514	520	-0.23979507	1972050	-0.51312133	2143372	0.09804613	experimental	BIOMOL	AC-103	METHOXY VERAPAMIL
1989 F06	X	874	880	0.23763257	633	640	0.18553319	2513266	0.47850762	2329258	0.40616786	experimental	BIOMOL	AG-200	acetyl-farnesyl-cysteine
1989 F07	X	632	640	-0.07668351	833	840	0.90037061	2446980	0.35705682	2549614	0.77142853	experimental	BIOMOL	KC-125	minoxidil
1989 F08	X	792	800	0.13112877	512	520	-0.24694344	2104167	-0.27105339	1814327	-0.44737372	experimental	BIOMOL	GR300	actinomycin D
1989 F09	X	753	760	0.08047453	755	760	0.62158402	2477207	0.41243946	2144602	0.10008496	experimental	BIOMOL	KC-130	minoxidil sulfate
1989 F10	X	674	680	-0.02213279	554	560	-0.111665	2189193	-0.11526671	1886501	-0.32773923	experimental	BIOMOL	VR101	Arvanil
1989 F11	X	554	560	-0.177992	315	320	-0.23622088	1456690	-1.45737629	1201339	-1.46345306	experimental	BIOMOL	AC-108	Nicardipine hydrochloride
1989 F12	X	313	320	-0.49100926	314	320	-0.95463249	1940161	-0.57154912	1740767	-0.56930563	experimental	BIOMOL	EI-277	AG1478
1989 F13	X	673	680	-0.02343161	515	520	-0.23622088	1818953	-0.11570644	1965139	-0.19739011	experimental	BIOMOL	CA-210	NIFEDIPINE
1989 F14	X	440	440	-0.33515005	434	440	-0.38276255	2502642	0.45904208	2249411	0.27638942	experimental	BIOMOL	AG-158	AG221 (Tyrphostin 47)
1989 F15	X	794	800	0.133022643	755	760	0.62158402	2382928	0.23969277	2240840	0.25960757	experimental	BIOMOL	AC-134	NIFLUMIC ACID
1989 F16	X	593	600	-0.12733776	394	400	-0.66869752	2697028	0.81520077	2290296	0.34158506	experimental	BIOMOL	EI-229	tyrphostin AG-370
1989 F17	X	229	240	-0.60011071	193	200	-1.38710912	1051491	-2.19979163	1044129	-1.7240419	experimental	BIOMOL	CA-216	NIQUILIPINE
1989 F18	X	1673	1680	1.27539518	955	960	1.33642143	2334000	0.15005215	2187025	0.17040466	experimental	BIOMOL	EI-272	AG-490
1989 F19	X	508	520	-0.23773804	432	440	-0.53287841	2433261	0.33192054	2322014	0.39416032	experimental	BIOMOL	CA-211	NIMODIPINE
1989 F20	X	712	720	0.02722263	832	840	0.89679642	1598326	-1.19786741	1764180	-0.53049661	experimental	BIOMOL	EI-258	AG-879
1989 F21	X	631	640	-0.07798234	712	720	0.46789397	2346636	0.17320414	2038010	-0.07660027	experimental	BIOMOL	CA-212	NITREDIPINE
1989 F22	E	840	0.18178302	548	840	0.93617972	2047111	1.37555523	72889232	1649663	0.72889232	empty			
1989 F23	E	491	1000	-0.25981809	990	1560	1.46151798	85509	-3.96968704	84428	-3.31482729	empty			
1989 F24	P	171448	172680	221.783714	192599	193560	686.30793	2139322	-0.20664155	2099005	0.02450408	empty			
1989 G01	N	517	520	-0.22604859	517	520	-0.22907251	2114283	-0.25251861	2159793	0.12526532	empty			
1989 G02	E	77	80	-0.79753238	77	80	-1.80171482	86579	-3.96772656	83711	-3.31601578	empty			
1989 G03	X	274	280	-0.54166351	475	480	-0.37918837	2588047	0.61552317	2471590	0.64209516	experimental	BIOMOL	L-108	1-octadecyl-2-methylglycero-3-PC
1989 G04	X	592	600	-0.12863659	432	440	-0.53287841	2624680	0.68264203	2194923	0.18349626	experimental	BIOMOL	RA101	LY-171883
1989 G05	X	673	680	-0.02343161	473	480	-0.34023989	2687738	0.79817941	2396381	0.9381723	experimental	BIOMOL	DG-125	1-octadecyl-2-acetylglcyrol
1989 G06	X	632	640	0.07668351	434	440	-0.52573004	2343319	0.16712665	2099201	0.02488289	experimental	BIOMOL	L101	LY-CL16-PAF
1989 G07	X	554	560	-0.177992	634	640	0.18910738	2773092	0.95456706	2380095	0.49043448	experimental	BIOMOL	DG-135	1-STEAROYL-2-LINOLEOYL-GLYCEROL
1989 G08	X	633	640	-0.07538469	594	600	0.0461399	2981631	1.33665722	1990805	-0.15484655	experimental	BIOMOL	LP100	lysophosphatidic acid
1989 G09	X	353	360	-0.43905619	593	600	0.04256571	2434899	0.33492172	2718519	1.05140082	experimental	BIOMOL	DG-130	1-STEAROYL-2-ARACHIDONOYL-GLYCEROL
1989 G10	X	394	400	-0.38580429	593	600	-0.24336922	2298298	0.08463809	2270773	0.30922404	experimental	BIOMOL	SL221	D-erythro-MAPP
1989 G11	X	354	360	-0.43775736	554	560	-0.09682759	2435283	0.33562533	2341884	0.42770952	experimental	BIOMOL	DM300	24,25-dihydroxyvitamin D3
1989 G12	X	555	560	-0.177992	434	440	-0.52573004	2426003	0.31862226	2265092	0.27638945	experimental	BIOMOL	SL222	MAPP, L-erythro
1989 G13	X	795	800	0.13502525	355	360	-0.80809702	2691050	0.2802560	2282650	0.32891117	experimental	BIOMOL	DM100	25-hydroxyvitamin
1989 G14	X	393	400	-0.38710312	394	400	-0.66869752	2541479	0.53020016	2216318	0.21896020	experimental	BIOMOL	FA004	MEAD ACID (20:3 n-9)
1989 G15	X	428	440	-0.34164418	429	440	-0.54360097	3011416	1.39123001	2711168	1.03921591	experimental	BIOMOL	FA028	2-arachidonylglycerol
1989 G16	X	674	680	-0.02213279	475	480	-0.37918837	2575791	0.59306743	2329760	0.40699997	experimental	BIOMOL	FA027	MEAD
1989 G17	X	634	640	-0.07408586	555	560	-0.09325234	3256248	1.83981708	2897332	1.34779845	experimental	BIOMOL	G231	2-FLUOROPALMITIC ACID
1989 G18	X	868	880	0.22983961	513	520	-0.24336922	2404381	0.27900591	2372857	0.47843688	experimental	BIOMOL	GR106	METHOPRENE ACID
1989 G19	X	833	840	0.18438067	433	440	-0.52930422	3492113	2.2719746	2669122	0.96952112	experimental	BIOMOL	G230	2-hydroxymyristic acid
1989 G20	X	548	560	-0.18578496	871	880	1.03618972	2808112	1.01873154	2482963	0.66094687	experimental	BIOMOL	PG-052	misoprostol
1989 G21	X	952	960	0.33894106	791	800	0.75025475	2676877	0.77827963	2046343	-0.06278762	experimental	BIOMOL	GR103	4-HYDROXYPHENYLETANAMIDE
1989 G22	X	828	840	0.17788654	710	720	0.4607456	2408071	0.28576682	1969991	-0.18934751	experimental	BIOMOL	SL-105	N,N-dimethylsphingosine
1989 G23	E	498	1200	-0.2507263	782	1240	0.71808707	88128	-3.96488844	83029	-3.31714625	empty			
1989 G24	P	238042	239160	308.277786	153426	154480	546.296299	2981442	1.33631093	2180981	0.16038622	empty			
1989 H01	N	597	600	-0.12214245	436	440	-0.51858166	2615571	0.66595333	1954342	-0.21528704	empty			
1989 H02	E	75	80	-0.80013004	116	120	-1.66232153	74569	-3.98973157	84709	-3.31436151	empty			
1989 H03	X	995	1000	0.39479061	673	680	0.32850067	2506005	0.46520385	2642756	0.92581725	experimental	BIOMOL	AC-132	N-PHENYLANTHRANILIC
1989 H04	X	951	960	0.33764223	1312	1320	2.61240622	3018083	1.40344545	3095951	1.67702621	experimental	BIOMOL	E1303	AG-1296
1989 H05	X	752	760	0.0791757	912	920	1.18273139	2130636	-0.22255625	1974760	-0.18144249	experimental	BIOMOL	CM-100	2-PHENYLPROPYLAMINO-5-NITROBENZIC ACID
1989 H06	X	473	480	-0.28319697	473	480	-0.38633674	3085459	1.52689338	2629455	0.90376972	experimental	BIOMOL	PD-152	Milrinone
1989 H07	X	273	280	-0.54296233	353	360	-0.81523919	1928260	-0.59335441	2348027	0.43727906	experimental	BIOMOL	KC-127	NS-1619
1989 H08	X	554	560	-0.177992	394	400	-0.66869752	3479052	2.24804392	3046709	1.59540344	experimental	BIOMOL	GR333	PRIMA-1
1989 H09	X	514	520	-0.22994508	474	480	-0.38276255	1960177	-0.53487532	1935681	-0.24621923	experimental	BIOMOL	KC-155	PAXILLINE
1989 H10	X	554	560	-0.177992	753	760	0.61443564	2745254	0.9108809	160932	0.87124294	experimental	BIOMOL	E1312	tanugamycin
1989 H11	X	394	400	-0.38580429	752	760	0.61086145	2428330	0.32288585	2141066	0.09422374	experimental	BIOMOL	KC-131	PCO-400
1989 H12	X	395	400	-0.38450546	714	720	0.47504235	2728353	0.87259519	2139090	0.09094835	experimental	BIOMOL	AP-101	4-Amino-1,8-naphthalimide
1989 H13	X	233</													

1989 107	X	674	680	-0.02213279	875	880	1.05048646	2988377	1.3490174	2406824	0.53474005	experimental	BIOMOL	HP005	5(S)-HPETE
1989 108	X	513	520	-0.2312439	474	480	-0.38276255	2611212	0.65796664	2198773	0.18987796	experimental	BIOMOL	FA-030	N-LINOLEOYLGLYCINE
1989 109	X	674	680	-0.02213279	395	360	-0.80089082	2753131	0.91799404	2466866	0.63426473	experimental	BIOMOL	EE56	5,6-EPOXYEICOSATRIENOIC ACID
1989 110	X	673	680	-0.0234161	513	520	-0.24338926	2242442	-0.01770261	2342775	0.42807615	experimental	BIOMOL	L100	PAF C16
1989 111	X	594	600	-0.12603893	754	800	-0.16203893	2266226	0.08815756	2349859	0.44031576	experimental	BIOMOL	ET004	5,8,11,14-eicosatetraenoic acid
1989 112	X	514	520	-0.22994508	552	560	-0.10397596	2252921	0.00149726	2261390	0.29367093	experimental	BIOMOL	L105	PAF C18
1989 113	X	635	640	-0.07278703	554	560	-0.09682759	2332565	0.14742291	2200559	0.19283841	experimental	BIOMOL	ET003	5,8,11-eicosatriynoic
1989 114	X	433	440	-0.33515005	514	520	-0.23979507	2182620	-0.12730992	2374724	0.48153159	experimental	BIOMOL	L107	PAF C18:1
1989 115	X	548	560	-0.18578496	469	480	-0.40063349	2367149	0.21078855	2541149	0.75739507	experimental	BIOMOL	K005	5-KETOEICOSATETRAENOIC ACID
1989 116	X	634	640	-0.07408586	435	440	-0.52215585	2215568	-0.0669418	2473010	0.64444893	experimental	BIOMOL	FA018	PALMITYLETHANOLAMIDE
1989 117	X	754	760	0.08177336	434	440	-0.52573004	2712158	0.84292232	2299759	0.35727078	experimental	BIOMOL	GR206	6-formylindolo-(3,2-beta)-carbazole
1989 118	X	551	560	-0.18188848	833	840	0.90037061	2206874	0.10035125	2348577	0.41017756	experimental	BIOMOL	LF103	PHOSPHATIDIC ACID, DIPALMITOYL
1989 119	X	831	840	0.18178302	832	840	0.89679642	2918989	1.22188305	2563104	0.79378734	experimental	BIOMOL	PG017	6-keto-prostaglandin F1a
1989 120	X	949	960	0.33504458	710	720	0.4607456	2628816	0.69022111	2452906	0.61112486	experimental	BIOMOL	PG001	prostaglandin A1
1989 121	X	792	800	0.13112877	793	800	0.75740312	2850538	1.09646548	2190279	0.17579844	experimental	BIOMOL	EI-112	7,7-dimethyleicosadienoic acid
1989 122	X	749	760	0.07527922	469	480	-0.40063349	2925461	1.2337412	2322588	0.39511177	experimental	BIOMOL	PG002	PROSTAGLANDIN A2
1989 123	E	653	1280	-0.04940815	976	1520	1.41147936	86207	-3.96840815	82849	-3.31744462	empty			
1989 124	P	211568	212880	273.892645	183708	184640	654.529832	2432852	0.33117116	2320425	0.39152642	empty			
1989 101	N	1037	1040	0.44934134	475	480	-0.37918837	1986867	-0.48597326	2204446	-0.09083375	empty			
1989 102	E	115	120	-0.74817697	115	120	-1.66589571	78767	-3.98203989	83392	-3.31654455	empty			
1989 103	X	595	600	-0.1247401	836	840	0.91109317	2468869	0.39716237	1880028	-0.33846877	experimental	BIOMOL	AC-118	pinacidil
1989 104	X	313	320	-0.49100926	593	600	0.04256571	2333814	0.14971136	2132453	0.07994697	experimental	BIOMOL	PD-150	8-methoxymethyl-IBMX
1989 105	X	513	520	-0.2312439	393	400	-0.67227171	2460885	0.3825339	2149233	0.10776123	experimental	BIOMOL	AC-127	PROCAINAMIDE
1989 106	X	1394	1400	0.91302251	1394	1320	2.61955599	2044250	-3.8083475	1722285	-0.5999411	experimental	BIOMOL	PD-149	MBCQ
1989 107	X	551	560	-0.18188848	231	240	-1.25129001	1511883	-1.35625035	1239857	-1.39960622	experimental	BIOMOL	AC-124	PROCAFENONE HYDROCHLORIDE
1989 108	X	514	560	-0.22994508	435	440	-0.52215585	2286533	0.06330508	1947777	-0.23204942	experimental	BIOMOL	G-581	quindine
1989 109	X	473	480	-0.28319697	395	400	-0.66572335	2433391	0.3881587	2374332	0.48088182	experimental	BIOMOL	AC-129	quindine
1989 110	X	513	520	-0.2312439	475	480	-0.37918837	2517778	0.48677462	2264165	0.29827072	experimental	BIOMOL	GR-244	BADGE
1989 111	X	555	560	-0.17669318	352	360	-0.81881338	1989860	-0.48048942	1806869	-0.45671918	experimental	BIOMOL	AC-122	QUININE
1989 112	X	314	320	-0.48971043	635	640	0.19268157	2324703	0.13301797	2111377	0.04501172	experimental	BIOMOL	CM110	bafilomycin A1
1989 113	X	554	560	-0.177992	514	520	-0.23979507	2337016	0.15557814	2297051	0.35278204	experimental	BIOMOL	NA-134	QX-314
1989 114	X	514	520	-0.22994508	475	480	-0.37918837	2503661	0.46090911	2434898	0.58127508	experimental	BIOMOL	CA-411	BAPTA-AM
1989 115	X	634	640	-0.07408586	433	440	-0.52930422	2351740	0.18255581	2258908	0.2895568	experimental	BIOMOL	CA-450	RYANODINE
1989 116	X	473	480	-0.28319697	395	400	-0.66572335	2343262	0.14142434	2186702	0.14142434	experimental	BIOMOL	EI-115	betanotins
1989 117	X	471	480	-0.28579463	351	360	-0.82238756	1658435	-1.08773426	1302216	-1.29624092	experimental	BIOMOL	NA-116	SDZ-201106
1989 118	X	513	520	-0.2312439	593	600	0.04256571	2576482	0.5943335	2680566	0.98849052	experimental	BIOMOL	CM-113	bongkrekic acid
1989 119	X	993	1000	0.39219296	712	720	0.46789397	1845789	-0.74445976	1619488	-0.77033581	experimental	BIOMOL	CA-230	SKF-96365
1989 120	X	471	480	-0.28579463	713	720	0.47146816	2565341	0.57392069	2213163	0.2137306	experimental	BIOMOL	AC-582	IB-MECA
1989 121	X	513	520	-0.2312439	471	480	-0.39348511	1287385	-1.76758098	1160614	-1.53095818	experimental	BIOMOL	CA-260	Tetrandrine
1989 122	X	509	520	-0.23643921	631	640	0.17838482	1791325	-0.84425001	1718775	-0.60575923	experimental	BIOMOL	G405	brefeldin A
1989 123	E	1400	1400	0.26880444	952	840	-0.14356989	84208	-0.9720707	81201	-0.32049624	empty			
1989 124	P	238382	239600	708.719387	149948	151200	533.865277	2451264	0.36490607	2108392	0.04006383	empty			
1989 K01	N	395	400	-0.38450546	717	720	0.48576491	2008972	-0.44547195	2048120	-0.0598421	empty			
1989 K02	E	156	160	-0.69492507	116	120	-1.66232153	84214	-3.97205977	84439	-3.31480906	empty			
1989 K03	X	795	800	0.13502525	355	360	-0.80089082	2746262	0.90540049	2123642	0.06534199	experimental	BIOMOL	EE89	8,9-EPOXYEICOSATRIENOIC ACID
1989 K04	X	834	840	0.1856795	635	640	0.19268157	2019327	-0.42649827	2416186	0.55025836	experimental	BIOMOL	PG003	prostaglandin B1
1989 K05	X	393	400	-0.38710312	274	280	-1.09759997	2671566	0.76054868	2193983	0.18193813	experimental	BIOMOL	PG049	8-EPI-PROSTAGLANDIN F2a
1989 K06	X	391	400	-0.38974077	514	520	-0.24338926	2531548	0.51200434	2365777	0.81141243	experimental	BIOMOL	PG057	PROSTAGLANDIN B2
1989 K07	X	514	520	-0.22994508	474	480	-0.38276255	2758857	0.688914656	2758857	1.15012258	experimental	BIOMOL	H0409	9(S)-HODE
1989 K08	X	473	480	-0.28319697	474	480	-0.38276255	2734116	0.8831543	2258800	0.28937778	experimental	BIOMOL	PG005	PROSTAGLANDIN D2
1989 K09	X	674	680	-0.02213279	435	440	-0.52215585	2743849	0.90098733	2608525	0.86907648	experimental	BIOMOL	HP019	9(S)-HPODE
1989 K10	X	594	600	-0.12603893	394	400	-0.66869752	2482220	0.4216244	2546057	0.7655305	experimental	BIOMOL	PG006	prostaglandin E1
1989 K11	X	394	400	-0.38580429	680	680	0.33564905	2580445	0.6015946	2373403	0.47934192	experimental	BIOMOL	FA025	9,10-octadecenoamide
1989 K12	X	475	480	-0.28059932	394	400	-0.66869752	2520712	0.49215036	2221204	0.22705924	experimental	BIOMOL	PG007	prostaglandin E2
1989 K13	X	554	560	-0.177992	435	440	-0.52215585	2811197	1.02438395	2320283	0.39129104	experimental	BIOMOL	PG031	9A,11B-prostaglandin F2
1989 K14	X	473	480	-0.28319697	353	360	-0.81523919	2475567	0.40961783	2433956	0.57971363	experimental	BIOMOL	PG010	prostaglandin F1a
1989 K15	X	714	720	0.02982028	675	680	0.33564905	2959352	1.2958371	2484742	0.66389571	experimental	BIOMOL	PG030	9,11A-prostaglandin
1989 K16	X	511	520	-0.23384156	431	440	-0.5364526	2672957	0.77109731	2497886	0.685683	experimental	BIOMOL	PG008	Dinoprost trometamol
1989 K17	X	1474	1480	0.101692865	1595	1600	3.62390116	2509004	0.47069868	2807838	1.1994546	experimental	BIOMOL	GR101	9-cis-retinoic
1989 K18	X	550	560	-0.11112434	550	560	-0.11112434	2687513	0.79776716	2577236	0.81721232	experimental	BIOMOL	PG011	PROSTAGLANDIN I2
1989 K19	X	553	560	-0.17929083	553	560	-0.10040177	2710492	0.83986984	2498393	0.6865234	experimental	BIOMOL	G200	acetyl-farnesyl-cysteine
1989 K20	X	513	520	-0.2312439	592	600	0.03899152	2727700	0.87139875	2697881	1.01719159	experimental	BIOMOL	PG033	prostaglandin
1989 K21	X	752	760	0.0791757	953	960	1.32927306	2767601	0.94450632	2365771	0.47332158	experimental	BIOMOL	FA011	adrenic
1989 K22	X	991	1000	0.38959531	910	920	1.17558301	2541304	0.52987952	2312614	0.37857903	experimental	BIOMOL	GR100	trans-retinoic acid
1989 K23	E	632	1240	-0.07668351	755	1480	0.62158402	85257	-3.97014876	82171	-3.31856846	empty			
1989 K24	P	204974	206280	265.328182	245460	246480	875.243033	2331947	0.1462906	2371574	0.4763102	empty			
1989 L01	N	637	640	-0.07018938	596	600	0.05328827	2173572	-0.14388788	2226015	0.23503388	empty			
1989 L02	E	117	120	-0.74557931	117	120	-1.65874734	75093	-3.98877148	81435	-3.31978844	empty			
1989 L03	X	114	120	-0.74947579	156	160	-1.51935404	928833	-2.44245286	950733	-1.87885365	experimental	BIOMOL	PE-180	THAPSIGARGIN
1989 L04	X	594	600	-0.12603893	514	520	-0.24338926	2436459	0.33777999	2262637	0.62332633	experimental	BIOMOL	CN-252	3-bromo-7-nitroindazole
1989 L05	X	553	560	-0.17929083	394	400	-0.66869752	2298008	0.08910675	2174774	0.18142434	experimental	BIOMOL	EI-110	TMB-8
1989 L06	X	634	640	-0.07408586	393	400	-0.67227171	2683106	0.78969255	2653127	0.94305779	experimental	BIOMOL	CN-115	Bromo-cAMP [8-Bromo-cAMP]
1989 L07	X	673	680	-0.02											

1989 M01	N	596	600	-0.12344128	636	640	0.19625575	1964595	-0.52678056	1915686	-0.27936263	empty							
1989 M02	E	116	120	-0.74687814	156	160	-1.51935404	83649	-3.97309498	80790	-3.32085758	empty							
1989 M03	X	518	520	-0.22474977	517	520	-0.22907251	2136862	-0.21114882	1995849	-0.14648569	BIOMOL	G221	AGC					
1989 M04	X	493	400	-0.38710312	714	720	0.47504235	1845231	-0.74548214	1991101	-0.15435559	experimental	E1209	REVA 5901					
1989 M05	X	794	800	-0.16237306	553	960	1.32927306	2237784	-0.02623711	2207203	0.93318853	experimental	G220	AGGC					
1989 M06	X	510	520	-0.23514038	747	760	0.59299052	2291874	0.07286789	1984615	-0.16510699	experimental	G-201	S-FARNESYL-L-CYSTEINE					
1989 M07	X	473	480	-0.28319697	593	600	0.04256571	2782303	0.97144367	2870913	1.30400673	experimental	CR108	AM-251					
1989 M08	X	754	760	0.08177336	633	440	-0.52930422	2371076	0.2198369	2816988	0.16157471	experimental	E1-155	SPHINGOSINE					
1989 M09	X	513	520	-0.2312439	435	640	0.19268157	2161456	-0.1660871	2330981	0.40902388	experimental	GR104	AM-580					
1989 M10	X	673	680	-0.02343161	474	400	-0.38276255	2169054	-0.15216587	2030418	-0.08918466	experimental	RA-103	SQ-29548					
1989 M11	X	794	800	-0.13726473	755	760	0.62158402	2023349	-0.41913007	2515614	0.71506866	experimental	FA026	anandamide(18:2,n-6)					
1989 M12	X	593	600	-0.12733776	394	400	-0.66869752	2162522	-0.16413395	2121768	0.05223568	experimental	L-126	TETRAHYDROCANNABINOL-7-OIC ACID					
1989 M13	X	514	520	-0.22994508	395	400	-0.66512333	2299401	0.08665904	2405034	0.53177298	experimental	FA019	anandamide(20:3,n-6)					
1989 M14	X	594	600	-0.12603893	514	520	-0.23979507	2363868	0.20477702	2216105	0.21860722	experimental	GR105	TNFB					
1989 M15	X	632	640	-0.07668351	474	480	-0.38276255	2694475	0.8105231	2246448	0.2689033	experimental	FA017	ANANDAMIDE (20:4, n-6)					
1989 M16	X	1033	1040	0.44414603	754	760	0.61800983	2479125	0.41595366	2069666	-0.02412778	experimental	PG023	U-46619					
1989 M17	X	752	760	0.0791757	673	680	0.32850067	2675008	0.7748552	2411228	0.54204005	experimental	FA020	anandamide(22:4,n-6)					
1989 M18	X	512	520	-0.23254273	513	520	-0.24336926	2572029	0.5861746	2393436	0.51254831	experimental	RA102	U-75302					
1989 M19	X	593	600	-0.12733776	394	400	-0.66869752	2162522	-0.16413395	2121768	0.05223568	experimental	FA022	ARACHIDONAMIDE					
1989 M20	X	671	680	-0.02602927	553	560	-0.10040177	2553015	0.5513367	2165026	0.13393946	experimental	CR-105	WIN 55,212-2					
1989 M21	X	752	760	0.0791757	713	720	0.47146816	2532438	0.51363502	2220220	0.22542818	experimental	FA003	ARACHIDONIC ACID					
1989 M22	X	670	680	-0.0273281	670	680	0.31777811	2477600	0.41315952	2441815	0.59274059	experimental	GR-200	WY-14643					
1989 M23	E	627	1160	-0.08317765	899	1480	1.13626695	84577	-3.97139467	80349	-3.32158858	empty							
1989 M24	P	179644	180840	232.428899	195962	197080	698.327921	2219123	-0.06042824	2328050	0.40411655	empty							
1989 N01	N	636	640	-0.07148821	475	480	-0.37918837	2108058	-0.26392924	1841150	-0.40291234	empty							
1989 N02	E	77	80	-0.79753738	117	117	-1.65874732	75288	7.9884142	79352	-3.32274291	empty							
1989 N03	X	155	160	-0.69623889	157	160	-0.5177986	1029324	-2.24040564	1019466	-0.76491793	experimental	PI-122	Tosyl-Phe-CMK (TPCK)					
1989 N04	X	396	400	-0.38320664	194	200	-1.38353494	1112491	-2.08802596	1093593	-1.64205115	experimental	BIOMOL	E1192	calyculin A				
1989 N05	X	550	560	-0.18318731	388	400	-0.69014264	2363493	0.20408994	2276846	0.31929055	experimental	PI-113	Thiorphan					
1989 N06	X	1634	1640	1.22474094	2953	2560	7.04797238	6072602	7.0000085	8864444	11.2387901	experimental	GR301	camptothecin					
1989 N07	X	391	400	-0.38970077	468	480	-0.40420768	1955550	-0.54353302	2098491	0.02365209	experimental	PI-112	Z-prolyl-prolinol canthanidin					
1989 N08	X	353	360	-0.66512333	395	400	-0.66512333	1445715	-1.47748495	1309228	-1.28461794	experimental	PR-105	NapSul-ile-Trp-CHO					
1989 N09	X	474	480	-0.28189815	394	400	-0.66869752	2062907	-0.34665095	1685030	-0.66169441	experimental	PI-125	7-epi-8-epi-arachidonic acid					
1989 N10	X	474	480	-0.28189815	394	400	-0.66512333	1445715	-1.47748495	1309228	-1.28461794	experimental	PI-110	3,4-dichloroisocoumarin					
1989 N11	X	433	440	-0.33515005	394	400	-0.66869752	1752379	-0.91560781	1418803	-1.10298813	experimental	NK101	capsazepine					
1989 N12	X	434	440	-0.33385122	555	560	-0.0932534	2101606	-0.2754571	1838632	-0.40780813	experimental	PI-128	Boc-GVV-CHO					
1989 N13	X	475	480	-0.28059932	555	560	-0.0932534	2131331	-0.22128285	2031253	-0.08780057	experimental	S-107	castanospermine					
1989 N14	X	273	280	-0.54296233	513	520	-0.24336926	2459379	0.37977457	2141910	0.09562274	experimental	E1-212	Bestatin					
1989 N15	X	474	480	-0.28189815	313	520	-0.23979507	1729394	-0.95772147	1546439	-0.89142069	experimental	E1-127	DIPYRIDAMOLE					
1989 N16	X	512	520	-0.23254273	553	560	-0.10040177	5417094	5.7989771	5115135	0.52399407	experimental	PI-123	18- α -Ala-Phe-CMK					
1989 N17	X	692	660	-0.28636569	672	672	0.32492646	1594441	-1.2049056	1141446	0.97807405	experimental	CM-119	CGP-37157					
1989 N18	X	434	440	-0.33385122	353	360	-0.8111665	2709572	0.83818419	2135648	0.085242957	experimental	PI-130	MDL-28170					
1989 N19	X	832	840	0.18308185	433	440	-0.52930422	2398848	0.26886822	2257702	0.28755775	experimental	E1225	chelerythrine					
1989 N20	X	952	960	0.33894106	794	800	0.76097731	2103607	-0.27207943	2332020	0.41074611	experimental	P-120	AC-Leu-Leu-Nle-CHO					
1989 N21	X	670	680	-0.0273281	591	600	0.03541733	1600992	-1.1929827	1418489	-1.10350861	experimental	FR102	CAPE					
1989 N22	P	868	880	0.22983961	909	920	1.17200883	1532037	-1.31932371	1433797	-1.07813431	empty							
1989 N23	E	806	1400	0.14931235	812	1360	0.82531268	82714	-3.9748081	78977	-3.32386278	empty							
1989 N24	P	204088	201660	259.397738	184071	185200	655.827462	2104970	-0.26606	216066	-1.05278413	empty							
1989 N01	N	640	640	-0.07408586	1116	1120	0.91186555	1765562	-0.8914536	1815334	-0.44205453	empty							
1989 O02	E	156	160	-0.69492507	155	160	-1.52292823	78492	-3.98254375	79653	-3.32274226	empty							
1989 O03	X	637	640	-0.07018938	316	320	-0.94748411	2133457	-0.21738754	2041348	-0.07106726	experimental	L102	arachidonoyl-PAF					
1989 O04	X	394	400	-0.38580429	635	640	0.19268157	2015077	-0.43428622	2215025	0.21681703	experimental	AC-119	tetrahydrocannabinol-7- <i>oic acid</i>					
1989 O05	X	475	480	-0.28059932	514	520	-0.23979507	1961264	-0.53288369	1888438	-0.32452849	experimental	BML-104	AMIDODARONE					
1989 O06	X	751	760	0.07787688	748	760	0.59656471	2111074	-0.25839821	2119037	0.05770882	experimental	SK-141	C2 DIHYDROCERAMIDE					
1989 O07	X	513	520	-0.2312439	554	560	-0.09687259	2344121	0.16859609	2290244	0.34149886	experimental	AC-126	ACONITINE					
1989 O08	X	674	680	-0.02213279	395	400	-0.66512333	2264798	0.0235859	1938011	-0.24235706	experimental	SL101	AM 92016					
1989 O09	X	554	560	-0.177992	435	440	-0.52215585	2256419	0.00790638	2043274	-0.06787475	experimental	AC-115	C2 DIHYDROCERAMIDE					
1989 O10	X	352	360	-0.44035502	394	400	-0.66869752	1660961	-1.08310606	1499096	-0.96898571	experimental	SL112	AM 92016					
1989 O11	X	394	400	-0.38580429	635	440	-0.52215585	2062640	-0.34714015	2197836	0.18832481	experimental	AC-133	C8-ceramide					
1989 O12	X	555	560	-0.17669318	515	520	-0.23622088	2163120	-0.16303828	1853473	-0.38248592	experimental	SL113	amantidine					
1989 O13	X	394	400	-0.38580429	313	320	-0.95820667	2410452	0.29012934	2039995	-0.07330997	experimental	AC-200	C8 DIHYDROCERAMIDE					
1989 O14	X	794	800	0.13372643	714	720	0.47504235	2002519	-0.45729529	1839317	-0.40595069	experimental	PG035	Amiloride hydrochloride dihydrate					
1989 O15	X	753	760	0.08047453	573	600	0.04256571	2353450	0.18568891	2196590	0.18685519	experimental	AC-105	CARBACLYLIN					
1989 O16	X	469	480	-0.28839228	469	480	-0.40063349	1406541	-1.54926049	1442544	-1.06363542	experimental	AC-105	AMIDODARONE					
1989 O17	X	954	960	0.34153871	1074	1080	1.76174969	2460700	0.38219494	2142778	0.09706153	experimental	GR205	ciglitazone					
1989 O18	X	193	200	-0.64686848	272	280	-1.10474834	1349173	-1.65437152	1276363	-1.33909445	experimental	AC-100	A-23187					
1989 O19	X	674	680	-0.02213279	635	640	0.19268157	2606414	0.64917563	2295591	0.35036197	experimental	E1160	clofibrate					
1989 O20	X	511	520	-0.23384156	552	560	-0.10397596	2											

1989 P19	X	675	680	-0.02083396	475	480	-0.37918837	1427700	-1.51049246	1298773	-1.30194798	experimental	BIOMOL	GR-336	Tanshinone IIA
1989 P20	X	515	520	-0.22864625	673	680	0.32850067	2387695	0.24843342	2104142	0.0330191	experimental	BIOMOL	PR-100	CYPROMETHIN
1989 P21	X	594	600	-0.12603893	1233	1240	2.33004544	1676637	-1.05438412	1358198	-1.20344603	experimental	BIOMOL	CA-421	Nigericin
1989 P22	X	869	880	0.23113844	987	1000	1.45079542	1858802	-0.72061703	1722244	-0.60000907	experimental	BIOMOL	T-108	cytochalasin B
1989 P23	E	1018	1920	0.42466363	1227	2240	2.30860032	75542	-3.98794882	75648	-3.327733	empty			
1989 P24	P	308330	309080	399.569724	346679	347240	1237.01867	1813047	-0.80445044	1669365	-0.68766047	empty			
1990 A01	N	678	680	-0.14044377	678	680	-0.13722651	1414587	-1.21116784	1519167	-1.06322631	empty			
1990 A02	E	114	120	-0.97914663	111	120	-0.2490238	79643	-3.79661208	76064	-3.78513609	empty			
1990 A03	X	1353	1360	0.86332296	2152	2160	0.15340702	1473749	-1.09658622	1565069	-0.97664822	experimental	BIOMOL	T-109	cytochalasin D
1990 A04	E	469	480	-0.45123969	468	480	-0.17863291	1562187	-0.92530449	1575682	-0.95663051	empty			
1990 A05	X	1676	1680	1.34364393	1595	1600	0.04358146	1415641	-1.20912651	1416804	-1.25629836	experimental	BIOMOL	ST-330	D609
1990 A06	E	511	520	-0.38878309	512	520	-0.16995278	1679467	-0.6991632	1674256	-0.47838944	empty			
1990 A07	X	834	840	0.09153787	795	800	-0.11415722	1276482	-1.47864182	1247700	-1.57525399	experimental	BIOMOL	EI-274	damnacanthal
1990 A08	E	554	560	-0.32483943	675	680	-0.13781803	1619228	-0.8148307	1680501	-0.75892607	empty			
1990 A09	X	516	520	-0.38134778	635	640	-0.14570496	1217291	-1.59327961	1065495	-1.91892009	experimental	BIOMOL	CN-223	YC-1
1990 A10	E	474	480	-0.44380438	635	640	-0.14570496	1805651	-0.45377715	1622123	-0.86903578	empty			
1990 A11	X	416	840	-0.53005397	510	520	-0.17035163	1787332	-0.48925635	1868238	-0.40482579	experimental	BIOMOL	A-230	decoyinine
1990 A12	E	143531	143560	214.997251	436	440	-0.18494246	1709974	-0.63907896	1764796	-0.5999933	experimental	BIOMOL	S-109	deoxymannojirimycin(1)
1990 A13	X	296	720	-0.70805138	436	440	-0.18494246	2029928	-0.0194101	1671534	-0.77583919	empty			
1990 A14	E	475	480	-0.44231732	435	440	-0.18513963	1908231	-0.25510599	1800887	-0.53336885	empty			
1990 A15	X	316	320	-0.67876015	756	760	-0.12184698	1822835	-0.42049614	2017667	-0.12298018	experimental	BIOMOL	S-110	deoxynorjirimycin(1)
1990 A16	E	634	640	-0.20587449	554	560	-0.161676	1804949	-0.45513674	1877804	-0.38678287	empty			
1990 A17	X	1110	1120	0.50196694	831	840	-0.10705898	1850895	-0.36615112	1876744	-0.38878219	experimental	BIOMOL	EI-126	dexamethasone
1990 A18	E	713	720	-0.08839661	614	620	-0.16956294	1632083	-0.78993386	1842026	-0.45426558	empty			
1990 A19	X	511	520	-0.38878309	572	680	-0.13840955	1899932	-0.27117902	1874046	-0.39387103	experimental	BIOMOL	CN-125	dibutyrylcyclic AMP
1990 A20	E	555	560	-0.3235237	675	680	-0.13781803	1753512	-0.55475702	1822261	-0.3863696	empty			
1990 A21	E	755	760	-0.02594001	554	560	-0.161676	1803093	-0.45873158	1885487	-0.3329158	experimental	BIOMOL	CN-215	dibutyrylcyclic GMP
1990 A22	E	549	560	-0.33227474	790	800	-0.11514309	1731843	-0.59672432	1724599	-0.6757506	empty			
1990 A23	E	1038	2080	0.39489849	1332	2120	-0.00827513	80869	-3.79423763	78034	-3.78142037	empty			
1990 A24	P	356303	357280	528.695915	269663	270200	52.8994493	1620575	-0.8122219	1716587	-0.69086244	empty			
1990 B01	N	596	600	-0.26238284	596	600	-0.15339472	1792478	-0.47928987	2058870	-0.04526511	empty			
1990 B02	E	153	160	-0.92115122	191	200	-0.23324993	84605	-3.78700195	83159	-3.77175385	empty			
1990 B03	X	1672	1680	1.33769568	2300	2320	0.18258868	1732665	-0.59513231	1855948	-0.42800659	experimental	BIOMOL	T101	Nocodazole
1990 B04	X	600	620	-0.3710521	391	400	-0.27130521	2127204	-0.4483775	1968621	-0.66862174	empty			
1990 B05	X	470	480	-0.44975263	814	880	-0.11041093	1705141	-0.64843924	1903224	-0.33883692	experimental	BIOMOL	ST315	OBAA
1990 B06	E	474	480	-0.44380438	513	520	-0.16976011	2177154	0.26572891	2626286	1.02496699	empty			
1990 B07	X	832	840	0.08856375	633	640	-0.14609931	1389577	-1.2596058	1393670	-1.29993257	experimental	BIOMOL	EI181	okadaic acid
1990 B08	E	554	560	-0.32483943	433	440	-0.18553398	2053711	0.02665147	2407668	0.61262049	empty			
1990 B09	X	473	480	-0.44529144	514	520	-0.16956294	1418368	-1.20384501	1436907	-1.21838107	experimental	BIOMOL	CM-111	OLIGOMYCIN (A shown)
1990 B10	E	713	720	-0.08839661	469	480	-0.17843574	2375023	0.64895042	2197735	0.21665521	empty			
1990 B11	E	640	640	-0.21181537	2314	2320	0.05333333	1808439	-0.4483775	1812382	0.38190152	experimental	BIOMOL	CC-200	olomoucine
1990 B12	E	1173	1600	0.59565183	349	360	-0.20299654	2271278	0.44802924	2714404	1.19117082	empty			
1990 B13	X	551	560	-0.32930062	555	560	-0.16147883	1443215	-1.15572275	1539000	-1.02581829	experimental	BIOMOL	CM109	ouabain
1990 B14	E	554	560	-0.32483943	475	480	-0.1772527	2046086	0.0118838	2273592	0.35973295	empty			
1990 B15	X	393	400	-0.56425639	393	400	-0.19342091	1575915	-0.89871687	1707714	-0.70759825	experimental	BIOMOL	L-133	PCA4248
1990 B16	E	590	600	-0.27130521	389	400	-0.19420961	2105701	0.12734277	2161825	0.14892354	empty			
1990 B17	X	2031	2040	1.87155087	2194	2200	0.16168831	1643214	-0.76837596	1770332	-0.58949127	experimental	BIOMOL	EI-360	PD 98059
1990 B18	E	665	680	-0.15977557	425	440	-0.18711137	2047589	0.01479472	1876322	0.27626067	empty			
1990 B19	E	1713	1720	-1.39860521	1538	1720	0.0324258	1603547	-0.8500077	1704507	-0.6345734	experimental	BIOMOL	EI-306	SU-4312
1990 B20	E	550	560	-0.33078768	589	600	-0.15477493	1265961	0.24405094	2448269	0.6892001	empty			
1990 B21	X	472	480	-0.4467785	673	680	-0.13821237	1942782	-0.18818956	2018789	-0.12086391	experimental	BIOMOL	PI-120	pepstatin
1990 B22	E	948	960	0.26106292	830	840	-0.10725616	2295719	0.49535891	2099748	0.03183696	empty			
1990 B23	E	1216	2200	0.65959549	736	1280	-0.12579045	87988	-3.78044995	83911	-3.77033546	empty			
1990 B24	P	333557	335360	494.871207	181877	183240	35.5903888	1946110	-0.18174408	1988334	-0.17830663	empty			
1990 C01	N	676	680	-0.14341789	436	440	-0.18494246	1674466	-0.70784885	1681453	-0.75713046	empty			
1990 C02	E	115	120	-0.97765957	147	160	-0.24192556	82628	-3.7908309	84327	-3.76985082	empty			
1990 C03	X	631	640	-0.21033567	3753	3880	0.46908157	226165	0.36065065	2485607	0.7596252	experimental	BIOMOL	GR-234	GW-9662
1990 C04	E	713	720	-0.08839661	40688	40760	7.75167956	2332581	0.56675115	2235999	0.28882689	empty			
1990 C05	X	715	720	-0.08542248	20198	20320	3.71159745	2199630	0.30925916	2259395	0.33295257	experimental	BIOMOL	D-100	6,7-ADTN
1990 C06	E	313	320	-0.68322133	216	280	-0.2283206	1827253	-0.41193961	2112729	0.05632109	empty			
1990 C07	X	713	720	-0.08839661	753	760	-0.1224385	2010499	-0.0570391	2226915	0.27169309	experimental	BIOMOL	FR-110	Hinokitiol
1990 C08	E	273	280	-0.74270381	633	640	-0.14609931	2163288	0.23887402	2278140	0.36831116	empty			
1990 C09	X	594	600	-0.26535696	394	400	-0.19322374	1698475	-0.66134958	1407135	-1.27453555	experimental	BIOMOL	CN-240	diphenylamineiodonium
1990 C10	E	873	880	-0.14953329	394	400	-0.19322374	2086811	0.09075768	2176390	0.17639533	empty			
1990 C11	X	431	440	-0.50774804	709	720	-0.13111413	1901934	-0.26730166	1694931	-0.73170892	experimental	BIOMOL	CA-420	2,5-diterbutylhydroquinone
1990 C12	E	952	960	0.26701117	474	480	-0.17744987	2333042	0.56764399	2116415	0.06327344	empty			
1990 C13	X	352	360	-0.62522592	475	480	-0.1772527	1443026	-1.15608879	1582372	-0.94401216	experimental	BIOMOL	GR-319	doxorubicin
1990 C14	E	553	560	-0.3263265	394	400	-0.19322374	2117742	0.1506631	2223691	0.26561214	empty			
1990 C15	X	994	1000	0.32946777	634	640	-0.14590213	1912887	-0.24608851	1937041	-0.27505296	experimental	BIOMOL	EI-231	DRB
1990 C16	E	512	520	-0.38729603	514	520	-0.16956294	2442638	0.77989753	3123286	0.27052556	empty			
1990 C17	X	589	600	-0.27279227	549	560	-0.16265187	2401587	0.70039808	2419306	0.6345734	experimental	BIOMOL	FR-107	Hydrochloride
1990 C18	E	832	840	0.08856375	419	600	-0.18829441	2275949	0.45706949	2408751	0.6146632	empty			
1990 C19	X	668	680	-0.15531439	61070	61080	11.7704669	1400406	-1.2386328	1564375	-0.97795721	experimental	BIOMOL	CA-302	E6 berbamine
1990 C20	E	792	800	0.02908128	418	600	-0.18849158	2372602	0.64426157	2198747	0.218564	empty			
1990 C21	X	551	560	-0.32930062	553	560	-0.16187318	1938273	-0.19629234	2006815	-0.14344868	experimental	BIOMOL	PI-107	E-64-d
1990 C22	E	909	920	0.20306751	790	800	-0.11514309	2414							

1990 D13	X	556	560	-0.32186531	435	440	-0.18513963	2307897	0.51894457	2389759	0.57884142	experimental	BIOMOL	GR334	cyclopamine
1990 D14	E	434	440	-0.50328685	435	440	-0.18513963	2560271	1.0077283	2607110	0.98879817	empty			
1990 D15	X	513	520	-0.38580897	594	600	-0.15378907	2318672	0.53981299	2125951	0.08125977	experimental	BIOMOL	EI-275	PP1
1990 D16	E	594	600	-0.26535996	594	600	-0.15378907	2703968	1.2840958	2383509	1.61384966	empty			
1990 D17	X	469	480	-0.45123969	511	514	520	-0.1756618	-0.60684301	1695314	-0.37098852	experimental	BIOMOL	AC-146	prazocin
1990 D18	E	912	920	0.2075287	594	600	-0.15378907	2452858	0.79969686	2848903	1.44485621	empty			
1990 D19	X	630	640	-0.21182274	298	480	-0.21215238	2064415	0.04738237	2187439	0.19723541	experimental	BIOMOL	AP401	Propidium iodide
1990 D20	E	871	880	0.14655916	633	640	-0.14609931	2613354	1.11053646	3064649	1.85178569	empty			
1990 D21	X	791	800	0.02759422	473	480	-0.17764704	1804856	-0.45531686	1863372	-0.4140038	experimental	BIOMOL	AR107	propranolol (S-)
1990 D22	E	747	760	-0.0378365	109	600	-0.15457776	2475568	0.84368031	2687134	1.13973549	empty			
1990 D23	E	1118	1880	0.51386343	515	1560	-0.07077908	87400	-3.78158876	84068	-3.77003934	empty			
1990 D24	P	258205	259600	382.818125	183747	184840	-0.35959103	1961137	-0.15264063	2418727	0.41459164	empty			
1990 E01	N	236	240	-0.79772509	436	440	-0.18494246	2060493	0.03978646	1869374	-0.40268313	empty			
1990 E02	E	117	120	-0.97468545	157	160	-0.23995383	83468	-3.78920403	84651	-3.76893971	empty			
1990 E03	X	555	560	-0.32335237	475	480	-0.1772527	2752539	1.38010212	2776031	1.30740864	experimental	BIOMOL	PD129	EHNA
1990 E04	E	554	560	-0.32483943	634	640	-0.14590213	2350111	0.60070227	2499603	0.78602376	empty			
1990 E05	X	514	520	-0.38432191	393	400	-0.19342091	2585927	1.05741739	2512284	0.80994204	experimental	BIOMOL	S620	Pregnenolone 16alpha carbonitrile
1990 E06	E	513	520	-0.38580897	794	800	-0.1143544	2399643	0.69663305	2479703	0.74848936	empty			
1990 E07	X	865	880	0.13763679	739	760	-0.12519893	2344574	0.58997852	2418727	0.63347944	experimental	BIOMOL	BL-093	Estradiol-17 beta
1990 E08	E	552	560	-0.32781356	1790	1800	0.08203027	2259088	0.42441406	2443063	0.6793808	empty			
1990 E09	X	951	960	0.26552411	899	920	-0.09365119	2429372	0.7542105	2942721	1.6218111	experimental	BIOMOL	GR307	etoposide
1990 E10	E	552	560	-0.32781356	914	400	-0.19381526	2627078	1.13711633	2598855	0.97322799	empty			
1990 E11	X	594	600	-0.26535996	391	920	-0.09069359	2827654	1.52558061	2442015	0.67740411	experimental	BIOMOL	CM120	FCCP
1990 E12	E	475	480	-0.44231732	353	360	-0.20130785	2455634	0.80507326	2425832	0.64688054	empty			
1990 E13	X	234	240	-0.80069922	435	440	-0.18513963	2979793	1.82023485	2257951	0.33023167	experimental	BIOMOL	CN100	forskolin
1990 E14	E	555	560	-0.32335237	354	435	-0.18513963	2523609	0.67672341	2159947	1.26551984	empty			
1990 E15	X	473	480	-0.44523444	354	360	-0.2011062	2737249	1.35048934	2340287	0.485977	experimental	BIOMOL	EI-280	geldanamycin
1990 E16	E	590	600	-0.27130521	472	480	-0.17784422	2673368	1.22676819	2626754	1.02584971	empty			
1990 E17	X	1754	1760	1.45963475	1314	1320	-0.01182425	2513566	0.91727269	2277522	0.36714552	experimental	BIOMOL	EI-147	genistein
1990 E18	E	629	640	-0.2133098	431	440	-0.18592832	2521649	0.93292739	2539851	0.86193756	empty			
1990 E19	X	831	840	0.08707669	632	640	-0.14629648	1192454	-1.64138251	1156365	-1.74752557	experimental	BIOMOL	EI-283	Ro 31-8220
1990 E20	E	871	880	0.14655916	713	720	-0.13032544	2402038	0.70127155	2861298	1.46823505	empty			
1990 E21	X	790	800	0.02610715	673	680	-0.13821237	1921596	-0.22922141	1949887	-0.25082347	experimental	BIOMOL	EI-300	GM6001
1990 E22	E	748	760	-0.03634944	630	680	-0.12809089	2345147	0.58997852	2418727	0.63347944	empty			
1990 E23	E	721	1360	-0.07650011	799	1320	-0.11336853	84834	-3.78655844	84689	-3.76886804	empty			
1990 E24	P	215246	216760	318.935347	175671	176640	34.366731	2270223	0.4459797	2429557	0.65390645	empty			
1990 F01	N	438	440	-0.49733861	637	640	-0.14531061	2086641	0.09042843	2174340	0.17252872	empty			
1990 F02	E	157	160	-0.91520298	76	80	-0.25592487	83601	-3.78894645	83816	-3.77051465	empty			
1990 F03	X	354	360	-0.6222518	274	280	-0.21688454	1086958	-1.84570121	1079994	-1.89157279	experimental	BIOMOL	GR-312	puromycin
1990 F04	E	554	560	-0.32483943	713	720	-0.13032544	2464030	0.82133416	2369710	0.54102599	empty			
1990 F05	X	794	800	-0.14787908	794	2341	14354	58420508	1.59070947	2625959	1.02435022	experimental	BIOMOL	EI314	SB-431542
1990 F06	E	745	760	-0.04081063	423	440	-0.18750571	2410599	0.71620180	2469262	0.78279606	empty			
1990 F07	X	3350	3360	3.83298541	3711	3720	0.46080029	3994954	3.78634141	4005740	3.62682516	experimental	BIOMOL	EI305	SP-600125
1990 F08	E	422	440	-0.52113159	769	800	-0.11928373	2641204	1.16447477	2689039	1.14332861	empty			
1990 F09	X	1433	1440	0.9822879	4432	4440	0.60296228	2190364	0.29131329	1883947	-0.37519625	experimental	BIOMOL	AC1142	benzamil
1990 F10	E	591	600	-0.26981815	582	600	-0.15615515	2687593	1.25431837	2724133	1.20952118	empty			
1990 F11	X	506	520	-0.3962184	703	720	-0.13269152	1884080	-0.30188028	1730306	-0.66489633	experimental	BIOMOL	A-275	rapamycin
1990 F12	E	594	600	-0.20587449	714	720	-0.13012826	2865929	1.59070947	27800	1.72864295	empty			
1990 F13	X	314	320	-0.68173427	431	440	-0.18533089	2119981	1.15499947	2131534	0.99179015	experimental	BIOMOL	AM-100	Cyclo [Arg-Gly-Asp-D-Phe-Val]
1990 F14	E	474	480	-0.44380438	593	600	-0.15398624	2574729	1.03572974	2540487	0.86313715	empty			
1990 F15	X	753	760	-0.02891413	672	680	-0.13840955	2445527	0.78549859	2604059	0.98304352	experimental	BIOMOL	ST-300	
1990 F16	E	554	560	-0.32483943	473	480	-0.17764704	2763773	1.4018595	2727267	1.30108249	empty			
1990 F17	X	351	360	-0.62671298	632	640	-0.14629648	2382500	0.66343146	2368111	0.53801003	experimental	BIOMOL	PR-112	RK-682
1990 F18	E	392	400	-0.56574345	513	520	-0.16976011	2577464	1.04102673	2479991	0.74903257	empty			
1990 F19	X	873	880	0.14953329	953	960	-0.08300383	1737858	-0.5850748	1958534	-0.23451393	experimental	BIOMOL	CC205	roscovitine
1990 F20	E	630	640	-0.21182274	471	480	-0.17804139	2279192	0.46353035	2791426	1.33644593	empty			
1990 F21	X	907	920	0.20009339	550	560	-0.1624647	1784959	-0.49385224	1751365	-0.62526589	experimental	BIOMOL	EI270	Rottlerin
1990 F22	E	1109	1120	0.50047987	831	840	-0.10705898	2312462	0.52778581	2728148	1.21709408	empty			
1990 F23	E	709	1480	-0.09434485	798	1240	-0.1135657	88744	-3.77898577	82933	-3.77218012	empty			
1990 F24	P	260434	261880	386.132786	147462	148600	28.8046677	2146169	0.20571891	2122982	0.07565979	empty			
1990 G01	N	357	360	-0.61779061	556	560	-0.16128166	2069488	0.05720747	2065735	-0.03231668	empty			
1990 G02	E	116	120	-0.97617251	195	200	-0.23246124	83755	-3.78864819	82524	-3.77295155	empty			
1990 G03	X	755	760	-0.02594001	835	840	-0.10627029	2764788	1.40382529	2625959	1.02435022	experimental	BIOMOL	EI-269	Go6976
1990 G04	E	513	520	-0.38580897	633	640	-0.14609931	2615880	1.11542868	2427744	0.31097973	empty			
1990 G05	X	554	560	-0.32483943	431	440	-0.18592832	2983874	1.8281387	2441145	0.67576316	experimental	BIOMOL	EI287	NIMESULIDE
1990 G06	E	551	560	-0.32930062	513	520	-0.16976011	2113781	0.14299166	2635765	1.04284582	empty			
1990 G07	X	1223	1240	0.67000492	1182	1200	-0.03785113	2699672	1.27771229	2465282	0.72128918	experimental	BIOMOL	EI-148	H7
1990 G08	E	792	800	0.02908128	591	600	-0.15438059	2475769	0.84406959	2428136	0.65122623	empty			
1990 G09	X	507	520	-0.39473134	459	480	-0.184040747	1740011	-0.580905	1981437	-0.19131542	experimental	BIOMOL	EI-196	H-89
1990 G10	E	640	660	-0.27725346	714	720	-0.13012826	247441284	0.8455508	3781886	1.32279019	empty			
1990 G11	X	3112	3120	3.47966477	4352	4360	0.58718841	2200379	0.31070978	2568233	0.99179015	experimental	BIOMOL	EI-195	H9
1990 G12	E	706	720	-0.09880604	542	560	-0.16404208	2592313	1.06978544	2427626	0.65026429	empty			
1990 G13	X	674	680	-0.14639202	713	720	-0.13032544	2801350	1.47463651	2704182	1.17189059	experimental	BIOMOL	EI-233	HA1077
1990 G14	E	592	600	-0.26833109	870	880	-0.09936922	2707800	1.29345415	2480072	0.74918535	empty			
1990 G15	X	950	960	0.26403705	1349	1360	-0.00492318	2899158	1.66406553	2628921	1.029937	experimental	BIOMOL	EI-184	HA-1004
1990 G16	E	513	520	-0.38580897	551	560	-0.16226752	2431558	0.75844422	2619911	1.01294278	empty			

1990 L01	N	517	520	-0.37986072	397	400	-0.19263222	2013903	-0.05044642	2020685	-0.11728777	empty				
1990 L02	E	156	160	-0.91669004	77	80	-0.25572769	79717	-3.79646876	82119	-3.77371544	empty				
1990 L03	X	514	520	-0.38432191	395	400	-0.19302657	1890288	-0.28985698	2362886	0.52815489	experimental	BIOMOL	EI-267		tyrphostin AG-825
1990 L04	E	640	640	-0.20587449	473	480	-0.17764704	2211180	0.33162854	2789558	1.34423965	empty				
1990 L05	X	554	560	-0.32483943	794	800	-0.16143544	2724004	0.25482938	2741750	1.24273064	experimental	BIOMOL	NA136		Kavain (+/-)
1990 L06	E	502	520	-0.40216665	698	720	-0.13328304	2782010	1.43717989	2544541	0.8707836	empty				
1990 L07	X	4475	4480	0.50592996	5315	5320	0.77706636	1472743	-1.09853458	1511758	-1.0772008	experimental	BIOMOL	AP-300		TPEN
1990 L08	E	694	720	-0.11665078	570	600	-0.15852123	2871563	1.61062109	2654260	1.07773018	empty				
1990 L09	X	3072	3080	3.41958222	3671	3680	0.45291336	1525830	-0.99571867	1441667	-1.20940299	experimental	BIOMOL	GR-309		trichostatin-A
1990 L10	E	627	600	-0.21628392	586	600	-0.15536645	2716386	1.31008303	2304192	0.41744916	empty				
1990 L11	X	144	144	0.93453478	177	200	-0.23601036	1030022	-1.95597164	1014617	-2.01488366	experimental	BIOMOL	CA-310		Trifluoperazine dihydrochloride
1990 L12	F	515	520	-0.38283485	555	560	-0.16147883	2568814	1.02427239	3190282	2.08946552	empty				
1990 L13	X	395	400	-0.56128226	555	560	-0.16147883	1771259	-0.52038563	1768006	-0.59387845	experimental	BIOMOL	CC-104		tunicamycin
1990 L14	E	474	480	-0.44380438	554	560	-0.161676	2736345	1.34873849	2715768	1.19374353	empty				
1990 L15	X	630	640	-0.21182274	593	600	-0.15398624	2337926	0.57710305	2834505	1.41769941	experimental	BIOMOL	EI-229		tyrphostin AG-370
1990 L16	E	713	720	-0.08839661	552	560	-0.16207035	2827262	1.52482141	2728754	1.21823709	empty				
1990 L17	X	473	480	-0.44529144	472	480	-0.17784422	2491579	0.87468951	2958303	1.6512011	experimental	BIOMOL	EI-263		tyrphostin AG-126
1990 L18	E	514	520	-0.38432191	674	680	-0.1380152	2981299	1.82315158	3103673	1.92539083	empty				
1990 L19	X	554	560	-0.32483943	354	360	-0.20111067	2634511	1.15151215	2637984	1.04703119	experimental	BIOMOL	EI-190		tyrphostin 1
1990 L20	E	592	600	-0.26833109	393	400	-0.19342091	2872306	1.61206009	2794909	1.34301539	empty				
1990 L21	X	631	640	-0.21033567	872	880	-0.09897487	1814280	-0.43706499	1895288	-0.35380542	experimental	BIOMOL	EI-215		tyrphostin A9
1990 L22	E	589	600	-0.27279227	748	760	-0.12342437	2888940	1.64427588	2906563	1.55361166	empty				
1990 L23	E	833	1720	0.09005081	969	1520	-0.07984906	85564	-3.78514462	82596	-3.77281575	empty				
1990 L24	P	301489	302960	447.184109	185833	186880	36.37040666	2272221	-0.04984931	2382588	0.56531583	empty				
1990 M01	N	477	480	-0.43934319	477	480	-0.17685835	2014592	-0.0499112	2302032	0.41337508	empty				
1990 M02	E	117	120	-0.97468545	117	120	-0.24784076	79928	-3.77443015	81800	-3.77443015	empty				
1990 M03	X	435	440	-0.50179979	475	480	-0.1772527	2598114	1.08171191	2738134	1.23592918	experimental	BIOMOL	CN242		L-NAME
1990 M04	E	554	560	-0.32483943	555	560	-0.16147883	2319404	0.54123068	2342721	0.49012066	empty				
1990 M05	X	274	280	-0.74121674	312	320	-0.20939195	2080149	0.0778551	1932320	-0.28395748	experimental	BIOMOL	ST420		LY-294002
1990 M06	E	475	480	-0.44231732	475	480	-0.1772527	2307342	0.51786968	2422144	0.63992441	empty				
1990 M07	X	143	160	-0.93602184	220	240	-0.2275319	984000	-2.04510445	1004797	-2.03340566	experimental	BIOMOL	CN-200		LY83583
1990 M08	E	514	520	-0.38432191	553	560	-0.16187318	2352550	0.60542599	2785857	1.32594195	empty				
1990 M09	X	506	520	-0.3962184	983	1000	-0.07708863	1836829	-0.39339335	2158072	0.14184482	experimental	BIOMOL	EI-293		5-iodotubercidin
1990 M10	E	534	560	-0.38432191	672	700	-0.16187318	2455881	0.60542599	2785857	1.32594195	empty				
1990 M11	X	355	360	-0.62076474	555	560	-0.16147883	2071428	0.06096475	2178515	-0.1804034	experimental	BIOMOL	EI177		Manoalide
1990 M12	E	356	360	-0.61927767	355	360	-0.2009135	2212121	0.33170795	2053615	-0.05517683	empty				
1990 M13	X	75	80	-1.03714205	195	200	-0.23246124	1118626	-1.78436841	1113501	-1.82837353	experimental	BIOMOL	G-236		manumycina
1990 M14	E	474	480	-0.44380438	474	480	-0.17744987	2271965	0.4493535	2458283	0.70808801	empty				
1990 M15	X	434	440	-0.50328685	633	640	-0.14609931	2439154	0.77315573	2589994	0.95651481	experimental	BIOMOL	G410		
1990 M16	E	553	560	-0.3262655	873	880	-0.0987777	2386199	0.67059547	2482527	0.75815855	empty				
1990 M17	X	880	880	0.15102035	632	640	-0.14629646	2573985	1.0342881	1.08657434	1.08657434	experimental	BIOMOL	FR103		MC1186
1990 M18	E	713	720	-0.08839661	635	640	-0.14570496	2463001	0.81934125	2472956	0.7357635	empty				
1990 M19	X	352	360	-0.62522592	194	200	-0.23265841	1330349	-1.37431525	1238593	-1.59243117	experimental	BIOMOL	PI129		Glotoxin
1990 M20	E	833	840	0.09005081	514	520	-0.16956294	2668480	1.21730139	2523582	0.83125177	empty				
1990 M21	X	1031	1040	0.38448905	870	880	-0.09936922	2477177	0.84679653	2577207	0.9323966	experimental	BIOMOL	EI-295		LFM-A13
1990 M22	E	709	720	-0.09434485	749	760	-0.1232272	2446500	0.78738305	2594680	0.96535331	empty				
1990 M23	E	571	1400	-0.29955938	918	1440	-0.0899049	83378	-3.78937834	81398	-3.77507536	empty				
1990 M24	P	281180	282560	416.98337	175645	176680	34.26165045	2711885	1.30136574	2488361	0.76485738	empty				
1990 N01	N	397	400	-0.55838814	557	560	-0.16108446	1978114	-1.11978054	2280828	0.37381114	empty				
1990 N02	E	117	120	-0.97468545	76	80	-0.2592487	78811	-3.79822345	78164	-3.78117517	empty				
1990 N03	X	434	440	-0.50328685	515	520	-0.16936576	2051306	0.0219936	1978054	-0.19769626	experimental	BIOMOL	ST-391		U73122
1990 N04	E	633	640	-0.20736155	433	440	-0.18553398	2701937	1.28209902	2192341	0.20648132	empty				
1990 N05	X	634	640	-0.20587449	754	760	-0.12224133	1817894	-0.43006559	1911029	-0.32411552	experimental	BIOMOL	EI282		U-0126
1990 N06	E	594	600	-0.26535696	513	520	-0.16976011	2375588	0.65004469	2365178	0.53247795	empty				
1990 N07	X	555	560	-0.32335237	515	520	-0.16936576	1511000	-1.02444058	1574487	-0.95888446	experimental	BIOMOL	KC-140		valinomycin
1990 N08	E	634	640	-0.20587449	553	560	-0.16187318	2345179	0.59115025	2427961	0.65089515	empty				
1990 N09	X	713	720	-0.08839661	952	960	-0.08320101	1571636	-0.9070042	1689258	-0.74240905	experimental	BIOMOL	T116		vinblastine
1990 N10	E	513	520	-0.38580897	594	600	-0.15418341	2297420	0.49865331	2751425	1.26099801	empty				
1990 N11	X	675	680	-0.14490495	554	360	-0.20111067	1327796	-1.37925975	1415565	-1.2586353	experimental	BIOMOL	CA-320		W7
1990 N12	E	434	440	-0.50328685	316	520	-0.16916859	2364442	0.62845774	2228735	0.27512589	empty				
1990 N13	X	395	400	-0.56128226	275	280	-0.21668737	2026142	-0.02674262	2012651	-0.13244111	experimental	BIOMOL	ST-415		wortmannin
1990 N14	E	915	920	0.21198988	635	640	-0.14570496	2414548	0.72550022	2229829	0.27718934	empty				
1990 N15	X	513	520	-0.38580897	432	440	-0.18571115	2407246	0.71135811	2167070	0.1588164	experimental	BIOMOL	EI-299		Y-27632
1990 N16	E	433	440	-0.50477391	712	720	-0.13052261	2499674	0.89036745	2377467	0.55565866	empty				
1990 N17	X	393	400	-0.56425639	594	600	-0.15378907	2275672	0.45653301	2326416	0.45936698	experimental	BIOMOL	AC-161		YOHIMBINE HYDROCHLORIDE
1990 N18	E	673	680	-0.14787908	353	360	-0.20130785	2821259	1.51319514	2406922	0.61121343	empty				
1990 N19	X	674	680	-0.14639202	635	640	-0.14570496	1344337	-1.34722408	1396521	-1.29455516	experimental	BIOMOL	ZW-9170		Z-Leu3-VS
1990 N20	E	550	560	-0.33087868	671	680	-0.13860672	2525647	0.94067049	2510949	0.80742403	empty				
1990 N21	X	1071	1080	0.44397153	1232	1240	-0.02799247	2061025	-0.02481681	1713413	0.170271	experimental	BIOMOL	EI-298		thrombin
1990 N22	E	840	840	0.08410257	553	560	-0.13114113	24239957	0.70553435	2540767	0.86362755	empty				
1990 N23	E	691	1200	-0.12111197	900	1400	-0.09345402	80033	-3.79585675	78918	-3.77953301	empty				
1990 N24	P	170620	172200	252.573816	168019	169200	32.8579604	2131415	0.17714419	2128519	0.08610341	empty				
1990 O01	N	516	520	-0.38134778	557	560	-0.16108448	1939374	-0.19478998	1900296	-0.34435957	empty				
1990 O02	E	115	120	-0.97765957	156	160	-0.240151	76667	-3.80237583	78982	-3.7796323	empty				
1990 O03	X	914	92													

1990 O19	X	311	320	-0.68619546	552	560	-0.16207035	2021539	-0.03565745	2466207	0.72303387	experimental	BIOMOL	A-248	monensin
1990 O20	E	714	720	-0.08690954	633	640	-0.14609931	2794708	1.46177266	2470509	0.73114809	empty			
1990 O21	X	672	680	-0.14936614	632	640	-0.14629648	2198478	0.30702803	2150903	0.128323	experimental	BIOMOL	A235	TACROLIMUS
1990 O22	E	749	760	-0.03486238	510	520	-0.17035163	2240792	0.3889799	2422667	0.64091087	empty			
1990 O23	E	749	1520	-0.03486238	804	1480	-0.11238266	82557	-3.79098641	79750	0.72783374	empty			
1990 O24	P	260268	262000	385.885934	228563	229760	44.7956242	2414692	0.72577911	2377365	0.55546447	empty			
1990 P01	N	718	720	-0.0809613	438	440	-0.18454811	1746062	-0.56918576	1725883	-0.67332878	empty			
1990 P02	E	75	80	-1.03714205	156	160	-0.240151	74870	-3.80585615	75230	-3.78670914	empty			
1990 P03	X	756	760	-0.02445295	874	880	-0.09858053	1754006	-0.55380027	1913257	-0.31991317	experimental	BIOMOL	P-416	zVAD-FMK
1990 P04	E	474	480	-0.44380438	1274	1280	-0.01971118	2066366	0.05116096	2112851	0.0565512	empty			
1990 P05	X	475	480	-0.44231732	633	640	-0.14609931	1714034	-0.63121578	1825314	-0.48578693	experimental	BIOMOL	EI-261	NS-398
1990 P06	E	595	600	-0.26389999	595	600	-0.15359189	2278290	0.46160341	2284869	0.26342987	empty			
1990 P07	X	716	720	-0.08393542	435	440	-0.18513963	1531206	-0.98530674	1613593	-0.88512464	experimental	BIOMOL	EI-216	AA-861
1990 P08	E	467	480	-0.45421381	507	520	-0.17094315	2123628	0.16206277	2205495	0.23129174	empty			
1990 P09	X	3194	3200	3.60100377	3475	3480	0.41426738	1939677	-0.19420315	1885042	-0.37313092	experimental	BIOMOL	A-249	Mycophenolic acid
1990 P10	E	548	560	-0.33376181	547	560	-0.16305622	2246627	0.40028029	2026153	-0.1069743	empty			
1990 P11	X	555	560	-0.32335237	515	520	-0.16936576	1643202	-0.76839921	1574438	-0.95897688	experimental	BIOMOL	CT115	Shikonin
1990 P12	E	556	560	-0.32186531	596	600	-0.15339472	2281606	0.46802565	2279321	0.37053871	empty			
1990 P13	X	396	400	-0.5597952	436	440	-0.18494246	2025219	-0.02853023	1828469	-0.47983612	experimental	BIOMOL	CA409	Xestospogin C
1990 P14	E	435	440	-0.50179979	474	480	-0.17744987	2306429	0.51610144	1982837	-0.18867481	empty			
1990 P15	X	834	840	0.09153787	914	920	-0.09069359	1842317	-0.38276451	1967713	-0.21720095	experimental	BIOMOL	EI211	CDC
1990 P16	E	1033	1040	0.38746318	633	640	-0.14609931	2202651	0.31511006	2177317	0.17814379	empty			
1990 P17	X	514	520	-0.38432191	675	680	-0.13781803	1458075	-1.12694274	1413506	-1.26251889	experimental	BIOMOL	G237	Ceruleinin
1990 P18	E	594	600	-0.26535696	594	600	-0.15378907	2328387	0.55862845	2182253	0.187453383	empty			
1990 P19	X	1036	1040	0.39192436	915	920	-0.09496422	2038350	-0.00309885	1964005	-0.2241948	experimental	BIOMOL	CA305	Phenoxybenzamine hydrochloride
1990 P20	E	594	600	-0.26535696	594	600	-0.15378907	2328387	0.55862845	2182253	0.187453383	empty			
1990 P21	X	314	320	-0.6813327	394	400	-0.19323774	962417	-2.08690519	2237423	-1.59152166	experimental	BIOMOL	T-126	Wisikostatin
1990 P22	E	750	760	-0.03337532	753	760	-0.1224385	2147401	0.26097808	2241373	0.29896306	empty			
1990 P23	E	1205	2440	0.64323781	930	1640	-0.08753882	78561	-3.79870763	78374	-3.78077908	empty			
1990 P24	P	423594	424360	628.761792	242250	242920	47.494336	1870342	-0.32848727	1840535	-0.45707783	empty			
2051 A01	N	1358	1360	1.04708588	1678	1680	2.54835781	4045506	0.27368483	2618912	-2.10139723	empty			
2051 A02	E	33	40	-2.30174898	32	40	-2.60521619	50710	-6.19255235	56397	-7.18989487	empty			
2051 A03	X	915	920	-0.0725623	916	920	0.16255988	3801981	-0.12050061	2696166	-1.9479906	experimental	NIH	SAM001247063	Nalbuphine
2051 A04	X	915	920	-0.0725623	916	920	0.16255988	3801981	-0.12050061	2696166	-1.9479906	experimental	NIH	SAM001247064	Cephalexin Monohydrate
2051 A05	X	913	920	-0.07761715	954	960	0.28153668	4031087	0.2503453	3059048	-1.32777383	experimental	NIH	SAM001246961	
2051 A06	X	752	760	-0.48453217	673	680	-0.59826544	4210562	0.54085523	3170704	-1.00567982	experimental	NIH	SAM001246756	Troxipide
2051 A07	X	833	840	-0.27981095	594	600	-0.84561195	2722602	-1.86765381	3229441	-0.8890432	experimental	NIH	SAM001247033	Flotidone
2051 A08	X	634	640	-0.78276803	713	720	-0.47302671	3991620	0.18646144	3230525	-0.88689066	experimental	NIH	SAM001246703	Levosulpiride
2051 A09	X	634	640	-0.78276803	713	720	-0.47302671	3991620	0.18646144	3230525	-0.88689066	experimental	NIH	SAM001246971	Salbutamol Sulfate
2051 A10	X	748	760	-0.49464186	947	960	0.2596199	3421043	-0.73711168	3303310	-0.74235833	experimental	NIH	SAM001246696	Alprazolam
2051 A11	X	670	680	-0.69178082	752	760	-0.69178082	2657455	-1.87019499	3992141	-3.85428793	experimental	NIH	SAM001247054	10h-phenothiazine, 2-chloro-10-[3-(4-methyl-1-piperazi
2051 A12	X	1073	1080	0.32677046	752	760	-0.35091894	3453755	-6.68416191	33262094	-0.82420272	experimental	NIH	SAM001246689	Doxetazone
2051 A13	X	831	840	-0.28486579	1074	1080	0.65725289	3535926	-0.55115457	3335498	-0.6784412	experimental	NIH	SAM001247052	Bifemelane
2051 A14	X	993	1000	0.12457666	912	920	0.15003601	3606196	-0.43741097	3473594	-0.40421796	experimental	NIH	SAM001246682	Methyltestosterone
2051 A15	X	673	680	-0.68419855	753	760	-0.34778797	3726135	-0.24326989	3469048	-0.41324515	experimental	NIH	SAM001247007	
2051 A16	X	952	960	0.02095233	914	920	0.15629794	3407831	-0.75849749	3221743	-0.90432946	experimental	NIH	SAM001246614	4-chloro-n-(2-morpholin-4-yl-ethyl)-benzamide
2051 A17	X	950	960	0.01589749	591	600	-0.85500485	3178088	-1.13037448	2915853	-1.51174855	experimental	NIH	SAM001247038	Pizotyline
2051 A18	X	1511	1520	1.45378153	1232	1240	-0.74542096	4004870	0.20790875	4592681	1.8299163	experimental	NIH	SAM001246685	Flubenzazole
2051 A19	X	1628	1640	0.29489997	1230	1240	-0.15468396	3591314	-0.46149995	32501336	-0.84794479	experimental	NIH	SAM001246693	Ketocanzole
2051 A20	X	991	1000	0.11952181	1191	1200	0.102357619	3415445	-0.74617297	3333407	-0.68259339	experimental	NIH	SAM001246720	Picidid
2051 A21	X	632	640	-0.78782288	1191	1200	0.102357619	3154961	-1.16780935	3245070	-0.85800802	experimental	NIH	SAM001247006	Prampixole
2051 A22	X	992	1000	0.12204923	1310	1320	1.39616143	3516433	-0.58270721	3039738	-1.26574471	experimental	NIH	SAM001246730	Gabaxete Mesylate
2051 A23	E	701	1240	-0.61343072	648	1160	-0.67653965	49360	-6.19473754	52524	-7.19758565	empty			
2051 A24	P	1837400	1842000	462.003463	174130	174440	542.490122	2594285	-2.07535607	2599734	-2.13947982	empty			
2051 B01	N	674	680	-0.68167113	593	600	-0.84874292	3116505	-1.23005674	3070171	-1.20531258	empty			
2051 B02	E	75	80	-2.19559723	35	40	-2.59832329	56989	-6.18238875	57931	-7.18684874	empty			
2051 B03	X	792	800	-0.38343527	832	840	-0.10044147	3385827	-0.79411459	3385429	-0.57929104	experimental	NIH	SAM001246723	Bupropion Hydrochloride
2051 B04	X	711	720	-0.5881565	712	720	-0.47615768	3982732	-0.17207474	3738752	0.12231783	experimental	NIH	SAM001246531	Nitrendipine
2051 B05	X	631	640	-0.7903503	631	640	-0.72976612	4345100	0.75862721	3849478	-0.05495744	experimental	NIH	SAM001246742	Pazufloxacin
2051 B06	X	871	880	-0.18376889	713	720	-0.47302671	3842756	-0.05449953	3856278	0.35569433	experimental	NIH	SAM001246528	Rutin
2051 B07	X	991	1000	0.11952181	512	520	-1.10235136	7978999	0.64069298	7710296	0.80878572	experimental	NIH	SAM001246651	Topotecan Hcl
2051 B08	X	631	640	-0.7903503	873	880	0.02792824	3310174	-0.91657147	3461494	-0.42824545	experimental	NIH	SAM001246783	Ritonavir
2051 B09	X	705	720	-0.60332103	626	640	-0.74542096	3180641	-1.12624203	3014007	-1.31683988	experimental	NIH	SAM001246658	Naftopidil
2051 B10	X	2668	2680	4.3580094	2510	2520	5.15332352	4288278	0.66665141	3858886	0.36087315	experimental	NIH	SAM001246605	Pterostilbene
2051 B11	X	1706	1720	1.92662892	1145	1160	0.87955165	3798056	-0.12685387	3833329	0.3101235	experimental	NIH	SAM001246610	Rosiglitazone Maleate
2051 B12	X	905	920	-0.09783653	670	680	-0.60765835	4684872	1.30860431	3645678	-0.06250326	experimental	NIH	SAM001246558	Ticlopidine Hcl
2051 B13	X	1070	1080	0.31918819	548	560	-0.98963649	3822093	-0.08794601	3731926	0.10876315	experimental	NIH	SAM001246612	Bicalutamide
2051 B14	X	871	880	-0.18376889	912	920	0.15003601	3164974	0.46706352	4322730	1.30180582	experimental	NIH	SAM001246992	Phystogimmine
2051 B15	X	591	600	-0.8914472	551	560	-0.98024359	3967765	0.14784818	3720862	0.08679288	experimental	NIH	SAM001246561	Flotafur
2051 B16	X	951	960	0.01842491	713	720	-0.47302671	3842756	-0.05449953	3856278	0.35569433	experimental	NIH	SAM001246615	Ziziphatrin Benzoate
2051 B18	X	948	960	0.01084264	1032	1040	0.52578222	3862629	-1.64099698	3651930	-0.05014797	experimental	NIH	SAM001246670	Isoquetartrin
2051 B17	X	666	680	-0.70189051	748	760	-0.36344281	3760442	-0.18773834	3535379	-0.28152879	experimental	NIH	SAM001246542	Itopride Hcl
2051 B19	X	1629	1640	1.73201739	1029	1040	0.51635931	3022274	-1.38258518	2810998	-1.71996369	experimental	NIH	SAM001246768	Doxorubicin Hydrochloride

2051 C13	X	826	840	-0.29750291	1312	1.40242337	4072396	0.31721074	3846255	0.33579122	experimental	NIH	SAM001246973		
2051 C14	X	552	560	-0.99001668	590	600	-0.85813582	4058311	0.29441184	3845553	0.33439723	experimental	NIH	SAM001246686	Tosufloxacin Tosylate
2051 C15	X	592	600	-0.88891978	713	720	-0.47302671	4698657	1.33091761	4315726	1.26804023	experimental	NIH	SAM001247014	D-cycloserine
2051 C16	X	789	720	-0.50321134	752	760	-0.35091894	4001636	0.20267399	3646663	-0.06564731	experimental	NIH	7AM0062345616	Haloperidol Mesylate Monohydrate
2051 C17	X	1391	1400	-1.30490883	671	680	-0.60452738	3896807	0.094299094	4198464	0.03518799	experimental	NIH	SAM001246532	Beta-estradiol
2051 C18	X	667	680	-0.69936309	710	720	-0.48241961	3680696	-0.31682041	3373637	-0.60270693	experimental	NIH	SAM001246677	Tacrolimus
2051 C19	X	749	760	-0.49211444	911	920	0.14690504	3795184	-0.13150267	3525981	-0.30019081	experimental	NIH	SAM001247047	Triptenamine Hydrochloride
2051 C20	X	791	800	-0.3859627	631	640	-0.72976612	3670539	-0.33326119	3935980	0.51396206	experimental	NIH	SAM001246716	1-(2-methyl-5-nitro-imidazol-1-yl)propan-2-ol
2051 C21	X	832	840	-0.28233837	991	1000	0.39738251	3609122	-0.43267475	4320488	1.27749634	experimental	NIH	SAM001247018	Lidocaine
2051 C22	X	389	400	-1.40198655	988	1000	0.38798961	1726352	-3.48024899	2449773	-2.43766106	experimental	NIH	SAM001246724	Oxiconazole Nitrate
2051 C23	E	665	1120	-0.70441793	631	1000	-0.72976612	54099	-6.18705669	57399	-7.18750801	empty			
2051 E24	P	154252	155040	387.474827	123899	124520	385.190269	3181921	-1.12417014	328392	-1.05002743	empty			
2051 D01	N	395	400	-1.38682202	915	920	0.15942891	3093864	-1.26670494	3039345	-1.26652511	empty			
2051 D02	E	77	80	-2.19054238	35	40	-2.59582329	56080	-6.18386011	57463	-7.18777807	empty			
2051 D03	X	513	520	-1.08858616	553	560	-0.97398165	3895982	0.03165554	3954321	0.55038258	experimental	NIH	SAM001246718	Irsogladine Maleate
2051 D04	X	711	720	-0.58815665	554	560	-0.97085068	2626767	-2.02277858	2716422	-1.90776737	experimental	NIH	SAM001246578	Saquinavir Mesylate
2051 D05	X	550	560	-0.99507153	571	680	-0.60452738	3944425	0.11006854	3967154	0.57586563	experimental	NIH	SAM001246745	Miglitol
2051 D06	X	632	640	-0.78722898	1152	1160	0.90146842	4462060	0.94794629	4436002	1.50687752	experimental	NIH	SAM001246580	Peniciliclovir
2051 D07	X	591	600	-0.8914472	671	680	-0.60452738	4233989	0.5787757	4214565	1.06716043	experimental	NIH	SAM001246539	Levetiracetam
2051 D08	X	1031	1040	0.22061871	752	760	-0.35091894	3101177	-1.25486764	3420142	-0.51035992	experimental	NIH	SAM001246780	Vinorelbine Bitartrate
2051 D09	X	990	1000	0.11699439	671	680	-0.60452738	4337094	0.74566817	3876383	0.3956177	experimental	NIH	SAM001246662	Nobletin
2051 D10	X	710	720	-0.59068392	912	920	0.15003601	4879251	1.62323883	4686875	2.00504697	experimental	NIH	SAM001246547	Roxatidine Acetate Hcl
2051 D11	X	700	800	-0.3859627	510	520	-1.10861329	4152235	0.44644335	3847960	0.63917691	experimental	NIH	SAM001246668	Escitalopram Oxalate
2051 D12	X	746	760	-0.49969671	832	840	-0.10044147	4811972	1.51433666	4619204	1.87066971	experimental	NIH	SAM001246594	Loxoprofen Sodium
2051 D13	X	2151	2160	3.05133195	750	760	-0.35718088	2993068	-1.42985991	3235298	-0.8774127	experimental	NIH	SAM001246672	Benidipine Hcl
2051 D14	X	787	800	-0.91556871	623	640	-1.22447086	42117086	0.5514154	3282962	-1.07411901	experimental	NIH	SAM001246577	Haloperidol Hydrochloride
2051 D15	X	712	720	-0.58562908	593	600	0.84874292	3456677	-0.69161882	3603202	-0.14571783	experimental	NIH	SAM001246769	Oligomycin C
2051 D16	X	671	680	-0.6892534	512	520	-1.10235136	3251407	-1.01169557	3692523	0.03051889	experimental	NIH	SAM001246620	Rifapentins
2051 D17	X	907	920	-0.09278168	672	680	-0.60139641	3949149	0.11771511	4167634	0.9739675	experimental	NIH	SAM001246763	Flumazenil
2051 D18	X	1471	1480	1.33268463	992	1000	0.40051348	4315576	0.71083774	4118430	0.87626097	experimental	NIH	SAM001246597	Rifaximin
2051 D19	X	749	760	-0.49211444	750	760	-0.35718088	3812105	-0.10411324	3839696	0.32276673	experimental	NIH	SAM001246764	Monoxidine Hcl
2051 D20	X	830	840	-0.28739322	632	640	-0.72663515	4193213	0.51277301	3899551	0.44162341	experimental	NIH	SAM001247080	Altanserin
2051 D21	X	870	880	-0.18629632	829	840	-0.10983437	3767437	-0.17641578	3272709	-0.80312405	experimental	NIH	SAM001246582	Lamivudine
2051 D22	X	1000	1000	0.12204927	712	720	-0.80765795	3702107	0.38068184	3702107	0.38068184	experimental	NIH	SAM001246873	Omidazole
2051 D23	E	383	720	-1.41715109	630	960	-0.73289709	56959	-6.18243731	58976	-7.18477364	empty			
2051 D24	P	112461	113360	281.851312	110063	110760	341.898369	3118338	-1.22708972	3171759	-1.00358486	empty			
2051 E01	N	997	1000	0.13468635	796	800	-0.21315633	4334471	0.74142241	2941778	-1.46026815	empty			
2051 E02	E	74	80	-2.19812465	76	80	-2.46745358	56589	-6.18303621	60369	-7.1820075	empty			
2051 E03	X	794	800	-0.37838043	475	480	-1.21819719	5332698	2.3572177	4187622	1.01365854	experimental	NIH	SAM001247069	Zacopride
2051 E04	X	1068	1080	0.31413335	741	480	-1.23072106	4531381	1.06015377	3889400	0.42146613	experimental	NIH	SAM001246575	Ramipril
2051 E05	X	1320	1320	0.82829782	752	760	-0.35718088	38347879	0.82891801	38347879	1.51493976	experimental	NIH	SAM001247051	Haloperidol Succinate
2051 E06	X	789	800	-0.39101754	479	760	-0.36031184	3448684	-0.69237016	3352501	0.61446776	experimental	NIH	SAM001246645	Azelastine Hcl
2051 E07	X	711	720	-0.58815665	631	640	-0.72976612	5200872	2.14383554	4606211	1.84486895	experimental	NIH	SAM001247003	Pancuronium
2051 E08	X	911	920	-0.08267199	832	840	-0.10044147	4761139	1.43205505	3848286	0.33982427	experimental	NIH	SAM001246649	Leptrozol
2051 E09	X	590	600	-0.89397462	751	760	-0.35404991	5614239	2.81293831	4089765	0.81933963	experimental	NIH	SAM001246693	Picrotin - Picrotoxinin
2051 E10	X	792	800	-0.38343527	831	840	-0.10357243	4245971	0.59817055	4117794	0.87499804	experimental	NIH	SAM001246702	Crotamiton
2051 E11	X	703	1040	0.22061871	873	880	0.02792824	4448974	0.92676443	4017660	0.67615759	experimental	NIH	SAM001247056	Clofibrate
2051 E12	X	1031	1040	0.49969671	627	640	-0.74228999	4111608	0.38068184	4028182	-1.18741904	experimental	NIH	SAM001246591	Tolterodine Tartrate
2051 E13	X	821	840	-0.31014002	788	800	-0.23820408	4521840	1.04471009	4519303	0.95280146	experimental	NIH	SAM001246679	Zincarnon
2051 E14	X	911	920	-0.08267199	552	560	-0.97711262	4225620	0.56522909	3906151	0.454272932	experimental	NIH	SAM001246687	Mecillinam
2051 E15	X	950	960	0.01589749	752	760	-0.35091894	4080837	0.33087389	4102573	0.84477304	experimental	NIH	SAM001246977	Fluvoxamine
2051 E16	X	911	920	-0.08267199	792	800	-0.2258602	3645885	-0.37316777	3674566	-0.0051391	experimental	NIH	SAM001246681	Triclabendazole
2051 E17	X	700	760	-0.4870596	631	640	-0.72976612	5463813	2.56944898	3937257	0.51649786	experimental	NIH	SAM001247019	N,n'-diacetyl-1,6-diaminohexane
2051 E18	X	746	760	-0.49969671	746	760	-0.36970475	3905080	0.04638215	4046863	0.73414726	experimental	NIH	SAM001246749	Valaciclovir Hydrochloride
2051 E19	X	831	840	-0.28486579	872	880	0.02479727	4621025	1.2052574	3563167	-0.22634895	experimental	NIH	SAM001246996	Pyrazinecarboxamide, 3,5-diamino-n-(aminoinimomethyl)
2051 E20	X	950	960	0.01589749	670	680	-0.60765835	4636033	1.22955032	3565404	-0.22190684	experimental	NIH	SAM001246717	Nifedipine Hcl
2051 E21	X	709	720	-0.59321134	1149	1160	0.89207552	4396539	0.84188972	3713248	0.07167343	experimental	NIH	SAM001246982	Indomethacin
2051 E22	X	749	760	-0.49211444	1028	1040	0.51322834	3566839	-0.50111677	3490362	-0.37092101	experimental	NIH	SAM001246731	Kitasamylin
2051 E23	E	625	1080	-0.80551484	697	1040	-0.5231222	56544	-6.18310905	57134	-7.18884318	empty			
2051 E24	P	153856	154600	386.473968	114440	115200	355.602617	3918821	0.06862423	3621984	-0.10955347	empty			
2051 F01	N	715	720	-0.57804681	515	520	-1.09295845	3709562	-0.27009602	3382963	-0.58418788	empty			
2051 F02	E	36	40	-2.59269232	36	40	-2.59269232	54378	-6.18661508	57879	-7.1869952	empty			
2051 F03	X	511	520	-1.093641	752	760	-0.35091894	3615000	-0.42316024	3821171	0.28598083	experimental	NIH	SAM001246733	Acarbose
2051 F04	X	1231	1240	0.72610322	1393	1400	1.65603181	3749541	-0.20538341	4086773	0.81339829	experimental	NIH	SAM001246775	Bifonazole
2051 F05	X	507	520	-1.1037507	349	360	-1.61269921	4090339	0.34625445	3927032	0.49619363	experimental	NIH	SAM001246737	Tranilast
2051 F06	X	1152	1160	0.52643684	1113	1120	0.77936066	4749144	1.41263916	4072948	2.03696382	experimental	NIH	SAM001246772	Calcitriol
2051 F07	X	830	840	-0.28739322	830	840	-0.1067034	4082103	0.33292312	4489006	1.61212987	experimental	NIH	SAM001246540	Pramipexole Hcl
2051 F08	X	791	800	-0.3859627	931	640	-0.72976612	4673998	1.29100295	4465833	1.56611424	experimental	NIH	SAM001246624	Linzolide
2051 F09	X	672	680	-0.68672598	631	600	-0.85500485	4523668	1.04766901	4227215	1.09228008	experimental	NIH	SAM001246541	Finasteride
2051 F10	X	551	560	-0.99261641	642	640	-0.72663515	4359119	0.78133927	4028182	-1.18741904	experimental	NIH	SAM001246556	Haloperidol Hydrochloride
2051 F11	X	907	920	-0.09278168	468	480	-1.24913997	3923375	0.07392663	4156975	0.95280146	experimental	NIH	SAM001246679	Zincarnon
2051 F12	X	2304	2320	3.438027											

2051 G07	X		712	720	-0.58562908	1072	1080	0.65099095	4792445	1.48272898	3995548	0.63224883	experimental	NIH	SAM001247010	Metronidazole
2051 G08	X		831	840	-0.28486579	829	840	-0.10983437	4304044	0.69217129	3932527	0.50710529	experimental	NIH	SAM001246650	Meropenem
2051 G09	X		671	680	-0.6892534	992	1000	0.40051348	4203546	0.52949868	4483443	1.60108318	experimental	NIH	SAM001247000	Terazosin
2051 G10	X		640	640	-0.7903533	711	720	-0.47928864	4290486	0.67022543	3845493	1.33626383	experimental	NIH	SAM001246659	Amifibutamide Hcl
2051 G11	X		670	680	-0.69178082	910	920	0.14377407	4217009	0.5539076	4270060	1.17329320	experimental	NIH	SAM001246987	Lorastidine
2051 G12	X		1105	1120	0.40764798	1347	1360	1.51200726	4102492	0.36592608	3291158	-0.76529762	experimental	NIH	SAM001246692	Carprofen
2051 G13	X		744	760	-0.50475155	826	840	-0.11922728	4746874	1.40896479	3736454	0.11775459	experimental	NIH	SAM001246975	Cisapride
2051 G14	X		592	600	-0.88891978	592	600	-0.85187388	3460868	-0.67264834	3536841	-0.27862564	experimental	NIH	SAM001246626	Atomoxetine Hcl
2051 G15	X		832	840	-0.28233837	631	640	-0.72976612	3910440	0.0550582	4039759	0.72004054	experimental	NIH	SAM001246976	Doxepin
2051 G16	X		671	680	-0.6892534	871	880	0.0216663	4057989	0.29389063	4173899	0.98640818	experimental	NIH	SAM001246617	Rofecoxib
2051 G17	X		711	720	-0.5881565	510	520	-1.10861329	4891550	1.64314679	3697650	0.04069998	experimental	NIH	SAM001247024	Diphenhydramine Hydrochloride
2051 G18	X		908	920	-0.09025426	1106	1120	0.75744388	3657248	-0.35477487	4245258	0.91239753	experimental	NIH	SAM001246748	Clarithromycin
2051 G19	X		829	840	-0.28992064	1111	1120	0.77309872	3769594	-0.17292432	3534716	-0.28284534	experimental	NIH	SAM001247002	9-amino-1,2,3,4-tetrahydroacridine Hydrochloride
2051 G20	X		908	920	-0.09025426	948	960	0.26275087	3661727	-0.34752487	3530404	-0.29140787	experimental	NIH	SAM001246721	Nategalid
2051 G21	X		1107	1120	0.41270283	1027	1040	0.51009737	4896289	1.65081765	4207619	1.05336745	experimental	NIH	SAM001246988	
2051 G22	X		947	960	0.00831522	1067	1080	0.63533611	3640795	-0.38140677	3724776	0.09456508	experimental	NIH	SAM001246732	Famciclovir
2051 G23	E		649	1120	-0.7448567	792	1240	-0.2256802	55081	-6.18547716	57807	-7.18709497	empty			
2051 G24	P	158653	159480	398.598013	150494	151280	468.486552	3434745	-0.71493273	3435827	-0.47921353	empty				
2051 H01	N		594	600	-0.88386493	1035	1040	0.5314512	3566455	-0.50173834	3253254	-0.30143587	empty			
2051 H02	E		116	120	-2.09197291	114	120	-2.34847678	53897	-6.18739366	59519	-7.18369538	empty			
2051 H03	X		592	600	-0.88891978	913	920	0.15316697	3114645	-1.23306746	3116959	-1.11240361	experimental	NIH	SAM001246739	Benpropine Phosphate
2051 H04	X		672	680	-0.68672598	629	640	-0.73602805	4817525	0.50356604	4953959	1.81982475	experimental	NIH	SAM001246579	Sumatriptan Succinate
2051 H05	X		551	560	-0.9925441	1031	1040	0.52262125	4050736	0.28215045	3775347	0.19498612	experimental	NIH	SAM001246652	Olanzapine
2051 H06	X		792	800	-0.38343527	1071	1080	0.64785998	4056261	0.29109357	4408652	1.45267444	experimental	NIH	SAM001246532	Difenphoxylate
2051 H07	X		470	480	-1.19726533	588	600	-0.86439776	4193040	0.51249298	3923517	0.48921374	experimental	NIH	SAM001246595	Risperidone
2051 H08	X		1080	1090	-0.32175654	1151	1160	0.89337346	3458560	0.67638422	3458560	0.57992413	experimental	NIH	SAM001246577	Alprazolone Dihd
2051 H09	X		909	920	-0.08772684	748	760	-0.35444281	4385022	0.61747556	3705114	0.05552139	experimental	NIH	SAM001246549	Zolopidine Tartrate
2051 H10	X		1030	1040	0.21809129	672	680	-0.60139641	4557464	1.10237342	3893201	0.42901394	experimental	NIH	SAM001246604	Analglidone Hcl
2051 H11	X		909	920	-0.08772684	790	800	-0.23194214	4700789	1.3343686	3491264	-0.36912987	experimental	NIH	SAM001246671	Latanoprost
2051 H12	X		1269	1280	0.82214528	909	920	0.1406431	4820357	1.52790916	4757543	2.14537549	experimental	NIH	SAM001246565	Terbinafine Hcl
2051 H13	X		1070	1080	0.31918819	910	920	0.14377407	4006347	0.21029952	3867457	0.37789296	experimental	NIH	SAM001246554	Carvastatin Na
2051 H14	X		551	560	-0.9925441	751	760	-0.35404991	4652715	1.25655289	3953049	0.54785672	experimental	NIH	SAM001247035	Milnacipran
2051 H15	X		511	520	-1.093641	952	960	0.27527474	4093881	0.35198776	4100007	0.83967762	experimental	NIH	SAM001246765	Oxymetolone
2051 H16	X		952	960	-0.08511994	1104	1120	-0.47649054	484369058	0.50114614	4224785	0.25939929	experimental	NIH	SAM001246528	911
2051 H17	X		951	960	0.01842491	952	960	-0.35091894	3621424	-0.41276194	3328493	-0.69235133	experimental	NIH	SAM001246776	Hydrosilone
2051 H18	X		909	920	-0.08772684	750	760	-0.35718088	4253414	0.61021827	3863628	0.37028954	experimental	NIH	SAM001246779	2',3'-dideoxycytidine
2051 H19	X		1028	1040	0.21303645	627	640	-0.74228999	4406345	0.85776235	3600788	-0.15164329	experimental	NIH	SAM001246571	Pefloxacin Mesylate
2051 H20	X		1308	1320	0.92071476	1469	1480	1.89388541	3758245	-0.19129455	3951339	0.54485824	experimental	NIH	SAM001246563	Indrubicin
2051 H21	X		1107	1120	0.41270283	1106	1120	0.75744388	3975250	0.15996389	3623178	-0.10718249	experimental	NIH	SAM001246538	Esomeprazole Mg
2051 H22	X		1188	1200	0.61742405	1148	1160	0.88894555	3600619	-0.44643826	3543108	-0.26618098	experimental	NIH	SAM001246893	Pirfenperone
2051 H23	E		1089	1100	-0.71958247	954	960	-0.71958247	55079	-6.1854804	55079	-7.18578247	empty			
2051 H24	P	141267	142080	354.656245	118911	119640	369.601177	3510227	-0.59275265	3358510	-0.63274527	empty				
2051 I01	N		1236	1240	0.73740333	835	840	-0.09104856	4678422	1.29816392	3168420	-1.01021526	empty			
2051 I02	E		73	80	-2.20065208	114	120	-2.34847678	57808	-6.18106306	60736	-7.18127873	empty			
2051 I03	X		953	960	0.02347976	912	920	0.15003601	5623617	2.82811815	4136862	0.9128622	experimental	NIH	SAM001246964	3'-deoxydenosine
2051 I04	X		868	880	-0.19135116	910	920	0.14377407	4511365	1.02775457	3708659	0.06256085	experimental	NIH	SAM001246751	19-nortestosterone
2051 I05	X		1070	1080	0.31918819	786	800	-0.24446601	3766984	-0.17714903	3043779	-1.25057165	experimental	NIH	SAM001247059	Duloxetine
2051 I06	X		798	800	-0.01589749	850	860	0.12660361	4186300	0.50114614	3047924	0.57798243	experimental	NIH	SAM001246760	Benzetone
2051 I07	X		791	800	-0.3859627	689	680	-0.61078932	4192837	0.51216439	3425417	-0.49988212	experimental	NIH	SAM001246678	Benzeneacetic Acid, Alpha-(hydroxymethyl)-, 9-methyl-
2051 I08	X		830	840	-0.28739322	750	760	-0.35718088	4000523	0.20087242	3775578	0.19580226	experimental	NIH	SAM001246637	Orlista
2051 I09	X		910	920	-0.08519941	1312	1320	1.40242337	4689845	1.31665393	3809340	0.2624875	experimental	NIH	SAM001247027	Diphenylcyclopropenone
2051 I10	X		829	840	-0.28992064	628	640	-0.73915902	4066678	0.30795521	3667416	-0.1933717	experimental	NIH	SAM001246638	Alfuzosin
2051 I11	X		871	880	-0.18376889	952	960	0.27527474	4268548	0.63471515	3763806	0.17206865	experimental	NIH	SAM001247037	Phenelzine Sulfate Salt
2051 I12	X		710	720	-0.59068392	949	960	-0.98650553	3768819	-0.17417878	3326749	-0.69635062	experimental	NIH	SAM001246633	Methyl Paroxetine
2051 I13	X		790	800	-0.38849012	592	1000	0.40051348	3578532	-0.48218972	3343574	-0.66240433	experimental	NIH	SAM001246981	Indralatine
2051 I14	X		952	960	0.02095233	712	720	-0.47615768	3541019	-0.54291071	3224785	-0.89828883	experimental	NIH	SAM001246528	Artesunate
2051 I15	X		622	640	-0.8130971	545	560	-0.9990294	3572987	-0.49116522	3454835	-0.44146852	experimental	NIH	SAM001247046	Trifluoperazine Dihydrochloride
2051 I16	X		1151	1160	0.52390942	591	600	-0.85500485	3987655	0.18004343	3767787	0.1799739	experimental	NIH	SAM001246618	Bisoprolol Fumarate
2051 I17	X		590	600	-0.89397462	552	560	-0.97711262	4239698	0.58801666	3417979	-0.51465509	experimental	NIH	SAM001246978	Galanthamine
2051 I18	X		910	920	-0.08519941	910	1000	0.39738251	3489957	-0.62556299	3200456	-0.94659998	experimental	NIH	SAM001246750	Aripiprazole
2051 I19	X		1149	1160	0.51885457	990	1000	0.39425154	3857292	-0.03097062	4051067	0.74249533	experimental	NIH	SAM001247008	Ethinylestradiol
2051 I20	X		1188	1200	0.61742405	947	960	0.2596199	3831313	-0.07302192	3674133	-0.00599893	experimental	NIH	SAM001246722	Megestrol Acetate
2051 I21	X		788	800	-0.39354496	1026	1040	0.51635931	3037315	-1.35823883	2961336	-1.42143098	experimental	NIH	SAM001246673	Paroxetine
2051 I22	X		867	880	-0.19387858	827	840	-0.11609631	3505113	-0.6010305	3502519	-0.34678033	experimental	NIH	SAM001246725	Sotalol Hydrochloride
2051 I23	E		524	880	-1.06078451	664	960	-0.62644416	56167	-6.18371929	57085	-7.18852868	empty			
2051 I24	P	119429	120160	299.462392	98634	99400	306.114531	3646006	-0.37297191	3445398	-0.46020798	empty				
2051 J01	N		713	720	-0.58310165	555	560	-0.96771972	3459521	-0.67482868	3106262	-1.13364511	empty			
2051 J02	E		75	80	-2.19559723	76	80	-2.46745358	54273	-6.186678504	57312	-7.18807791	empty			
2051 J03	X		831	840	-0.28486579	712	720	-0.47615768	3695490	-0.29287388	3603291	-0.14667298	experimental	NIH	SAM001246740	Phenprobamate
2051 J04	X		1349	1360	1.02433943	1026	1040	0.5060964	4042192	0.268320						

2051 K01	N	1156	1160	0.53654653	636	640	-0.71411127	4426306	0.89007253	3440011	-0.47090518	empty		
2051 K02	E	34	40	-2.2992155	636	40	-2.59269232	57040	-6.1823062	58407	-7.18590352	empty		
2051 K03	X	872	880	-0.18124147	632	640	-0.72663515	4560366	1.10707078	4948086	2.52374502	experimental	NIH	SAM001246965
2051 K04	X	981	1000	0.09424759	1146	1160	0.08268261	4532357	1.06319038	4235727	1.10920259	experimental	NIH	SAM001246752
2051 K05	X	1030	1040	0.21809129	706	720	-0.49494349	4625311	1.213129499	4453116	1.25215488	experimental	NIH	SAM001247060
2051 K06	X	870	880	-0.18629632	831	840	-0.10357243	4242351	0.59231098	3801971	0.24785455	experimental	NIH	SAM001246642
2051 K07	X	550	560	-0.99507153	790	800	-0.23194214	3517808	-0.58048155	3763467	0.17139548	experimental	NIH	SAM001246968
2051 K08	X	991	1000	0.11952181	671	680	-0.60452738	3790448	-0.13916867	3493587	-0.36451699	experimental	NIH	SAM001246631
2051 K09	X	831	840	-0.28486579	1032	1040	0.52575222	4633089	1.22478497	4246495	1.1314588	experimental	NIH	SAM001247016
2051 K10	X	625	640	-0.80551483	628	640	-0.73915902	4243635	0.59938934	3925803	0.489375315	experimental	NIH	SAM001246639
2051 K11	X	2712	2720	4.46921599	1470	1480	1.89711638	4617366	1.1953347	4434824	1.50453832	experimental	NIH	SAM001246997
2051 K12	X	666	680	-0.70189073	829	840	-0.10983437	3425870	-0.72929839	3325137	-0.60377923	experimental	NIH	SAM001246634
2051 K13	X	751	760	-0.48705956	552	560	-0.97711262	4328425	0.73163596	4031365	0.70337221	experimental	NIH	SAM001247045
2051 K14	X	911	920	-0.08267199	753	760	-0.34778797	4017064	0.22764676	3726026	0.09704726	experimental	NIH	SAM001246679
2051 K15	X	781	800	-0.41123692	864	880	-0.00025048	3917201	0.066002	3883735	0.41021689	experimental	NIH	SAM001247023
2051 K16	X	710	720	-0.59068392	1030	1040	0.51949028	3730725	-0.23584021	3836738	0.3168929	experimental	NIH	SAM001246623
2051 K17	X	911	920	-0.08267199	672	680	-0.60139641	4483820	0.98316844	3913707	0.463973359	experimental	NIH	SAM001246980
2051 K18	X	988	1000	0.11193954	750	760	-0.35718088	3657644	-0.35413388	3782806	0.20979778	experimental	NIH	SAM001246747
2051 K19	X	1469	1480	1.32762978	1309	1320	1.39303046	458140	1.10348764	4445553	1.52584336	experimental	NIH	SAM001247012
2051 K20	X	909	920	-0.08772684	1068	1080	0.63846708	3960769	0.136524	3651896	-0.05015591	experimental	NIH	SAM001246728
2051 K21	X	790	800	-0.38849012	749	760	-0.36031184	3987985	0.18057759	3575754	-0.2013544	experimental	NIH	SAM001247031
2051 K22	X	787	800	-0.39607239	1229	1240	1.14255299	3892260	0.02563087	4100318	0.84029518	experimental	NIH	SAM001246726
2051 K23	E	521	880	-1.06836678	500	840	-1.13992298	55238	-6.18522303	58470	-7.18577842	empty		
2051 K24	P	120782	121480	302.881995	113386	114160	352.302577	387165	-0.00773792	3531929	-0.28837651	empty		
2051 L01	N	712	720	-0.58562908	835	840	-0.09104896	3785536	-0.14741092	3608030	-0.13726254	empty		
2051 L02	E	115	115	-0.09450323	75	120	-2.0945045	52489	-6.1886227	55216	-7.19429403	empty		
2051 L03	X	784	800	-0.40365453	670	680	-0.60765835	3706001	-0.27586009	3689011	0.02354496	experimental	NIH	SAM001246743
2051 L04	X	3310	3320	5.98061467	2311	2320	4.53026081	2717504	-1.87590576	2902972	-1.53732692	experimental	NIH	SAM001246708
2051 L05	X	501	520	-1.11891523	707	720	-0.49181252	4379967	0.8150652	3991181	0.62357709	experimental	NIH	SAM001246654
2051 L06	X	872	880	-0.18124147	911	920	0.14690504	3991820	0.18678517	4153418	0.94573817	experimental	NIH	SAM001247013
2051 L07	X	711	720	-0.5881565	671	680	-0.60452738	3836013	-0.06541419	4115750	0.87093918	experimental	NIH	SAM001246552
2051 L08	X	793	800	-0.38090785	872	880	0.02479727	3744129	-0.21414362	3254550	-0.83918317	experimental	NIH	SAM001246548
2051 L09	X	431	440	-1.29583481	591	600	-0.85500485	3826153	-0.08137423	3899692	0.4419034	experimental	NIH	SAM001246601
2051 L10	X	390	400	-0.38343327	600	610	-0.85500485	4105503	-0.2648424	3789242	-1.0642081	experimental	NIH	SAM001246594
2051 L11	X	865	880	-0.19893343	909	920	0.1406431	3278724	-0.96747849	3408611	-0.53325753	experimental	NIH	SAM001246666
2051 L12	X	830	840	-0.28739322	910	920	0.14377407	4007325	0.21188258	4080991	0.81800124	experimental	NIH	SAM001246581
2051 L13	X	831	840	-0.28486579	752	760	-0.35091894	3885698	0.01500919	3728905	0.10276421	experimental	NIH	SAM001246562
2051 L14	X	749	760	-0.49211444	692	600	-0.85187388	4039957	0.26470286	4415138	1.46544697	experimental	NIH	SAM001247022
2051 L15	X	1112	1120	0.42533994	572	680	-0.60139641	3645438	-0.37389131	3574857	-0.20313561	experimental	NIH	SAM001246720
2051 L16	X	790	800	-0.38849012	751	760	-0.35404991	4357832	0.77923605	3666193	-0.02176574	experimental	NIH	SAM001246755
2051 L17	X	951	960	-0.11952181	813	820	-0.25813851	3712953	-0.26460389	3712953	0.13378256	experimental	NIH	SAM001246633
2051 L18	X	708	720	-0.59573877	870	880	0.01853533	4282963	0.65804821	3869834	0.38261307	experimental	NIH	SAM001247077
2051 L19	X	949	960	0.01337007	1068	1080	0.63846708	4025255	0.24090524	3488806	-0.37401083	experimental	NIH	SAM001246591
2051 L20	X	749	760	-0.49211444	868	880	0.0122734	4220079	0.55626007	3973910	0.58928131	experimental	NIH	SAM001246871
2051 L21	X	790	800	-0.38849012	710	720	-0.48241961	3423242	-0.73355224	3442013	-0.466692972	experimental	NIH	SAM001246567
2051 L22	P	1069	1080	0.31666077	948	960	0.26275087	4035658	0.25774422	3747613	0.1399135	experimental	NIH	SAM001246867
2051 L23	E	493	880	-1.13913661	798	1160	-0.20689439	54774	-6.18597409	58508	-7.18570296	empty		
2051 L24	P	130084	130760	326.392079	121890	122520	378.926028	3395020	-0.77923421	311133	-1.0642081	empty		
2051 M01	N	1394	1400	1.3807309	875	880	0.03419018	4190330	0.5081064	3270337	-0.8078423	empty		
2051 M02	E	72	80	-2.2031795	75	80	-2.47058455	53015	-6.18882132	56326	-7.19003586	empty		
2051 M03	X	1149	1160	0.51885457	555	560	-0.96771972	4472319	0.96455217	3506044	-0.33978058	experimental	NIH	SAM001246962
2051 M04	X	1260	1280	0.79939847	628	640	-0.73915902	3936672	0.09751902	3851861	0.3469233	experimental	NIH	SAM001246753
2051 M05	X	1429	1440	1.22653288	631	640	-0.72976612	4307180	0.62724742	3475999	-0.39944224	experimental	NIH	SAM001247057
2051 M06	X	708	720	-0.59573877	831	840	-0.10357243	3773073	-0.16729298	3455638	-0.43987397	experimental	NIH	SAM001246643
2051 M07	X	871	880	-0.18376889	551	560	-0.98024359	3617312	-0.41941789	3630952	-0.09174532	experimental	NIH	SAM001246969
2051 M08	X	390	400	-1.39945913	712	720	-0.47615768	3790728	-0.13871545	3726101	0.09719519	experimental	NIH	SAM001246694
2051 M09	X	673	680	-0.68419855	672	680	-0.60139641	3304393	-0.92592898	3384425	-0.58164216	experimental	NIH	SAM001247051
2051 M10	X	832	840	-0.28233837	952	960	0.27527474	3449251	-0.69145237	3483785	-0.38398125	experimental	NIH	SAM001246632
2051 M11	X	749	760	-0.49211444	709	720	-0.48555058	3293099	-0.94421018	2823400	-1.6953365	experimental	NIH	SAM001247004
2051 M12	X	951	960	0.01842491	871	880	0.0216663	4210290	0.54041495	3702792	0.05091049	experimental	NIH	SAM001246635
2051 M13	X	828	840	-0.29244806	790	800	-0.23194214	4000537	0.20089508	3656193	-0.04162317	experimental	NIH	SAM001246995
2051 M14	X	752	760	-0.48453217	632	640	-0.72663515	4045809	0.27417529	3539711	-0.27292655	experimental	NIH	SAM001246674
2051 M15	X	551	560	-0.9925441	631	640	-0.72976612	3833565	-0.06937669	3764524	0.17349441	experimental	NIH	SAM001247049
2051 M16	X	632	640	-0.78782288	671	680	-0.60452738	4113264	0.3836235	3915008	0.47231705	experimental	NIH	SAM001246625
2051 M17	X	629	640	-0.79540515	1191	1200	1.02357619	3516931	-0.58190112	3552023	-0.24847808	experimental	NIH	SAM001247028
2051 M18	X	1070	1080	0.31918819	988	1000	0.38798961	3675501	-0.32522938	3799509	0.24296565	experimental	NIH	SAM001246746
2051 M19	X	708	720	-0.59573877	987	1000	0.38485864	3569804	-0.49631743	3593537	-0.16604192	experimental	NIH	SAM001246985
2051 M20	X	1111	1120	0.42281252	1149	1160	0.89207552	3704190	-0.28789149	3861334	0.365737425	experimental	NIH	SAM001246738
2051 M21	X	828	840	-0.29244806	989	1000	0.39112057	3718016	-0.25641183	3754514	0.15361712	experimental	NIH	SAM001247020
2051 M22	X	1269	1280	0.82214528	670	680	-0.60139641	3518276	-0.57972401	3718223	0.14628074	experimental	NIH	SAM001246778
2051 M23	X	669	680	-0.90026024	574	580	-0.86126132	4058378	-0.38791809	56330	-7.19002791	empty		
2051 M24	P	110126	111040	275.94978	101615	102360	315.447948	3444220	-0.69959588	3269162	-0.81016748	empty		
2051 N01	N	1151	1160	0.52390942	834	840	-0.09417953	3457337	-0.67836385	2980274	-1.38382497	empty		
2051 N02	E	71	80	-2.20570692	76	80	-2.46745358	50276	-6.19325485	53938	-7.19477781	empty		
2051 N03	X	1749	1760	2.03530809	474	480	-1.22132816	2715737	-1.87876594	3000167	-1.34432257	experimental	NIH	SAM001246736
2051 N04	X	1064	1080	0.30402366	592									

2051 N19	X	988	1000	0.11193954	1189	1200	1.01731426	3605556	-0.43844691	3653645	-0.04668285	experimental	NIH	SAM001246583	Fluticasone Propionate
2051 N20	X	868	880	-0.19135116	747	760	-0.36657378	3772544	-0.16814925	3551721	-0.24907777	experimental	NIH	SAM001246897	Delta1-hydrocortisone 21-hemisuccinate Sodium Salt
2051 N21	X	989	1000	0.11446697	1030	1040	0.51949028	3187505	-1.11513151	3338034	-0.67340535	experimental	NIH	SAM001246576	Tropisetron Hcl
2051 N22	X	986	1000	0.1068847	708	720	-0.48686155	3737185	-0.22538364	3184155	-0.95812115	experimental	NIH	SAM001246588	Benactyzine Hydrochloride
2051 N23	E	738	1280	-0.51991609	764	1160	-0.31334732	54001	181272532	56255	-7.19017486	empty			
2051 N24	P	183220	184000	460.689203	133088	133800	413.988916	3471994	-0.65463907	3360123	-0.62954226	empty			
2051 O01	N	1513	1520	1.43883637	1154	1160	0.90773036	3625966	-0.40540996	3155811	-1.0352535	empty			
2051 O02	E	111	120	-2.10461002	74	80	-2.47371552	53754	-6.18762513	56363	-7.18996238	empty			
2051 O03	X	1347	1360	1.01928423	754	760	-0.344657	3961447	0.13762145	3314640	-0.71985984	experimental	NIH	SAM001246963	Nifedipine
2051 O04	X	1344	1360	1.01170197	711	720	-0.47928864	3538920	-0.54630829	3332962	-0.68347704	experimental	NIH	SAM001246754	Trileptal
2051 O05	X	1426	1440	1.21895061	711	720	-0.47928864	3895711	0.03121688	3593229	-0.16665353	experimental	NIH	SAM001247039	Progesterone
2051 O06	X	903	920	-0.10289137	710	720	-0.48241961	3366517	-0.82537102	362345	-0.10905505	experimental	NIH	SAM001246700	Idebenone
2051 O07	X	1310	1320	0.9257696	671	680	-0.60452738	3453337	-0.68483851	3457245	-0.43668288	experimental	NIH	SAM001246970	Capsaicin
2051 O08	X	826	840	-0.29750291	672	680	-0.60139641	3487980	-0.62876309	3225606	-0.89665853	experimental	NIH	SAM001246695	Cetaxate Hcl
2051 O09	X	1190	1200	0.6224789	711	720	-0.47928864	3672543	-0.33001739	3737274	0.1193829	experimental	NIH	SAM001247053	3(2h)-pyridazinone, 6-[4-(difluoromethoxy)-3-methoxy]
2051 O10	X	789	800	-0.39101754	871	880	0.0216663	3222319	-1.0587793	3217672	-0.91241342	experimental	NIH	SAM001246688	Perospirone Hcl
2051 O11	X	946	960	0.0057878	988	1000	0.38798961	3517975	-0.58021123	3383510	-0.58310168	experimental	NIH	SAM001247026	Normeticine
2051 O12	X	750	760	-0.48958702	671	680	-0.60452738	3378983	-0.80519274	3267376	-0.81371402	experimental	NIH	SAM001246636	Terazosolone
2051 O13	X	786	800	-0.39859981	508	520	-1.11487523	3234010	-1.03985549	3280493	-0.93064056	experimental	NIH	SAM001247001	Urapidil Hydrochloride
2051 O14	X	752	760	-0.48453217	1030	1040	0.51949028	3128295	-1.21097268	3279442	-0.78975404	experimental	NIH	SAM001246680	Bufomedil Hydrochloride
2051 O15	X	827	840	-0.29497548	1625	1640	2.38241648	2998650	-1.42082452	3077363	-1.19103111	experimental	NIH	SAM001246989	Maprotiline Hcl
2051 O16	X	1547	1560	1.52476874	1748	1760	2.76752556	2584197	-2.09168516	2665935	-2.00802161	experimental	NIH	SAM001246676	Idarubicin Hcl
2051 O17	X	1665	1680	1.8230046	827	840	-0.11609631	3216288	-1.06854147	3483634	-0.38428109	experimental	NIH	SAM001246994	Piribedil
2051 O18	X	1546	1560	1.52224136	989	1000	0.39112057	3117838	-1.22789906	3117840	-1.11065417	experimental	NIH	SAM001246719	Nisoldipine
2051 O19	X	1107	1120	0.41270283	908	920	0.13751213	3248933	-1.01570015	3320902	-0.70742511	experimental	NIH	SAM001247043	Trmp
2051 O20	X	869	880	-0.18882374	710	720	-0.48241961	3299818	-0.93335137	3481361	-0.26242566	experimental	NIH	SAM001246759	Stavudine
2051 O21	X	908	920	-0.09025426	868	880	0.0122734	3654468	-0.35924563	327721	-0.79418423	experimental	NIH	SAM001246785	Oxirane-carboxylic Acid, 2-[6-(4-chlorophenoxy)hexyl]-,
2051 O22	X	1427	1440	1.22147804	948	960	0.26275087	3089739	-1.27338193	3228894	-0.88995069	experimental	NIH	SAM001246872	Alsetron Hcl
2051 O23	E	692	1160	-0.63617753	897	1320	0.10307148	53146	-6.18860928	56252	-7.1901828	empty			
2051 O24	P	155821	157240	391.440353	141562	142480	440.520743	3043037	-1.34897683	3206432	-0.93473318	empty			
2051 P01	N	995	1000	0.1296315	1036	1040	0.53827609	2817278	-1.71440506	3023131	-1.29872195	empty			
2051 P02	E	73	80	-2.20065208	115	120	-2.34534582	51639	-6.19104861	57637	-7.18743256	empty			
2051 P03	X	1272	1280	0.82972754	755	760	-0.34152603	3124655	-1.21686462	3148724	-1.05529795	experimental	NIH	SAM001246741	Lomifylline
2051 P04	X	1486	1520	1.32762978	874	880	-0.48202523	3802826	-0.59092699	3495169	-0.91496172	experimental	NIH	SAM001246577	Quetiapine Hemifumarate
2051 P05	X	1146	1160	0.5112723	912	920	-0.47615768	3064436	-1.31433902	3050343	-1.2446859	experimental	NIH	SAM001246656	Pravastatin Sodium
2051 P06	X	1952	1960	2.54837487	1193	1200	1.02983813	3540966	-0.5429965	3807857	0.25954264	experimental	NIH	SAM001246596	Toradol
2051 P07	X	707	720	-0.59826619	953	960	0.27840571	3282958	-0.96062506	3547453	-0.25755292	experimental	NIH	SAM001246603	Valdecobix
2051 P08	X	1032	1040	0.22314614	873	880	-0.59826544	3277241	-0.96987897	3444159	-0.46266832	experimental	NIH	SAM001246555	Ethylestrenol
2051 P09	X	1070	1080	0.31918819	673	680	0.02792824	3205013	-1.08679192	3140964	-1.06473584	experimental	NIH	SAM001246665	Fenoldopam Mesylate
2051 P10	X	1108	1120	0.41523025	110	920	0.14377407	3029005	-1.37168994	3184021	-0.97923568	experimental	NIH	SAM001246599	Citalopram Hydrobromide
2051 P11	X	2191	2200	-0.2422895	1212	1220	-0.2422895	3258808	-2.0842125	3278242	-0.91496172	experimental	NIH	SAM001246559	Epinuridine Hydrochloride
2051 P12	X	987	1000	0.10941212	669	680	-0.61078932	3236174	-1.03635269	3342973	-0.66359777	experimental	NIH	SAM001246629	Glycopyrrate
2051 P13	X	1673	1680	1.84322398	1274	1280	1.28344657	3253436	-1.0084113	3161965	-1.02303324	experimental	NIH	SAM001246608	Rosiglitazone Hcl
2051 P14	X	629	640	-0.79540515	829	840	-0.10983437	3155266	-1.16731566	3167769	-1.01150798	experimental	NIH	SAM001246675	Formoterol Fumarate Dihydrate
2051 P15	X	1313	1320	0.93335187	1310	1320	1.39616143	3278673	-0.96756104	3158942	-1.02903614	experimental	NIH	SAM001246713	Mosapride Citrate
2051 P16	X	949	960	0.01337007	1028	1040	0.51322834	3556890	-0.51722087	3473023	-0.40535182	experimental	NIH	SAM001246602	Telmisartan
2051 P17	X	830	840	-0.28739322	1111	1120	0.177309872	3233341	-1.04093837	3330616	-0.6881356	experimental	NIH	SAM001246587	Mofadalin
2051 P18	X	750	760	-0.48958702	1071	1080	0.64785998	3407505	-0.75902517	3481626	-0.26242566	experimental	NIH	SAM001247074	Adimav Sulphate
2051 P19	X	912	920	-0.08014457	871	880	0.02146663	1121814	-1.22146204	3072898	-1.19989784	experimental	NIH	SAM001246588	Diazoxide
2051 P20	X	952	960	0.02095233	991	1000	0.39738251	3485440	-0.6328745	3300441	-0.74805541	experimental	NIH	SAM001246872	Ranolazine Dihydrochloride
2051 P21	X	871	880	-0.18376889	991	1000	0.39738251	3032729	-1.36566203	2977452	-1.38942874	experimental	NIH	SAM001246534	Dichloroacetic Acid
2051 P22	X	1228	1240	0.71852095	1270	1280	1.27092227	3151857	-1.17283369	3070605	-1.20445077	experimental	NIH	SAM001246870	
2051 P23	E	790	1680	-0.38849012	825	1360	-0.12235825	54221	-6.18686921	57642	-7.18742262	empty			
2051 P24	P	304500	304960	767.215008	181704	182120	566.204077	2819164	-1.71135226	2840330	-1.66171786	empty			
2052 A01	N	1674	1680	0.61709919	2198	2200	2.22940244	2551811	-1.56124526	2859326	-1.50151987	empty			
2052 A02	E	110	120	-1.87295017	29	40	-2.48202533	52977	-5.8647315	52062	-6.19509352	empty			
2052 A03	X	1594	1600	0.48973093	1635	1640	1.00647305	2143871	-2.2637986	2415953	-2.24282124	experimental	NIH	SAM001246806	Bestatin
2052 A04	E	72	80	-1.93345009	70	80	-2.39296653	55869	-5.8597509	55621	-6.18914309	empty			
2052 A05	X	1232	1240	-0.08661041	1677	1680	1.09770402	2927859	-0.91361625	3459736	-0.49767108	experimental	NIH	SAM001246862	Tryptoline
2052 A06	E	33	40	-1.99554211	31	40	-2.477681	54236	-5.86256325	55548	-6.18926515	empty			
2052 A07	X	911	920	-0.59767553	1554	1560	0.83052762	2926539	-0.91588955	3777228	0.03315612	experimental	NIH	SAM001246891	Mepirizole
2052 A08	E	72	80	-1.93345009	69	80	-2.39513869	56225	-5.8591378	57156	-6.18657667	empty			
2052 A09	X	1629	1640	0.54545455	1071	2000	1.78193627	34486056	-0.02117855	3945964	0.31527239	experimental	NIH	SAM001246869	Homoveratrylamine
2052 A10	E	69	80	-1.9382264	108	120	-2.31042422	53209	-5.8643195	57019	-6.18680572	empty			
2052 A11	X	1912	1920	0.99601974	1396	2000	1.79062493	3406685	-0.0889832	3439000	-0.5323404	experimental	NIH	SAM001246857	Dehydrochloric Acid
2052 A12	E	107	120	-1.87772648	70	80	-2.39296653	54594	-5.8619467	53688	-6.19237495	empty			
2052 A13	X	2437	2440	1.83187391	1519	1520	0.75450181	3617397	0.27390453	3526079	-0.38674964	experimental	NIH	SAM001246906	Medroxyprogesterone
2052 A14	E	68	80	-1.9398185	0	0	-2.54501814	54214	-5.86260114	56286	-6.18803126	empty			
2052 A15	X	1557	1560	0.43082312	1398	1400	0.49166974	3294950	-0.28141296	3904432	0.24583342	experimental	NIH	SAM001247092	Nafadotride
2052 A16	E	110	120	-1.87295017	67	70	-2.39707856	4907143	-5.87017364	49817	-6.20110166	empty			
2052 A17	X	1996	2000	1.12975641	1436	1440	0.57421205	3678669	-0.37942703	2970261	-5.16204333	experimental	NIH	SAM001247091	Methanesulfonamide, N-[4-[1-[2-(6-methyl-2-pyridinyl)]
2052 A18	E	110	120	-1.87295017	112	120	-2.30173556	55220	-5.86086861	53681	-6.19238666</				

2052 B13	X		910	920	-0.59926763	193	200	-2.12579013	2213213	-2.14437797	1781971	-3.30279151	experimental	NIH	SAM001247099	
2052 B14	E		74	80	-1.93026588	77	80	-2.37776137	62503	-5.84832584	60038	-6.18175814	empty			
2052 B15	E		990	1000	-0.47189938	632	640	-1.17220991	3878071	0.7228367	4158378	0.6704156	empty			
2052 B16	E		33	40	-1.99554641	114	120	-2.29739123	60300	-5.85211986	57574	-6.18507778	empty			
2052 B17	E		1191	1200	-0.15188664	1153	1160	-0.04051089	3884892	0.73458381	4241626	0.80960116	empty			
2052 B18	E		113	120	-1.86817386	73	80	-2.38645003	61138	-5.85067664	59598	-6.18249379	empty			
2052 B19	E		872	880	-0.65976755	953	960	-0.47494407	3586610	0.22088322	3988297	0.38605057	empty			
2052 B20	E		155	160	-1.80130552	153	160	-2.21267676	62357	-5.84857728	58947	-6.18358223	empty			
2052 B21	E		753	760	-0.84922783	1232	1240	0.13109021	3382079	-0.1313596	3802681	0.07571198	empty			
2052 B22	E		155	160	-1.80130552	192	200	-2.12796228	58609	-5.85503208	59288	-6.18303121	empty			
2052 B23	E	489	800	-1.26954307	637	1120	-1.16134488	60791	-5.85127424	59401	-6.18444951	empty				
2052 B24	P	104633	105360	164.538499	163270	164240	352.104503	2720783	-1.27024207	3111958	-0.99680035	empty				
2052 C01	N		951	960	-0.5339914	1395	1400	0.48515325	3350091	-0.18644926	3517585	-0.40095109	empty			
2052 C02	E		37	40	-1.9891737	35	40	-2.46899233	60556	-5.85167896	57399	-6.18617039	empty			
2052 C03	X		28	40	-2.00350263	71	80	-2.39079436	1311332	-3.69759537	1475378	-3.81539625	experimental	NIH	SAM001246774	Toremifene Citrate
2052 C04	E		76	80	-1.92708167	76	80	-2.37993353	58504	-5.85521291	58186	-6.18485457	empty			
2052 C05	X	1187	1200	-0.15825505	1154	1160	-0.03833873	1943210	-2.60937652	2664412	-1.82740415	experimental	NIH	SAM001246863	Fluphenazine Hydrochloride	
2052 C06	E		34	40	-1.99395001	33	40	-2.47333666	58559	-5.85511819	57933	-6.18527757	empty			
2052 C07	X		587	600	-1.11351696	1191	1200	0.04203141	2855217	-1.03872014	3907877	0.25159325	experimental	NIH	SAM001246876	6-azauridine
2052 C08	E		76	80	-1.92708167	111	120	-2.30390773	58289	-5.85558318	57005	-6.18682913	empty			
2052 C09	X		745	760	-0.86196466	1709	1720	1.16721333	3495158	0.0633848	4150591	0.65739621	experimental	NIH	SAM001246913	Tinidazole
2052 C10	E		74	80	-1.93026588	72	80	-2.3886222	55770	-5.8599214	56226	-6.18813157	empty			
2052 C11	X	1149	1160	-0.21875498	833	840	-0.73560397	3648129	0.32683111	3998842	0.40368117	experimental	NIH	SAM001246884	Cefaclor	
2052 C12	E		113	120	-1.86817386	75	80	-2.3821057	57228	-5.85741043	56241	-6.18810649	empty			
2052 C13	X	953	960	-0.5308072	677	680	-1.07446185	3777667	0.54992116	4046768	0.48381051	experimental	NIH	SAM001246907	Pinacidil Monohydrate	
2052 C14	E		73	80	-1.93450999	114	120	-2.38427786	57642	-5.85665749	57398	-6.19204056	empty			
2052 C15	X	1635	1640	0.55500716	1195	1200	0.05072007	4375831	-0.08097784	4668951	1.52406202	experimental	NIH	SAM001246885	Desoximetasone	
2052 C16	E		112	120	-1.86976596	73	80	-2.38645003	55811	-5.85985079	55496	-6.18935209	empty			
2052 C17	X	954	960	-0.52921509	874	880	-0.64654517	3676556	0.37578802	4100372	0.57343312	experimental	NIH	SAM001247076	2h-indol-2-one, 1,3-dihydro-1-phenyl-3,3-bis(4-pyridiny	
2052 C18	E		73	80	-1.93185798	75	80	-2.3821057	59222	-5.85397637	57275	-6.18637771	empty			
2052 C19	X	995	1000	-0.46393886	755	760	-0.90503291	4111130	1.12421038	4393387	1.06333627	experimental	NIH	SAM001246815	Chlordiazepoxide	
2052 C20	E		153	160	-1.80448973	194	200	-2.12361796	57768	-5.85648045	58559	-6.18423094	empty			
2052 C21	X	1074	1080	-0.33816271	912	920	-0.56400287	2889925	-0.9789461	3248640	-0.85061068	experimental	NIH	SAM001246883	Cyproheptadine Hydrochloride	
2052 C22	E		115	120	-1.86658175	154	160	-2.21050459	56893	-5.85805213	57114	-6.18699545	empty			
2052 C23	E		429	720	-1.36506926	660	1040	-1.11138867	57265	-5.85734671	58431	-6.18444495	empty			
2052 C24	P	98597	99120	154.928515	128336	129160	276.222061	2709787	-1.28917935	3510920	-0.41209456	empty				
2052 D01	N		1314	1320	0.04394205	993	1000	-0.38805743	3433587	-0.04265264	3212784	-0.91055972	empty			
2052 D02	E		110	120	-1.87295017	113	120	-2.29956339	61508	-5.85003943	61459	-6.17938232	empty			
2052 D03	X	2116	2120	1.32080879	1156	1160	-0.0339944	3408379	-0.0860658	3242478	-0.86091317	experimental	NIH	SAM001246570	Vincristine Sulfate	
2052 D04	E		68	80	-1.93185798	114	120	-2.29739123	60368	-5.85200273	60313	-6.18129836	empty			
2052 D05	X	1714	1720	0.68077618	155	160	-2.29739123	5592385	3.67524217	6474266	1.55360382	experimental	NIH	SAM001246598	Irinotecan Hcl (trihydrate)	
2052 D06	E		70	80	-1.93663429	115	160	-2.0833243	71267	-5.8323235	58558	-6.18423261	empty			
2052 D07	X	1635	1640	0.55500716	913	920	-0.5618307	4245355	1.35537237	4262752	0.84492254	experimental	NIH	SAM001246851	Huperzine A	
2052 D08	E		72	80	-2.38427786	74	80	-2.38427786	59121	-5.85415031	61260	-6.17971503	empty			
2052 D09	X	1075	1080	-0.33657061	991	1000	-0.39240176	3957528	0.85967736	4455455	1.16711017	experimental	NIH	SAM001247102	Metylperon	
2052 D10	E		74	80	-1.93026588	114	120	-2.29739123	56627	-5.85844547	57269	-6.18638774	empty			
2052 D11	X	993	1000	-0.46712307	1075	1080	-0.20993983	3837486	0.65294313	4413516	1.09699073	experimental	NIH	SAM001247065		
2052 D12	E		73	80	-1.93185798	674	80	-2.38427786	59362	-5.85373526	57547	-6.18609545	empty			
2052 D13	X	1154	1160	-0.21075446	1076	680	-0.08097834	3998605	0.95214288	4577409	1.10097979	experimental	NIH	SAM001247101	Thiophene, 5-bromo-2-(4-fluorophenyl)-3-[4-(methylsul	
2052 D14	E		114	120	-1.86658175	75	80	-2.3821057	62099	-5.84902161	63740	-6.17556862	empty			
2052 D15	E		592	600	-1.10555644	873	880	-0.64871734	3680272	0.38218771	4394341	1.0649313	empty			
2052 D16	E		76	80	-1.92708167	114	120	-2.29739123	58323	-5.85552463	56921	-6.18696957	empty			
2052 D17	E		633	640	-1.04028021	874	880	-0.64654517	3309883	-0.25569539	4158275	0.67024339	empty			
2052 D18	E		196	200	-1.73602929	115	120	-2.29521906	62900	-5.84764213	60383	-6.18118132	empty			
2052 D19	E		633	640	-1.04028021	594	600	-1.25475161	3368989	-0.15390317	3869972	0.18821841	empty			
2052 D20	E		115	120	-1.86498965	154	160	-2.21050459	60643	-5.85152913	61785	-6.17883726	empty			
2052 D21	E		910	920	-0.59926763	1071	1080	-0.21862849	3326419	-0.22721712	3791619	0.05721699	empty			
2052 D22	E		155	160	-1.80130552	234	240	-2.03673132	61078	-5.85077997	57576	-6.18587445	empty			
2052 D23	E		339	560	-1.50835854	327	680	-1.8347199	62254	-5.84875467	59040	-6.18342674	empty			
2052 D24	P	74186	74720	116.063684	118688	119480	255.265004	3074544	-0.66099568	3408838	-0.58276942	empty				
2052 E01	N		1153	1160	-0.21238656	1033	1040	-0.3011708	3163541	-0.50772525	3118141	-1.06879702	empty			
2052 E02	E		73	80	-1.93185798	73	80	-2.38645003	60925	-5.85104347	62492	-6.1776552	empty			
2052 E03	X	1069	1080	-0.34612323	1192	1200	0.04420358	3672546	0.36888201	4471296	1.19355335	experimental	NIH	SAM001246784	Goserelin Acetate	
2052 E04	E		74	80	-1.93026588	32	40	-2.47550883	57702	-5.85594111	59211	-6.18314083	empty			
2052 E05	X	703	720	-0.92883299	1269	1280	0.21146035	2849881	-1.04790978	3376918	-0.63613771	experimental	NIH	SAM001246791	Palonosetron Hcl	
2052 E06	E		75	80	-1.92867378	33	40	-2.47333666	53158	-5.86441978	57952	-6.18524581	empty			
2052 E07	X	951	960	-0.5339914	1395	1400	-0.29682647	2827870	-1.08581708	4366530	1.01843301	experimental	NIH	SAM001246889	Reichstein◆◆s Substance◆◆s	
2052 E08	E		74	80	-1.93026588	74	80	-2.38427786	50509	-5.86898188	57614	-6.18581092	empty			
2052 E09	X	832	840	-0.72345168	1073	1080	-0.21428416	3665616	0.35694718	4048468	0.48665298	experimental	NIH	SAM001246912	Xanthinol Nicotinate	
2052 E10	E		74	80	-1.93185798	74	80	-2.38427786	50922	-5.86827061	51532	-6.18761116	empty			
2052 E11	X	993	1000	-0.46712307	712	720	-0.98843604	4652707	0.8591305	4235830	0.7999106	experimental	NIH	SAM001246858	1-benzylimidazole	
2052 E12	E		114	120	-1.86658175	114	120	-2.29739123	47587	-5.87401414	55490	-6.18936212	empty			
2052 E13	X	793	800	-0.7855437	1075	1080	-0.20993983	3606502	0.25514118	3934897	0.29676904	experimental	NIH	SAM001246908	7-nitroindazole	
2052 E14	X		74	80	-1.93026588	33	40	-2.47333666	52778	-5.86507421	57348	-6.18625566	empty			
2052 E15	X	1035	1040	-0.40025474	1114	1120	-0.12522536	4216047	1.3048982	4656365	1.5030194	experimental	NIH	SAM001246557	Dexchlorpheniramine Maleate	
2052 E16	E		74	80	-1.9											

2052 F07	X	1475	1480	0.30027066	795	800	-0.81814627	4095855	1.09790381	3777713	0.03396701					
2052 F08	E	71	80	-1.93504219	34	40	-2.4711645	50679	-5.86868911	55022	-6.19014459		experimental	NIH	SAM001246592	Sibutramine Hcl
2052 F09	X	1555	1560	0.42763891	1154	1160	-0.03833873	4692253	2.12501909	4674497	1.53333499		empty	NIH	SAM001246773	Parecoxib Na
2052 F10	E	120	120	-1.86976596	112	120	-2.30173556	50938	-5.86824306	55930	-6.18862647		experimental	NIH	SAM001247067	
2052 F11	X	1112	1120	-0.27766579	1473	1480	0.6545833	3949742	0.84638833	3876389	0.19894724		empty			
2052 F12	E	73	80	-1.93185798	73	80	-2.38645003	51267	-5.86767645	56729	-6.18729059		empty			
2052 F13	X	1032	1040	-0.40503105	833	840	-0.73560397	2837639	-1.06899293	3235046	-0.87333901		experimental	NIH	SAM001247103	5-nonyloxytryptamine
2052 F14	E	114	120	-1.86658175	35	40	-2.46899233	50452	-5.86908004	55401	-6.18951092		empty			
2052 F15	E	794	800	-0.7839516	873	880	-0.64871734	3887426	0.73894786	4032957	0.46071936		empty			
2052 F16	E	75	80	-1.92867378	114	120	-2.29739123	49009	-5.87156518	56209	-6.18815999		empty			
2052 F17	E	753	760	-0.84922783	1113	1120	-0.12739753	3742853	0.48996456	4212227	0.76044783		empty			
2052 F18	E	173	120	-1.86335795	115	120	-2.29956339	51256	-5.86769554	57312	-6.18578083		empty			
2052 F19	E	474	480	-1.29342461	1033	1040	-0.3011708	3430695	-0.04763323	3740051	-0.02900155		empty			
2052 F20	E	156	160	-1.79971342	114	120	-2.29739123	61139	-5.85067492	58122	-6.18496158		empty			
2052 F21	E	748	760	-0.85718835	710	720	-1.00278037	3574913	0.20073868	3505540	-0.4210896		empty			
2052 F22	E	275	280	-1.61025314	234	240	-2.03673132	59218	-5.85398326	60170	-6.18153745		empty			
2052 F23	E	363	680	-1.47014807	436	840	-1.59795382	56515	-5.85863836	59522	-6.18262086		empty			
2052 F24	P	107085	107680	168.442286	136560	137400	294.085953	3043327	-0.71475752	3365173	-0.65577463		empty			
2052 G01	N	513	520	-1.23132559	914	920	-0.55965854	3391904	-0.11443901	3604548	-0.23555428		empty			
2052 G02	E	76	80	-1.92708167	73	80	-2.38645003	59483	-5.85352688	58703	-6.18399018		empty			
2052 G03	X	753	760	-0.84922783	1312	1320	0.30486348	3318274	-0.24124442	3923827	0.27826068		experimental	NIH	SAM001246678	Secoisolaricresinol
2052 G04	E	35	40	-1.9923579	74	80	-2.38427786	51964	-5.86647608	64886	-6.17365258		empty			
2052 G05	X	704	720	-0.92724089	789	800	-0.83117927	3226660	-0.39902185	4215834	0.76647852		experimental	NIH	SAM001246874	Naproxen Sodium
2052 G06	E	36	40	-1.9907658	67	80	-2.3821057	48725	-5.87205428	57168	-6.18655661		empty			
2052 G07	X	472	480	-1.29660882	754	680	-1.08097834	3380150	-0.13468172	3972811	0.36015893		experimental	NIH	SAM001246894	3-pyridinemethanol
2052 G08	E	76	80	-1.92708167	73	80	-2.46899233	49887	-5.8689912	55701	-6.18815915		empty			
2052 G09	X	792	800	-0.78713581	954	960	-0.47277119	3843521	0.6333477	4006116	0.15842885		experimental	NIH	SAM001246896	Synephrine
2052 G10	E	33	40	-1.99554211	72	80	-2.3886222	48074	-5.87317543	57152	-6.18658336		empty			
2052 G11	X	1393	1400	0.1697182	1472	1480	0.65241002	3226976	-0.39847763	3080495	-1.13173883		experimental	NIH	SAM001246523	Duloxetine Hcl
2052 G12	E	71	80	-1.93504219	34	40	-2.47550883	48011	-5.87328393	55495	-6.18935376		empty			
2052 G13	X	1674	1680	0.61709919	1074	1080	-0.212112	3930498	0.81312636	4004224	0.41267954		experimental	NIH	SAM001246909	5-methoxytryptamine
2052 G14	E	72	80	-1.93345009	73	80	-2.38645003	49560	-5.87061624	56237	-6.18811318		empty			
2052 G15	X	995	1000	-0.46393886	1235	1240	0.13760671	4203851	1.28389427	4611611	1.42819345		experimental	NIH	SAM001247088	Guanidine, N-cyano-n'-(1,1-dimethylpropyl)-n"-3-pyridi
2052 G16	E	73	80	-1.93185798	34	40	-2.4711645	45379	-5.87181725	52727	-6.18719024		empty			
2052 G17	X	1275	1280	-0.01814998	1115	1120	-0.12305532	3577807	0.20572272	3738309	-0.03191407		experimental	NIH	SAM001246900	Guanzoline
2052 G18	E	153	160	-1.80448973	113	120	-2.29956339	49225	-5.87119318	56882	-6.18703478		empty			
2052 G19	X	876	880	-0.65339914	1154	1160	-0.03833873	3474548	0.0278903	4214295	0.7639054		experimental	NIH	SAM001246818	Cefdinir
2052 G20	E	73	80	-1.93185798	152	160	-2.21484893	52956	-5.86476766	58259	-6.18473252		empty			
2052 G21	X	1395	1400	0.1729024	1074	1080	-0.212112	3354905	-0.1781586	3394570	-0.60662465		experimental	NIH	SAM001246879	Corticosterone
2052 G22	E	232	240	-1.67871358	193	200	-2.12579013	58971	-5.85440864	57820	-6.18544665		empty			
2052 G23	E	589	640	-1.20745104	493	880	-1.47141623	68030	-5.83880725	55727	-6.14040263		empty			
2052 G24	P	119428	120000	188.093616	144827	145560	312.043248	3245485	-0.36660147	3679696	-0.12991142		empty			
2052 H01	N	1036	1040	-0.39866263	634	640	-1.16786498	3610108	0.26135143	3467359	-0.48492589		empty			
2052 H02	E	74	80	-1.93026588	75	80	-2.3821057	59035	-5.85429842	58199	-6.18483284		empty			
2052 H03	X	954	960	-0.52921509	1032	1040	-0.30334296	3691884	0.40218587	3680064	-0.12929615		experimental	NIH	SAM001246659	Mirtazapine
2052 H04	E	34	40	-1.99395001	74	80	-2.38427786	50716	-5.86862538	57748	-6.18558688		empty			
2052 H05	X	1155	1160	-0.20920236	834	840	-0.7334318	3002158	-0.78565868	3067791	-1.15297914		experimental	NIH	SAM001246545	8-chloro-11-piperidin-4-ylidene-6,11-dihydro-5h-benzo[
2052 H06	E	73	80	-1.93185798	34	40	-2.4711645	48887	-5.87177528	51817	-6.18717021		empty			
2052 H07	X	1036	1040	-0.39866263	1075	1080	-0.20993983	3991335	0.918997	4150524	0.65277918		experimental	NIH	SAM001246833	Lorazepam
2052 H08	E	73	80	-1.93185798	74	80	-2.38427786	48325	-5.87274316	53150	-6.19327446		empty			
2052 H09	X	1109	1120	-0.2824391	868	880	-0.65957817	4148594	1.18873079	3838366	0.13537511		experimental	NIH	SAM001247070	Pergolide Mesylate Salt
2052 H10	E	32	40	-1.99713421	74	80	-2.38427786	48283	-5.87281549	55448	-6.18943234		empty			
2052 H11	X	1313	1320	0.04234994	1072	1080	-0.21645633	3832182	0.64380677	4299248	0.90594162		experimental	NIH	SAM001246590	Stanozolol
2052 H12	E	113	120	-1.86817386	114	120	-2.29739123	49700	-5.87037514	54475	-6.19105914		empty			
2052 H13	X	911	920	-0.59767553	1033	1040	-0.3011708	2757683	-1.20669297	3311672	-0.74522503		experimental	NIH	SAM001247096	Salmeterol
2052 H14	E	75	80	-1.92867378	114	120	-2.29739123	49014	-5.87155656	54728	-6.19063614		empty			
2052 H15	E	713	720	-0.91291196	672	680	-1.08532668	3426578	-0.05472352	4229968	0.7901097		empty			
2052 H16	E	75	80	-1.92867378	116	120	-2.2930469	47730	-5.87376787	56725	-6.18729727		empty			
2052 H17	E	673	680	-0.97659608	553	560	-1.34381041	3468989	0.01831661	4305695	0.91672061		empty			
2052 H18	E	35	40	-1.9923579	116	120	-2.2930469	52314	-5.86587331	56838	-6.18710835		empty			
2052 H19	E	754	760	-0.84763573	713	720	-0.99626387	3230469	-0.392462	4006568	0.41659857		empty			
2052 H20	E	75	80	-1.92867378	234	240	-2.03673132	49401	-5.87089007	57529	-6.18595304		empty			
2052 H21	E	632	640	-1.04187231	952	960	-0.47711623	3603396	0.24979204	3843373	0.14404263		empty			
2052 H22	E	75	80	-1.92867378	193	200	-2.12579013	60981	-5.85094702	59517	-6.18262922		empty			
2052 H23	E	379	640	-1.44467441	542	880	-1.36770424	61077	-5.85078169	60609	-6.18080346		empty			
2052 H24	P	88687	89040	139.150772	113998	114720	245.077546	3016658	-0.76068681	3375435	-0.6386172		empty			
2052 I01	N	634	640	-1.03868811	1035	1040	-0.29682647	3251724	-0.35585668	3667226	-0.15076005		empty			
2052 I02	E	34	40	-1.99395001	113	120	-2.29956339	56898	-5.85797876	58537	-6.18426772		empty			
2052 I03	X	1154	1160	-0.21079446	1194	1200	0.04854739	3200459	-0.44414515	3748569	-0.01479998		experimental	NIH	SAM001246796	Raltitrexed
2052 I04	E	34	40	-1.99395001	73	80	-2.38645003	49423	-5.8708521	57435	-6.1861102		empty			
2052 I05	X	834	840	-0.72026747	1034	1040	-0.29899863	3084051	-0.64462274	4201617	0.67208556		experimental	NIH	SAM001246875	Mepivacaine Hydrochloride
2052 I06	E	35	40	-1.9923579	34	40	-2.4711645	49552	-5.87063002	56562	-6.1875698		empty			
2052 I07	X	592	600	-1.10555644	994	1000	-0.38588527	2520852	-1.61456278	3590670	-0.27875744		experimental	NIH	SAM001246979	Haloperidol
2052 I08	E	149	160	-1.81085814	108	120	-2.31042422	48594	-5.87227989	54034	-6.19179646		empty			
2052 I09	X	2952	2960	2.65180704	3035	3040	0.404750527	3491838	0.0576671	4218699	0.77126862		experimental	NIH	SAM001246888	Resveratrol
2052 I10																

2052 M19	X	795	800	-0.7823595	914	920	-0.55965854	3081271	-0.64941045	3872851	0.19303192				
2052 M20	E	74	80	-1.93026588	74	80	-2.38427786	52319	-5.8658647	59510	-6.18264092	experimental	NIH	SAM001246802	Olopatadine Hcl
2052 M21	X	1033	1040	-0.40343894	1033	1040	-0.3011708	3239145	-0.37752021	3533405	-0.37450102	experimental	NIH	SAM001246860	Nicotinamide
2052 M22	E	195	200	-1.7376214	313	320	-1.06513022	59968	-5.85269161	59649	-6.18240853	empty			
2052 M23	X	492	523	-1.64527941	492	840	-4.761253	61659	-5.84977937	59348	-6.18240853	empty			
2052 M24	P	90989	91240	142.815794	117478	118120	252.636684	2961787	-0.85518553	3414358	-0.57354032	empty			
2052 N01	N	994	1000	-0.46553097	952	960	-0.47711623	3570159	0.19255135	3497765	-0.43408892	empty			
2052 N02	E	113	120	-1.86817386	34	40	-2.4711645	55458	-5.86045872	54507	-6.19100563	empty			
2052 N03	X	1274	1280	-0.01974208	1114	1120	-0.12522536	2785516	-1.15875904	2731329	-1.71552302	experimental	NIH	SAM001246705	Amlodipine Base
2052 N04	X	72	80	-1.93345009	34	40	-2.4711645	48697	-5.8721025	53160	-6.19325774	empty			
2052 N05	E	1395	1400	0.1729024	910	920	-0.5683472	3620949	0.28002177	3678194	-0.13242267	experimental	NIH	SAM001246880	Etoposide
2052 N06	E	73	80	-1.93663429	113	120	-2.29956339	47501	-5.87416225	54763	-6.19057762	empty			
2052 N07	X	1914	1920	0.99920395	1273	1280	0.22014901	2378931	-1.8589788	2491838	-2.11593732	experimental	NIH	SAM001246646	Amiodarone Hydrochloride
2052 N08	E	109	120	-1.87454227	72	80	-2.3886222	47107	-5.8748408	53695	-6.19236325	empty			
2052 N09	X	1594	1600	0.48973093	1274	1280	0.22232118	4044981	1.01028872	4006370	0.41626752	experimental	NIH	SAM001247071	Ebselen
2052 N10	E	72	80	-1.93345009	113	120	-2.29956339	47418	-5.87430519	52847	-6.19378105	empty			
2052 N11	X	1233	1240	-0.08501831	873	880	-0.64871734	3519242	0.10486221	4011663	0.4251171	experimental	NIH	SAM001246921	Testosterone
2052 N12	E	114	120	-1.86658175	73	80	-2.38645003	48822	-5.87188723	59927	-6.18194373	empty			
2052 N13	E	670	680	-0.98137239	1354	1360	0.39609445	4115287	1.13309175	4249145	0.82217247	empty			
2052 N14	E	34	40	-1.99395001	73	80	-2.38645003	50117	-5.86965698	51502	-6.19602981	empty			
2052 N15	E	913	920	-0.59449132	793	800	-0.82249061	3341546	-0.20116544	3832703	0.12590692	empty			
2052 N16	E	75	80	-1.92867378	115	120	-2.29521906	49717	-5.87034586	53124	-6.19331793	empty			
2052 N17	E	671	680	-0.97978029	830	840	-0.74212047	3311089	-0.25361841	3988696	0.38671768	empty			
2052 N18	E	35	40	-1.9923579	114	120	-2.29739123	47091	-5.87486835	53191	-6.19320591	empty			
2052 N19	E	1035	1040	-0.40025474	914	920	-0.55965854	3396574	-0.10639634	3896362	0.23234088	empty			
2052 N20	E	73	80	-1.93185798	113	120	-2.29739123	57363	-5.85717794	57363	-6.18000762	empty			
2052 N21	E	1152	1160	-0.21397867	1072	1080	-0.21649533	3005193	0.1818181	3721415	-0.0601598	empty			
2052 N22	E	193	200	-1.7408056	233	240	-0.03890349	84729	-5.81004827	55037	-6.19011951	empty			
2052 N23	E	471	720	-1.29820092	515	840	-1.42635272	56750	-5.85823364	56474	-6.18771693	empty			
2052 N24	P	84087	84600	131.827098	109018	109960	234.260116	2967737	-0.84493845	3272290	-0.81106933	empty			
2052 O01	N	1073	1080	-0.33975482	1234	1240	0.13534544	3150070	-0.53092497	3245807	-0.85534728	empty			
2052 O02	E	74	80	-1.93026588	33	40	-2.47333666	57906	-5.85624278	58720	-6.18396176	empty			
2052 O03	X	627	640	-1.04983283	947	960	-0.48797706	3234984	-0.38468627	3712370	-0.07528249	experimental	NIH	SAM001246865	Brucine
2052 O04	E	66	80	-1.99076588	67	80	-2.3886222	52342	-5.8582222	56422	-6.18744612	empty			
2052 O05	X	588	600	-1.11192485	1593	1600	0.91524209	2931782	-0.90686007	3496302	-0.43653497	experimental	NIH	SAM001246892	Rolitetraycline
2052 O06	E	75	80	-1.92867378	112	120	-2.30173556	55843	-5.85979568	53557	-6.19259398	empty			
2052 O07	X	1069	1080	-0.34612323	951	960	-0.4792884	2993529	-0.80051953	3724981	-0.05419767	experimental	NIH	SAM001246887	Oxyphenonium Bromide
2052 O08	X	112	120	-1.86976596	94	80	-2.38427786	54004	-5.8629628	54497	-6.19102235	empty			
2052 O09	E	1269	1280	-0.0277026	712	920	-0.56400287	3491951	0.05786171	3763365	0.00997803	experimental	NIH	SAM001246856	Enrofloxacin
2052 O10	E	33	40	-1.99554211	73	80	-2.38645003	51791	-5.86677402	55867	-6.1887318	empty			
2052 O11	X	920	920	-0.5960343	1234	1240	0.13534544	3646340	0.32179449	3127495	-1.05315771	experimental	NIH	SAM001246984	Ketotifen Fumarate
2052 O12	E	73	80	-1.93185798	33	40	-2.47333666	56362	-5.85890186	57185	-6.18652818	empty			
2052 O13	X	1114	1120	-0.27447859	1074	1080	-0.212112	3010401	-0.77146261	3222865	-0.8937049	experimental	NIH	SAM001247094	Rimazole
2052 O14	E	112	120	-1.86976596	113	120	-2.29956339	57206	-5.85744832	56533	-6.18761829	empty			
2052 O15	X	1433	1440	0.23340232	1274	1280	0.22232118	3237906	-0.37965401	3495847	-0.4372957	experimental	NIH	SAM001247083	Benzo[a]phenanthridine-10,11-diol, 5,6,6a,7,8,12b-hex-
2052 O16	E	110	120	-1.87295017	29	40	-2.48202533	63115	-5.84727185	55064	-6.19007436	empty			
2052 O17	X	1875	1880	0.93711192	2194	2200	2.22071377	2718243	-1.27461645	2710691	-1.75002849	experimental	NIH	SAM001246846	Dactinomycin
2052 O18	E	73	80	-1.93345009	113	120	-2.30679989	55578	-5.85852986	55699	-6.18736582	empty			
2052 O19	X	873	880	-0.65817545	2184	920	-0.55965854	2850976	-1.04085298	3409983	-0.58085055	experimental	NIH	SAM001246803	Itavastatin Ca
2052 O20	E	112	120	-1.86976596	153	160	-2.21267676	56578	-5.85852986	56415	-6.18781558	empty			
2052 O21	X	1592	1600	0.48654673	1354	1360	0.39609445	2920089	-0.92699773	3438388	-0.53336363	experimental	NIH	SAM001246861	Nialamide
2052 O22	E	192	200	-1.74239771	151	160	-2.21072109	58874	-5.8545757	56851	-6.18708661	empty			
2052 O23	E	388	640	-1.43034549	636	1240	-1.16352065	63244	-5.84704969	56448	-6.1877604	empty			
2052 O24	P	84591	85240	132.629518	205726	206560	444.325977	3051453	-0.70076294	3512478	-0.40948968	empty			
2052 P01	N	1477	1480	0.30345486	996	1000	-0.38154093	3330793	-0.21968423	3048657	-1.18497002	empty			
2052 P02	E	66	80	-1.94300271	67	80	-2.39483302	53604	-5.86365168	55022	-6.19014459	empty			
2052 P03	X	3198	3200	0.30434644	3277	3280	4.57316941	2924734	-0.91899812	2913611	-1.41075867	experimental	NIH	SAM001246619	Rabeprazole
2052 P04	E	103	120	-1.88409489	107	120	-2.31259639	53358	-5.86407534	53768	-6.1922412	empty			
2052 P05	X	2558	2560	0.02451839	1235	1240	0.13760671	3604704	0.25204467	3494011	-0.44036538	experimental	NIH	SAM001247105	Sibutramine
2052 P06	E	68	80	-1.9398185	111	120	-2.30390773	52856	-5.86493988	52188	-6.19488286	empty			
2052 P07	X	1556	1560	0.42923101	1757	1760	1.27147729	3623555	0.28450982	3307613	-0.75201143	experimental	NIH	SAM001246644	Mevastatin
2052 P08	E	110	120	-1.87295017	71	80	-2.39079436	55179	-5.86093922	53493	-6.19270098	empty			
2052 P09	X	1876	1880	0.93870403	1197	1200	0.0550644	2932393	-0.90580781	3127495	-1.05315771	experimental	NIH	SAM001247066	Flutamide
2052 P10	E	110	120	-1.87295017	33	40	-2.47333666	53397	-5.86400817	54593	-6.19086185	empty			
2052 P11	X	1517	1520	0.36713899	996	1000	-0.38154093	3358613	-0.17177269	3395845	-0.60449292	experimental	NIH	SAM001246922	Dehydroepiandrosterone
2052 P12	E	112	120	-1.86976596	75	80	-2.3821057	53161	-5.86441461	54223	-6.19148047	empty			
2052 P13	E	1276	1280	-0.01655787	636	640	-1.16352065	3335463	-0.21164157	3812917	0.09282594	empty			
2052 P14	E	33	40	-1.99554211	74	80	-2.38427786	54021	-5.86293352	53327	-6.19297852	empty			
2052 P15	E	1155	1160	-0.20920236	1196	1200	0.05289224	3040233	-0.720086	3334438	-0.70716167	empty			
2052 P16	E	114	120	-1.86658175	74	80	-2.38427786	56893	-5.85796737	56893	-6.18698964	empty			
2052 P17	E	794	800	-0.78319516	913	920	-0.5163077	3117998	-0.53851593	3918984	0.27016348	empty			
2052 P18	E	74	80	-1.93026588	74	80	-2.38427786	55858	-5.85976984	55238	-6.18978345	empty			
2052 P19	E	1037	1040	-0.39707053	957	960	-0.4662554	3114946	-0.59141544	3268012	-0.81822188	empty			
2052 P20	E	113	120	-1.86817386	154	160	-2.21050459	57631	-5.85671639	56056	-6.1884158	empty			
2052 P21	E	1115	1120	-0.27288648	835	840	-0.73125964	2834694	-1.0740648	3259219	-0.83292324	empty			
2052 P22	E	153	160	-1.80448973	194	200	-2.12361796	57960	-5.85614978	58644	-6.18408882	empty			
2052 P23	E	596	1000	-1.09918803	644	1160	-1.14614332	57320	-5.85725199	57564	-6.18589452	empty			
2052 P24	N	138930	138880												

2089 A13	X	435	440	-0.21540474	274	280	-0.89381533	2000584	-0.51619652	2401982	0.86918354	BIOMOL	A-240	Lincomycin
2089 A14	X	477	480	-0.08139498	397	400	-0.4296819	1908622	-0.85082197	2281224	0.39998295	BIOMOL	AC-734	Acetylcholine Cl
2089 A15	X	356	360	-0.46747073	437	440	-0.2787442	1984197	-0.57582449	1963006	-0.83644091	BIOMOL	A245	Lomofungin
2089 A16	X	315	320	-0.59828978	354	360	-0.59193993	1847644	-1.07270482	2047103	-0.50965623	BIOMOL	AC-735	Atropine sulfate
2089 A17	X	917	920	-1.32516883	835	840	1.22308592	19687242	1.96202422	1523866	1.35349908	BIOMOL	A-249	Mycophenolic acid
2089 A18	X	355	360	-0.47066143	555	560	0.16652202	1901955	-0.87508143	2265565	0.33914051	BIOMOL	AC-737	Decamethonium 2Br
2089 A19	X	395	400	-0.34033309	394	400	-0.44100223	1903379	-0.86989987	2111548	-0.25928665	BIOMOL	A-256	Novobincin B
2089 A20	X	316	320	-0.59509907	596	600	0.32123316	2882088	2.6913639	12172006	-0.02437941	BIOMOL	AC-741	Mecamylamine HCl
2089 A21	X	476	480	-0.08458569	394	400	-0.44100223	1634583	-1.84797757	2083010	-0.37016996	BIOMOL	A-275	Rapamycin
2089 A22	X	636	640	0.4259277	1156	1160	2.43436097	1705428	-1.59019131	1964164	-0.83194154	BIOMOL	AC-743	Neostigmine Br
2089 A23	E	464	680	-0.12287419	377	680	-0.50515075	89642	-7.46961015	92477	-8.10430973	empty		
2089 A24	X	72928	73160	231.086366	102251	102560	383.910532	1661580	-1.74974261	1692466	-1.88807997	empty		
2089 B01	N	635	640	0.42273699	278	280	-0.87872156	1504397	-2.32169007	1885156	-1.1389241	empty		
2089 B02	E	77	80	-1.35767844	78	80	-1.63341006	93376	-7.45602311	95422	-8.09286704	empty		
2089 B03	X	434	440	-0.21859545	277	280	-0.882495	1920465	-0.80772842	2150914	-0.10633157	BIOMOL	AR-103	Tizanidine HCl
2089 B04	X	274	280	-0.72910884	316	320	-0.73533074	1945616	-0.71621057	2427753	0.96931577	BIOMOL	EI-217	Tranlylcypromine
2089 B05	X	315	320	-0.59828978	515	320	-0.73910418	1940080	-0.73635461	2151811	-0.10284631	BIOMOL	DL-549	Meglumine
2089 B06	X	314	320	-0.60148049	395	400	-0.43722878	2035329	-0.38976884	2369091	0.74138682	BIOMOL	EI-219	Proxicam
2089 B07	X	594	600	0.25191793	636	640	0.47217085	2125494	-0.061682	2100797	-0.30105925	BIOMOL	AR-107	Propranolol HCl s(-)
2089 B08	X	275	280	-0.72591813	274	280	-0.89381533	1850198	-1.06341149	2107771	-0.27396204	BIOMOL	EI-240	Desprenyl HCl r (-)
2089 B09	X	355	360	-0.47066143	395	400	-0.43722878	1833673	-1.1235416	1935161	-0.94463159	BIOMOL	AR-112	Carvedilol
2089 B10	X	435	440	-0.21540474	394	400	-0.44100223	2040522	-0.37087268	2109129	-0.26868558	BIOMOL	EI-249	Troleanodolmycin
2089 B11	X	393	400	-0.3494145	595	600	0.31745972	1707018	-1.58440572	1892439	-1.11062628	BIOMOL	DL-223	Cervastatin
2089 B12	X	474	480	-0.0909671	272	280	-0.90136221	2013211	-0.4702502	1975541	-0.78773664	BIOMOL	EI-265	Acaridazole
2089 B13	X	795	800	0.93235037	1356	1360	3.18904947	1534026	-2.21387796	1620735	-2.16632177	BIOMOL	AW8655	Carlubacin
2089 B14	X	400	400	0.74622338	375	400	0.29761147	204935	-0.50936438	2104937	-0.06703789	BIOMOL	EI-287	Kitesulide
2089 B15	X	435	440	-0.21540474	394	400	-0.44100223	1961835	-0.65719394	2048386	-0.50470018	BIOMOL	B-100	Flumazenil
2089 B16	X	395	400	-0.34033309	714	720	0.76649938	1966617	-0.63979347	2023091	-0.60298294	BIOMOL	EI-288	Ketoprofen
2089 B17	X	313	320	-0.6046712	672	680	0.60801479	1690923	-1.64297118	1642006	-2.08367412	BIOMOL	GR-103	Fenretinide
2089 B18	X	514	520	0.03666124	513	520	0.00803743	1896556	-0.89472696	2055718	-0.47621198	BIOMOL	EI-292	Meloxicam
2089 B19	X	955	960	1.44376376	954	960	1.67212558	1776117	-1.3329727	1849683	-1.27675308	BIOMOL	DL-269	Gefitinib
2089 B20	X	354	360	-0.47385214	513	520	0.00803743	1903868	-0.86812052	2414252	0.91685815	BIOMOL	EI-318	Terbinafine HCl
2089 B21	X	515	520	0.03981595	474	480	-0.13912683	1863066	-1.01658823	2050235	-0.49751597	BIOMOL	DL-270	Ibudilast
2089 B22	X	400	400	0.60406723	391	400	0.65232255	2063086	-0.88978412	2011997	-0.58479525	BIOMOL	EI320	Sodium phenylbutyrate
2089 B23	E	406	640	-0.30793529	648	960	0.51745217	94322	-7.45258086	98888	-8.07940003	empty		
2089 B24	P	78879	79280	250.076545	105222	105880	395.121429	1805777	-1.22504779	1847039	-1.28702625	empty		
2089 C01	N	637	640	0.42911841	278	280	-0.87872156	2284054	0.515276	1806197	-1.44571627	empty		
2089 C02	E	74	80	-1.36725057	118	120	-1.48247236	93806	-7.45445845	97123	-8.08625787	empty		
2089 C03	X	1116	1120	1.95746785	317	320	-0.7315573	2288859	0.53276012	2303989	0.48843549	BIOMOL	A-280	Spectinomycin
2089 C04	X	633	640	0.41635557	316	320	-0.73533074	1979001	-0.59473196	2332614	0.59965683	BIOMOL	AC-745	Strychnine HCl
2089 C05	X	674	680	0.74635214	475	480	0.54717463	2097755	-0.1626169	2141338	-0.27456445	BIOMOL	AC-746	Copaxone
2089 C06	X	434	440	-0.21859545	515	520	0.01559432	2191457	0.01559432	2202266	0.09319466	BIOMOL	AC-746	Tubocurarine Cl (+)
2089 C07	X	874	880	1.18531636	313	320	-0.74665107	1977118	-0.6015831	2168315	-0.03872065	BIOMOL	AC-105	Amiodarone
2089 C08	X	474	480	-0.0909671	476	480	-0.13157994	1983348	-0.57891378	1938973	-0.92982021	BIOMOL	AC-747	Butaclamol (+)
2089 C09	X	315	320	-0.59828978	435	440	-0.28629108	1960564	-0.66181874	2035621	-0.5542981	BIOMOL	AC-108	Nicaridine
2089 C10	X	514	520	0.03666124	475	480	-0.13535338	1930266	-0.77206517	1862475	-1.22705026	BIOMOL	AC-748	Apomorphine r (-)
2089 C11	X	995	1000	1.57139211	435	440	-0.28629108	2005908	-0.49682389	1976346	-0.78460885	BIOMOL	AC-109	Pimozide
2089 C12	X	474	480	-0.0909671	395	400	-0.8626844	1978928	-0.59496999	2458008	-0.03983579	BIOMOL	AC-749	Chlorpromazine HCl
2089 C13	X	314	320	-0.60148049	493	400	-0.44477567	2062088	-0.29240334	1896277	-0.09573717	BIOMOL	AC-110	Loperamide
2089 C14	X	475	480	-0.0877664	475	480	-0.13535338	2026029	-0.42360888	1956133	-0.86314568	BIOMOL	AC-751	Domperidone
2089 C15	X	595	600	0.29510864	514	520	0.01181088	1918942	-0.81327022	1946919	-0.89894633	BIOMOL	AC-116	Fusipirine
2089 C16	X	674	680	0.54717463	594	600	0.91743708	1938168	-0.74331188	1947121	-0.89816147	BIOMOL	AC-753	Fluphenazine 2HCl
2089 C17	X	595	600	0.31368628	754	600	0.31368628	2042117	-0.3650689	2168326	-0.03867791	BIOMOL	AC-117	Tolbutamide
2089 C18	X	394	400	-0.3462238	394	360	-0.59193993	1902579	-0.87281085	1933466	-0.95121745	BIOMOL	AC-755	Pergolide mesylate
2089 C19	X	554	560	0.16428959	674	680	0.61556168	1989326	-0.55716141	2143018	-0.13701117	BIOMOL	AC-118	Pimozidil
2089 C20	X	434	440	-0.21859545	474	480	-0.15044715	1963112	-0.65254724	2011508	-0.64798824	BIOMOL	AC-757	Raclopride l-tartrate s(-)
2089 C21	X	514	520	0.03666124	714	720	0.76649938	2020338	-0.44431693	2161985	-0.06331562	BIOMOL	AC-120	Glipizide
2089 C22	X	595	600	0.29510864	433	440	-0.29383797	1931347	-0.76813169	1979912	-0.77075329	BIOMOL	AC-758	Risperidone
2089 C23	E	328	520	-0.55681057	396	760	-0.43345534	98793	-7.43631208	99567	-8.07676118	empty		
2089 C24	P	64154	64560	203.09336	123082	123680	462.515113	2010621	-0.47967453	2076699	-0.39469111	empty		
2089 D01	N	316	320	-0.59509907	278	280	-0.87872156	2212745	0.25580136	2379167	0.78053673	empty		
2089 D02	E	78	80	-1.35448773	118	120	-1.48247236	94784	-7.45089977	97048	-8.08654928	empty		
2089 D03	X	354	360	-0.47385214	317	320	-0.7315573	1876902	-0.96624268	2114492	-0.24784785	BIOMOL	DL-271	Imatinib
2089 D04	X	475	480	-0.09415781	235	240	-1.04097959	2217124	0.27173539	2636756	1.78138893	BIOMOL	FR-111	Ergothioneine
2089 D05	X	795	800	0.93235037	635	640	0.46839742	1565674	-2.09871924	1703579	-1.84443458	BIOMOL	DL-548	Idarubicin
2089 D06	X	352	360	-0.48023356	554	560	0.16274858	2456802	1.14386038	2373092	2.31111723	BIOMOL	FR-112	Ambroxol
2089 D07	X	593	600	0.28872723	715	720	0.77027282	2066434	-0.27658575	2345773	0.65078562	BIOMOL	DL-273	Montelukast
2089 D08	X	554	560	0.16428959	394	400	-0.44100223	2264034	0.4424285	2803136	2.42785205	BIOMOL	FR114	Idebeneone
2089 D09	X	474	480	-0.0909671	395	400	-0.43722878	2059571	-0.3015584	2305536	0.4944463	BIOMOL	EI-240	Selegiline
2089 D10	X	475	480	-0.0877664	394	400	-0.44100223	2285258	0.53057324	2321926	0.55812901	BIOMOL	G-233	Mevastatin
2089 D11	X	354	360	-0.47385214	356	360	-0.58439251	2073828	-0.2468094	1997088	-0.09416166	BIOMOL	DL-275	Vatalanid
2089 D12	X	194	200	-0.98436553	197	200	-1.1843704	2399973	0.93707465	2384168	0.79996792	BIOMOL	G-244	Simvastatin
2089 D13	X	397	400	-0.33665167	276	280	-0.88626844	1996181	-0.53221788	2138011	-0.15646568	BIOMOL	CT-100	Fumagillone
2089 D14	X	435	440	-0.21540474	435	440	-0.28629108	2099959	-0.15459712	2750220	2.22224895	BIOMOL	G-430	Suramin sodium
2089 D15	X	275	280	-0.72591813	435	440	-0.28629108	2123776	-0.06793335	2157482	-0.08081185	BIOMOL	DL-239	Efaroxan
2089 D16	X	355	360	-0.47066143	355	360	-0.58816648	2159793	0.06312301	2498339	1.24357497	BIOMOL	DL-282	Gos

2089 E07	X		554	560	0.16428959	475	480	-0.13535338	2202031	0.21681595	2106603	-0.27850026	experimental	BIOMOL	AC-123	Flufenamic acid
2089 E08	X		354	360	-0.47385214	395	400	-0.43722878	1909638	-0.84712502	1780112	-1.54706854	experimental	BIOMOL	AC-765	Promethazine HCl
2089 E09	X		715	720	0.67799368	434	440	-0.29006453	2037491	-0.38190169	2156308	-0.08537339	experimental	BIOMOL	AC-124	Propafenone
2089 E10	X		514	520	0.03665124	675	680	0.61935514	2139865	-0.00838972	2077871	-0.39013735	experimental	BIOMOL	AC-766	Ranitidine HCl
2089 E11	X		475	480	-0.28629108	435	440	-0.28629108	2100229	-0.15338904	2100529	-0.30210055	experimental	BIOMOL	AC-125	Naltrindole HCl
2089 E12	X		677	680	0.55674675	195	200	-1.19191729	1933891	-0.75887475	1934777	-0.94612361	experimental	BIOMOL	AC-770	Naltrindole HCl
2089 E13	X		195	200	-0.98117482	476	480	-0.13157994	2114429	-0.10194461	2268397	0.35014413	experimental	BIOMOL	AC-127	Procainamide
2089 E14	X		395	400	-0.34303309	435	440	-0.28629108	2058735	-0.30460038	2057893	-0.4677611	experimental	BIOMOL	AC-806	Idazoxan
2089 E15	X		476	480	-0.08458569	355	360	-0.58816648	2284689	0.51758659	2427861	0.9697354	experimental	BIOMOL	AC-128	Lidocaine
2089 E16	X		393	400	-0.3494145	354	360	-0.59193993	2016067	-0.45985797	1756436	-1.63906073	experimental	BIOMOL	AC-807	Sipiperone
2089 E17	X		435	440	-0.21540474	714	720	0.76649938	2443861	1.0967715	2274186	0.37263707	experimental	BIOMOL	AC-130	Flecainide
2089 E18	X		394	400	-0.3462238	594	600	0.31368628	2154612	0.04427072	2078755	-0.39762075	experimental	BIOMOL	AC-808	Epinephrine-(+)-tartrate l (-)
2089 E19	X		1075	1080	1.8266488	915	920	1.52496132	2245112	0.37357634	2264114	0.3335207	experimental	BIOMOL	AC-131	Phenamil
2089 E20	X		473	480	-0.09415781	351	360	-0.60326025	2271606	0.46998101	2140590	-0.14644507	experimental	BIOMOL	AC-809	Xylazine HCl
2089 E21	X		554	560	0.16428959	714	720	0.76649938	2528336	1.40415373	2405906	0.88443009	experimental	BIOMOL	AC-136	Cirazoline HCl
2089 E22	X		512	520	0.03027983	471	480	-0.15044715	2182353	0.1452129	2116109	-0.24156506	experimental	BIOMOL	AC-810	Norepinephrine-(+)-tartrate l (-)
2089 E23	E		285	480	-0.69401104	290	520	-0.83344025	96820	-7.4434913	97832	-0.08350308	empty			
2089 E24	P		65516	65920	207.439105	77108	77640	289.034867	2305490	0.59327594	2459615	1.09311435	empty			
2089 F01	N		435	440	-0.21540474	438	440	-0.27497076	2210924	0.24917523	2074889	-0.40172379	empty			
2089 F02	E		77	80	-1.35767844	78	80	-1.63341006	90962	-7.46480702	93310	-8.10107314	empty			
2089 F03	X		355	360	-0.47066143	196	200	-1.18814384	1963645	-0.65067078	1909206	-1.04547875	experimental	BIOMOL	DL-278	Dofetilide
2089 F04	X		354	360	-0.47385214	436	440	-0.28251764	2258739	0.42316139	2316249	0.53607125	experimental	BIOMOL	GR-211	Bezafibrate
2089 F05	X		474	480	-0.0909671	434	440	-0.29006453	2054771	-0.31902433	1865937	-1.21359879	experimental	BIOMOL	DL-279	Erolotinib
2089 F06	X		514	520	0.03666124	395	400	-0.43722878	1823657	-1.15998718	1849091	-1.27905328	experimental	BIOMOL	GR243	Raloxifene HCl
2089 F07	X		434	440	-0.21859545	395	400	-0.43722878	2332180	0.69039381	2056359	-0.47372124	experimental	BIOMOL	AC-227	Lobeline
2089 F08	X		394	400	-0.3462238	594	600	0.31368628	2154612	0.04427072	2078755	-0.39762075	experimental	BIOMOL	AC-301	Amptopothecin
2089 F09	X		394	400	-0.3462238	435	440	-0.28629108	2065795	-0.2789109	1957355	-0.85839765	experimental	BIOMOL	NS-520	Melatonin
2089 F10	X		515	520	0.03985195	434	440	-0.29006453	1837167	-1.11082786	1743120	-1.69079954	experimental	BIOMOL	GR-305	Plicamycin
2089 F11	X		275	280	-0.72591813	395	400	-0.43722878	2297389	0.56379854	2085250	-0.36146652	experimental	BIOMOL	PG-008	Dinoprost
2089 F12	X		275	280	-0.72591813	394	440	-0.28251764	2127557	-0.05417529	2094943	-0.32380474	experimental	BIOMOL	GR-306	Rifampicin
2089 F13	X		236	240	-0.85035576	435	440	-0.28629108	2107184	-0.12830726	2000862	-0.68935287	experimental	BIOMOL	EI-233	Fasudil
2089 F14	X		475	480	-0.0877764	595	600	0.31745972	2324471	0.66234279	2075498	-0.39935755	experimental	BIOMOL	GR-307	Etosipide
2089 F15	X		433	440	-0.22178616	474	480	-0.13912683	2173254	0.11210404	2039107	-0.54075338	experimental	BIOMOL	C-106	Hydroxytacrine maleate
2089 F23	E		440	440	-0.94607702	82582	83120	-0.01460322	9394861	7.45630329	2108888	-0.26962198	empty			
2089 F24	P		78015	78440	247.319773	82582	83120	309.690691	1847173	0.0741867	1810999	-1.42750822	empty			
2089 G01	N		878	880	1.19807919	398	400	-0.42590846	2244594	0.37169147	1926530	-0.97816701	empty			
2089 G02	E		35	40	-1.4916882	37	40	-1.7881212	92759	-7.45826821	96516	-0.08861635	empty			
2089 G03	X		716	720	0.68118439	397	400	-0.4296819	2231625	0.3245007	2285920	0.41822908	experimental	BIOMOL	AC-138	Oxymetazoline HCl
2089 G04	X		666	680	0.52164896	390	400	-0.456096	2224104	0.29713377	2256123	0.30245398	experimental	BIOMOL	DL-557	Quetiapine fumarate
2089 G05	X		834	840	1.05768801	555	560	0.16652202	2239342	0.35258083	2379420	0.78151975	experimental	BIOMOL	AC-142	Ifenprodil
2089 G06	X		433	440	-0.22178616	275	280	-0.72591813	2247791	0.38332451	4030368	0.39160509	experimental	BIOMOL	AC-812	Alprenolol HCl
2089 G07	X		514	520	0.03666124	275	280	-0.89004209	211045	-0.2852022	2155425	-0.08880245	experimental	BIOMOL	AC-144	Naftopidil 2HCl
2089 G08	X		555	560	0.1674803	276	280	-0.88626844	2059842	-0.3005723	2083546	-0.36808735	experimental	BIOMOL	AC-813	Imipramine HCl
2089 G09	X		595	600	0.29510864	315	320	-0.73910418	2349681	0.75407533	2195527	0.06701054	experimental	BIOMOL	AC-146	Prazosin HCl
2089 G10	X		394	400	-0.3462238	556	560	0.17029546	1946814	-0.71185136	1975945	-0.78616692	experimental	BIOMOL	AC-814	Amoxapine
2089 G11	X		356	360	-0.46747073	315	320	-0.73910418	2404123	0.9521754	2257058	0.30608688	experimental	BIOMOL	AC-152	Clonidine HCl
2089 G12	X		476	480	-0.08458569	475	480	-0.13535338	2246525	0.37871787	2228013	0.19323365	experimental	BIOMOL	AC-834	Mesulergine HCl
2089 G13	X		435	440	-0.21540474	355	360	-0.58816648	2069014	-0.26719781	2034069	-0.56032834	experimental	BIOMOL	AC-153	Guanabenz acetate
2089 G14	X		595	600	0.29510864	394	400	-0.44100223	2214048	0.26054264	2108888	-0.26962198	experimental	BIOMOL	DL-558	Amfebutamone
2089 G15	X		594	600	0.29191793	474	480	-0.13912683	2171593	0.1060601	2153413	-0.0966218	experimental	BIOMOL	AC-154	Rilmenidine hemifumarate
2089 G16	X		473	480	-0.09415781	634	640	0.46462398	2413088	0.98479667	1983910	-0.75521921	experimental	BIOMOL	AC-840	Metolopramide HCl
2089 G17	X		714	720	0.67480297	633	640	0.46085053	2496307	1.28706865	2233625	0.21503886	experimental	BIOMOL	AC-160	Spiroaxtrine
2089 G18	X		434	440	-0.21859545	635	640	0.46839742	2126111	-0.0594369	2062084	-0.45147713	experimental	BIOMOL	AC-858	Naltriben mesylate
2089 G19	X		515	520	0.03985195	483	480	-0.14290027	2233592	0.3316581	2308962	0.50775789	experimental	BIOMOL	AC-161	Yohimbine HCl
2089 G20	X		475	480	-0.0877764	514	520	0.01181088	2283455	0.51309639	2135639	-0.16568199	experimental	BIOMOL	DL-124	Vitamin a (acetate)
2089 G21	X		394	400	-0.3462238	714	720	0.76649938	2102315	-0.14603426	1998035	-0.70033707	experimental	BIOMOL	AC-164	Dihydroergotamine mesylate
2089 G22	X		552	560	0.15790817	471	480	-0.15044715	2092502	-0.18173118	2046783	-0.42092858	experimental	BIOMOL	AC-891	Levallophan tartrate
2089 G23	E		522	760	0.06218691	483	800	-0.10516584	96816	-7.44350586	98854	-8.07953214	empty			
2089 G24	P		80049	80480	253.809674	107050	107640	402.019282	1983461	-0.5785026	2223417	0.17537607	empty			
2089 H01	N		316	320	-0.59509907	317	320	-0.7315573	2163266	0.07576034	2191638	0.05189998	empty			
2089 H02	E		38	40	-1.48211608	158	160	-1.33153466	93494	-7.45559374	96081	-0.09030652	empty			
2089 H03	X		347	360	-0.4961871	312	320	-0.75042451	2187284	0.16315955	2284959	0.41449515	experimental	BIOMOL	C-115	Galanthamine HBr
2089 H04	X		304	320	-0.724706	312	320	-0.75042451	2187284	0.16315955	2284959	0.41449515	experimental	BIOMOL	GR-318	Galantamine HBr
2089 H05	X		414	440	-0.28240962	342	360	-0.63721254	1714361	-1.4594061	1770791	-1.58285753	experimental	BIOMOL	CA-200	Amiloride
2089 H06	X		4154	4160	11.6508408	3355	3360	10.7321611	1869393	-0.99356595	1839869	-1.31488501	experimental	BIOMOL	GR-319	Doxorubicin HCl
2089 H07	X		423	440	-0.25369325	346	360	-0.62212747	2347639	0.74664503	2438048	1.0093166	experimental	BIOMOL	CA-202	Doxorubicin HCl
2089 H08	X		395	400	-0.34303309	436	440	-0.28251764	1993501	-0.54196969	2022725	-0.60440502	experimental	BIOMOL	GR336	Amiodipine
2089 H09	X		234	240	-0.85673718	335	340	-0.28629108	2193956	0.18743315	2479594	1.17074199	experimental	BIOMOL	CA-205	Amiodipine
2089 H10	X		476	480	-0.08458569	435	320	-0.73910418	2272562	0.47345964	2270187	0.35709911	experimental	BIOMOL	DL-284	Lapatinib
2089 H11	X		355	360	-0.47066143	435	440	-0.28629108	2237195	0.34476846	2089605	-0.34454534	experimental	BIOMOL	CA-210	Nifedipine
2089 H12	X		394	400	-0.3462238	594	600	0.31368628	2154612	0.04427072	2078755	-0.39762075	experimental	BIOMOL	DL-285	Methsallylclyate
2089 H13	X		316	320	-0.59509907	354	360	-0.59193993								

2089 I01	N	598	600	0.30468077	558	560	0.17784235	2644363	1.82634536	2018402	-0.62120187	empty					
2089 I02	E	116	120	-1.232408	471	120	-1.4862458	91017	-7.46460689	94518	-8.0963795	empty					
2089 I03	X	716	720	0.68118439	316	320	-0.73532074	2403616	0.95033056	2425226	0.95949721	experimental	BIOMOL	AC-165			Nicergoline
2089 I04	X	505	520	0.00794486	471	480	-0.15044715	2565157	1.53085816	2399267	0.84669781	experimental	BIOMOL	AC-893			Sulbutamol HCl
2089 I05	X	831	840	0.04811589	314	480	-0.13912683	2485006	2.4648729	2403219	0.87607533	experimental	BIOMOL	DL-564			Emtricitabine
2089 I06	X	822	840	0.10193951	385	400	-0.47496321	2386973	0.88977108	2321074	0.5548186	experimental	BIOMOL	AC-911			Carbamylcholine Cl
2089 I07	X	754	760	0.80243132	676	680	0.62310856	2330465	0.68415338	2273968	0.37179004	experimental	BIOMOL	AC-169			Betaxolol HCl
2089 I08	X	475	480	-0.0877764	393	400	-0.44477567	2421155	1.01415035	2404847	0.88031538	experimental	BIOMOL	AC-912			Carbamyl-beta-methylcholine Cl
2089 I09	X	475	480	-0.0877764	635	640	0.46839742	2265618	0.44819226	2266812	0.11085797	experimental	BIOMOL	AC-171			Practolol
2089 I10	X	474	480	-0.0909671	434	440	-0.29006453	2294409	0.55295511	2449531	1.05393336	experimental	BIOMOL	AC-915			Butyrylcholine
2089 I11	X	556	560	0.17067101	555	560	0.16652202	2287661	0.52840092	2372581	0.75494708	experimental	BIOMOL	AC-172			Timolol maleate (s)
2089 I12	X	315	320	-0.59828978	432	440	-0.29761141	2176210	0.12286014	2321919	0.57170093	experimental	BIOMOL	AC-925			Famotidine
2089 I13	X	355	360	-0.47066143	393	400	-0.44477567	2116574	-0.09413952	2210980	0.12705258	experimental	BIOMOL	AC-173			Xamoterol hemifumarate
2089 I14	X	756	760	0.80881274	434	440	-0.29006453	2056754	-0.31180872	2070836	-0.41747157	experimental	BIOMOL	AC-928			Terfenadine
2089 I15	X	514	520	0.03666124	474	480	-0.13912683	2121172	-0.07740862	2181714	0.01334066	experimental	BIOMOL	AC-174			Clenbuterol
2089 I16	X	674	680	0.54717463	593	600	0.30991283	2298515	0.56789576	2254469	0.29602742	experimental	BIOMOL	AC-986			Isoniazid
2089 I17	X	914	920	1.31294471	473	480	-0.14290027	2349054	0.75179384	2098053	-0.31172096	experimental	BIOMOL	AC-175			Procaterol hcl
2089 I18	X	473	480	-0.09415781	594	600	0.31368628	2209083	0.24247631	2105095	-0.28435954	experimental	BIOMOL	AC-993			Ticlopidine HCl
2089 I19	X	314	320	-0.60148049	592	600	0.30613939	2080090	-0.22689517	2301766	0.477939811	experimental	BIOMOL	AC-176			Salbutamol sulfate
2089 I20	X	555	560	0.1674803	1154	1160	2.42681408	2346688	0.74318459	2417148	0.92811045	experimental	BIOMOL	DL-246			Amorolfine
2089 I21	X	474	480	-0.0909671	270	280	-0.9089091	2321159	0.6502913	2051251	-0.49356834	experimental	BIOMOL	AC-181			Pindolol
2089 I22	X	514	520	0.03666124	475	480	-0.13535338	2059082	-0.30333774	2059958	-0.45973762	experimental	BIOMOL	DL-247			Clemastine fumarate
2089 I23	E	361	560	-0.45151718	431	720	-0.30138485	98638	-7.43687608	101357	-8.06980683	empty					
2089 I24	P	66531	67000	210.677675	96983	97640	364.032037	1949895	-0.70064042	2147078	-0.1212362	empty					
2089 J01	N	317	320	-0.59190836	277	280	-0.882495	2265800	0.41530536	1952034	-0.87907219	empty					
2089 J02	E	117	120	-1.23005009	118	120	-1.48247236	92493	-7.4592361	92493	-8.09458244	empty					
2089 J03	X	315	320	-0.59828978	317	320	0.7135573	2092023	1.18137413	1183472	0.20201713	experimental	BIOMOL	CA-234			Gabapentin
2089 J04	X	432	440	-0.22497687	474	480	-0.13912683	2252935	0.40204217	2085449	1.28324554	experimental	BIOMOL	DL-291			Sulindac
2089 J05	X	1193	1200	2.20315242	794	800	1.06837478	2281713	0.50675772	2322075	0.55870795	experimental	BIOMOL	CA-236			Felodipine
2089 J06	X	592	600	0.28553652	795	800	1.07214822	2227678	0.31013861	2397052	0.85002821	experimental	BIOMOL	DL-292			Valproic acid
2089 J07	X	394	400	-0.3462238	313	320	-0.74665107	2243810	0.3688387	2301881	0.48024493	experimental	BIOMOL	CA-237			Cilnidipine
2089 J08	X	234	240	-0.85673718	555	560	0.16652202	2460550	1.15749836	2166477	-0.04586213	experimental	BIOMOL	DL-547			Calciprotiene
2089 J09	X	556	560	0.17067101	394	400	-0.44102223	2265047	0.44611454	2150833	-0.10664629	experimental	BIOMOL	CA-305			Phenoxylbenzamine HCl
2089 J10	X	432	440	-0.03981599	515	520	0.15589430	2309393	0.3093953	2227456	0.22193277	experimental	BIOMOL	DL-294			Sildenafil
2089 J11	X	274	280	-0.72910884	432	440	-0.29761141	2152959	0.03825589	2188319	0.03900413	experimental	BIOMOL	CA-310			Trifluoperazine
2089 J12	X	356	360	-0.46747073	1233	1240	2.72491604	2280454	0.50217655	2375077	0.76464519	experimental	BIOMOL	DL-295			Zileuton
2089 J13	X	316	320	-0.59509907	1032	1040	1.9664541	2239848	0.35442203	2536743	1.39279224	experimental	BIOMOL	DL-218			Denbutylline
2089 J14	X	193	200	-0.98755624	712	720	0.75895249	2138229	-0.01534269	2161579	-0.06489312	experimental	BIOMOL	PR-11579			Pentamidine
2089 J15	X	275	280	-0.72591813	672	680	0.60801479	2090902	-0.18755316	2154192	-0.09359502	experimental	BIOMOL	DL-131			Miltefosine
2089 J16	X	475	480	-0.0877764	1033	1040	1.97022754	1281792	-3.13169092	1238535	-3.65134524	experimental	BIOMOL	DL-297			Bortezomib
2089 J17	X	320	320	-1.00148049	752	760	-0.15044715	1945585	-0.71633337	2163322	-0.3311841	experimental	BIOMOL	DL-281			Docetaxil
2089 J18	X	352	360	-0.48023356	632	640	0.45707709	2437898	0.07507371	2643193	1.80639961	experimental	BIOMOL	DL-161			Bambuterol
2089 J19	X	715	720	0.67799368	593	600	0.30991283	1763812	-1.37747435	1728363	-1.7481373	experimental	BIOMOL	CM-109			Ubain
2089 J20	X	474	480	-0.0909671	630	640	0.44953021	2764160	2.26225503	2180032	0.00680531	experimental	BIOMOL	DL-186			Fentiazac
2089 J21	X	594	600	0.29191793	1154	1160	2.42681408	2235365	0.33810957	2156649	-0.08404844	experimental	BIOMOL	CM-112			Clopidamide
2089 J22	X	513	520	0.03347053	390	400	-0.456096	2748213	2.2042281	2212665	0.13359958	experimental	BIOMOL	J120			Mefenpytoin
2089 J23	E	409	680	-0.29836317	527	840	0.06086563	97462	-7.44115523	97179	-8.08604029	empty					
2089 J24	P	91585	92000	290.617689	105667	106240	396.806616	1857775	-1.03584079	1857775	-0.49129146	empty					
2089 K01	N	278	440	-0.209032	278	280	-0.882495	2766876	2.2705004	1954120	-0.87096712	empty					
2089 K02	E	117	120	-1.23005009	118	120	-1.48247236	90310	-7.46717947	94942	-8.09473206	empty					
2089 K03	X	476	480	-0.08458569	277	280	-0.882495	2617624	1.72904919	2431656	0.98448073	experimental	BIOMOL	AC-183			Cimaterol
2089 K04	X	875	880	1.18850707	316	320	-0.73533074	2539466	1.44465286	1955192	-0.8668019	experimental	BIOMOL	DL-248			Vardenafil
2089 K05	X	632	640	-0.41316486	234	240	-1.04475303	2723202	2.11321967	2323744	0.56519278	experimental	BIOMOL	AC-185			Dobutamine HCl
2089 K06	X	474	480	-0.0909671	275	280	-0.89004189	2425674	1.0305938	2113812	-0.25048997	experimental	BIOMOL	DL-249			Linezolid
2089 K07	X	515	520	0.03981595	356	360	-0.58439304	2332822	0.69272988	2456345	1.08040889	experimental	BIOMOL	AC-189			Pronethalol HCl
2089 K08	X	516	520	0.04304266	595	600	0.31745972	2457937	1.14799034	2111053	-0.26120996	experimental	BIOMOL	DL-250			Docetaxil
2089 K09	X	275	280	-0.72591813	475	480	-0.13535338	2690432	1.99397829	2101070	-0.29999852	experimental	BIOMOL	AC-192			Sotalol HCl
2089 K10	X	435	440	-0.21540474	355	360	-0.58816648	2163384	0.07618971	2120746	-0.22354817	experimental	BIOMOL	DL-251			Olopatadine
2089 K11	X	556	560	0.17067101	395	400	-0.43722878	2305328	0.59268647	2082914	-0.37054296	experimental	BIOMOL	AR-111			Maprotiline HCl
2089 K12	X	355	360	-0.47066143	433	440	-0.29383797	1956969	-0.6749	2014088	-0.63796375	experimental	BIOMOL	DL-258			Mindipine
2089 K13	X	594	600	0.29191793	274	280	-0.89381533	2305147	0.59202786	2236684	0.22692449	experimental	BIOMOL	AC-194			Nisoxetine HCl
2089 K14	X	915	920	1.31613541	475	480	-0.13535338	1995828	-0.53350235	1943080	-0.91386262	experimental	BIOMOL	DL-252			Tolcapone
2089 K15	X	475	480	-0.0877764	554	560	0.16274858	2326139	0.67568968	2177655	-0.00239158	experimental	BIOMOL	DL-553			Cantaxanthin
2089 K16	X	275	280	-0.72591813	393	400	-0.44477567	2143153	0.00257444	2029169	-0.5793671	experimental	BIOMOL	DL-253			Gastritron
2089 K17	X	474	480	-0.0909671	513	520	0.00803743	2539670	1.44539516	2421750	0.94599134	experimental	BIOMOL	AC-214			Pilocarpine HCl
2089 K18	X	1075	1080	1.8266488	674	680	0.61556168	2418918	1.0060105	2258781	0.31278153	experimental	BIOMOL	DL-254			Olmesartan
2089 K19	X	473	480	-0.09415781	431	440	-0.30138485	2954987	2.95662412	2454307	1.07249032	experimental	BIOMOL	AC-218			Ipratropium Br
2089 K20	X	355	360	-0.47066143	633	640	0.46085053	2340113	0.7192599	2054935	-0.4792545	experimental	BIOMOL	DL-255			Nisoldipine
2089 K21	X	434	440	-0.21859545	876	880	1.35892985	3308162	4.24173474	2114921	-0.24618099	experimental	BIOMOL	AC-220			Prenzipine 2HCl
2089 K22	X	594	600	0.29191793	912	920	1.51364999	2462528	1.16468578	2062730	-0.44896712	experimental	BIOMOL	DL-256			

2089 L19	X	396	400	-0.33984238	1074	1080	2.12493868	1962341	-0.65535271	2237550	0.2302893	experimental	BIOMOL	D-111	Remoxipride
2089 L20	X	235	240	-0.85354647	472	480	-0.14667371	2319693	0.64495691	2388196	0.81561856	experimental	BIOMOL	DL-172	Levetiracetam
2089 L21	X	475	480	-0.0877764	433	440	-0.29383797	1866347	-0.99737207	1993896	-0.71641899	experimental	BIOMOL	DM100	Calcitriol
2089 L22	X	400	400	-0.3494145	592	600	0.30613939	2437005	1.07182432	2312758	0.5225507	experimental	BIOMOL	DL-300	Ezetimibe
2089 L23	E	464	464	-0.12287419	471	760	-0.15044715	91250	-7.46375906	4051	-8.09819401	empty			
2089 L24	P	58883	59320	186.275135	96801	97480	363.34527	2009212	-0.48480151	2024614	-0.59706538	empty			
2089 M01	N	398	400	-0.33346096	318	320	-0.72778386	2635495	1.79407705	2066891	-0.43279972	empty			
2089 M02	E	75	80	-1.36405986	117	120	-1.4862458	99910	-7.43224761	97739	-8.08386443	empty			
2089 M03	X	1116	1120	1.95746785	436	440	-0.28251764	2564209	1.53468611	2646930	1.82091961	experimental	BIOMOL	AC-221	Telenzepine 2HCl
2089 M04	X	553	560	0.16109888	635	640	0.46839742	2267160	0.45380319	2121754	-0.21963163	experimental	BIOMOL	DL-257	Olanzapine
2089 M05	X	594	600	0.29191793	353	360	-0.59571337	2265503	0.4477738	2192487	0.05519873	experimental	BIOMOL	AC-222	Tropicamide
2089 M06	X	595	600	0.29510864	436	440	-0.28251764	2228361	0.50262387	2471302	1.13852763	experimental	BIOMOL	G-226	Lovastatin
2089 M07	X	595	600	0.29510864	315	320	-0.73910418	2134018	-0.03066541	2244754	0.25828016	experimental	BIOMOL	AC-232	Pancuronium Br
2089 M08	X	514	520	0.03666124	555	560	0.16652202	2261727	0.43403394	2450395	1.05729039	experimental	BIOMOL	NA-137	Lamotrigine
2089 M09	X	515	520	0.03985195	475	480	-0.13535338	2171775	0.10672235	2161073	-0.06685916	experimental	BIOMOL	AC-238	Ivermectin
2089 M10	X	675	680	0.55036534	555	560	0.16652202	1919689	-0.81055208	2107096	-0.27658473	experimental	BIOMOL	DL-260	Ractopamine
2089 M11	X	471	480	-0.10053923	594	600	0.31368628	2070318	-0.2624529	2252506	0.28840026	experimental	BIOMOL	AC-241	Physostigmine sulfate
2089 M12	X	1356	1360	2.72323793	434	440	-0.2906453	2206807	0.23419455	2076251	-0.39643179	experimental	BIOMOL	DL-261	Sildenafil
2089 M13	X	232	240	-0.8631186	476	480	-0.13157994	1974645	-0.61058117	2220490	0.16400332	experimental	BIOMOL	DL-554	Nitroglycerin
2089 M14	X	475	480	-0.0877764	396	400	-0.43345534	1931931	-0.76600667	2105026	-0.28462763	experimental	BIOMOL	DL-262	Atovaquone
2089 M15	X	395	400	-0.34303309	555	560	-0.58816648	2166420	0.08723691	2150141	-0.10933503	experimental	BIOMOL	AC-250	Haloperidol HCl
2089 M16	X	395	400	-0.34303309	594	600	0.31368628	1981786	-0.58459748	2101004	-0.30025496	experimental	BIOMOL	DL-208	Sertaconazole
2089 M17	X	436	440	-0.21221403	952	960	1.6645787	2029427	-0.41124446	2189580	0.0439037	experimental	BIOMOL	AC-259	Piribedil HCl
2089 M18	X	356	360	-0.46747073	793	880	1.36647674	1914159	-0.83067429	2354199	0.68515641	experimental	BIOMOL	DL-191	Cefepime
2089 M19	X	355	360	-0.47066143	871	800	1.05705445	2333037	0.69351221	2795577	2.39848184	experimental	BIOMOL	AC-277	Mepyramine maleate
2089 M20	X	395	400	-0.34303309	593	593	0.30613939	1949707	-0.7158794	2052544	-0.45142214	experimental	BIOMOL	DL-178	Atipripazine
2089 M21	X	634	640	0.41954628	473	480	-0.14290027	2573653	0.50865033	3968989	0.74487595	experimental	BIOMOL	AC-279	Trisartan
2089 M22	X	754	760	0.80243132	793	800	1.06460134	1936770	-0.74839883	2146522	-0.12339651	experimental	BIOMOL	DL-264	Candesartan
2089 M23	E	298	520	-0.65253183	484	880	-0.1013924	91330	-7.46346796	95924	-8.09091654	empty			
2089 M24	P	74320	74720	235.530104	133820	134360	503.034338	2133806	-0.03143682	2123998	-0.21091265	empty			
2089 N01	N	277	280	-0.71953671	318	320	-0.72778386	2217630	0.27357659	2180706	0.00942411	empty			
2089 N02	E	37	40	-1.48530679	117	120	-1.4862458	87873	-7.47604707	92067	-8.10590277	empty			
2089 N03	X	394	400	0.3462238	357	360	0.5806196	1745738	-1.44351386	1920840	-1.00027528	experimental	BIOMOL	DM200	Calcitriol
2089 N04	X	394	400	-0.47066143	354	360	-0.5806196	1745738	-1.44351386	1920840	-1.00027528	experimental	BIOMOL	DL-301	Amoxicillin
2089 N05	X	513	520	0.03347053	475	560	0.17029546	2145246	0.01019032	2360460	0.7078514	experimental	BIOMOL	EI-107	Ketconazole
2089 N06	X	355	360	-0.47066143	395	400	-0.43722878	2275944	0.48576585	2469424	1.13122685	experimental	BIOMOL	DL-222	Alfacalcidol
2089 N07	X	354	360	-0.47385214	395	400	-0.43722878	2203126	0.22080036	2165630	-0.04915311	experimental	BIOMOL	EI-114	Oxatome
2089 N08	X	714	720	0.67480297	555	560	0.16652202	2177100	0.12609862	2234848	0.21979078	experimental	BIOMOL	DL-151	Anethole-trithione (anetholtrithion)
2089 N09	X	314	320	-0.60148049	275	280	-0.89004189	2175748	0.121117905	2111767	-0.25843574	experimental	BIOMOL	EI-121	Diosithion cromoglycate
2089 N10	X	394	400	-0.3462238	435	440	-0.28629108	1986994	-0.56564695	2325283	0.57117251	experimental	BIOMOL	DL-144	Anastrozole
2089 N11	X	396	400	0.42512977	455	560	0.16652202	2157876	0.27778297	2083263	-0.36763275	experimental	BIOMOL	EI-125	Capsaicin
2089 N12	X	392	400	-0.35260521	473	480	-0.1832871	2183471	0.18281181	2331597	0.59570531	experimental	BIOMOL	DL-162	Bicalutamide
2089 N13	X	356	360	-0.46747073	235	240	-1.04097959	2075230	-0.24457943	2088643	-0.34828315	experimental	BIOMOL	EI-126	Dexamethasone
2089 N14	X	475	480	-0.0877764	275	280	-0.89004189	2042498	-0.36368254	2312841	0.52282959	experimental	BIOMOL	DL-180	Clodranone disodium
2089 N15	X	435	440	-0.21540474	356	360	-0.58439304	2647046	1.83610809	2835124	2.5521402	experimental	BIOMOL	EI-127	Dipyridamide
2089 N16	X	516	520	0.04304266	312	320	-0.74287763	2058903	-0.30398907	2111436	-0.25972182	experimental	BIOMOL	DL-102	Clindamycin palmitate
2089 N17	X	236	240	-0.85035576	754	760	0.91743708	1946790	-0.71193869	1915904	-1.01945392	experimental	BIOMOL	EI-128	Ethacrynic acid
2089 N18	X	195	200	-0.98117462	312	320	-0.74287763	2156583	0.05071492	2472762	-1.14221493	experimental	BIOMOL	DL-164	Indinavir
2089 N19	X	515	520	0.03985195	512	520	0.00426399	1947609	-0.7805857	2397392	-0.02811385	experimental	BIOMOL	EI-131	Indomethacin
2089 N20	X	555	560	0.1674803	753	760	0.91366364	2386981	0.88890919	2397246	0.85078199	experimental	BIOMOL	DL-302	Didanosine
2089 N21	X	394	400	-0.3462238	472	480	-0.14667371	1985396	-0.57146165	2132241	-0.17888479	experimental	BIOMOL	EI-133	Naproxen
2089 N22	X	513	520	0.03347053	472	480	-0.14667371	2094182	-0.1756181	2304238	0.48940297	experimental	BIOMOL	DL-199	Dolasetron
2089 N23	E	369	600	-0.42599151	459	720	-0.19572846	89526	-7.47003224	93123	-8.10179972	empty			
2089 N24	P	77756	78016	246.493379	87315	88000	327.550394	1890215	-0.91780019	1859795	-1.2374633	empty			
2089 O01	N	478	480	-0.07820427	358	360	-0.57684616	2341352	0.7237683	1973864	-0.79425256	empty			
2089 O02	E	116	120	-1.2332408	78	80	-1.63341006	86687	-7.48036261	96478	-8.08876399	empty			
2089 O03	X	597	600	0.30149006	237	240	-1.0334327	2855376	2.59416598	2442858	1.02800567	experimental	BIOMOL	AC-280	Cimetidine
2089 O04	X	353	360	-0.47704285	396	400	-0.43345534	2388506	0.89534926	2189426	0.04330534	experimental	BIOMOL	DL-101	Butenafine
2089 O05	X	1115	1120	1.95427714	354	360	-0.59193993	2867918	2.36980301	2808975	2.45053926	experimental	BIOMOL	AC-282	Tiotidine
2089 O06	X	393	400	-0.3494145	356	360	-0.58439304	2268222	0.45766753	2200479	0.08625134	experimental	BIOMOL	DL-200	Dorzolamide
2089 O07	X	554	560	0.16428959	275	280	-0.89004189	2819952	2.46526739	2453054	1.06762184	experimental	BIOMOL	DL-555	Zonisamide
2089 O08	X	953	960	1.43738234	555	560	0.16652202	2138078	-0.01589214	1906444	-1.05621039	experimental	BIOMOL	DL-212	Escitalopram
2089 O09	X	594	600	0.29191793	355	360	-0.58816648	2532340	1.41872323	2083563	-0.36763275	experimental	BIOMOL	EI-556	Zoledronic acid
2089 O10	X	514	520	0.03666124	435	440	-0.28629108	2082370	-0.21859885	1933011	-0.95296201	experimental	BIOMOL	DL-209	Eprosartan
2089 O11	X	234	240	-0.85673718	315	320	-0.73910418	2459471	-1.15357217	2118081	-0.23390293	experimental	BIOMOL	AC-322	Naltrexone HCl
2089 O12	X	396	400	-0.33984238	514	520	0.01181088	2065421	-0.28027179	2046369	-0.51253716	experimental	BIOMOL	DL-119	Sodium phenylacetate
2089 O13	X	395	400	-0.34303309	554	560	0.16274858	2402789	0.94732133	2418971	0.93519365	experimental	BIOMOL	DL-560	zolmitriptan
2089 O14	X	435	440	-0.21540474	794	800	1.06837478	2123200	-0.07068223	1995091	-0.71177587	experimental	BIOMOL	DL-551	Ozagrel
2089 O15	X	434	440	-0.21859545	514	520	0.01181088	2806027	2.41459799	2516098	1.31257689	experimental	BIOMOL	AC-408	Memantine HCl
2089 O16	X	400	400	-0.34303309	315	320	-0.74287763	2048979	-0.3409098	2052544	-0.48854443	experimental	BIOMOL	DL-217	Entacapone
2089 O17	X	316	320	0.59509907	473	480	-0.13525338	2183471	1.42574963	2297498	2.71678275	experimental	BIOMOL	AC-439	Acetylsalicylic acid
2089 O18	X	596	600	0.29829935	513	520	0.00803743	2120317	-0.08051974	2225543	0.18363656	experimental	BIOMOL	AP-302	Bleomycin sulfate
2089 O19	X	434	440	-0.21859545	992	1000	1.8155164	2674666	1.93660998	3045506	3.3695714	experimental	BIOMOL	AC-501	Riluzole HCl
2089 O20	X	555	560	0.1674803	871	880	1.3589298								

2089 P13	X	517	520	0.04623337	435	440	-0.28629108	1794081	-1.26706644	2074670	-0.40257471								
2089 P14	X	474	480	-0.0909671	595	600	0.31745972	1890519	-0.91669401	2611023	1.68140434			experimental	BIOMOL	EI-168		Bumetanide	
2089 P15	X	956	960	1.44695447	515	520	0.01558432	1873905	-0.97714797	2064500	-0.44208985			experimental	BIOMOL	DL-166		Granisetron	
2089 P16	X	396	400	-0.33964238	677	680	0.626882	1890337	-0.91735626	2640707	-1.79674039			experimental	BIOMOL	EI-180		Neomycin sulfate	
2089 P17	X	116	120	-0.3332408	155	160	-1.16285499	997996	-0.16434967	113345	-0.06803405			experimental	BIOMOL	3I-105		Nidaplatin	
2089 P18	X	557	560	0.17386171	636	640	0.47217086	1821248	-1.1687529	2215092	0.1430296			experimental	BIOMOL	EI-205		Aurofinin	
2089 P19	X	316	320	-0.59509907	714	720	0.76649938	1871659	-0.98532057	1973472	-0.79577566			experimental	BIOMOL	DL-303		Oxaliplatin	
2089 P20	X	436	440	-0.21221403	593	600	0.30991283	2269504	0.46232339	2426658	0.96506119			experimental	BIOMOL	EI-213		Captopril	
2089 P21	X	516	520	0.04304266	674	680	0.61556168	1910104	-0.84542937	2089552	-0.34475127			experimental	BIOMOL	DL-174		Anethole, trans-	
2089 P22	X	434	440	-0.21859545	713	720	0.76272593	2200276	0.21042996	2598976	1.63459618			experimental	BIOMOL	EI-216		Docetaxone	
2089 P23	E	535	880	0.10366612	392	800	-0.44854911	85442	-7.48489284	91594	-8.10774059			empty		DL-546		Atazanavir	
2089 P24	P	118051	118240	375.062985	138944	139240	522.369498	1822666	-1.16359317	2161265	-1.04088225			empty					
2090 A01	N	518	520	-0.78254367	798	800	-0.15687962	1984136	-0.308528096	1920791	-0.388874263			empty					
2090 A02	E	71	80	-2.11958603	70	80	-1.9995444	80409	-8.11756994	89308	-9.27866291			empty					
2090 A03	X	2592	2600	5.42109356	2669	2680	4.5788701	2245394	-2.39467471	2451270	-2.3275818			experimental	BIOMOL	DL-545		Mycophenolate mofetil	
2090 A04	X	1027	1040	0.73994975	1385	1400	1.32889541	2285621	-2.28833914	2623664	-1.82023888			experimental	BIOMOL	DL-363		Clobetasol propionate	
2090 A05	X	871	880	0.27333094	1751	1760	2.25529007	2652653	-1.31813118	2778004	-1.36602757			experimental	BIOMOL	DL-544		Etoricoxib	
2090 A06	X	1352	1360	1.71207227	1027	1040	0.42274982	1886830	-3.34249846	2020871	-3.59421452			experimental	BIOMOL	DL-364		Cislosetal	
2090 A07	X	1073	1080	0.87754247	1832	1840	2.46031184	2587277	-1.49094531	2961023	-0.82741606			experimental	BIOMOL	DL-103		Clofarabine	
2090 A08	X	473	480	-0.91714525	1030	1040	0.43034322	2717365	-1.14707226	2669033	-1.68672124			experimental	BIOMOL	DL-365		Corticosterone	
2090 A09	X	714	720	-0.19627901	952	960	0.23291485	2462130	-1.82175738	2825668	-1.22575591			experimental	BIOMOL	DL-219		Cabergoline	
2090 A10	X	875	880	0.28529553	714	720	-0.36949479	2779441	-0.98298131	2826600	-1.22460228			experimental	BIOMOL	DL-366		Crotamiton	
2090 A11	X	474	480	-0.9141541	634	640	-0.57198542	2538120	-1.62088633	2970684	-0.79898445			experimental	BIOMOL	DL-207		Dilazep	
2090 A12	X	913	920	0.39895908	754	760	-0.26824947	2742137	-1.08159026	2726617	-1.51725575			experimental	BIOMOL	DL-367		Cyclophosphamide monohydrate	
2090 A13	X	832	840	0.15667624	669	680	-0.48339577	2802033	-0.92326189	2664496	-1.70007033			experimental	BIOMOL	DL-213		Ibuprofen	
2090 A14	X	954	960	0.521569718	993	1000	0.3366269	2670592	-1.27071145	2732529	-1.50623296			experimental	BIOMOL	DL-468		Cyclopropane acetate	
2090 A15	X	512	520	-0.80490555	905	920	0.139516	2598355	-0.46168185	2913337	-0.87946467			experimental	BIOMOL	DL-202		Insipiden	
2090 A16	X	875	880	0.28529553	3231	3240	6.00136681	2539650	-1.61684195	2836961	-1.19252144			experimental	BIOMOL	DL-369		Cyclocytidine HCl	
2090 A17	X	670	680	-0.32788945	785	800	-0.18978435	2772413	-1.00155904	2862678	-1.11683819			experimental	BIOMOL	DL-156		Lomustine	
2090 A18	X	1752	1760	2.90853075	1072	1080	0.5366508	2942587	-0.5517231	2856516	-1.13497251			experimental	BIOMOL	DL-370		Cytarabine	
2090 A19	X	949	960	0.50664034	1069	1080	0.52905741	3047865	-0.27343255	2801383	-1.29722489			experimental	BIOMOL	DL-543		Iloprost	
2090 A20	X	712	720	-0.20226131	1152	1160	0.73914144	2620848	-1.40220414	2881530	-1.06135814			experimental	BIOMOL	DL-371		Dacarbazine	
2090 A21	X	1071	1080	0.87156018	1111	1120	0.6356499	2476770	-1.78305818	2484402	-2.2311362			experimental	BIOMOL	DL-244		Lomerizine HCl	
2090 A22	X	1560	1570	1.30710326	952	960	-0.4859269	2624281	-0.90812916	2913129	-1.674255			experimental	BIOMOL	DL-372		Danzol	
2090 A23	E	468	800	-0.93210098	480	800	-0.96177989	88639	-8.09581486	93114	-9.26746213			empty					
2090 A24	P	112247	112560	333.415231	108758	109040	273.104232	2293035	-2.26874107	2565746	-1.99068731			empty					
2090 B01	N	476	480	-0.90817181	475	480	-0.97443556	2694916	-1.20641368	2642287	-1.76543276			empty					
2090 B02	E	73	80	-2.11360373	111	120	-1.89576795	87063	-8.09998084	95411	-9.26070223			empty					
2090 B03	X	1787	1800	3.01322087	2348	2360	3.76637643	2640930	-1.34911962	3240556	-0.00477093			experimental	BIOMOL	DL-439		Mebendazol	
2090 B04	X	1029	1040	0.74593204	706	720	-0.38974285	3489808	0.89479424	3032878	-1.61595206			experimental	BIOMOL	DL-514		Tetracycline	
2090 B05	X	690	690	0.71818114	914	920	-0.58712306	2807701	-0.90877917	2951248	-0.65182703			experimental	BIOMOL	DL-440		Hydroxyprogesterone 17-acetate	
2090 B06	X	950	960	0.50963149	795	1000	0.31629004	3567792	-1.10093621	3244816	0.00778559			experimental	BIOMOL	DL-169		Tenatoprostol	
2090 B07	X	711	720	-0.20525245	788	800	-0.18219095	3012382	-0.36722788	3096652	-0.42826985			experimental	BIOMOL	DL-441		Mefenamic acid	
2090 B08	X	512	520	-0.80049055	550	560	-0.78460059	3203324	0.13750589	3037502	-0.60234397			experimental	BIOMOL	DL-190		Tenolamide	
2090 B09	X	632	640	-0.441553	872	880	0.03042422	3035719	-0.30553914	2899409	-1.00874155			experimental	BIOMOL	DL-442		Melphalan	
2090 B10	X	510	520	-0.80647284	552	560	-0.77953832	3072143	-0.20925638	3245917	0.0110061			experimental	BIOMOL	DL-206		Tibolone	
2090 B11	X	392	400	-1.15942809	712	720	-0.37455705	3364679	0.56402976	2980788	-0.76924912			experimental	BIOMOL	DL-443		Methyldopa	
2090 B12	X	1112	1120	0.994169718	668	680	-0.4859269	3102272	-0.12961374	3173782	-0.36623296			experimental	BIOMOL	DL-515		Ticozanolol	
2090 B13	X	830	840	-1.5069395	702	2080	3.06778331	3056710	-0.0652653	2777800	-0.36633251			experimental	BIOMOL	DL-444		Methylprednisolone	
2090 B14	X	550	560	-0.68682699	866	880	0.01523742	3346037	0.51475172	3196149	-0.13545747			experimental	BIOMOL	DL-516		Tinidazole	
2090 B15	X	913	920	0.39895908	868	880	0.02029969	3238436	0.23032053	2835737	-1.19612358			experimental	BIOMOL	DL-445		Metoprolol tartrate	
2090 B16	X	669	680	-0.33088059	746	1480	1.52632378	3101632	-0.13130551	3328300	0.25345324			experimental	BIOMOL	DL-517		Tobramycin (free base)	
2090 B17	X	831	840	0.15368509	1093	720	-0.38215045	3050422	-0.26667341	2927586	-0.92581871			experimental	BIOMOL	DL-446		Methimazole	
2090 B18	X	946	960	0.49766691	708	720	-0.38468158	3222037	0.18697161	2864272	-1.11214717			experimental	BIOMOL	DL-188		Tosufloxacin	
2090 B19	X	1231	1240	1.35014358	1390	1400	1.34155108	2728439	-1.11779938	3202930	-1.11550149			experimental	BIOMOL	DL-447		Metronidazole	
2090 B20	X	710	720	-0.2082436	627	640	-0.58970335	3422981	0.72078795	3781269	1.58650782			experimental	BIOMOL	DL-518		Topotecan	
2090 B21	X	989	1000	0.62628619	830	840	-0.07588337	2880781	-0.71510038	2818658	-1.24638583			experimental	BIOMOL	DL-448		Miconazole	
2090 B22	X	1068	1080	0.86258674	791	800	-0.17459755	3205455	-0.14313895	3013580	-0.67274466			experimental	BIOMOL	DL-519		Toremifene	
2090 B23	E	362	680	-1.24916248	274	560	-1.48319328	90420	-8.09110698	98764	-9.25083459			empty					
2090 B24	P	106592	107240	316.500299	96120	96680	241.115774	2925111	-0.59791899	2766955	-1.39854397			empty					
2090 C01	N	636	640	-0.42958842	677	680	-0.4631467	2644266	-1.34030128	2368462	-2.57127967			empty					
2090 C02	E	35	40	-2.22726729	76	80	-1.9843576	90295	-8.09143741	92695	-9.26869521			empty					
2090 C03	X	752	760	-0.08261546	588	600	-0.68841754	2670916	-1.26985499	2901092	-1.00378861			experimental	BIOMOL	DL-138		Lofexidine	
2090 C04	X	432	440	-0.03978224	552	560	-0.77953832	3278643	0.33660323	3008355	-0.68812146			experimental	BIOMOL	DL-373		Dehydroepiandrosterone	
2090 C05	X	509	520	-0.80946399	631	640	-0.57957882	3567573	1.10035731	3708416	-1.57081996			experimental	BIOMOL	DL-167		Mercopron	
2090 C06	X	632	640	-0.441553	751	520	-0.88331477	2348323	-2.12259343	2165948	-3.16726354			experimental	BIOMOL	DL-154		Desloratadine	
2090 C07	X	631	640	-0.44454415	511	760	-0.27584287	3277199	0.33278618	3056729	-0.54576032			experimental	BIOMOL	DL			

2090 D07	X	872	880	0.27632209	951	960	0.23038372	2976910	-0.46099414	2950395	-0.85869349	experimental	BIOMOL	T-104	Taxol	
2090 D08	X	751	760	-0.0856066	671	680	-0.4783335	3618835	1.23586266	3592898	1.03214577	experimental	BIOMOL	DL-522	Toilrazuril	
2090 D09	X	512	520	-0.80049055	672	680	-0.47580237	3679793	1.3969983	3176006	-0.19473685	experimental	BIOMOL	DL-452	Myclobutanil	
2090 D10	X	470	480	-0.92611869	714	720	-0.36946479	30640262	-0.23071276	3219022	-0.09463025	experimental	BIOMOL	DL-523	Tramadol HCl	
2090 D11	X	673	680	-0.31891601	511	520	-0.89331477	3560217	1.08091155	3414869	0.50822606	experimental	BIOMOL	DL-453	Nadifloxacin	
2090 D12	X	786	800	0.01908351	707	720	-0.38721272	3359127	0.54935367	3594608	1.03717817	experimental	BIOMOL	DL-524	Triamcinolone	
2090 D13	X	2909	2920	0.36928691	2669	2680	4.5788701	3349348	0.52350397	3481941	0.70560744	M	experimental	BIOMOL	DL-454	Nabumetone
2090 D14	X	826	840	0.13872936	905	920	0.1139516	3493315	0.90406461	3181337	-0.1790481	experimental	BIOMOL	DL-525	Trimethoprim	
2090 D15	X	910	920	0.38998564	787	800	-0.18472208	3302820	0.40051242	3259120	0.05012643	experimental	BIOMOL	DL-455	Naphazoline HCl	
2090 D16	X	830	840	0.15069395	1031	1040	0.43287435	3024828	-0.33432828	3260671	0.05442605	experimental	BIOMOL	DL-518	Tropisetron HCl	
2090 D17	X	1110	1120	0.98821488	631	640	-0.57957882	3088059	-0.16718422	3163601	-0.23124385	experimental	BIOMOL	DL-456	Nefazodone	
2090 D18	X	709	720	-0.21123475	828	840	-0.08094563	3605432	1.20043333	3237449	-0.01008879	experimental	BIOMOL	DL-526	Tylosin tartrate	
2090 D19	X	870	880	0.27033979	1386	1400	1.33142655	3428798	0.73352115	3280557	0.12913518	experimental	BIOMOL	DL-457	Niflumic acid	
2090 D20	X	670	680	-0.32788945	748	760	-0.28343627	3217614	0.17527991	3066693	-0.516437	experimental	BIOMOL	DL-527	Valaciclovir	
2090 D21	X	1111	1120	0.99120603	709	720	-0.38215045	3115007	-0.0959502	3325718	0.2458546	experimental	BIOMOL	DL-458	Norethindrone	
2090 D22	X	790	800	0.0310481	950	960	0.22785259	3668946	1.36832547	3105063	-0.4035169	experimental	BIOMOL	DL-528	Acyclovir Br	
2090 D23	E	356	600	-1.26710936	414	640	-1.12883467	93785	-0.80221198	97658	-9.25408947	empty				
2090 D24	P	81562	82120	241.63191	75412	75880	188.701073	3126305	-0.0660852	3175250	-0.1969617	empty				
2090 E01	N	596	600	-0.54923427	437	440	-1.07061861	2594409	-1.47209267	2731170	-1.5038566	empty				
2090 E02	E	35	40	-2.22726729	77	80	-1.98182647	92638	-0.08524395	94403	-9.2636687	empty				
2090 E03	X	754	760	-0.07663317	554	560	-0.77447606	3488268	0.89072343	3507259	0.78011646	experimental	BIOMOL	DL-187	Rocuronium bromide	
2090 E04	X	670	680	-0.32788945	470	480	-0.98709122	2959397	-0.50728779	3127081	-0.33871954	experimental	BIOMOL	DL-181	Doxofylline	
2090 E05	X	987	1000	0.6203039	989	1000	0.32656677	3978658	2.18701444	3471884	0.67601043	experimental	BIOMOL	DL-184	Ricobendazole	
2090 E06	X	671	680	-0.3248983	910	920	0.12660727	2917152	-0.61895772	3323654	0.2397804	experimental	BIOMOL	DL-381	Doxycycline HCl	
2090 E07	X	592	600	-0.56119885	911	920	0.1291384	3463815	0.82608666	4134475	2.6259672	experimental	BIOMOL	DL-176	Sulbactam	
2090 E08	X	709	720	-0.14927016	752	760	-0.25962217	3095435	-0.14742225	3275527	-0.49932582	experimental	BIOMOL	DL-152	Enalapril	
2090 E09	X	553	560	-0.67785555	592	600	-0.678293	4103970	1.51826285	3854577	1.80224809	experimental	BIOMOL	DL-143	Triamphenicol glycinate	
2090 E10	X	593	600	-0.55820771	590	600	-0.68335527	3070702	-0.2130655	3521550	0.82217383	experimental	BIOMOL	DL-383	Enoxacin	
2090 E11	X	472	480	-0.9201364	913	920	0.13420067	3647841	1.31253677	3221387	-0.06118389	experimental	BIOMOL	DL-175	Tulobuterol	
2090 E12	X	671	680	-0.3248983	749	760	-0.28090513	3019464	-0.34850741	2875829	-1.07813576	experimental	BIOMOL	DL-384	Enoxifloxacin	
2090 E13	X	1186	1200	1.215542	1585	1600	1.835122	3224886	0.19450263	3037580	-0.60211442	experimental	BIOMOL	NP-461	Vinorelbine	
2090 E14	X	549	560	-0.68981814	825	840	-0.08853903	2919433	-0.61292815	2789225	-1.33300499	experimental	BIOMOL	DL-385	Ethisterone	
2090 E15	X	1152	1160	1.11384302	1630	1640	1.94902298	3481253	0.87218006	3339431	0.28621096	experimental	BIOMOL	DL-220	Vindesine	
2090 E16	X	592	600	-0.68981814	788	800	-0.22149023	3021408	-0.64840514	2735655	-0.80252032	experimental	BIOMOL	DL-386	Gemeprozole potassium	
2090 E17	X	1030	1040	0.74892319	949	440	-1.08580541	3310301	0.42028761	2763039	-1.41006847	experimental	BIOMOL	DL-210	Salmeterol	
2090 E18	X	788	800	0.02505681	947	960	0.22025919	2987454	-0.43312226	3225085	-0.05030095	experimental	BIOMOL	BL-093	Estradiol	
2090 E19	X	1469	1480	0.26203637	2387	2400	3.86509061	3195010	0.11552877	3796251	1.63059875	experimental	BIOMOL	T-117	Vincristine sulfate	
2090 E20	X	949	960	0.50664034	1106	1120	0.62270932	3118111	-0.08774512	3044127	-0.58284708	experimental	BIOMOL	DL-388	Estril	
2090 E21	X	868	880	0.2643575	909	920	0.12407614	4004623	2.25565	3196409	-0.13469231	experimental	BIOMOL	DL-312	Acemetacin	
2090 E22	X	792	800	0.03703039	1109	1120	0.63030272	2901235	-0.66103252	2940137	-0.88888203	experimental	BIOMOL	BL-090	Estrone	
2090 E23	X	520	530	-0.3409991	409	420	-0.27311173	93966	-0.0817335	2731874	-9.25250322	empty				
2090 E24	P	81180	81680	240.489522	76914	77320	192.502835	3665072	1.35808499	3422052	0.52938585	empty				
2090 F01	N	515	520	-0.79151711	357	360	-1.27310924	2912902	-0.63019212	3278393	0.10658059	empty				
2090 F02	E	116	120	-1.98498445	77	80	-1.98182647	87587	-0.0985957	96209	-9.25835377	empty				
2090 F03	X	713	720	-0.19927016	553	560	-0.77007719	3073940	-0.20450621	3035271	-0.60890964	experimental	BIOMOL	DL-459	Norflloxacin	
2090 F04	X	951	960	0.51262264	1113	1120	0.64042726	3287783	0.3607638	3698688	1.34347798	experimental	BIOMOL	DL-529	Norfloxacin HCl	
2090 F05	X	1030	1040	0.74892319	710	720	-0.37961932	3217175	0.17411946	3465903	0.65840878	experimental	BIOMOL	DL-460	Nystatin	
2090 F06	X	870	880	0.03033979	752	760	-0.27311173	93966	-0.0817335	386671	0.42523481	experimental	BIOMOL	DL-530	Vidarabine	
2090 F07	X	512	520	-0.80049055	591	600	-0.68082414	3457105	0.80083475	3310458	0.38024640	experimental	BIOMOL	DL-461	Acyclovir	
2090 F08	X	513	520	-0.7974994	632	640	-0.57704769	3647103	1.3105895	4050983	2.38025636	experimental	BIOMOL	DL-531	Iproniazid	
2090 F09	X	632	640	-0.441553	750	760	-0.278374	3334425	0.4840567	3216777	-0.07475078	experimental	BIOMOL	DL-106	Tipiraz	
2090 F10	X	1032	1040	0.75490548	1072	1080	0.5366508	3847916	1.84141261	3518665	0.81368349	experimental	BIOMOL	NA-103	Benamil	
2090 F11	X	832	840	-0.15667624	670	680	-0.48086464	3403297	0.66611211	3417886	0.51709827	experimental	BIOMOL	DL-462	Omeprazole	
2090 F12	X	748	760	-0.09458004	946	960	-0.79472512	4292524	0.301668403	3372554	0.38368952	experimental	BIOMOL	NA-139	Bupivacaine HCl	
2090 F13	X	591	600	-0.564419	589	1000	0.32656677	3255007	0.27412411	3107969	-0.39496475	experimental	BIOMOL	DL-463	Oxcarbazepine	
2090 F14	X	632	640	-0.441553	869	880	0.02283082	2842293	-0.81683909	2775676	-1.37287871	experimental	BIOMOL	NH-101	Astemizole	
2090 F15	X	831	840	0.15368509	899	1000	0.32656677	3250080	0.26110014	3135951	-0.31261578	experimental	BIOMOL	DL-464	Oxiconazole nitrate	
2090 F16	X	631	640	-0.44454415	871	880	0.02789308	3981301	2.19400091	4025395	2.30495275	experimental	BIOMOL	NH-106	Ketotifen fumarate	
2090 F17	X	831	840	0.15368509	751	760	-0.27584287	3123113	-0.07452289	3275772	0.09886718	experimental	BIOMOL	DL-465	Oxalicillin sodium monohydrate	
2090 F18	X	871	880	0.27333094	871	880	0.02789308	3458334	0.81159625	3557861	0.92903444	experimental	BIOMOL	NH-107	Levocastastine HCl	
2090 F19	X	985	1000	0.61432161	903	920	0.10888934	2974744	-0.46671972	3158240	-0.24702088	experimental	BIOMOL	DL-466	Oxifenazole	
2090 F20	X	827	840	0.14172051	868	880	0.02029969	3765517	1.62360009	3367751	0.36955464	experimental	BIOMOL	NO-101	Naloxone HCl	
2090 F21	X	1190	1200	1.22750658	752	760	-0.27311173	93966	-0.0817335	2539870	-2.06683849	experimental	BIOMOL	DL-467	Oxibendazole	
2090 F22	X	709	720	-0.21123475	1190	1200	0.83532449	3632862	1.27335867	3142404	-0.29362507	experimental	BIOMOL	NO-102	Naloxonazine 2HCl	
2090 F23	E	493	560	-0.85732233	368	560	-1.24526678	93191	-0.08378215	99448	-9.24882163	empty				
2090 F24	P	89600	90120	265.674743	63317	63800	158.08702	2933336	-0.57617713	2791291	-1.3269249	empty				
2090 G01	N	837	840	-0.17163197	517	520	-0.86812797	2812039	-0.89681215	2765325	-1.40334094	empty				
2090 G02	E	75	80	-2.10762144	76	80	-1.9843576	90140	-0.09184713	94080	-9.26461926	empty				
2090 G03	X	593	600	-0.55820771	754	760	-0.26824947	3377092	0.59684213	3341793	0.29316215	experimental	BIOMOL	DL-313	Acetylsalicylic acid	
2090 G04	X	750	760	-0.09138989	599	600	-0.38215045	3123203	-0.07428489	3117488	0.22163421	experimental	BIOMOL	DL-390	Acetaminofen 2Na	
2090 G05	X	550	560	-0.68682699	511	520	-0.89331477	3911221	0.63419056	3891055	0.78245658	experimental	BIOMOL	DL-314	Acipimox	
2090 G06	X	1151	1160	1.11085188	672	680	-0.47580237	3280603	0.34178427	3266235	0.07080049	experimental	BIOMOL	DL-170	Ethretinate	
2090 G07	X	752	760	-0.08261546	793	800	-0.16953528	3514276	0.95947266	3522135	0.82389544	experimental	BIOMOL	DL-315	Acedofenac	
2090 G08	X	593	600	-0.55												

2090 H01	N	596	600	-0.54923427	516	520	-0.87065911	2787156	-0.96258758	2785093	-1.34516516	empty					
2090 H02	E	76	80	-2.10463029	75	80	-1.98688873	85848	-8.10319255	93053	-9.26764165	empty					
2090 H03	X	712	720	-0.20226131	871	880	0.02789308	3134934	-0.04327541	3177339	-0.19081392	experimental	BIOMOL	DL-468			Pantoprazole
2090 H04	X	1512	1520	2.19065566	1310	1320	1.13906044	3234447	0.21976066	3666312	1.25707257	experimental	BIOMOL	AC-1053			Harmaline
2090 H05	X	429	440	-0.04875568	871	880	0.02789308	3054506	-0.25677787	3036675	-0.60477787	experimental	BIOMOL	NS-109			Paroxetine HCl
2090 H06	X	792	800	0.03703039	512	520	-0.88078364	3281527	0.34422676	3677559	1.28129689	experimental	BIOMOL	NS-102			Cinanserin
2090 H07	X	512	520	-0.80049055	512	520	-0.88078364	3520306	0.97541229	3486681	0.71955692	experimental	BIOMOL	DL-470			Pazufloxacin
2090 H08	X	473	480	-0.91714525	631	640	-0.57957882	3594185	1.17070315	3819524	1.69908948	experimental	BIOMOL	NS-107			Dibenzepine HCl
2090 H09	X	714	720	-0.19627901	751	760	-0.27584287	3532068	1.00650382	3586428	1.01310503	experimental	BIOMOL	DL-471			Pefloxacin mesylate
2090 H10	X	433	440	-1.03679111	549	560	-0.78713172	3461479	0.81990971	3142221	-0.29416363	experimental	BIOMOL	NS-108			Dihydroergocristine mesylate
2090 H11	X	393	400	-1.15643695	872	880	0.03042422	3590666	1.16140106	3488818	0.72584595	experimental	BIOMOL	DL-472			Penciclovir
2090 H12	X	827	840	0.14172051	621	640	-0.60489015	3291397	0.3703117	3174968	-0.19379511	experimental	BIOMOL	NS-109			Fluperlapine
2090 H13	X	513	520	0.79749994	992	1000	0.33416017	3542089	1.03299321	3605874	1.07033318	experimental	BIOMOL	DL-473			Pentoxifylline
2090 H14	X	552	560	-0.6808447	870	880	0.02536195	3039260	-0.2961789	3280565	0.11297263	experimental	BIOMOL	NS-140			Fluoxetine HCl
2090 H15	X	591	600	-0.56419	671	680	-0.4783335	3518042	0.96942766	3667111	1.25054919	experimental	BIOMOL	DL-474			Pencilin v potassium
2090 H16	X	1231	1240	1.35014358	1151	1160	0.73661031	3200056	0.1288673	3609110	1.07985649	experimental	BIOMOL	NS-145			Ondansetron
2090 H17	X	751	760	-0.0856066	990	1000	0.3290979	3379737	0.60383389	3326986	0.24958623	experimental	BIOMOL	DL-475			Phenylbutazone
2090 H18	X	351	360	-1.28206509	750	760	-0.278374	3081096	-0.18599013	3353004	0.3261553	experimental	BIOMOL	NS-515			Ketanserin tartrate
2090 H19	X	748	760	-0.09458004	828	840	-0.08094563	3728894	1.52679129	3174968	-0.1977916	experimental	BIOMOL	DL-476			Piperacilin
2090 H20	X	1070	1080	0.86856904	870	880	0.02536195	3721128	1.50626274	3800851	1.64413621	experimental	BIOMOL	DL-562			Tiotropium Br
2090 H21	X	788	800	0.02506581	667	680	-0.48845803	3195132	0.11585126	3432894	0.56126572	experimental	BIOMOL	DL-477			Pravastatin lactone
2090 H22	X	1191	1200	1.23049773	1191	1200	0.83785562	3055881	-0.25224315	3105235	-0.40301071	experimental	BIOMOL	NS-531			Mesoridazine besylate
2090 H23	E	390	760	-1.16541039	478	800	-0.96684216	91849	-8.08732958	97631	-9.25416893	empty					
2090 H24	P	124528	125040	370.149497	108065	108600	271.350157	3563349	1.08919164	3163429	0.23175004	empty					
2090 I01	N	597	600	-0.54624312	676	680	-0.46567784	2782621	-0.97457534	2735246	-1.49186123	empty					
2090 I02	E	36	40	-2.224214	75	80	-1.98688873	87440	-8.09898228	93543	-9.27502835	empty					
2090 I03	X	473	480	-0.91714525	832	840	-0.0708211	3399665	0.65651133	3930786	0.2320245	experimental	BIOMOL	GR-341			Amifostine
2090 I04	X	990	1000	0.62927734	950	960	0.22785259	3034888	-0.3077358	3275166	0.09708965	experimental	BIOMOL	DL-399			5-fluorouracil
2090 I05	X	791	800	0.03403924	711	720	-0.37708818	3566588	1.09775357	4008462	2.25512017	experimental	BIOMOL	DL-324			Di-aminoglutethimide
2090 I06	X	791	800	0.03403924	752	760	-0.27331173	3116005	-0.0933121	3431712	0.55778718	experimental	BIOMOL	DL-400			Flurbiprofen
2090 I07	X	872	880	0.27632209	870	880	0.02536195	3750292	1.58335451	4338094	3.22520299	experimental	BIOMOL	DL-325			4-aminosalicylic acid
2090 I08	X	552	560	-0.6808447	1151	1160	0.73661031	3703165	1.45877956	3738487	1.46060353	experimental	BIOMOL	DL-401			Floxacin
2090 I09	X	633	640	-0.43856186	748	760	-0.28343627	4208616	2.79488264	3394919	0.31560491	experimental	BIOMOL	DL-326			5-aminosalicylic acid
2090 I10	X	640	650	-0.09462431	748	760	-0.09462431	4208616	2.79488264	3394919	0.31560491	experimental	BIOMOL	DL-402			Fluorouracil
2090 I11	X	751	760	-0.0856066	703	720	-0.39733725	3532306	1.00713294	3266671	0.07208361	experimental	BIOMOL	DL-327			Ampicillin trihydrate
2090 I12	X	1352	1360	1.71207227	2552	2560	4.28272755	3421740	0.71486411	3051096	-0.56233782	experimental	BIOMOL	DL-403			Floxuridine
2090 I13	X	470	480	-0.92611869	666	680	-0.49098917	3358791	0.54846549	3616078	1.10036281	experimental	BIOMOL	DL-328			Amproxicam
2090 I14	X	753	760	-0.07962431	672	680	-0.47580237	3325300	0.45993578	3363948	0.35863269	experimental	BIOMOL	DL-404			Fluocinonone acetonide
2090 I15	X	509	520	-0.80946399	432	440	-1.08327427	3498261	0.9171388	3367043	0.36747105	experimental	BIOMOL	DL-329			Apramycin
2090 I16	X	991	1000	0.63226849	792	800	-1.17206642	2917548	-0.61791094	2960197	-0.82984692	experimental	BIOMOL	DL-405			Flubendazole
2090 I17	X	640	650	-0.09462431	549	560	-0.4707401	30771798	-0.47460714	3374987	-0.42447261	experimental	BIOMOL	NP-015			Terminin
2090 I18	X	873	880	0.27931323	950	1000	0.33416017	3324562	0.45798496	3420044	0.52344911	experimental	BIOMOL	DL-406			Flutamide
2090 I19	X	831	840	0.15368509	870	880	0.02536195	4054576	2.36469769	3420453	0.52465276	experimental	BIOMOL	AC-166			Atenolol
2090 I20	X	790	800	0.0310481	910	920	0.12660727	3372571	0.58489137	3460399	0.64221092	experimental	BIOMOL	DL-407			Fluconazole
2090 I21	X	871	880	0.27333094	831	840	-0.07335223	3015262	-0.35961493	3328810	0.25495413	experimental	BIOMOL	DL-332			Atorcium besylate
2090 I22	P	669	680	-0.33088059	869	880	0.02283082	3118986	-0.08543216	3124354	-0.34674449	experimental	BIOMOL	DL-408			Formestane
2090 I23	E	365	600	-1.24018904	398	680	-1.16933279	92183	-8.08644669	96860	-9.25643792	empty					
2090 I24	P	78229	78860	231.662449	94370	95000	236.686591	3465743	0.6338245	318072	-0.38478511	empty					
2090 J01	N	355	360	-0.770105	636	640	-0.5692315	2750933	-1.0593902	2857786	-1.1079355	empty					
2090 J02	E	117	120	-1.9819933	75	80	-1.98688873	86883	-8.10045665	94163	-9.264375	empty					
2090 J03	X	514	520	-0.79450826	674	680	-0.4707401	3179594	0.0747783	3523688	0.82846581	experimental	BIOMOL	DL-478			Pranoprofen
2090 J04	X	632	640	-0.441553	632	640	-0.57704769	2431922	-1.90160885	2338621	-2.65909955	experimental	BIOMOL	NS-835			Thioridazine HCl
2090 J05	X	870	880	0.27033979	629	640	-0.58464109	3383458	0.61366994	3288949	0.13764613	experimental	BIOMOL	DL-479			Prindolone
2090 J06	X	631	640	-0.44454415	631	640	-0.57957882	3327471	0.46567458	3515347	0.80391885	experimental	BIOMOL	PD-125			Clostatone
2090 J07	X	712	720	-0.20226131	1031	1040	0.43287435	3257072	0.27958271	3667368	1.25130552	experimental	BIOMOL	DL-480			Progesterone
2090 J08	X	754	760	-0.07663317	989	1000	0.32656677	3409999	0.6838281	3701333	1.35126203	experimental	BIOMOL	PD-130			Etazolate
2090 J09	X	512	520	-0.80049055	551	560	-0.78206945	3828932	1.79123053	3558573	0.93112981	experimental	BIOMOL	DL-481			Procabazine HCl
2090 J10	X	713	720	-0.19927016	790	800	-0.17712868	3174138	0.06035597	3610936	1.08523028	experimental	BIOMOL	PD-140			Isobutylmethylxanthine
2090 J11	X	673	680	-0.31891601	911	920	0.1291384	3185556	0.09053818	3320108	0.22934478	experimental	BIOMOL	DL-482			Prothionamide
2090 J12	X	510	520	-0.80647284	546	560	-0.79472512	3337282	0.49160886	3522515	0.82501375	experimental	BIOMOL	PD-141			Irsogladine maleate
2090 J13	X	789	800	0.02805695	712	720	-0.37455705	3366462	0.56874292	3450043	0.61173397	experimental	BIOMOL	DL-483			Prindolone
2090 J14	X	949	960	0.50664034	592	600	-0.678293	3129889	-0.0566113	3664768	1.24365391	experimental	BIOMOL	PD-152			Milrinone
2090 J15	X	1352	1360	1.71207227	753	760	-0.2707806	3381569	0.60894092	3374987	0.39084966	experimental	BIOMOL	DL-484			Prindolone
2090 J16	X	789	800	0.02805695	591	600	-0.68082414	3522942	0.9823829	3716401	1.39550605	experimental	BIOMOL	PD-175			Rolipram
2090 J17	X	672	680	-0.32190715	913	920	0.13420067	2903446	-0.65518799	2868171	-1.10067227	experimental	BIOMOL	DL-485			Primaquine phosphate
2090 J18	X	712	720	-0.20226131	590	600	-0.68335527	3412332	0.68999512	3645382	1.18660233	experimental	BIOMOL	PD-179			Siguzadon
2090 J19	X	591	600	-0.56419	829	840	-0.0784145	3411388	0.68749976	3307384	0.19189898	experimental	BIOMOL	DL-486			Praziquantel
2090 J20	X	752	760	-0.08261546	951	960	0.23038372	3729145	1.52745478	3194017	-0.14173179	experimental	BIOMOL	DL-487			Triquinsin
2090 J21	X	750	760	-0.08859775	789	800	-0.17965982	3062886	-0.23372622	3085619	-0.46073916	experimental	BIOMOL	DL-480			Pyrantel pamoate
2090 J22	X	1111	1120	0.99120603	988	1000	0.32403564	3197745	0.12275843	3148029	-0.27707111</						

2090 K19	X	793	800	0.04002154	1431	1440	1.44532753	3448742	0.78624088	3199231	-0.12638737	experimental	BIOMOL	DL-341	Bupirone HCl
2090 K20	X	551	560	-0.68383585	709	720	-0.38215045	3172300	0.05549743	3393868	0.44641506	experimental	BIOMOL	DL-417	Guiafenines
2090 K21	X	832	840	0.15667624	910	920	0.12660727	3183006	0.08379754	3215822	-0.07756128	experimental	BIOMOL	DL-342	Canrenone
2090 K22	X	950	960	0.50963149	1550	1560	1.74652335	2861862	-0.76511064	3413610	0.52217188	experimental	BIOMOL	DL-418	Hexestrol
2090 K23	E	486	840	-0.8782635	486	760	-0.9465931	91216	-0.08900285	98497	-9.25162035	empty			
2090 K24	P	119041	119600	353.730778	90941	91480	228.007037	3526498	0.99178015	3219331	-0.067233455	empty			
2090 L01	N	556	560	-0.66888011	476	480	-0.97190442	2745271	-1.07330588	3019078	-0.65656445	empty			
2090 L02	E	116	120	-1.98498445	155	160	-1.7843981	81588	-8.11445338	88360	-9.2814528	empty			
2090 L03	X	794	800	0.04301268	914	920	0.1367318	2043588	-2.92812626	2462239	-2.92500654	experimental	BIOMOL	DL-488	Quinacrine 2HCl dihydrate
2090 L04	X	471	480	-0.92312754	711	720	-0.37708818	3586152	1.14946881	3513317	0.79794471	experimental	BIOMOL	PD-190	Zaprinas
2090 L05	X	671	680	0.3248983	830	840	-0.07588337	2905935	-0.6486086	3009809	-0.68384244	experimental	BIOMOL	DL-489	Quinapril HCl
2090 L06	X	512	520	-0.80049055	593	600	-0.67576187	3627394	1.25948742	3475479	0.58659025	experimental	BIOMOL	PD-195	Zardaverine
2090 L07	X	554	560	-0.67486241	474	480	-0.97696669	3253464	0.27004537	3289137	0.1381994	experimental	BIOMOL	DL-159	Racecadotril
2090 L08	X	554	560	-0.67486241	432	440	-1.08327427	3411534	0.6878857	3484147	0.71209954	experimental	BIOMOL	PG-006 PGE1	Alprostadi
2090 L09	X	354	360	-1.27309165	833	840	-0.06828997	2994288	-0.41505735	3151170	-0.26782737	experimental	BIOMOL	DL-490	Ranolazine 2HCl
2090 L10	X	434	440	-1.03379995	631	640	-0.57957882	3047139	-0.27535165	3405087	0.47943175	experimental	BIOMOL	PG-051	Misoprostol
2090 L11	X	595	600	-0.55222541	991	1000	0.33162904	3359296	0.5498004	3383623	0.41626477	experimental	BIOMOL	DL-491	Ramipril
2090 L12	X	474	480	-0.9141541	751	760	-0.27584287	3080798	-0.18637786	3555930	0.92335165	experimental	BIOMOL	PI-146	Argatroban
2090 L13	X	391	400	-1.16241924	872	880	0.03042422	3028491	-0.32464555	3219383	-0.06708151	experimental	BIOMOL	DL-147	Rebamipide
2090 L14	X	352	360	-1.27907394	710	720	-0.37961932	3806696	1.73245216	3798224	1.63640514	experimental	BIOMOL	PI-153	Cilastatin
2090 L15	X	712	720	-0.20226131	1032	1040	0.43540549	3058296	-0.24585937	3114579	-0.37551201	experimental	BIOMOL	DL-492	Ribavirin
2090 L16	X	752	760	-0.08261546	671	680	-0.4783335	3568991	1.10410563	3125725	-0.34271015	experimental	BIOMOL	PR-117	Artresunate
2090 L17	X	392	400	-1.15942809	952	960	0.23291485	2008130	-3.02185551	2231015	-2.97577612	experimental	BIOMOL	DL-566	Nelfinavir Mesylate
2090 L18	X	713	720	-0.37708818	711	720	-0.37708818	3744183	1.56720605	3549258	0.90371644	experimental	BIOMOL	RA-104	Picotamide
2090 L19	X	592	600	-0.56119885	750	760	-0.278374	3201834	0.13356275	3367556	0.3960557	experimental	BIOMOL	DL-494	Rimantadine HCl
2090 L20	X	833	840	0.15966739	872	880	-0.47502337	3340940	-0.29173801	334767	0.04222498	experimental	BIOMOL	SI-04	Condulrot b epoxide
2090 L21	X	512	520	-0.80049055	511	520	-0.8833147	2849528	-0.79774118	3138529	-0.30502895	experimental	BIOMOL	ST-405	Proramipid
2090 L22	X	591	600	-0.56419	629	640	-0.58464109	3108478	-0.11320888	3521437	0.82184128	experimental	BIOMOL	S-510	Mifepristone
2090 L23	E	524	800	-0.76459679	490	720	-0.93646856	87671	-8.09837366	97436	-9.2547428	empty			
2090 L24	P	92153	92960	273.311139	76528	77160	191.525818	3271195	0.31691528	2964931	-0.81591511	empty			
2090 M01	N	437	440	-1.02482651	637	640	-0.56439202	2550999	-1.58684214	2675504	-1.66767756	empty			
2090 M02	E	36	40	-2.2427614	116	120	-1.88311228	84467	-8.10684307	93295	-9.26692946	empty			
2090 M03	X	792	800	0.03703039	593	600	-0.67576187	2740271	-1.08652282	3043216	-0.58552809	experimental	BIOMOL	DL-343	Carbadox
2090 M04	X	1240	1250	1.35313472	633	640	-0.47502337	3049940	-0.29173801	3389582	0.056897149	experimental	BIOMOL	DL-419	Hydrocotilone
2090 M05	X	710	720	0.2082436	392	400	-1.18451959	2738445	-1.09134965	3183889	-0.17153775	experimental	BIOMOL	DL-344	Carboplatin
2090 M06	X	753	760	-0.07962431	592	600	-0.678293	2716534	-1.14926892	3101950	-0.41267823	experimental	BIOMOL	DL-420	Hydrocortisone 21-acetate
2090 M07	X	553	560	-0.67785355	594	600	-0.67323074	3658507	1.34073115	3386295	0.42412827	experimental	BIOMOL	DL-345	Carbamazepine
2090 M08	X	554	560	-0.67486241	472	480	-0.98202896	3083819	-0.17839218	3319808	0.2284619	experimental	BIOMOL	DL-421	17- hydroxyprogesterone
2090 M09	X	514	520	-0.79450826	712	720	-0.37455705	3285078	0.35361343	3432172	0.55914092	experimental	BIOMOL	DL-346	Cefoperazone acide
2090 M10	X	875	880	0.28529553	791	800	-0.17459755	2912688	-0.6307578	3397413	0.45684773	experimental	BIOMOL	DL-422	Idoxuridine
2090 M11	X	460	460	-1.15643695	870	880	-0.47502337	3161723	0.04220912	3612260	0.17517038	experimental	BIOMOL	DL-347	Saralofloxacin acid
2090 M12	X	354	360	-1.27309165	712	720	-0.37455705	3088677	-0.1655506	3811292	-0.179187054	experimental	BIOMOL	DL-423	Ifofosamide
2090 M13	X	474	480	-0.9141541	511	520	-0.88331477	3152162	0.00226488	3255800	0.04009105	experimental	BIOMOL	DL-348	Ceftazidime
2090 M14	X	993	1000	0.63825078	952	960	0.23291485	3073199	-0.20646496	2953939	-0.84826376	experimental	BIOMOL	DL-424	Inequidam
2090 M15	X	1031	1040	0.75191433	670	680	-0.48086464	3014060	-0.36279228	2803754	-1.29024721	experimental	BIOMOL	DL-349	Chloramphenicol
2090 M16	X	832	840	0.15667624	553	560	-0.77700719	3136870	-0.03815781	3170328	-0.21144678	experimental	BIOMOL	DL-425	Indapamide
2090 M17	X	552	560	-0.6808447	551	560	-0.78206945	2974585	-0.46714002	3320674	0.23101048	experimental	BIOMOL	DL-350	Chlormadinone acetate
2090 M18	X	729	730	-0.31891695	672	680	-0.47502337	3040940	-0.29173801	334767	0.04222498	experimental	BIOMOL	DL-426	Isopride HCl
2090 M19	X	552	560	-0.6808447	871	880	0.02789308	3226142	0.19782722	3292246	0.39224166	experimental	BIOMOL	DL-427	Chlorambucil
2090 M20	X	873	880	0.27931323	952	960	0.23291485	3290529	0.36802254	3302180	0.17658399	experimental	BIOMOL	DL-427	Itraconazole
2090 M21	X	552	560	-0.6808447	871	880	0.02789308	3370729	0.58002225	3134830	-0.31591478	experimental	BIOMOL	DL-352	Chlorpheniramine maleate
2090 M22	X	831	840	0.15368509	1111	1120	0.63356499	2832063	-0.84388095	2914502	-0.96432396	experimental	BIOMOL	EI-288	Ketoprofen (s)
2090 M23	E	615	1080	-0.49240249	546	920	-0.79472512	90860	-8.08994389	96200	-9.25838026	empty			
2090 M24	P	157722	158240	469.437605	125519	126160	315.528551	3596710	1.17737777	3143419	-0.290638	empty			
2090 N01	N	436	440	-1.02781766	556	560	-0.76941379	2551383	-1.6850863	3096330	-0.42521748	empty			
2090 N02	E	117	120	-1.98199335	116	120	-1.88311228	82574	-8.111847	90295	-9.27575824	empty			
2090 N03	X	634	640	-0.43557071	594	600	-0.67323074	2770640	-1.00624577	2894287	-1.02381522	experimental	BIOMOL	DL-496	Roxatidine acetate HCl
2090 N04	X	591	600	-0.56419	591	600	-0.68082414	2934080	-0.57421045	3064570	-0.52268483	experimental	BIOMOL	S-515	Megestrol acetate
2090 N05	X	872	880	0.27632209	712	720	-0.37455705	3054898	-0.2548416	3242287	0.00032328	experimental	BIOMOL	DL-497	Roxithromycin
2090 N06	X	632	640	-0.441553	1032	1040	0.43540549	3198494	0.12473833	3402699	0.47240404	experimental	BIOMOL	S-520	Melengestrol acetate
2090 N07	X	553	560	-0.67785355	551	560	-0.78206945	3229013	0.20541189	3051040	-0.56250263	experimental	BIOMOL	DL-498	Rufloxacin
2090 N08	X	514	520	-0.79450826	1113	1120	0.64042726	2882335	-0.71099256	3366130	0.36478416	experimental	BIOMOL	S-650	Tamoxifen citrate
2090 N09	X	353	360	-1.27608279	672	680	-0.68082414	3307587	0.41131345	3368670	0.37225919	experimental	BIOMOL	DL-499	Saralofloxacin HCl
2090 N10	X	513	520	-0.79749994	753	760	-0.27584287	3554624	1.06612808	3487702	0.72256164	experimental	BIOMOL	DL-532	Ampranavir
2090 N11	X	674	680	-0.31592486	912	920	0.13166954	3220312	0.18241177	3189965	-0.15365653	experimental	BIOMOL	DL-500	Scopolamine n-butylbromide
2090 N12	X	589	600	-0.57017229	546	560	-0.79472512	3387600	0.62461885	3153217	-0.2618032	experimental	BIOMOL	DL-533	Aprepitant
2090 N13	X	393	400	-1.15643695	513	520	-0.87825251	3013769	-0.36356151	3233230	-0.02633081	experimental	BIOMOL	DL-501	Scopolamine HBr
2090 N14	X	592	600	-0.56119885	672	680	-0.4783335	3225990	0.19742093	3174918	-0.19793875	experimental	BIOMOL	DL-534	Bosentan
2090 N15	X	432	440	-1.03978224	1033	1040	0.43793662	3238824	0.23134617	3607371	1.07473874	experimental	BIOMOL	DL-502	Secnidazole
2090 N16	X	551	560	-0.68383585	512	520	-0.88331477	3364132	0.56258382	329499	0.056897149	experimental	BIOMOL	DL-535	Tafaviren
2090 N17	X	994	1000	0.64124912	753	760	-0.2707806	2070114	-0.21651981	3116150	-0.37088867	experimental	BIOMOL	DL-503	Sibutramine HCl
2090 N18	X	551	560	-0.68383585	712	720	-0.37455705	2895890	-0.67516143	3124356	-0.34673901	experimental	BIOMOL	DL-536	Taurocholic acid, sodium salt hydrate
2090 N19	X	754	760	-0.07663317	751	760	-0.27584287	3269948	0.31361897	3184594	-0.16946299	experimental	BIOMOL	DL-149	Sparfloxacin
2090 N20															

2090 O13	X	707	720	-0.21721704	667	680	-0.48845803	3078448	-0.19258982	3345981	0.30548713	experimental	BIOMOL	DL-358	Climbazole
2090 O14	X	793	800	0.04002154	752	760	-0.27331173	2831316	-0.84585556	2942921	-0.88068892	experimental	BIOMOL	DL-434	Lisinopril
2090 O15	X	471	480	-0.92312754	591	600	-0.68082414	3225810	0.19694512	2989361	-0.74401941	experimental	BIOMOL	DL-359	Clinafloxacin HCl
2090 O16	X	914	920	0.40195023	511	520	-0.86331477	2896483	-0.6735939	3062138	-0.51219035	experimental	BIOMOL	DL-435	Lumefantrone HCl
2090 O17	X	551	560	-0.68383585	572	580	-0.27331173	3216692	0.1728427	3305453	-0.18623385	experimental	BIOMOL	DL-360	Clomiphene citrate
2090 O18	X	550	560	-0.68682699	506	520	-0.89597044	2670451	-1.27108416	2961557	-0.82584454	experimental	BIOMOL	DL-436	Loratadine
2090 O19	X	510	520	-0.80647284	1030	1040	0.43034322	2892565	-0.6839507	3541419	0.88064684	experimental	BIOMOL	DL-361	Clopidol
2090 O20	X	913	920	0.39895908	869	880	0.02283082	2955567	-1.46903163	3013266	-0.67366874	experimental	BIOMOL	DL-437	Lorglumidol
2090 O21	X	628	640	-0.45351759	630	640	-0.58210995	3009457	-0.37495979	3361902	0.35234146	experimental	BIOMOL	AC-1290	Clopidogrel sulfate
2090 O22	X	1030	1040	0.74892319	1230	1240	0.93656981	2621765	-1.39978015	3184425	-0.16996305	experimental	BIOMOL	DL-438	Losartan potassium
2090 O23	E	683	1200	-0.28904555	610	920	-0.63273261	89090	-8.09462269	94637	-9.26298005	empty			
2090 O24	P	175176	175880	521.645071	101871	102960	255.67232	308402	-0.17156431	3188156	-0.15898029	empty			
2090 P01	N	838	840	0.17462312	1478	1480	1.56429078	2423596	-1.92361769	2485949	-2.22552404	empty			
2090 P02	E	76	80	-2.10463029	114	120	-1.88817455	80682	-8.11684829	88339	-9.2815146	empty			
2090 P03	X	636	640	-0.42958842	635	640	-0.56945429	2707612	-1.17285323	2834920	-1.19852795	experimental	BIOMOL	DL-505	Stanozolol
2090 P04	X	554	560	-0.67486241	993	1000	0.3366913	2868262	-0.74819295	3325455	0.24508061	experimental	BIOMOL	DL-538	Methysergide
2090 P05	X	1114	1120	1.00017947	752	760	-0.27331173	2687979	-1.22475086	3139776	-0.30135908	experimental	BIOMOL	DL-506	Streptomycin sulfate
2090 P06	X	751	760	-0.0856066	833	840	-0.06828997	3166638	0.04053056	3165219	-0.5264822	experimental	BIOMOL	DL-107	Esmolol
2090 P07	X	1273	1280	1.47577172	794	800	-0.16700415	2752120	-1.05520132	3188156	-0.15898029	experimental	BIOMOL	DL-507	Sulfadoxime
2090 P08	X	913	920	0.39895908	634	640	-0.57198542	3165530	0.03760169	3651862	1.2056725	experimental	BIOMOL	DL-123	Pantothenic acid
2090 P09	X	594	600	-0.55521656	715	720	-0.36696365	2759982	-1.034419	2928325	-0.92364388	experimental	BIOMOL	DL-508	Sulfadiazine
2090 P10	X	514	520	-0.79450826	715	720	-0.36696365	3146872	-0.01171864	3351774	0.3225355	experimental	BIOMOL	DL-146	Phloridzin
2090 P11	X	875	880	0.28529553	394	400	-1.17945733	1997306	-3.05046754	3106187	-0.40020905	experimental	BIOMOL	DL-509	Sulfamidmethoxine
2090 P12	X	468	480	-0.93210098	1029	1040	0.42781209	2792696	-0.94794321	3601482	1.05740785	experimental	BIOMOL	DL-225	Phenylpropanolamine
2090 P13	X	954	960	-0.52159608	553	560	-0.77700719	2512272	-1.68921262	2856990	-1.13357756	experimental	BIOMOL	DL-510	Sulfasalazine
2090 P14	X	712	720	-0.20226131	874	880	-0.47074401	3984089	-0.44201726	3658296	0.72540066	experimental	BIOMOL	DL-234	Succinylcholine
2090 P15	X	955	960	-0.5245822	753	760	0.2707806	2827176	-0.8579149	2870702	-1.09322415	experimental	BIOMOL	DL-160	Tamsulosin HCl
2090 P16	X	552	560	-0.6808447	1193	1200	0.84291789	2764679	-1.02200301	3315123	0.21467429	experimental	BIOMOL	DL-195	Trifluoperidol 2HCl
2090 P17	X	792	800	0.03703039	987	1000	0.32150451	2567128	-1.54420694	3099118	-0.4210126	experimental	BIOMOL	DL-511	Telmisartan
2090 P18	X	1673	1680	2.6722302	2432	2440	3.9789916	3006232	-0.38348472	3190351	-0.15252056	experimental	BIOMOL	DL-540	L-thyroxine [[3-[4-(4-hydroxy-3,5-diiodophenoxy)-3,5-c
2090 P19	X	1192	1200	1.23348887	1265	1280	1.02515946	2544984	-1.60274212	2917146	-0.95654286	experimental	BIOMOL	DL-512	Tenoxicam
2090 P20	X	670	680	-0.32788945	1592	1600	1.85283993	2300775	-2.24828124	2914207	-0.96519212	experimental	BIOMOL	DL-136	Cyproheptadine
2090 P21	X	1474	1480	2.07699221	670	680	-0.48086464	2598358	-1.46165393	2896614	-1.01696703	experimental	BIOMOL	DL-513	Terazosin HCl
2090 P22	X	840	840	0.15069392	1070	1070	0.15069392	3273354	0.15069392	3273354	0.15069392	experimental	BIOMOL	DL-513	Benzydamine
2090 P23	E	459	920	-0.9590213	922	1600	0.15698086	83161	-8.11029534	93109	-9.26747684	empty			
2090 P24	P	156688	157200	466.34476	231857	232160	584.684165	2387174	-2.01989517	2679043	-1.65726254	empty			
2091 A01	N	599	600	0.34611629	398	400	-0.86758332	2140856	0.72095797	1662093	0.28651379	empty			
2091 A02	E	116	120	-1.79679885	156	160	-1.95228994	72419	-0.91804505	72727	-0.91688629	empty			
2091 A03	X	477	480	-0.19515834	556	560	-0.15938643	2188608	0.75879605	1640557	0.2702077	experimental	Microsource	200046	Griseofulvin
2091 A04	X	552	560	0.13759245	755	760	0.73258306	1994588	0.60550708	1811811	0.39987353	experimental	Microsource	1500161	Carbinopamine maleate
2091 A05	X	435	440	-0.28309588	436	440	-0.28309588	2124130	0.7077045	1951430	0.53086968	experimental	Microsource	1500162	Carbinopamine maleate
2091 A06	X	516	520	-0.02212793	636	640	0.19919427	2299515	0.84667733	2301058	0.77030926	experimental	Microsource	1500162	Carbinopamine maleate
2091 A07	X	436	440	-0.37706211	555	560	-0.16386869	1868068	0.50480425	2208192	0.6999954	experimental	Microsource	210369	Gallic acid
2091 A08	X	596	600	0.33280626	475	480	-0.52244939	2266480	0.82050082	2377976	0.82854821	experimental	Microsource	1500163	Cefadroxil
2091 A09	X	556	560	0.15533916	596	600	0.01990392	2307627	0.85310518	2350816	0.80798388	experimental	Microsource	211468	Danthron
2091 A10	X	475	480	-0.2040317	595	600	0.01542166	2130570	0.71280748	2122128	0.63483161	experimental	Microsource	1500164	Cefazolin sodium
2091 A11	X	555	560	0.15090249	554	560	-0.16835095	2249743	0.80723864	2709527	0.60257604	experimental	Microsource	300024	Hydrocortisone
2091 A12	X	709	720	0.86077085	836	840	0.86077085	2055356	0.65320887	2055356	0.60984472	experimental	Microsource	1500165	Hydrocortisone sodium
2091 A13	X	475	480	-0.2040317	395	400	0.88103009	1953116	0.81260471	2014553	0.5533836471	experimental	Microsource	300029	Desoxycorticosterone acetate
2091 A14	X	476	480	-0.19959502	516	520	-0.33867678	1956868	0.60592871	1958502	0.51094136	experimental	Microsource	1500166	Cephalothin sodium
2091 A15	X	355	360	-0.73643297	395	400	-0.88103009	2204723	0.77156537	1946918	0.50217047	experimental	Microsource	300034	Testosterone propionate
2091 A16	X	635	640	0.50583667	635	640	-0.70173974	2427635	0.94819798	1947431	0.50255889	experimental	Microsource	1500167	Cephapirin sodium
2091 A17	X	833	840	1.38429878	475	480	0.37400236	2232661	0.79370308	1931885	0.49078816	experimental	Microsource	300548	Sparteine sulfate
2091 A18	X	874	880	1.56620255	715	720	0.55329271	2243980	0.80267211	2152742	0.65801115	experimental	Microsource	1500168	Cephadrine
2091 A19	X	593	600	0.31949622	474	480	-0.52693165	2118280	0.70306904	2296662	0.7669809	experimental	Microsource	300607	Rutroside (rutin)
2091 A20	X	994	1000	2.05860382	914	920	1.44526221	1653933	0.33512642	1926376	0.48661699	experimental	Microsource	1500169	Cetylpyridinium chloride
2091 A21	X	913	920	0.73923296	1153	1160	2.51652205	2214630	0.77941555	2205624	0.69805102	experimental	Microsource	300618	Salicylanilide
2091 A22	X	712	720	0.84746082	990	1000	1.78591387	1958804	0.5767023	2722845	1.08966751	experimental	Microsource	1500171	Chlorambucil
2091 A23	E	749	1160	1.01161788	805	1440	0.956696	75192	-0.91584776	77869	-0.91298939	empty			
2091 A24	P	139725	140200	617.603283	216854	217280	969.344221	1639020	0.32330955	1990096	0.53486291	empty			
2091 B01	N	356	360	-0.7319963	357	360	-1.05135593	1830772	0.47525138	2322173	0.78629669	empty			
2091 B02	E	157	160	-1.61489508	277	280	-1.40993663	75741	-0.91541274	81765	-0.91003952	empty			
2091 B03	X	472	480	-0.21734173	514	520	-0.3476413	2145482	0.72462356	2685694	1.06153844	experimental	Microsource	1500263	Dopamine hydrochloride
2091 B04	X	1554	1560	4.58314311	674	680	0.3695201	1455486	0.17787955	1514845	0.17502422	experimental	Microsource	1500375	Mechlorethamine
2091 B05	X	472	480	-0.21734173	315	320	-1.2396108	2195483	0.76424371	2268676	0.74579116	experimental	Microsource	1500264	Doxepin hydrochloride
2091 B06	X	355	360	-0.73643297	433	440	-0.71070426	2231280	0.79260879	2742432	1.10449791	experimental	Microsource	1500376	Mecizline hydrochloride
2091 B07	X	315	320	-0.91390007	433	440	-0.71070426	2694921	1.15999199	3017387	1.31268147	experimental	Microsource	1500266	Doxycycline hydrochloride
2091 B08	X	395	400	-0.55896588	594	600	-0.16835095	2340518	0.87916759	2526390	0.94092062	experimental	Microsource	1500377	Meclofenamate sodium
2091 B09	X	355	360	-0.73643297	394	400	-0.88551235	2524964	1.02532024	2482355	0.90757269	experimental	Microsource	1500267	Doxylamine succinate
2091 B10	X	445	450	-0.38149879	554	560	-0.16835095	2485424	0.99398925	2581399	1.15823093	experimental	Microsource	1500378	Dicycloxypropionate acetate
2091 B11	X	475	480	-0.2040317	754	760	0.7281008	2269207	0.82261417	2958871	0.726519432	experimental	Microsource	1500268	Dicyclonine hydrochloride
2091 B12	X	554	560	0.14646581	473	480	-0.53141391	2486749	0.95039116	2708481	1.07879173	experimental	Microsource	1500380	Medrysone
2091 B13	X	474	480	-0.20846837	473	480	-0.52693165	2470058	0.9818134						

2091 C07	X		556	560	0.15533916	753	760	0.72361855	4734589	2.77619882	4963859	2.78646255			experimental	Microsource	310006		Hydrastinine hydrochloride
2091 C08	X		395	400	-0.55896588	834	840	1.08668151	2576337	1.06602755	2740062	1.10270345			experimental	Microsource	1500174		Chloramphenicol
2091 C09	X		196	200	-1.44186466	194	200	-1.78196411	1909231	-0.11154384	1026425	-0.19478544			experimental	Microsource	310035		Sanguinarine sulfate
2091 C10	X		276	280	-1.08693048	355	360	-1.06032045	2177113	0.74669756	2314151	0.78022279			experimental	Microsource	1500175		Chlorcyclizine hydrochloride
2091 C11	X		275	280	-1.09136716	194	400	-0.88551235	2082442	2.254546	2445182	0.87493584			experimental	Microsource	150039		Alpha-tocopherol
2091 C12	X		515	520	-0.02656461	434	440	-0.706222	2366155	0.89484802	2298845	0.76863377			experimental	Microsource	1500177		Chlorhexidine
2091 C13	X		474	480	-0.20846837	475	480	-0.52244939	2469030	0.98099885	2211887	0.70279309			experimental	Microsource	310040		Alpha-tocopheryl acetate
2091 C14	X		554	560	0.14646581	514	520	-0.3476413	2697034	1.1616663	2325433	0.78876501			experimental	Microsource	1500178		Chlorocresol
2091 C15	X		634	640	0.50139999	354	364	-1.0648027	2689759	1.15590169	2627853	1.01774384			experimental	Microsource	310050		Quinine ethyl carbonate
2091 C16	X		473	480	-0.21290505	434	440	-0.706222	2479834	0.98955988	2568723	0.97297326			experimental	Microsource	1500179		Chloroquine diphosphate
2091 C17	X		673	680	0.67443041	632	640	0.18126523	2377272	0.90829099	2059636	0.97551547			experimental	Microsource	330001		Dactinomycin
2091 C18	X		594	600	0.3239329	914	920	1.44526221	2850799	1.28350772	263269	1.01587821			experimental	Microsource	1500180		Chlorothiazide
2091 C19	X		433	440	-0.39037214	393	400	-0.88999461	1571403	0.2697307	1450492	0.12629903			experimental	Microsource	330002		Mitomycin c
2091 C20	X		555	560	0.15090249	434	440	-0.706222	2874987	1.30267399	2440252	0.8757008			experimental	Microsource	1500181		Chlorocyanisene
2091 C21	X		472	480	-0.21734173	632	640	0.18126523	2885295	1.31084191	2790873	1.14117525			experimental	Microsource	330018		Dichlorvos
2091 C22	X		673	680	0.67443041	671	680	0.35607333	2451766	0.96731908	2690772	1.06538328			experimental	Microsource	1500182		Chloroxylenol
2091 C23	E		451	760	-0.31051195	774	1200	0.81774598	83193	-0.90950787	84126	-0.90825188			empty				
2091 C24	P	103499	104240	456.880211	143327	141460	639.777181	2374878	0.90639401	2353348	0.80990099			empty					
2091 D01	N		276	280	-1.08693048	557	560	-0.15490417	1921169	0.54688808	2200656	0.69428948			empty				
2091 D02	E		237	240	-1.2599609	156	160	-1.95228994	82073	-0.91039534	82431	-0.90953525			empty				
2091 D03	X		355	360	-0.73643297	435	440	-0.70173974	2421193	0.94309343	2692515	1.06874732			experimental	Microsource	1500279		Erythromycin ethylsuccinate
2091 D04	X		236	240	-1.26439757	554	560	-0.16835095	2438778	0.95702755	2708368	1.07870618			experimental	Microsource	1500390		Metaprotenerol
2091 D05	X		316	320	-0.90946339	835	840	1.09116376	2285161	0.83530341	2963366	1.2717792			experimental	Microsource	1500280		Erythromycin
2091 D06	X		396	400	-0.5545292	433	440	-0.71070426	2440131	0.95809965	2706280	1.07712524			experimental	Microsource	1500391		Methacholine chloride
2091 D07	X		395	400	-0.55896588	354	360	-1.0648027	2675281	1.14442951	2921730	1.24025429			experimental	Microsource	1500282		Estradiol
2091 D08	X		520	520	-0.02212793	394	400	-0.706222	2658631	1.13123626	3343275	1.53262592			experimental	Microsource	1500394		Methamphetamine
2091 D09	X		316	320	-0.90946339	395	400	-0.88103009	2655572	0.04933303	3101875	0.67507727			experimental	Microsource	1500283		Estradiol cypionate
2091 D10	X		396	400	-0.5545292	395	400	-0.88103009	2664373	1.13578615	2863248	1.19597435			experimental	Microsource	1500295		Methicillin sodium
2091 D11	X		436	440	-0.37706211	515	520	-0.34315904	2531817	1.03075047	2608833	1.00334275			experimental	Microsource	1500284		Estradiol valerate
2091 D12	X		395	400	-0.55896588	555	560	-0.16386869	2642266	1.11826884	3179433	1.43537541			experimental	Microsource	1500396		Methimazole
2091 D13	X		436	440	-0.37706211	354	360	-1.0648027	2558799	1.05213066	2677100	1.05530145			experimental	Microsource	1500285		Estril
2091 D14	X		275	280	-1.09136716	595	600	0.01542166	2651548	1.12562378	2844062	1.18144757			experimental	Microsource	1500397		Methocarbamol
2091 D15	X		514	520	-0.03100128	394	400	-0.88551235	2990406	1.39413053	3079921	1.3600294			experimental	Microsource	1500286		Estrone
2091 D16	X		640	640	-0.68119281	394	400	-0.706222	2907738	0.6747377	3560625	0.69548542			experimental	Microsource	1500398		Methoxetate(+/-)
2091 D17	X		354	360	-0.74086965	993	1000	1.79936065	2688409	1.15483197	2562130	0.96798134			experimental	Microsource	1500287		Acetyric acid
2091 D18	X		434	440	-0.38593547	750	760	0.71017177	3056078	1.44616818	2626213	1.0165021			experimental	Microsource	1500399		Methoxamine hydrochloride
2091 D19	X		555	560	0.15090249	472	480	-0.53589617	2970913	1.37868452	2693797	1.06767367			experimental	Microsource	1500288		Ethambutol hydrochloride
2091 D20	X		473	480	-0.21290505	512	520	-0.35660582	3138579	1.51154091	2625887	1.01625527			experimental	Microsource	1500400		Methoxsalen
2091 D21	X		834	840	1.38873545	953	960	1.62007073	2745233	1.19985858	2532040	0.94519854			experimental	Microsource	1500291		Ethyl estradiol
2091 D22	X		472	480	-0.21734173	630	640	0.17230072	2854303	1.28628425	2477692	0.90404868			experimental	Microsource	1500401		Methscopolamine bromide
2091 D23	E		367	640	-0.68119281	394	400	-0.706222	2907738	0.6747377	3560625	0.69548542			empty				
2091 D24	P	91712	92280	404.585095	139925	140720	624.528536	2393162	0.92088022	2353812	0.90568022			empty					
2091 E01	N		398	400	-0.54565585	357	360	-1.05135593	3160825	1.52916836	2093616	0.6132436			empty				
2091 E02	E		156	160	-1.61933176	157	160	-1.94780768	84613	-0.90838268	87326	-0.90582898			empty				
2091 E03	X		636	640	0.51027335	436	440	-0.69725749	3346199	1.67605635	2323515	0.78731279			experimental	Microsource	330062		Temefos
2091 E04	X		394	400	-0.56340256	314	320	-1.24409306	2969415	1.37749753	2099967	0.61737085			experimental	Microsource	1500183		Chlorpheniramine (s) maleate
2091 E05	X		476	480	-0.19959502	395	400	-0.88103009	3291678	1.6328546	2766403	1.2264767			experimental	Microsource	330071		Lindane
2091 E06	X		355	360	-0.73643297	394	400	-0.88551235	2083926	0.6747377	2742745	0.55920772			experimental	Microsource	3500184		Methylpromazine
2091 E07	X		366	360	-0.7319963	393	600	-0.00647810	2863451	1.29353303	3040816	1.12647053			experimental	Microsource	1500382		Mitomycin
2091 E08	X		395	400	-0.55896588	514	520	-0.3476413	2664988	1.13627346	2693012	1.0670793			experimental	Microsource	1500185		Chlorpropamide
2091 E09	X		395	400	-0.55896588	514	520	-0.3476413	2614471	1.09624444	2561064	0.96717421			experimental	Microsource	330086		Dibutyl phthalate
2091 E10	X		475	480	-0.2040317	515	520	-0.34315904	2687280	1.15393736	2364844	0.81860525			experimental	Microsource	1500186		Chlortetracycline hydrochloride
2091 E11	X		395	400	-0.55896588	394	400	-0.88551235	2742747	1.1978887	2610265	1.004427			experimental	Microsource	1300027		Ivermectin
2091 E12	X		356	360	-0.7319963	434	440	-0.706222	2724284	1.18325886	2009271	0.54938136			experimental	Microsource	1500187		Chlorthalidone
2091 E13	X		315	320	-0.91390007	435	440	-0.70173974	2623541	1.10343139	2425837	0.86478641			experimental	Microsource	1500037		Sodium nitroprusside
2091 E14	X		355	360	-0.73643297	393	400	-0.88999461	2807032	1.24882731	2432363	0.8697276			experimental	Microsource	1500188		Chlorzoxazone
2091 E15	X		714	720	0.85633418	714	720	0.54881045	3044909	1.43731801	2668253	1.0483329			experimental	Microsource	1300038		Sodium oxybate
2091 E16	X		674	680	0.67886709	673	680	0.36503784	2572939	1.06333501	2561639	0.96760957			experimental	Microsource	1500189		Ciclopirox olamine
2091 E17	X		513	520	-0.03543796	550	560	-0.18627999	3218421	1.57480669	2793701	1.14331649			experimental	Microsource	1400151		Ethyl paraben
2091 E18	X		715	720	0.86077085	992	1000	1.79487839	2900492	1.32288382	2764079	1.12088804			experimental	Microsource	1500190		Cinoxacin
2091 E19	X		433	440	-0.39037214	909	920	1.42285091	2704093	1.16725977	2746199	1.10735011			experimental	Microsource	1400208		Coumarin
2091 E20	X		554	560	0.14646581	793	800	0.9029089	2202395	0.76972069	2509096	0.92782638			experimental	Microsource	1500191		Clemastine
2091 E21	X		593	600	0.31949622	470	480	-0.54486569	2488676	0.99565609	3648586	1.79059697			experimental	Microsource	1600716		2,6-di-t-butyl-4-methylphenol
2091 E22	X		552	560	0.13759245	711	720	0.53536368	2565008	1.05705059	2809720	1.15544535			experimental	Microsource	1500192		Clidinium bromide
2091 E23	E		450	720	-0.31494863	777	1160	0.83119276	84937	-0.90812594	88579	-0.90488026			empty				
2091 E24	P	96068	91240	399.687004	128912	129640	575.16542	2579489	1.06852515	2818796	1.16231729			empty					
2091 F01	N		317	320	-0.90502671	477	480	-0.51348488	215187										

2091 G01	N	477	480	-0.19515834	437	440	-0.69277523	2859219	1.29017962	2162909	0.66570915	empty			
2091 G02	E	197	200	-1.43742799	196	200	-1.77299959	82298	-0.91021705	85132	-0.90749018	empty			
2091 G03	X	396	400	-0.5545292	316	320	-1.23512854	3375473	1.69925269	2027323	0.56304952	experimental	Microsource	1500101	Acetaminophen
2091 G04	X	275	280	-1.09136718	434	440	-0.706222	2876378	1.3037762	216403	0.55478139	experimental	Microsource	1500193	Clindamycin hydrochloride
2091 G05	X	396	400	-0.5545292	316	320	-1.23512854	3375473	1.69925269	2027323	0.56304952	experimental	Microsource	1500102	Acetazolamide
2091 G06	X	395	400	-0.55896588	514	520	-0.3476413	3047046	1.43901134	3238059	1.47976439	experimental	Microsource	1500196	Clomiphene citrate
2091 G07	X	436	440	-0.37706211	712	720	0.53984594	3060006	1.44928067	3042208	1.33147481	experimental	Microsource	1500103	Acetohydroxamic acid
2091 G08	X	395	400	-0.55896588	514	480	-0.53141391	2835021	1.27100544	2735169	1.09899869	experimental	Microsource	1500198	Clonidine hydrochloride
2091 G09	X	476	480	-0.19959502	473	520	-0.3476413	2746350	1.20074367	2558868	0.9655115	experimental	Microsource	1500104	Acetylcholine
2091 G10	X	395	400	-0.55896588	514	480	-0.52693165	2613678	1.09561608	2693370	1.06735036	experimental	Microsource	1500200	Clotrimazole
2091 G11	X	275	280	-1.09136718	434	560	-0.16835095	2955225	1.36625355	2409384	0.85232893	experimental	Microsource	1500105	Acetylcysteine
2091 G12	X	474	480	-0.20846837	394	400	-0.88551235	2399528	0.92592636	262623	1.01335234	experimental	Microsource	1500201	Cloxacillin sodium
2091 G13	X	755	760	1.03823795	434	440	-0.706222	2529248	1.02871482	2336877	0.79742989	experimental	Microsource	1500107	Adenosine
2091 G14	X	474	480	-0.20846837	394	720	0.54432819	2609397	1.09222387	2133649	0.64355479	experimental	Microsource	1500202	Cloxyquin
2091 G15	X	512	520	-0.03987464	551	560	-0.18179773	3008974	1.40884357	2689737	1.06459962	experimental	Microsource	1500108	Allopurinol
2091 G16	X	1274	1280	3.34087347	1114	1120	2.34171396	2490506	0.99801616	2420489	0.86073714	experimental	Microsource	1500205	Colchicine
2091 G17	X	752	760	1.02492792	550	560	-0.18627999	2389044	0.91761897	2726910	1.092274534	experimental	Microsource	1500109	Alverine citrate
2091 G18	X	514	520	-0.03101028	553	560	-0.17283321	2409104	0.93351426	2834897	1.17450825	experimental	Microsource	1500206	Colistimethate sodium
2091 G19	X	514	520	-0.03101028	710	720	0.53088142	2533175	1.16032653	2299160	0.84458778	experimental	Microsource	1500110	Amantadine hydrochloride
2091 G20	X	554	560	0.14646581	833	840	1.08219925	2344061	0.88197501	2687773	1.06311257	experimental	Microsource	1500207	Cortisone acetate
2091 G21	X	633	640	0.49696332	631	640	0.17678298	2481928	0.99121906	2443436	0.87811158	experimental	Microsource	1500111	Amikacin sulfate
2091 G22	X	431	440	-0.3992455	711	720	0.53536368	2324597	0.86655199	2568926	0.97312696	experimental	Microsource	1500208	Cotinine
2091 G23	E	613	920	0.40822977	481	840	-0.49555584	83725	-0.90908632	86067	-0.90678224	empty			
2091 G24	P	103219	103920	55.637941	120591	121320	57.868545	2454056	0.96913365	2400126	0.84531919	empty			
2091 H01	N	357	360	-0.72755962	436	440	-0.69275479	2056364	0.65400759	2443283	0.87799573	empty			
2091 H02	E	157	160	-1.41480908	236	236	-1.59370924	77942	-0.91365869	81782	-0.90302665	empty			
2091 H03	X	360	360	-0.72755962	515	520	-0.34315904	2470033	0.88019362	2602340	0.99856344	experimental	Microsource	1500309	Furazolidone
2091 H04	X	315	320	-0.91390007	874	880	1.26597186	2605343	1.08901153	2870232	1.20126232	experimental	Microsource	1500418	Moxalactam disodium
2091 H05	X	436	440	-0.37706211	553	560	-0.17283321	2434167	0.95337386	2972468	1.27867082	experimental	Microsource	1500310	Furosemide
2091 H06	X	436	440	-0.37706211	433	440	-0.71070426	2775249	1.22364287	3018134	1.31324706	experimental	Microsource	1500419	Nadide
2091 H07	X	315	320	-0.91390007	633	640	0.18574749	2494116	1.00087668	2868070	1.19866906	experimental	Microsource	1500311	Fusidic acid
2091 H08	X	396	400	-0.5545292	554	560	-0.16835095	2953940	1.36523533	3153579	1.41579993	experimental	Microsource	1500420	Nafcillin sodium
2091 H09	X	235	240	-1.26883425	434	440	-0.706222	2552984	1.04752293	3109728	1.38259792	experimental	Microsource	1500312	Gallamine triethiodide
2091 H10	X	474	480	-0.20846837	474	560	-0.49746142	2594966	1.27009656	2700966	0.93439848	experimental	Microsource	1500421	Minoxidil hydrochloride
2091 H11	X	395	400	-0.55896588	473	480	-0.52693165	2499902	1.00546143	2861428	1.19459633	experimental	Microsource	1500313	Gemfibrozil
2091 H12	X	474	480	-0.20846837	475	480	-0.52244939	2724014	1.18304491	2804802	1.15172167	experimental	Microsource	1500425	Naproxen(+)
2091 H13	X	474	480	-0.20846837	554	560	-0.16835095	2422785	0.94435491	2763283	1.12028535	experimental	Microsource	1500314	Gentamicin sulfate
2091 H14	X	394	400	-0.56340256	713	720	0.54432819	2665019	1.13629803	2908417	1.23017428	experimental	Microsource	1500427	Neomycin sulfate
2091 H15	X	434	440	-0.38593547	634	640	0.19022975	1470801	0.19001496	1392665	0.08251502	experimental	Microsource	1500315	Gentian violet
2091 H16	X	512	520	-0.03987464	512	520	-0.35660582	2734079	1.19102029	2754206	1.11341265	experimental	Microsource	1500433	Nitrofurantoin
2091 H17	X	474	480	-0.20846837	754	760	-0.72810704	2784921	1.09948111	2879561	0.38162699	experimental	Microsource	1500435	Netilmicin hydrochloride
2091 H18	X	394	400	-0.56340256	473	480	-0.53141391	2510067	1.01351605	2909082	1.23067739	experimental	Microsource	1500428	Netogistamine bromide
2091 H19	X	275	280	-1.09136718	392	400	-0.89447687	1369565	0.10979685	1301384	0.01340115	experimental	Microsource	1500319	Grammidin
2091 H20	X	313	320	-0.92277342	633	640	0.18574749	2547497	1.0431751	2779781	1.13277689	experimental	Microsource	1500431	Nifedipine
2091 H21	X	953	960	1.91670005	552	560	-0.17731547	2445265	0.96216777	2612993	1.00649251	experimental	Microsource	1500321	Guaifenesin
2091 H22	X	752	760	1.02492792	749	760	0.70568951	2380232	0.91063645	2949234	1.26107908	experimental	Microsource	1500430	Niacin
2091 H23	E	498	840	-0.10198812	663	1080	0.32021526	83914	-0.90893656	84646	-0.90785815	empty			
2091 H24	P	115170	115760	508.606671	140427	141240	526.79863	2291913	0.84041589	217776	0.93439848	empty			
2091 I01	N	437	440	-0.37262543	637	640	0.2036753	2818866	1.25808922	2162800	0.65656344	empty			
2091 I02	E	117	120	-1.79236217	116	120	-2.13158029	80023	-0.91201974	83023	-0.90908702	empty			
2091 I03	X	117	320	-0.90502671	435	440	-0.70173974	3334034	1.66641696	2166646	0.67005294	experimental	Microsource	1500112	Amiloride hydrochloride
2091 I04	X	476	480	-0.19959502	552	560	-0.17731547	2913516	1.33320387	2376842	0.82768959	experimental	Microsource	1500209	Cresol
2091 I05	X	275	280	-1.09136718	633	640	0.18574749	3112878	1.49117577	2425853	0.86479852	experimental	Microsource	1500113	Potassium p-aminobenzoate
2091 I06	X	356	360	-0.7319963	713	720	0.54432819	2808038	1.24962445	2980230	1.28454786	experimental	Microsource	1500210	Cromolyn sodium
2091 I07	X	355	360	-0.73643297	793	800	0.9029089	2759886	1.21146943	2724151	1.09065635	experimental	Microsource	1500114	Aminocaproic acid
2091 I08	X	556	560	0.15533916	513	520	-0.35212356	2694969	1.16003003	3019061	1.31394895	experimental	Microsource	1500211	Cyclizine
2091 I09	X	355	360	-0.73643297	474	440	-0.706222	2715781	1.17652119	2735492	1.09924325	experimental	Microsource	1500115	Aminoglutethimide
2091 I10	X	395	400	-0.55896588	594	600	0.0109394	2481777	0.99109941	2812276	1.15738064	experimental	Microsource	1500212	Cyclopentolate hydrochloride
2091 I11	X	434	440	-0.38593547	674	680	0.3695201	2786619	1.23265231	2548600	0.95773703	experimental	Microsource	1500116	Aminosalicylate sodium
2091 I12	X	675	680	0.68330376	434	440	-0.706222	2503797	1.00854778	2621098	1.01262926	experimental	Microsource	1500213	Cyclophosphamide hydrate
2091 I13	X	394	400	-0.56340256	434	440	-0.706222	2357879	0.89292422	2599534	0.99630196	experimental	Microsource	1500117	Amitriptyline hydrochloride
2091 I14	X	595	600	0.32836958	434	440	-0.706222	2413995	0.93738982	2521704	0.93737259	experimental	Microsource	1500215	Cycloserine
2091 I15	X	553	560	0.14202913	354	360	-1.0648027	1765296	0.42461642	1692351	0.30842379	experimental	Microsource	1500119	Amiodiaquine dihydrochloride
2091 I16	X	513	520	-0.03543796	354	360	-1.0648027	2322232	1.02315544	2474116	0.90134109	experimental	Microsource	1500216	Cyproterone acetate
2091 I17	X	553	560	0.14202913	473	480	-0.53141391	2453011	0.96830556	2549556	0.95573511	experimental	Microsource	1500120	Amoxicillin
2091 I18	X	914	920	1.74366964	793	800	0.9029089	2746309	0.98676664	2341132	0.80065159	experimental	Microsource	1500217	Cytarabine
2091 I19	X	593	600	0.31949622	873	880	1.2614896	2504116	1.00880055	2563192	0.96878544	experimental	Microsource	1500122	Amphotericin b
2091 I20	X	674	680	0.67886709	632	640	0.18126523	2294476	0.82468445	2701293	1.0733493	experimental	Microsource	1500218	Oracarbazine
2091 I21	X	592	600	0.31505955	710	720	0.53088142	2518377	1.02010078	2586075	0.98611442	experimental	Microsource	1500123	Ampicillin sodium
2091 I22	X	474	480	-0.03987464	1349	1360	-0.39504477	2198645	0.76474924	2174374	0.89396489	experimental	Microsource	1500220	Danzol
2091 I23	X	467	760	-0.23952512	770	1240	0.79981694	85919	-0.90734782	86592	-0.90638473	empty			
2091 I24	P	98487	99080	434.643584	157610	158480	703.797283	2346142	0.88362397	2688657	1.06378189	empty			
2091 J01	N	717	720	0.86964421	556	560	-0.15938643	2186610	0.75721286	2404883	0.84892098				

2091 J19	X	474	480	-0.20846837	553	560	-0.17283321	2393658	0.92127504	2624584	1.0152687	experimental	Microsource	1500332	Homatropine bromide
2091 J20	X	513	520	-0.03543796	632	640	0.18126523	2211814	0.77718418	2412445	0.85464659	experimental	Microsource	1500442	Nortriptyline
2091 J21	X	673	680	0.67443041	870	880	1.24804282	2410055	0.93426782	2690422	1.06511827	experimental	Microsource	1500333	Homatropine methylbromide
2091 J22	X	472	480	-0.21734173	1187	1200	2.66891885	2079837	0.6726073	2173790	0.63881572	experimental	Microsource	1500443	Noscapine hydrochloride
2091 J23	E	458	720	-0.27945521	812	1280	0.98807181	82191	-0.0303184	84435	-0.90801791	empty			
2091 J24	P	87580	88200	386.252745	157111	157960	701.560636	2191852	0.76136655	2710608	1.0804022	empty			
2091 K01	N	516	520	-0.02212793	596	600	0.01990392	3438818	1.74944646	1994156	0.53793696	empty			
2091 K02	E	196	160	-1.61933176	276	280	-1.41441889	81637	-0.91074082	87362	-0.90580172	empty			
2091 K03	X	356	400	-0.5545292	275	380	-1.41890115	3079417	1.4646617	2437771	0.87382229	experimental	Microsource	1500124	Amprolium
2091 K04	X	355	360	-0.73643297	374	360	-1.0648027	2690012	1.15610216	1999280	0.54181662	experimental	Microsource	1500222	Dapsone
2091 K05	X	392	400	-0.57227591	450	480	-0.54486069	2859638	1.29051163	2535727	0.94799017	experimental	Microsource	1500126	Antiazoline phosphate
2091 K06	X	1716	1720	5.30188483	2114	2120	6.82397273	1886950	0.51976611	2029153	1.24587465	experimental	Microsource	1500223	Daunorubicin
2091 K07	X	431	440	-0.3992455	469	480	-0.54934295	2704942	1.1679325	2932813	1.24864584	experimental	Microsource	1500127	Anthrakin
2091 K08	X	275	280	-1.09136716	434	440	-0.706222	2797282	1.24110154	2677234	1.05513291	experimental	Microsource	1500224	Deferoxamine mesylate
2091 K09	X	394	400	-0.56340256	474	680	0.3695201	2460923	0.97457497	2834530	1.17423037	experimental	Microsource	1500128	Antipyrine
2091 K10	X	874	880	1.56620255	672	480	-0.53589617	2800330	1.24351673	2541308	0.95221586	experimental	Microsource	1500225	Sodium hydrochlorolate
2091 K11	X	832	840	1.3798621	633	640	0.18574749	2441366	0.95907825	1947579	0.52311414	experimental	Microsource	1500129	Apomorphine hydrochloride
2091 K12	X	274	280	-1.09580383	434	440	-0.706222	2361075	0.89545669	2432005	0.86945654	experimental	Microsource	1500226	Demeclocycline hydrochloride
2091 K13	X	515	520	-0.02656461	512	520	-0.35660582	2729591	1.18748406	2929153	1.24587465	experimental	Microsource	1500130	Aspirin
2091 K14	X	675	680	0.68330376	994	1000	1.80384291	2444825	0.96181912	2238799	0.72316964	experimental	Microsource	1500227	Desipramine hydrochloride
2091 K15	X	472	480	-0.21734173	712	720	0.53984594	2585079	1.0729546	3117445	1.38844089	experimental	Microsource	1500131	Atropine sulfate
2091 K16	X	713	720	0.8518975	552	560	-0.17731547	2465740	0.9783919	2664853	1.04575857	experimental	Microsource	1500230	Dexamethasone
2091 K17	X	554	560	0.14646581	472	480	-0.53589617	2391919	0.91989708	2535093	0.94751014	experimental	Microsource	1500132	Aurothioglucose
2091 K18	X	394	400	-0.56340256	914	920	1.44526221	2495185	1.00172374	2639771	1.02676761	experimental	Microsource	1500232	Dexamethasone sodium phosphate
2091 K19	X	474	480	-0.20846837	473	480	-0.53141391	2874192	1.30204404	2593911	0.99204448	experimental	Microsource	1500133	Azathioprine
2091 K20	X	474	480	-0.03180428	593	600	-0.44569507	0.96199503	1.348295601			experimental	Microsource	1500233	Metamorphoran hydrobromide
2091 K21	X	673	680	0.67443041	912	920	-1.43629769	2570557	0.61444755	3273250	1.50900473	experimental	Microsource	1500134	Bacitracin
2091 K22	X	672	680	0.66999373	828	840	1.05978795	2481831	0.9911422	2634189	1.02254117	experimental	Microsource	1500235	Dibenzothioephene
2091 K23	E	622	960	0.44815987	685	1080	0.41882495	82766	-0.90984622	86478	-0.90647105	empty			
2091 K24	P	113796	114400	502.564677	132729	133520	592.274202	2527686	1.02747712	2666067	1.04667776	empty			
2091 L01	N	397	400	-0.55009253	516	520	-0.33867678	2134645	0.71603646	2554959	0.96255178	empty			
2091 L02	E	196	200	-1.44186466	236	240	-1.59370924	76585	-0.91474396	77486	-0.91327938	empty			
2091 L03	X	596	600	0.33280626	517	520	-0.33419452	2172473	0.74601088	2262109	0.74081893	experimental	Microsource	1500334	Hydralazine hydrochloride
2091 L04	X	236	240	-0.91390007	593	600	-0.39610114	289148233	0.91281007	310198387	1.02683807	experimental	Microsource	1500335	Hydrochlorothiazide
2091 L05	X	315	320	-0.91390007	555	560	-0.16386869	2390648	0.91888996	2662587	1.04404286	experimental	Microsource	1500445	Nylidrin hydrochloride
2091 L06	X	311	320	-0.93164677	509	520	-0.37005259	2896760	1.31992663	3378183	1.58585998	experimental	Microsource	1500338	Hydrocortisone acetate
2091 L07	X	635	640	0.50583667	675	680	0.37400236	2531075	1.03016252	2729212	1.09448832	experimental	Microsource	1500446	Nystatin
2091 L08	X	355	360	-0.73643297	433	440	-0.71070426	2879336	1.30612008	3503175	1.6804983	experimental	Microsource	1500447	Hydrocortisone hemisuccinate
2091 L09	X	355	360	-0.73643297	552	560	-0.17731547	2216050	0.78054074	2712923	1.08215502	experimental	Microsource	1500339	Orphenadrine citrate
2091 L10	X	352	360	-0.74974301	873	880	1.2614896	2518316	1.02005245	3309999	1.53423412	experimental	Microsource	1500448	Oxacillin sodium
2091 L11	X	1120	1120	2.63110925	833	840	-0.34932819	28549618	0.95249718	2643968	1.03120207	experimental	Microsource	1500449	Oxidopamine hydrochloride
2091 L12	X	354	360	-0.74086965	713	720	0.54330819	2684356	1.15162042	2930486	1.24688394	experimental	Microsource	1500450	Hydroxyprogesterone caproate
2091 L13	X	314	320	-0.91833674	434	440	-0.706222	2189181	0.75925008	2791614	1.1417363	experimental	Microsource	1500451	Oxybenzone
2091 L14	X	514	520	-0.03100128	473	480	-0.53141391	2953513	1.36489698	3143839	1.40842524	experimental	Microsource	1500343	Oxyphenbutazone
2091 L15	X	434	440	-0.38593547	511	520	-0.36108808	2272283	0.82509905	2535607	0.94789931	experimental	Microsource	1500452	Oxytetracycline hydrochloride
2091 L16	X	594	600	0.3239329	1073	1080	2.15794135	3474360	1.77760948	3463273	1.6502863	experimental	Microsource	1500453	Hydroxyzine pamoate
2091 L17	X	514	520	-0.03100128	592	600	0.00197488	2364153	0.89789566	2748991	1.10946409	experimental	Microsource	1500454	Oxyphenbutazone
2091 L18	X	794	800	0.38593547	474	480	-0.53141391	2748563	1.20249723	3509920	1.56521766	experimental	Microsource	1500455	Oxyphenbutazone
2091 L19	X	467	480	-0.23952512	593	600	0.00645714	2364633	0.8982726	3215285	1.46252094	experimental	Microsource	1500456	Oxyquinoline hemisulfate
2091 L20	X	593	600	0.31949622	631	640	0.17678298	2289665	0.83887232	2523385	0.93864537	experimental	Microsource	1500457	
2091 L21	X	671	680	0.66555705	831	840	1.07323473	2340889	0.87946156	2647455	1.03258559	experimental	Microsource	1500458	
2091 L22	E	687	1040	0.73654389	541	880	-0.22662031	81700	-0.9106909	82873	-0.90920059	empty			
2091 L23	P	118928	119600	525.333705	113391	114200	505.596282	2268963	0.82246832	2488650	0.91234559	empty			
2091 M01	N	477	480	-0.19515834	436	440	-0.69725749	2711016	1.17274546	2133088	0.64085856	empty			
2091 M02	E	236	240	-1.26439757	197	200	-1.76851733	79024	-0.91281133	83984	-0.90835939	empty			
2091 M03	X	396	400	-0.5545292	276	280	-1.41441889	2746926	1.20120009	1982156	0.5288511	experimental	Microsource	1500135	Baclofen
2091 M04	X	355	360	-0.73643297	316	320	-1.23512854	2400886	0.92700242	2115880	0.6301009	experimental	Microsource	1500236	Dibucaine hydrochloride
2091 M05	X	555	560	0.15090249	355	360	-1.06032045	2641713	1.11783065	2413565	0.85549446	experimental	Microsource	1500136	Betmethasone dipropionate
2091 M06	X	355	360	-0.73643297	474	480	-0.52693165	2469732	0.98155511	2637069	1.02472178	experimental	Microsource	1500237	Diclofenac sodium
2091 M07	X	635	640	0.50583667	393	400	-0.88999461	2466468	0.97896876	2597110	0.99446662	experimental	Microsource	1500137	Benserazide hydrochloride
2091 M08	X	473	480	-0.21290505	594	600	0.0109394	2550923	1.04588982	2821116	1.16407389	experimental	Microsource	1500238	Dicloxacillin sodium
2091 M09	X	555	560	0.15090249	713	720	0.54330819	2319519	0.86252825	2219997	0.70893367	experimental	Microsource	1500138	Benzethonium chloride
2091 M10	X	475	480	-0.2040317	553	560	-0.17283321	2735522	1.1921637	2448362	0.88184132	experimental	Microsource	1500239	Dicumarol
2091 M11	X	513	520	-0.03543796	712	280	-1.43234792	2251313	0.80848269	2054126	0.58334355	experimental	Microsource	1500139	Benzocaine
2091 M12	X	314	320	-0.91833674	595	600	0.01542166	2356178	0.89157637	3239041	0.79149683	experimental	Microsource	1500240	Dicyclomine hydrochloride
2091 M13	X	675	680	0.68330376	355	360	-1.06032045	2298439	0.84582473	2140396	0.64866331	experimental	Microsource	1500141	Difenhydramine
2091 M14	X	474	480	-0.20846837	394	400	-0.88551235	2214133	0.77902173	2148590	0.65486744	experimental	Microsource	1500241	Dienestrol
2091 M15	X	434	440	-0.38593547	874	880	1.26597186	2237370	0.79743443	2165668	0.66779814	experimental	Microsource	1500142	Benzotropine
2091 M16	X	494	400	-0.56340256	712	720	0.53984594	2347491	0.8645929	2354943	0.87168106	experimental	Microsource	1500242	Diethylcarbamazine citrate
2091 M17	X	515	520	-0.02656461	434	440	-0.706222	2220967	0.7844369	2180762	0.67922664	experimental	Microsource	1500143	Beta-carotene
2091 M18	X	231	240	-1.28658096	471	480	-0.54037843	1590469	0.28483835	2662447	1.04393686	experimental	Microsource	1500244	Diethylstilbestrol
2091 M19	X	788	800	1.1846483	512	520	-0.35660582	2363255	0.89718409	2492279	0.9150933	experimental	Microsource	1500146	Bethanechol chloride
2091 M20	X	2633	2640	9.37031792	873	880	1.2614896	2430253	0.95027245	2864467</					

2091 N13	X	435	440	-0.38149879	315	320	-1.2396108	2294603	0.84278513	2691740	1.0661162	experimental	Microsource	1500352	Inositol	
2091 N14	X	274	280	-1.09580383	434	440	-0.706222	2168339	0.74273515	2466260	0.89539288	experimental	Microsource	1500467	Penicillin v potassium	
2091 N15	X	674	680	0.67886709	594	600	0.0109394	2416716	0.93954591	2644414	1.03005594	experimental	Microsource	1500353	Iodoquinol	
2091 N16	X	513	520	-0.03543796	394	400	-0.88551235	2362663	0.896715	2189944	0.69137603	experimental	Microsource	1500472	Phenacetamide	
2091 N17	X	672	680	0.66999373	391	400	-0.89895913	2359474	0.89418887	2790959	1.07922937	experimental	Microsource	1500354	Ipratropium bromide	
2091 N18	X	1315	1320	3.52277724	1593	1600	4.48871591	2301879	0.84855054	2358259	0.81361938	W	experimental	Microsource	1500473	Phenazopyridine hydrochloride
2091 N19	X	471	480	-0.22177841	788	800	0.8804976	2444318	0.96141738	2692298	1.06653869	experimental	Microsource	1500355	Isotiazid	
2091 N20	X	387	400	-0.5944593	831	840	1.07323473	2350785	0.88730303	2503633	0.92369004	experimental	Microsource	1500476	Phenelzine sulfate	
2091 N21	X	674	680	0.67886709	672	680	0.36055558	2358186	0.89316748	2604461	1.00003247	experimental	Microsource	1500356	Isopropamide iodide	
2091 N22	X	551	560	0.13315578	571	680	0.35607333	2013776	0.62026141	2351044	0.80815651	experimental	Microsource	1500477	Phenindione	
2091 N23	E	745	1200	0.99387117	646	960	-0.20420902	77506	-0.91401417	80076	-0.91131835	empty				
2091 N24	P	153821	154560	680.142686	138875	139840	619.822185	2380583	0.91091458	2304028	0.78483765	empty				
2091 O01	N	517	600	0.33724293	556	560	-0.15938643	2478456	0.98846789	1946525	0.50187291	empty				
2091 O02	E	126	120	-1.79679885	355	360	-1.06032045	74577	-0.91633508	80846	-0.91073534	empty				
2091 O03	X	395	400	-0.55896588	634	640	0.19022975	3163057	1.53093697	1909199	0.47361134	experimental	Microsource	1500147	Bisacodyl	
2091 O04	X	354	360	-0.74086965	314	320	-1.24409306	1741455	0.40447773	1561238	0.21015092	experimental	Microsource	1500247	Digoxin	
2091 O05	X	674	680	0.67886709	594	600	-0.88551235	1902318	0.53194351	1672966	0.29474634	experimental	Microsource	1500148	Bithioniate sodium	
2091 O06	X	672	680	0.66999373	792	800	0.89842664	2273867	0.82635419	2421708	0.86166011	experimental	Microsource	1500249	Dihydrostreptomycin sulfate	
2091 O07	X	474	480	-0.20846837	673	680	0.36503784	2052385	0.65085468	2304028	0.77253811	experimental	Microsource	1500151	Bromocriptine mesylate	
2091 O08	X	672	680	0.66999373	393	400	-0.89899461	2498620	1.00444559	2341897	0.80123081	experimental	Microsource	1500251	Dimenhydrinate	
2091 O09	X	672	680	0.66999373	513	520	-0.35212356	2115417	0.70080043	2442758	0.87759823	experimental	Microsource	1500152	Busulfan	
2091 O10	X	1074	1080	2.45353801	394	400	-0.88551235	2227870	0.78990675	2133005	0.64306718	experimental	Microsource	1500253	Dimefethadione	
2091 O11	X	793	800	-1.20683168	433	440	-0.71070426	2554008	1.04833433	2252243	0.73334883	experimental	Microsource	1500155	Caffeine	
2091 O12	X	394	400	-0.56340256	555	560	-0.16386869	2163470	0.73887702	2144957	0.6521167	experimental	Microsource	1500255	Dioxibenzone	
2091 O13	X	435	440	-0.38149879	394	400	-0.88551235	2258608	0.81426315	2122248	0.63492247	experimental	Microsource	1500156	Camphor (1r)	
2091 O14	X	565	560	-0.15090249	695	695	0.15090249	11912209	0.7107441	2392307	0.57203998	experimental	Microsource	1500256	Diphenhydramine hydrochloride	
2091 O15	X	673	680	0.67443041	513	520	-0.35212356	2251121	0.76394973	2399355	0.8423733	experimental	Microsource	1500155	Carbamoyl sulfate	
2091 O16	X	713	720	0.8518975	474	480	-0.52693165	2048523	0.64779448	2066346	0.59259598	experimental	Microsource	1500258	Diphenylpicrylamine hydrochloride	
2091 O17	X	473	480	-0.21290505	594	600	0.0109394	2459675	0.97358607	2369191	0.8218966	experimental	Microsource	1500158	Carbachol	
2091 O18	X	432	440	-0.39480882	628	640	0.1633362	3802452	2.03758539	4266685	2.25859374	experimental	Microsource	1500259	Dipyridamole	
2091 O19	X	474	480	-0.20846837	1312	1320	3.2292012	2342838	0.88100593	2645175	1.03085928	experimental	Microsource	1500159	Carbamazepine	
2091 O20	X	514	520	-0.03100128	630	640	0.17230072	1563149	0.26319034	1607882	0.24546766	experimental	Microsource	1500260	Pyritnone zinc	
2091 O21	X	592	600	0.31505955	712	720	0.53984594	2102469	0.6905406	2706001	1.07691399	experimental	Microsource	1500160	Carbenicillin disodium	
2091 O22	X	674	680	0.6655705	909	909	0.6655705	1912209	0.93770232	2392350	0.65770232	experimental	Microsource	1500262	Dulcifram	
2091 O23	E	713	1120	0.8518975	809	1360	0.97462504	78679	-0.9130847	81303	-0.91038932	empty				
2091 O24	P	136426	137320	602.966684	186246	187240	832.151245	2266945	0.82086928	2306076	0.77410876	empty				
2091 P01	N	798	800	1.22901507	638	640	0.20815879	1533017	0.23931412	1741404	0.34656451	empty				
2091 P02	E	195	200	-1.44630134	274	280	-1.42338341	71970	-0.91840083	73865	-0.91602104	empty				
2091 P03	X	877	880	1.57951258	916	920	1.45422673	1714449	0.38307852	2029972	0.56505523	experimental	Microsource	1500357	Isoproterenol hydrochloride	
2091 P04	X	435	440	-0.38149879	395	440	-0.70173974	2026200	0.63010602	2374975	0.82627599	experimental	Microsource	1500478	Pheniramine maleate	
2091 P05	X	435	440	-0.38149879	435	440	-0.38149879	1783079	0.4418383	2191919	0.56510519	experimental	Microsource	1500358	Phenylephrine	
2091 P06	X	1155	1160	0.81290887	594	600	0.0109394	2155280	0.73238737	2497055	0.91870947	experimental	Microsource	1500480	Phenolphthalein	
2091 P07	X	513	520	-0.03543796	674	680	0.3695201	1823868	0.46978074	2019436	0.55707784	experimental	Microsource	1500359	Isosuxprine hydrochloride	
2091 P08	X	635	640	0.50583667	713	720	0.54432819	1976744	0.59091772	2604488	1.00005291	experimental	Microsource	1500482	Phenylbutazone	
2091 P09	X	475	480	-0.2040317	1194	1200	2.70029466	1846047	0.48735509	2311338	0.77809291	experimental	Microsource	1500360	Kanamycin a sulfate	
2091 P10	X	474	480	-0.20846837	714	720	0.54881045	2127950	0.71073142	2692162	1.06643572	experimental	Microsource	1500483	Phenylephrine hydrochloride	
2091 P11	X	475	480	-0.2040317	635	640	0.19471201	1740058	0.40337076	1934762	0.4929665	experimental	Microsource	1500362	Ketocanzole	
2091 P12	X	476	480	-0.19959502	495	480	-0.52244939	1996282	0.60639938	2025266	0.92061826	experimental	Microsource	1500484	Levonordrin	
2091 P13	X	476	480	-0.19959502	556	560	-0.15938643	2974367	0.58989427	2376898	0.6827733	experimental	Microsource	1500365	Levonordrin	
2091 P14	X	476	480	-0.19959502	515	520	-0.34315904	1925198	0.55007333	2279127	0.75370419	experimental	Microsource	1500485	Phenylephrine hydrochloride	
2091 P15	X	395	400	-0.55896588	676	680	0.37848462	1929894	0.55379438	2317903	0.78306363	experimental	Microsource	1500372	Mefenidine hydrochloride	
2091 P16	X	595	600	0.32836958	475	480	-0.52244939	2121552	0.70566713	2362503	0.81683275	experimental	Microsource	1500486	Phystostigmine salicylate	
2091 P17	X	635	640	0.50583667	615	620	-0.34315904	1953341	0.57237348	2118661	0.63220655	experimental	Microsource	1500373	Maprotiline hydrochloride	
2091 P18	X	475	480	-0.2040317	673	640	0.19471201	2120928	0.70516728	2410721	0.85334125	experimental	Microsource	1500487	Pilocarpine nitrate	
2091 P19	X	515	520	-0.02654661	635	680	0.36503784	1930532	0.55429992	2301539	0.77067355	experimental	Microsource	1500374	Mecamylamine hydrochloride	
2091 P20	X	755	760	1.03823795	554	560	-0.16835095	2020419	0.62552523	2392350	0.83958299	experimental	Microsource	1500488	Pindolol	
2091 P21	X	754	760	1.03823795	633	640	0.18574749	1917230	0.54375959	2207086	0.69915798	experimental	Microsource	1500364	Leucovorin calcium	
2091 P22	X	672	680	0.66999373	992	1000	1.79487839	1936768	0.55924125	2343986	0.80281251	experimental	Microsource	1500489	Piperacillin sodium	
2091 P23	E	871	1320	1.55289251	648	1240	0.25298137	72684	-0.91783507	75579	-0.91472328	empty				
2091 P24	P	152839	153240	675.785869	201534	202080	900.676017	1728782	0.39443581	1864761	0.43996489	empty				
2092 A01	N	557	560	-0.18284368	1158	1160	0.57416205	1570969	0.25065867	1670470	0.30034044	empty				
2092 A02	E	157	160	-0.88362509	235	240	-0.50021162	75067	-0.90955516	73013	-0.91390346	empty				
2092 A03	X	397	400	-0.46315624	436	440	-0.26247225	1828213	0.45017579	1941169	0.50610157	experimental	Microsource	1500490	Piperazine	
2092 A04	X	555	560	-0.18634759	555	560	-0.12753104	1989199	0.57035669	1996776	0.54836904	experimental	Microsource	1500592	Trihexyphenidyl hydrochloride	
2092 A05	X	755	760	1.16404312	596	600	-0.08000697	1950132	0.54473553	1975470	0.53217412	experimental	Microsource	1500491	Piroxicam	
2092 A06	X	554	560	-0.18809954	395	400	-0.31397133	1872251	0.48433143	1756908	0.36604285	experimental	Microsource	1500593	Trimiprazine tartrate	
2092 A07	X	674	680	0.67886709	556	560	-0.12656704	1954945	0.54846847	2124999	0.64583269	experimental	Microsource	1500492	Polymyxin b sulfate	
2092 A08	X	955	960	0.51443382	635	640	-0.0346109	2001262	0.58439169	2035770	0.57800879	experimental	Microsource	1500594	Trimethoprim hydrochloride	
2092 A09	X	434	440	-0.12889504	556	560	-0.12889504	2254537	0.78083047	2039092	0.58053388	experimental	Microsource	1500494	Prizabiquantel	
2092 A10	X	636	640	-0.04443935	835	840	-0.19815947	2254451	0.7807337	2329256	0.78175776	experimental	Microsource	1500595	Trimethoprim	
2092 A11	X	472	480	-0.33175973	551	560	-0.13288705	1939573	0.69166499	2626073	1.02670431	experimental	Microsource	1500495	Zalcitabine hydrochloride	
2092 A12	X	476	480	-0.32475191	675	680	0.01194918	2162400	0.70936949	2122027	0.64357364	experimental	Microsource	1500596	Trioxsalen	
2092 A13	X	516	520	-0.25467377	635	640	-0.034									

2092 B07	X		394	400	-0.4684121	314	320	-0.40825547	2524798	0.9904435	2630185	1.02982989	experimental	Microsource	1501011	Fenoprofen	
2092 B08	X		434	440	-0.39833396	475	480	-0.22085118	2407444	0.8994235	2930863	1.2583784	experimental	Microsource	1502042	Cefoperazone sodium	
2092 B09	X		394	400	-0.4684121	594	600	-0.08233497	2534705	0.99812732	3107886	1.39293544	experimental	Microsource	1501015	Flufenamic acid	
2092 B10	X		511	520	-0.26343354	550	560	-0.13351005	2749674	1.1648561	2763668	1.13130692	experimental	Microsource	1502044	Ofloxacin	
15564			1564	1560	-0.3835398	1634	1640	-1.1282699	2855823	2.4718477	2289252	0.77068313	experimental	Microsource	1501016	Fenbendazole	
2092 B12	X		512	520	-0.26168159	510	520	-0.18011112	2713550	1.13683857	2609317	1.0139679	experimental	Microsource	1502046	Bezafibrate	
2092 B13	X		352	360	-0.54199415	672	680	0.00845717	2439643	0.92439772	2412403	0.8642915	experimental	Microsource	1501021	Fenpropiridone hydrochloride	
2092 B14	X	1433	1440	1.3518676	1112	920	0.2878176	2432541	0.91888945	2596008	1.00385159	2479635	0.91539525	experimental	Microsource	1502047	Lithionazole (- isomer) sodium
2092 B15	X		790	800	0.22536149	914	1120	0.52294597	2422853	0.91137549	2479635	0.91539525	experimental	Microsource	1501100	Mebendazole	
2092 B16	X		871	880	0.36726972	512	520	-0.17778312	2762558	1.17484892	3005856	1.31538137	experimental	Microsource	1502006	Carprofen	
2092 B17	X		711	720	0.08695716	353	360	-0.3628594	2297253	0.81396078	2345529	0.81345987	experimental	Microsource	1501103	Mefenamic acid	
2092 B18	X		951	960	-0.1933554	434	440	-0.26937526	2696285	1.12244793	2480227	0.90309134	experimental	Microsource	1502053	Alrestatin	
2092 B19	X		514	520	-0.25817768	551	560	-0.13238705	2541350	1.00328114	2613715	1.01731087	experimental	Microsource	1501104	Methacycline hydrochloride	
2092 B20	X		395	400	-0.46666015	515	520	-0.17429111	2212101	0.74791733	2704375	0.60735286	experimental	Microsource	1502084	Proadifen hydrochloride	
2092 B21	X		354	360	-0.53849024	314	320	-0.40825547	1655727	0.31639654	1519815	0.18582596	experimental	Microsource	1501105	Puromycin hydrochloride	
2092 B22	X		632	640	-0.05144717	512	520	-0.17778312	2489341	0.96294323	2417624	0.86826003	experimental	Microsource	1502106	Carboplatin	
2092 B23	E		486	840	-0.30723238	695	1080	0.03522921	81574	-0.90450836	83196	-0.90616326	empty				
2092 B24	P	118858	119640	207.075009	128794	129800	149.142696	1878165	0.4889183	1949530	0.51245686	empty					
2092 C01	N		475	480	-0.32650387	597	600	-0.07084295	2015972	0.59580069	2408027	0.58732546	empty				
2092 C02	E		195	200	-0.81705085	156	160	-0.59216776	80160	-0.90560505	79961	-0.90862222	empty				
2092 C03	X		915	920	0.44435568	436	440	-0.26624725	2689322	1.11804746	2674367	1.06341309	experimental	Microsource	1500502	Probenecid	
2092 C04	X		432	440	-0.40183787	353	360	-0.3628594	2594538	1.04453348	2501083	0.9316981	experimental	Microsource	1500602	Tubocurarine chloride	
2092 C05	X		914	920	0.44260373	635	640	-0.0346109	2630259	1.0722385	2723497	1.10075732	experimental	Microsource	1500503	Procainamide hydrochloride	
2092 C06	X		469	480	-0.33701559	474	480	-0.22201519	1590901	0.26611783	1571984	0.22548017	experimental	Microsource	1500603	Tyrothricin	
2092 C07	X		394	400	-0.4684121	755	760	0.10506932	2725454	1.14607125	2589934	0.99923468	experimental	Microsource	1500504	Procaine hydrochloride	
2092 C08	X		494	480	-0.38333561	313	320	-0.40941945	2589718	1.04979531	2452208	1.05419115	experimental	Microsource	1501105	Urea	
2092 C09	X		715	720	0.09396498	394	400	-0.31513533	1902356	0.50768071	2283153	0.76504721	experimental	Microsource	1500505	Prochlorperazine edisylate	
2092 C10	X		352	360	-0.54199415	473	480	-0.22317919	2270907	0.79352696	2664793	1.05613579	experimental	Microsource	1500605	Ursodiol	
2092 C11	X		552	560	-0.19160345	511	520	-0.17894712	2605830	1.0532915	2455720	0.8972172	experimental	Microsource	1500507	Procydiline hydrochloride	
2092 C12	X		354	360	-0.53849024	433	440	-0.26973926	2531972	0.99600762	3052903	1.35114229	experimental	Microsource	1500606	Valproate sodium	
2092 C13	X		355	360	-0.53673829	634	640	-0.0357749	2893106	1.27610127	2481316	0.91667299	experimental	Microsource	1500508	Progesterone	
2092 C14	X		551	560	-0.1933554	433	440	-0.26973926	2712260	1.13583805	2569318	0.98356424	experimental	Microsource	1500607	Vancocycin hydrochloride	
2092 C15	X		432	440	-0.40183787	193	200	-0.54909969	2007400	0.58915229	2210257	0.71063819	experimental	Microsource	1500509	Promazine hydrochloride	
2092 C23	E		497	480	-0.38333561	515	520	-0.17429111	2065326	1.09979531	2589915	0.99923468	experimental	Microsource	1500510	Meperidine	
2092 C17	X		1112	1120	0.78949052	594	600	-0.08233497	2094312	0.65656079	2526277	0.95084832	experimental	Microsource	1500510	Promethazine hydrochloride	
2092 C18	X		832	840	0.29894354	671	680	0.00729317	2335193	0.84338684	2319853	0.79394327	experimental	Microsource	1500611	Vinblastine sulfate	
2092 C19	X		513	520	-0.25992963	1633	1640	-1.1270629	2866410	1.25539599	2593502	1.00194675	experimental	Microsource	1500511	Procaine hydrochloride	
2092 C20	X		515	520	-0.25642573	431	440	-0.27206726	2676650	1.10821912	2990162	1.30345219	experimental	Microsource	1500613	Warfarin	
2092 C21	X		434	440	-0.39833396	354	360	-0.3616954	2182504	0.72496205	2550010	0.96888803	experimental	Microsource	1500514	Dexpropranolol hydrochloride	
2092 C22	X		552	560	-0.19160345	512	520	-0.17778312	2410206	0.90156654	2480361	0.91609911	experimental	Microsource	1500614	Xylometazoline hydrochloride	
2092 C23	E		497	480	-0.38333561	515	520	-0.17429111	2065326	1.09979531	2589915	0.99923468	experimental	Microsource	1500510	Meperidine	
2092 C24	P	101780	102480	177.155147	142715	143520	165.344765	2008370	0.58990462	2145474	0.66160118	empty					
2092 D01	N		756	760	0.16579507	436	440	-0.26624725	2169136	0.7145939	2004481	0.55422569	empty				
2092 D02	E		275	280	-0.67689457	236	240	-0.49904761	84280	-0.9024096	82769	-0.90648783	empty				
2092 D03	X		553	560	-0.18985149	436	440	-0.26624725	2665887	1.0998714	2925937	1.25463409	experimental	Microsource	1501108	Mefexamide	
2092 D04	X		514	520	-0.25817768	355	360	-0.3605314	2412908	0.9036622	2491692	0.9245599	experimental	Microsource	1502107	Cisplatin	
2092 D05	X		429	440	-0.40709373	395	400	-0.31397133	2502392	0.97306552	2588102	0.99784216	experimental	Microsource	1501109	Probucol	
2092 D06	X		515	520	-0.19639919	380	380	-0.45481555	2665789	1.09979539	2808265	0.96195126	experimental	Microsource	1502109	Zidovudine [azt]	
2092 D07	X		590	600	-0.12502921	514	520	-0.17545511	1746197	0.16715942	3001336	1.3194456	experimental	Microsource	1501136	Procaine hydrochloride	
2092 D08	X		509	520	-0.26693745	701	720	0.04221322	2033253	0.60920375	1945542	0.50942554	experimental	Microsource	1502111	Azaticidin	
2092 D09	X		593	600	-0.11977335	632	640	-0.0381029	2663934	1.09835666	2845310	1.19334866	experimental	Microsource	1501117	Mebeverine hydrochloride	
2092 D10	X		795	800	0.23412126	994	1000	0.38326575	2030650	0.60718487	2196573	0.70023684	experimental	Microsource	1502112	Cycloheximide	
2092 D11	X		312	320	-0.61032034	432	440	-0.27090326	2560505	1.01813766	2924783	1.25375693	experimental	Microsource	1501118	Mecloxyline sulfosalicylate	
2092 D12	X		555	560	-0.18634759	755	760	0.10506932	3042149	1.39169825	3064377	1.35988638	experimental	Microsource	1502113	Azaserine	
2092 D13	X		593	600	-0.11977335	473	480	-0.22317919	2832906	1.22941047	2424727	0.87365991	experimental	Microsource	1501119	Progulimide	
2092 D14	X		713	720	0.09046107	515	520	-0.17429111	2667294	1.10096286	2589915	0.99923468	experimental	Microsource	1502127	Tindazole	
2092 D15	X		552	560	-0.19160345	354	360	-0.3616954	3367767	1.64424588	3289414	1.53091679	experimental	Microsource	1501120	Minaprine hydrochloride	
2092 D16	X		633	640	-0.04969521	515	520	-0.17429111	2479444	0.95526717	3192301	1.45710017	experimental	Microsource	1502150	Carbidopa	
2092 D17	X		387	400	-0.48067578	423	440	-0.28137928	2429957	0.91688531	2473641	0.91083914	experimental	Microsource	1501121	Mefenamic acid	
2092 D18	X		554	560	-0.18809954	514	520	-0.17545511	2685931	1.11541742	2602474	1.00876646	experimental	Microsource	1502195	Piracetam	
2092 D19	X		674	680	0.02213488	670	680	0.00612917	2358908	0.86178008	2897589	1.23308648	experimental	Microsource	1501127	Atenolol	
2092 D20	X		474	480	-0.32825582	634	640	-0.0357749	2549320	1.00946264	3040405	1.34164243	experimental	Microsource	1502196	Ethosuximide	
2092 D21	X		474	480	-0.32825582	634	640	-0.0357749	2393524	0.88862807	2650016	1.04490364	experimental	Microsource	1501128	Capsaicin	
2092 D22	X		713	720	0.09046107	632	640	-0.0381029	2635602	1.07538251	3429340	1.63727601	experimental	Microsource	1502197	Piperidolate hydrochloride	
2092 D23	E		442	800	-0.38431833	607	1040	-0.06720295	86339	-0.90081265	82722	-0.90652355	empty				
2092 D24	P	120663	121200	210.237285	146300	146960	169.519711	2287014	0.80601946	2238415	0.73204139	empty					
2092 E01	N		556	560	-0.18459563	517	520	-0.17196311	2085477	0.64970841	2055771	0.59321176	empty				
2092 E02	E		235	240	-0.74697271	196	200	-0.54560769	81397	-0.90464564	83604	-0.90585313	empty				
2092 E03	X		714	720	0.09221302	435	440	-0.26741126	2745111	1.16131712	2652095	1.04648391	experimental	Microsource	1500515	Propylthiouracil	
2092 E04	X		513	520	-0.25992963	514	520	-0.17429111	2644864	1.08956607	2452232	0.88659483	experimental	Microsource	1500516	Zomepirac sodium	
2092 E05	X		274	280	-0.67864652	434	440	-0.26857526	167900091	0.7090091	2700937	1.08360922	experimental	Microsource</			

2092 F01	N		516	520	-0.25467377	517	520	-0.17196311	2188278	0.72944033	2412182	0.86412351	empty			
2092 F02	E		235	240	-0.74697271	236	240	-0.49904761	83199	-0.90324802	79927	-0.90864806	empty			
2092 F03	X		753	760	0.16053921	554	560	-0.12889504	2660371	1.09559321	2844804	1.19296405	experimental	Microsource	1501129	Carbetapentane citrate
2092 F04	X		992	1000	0.5792561	874	880	-0.24358554	2872007	1.2597373	3087429	1.37358531	experimental	Microsource	1501129	Anisidione
2092 F05	X		714	720	0.09221302	514	520	-0.17545511	103994041	0.03994011	3023551	3.28831552	experimental	Microsource	1501130	Fampridine
2092 F06	X		432	440	-0.40183787	354	360	-0.3616954	2845573	1.23923493	2408258	0.86114084	experimental	Microsource	1502202	Cyclosporine
2092 F07	X	1034	1040	0.65283815	472	480	-0.22434319	3000252	1.35920316	2927993	1.25619688		experimental	Microsource	1501133	Nicergoline
2092 F08	X	588	600	-0.12853312	542	560	-0.14286306	2947495	1.3182851	2681228	1.06862821		experimental	Microsource	1502203	Troleanomycin
2092 F09	X	634	640	-0.04794326	394	400	-0.31513533	2849478	1.24226362	2797576	1.15706555		experimental	Microsource	1501134	Pimozide
2092 F10	X	473	480	-0.33000778	474	480	-0.22201519	2958459	1.32678872	3037142	1.33916219		experimental	Microsource	1502230	Ascorbic acid
2092 F11	X	554	560	-0.18809954	595	600	-0.08117097	2926338	1.30187584	2806735	1.1640274		experimental	Microsource	1501137	Neofepam
2092 F12	X	674	680	0.02213488	394	400	-0.31513533	1964500	0.55587928	1783213	0.38606036		experimental	Microsource	1502254	Menadiolone
2092 F13	X	472	480	-0.33175973	595	600	-0.08117097	2342498	0.84905256	2794000	1.14324978		experimental	Microsource	1501138	Pirenzepine hydrochloride
2092 F14	X	553	560	-0.18985149	474	480	-0.22201519	2714399	1.13749705	3041757	1.3426701		experimental	Microsource	1502255	Salicin
2092 F15	X	433	440	-0.40008592	594	600	-0.08233497	2934091	1.30788903	2567646	0.98229333		experimental	Microsource	1501139	Pramoxine hydrochloride
2092 F16	X	511	520	-0.26343354	313	320	-0.40941948	2551308	1.01100452	2639532	1.03693464		experimental	Microsource	1502258	Monensin sodium (monensin a is shown)
2092 F17	X	709	720	0.08345325	743	760	0.09110113	2560026	1.01776615	2980227	1.29590005		experimental	Microsource	1501140	Mephesisin
2092 F18	X	313	320	-0.61032034	634	640	-0.0357749	2641025	1.08058856	3145052	1.42118571		experimental	Microsource	1503001	Benzoic acid
2092 F19	X	754	760	0.16229116	513	520	-0.17661911	2395501	0.89016142	2438463	0.98409998		experimental	Microsource	1501142	Sulfachlorpyridazine
2092 F20	X	553	560	-0.18985149	633	640	-0.0369389	2740629	1.1578409	3015143	1.32244051		experimental	Microsource	1503002	Benzyd benzoate
2092 F21	X	592	600	-0.12152531	753	760	0.10274132	2522304	0.98850917	2415645	0.86675577		experimental	Microsource	1501144	Sulfadimethoxine
2092 F22	X	750	760	0.15528335	588	600	-0.08931898	2635757	1.07650272	2405928	0.85936978		experimental	Microsource	1503004	Benzoyl peroxide
2092 F23	E	511	840	-0.26343354	399	720	-0.30931532	86540	-0.90065676	83668	-0.90580449		empty			
2092 F24	P	110017	110560	191.585988	107790	108360	124.694002	2198663	0.73749488	2198712	0.70186272		empty			
2092 G01	N	556	560	-0.18489563	317	320	-0.40476347	2077653	0.64364016	2046087	0.58585085		empty			
2092 G02	E	196	200	-0.81527775	156	160	-0.52167776	82170	-0.90404611	7854	-0.90962428		empty			
2092 G03	N	354	360	-0.53849024	556	560	-0.12650404	2623542	0.6702883	2703318	1.08541905		experimental	Microsource	1500525	Racephedrine hydrochloride
2092 G04	X	593	600	-0.11977335	352	360	-0.3640234	2636656	1.07719998	2724138	1.10124455		experimental	Microsource	1500649	Theobromine
2092 G05	X	353	360	-0.5402422	393	400	-0.31397133	2594103	1.0441961	2553031	0.97118432		experimental	Microsource	1500526	Reserpine
2092 G06	X	555	560	-0.18634759	435	440	-0.26973926	2751656	1.16639339	2695525	1.07949551		experimental	Microsource	1500651	Strychnine
2092 G07	X	472	480	-0.33175973	1394	1400	0.84886647	2611724	1.05786265	2719352	1.09760666		experimental	Microsource	1500527	Resorcinol
2092 G08	X	514	520	-0.25817768	551	560	-0.13238705	2749016	1.16434582	2741104	1.11414059		experimental	Microsource	1500663	Yohimbine hydrochloride
2092 G09	X	594	600	-0.1180214	474	480	-0.22201519	2932585	1.30672098	2422541	0.8719975		experimental	Microsource	1500529	Rifampin
2092 G10	X	674	680	0.02213488	394	400	-0.31513533	1964500	0.55587928	1783213	0.38606036		experimental	Microsource	1500667	Acetazolol hydrochloride
2092 G11	X	594	600	-0.1180214	354	360	-0.3616954	2610159	0.05664905	2571297	0.9850685		experimental	Microsource	1500530	Roxarsone
2092 G12	X	513	520	-0.25992963	355	360	-0.3605314	2603294	1.05132459	2728743	1.10474486		experimental	Microsource	1500655	Acotinine
2092 G13	X	513	520	-0.25992963	355	360	-0.3605314	2342716	0.84922164	2684495	1.07111149		experimental	Microsource	1500531	Salicyl alcohol
2092 G14	X	833	840	0.30069549	434	440	-0.26857526	2424734	0.91283438	2885625	1.22399252		experimental	Microsource	1500667	Adenosine phosphate
2092 G15	X	511	520	-0.26343354	714	720	0.05734525	2330109	0.83944372	2949634	1.27264643		experimental	Microsource	1500532	Sulcylamide
2092 G16	X	1313	1320	1.14163318	594	600	-0.08233497	2754559	1.16864494	2598308	1.00559984		experimental	Microsource	1500668	Ketotifen fumarate
2092 G17	X	391	400	-0.47191601	554	560	-0.13238705	2749016	1.16434582	2741104	1.11414059		experimental	Microsource	1500533	Ranididine
2092 G18	X	555	560	-0.18634759	554	560	-0.12889504	2624069	0.6743757	2563042	0.97879379		experimental	Microsource	1500530	Betahistine hydrochloride
2092 G19	X	513	520	-0.25992963	474	480	-0.22201519	2646390	1.08474962	2707429	1.08854386		experimental	Microsource	1500534	Scopolamine hydrobromide
2092 G20	X	674	680	0.02213488	674	680	0.01078518	2608629	1.05546239	2636844	1.03489146		experimental	Microsource	1500673	Molsidomine
2092 G21	X	711	720	0.08695716	508	520	-0.18243912	2428213	0.91553267	2743749	1.11594585		experimental	Microsource	1500536	Sisomicin sulfate
2092 G22	X	1391	1400	1.27828555	2112	2120	1.68461976	2309871	0.82374723	2432719	0.87973339		experimental	Microsource	1500674	Misophenolic acid
2092 G23	E	929	1240	0.46888303	622	960	-0.04974292	83285	-0.90318132	82836	-0.90643629		empty			
2092 G24	P	10368	10433	180.489145	112367	113040	130.044918	2398178	0.89223768	218922768	0.91261628		empty			
2092 H01	N	357	360	-0.18284368	317	320	-0.40941948	2159817	0.7073865	2613395	1.070633		empty			
2092 H02	E	236	240	-0.74522076	197	200	-0.54443668	84859	-0.90196053	81257	-0.90763711		empty			
2092 H03	X	555	560	-0.18634759	393	400	-0.31629933	2590991	1.04178245	2595964	1.00381814		experimental	Microsource	1501145	Sulfaquinoxaline sodium
2092 H04	X	594	600	-0.1180214	913	920	0.28898161	3019037	1.3737727	2551336	0.96898953		experimental	Microsource	1503007	Betaine hydrochloride
2092 H05	X	475	480	-0.32650387	514	520	-0.17545511	2644216	1.08306348	2677942	1.06613049		experimental	Microsource	1501146	Sulfaguandine
2092 H06	X	274	280	-0.67864652	234	240	-0.50137562	1195627	-0.04045463	1180632	-0.0719906		experimental	Microsource	1502260	Abametin
2092 H07	X	714	720	0.09221302	431	440	-0.27206726	2932953	1.3070064	2800498	1.15928659		experimental	Microsource	1501147	Sulfamonomethoxine
2092 H08	X	394	400	-0.4684121	795	800	0.15162939	2898563	1.28033369	2911564	1.24370903		experimental	Microsource	1503009	Biotin
2092 H09	X	353	360	-0.5402422	433	440	-0.26973926	1659313	0.31917782	1763035	0.37070005		experimental	Microsource	1501148	Sulconazole nitrate
2092 H10	X	434	440	-0.39833396	594	600	-0.08233497	3041437	1.39114603	2844435	1.19268357		experimental	Microsource	1503014	Aklamide
2092 H11	X	474	480	-0.32825582	514	520	-0.17545511	2601754	1.05013017	2555233	0.97285808		experimental	Microsource	1501149	Ritodrine hydrochloride
2092 H12	X	594	600	-0.1180214	435	440	-0.26741126	3061598	1.40678279	3159275	1.43199676		experimental	Microsource	1503038	Nicotinyl alcohol tartrate
2092 H13	X	713	720	0.09046107	475	480	-0.22085118	2743096	1.1597543	2814564	1.16997831		experimental	Microsource	1501150	Sulpiride
2092 H14	X	793	800	0.23061735	595	600	-0.08117097	2703223	1.128829	3061718	1.35784266		experimental	Microsource	1503059	Floxuridine
2092 H15	X	392	400	-0.47191601	314	320	-0.40825547	2484522	0.95920564	2717386	1.09611228		experimental	Microsource	1501151	Ranididine
2092 H16	X	632	640	-0.05144717	434	440	-0.26857526	2687911	1.1169531	2997123	1.30874332		experimental	Microsource	1500684	Atretamine
2092 H17	X	554	560	-0.18809954	594	600	-0.08233497	2127325	0.6821655	2339733	0.80905426		experimental	Microsource	1501152	Sipiperone
2092 H18	X	434	440	-0.39833396	433	440	-0.26973926	2625646	1.06866068	2943445	1.26794211		experimental	Microsource	1503069	Aminohippuric acid
2092 H19	X	515	520	-0.25642573	475	480	-0.22085118	2260995	0.78583926	2266859	0.75366197		experimental	Microsource	1501153	Sulctodil
2092 H20	X	434	440	-0.39833396	394	400	-0.31513533	2380302	0.87837315	2637564	1.03543874		experimental	Microsource	1501150	Mefloquine
2092 H21	X	433	440	-0.40008592	591	600	-0.08582697	2407102	0.89915909	2448393	0.89164787		experimental	Microsource	1501157	Ronidazole
2092 H22	X	550	560	-0.1933554	720	730	0.05036124	2580728	1.03382252	2740576	1.11373925		experimental	Microsource	1503073	Adiphenine hydrochloride
2092 H23	X	519	520	-0.24941917	536	540	-0.14984707	83977	0.90264461	8234	-0.90061315		empty			
2092 H24	P	107474	1													

2092 I19	X	474	480	-0.32825582	394	400	-0.31513533	2630195	1.07218887	2928498	1.25658074	experimental	Microsource	1500548	Sulfamethazine
2092 I20	X	593	600	-0.11977335	472	480	-0.22434319	2622504	1.06622377	2756830	1.12609408	experimental	Microsource	1500689	Lidocaine hydrochloride
2092 I21	X	754	760	0.16229116	1314	1320	0.75574633	2510225	0.97914076	3009632	1.31825155	experimental	Microsource	1500549	Sulfamethazine
2092 I22	X	471	480	-0.33511658	550	560	-0.12355105	2306371	0.82103265	2610789	1.01508438	experimental	Microsource	1500561	Phentolamine hydrochloride
2092 I23	E	612	960	0.08648624	473	760	-0.22317919	80604	-0.96526069	1069699	-0.90806125	empty			
2092 I24	P	117258	117840	204.271884	96061	96680	111.041425	2310314	0.82409082	2214856	0.71413394	empty			
2092 J01	N	556	560	-0.18459563	277	280	-0.45132354	2247650	0.77548895	2180334	0.68789341	empty			
2092 J02	E	316	320	-0.60506448	317	320	-0.40476347	82366	-0.90389409	81797	-0.90722665	empty			
2092 J03	X	354	360	-0.53849024	394	400	-0.31513533	2529909	0.99440756	2461012	0.90123971	experimental	Microsource	1501155	Sulfamer
2092 J04	X	553	560	-0.18985149	353	360	-0.3628594	2523668	0.98956708	2711556	1.09168084	experimental	Microsource	1503076	Quinapril hydrochloride
2092 J05	X	594	600	-0.1180214	555	560	-0.12773104	2822505	1.2213435	2734465	1.10909421	experimental	Microsource	1501156	Sulfamethoxypridazine
2092 J06	X	671	680	0.01687906	470	480	-0.22657119	2773063	1.18299655	2656217	1.05751463	experimental	Microsource	1503083	Amipriose
2092 J07	X	792	800	0.2288654	433	440	-0.26973926	2915756	1.2936685	2992507	1.30523465	experimental	Microsource	1501161	Suprofen
2092 J08	X	394	400	-0.4684121	315	320	-0.40709147	2838155	1.23348156	2927886	1.25611555	experimental	Microsource	1503086	Tiaprofen hydrochloride
2092 J09	X	473	480	-0.33000778	394	400	-0.31513533	3010484	1.36713904	2971779	1.28947908	experimental	Microsource	1501171	Saccharin
2092 J10	X	554	560	-0.18809954	514	520	-0.17545511	2743685	1.16021112	2941264	1.26628431	experimental	Microsource	1503092	Glucosylactone
2092 J11	X	635	640	-0.04619131	513	520	-0.17661911	2837590	1.23304335	2884240	1.22293977	experimental	Microsource	1501173	Acetanilide
2092 J12	X	472	480	-0.33175973	794	800	0.15046539	2844841	1.23866719	3066109	1.36118031	experimental	Microsource	1503101	Azlocillin sodium
2092 J13	X	594	600	-0.1180214	633	640	-0.0369389	2704151	1.12959476	2593205	1.0011721	experimental	Microsource	1501175	Flurandrenolide
2092 J14	X	513	520	-0.25992963	713	720	0.05618125	2652231	1.08927987	2811478	1.1676326	experimental	Microsource	1503102	Bacampicillin hydrochloride
2092 J15	X	632	640	-0.05144717	513	520	-0.17661911	2504377	0.97460508	3069036	1.36340515	experimental	Microsource	1501176	Erythromycin estolate
2092 J16	X	834	840	0.30244744	755	760	0.10506932	2547798	1.00828218	3011777	1.31988198	experimental	Microsource	1503104	Bendroflumethiazide
2092 J17	X	433	440	-0.40008592	393	400	-0.31629933	2529774	0.99430286	2911749	1.24384965	experimental	Microsource	1501179	Estradiol propionate
2092 J18	X	433	440	-0.40008592	554	560	-0.12889504	2299979	0.81607505	2403675	0.85765725	experimental	Microsource	1503106	Bepidril hydrochloride
2092 J19	X	554	560	-0.18809954	554	560	-0.12889504	2629284	1.0714823	2720023	1.0981167	experimental	Microsource	1501182	Estradiol benzoate
2092 J20	X	474	480	0.02212488	534	540	-0.08349874	2795750	1.3023505	2657331	1.06189311	experimental	Microsource	1503107	Thioridazine hydrochloride
2092 J21	X	551	560	-0.1933554	430	440	-0.17323126	2264577	0.78295325	2399593	0.84799093	experimental	Microsource	1501184	Estradiol acetate
2092 J22	X	807	840	0.2551447	754	800	0.10390532	2617261	1.06215732	2425997	0.87462444	experimental	Microsource	1503110	Carmustine
2092 J23	E	606	880	-0.09699796	552	840	-0.13122304	81164	-0.90482636	81220	-0.90766524	empty			
2092 J24	P	91360	92000	158.899791	96352	96880	111.380149	2257789	0.7833527	2247485	0.73893559	empty			
2092 K01	N	715	720	0.09396498	470	480	-0.22667119	2163547	0.7102591	2083280	0.61412164	empty			
2092 K02	E	195	200	-0.81705085	195	200	-0.54677169	84880	-0.90194425	79527	-0.9089521	empty			
2092 K03	X	435	440	-0.39658201	595	600	-0.08117097	3176255	1.49571017	2850721	1.19746162	experimental	Microsource	1500550	Sulfamethoxazole
2092 K04	X	435	440	-0.39658201	595	600	-0.08117097	3176255	1.49571017	2850721	1.19746162	experimental	Microsource	1500550	Sulfamethoxazole
2092 K05	X	546	560	-0.20211517	350	360	-0.36635141	2719002	1.14106711	2785260	1.14770403	experimental	Microsource	1500551	Sulfapyridine
2092 K06	X	1513	1520	1.49202388	1714	1720	1.22134705	2463463	0.94287239	2610001	1.01448782	experimental	Microsource	1500767	Butamben
2092 K07	X	630	640	-0.05495107	791	800	0.14697339	3002274	1.36077141	2860638	1.1634976	experimental	Microsource	1500552	Sulfasalazine
2092 K08	X	514	520	-0.25817768	554	560	-0.12889504	2610667	1.05704305	2782845	1.14586836	experimental	Microsource	1500771	Cefaclor
2092 K09	X	512	520	-0.26168159	554	560	-0.12889504	2909016	1.28844099	3504169	1.69415432	experimental	Microsource	1500553	Sulfathiazole
2092 K10	X	434	440	-0.39833396	714	720	0.05734525	2727861	1.14793811	2751410	1.12197429	experimental	Microsource	1500772	Idopamide
2092 K11	X	914	920	0.61201229	534	540	-0.26857526	3438837	1.69921229	2655904	1.04937917	experimental	Microsource	1500554	Tolazamide
2092 K12	X	914	920	0.61201229	534	540	-0.26857526	3438837	1.69921229	2655904	1.04937917	experimental	Microsource	1500554	Tolazamide
2092 K13	X	432	440	-0.40183787	433	440	-0.26973926	3075459	1.41753331	3201061	1.46375874	experimental	Microsource	1500555	Sulfisoxazole
2092 K14	X	554	560	-0.18809954	874	880	0.24358554	2477557	0.95380362	2323109	0.79641819	experimental	Microsource	1500778	Liothyronine
2092 K15	X	553	560	-0.18985149	513	520	-0.17661911	3112492	1.44625592	3274742	1.51976445	experimental	Microsource	1500556	Sulindac
2092 K16	X	554	560	-0.18809954	553	560	-0.13005904	2611307	1.05753943	2910824	1.24314654	experimental	Microsource	1500801	Allantoin
2092 K17	X	472	480	-0.33175973	515	520	-0.17429111	2356327	0.85977827	2199481	0.70244724	experimental	Microsource	1500557	Tamoxifen citrate
2092 K18	X	995	1000	0.58451186	434	440	-0.26857526	2795750	1.20058316	2958381	0.97129083	experimental	Microsource	1500558	Thiazidiazole
2092 K19	X	392	400	-0.47191001	553	560	-0.13005904	4098694	1.45446603	3188824	1.45446603	experimental	Microsource	1500558	Terbutaline hemisulfate
2092 K20	X	513	520	-0.25992963	792	800	0.14813739	2778502	1.18721501	2799111	1.15199941	experimental	Microsource	1500807	Adenine
2092 K21	X	688	720	0.04666223	794	840	0.15046539	2453794	0.93537317	3239667	1.49310357	experimental	Microsource	1500564	Tetracaine hydrochloride
2092 K22	X	9551	9560	15.5742262	14149	14160	15.6957094	2473984	0.95103242	2411003	0.86322734	experimental	Microsource	1500810	Aminacrine
2092 K23	E	511	840	-0.26343354	868	1160	0.23660152	82314	-0.90393442	84160	-0.90543051	empty			
2092 K24	P	101714	102280	177.039518	84399	85000	97.466836	2458730	0.9392015	2399026	0.8541235	empty			
2092 L01	N	835	840	0.3041994	2875	2880	0.52725314	2485021	0.95959266	2269449	0.75563066	empty			
2092 L02	E	195	200	-0.81705085	229	240	-0.50719563	83677	-0.90287729	78578	-0.90967345	empty			
2092 L03	X	475	480	-0.32650387	515	520	-0.17429111	1781718	0.41411451	1471078	0.14878046	experimental	Microsource	1501185	Econazole nitrate
2092 L04	X	429	440	-0.40709373	393	400	-0.31629933	2912188	1.29090117	2881869	1.22113754	experimental	Microsource	1503111	Ceftriaxone sodium trihydrate
2092 L05	X	1753	1760	1.91249273	715	720	0.05850925	2475204	0.95197865	2518957	0.94528431	experimental	Microsource	1501187	Flunisolide
2092 L06	X	586	600	-0.13203703	430	440	-0.27323126	3246549	1.55022983	3149379	1.42444741	experimental	Microsource	1503115	Xylazine
2092 L07	X	592	600	-0.12152531	512	520	-0.17778312	2442464	0.92658568	2502894	0.93307466	experimental	Microsource	1501200	Xylazine
2092 L08	X	352	360	-0.54199415	393	400	-0.31629933	2806116	1.20863228	3057346	1.35451946	experimental	Microsource	1503117	Trimipramine maleate
2092 L09	X	1234	1240	1.00322885	471	480	-0.22550719	2557731	1.01598616	2655904	1.04937917	experimental	Microsource	1501201	Tolazamide
2092 L10	X	512	520	-0.26168159	553	560	-0.13005904	2523712	0.9896012	2410137	0.86256909	experimental	Microsource	1503118	Trifluoroacetyl hydrochloride
2092 L11	X	594	600	-0.1180214	473	480	-0.22317919	2845949	1.23952655	2646547	1.04226682	experimental	Microsource	1501202	Galanthamine hydrobromide
2092 L12	X	672	680	0.01863097	554	560	-0.12889504	3380829	1.6543767	2966921	1.28578646	experimental	Microsource	1503121	Trazodone hydrochloride
2092 L13	X	634	640	-0.04794326	274	280	-0.45481555	2406264	0.89850914	2412744	0.86455069	experimental	Microsource	1501203	Retinol
2092 L14	X	553	560	-0.18985149	514	520	-0.17545511	2868305	1.25686575	3356651	1.58202434	experimental	Microsource	1503134	Menthyl(-)
2092 L15	X	594	600	-0.1180214	474	480	-0.22201519	2147529	0.69783652	2079254	0.61106144	experimental	Microsource	1501205	Lanatoside c
2092 L16	X	554	560	-0.18809954	554	560	-0.12889504	3120130	1.45217991	2435583	1.10994402	experimental	Microsource	1503135	Thiozylamine hydrochloride
2092 L17	X	675	680	0.02388684	394	400	-0.31513533	2484622	0.9592832	2471491	0.90204931	experimental	Microsource	1501214	Enalapril maleate
2092 L18	X	432	440	-0.40183787	474	480	-0.22201519	2901608	1.28269538	2848758	1.19596952	experimental	Microsource	1503136	Thiamphenicol
2092 L19	X	554	560	-0.18809954	672	680	0.00845717	2309100	0.82314925	2475161					

2092 M13	X	273	280	-0.68039848	555	560	-0.12773104	2133543	0.68698815	2020193	0.56616855	experimental	Microsource	1500575	Thioridazine hydrochloride
2092 M14	X	515	520	-0.25642573	553	560	-0.13005904	2489160	0.96280285	2158950	0.94527899	experimental	Microsource	1500839	Cinchonidine
2092 M15	X	514	520	-0.25817768	474	480	-0.22201519	2161619	0.70876375	2349055	0.81614002	experimental	Microsource	1500576	Thiothixene
2092 M16	X	394	400	-0.46841121	674	680	-0.17545511	2550609	1.01046238	2617013	1.01981771	experimental	Microsource	1500814	Cinchonine
2092 M17	X	394	400	0.46841121	474	480	0.01078518	2453221	0.77368259	2677713	0.94433874	experimental	Microsource	1500579	Tibramycin
2092 M18	X	474	480	-0.32825582	672	680	0.00845717	2427155	0.91471209	2813014	1.16880013	experimental	Microsource	1500844	Coenzym b12
2092 M19	X	552	560	-0.19160345	913	920	0.28898161	2386122	0.88288711	2565128	0.98037938	experimental	Microsource	1500580	Tolazoline hydrochloride
2092 M20	X	1113	1120	0.79124247	612	520	-0.17778312	2454379	0.93582689	2723925	1.10108265	experimental	Microsource	1500847	Cholesterol
2092 M21	X	627	640	-0.06020693	530	640	-0.0404309	2204955	0.74237493	2352646	0.81886957	experimental	Microsource	1500581	Tolbutamide
2092 M22	X	2111	2120	2.53969208	1710	1720	1.21669104	2371854	0.87182093	2349368	0.81637793	experimental	Microsource	1500873	Piperine
2092 M23	E	649	1000	-0.02166396	625	1040	-0.04625091	83079	-0.90334109	81554	-0.90741136	empty			
2092 M24	P	116344	117000	202.670598	138840	139600	160.836258	240870	0.77023042	2405274	0.77156333	empty			
2092 N01	N	1035	1040	0.6545901	755	760	0.10506932	1969001	0.55937023	1968329	0.52674618	empty			
2092 N02	E	194	200	-0.81880281	275	280	-0.45365154	77420	-0.90773018	73902	-0.91322773	empty			
2092 N03	X	514	520	-0.25817768	554	360	-0.3616954	2616261	1.06138173	2366296	0.82924508	experimental	Microsource	1502004	Bumetanide
2092 N04	X	552	560	-0.19160345	313	520	-0.17661911	1992989	0.5779752	2205898	0.70732487	experimental	Microsource	1503202	Chloroxine
2092 N05	X	513	520	-0.25992963	632	640	-0.0381029	2595405	1.04520592	2575300	0.98811578	experimental	Microsource	1502005	Chlorobenzoxolone sodium
2092 N06	X	432	440	-0.04183787	513	520	-0.17661911	1923409	0.52400931	2011572	0.55961563	experimental	Microsource	1503203	Chloroprothixene hydrochloride
2092 N07	X	792	800	0.2288654	552	560	-0.13122304	2471309	0.94895771	2405274	0.95887267	experimental	Microsource	1502013	Isotretinoin
2092 N08	X	513	520	-0.25992963	473	480	-0.22317919	2589040	1.04026926	2223496	0.7207013	experimental	Microsource	1503204	Cinnarazine
2092 N09	X	471	480	-0.33351168	511	520	-0.17894712	2569455	1.02507924	2705885	1.08737025	experimental	Microsource	1502104	Mesna
2092 N10	X	1152	1160	0.85956866	591	600	-0.08582697	2157781	0.70578702	2167202	0.67791164	experimental	Microsource	1503207	Cyclobenzaprine hydrochloride
2092 N11	X	1231	1240	0.99797299	1433	1440	0.89426254	2753314	1.16767932	2384906	0.84339074	experimental	Microsource	1502016	Tretinoin
2092 N12	X	592	600	-0.12152531	391	400	-0.31862733	2463212	0.94267772	1939521	0.50484891	experimental	Microsource	1503209	Dantrolene sodium
2092 N13	X	634	640	-0.04794326	473	480	-0.22317919	2650002	1.08755107	2317553	0.79219501	experimental	Microsource	1502018	Bretylium tosylate
2092 N14	X	513	520	-0.25992963	634	640	-0.28898161	2220825	0.75463362	2057416	0.37290636	experimental	Microsource	1503205	Tamethasonone 17,21-dipropionate
2092 N15	X	713	720	0.09046107	591	600	-0.08582697	2295916	0.001595	2587840	0.99764301	experimental	Microsource	1502019	Foscarnet sodium
2092 N16	X	634	640	-0.04794326	474	480	-0.22201519	2217458	0.75207219	2372467	0.83393572	experimental	Microsource	1503212	Dobutamine hydrochloride
2092 N17	X	473	480	-0.33000778	512	520	-0.1778312	2524469	0.99018833	2609811	1.0143434	experimental	Microsource	1502020	Folic acid
2092 N18	X	633	640	-0.04969521	833	840	-0.19586146	2093304	0.65577899	2589777	0.99911534	experimental	Microsource	1503214	Edoxudine
2092 N19	X	591	600	-0.12327726	591	600	-0.08582697	2348640	0.85381627	2844741	1.19291616	experimental	Microsource	1502021	Phthalylsulfathiazole
2092 N20	X	751	760	0.1570353	554	560	-0.12889504	2185957	0.72764018	2544124	0.96441402	experimental	Microsource	1503215	Enoxacin
2092 N21	X	632	640	-0.05144717	553	560	-0.13005904	2424094	0.912338	2377079	0.83744135	experimental	Microsource	1502025	Succinylsulfathiazole
2092 N22	X	624	640	-0.06546279	624	640	-0.06546279	2087811	0.75151763	2583698	0.79088764	experimental	Microsource	1503221	Ethisterone
2092 N23	E	797	1160	0.23762516	670	1120	0.00612917	80489	-0.90534988	78669	-0.90960428	empty			
2092 N24	P	122281	122960	213.071946	151053	152040	175.052212	2289479	0.8079313	2262495	0.75034485	empty			
2092 O01	N	794	800	0.2323693	475	480	-0.22085118	2062939	0.63222805	1892568	0.46915944	empty			
2092 O02	E	314	320	-0.60856838	315	320	-0.40709147	80230	-0.90555076	75714	-0.91185041	empty			
2092 O03	X	713	720	0.09046107	634	640	-0.0357749	2434594	0.92048174	2507823	0.93682124	experimental	Microsource	1500582	Tolmetin sodium
2092 O04	X	873	880	0.37077363	792	800	0.14813739	2150393	0.70005692	2268474	0.75488955	experimental	Microsource	1500903	Etoposide
2092 O05	X	590	600	-0.1745782	612	620	-0.1745782	2465508	0.9445584	2352464	0.95234642	experimental	Microsource	1500583	Tolmetin sodium
2092 O06	X	633	640	-0.04969521	671	680	0.00729317	2303020	0.81843363	2114340	0.63773067	experimental	Microsource	1500907	Dehydrolic acid
2092 O07	X	752	760	0.15878726	830	840	0.19236946	2322147	0.83326843	2368300	0.82737065	experimental	Microsource	1500584	Tranlycypromine sulfate
2092 O08	X	632	640	-0.05144717	473	480	-0.22317919	2340730	0.84768131	2131949	0.65111546	experimental	Microsource	1500992	Flumequine
2092 O09	X	672	680	0.01863097	473	480	-0.22317919	2420555	0.90959317	2341470	0.81037458	experimental	Microsource	1500585	Triacetin
2092 O10	X	631	640	-0.05319912	673	680	0.00962117	2204952	0.74237216	2034530	0.57706625	experimental	Microsource	1500993	Flunarizine hydrochloride
2092 O11	X	711	720	0.08695716	669	680	0.00496517	2137762	0.69026039	2451993	0.89438427	experimental	Microsource	1500586	Triamcinolone
2092 O12	X	354	360	-0.54024262	634	640	-0.0357749	1743788	0.38469619	1309415	0.32925882	experimental	Microsource	1500994	Fluphenazine hydrochloride
2092 O13	X	513	520	-0.25992963	673	680	0.00962117	2204952	0.89048329	2384680	0.84716666	experimental	Microsource	1500587	Triamcinolone acetonide
2092 O14	X	592	600	-0.12152531	670	680	0.00612917	2138805	0.69106933	2312964	0.78870687	experimental	Microsource	1500995	Flutamide
2092 O15	X	792	800	0.2288654	1073	1080	0.47522189	2633703	1.07490965	2465141	0.90437821	experimental	Microsource	1500588	Triamcinolone diacetate
2092 O16	X	591	600	-0.12327726	551	560	-0.13238705	2091923	0.65470789	2332262	0.80337548	experimental	Microsource	1501002	Droperidol
2092 O17	X	793	800	0.23061735	914	920	0.29014561	7144938	4.57380012	6295992	3.81624837	experimental	Microsource	1500589	Triamterene
2092 O18	X	711	720	0.08695716	511	520	-0.17894712	2232817	0.76400006	2244133	0.7363877	experimental	Microsource	1501003	Famotidine
2092 O19	X	1152	1160	0.85956866	673	680	0.00962117	2412464	0.90331783	2764450	1.13188613	experimental	Microsource	1500590	Trichlormethiazide
2092 O20	X	589	600	-0.12678117	513	520	-0.17661911	2220611	0.75451764	2583698	0.99449463	experimental	Microsource	1501005	Etodolac
2092 O21	X	590	600	-0.12502921	469	480	-0.22783519	1319496	0.05561752	1446134	0.12982026	experimental	Microsource	1500591	Trifluoperazine hydrochloride
2092 O22	X	1432	1440	1.35011565	869	880	0.23776553	2085231	0.64951761	2206484	0.70777703	experimental	Microsource	1501007	Fenoterol hydrobromide
2092 O23	E	572	920	-0.15656438	850	1440	0.21564949	79790	-0.90589202	77964	-0.91014016	empty			
2092 O24	P	115546	116400	201.272539	198930	200040	230.781126	2019248	0.59834154	2243605	0.73598636	empty			
2092 P01	N	837	840	0.3077033	598	600	-0.07767896	1640717	0.30475486	1565682	0.22068995	empty			
2092 P02	E	195	200	-0.81705085	276	280	-0.45248754	75569	-0.90916581	72661	-0.91417102	empty			
2092 P03	X	596	600	-0.11451749	516	520	-0.17312711	2015844	0.59570142	2015362	0.56249645	experimental	Microsource	1502026	Tranexamic acid
2092 P04	X	433	440	-0.40008592	435	440	-0.26741126	1287683	0.03094352	1161400	-0.08660221	experimental	Microsource	1503223	Parosaraniline pamoate
2092 P05	X	875	880	0.37427754	554	560	-0.12889504	2168486	0.71408976	2094943	0.62298681	experimental	Microsource	1502028	Cephalexin
2092 P06	X	434	440	-0.39833396	551	560	-0.13238705	2019345	0.59841677	2175396	0.68413998	experimental	Microsource	1503227	Perhexiline maleate
2092 P07	X	715	720	0.09396498	1874	1880	1.40758734	2244395	0.77296439	2118605	0.64097254	experimental	Microsource	1502029	Cefsulodin sodium
2092 P08	X	634	640	-0.04794326	675	680	0.00729317	2416077	0.90612006	2219516	0.71767606	experimental	Microsource	1503229	Methapyrilene hydrochloride
2092 P09	X	875	880	0.37427754	671	680	0.01194918	2205981	0.74317069	2014458	0.56180931	experimental	Microsource	1502030	Oxolinic acid
2092 P10	X	514	520	-0.39833396	513	520	-0.16619111	1217978	-0.02311391	1193306	0.06235696	experimental	Microsource	1503239	Hycaonitine
2092 P11	X	715	720	0.09396498	1035	1040	0.43098983	2152612	0.7078271	1200442	0.62716666	experimental	Microsource	1502031	Cefamandole sodium
2092 P12	X	714	720	0.09221302	433	440	-0.26973926	2311335	0.8248827	2130814	0.65025273	experimental	Microsource	1503234	Beta-proiolactone
2092 P13	X	914	920	0.44260373	754	760	0.1039053								

2093 A07	X	316	320	-0.46830557	436	440	-0.32037849	1675688	0.30493004	1970256	0.46152404	experimental	Microsource	1503253	Methylbenzethonium chloride
2093 A08	X	556	560	-0.03224995	475	480	-0.25674639	2119095	0.6426045	2288181	0.69175168	experimental	Microsource	1504148	Mepivacaine hydrochloride
2093 A09	X	595	600	0.03860909	956	960	0.52804952	2011891	0.56096381	2500076	0.84519694	experimental	Microsource	1503255	Methylprednisolone sodium succinate
2093 A10	X	716	720	0.2584538	355	360	-0.42523747	2281553	0.7666236	2605094	0.48657523	experimental	Microsource	1504152	Miliumamide
2093 A11	X	515	520	-0.10674278	356	360	-0.45090588	1588169	0.23545037	1453452	0.6828538	experimental	Microsource	1503256	Amtracaine
2093 A12	X	675	680	0.18396097	392	400	-0.39216855	2255731	0.74665898	1873430	0.39140681	experimental	Microsource	1504171	Vanflaxine
2093 A13	X	636	640	0.11310193	1836	1840	1.96385077	2196277	0.70138208	1969541	0.46100627	experimental	Microsource	1503257	Midoxifene hydrochloride
2093 A14	X	315	320	-0.47012247	391	400	-0.39380014	1818930	0.41401529	2050619	0.51971948	experimental	Microsource	1504172	Citalopram
2093 A15	X	556	560	-0.03224995	676	680	0.07120367	2113858	0.63861628	2432759	0.79644886	experimental	Microsource	1503260	Nadolol
2093 A16	X	355	360	-0.39744653	595	600	-0.06095531	1699829	0.3233145	2442572	0.80355501	experimental	Microsource	1504173	Fluoxetine
2093 A17	X	676	680	0.18577786	635	640	0.00430838	2277929	0.76356376	2245950	0.6611698	experimental	Microsource	1503262	Naltrexone hydrochloride
2093 A18	X	714	720	0.11258482	594	600	-0.06258669	1980765	0.53725995	248845	0.83692634	experimental	Microsource	1504174	Bupropion
2093 A19	X	835	840	0.47466471	754	760	0.19846787	1953927	0.5168216	2453105	0.81118255	experimental	Microsource	1503263	Cyclothiazide
2093 A20	X	631	640	0.10401743	870	880	0.38773258	2172048	0.6829306	2814138	1.07262715	experimental	Microsource	1504175	Cefuroxime axetil
2093 A21	X	1475	1480	1.63747971	1714	1720	1.7647965	1532970	0.19624384	1590672	0.18664561	experimental	Microsource	1503265	Nicosamide
2093 A22	X	670	680	0.17487647	989	1000	0.58189207	2085848	0.6172854	2324599	0.71812403	experimental	Microsource	1504179	Fexofenadine hydrochloride
2093 A23	E	754	1200	0.32749594	656	1080	0.03857182	77762	-0.91196278	78697	-0.90826176	empty			
2093 A24	P	152009	152360	275.142468	143812	144240	233.610803	1568452	0.22326498	1886737	0.40104317	empty			
2093 B01	N	357	360	-0.39381273	516	520	-0.1988511	1813444	0.40983746	2283348	0.68823182	empty			
2093 B02	E	157	160	-0.75719242	276	280	-0.58143326	80167	-0.91013127	81598	-0.90616098	empty			
2093 B03	X	316	320	-0.46830557	436	440	-0.32037849	2412042	0.86596987	2597470	0.91572549	experimental	Microsource	1505305	Pefloxacin mesylate
2093 B04	X	316	320	-0.46830557	354	360	-0.45416906	2243339	0.73722191	2202607	0.62978266	experimental	Microsource	1505622	Rifaxime hydrochloride
2093 B05	X	355	360	-0.39744653	395	400	-0.38727378	2300556	0.78079524	2566890	0.89358077	experimental	Microsource	1505306	Alaroxane dihydrochloride
2093 B06	X	394	400	-0.32658749	354	360	-0.45416906	2483428	0.92006653	2861269	1.1067574	experimental	Microsource	1505636	Zimelidine dihydrochloride
2093 B07	X	315	320	-0.47012247	355	360	-0.45253747	1968008	0.52754492	2425141	0.79993223	experimental	Microsource	1505308	Chlorophyllide cu complex na salt
2093 B08	X	440	440	0.25391156	475	480	-0.25391156	2463197	0.9046531	3093216	0.27407211	experimental	Microsource	1505637	Ipefodopamide proxetil
2093 B09	X	514	520	-0.10855968	592	600	-0.06585009	1904323	0.47904592	2255613	0.66816733	experimental	Microsource	1505299	Bifonazole
2093 B10	X	394	400	-0.32658749	474	480	-0.25837798	2412739	0.86622767	2826369	1.08148432	experimental	Microsource	1505650	Aminopentamide
2093 B11	X	275	280	-0.54279841	555	560	-0.126219	2890322	1.22992869	2949743	1.17082647	experimental	Microsource	1505312	Tylosin tartrate
2093 B12	X	395	400	-0.32477059	514	520	-0.19311429	2817629	1.17456969	3105898	1.28390721	experimental	Microsource	1505652	Arsenic acid
2093 B13	X	513	520	-0.11037658	550	560	-0.13437697	2596218	1.00595521	2735682	1.01581268	experimental	Microsource	1505314	Sarrafloxacin hydrochloride
2093 B14	X	555	560	-0.03406685	514	520	-0.19311429	3033088	1.33865145	3156923	1.32085733	experimental	Microsource	1505656	Panthenol
2093 B15	X	674	680	0.18214407	514	520	-0.19311429	2723553	1.10292656	3124799	1.29759451	experimental	Microsource	1505319	Clopidol
2093 B16	X	440	440	0.25391156	475	480	-0.25391156	2463197	0.9046531	3093216	0.27407211	experimental	Microsource	1505661	Nimetozine
2093 B17	X	354	360	-0.39926343	593	600	-0.0642185	2211555	0.71301966	2783659	1.05055557	experimental	Microsource	1505321	Rifaximin
2093 B18	X	528	560	-0.0831231	648	680	0.02551908	2417612	0.86993867	2770216	1.04082072	experimental	Microsource	1505665	Phthalylsulfathiazole
2093 B19	X	472	480	-0.18486941	431	440	-0.32853645	2434362	0.88269456	2275916	0.68286989	experimental	Microsource	1505327	Chloramidine acetate
2093 B20	X	833	840	0.47103092	993	1000	0.58841844	2843584	1.19433559	2437176	0.79964746	experimental	Microsource	1505668	Ronnel
2093 B21	X	470	480	-0.18850321	348	360	-0.46395861	1391319	0.08883702	1486025	0.11086474	experimental	Microsource	1505330	Oxicanazole nitrate
2093 B22	X	712	720	0.25118621	951	960	0.51989156	2139970	0.65880175	2410843	0.78057823	experimental	Microsource	1505672	Vincristine sulfate
2093 B23	E	604	660	0.05494537	766	840	0.05494537	84649	0.9671802	484949	0.90262565	empty			
2093 B24	P	119301	120040	215.715354	145943	146680	237.087726	2163533	0.67544004	2339528	0.72893877	empty			
2093 C01	N	277	280	-0.53916461	397	400	-0.38401059	2162010	0.67528621	2013249	0.49265773	empty			
2093 C02	E	157	160	-0.75719242	276	280	-0.58143326	77540	-0.91213184	82886	-0.90522827	empty			
2093 C03	X	397	400	-0.3211368	315	320	-0.51780116	2971434	1.29169914	2207352	0.63321878	experimental	Microsource	1503267	Nomifensine maleate
2093 C04	X	475	480	-0.17941872	636	640	0.00593998	2534866	0.95923289	2351099	0.73731419	experimental	Microsource	1504190	Avobezone
2093 C05	X	395	400	-0.32477059	394	400	-0.38890537	2737522	1.11356459	2436347	0.79904713	experimental	Microsource	1503269	Pergolide mesylate
2093 C06	X	440	440	0.25391156	475	480	-0.25391156	2463197	0.9046531	3093216	0.27407211	experimental	Microsource	1504815	Ammoniolevulinic acid hydrochloride
2093 C07	X	474	480	-0.18123562	514	520	-0.19311429	2880004	1.22209924	3047328	1.24106688	experimental	Microsource	1503270	Pirlicaine hydrochloride
2093 C08	X	515	520	-0.10674278	354	360	-0.45416906	2689373	0.70689695	2787597	1.0534073	experimental	Microsource	1504188	Pirenperone
2093 C09	X	554	560	-0.03588374	675	680	0.06957208	2679662	1.06950159	3153868	1.31864503	experimental	Microsource	1503273	Hydrocortisone butyrate
2093 C10	X	595	600	0.03860909	514	520	-0.19311429	2421634	0.87300611	2209108	0.6344904	experimental	Microsource	1504210	Atovaquone
2093 C11	X	355	360	-0.39744653	434	440	-0.32364167	2845784	1.19601099	2461490	0.81725461	experimental	Microsource	1503276	Ritonavir
2093 C12	X	354	360	-0.39926343	394	400	-0.38890537	2727543	1.10596513	2266129	0.67578256	experimental	Microsource	1504211	Chloroquinidone hydrochloride
2093 C13	X	755	760	0.32931284	594	600	-0.06258669	1920672	0.49149642	1671583	0.24523788	experimental	Microsource	1503278	Mitoxanthrone hydrochloride
2093 C14	X	314	320	-0.47193937	673	680	0.06530889	2964871	1.28670112	2992658	1.20190367	experimental	Microsource	1504774	Trimetozine
2093 C15	X	394	400	-0.32658749	473	480	-0.26009557	2519812	0.94776859	3093719	1.27508771	experimental	Microsource	1503279	Oxethazaine
2093 C16	X	515	520	-0.10674278	593	600	-0.0642185	2633479	1.03433115	2762163	1.03498909	experimental	Microsource	1504216	Zoxazolamine
2093 C17	X	449	480	-0.22665808	568	600	-0.1050083	2540955	0.96386994	3054264	1.24651609	experimental	Microsource	1503298	Dipyron
2093 C18	X	9434	9440	16.0981743	9273	9280	14.0980029	2737030	1.11318991	2478712	0.82972604	experimental	Microsource	1504218	Arsinorcin
2093 C19	X	607	640	0.06041187	689	720	0.09241437	2914539	1.24837103	2977177	1.19069299	experimental	Microsource	1503301	Sulfanilic acid zinc
2093 C20	X	713	720	0.25300311	632	640	-0.00058639	2241517	0.73583438	2327415	0.72016325	experimental	Microsource	1504226	Cysteamine hydrochloride
2093 C21	X	513	520	-0.11037658	594	600	-0.06258669	2538335	0.96187469	2939152	1.16135692	experimental	Microsource	1503304	Urethane
2093 C22	X	672	680	0.17851027	630	640	-0.00384958	2258956	0.74911497	2628401	0.93812439	experimental	Microsource	1504229	Metaxalone
2093 C23	E	578	880	0.00772182	796	1120	0.26699475	81433	-0.90916715	86473	-0.90263072	empty			
2093 C24	P	101235	101880	182.891267	108400	109160	175.832855	2365995	0.830663	2510967	0.85308373	empty			
2093 D01	N	357	360	-0.39381273	277	280	-0.57980167	1999460	0.55149704	2494501	0.84115976	empty			
2093 D02	E	317	320	-0.46648867	237	240	-0.64506336	82388	-0.90843987	84624	-0.90396988	empty			
2093 D03	X	235	240	-0.61547434	475	480	-0.25674639	2731423	1.10891992	2753619	1.02880169	experimental	Microsource	1505332	Azaperone
2093 D04	X	440	440	0.25027176	395	400	-0.38727378	2550896	0.9395241	3934424	1.41825718	experimental	Microsource	1505373	Flotizone
2093 D05	X	315	320	-0.47012247	315	320	-0.51780116	2014836	0.86320656	2087916	0.5401181	experimental	Microsource	1505340	Azetastine hydrochloride
2093 D06	X	434	440	-0.25391156	434	440	-0.32364167	2562365	0.98017462	2928563	1.15548882	experimental	Microsource	1505675	Trientine hydrochloride
2093 D07	X	715	720	0.2566369	594	600	-0.06258669	3597618	1.768						

2093 E01	N	437	440	-0.24846086	437	440	-0.3187469	2219059	0.7187316	2030674	0.50527616	empty							
2093 E02	E	236	240	-0.61365744	156	160	-0.77722434	83384	-0.90768137	86386	-0.90269372	empty							
2093 E03	X	396	400	-0.3229537	596	600	-0.05932372	2431544	0.88054852	2445306	0.80553485	experimental							
2093 E04	X	394	400	-0.47012247	394	400	-0.38890537	2627722	1.02994693	2118679	0.56900561	experimental	Microsource	1503322	Thiram				
2093 E05	X	436	440	-0.25027776	436	440	-0.25027776	2759026	1.12996066	2623075	0.93426753	experimental	Microsource	1504235	Rifedoxil				
2093 E06	X	434	440	-0.25391156	474	280	-0.58469645	2679993	1.06975366	2395484	0.7694559	experimental	Microsource	1504236	Nicotinamide				
2093 E07	X	634	640	0.10946813	274	480	-0.25837798	3205632	1.4700515	3428148	1.51726683	experimental	Microsource	1503330	Simvastatin				
2093 E08	X	555	560	-0.03406685	635	640	0.00430838	2554517	0.97419802	2718827	1.00360702	experimental	Microsource	1504237	Quinacrine				
2093 E09	X	355	360	-0.39744653	434	440	-0.32364167	2886610	1.22710183	2980768	1.19329344	experimental	Microsource	1503339	Hydroquinone				
2093 E10	X	516	520	-0.10492588	395	400	-0.38727378	2690349	1.07764022	2657119	0.95892073	experimental	Microsource	1504243	Sulfanilamide				
2093 E11	X	394	400	-0.32658749	513	520	-0.19474588	3295861	1.53876496	2882943	1.122452078	experimental	Microsource	1503393	Oxcarbazepine				
2093 E12	X	675	680	0.18396097	515	520	-0.1914827	2523227	0.95501469	2382362	0.69104273	experimental	Microsource	1504257	Pipobroman				
2093 E13	X	394	400	-0.32658749	394	400	-0.38890537	3237822	1.49456564	2844179	1.09438155	experimental	Microsource	1503412	Carvedilol				
2093 E14	X	595	600	0.03860909	593	600	-0.0642185	2976696	1.29570639	3040214	1.23634168	experimental	Microsource	1504258	Etanidazole				
2093 E15	X	434	440	-0.25391156	593	600	-0.0642185	3032369	1.3381039	3075087	1.26159521	experimental	Microsource	1503419	Nafrolin				
2093 E16	X	434	440	-0.25391156	513	520	-0.19474588	2450518	0.89499808	2455034	0.81257945	experimental	Microsource	1504259	Irbesartan				
2093 E17	X	674	680	0.18214407	752	760	0.19520468	2677451	1.06781781	2988621	1.19898025	experimental	Microsource	1503420	Quipazine maleate				
2093 E18	X	632	640	0.10583433	712	720	0.12994099	2778130	1.14448942	2867470	1.11124789	experimental	Microsource	1504260	Levofloxacin				
2093 E19	X	673	680	0.18032717	512	520	-0.19637747	3051177	1.35242704	2582664	0.90500362	experimental	Microsource	1503421	Ritanserin				
2093 E20	X	832	840	0.46921402	792	800	0.26046838	2614119	1.01958763	2728457	1.01058065	experimental	Microsource	1504261	Candesartan cilextil				
2093 E21	X	753	760	0.32567904	1432	1440	1.30468747	2509068	0.93958655	3007480	1.21263712	experimental	Microsource	1504262	Semustine				
2093 E22	X	472	480	-0.18486941	590	600	-0.06911327	2359286	0.82552079	2637248	0.94466136	experimental	Microsource	1504268	Losartan				
2093 E23	E	495	760	-0.14308075	517	760	-0.18821951	86117	-0.90560007	90464	-0.89974061	empty							
2093 E24	P	88394	89808	159.560474	89814	81520	130.986099	2298070	0.77890814	2567191	0.89379874	empty							
2093 F01	N	477	480	-0.17578492	437	440	-0.3187469	2131875	0.65233704	2758480	0.90197375	empty							
2093 F02	E	196	200	-0.68633338	196	200	-0.68633338	84325	-0.90647676	8384	-0.90453255	empty							
2093 F03	X	476	480	-0.1776582	435	440	-0.32201008	2531301	0.95651798	2812952	1.0717683	experimental	Microsource	1505374	Vardenafil hydrochloride				
2093 F04	X	275	280	-0.54279841	475	480	-0.25674639	2616065	1.02106996	2752513	1.02800097	experimental	Microsource	1505803	Pravastatin sodium				
2093 F05	X	434	440	-0.25391156	514	520	-0.19311429	2854828	1.20289841	3104177	1.28266094	experimental	Microsource	1505376	Acedapone				
2093 F06	X	434	440	-0.25391156	755	760	0.20009946	3045899	1.3484076	3173983	1.33321145	experimental	Microsource	1505805	Gabapentin				
2093 F07	X	515	520	-0.10674278	514	520	-0.19311429	2945348	1.27183347	2847994	1.09714421	experimental	Microsource	1505384	Methylglutamate hydrochloride				
2093 F08	X	435	440	-0.25209466	393	400	-0.39053696	2857238	1.20473373	3201425	1.35308377	experimental	Microsource	1505814	Metformin hydrochloride				
2093 F09	X	316	320	-0.4630557	795	800	0.26536315	2820489	1.17674771	3140094	1.30867049	experimental	Microsource	1505385	Atomoxetine hydrochloride				
2093 F10	X	545	550	-0.15429185	392	400	-0.39216864	2896179	0.9921556	2982156	1.0446922	experimental	Microsource	1505391	Pravastatin sodium				
2093 F11	X	555	560	-0.03406685	955	960	0.52641793	2395293	0.85294175	2596856	0.91528086	experimental	Microsource	1505387	Duloxetine hydrochloride				
2093 F12	X	514	520	-0.10855968	433	440	-0.32527327	2924572	1.25601161	3335153	1.44992384	experimental	Microsource	1505817	Ramelteon				
2093 F13	X	354	360	-0.39926343	474	480	-0.25837798	2376442	0.83858586	2933558	1.15910599	experimental	Microsource	1505389	Tramadol hydrochloride				
2093 F14	X	554	560	-0.03588374	634	640	0.00267679	2700291	1.0852115	3299798	1.42432127	experimental	Microsource	1505818	Pantoprazole				
2093 F15	X	395	400	-0.32477059	513	520	-0.19474588	2458165	0.90082162	2659530	0.96066668	experimental	Microsource	1505390	Nisoldipine				
2093 F16	X	314	320	-0.47193937	433	440	-0.32527327	3212155	1.47501906	3308085	1.23479995	experimental	Microsource	1505819	Eletriptan hydrobromide				
2093 F17	X	593	600	-0.12770654	712	720	0.12994099	2778130	1.14448942	2867470	1.11124789	experimental	Microsource	1505391	Thalidomide				
2093 F18	X	983	1000	0.76173467	789	800	0.2555737	642622	0.93515558	6869301	4.00302027	experimental	Microsource	1505820	Tobacatin hydrochloride				
2093 F19	X	431	440	-0.25936225	873	880	0.39262736	2406951	0.86181984	2495267	0.84171446	experimental	Microsource	1505393	Desloratadine				
2093 F20	X	832	840	0.46921402	510	520	-0.19964066	2959158	1.28235041	2920418	1.14959056	experimental	Microsource	1505391	Sitagliptin				
2093 F21	X	671	680	0.17669337	871	880	0.38936417	4938439	2.78966229	5346861	2.90671639	experimental	Microsource	1505396	Fluorescein				
2093 F22	X	792	800	-0.06748168	591	600	-0.06748168	2425344	0.87582694	2556407	0.88598943	experimental	Microsource	1505851	Aripiprazole				
2093 F23	E	564	960	-0.01771476	561	840	-0.11642945	83914	-0.90727776	90649	-0.89960664	empty							
2093 F24	P	137000	134200	241.876867	93327	93800	151.239864	2341186	0.81173682	2600118	0.77925664	empty							
2093 G01	N	440	440	-0.24846086	357	360	-0.44927428	2171905	0.5680219	2210754	0.5680219	empty							
2093 G02	E	115	120	-0.83350215	197	200	-0.71032906	77577	-0.91210367	82198	-0.90572649	empty							
2093 G03	X	435	440	-0.25209466	356	360	-0.45090588	2564810	0.9820366	2325930	0.71908788	experimental	Microsource	1503423	Spiramycin				
2093 G04	X	354	360	-0.39926343	435	360	-0.45253747	2677825	1.06810263	2257744	0.66971051	experimental	Microsource	1504269	Lithium citrate				
2093 G05	X	794	800	0.40017188	355	440	-0.32201008	2836838	1.18919821	2849211	1.09802551	experimental	Microsource	1503428	Choline chloride				
2093 G06	X	554	560	-0.03588374	354	360	-0.45416906	2865441	1.21098069	3133483	1.30388309	experimental	Microsource	1504272	Gatifloxacin				
2093 G07	X	354	360	-0.39926343	395	400	-0.38727378	3038291	1.34261377	3261270	1.39642095	experimental	Microsource	1503429	Clofibrate				
2093 G08	X	475	480	-0.17941872	435	440	-0.32201008	2828506	1.18028301	3193150	1.34709137	experimental	Microsource	1504273	Miglitol				
2093 G09	X	355	360	-0.39744653	393	400	-0.39053696	2652897	1.04911883	3035746	1.23310615	experimental	Microsource	1503500	Resorcinol monoacetate				
2093 G10	X	314	320	-0.47193937	515	520	-0.1914827	2724809	1.10388307	2818193	1.07556361	experimental	Microsource	1504300	Orlistat				
2093 G11	X	395	400	-0.32477059	433	440	-0.32527327	2624919	1.02781232	2683607	0.97810221	experimental	Microsource	1503600	Nimodipine				
2093 G12	X	515	520	-0.10674278	395	400	-0.38727378	2954503	1.27880542	3045901	1.24045996	experimental	Microsource	1504303	Moxifloxacin hydrochloride				
2093 G13	X	434	440	-0.25391156	434	440	-0.32364167	2627427	1.02972227	2770969	1.04136601	experimental	Microsource	1503604	Retinyl palmitate				
2093 G14	X	554	560	-0.03588374	594	600	-0.0625869	2632825	1.03383309	2757638	1.03171228	experimental	Microsource	1504401	Pioglitazone hydrochloride				
2093 G15	X	434	440	-0.25391156	593	600	-0.0642185	3086492	1.37932101	2990716	1.20049736	experimental	Microsource	1503607	Thalidomide				
2093 G16	X	755	760	0.32931284	634	640	0.00267679	2558364	0.97712768	2835525	1.0881147	experimental	Microsource	1504402	Tolterodine tartrate				
2093 G17	X	552	560	-0.03951754	709	720	0.12504621	2848719	1.19824613	3026008	1.22605431	experimental	Microsource	1503609	Nitrendipine				
2093 G18	X	633	640	0.10765123	1313	1320	1.11052798	2345557	0.81506554	2748198	1.02487623	experimental	Microsource	1504403	Donepezil hydrochloride				
2093 G19	X	674	680	0.18214407	430	440	-0.33016804	1828901	0.42160866	2									

2093 H19	X		434	440	-0.25391156	544	560	-0.14416652	2580826	0.99423351	2545580	0.87814898	experimental	Microsource	1505417	Capoebnic acid
2093 H20	X		473	480	-0.18305252	3832	3840	5.22050905	2658815	1.05362565	3433974	1.52148577	experimental	Microsource	1505957	Arsenic trioxide
2093 H21	X		593	600	0.03497529	763	680	0.04999297	2772601	1.14027883	2619693	0.93181843	experimental	Microsource	1505425	Acetohexamide
2093 H22	X		750	760	0.32386214	671	750	0.32386214	2514022	0.94359224	2752330	1.03293755	experimental	Microsource	1505111	Clonazepam
2093 H23	E		581	582	0.01317251	656	1040	0.20173105	84496	-0.906883454	87434	-0.9019348	empty			
2093 H24	P	114198	114680	206.443721	94803	95400	153.648095	2515038	0.94413297	2444076	0.80464414		empty			
2093 I01	N		317	320	-0.46648867	477	480	-0.2534832	2323881	0.79855829	2282365	0.68753998	empty			
2093 I02	E	195	200	-0.68815028	196	160	-0.77722434	78202	-0.9116277	81539	-0.90620371		empty			
2093 I03	X	434	440	-0.25391156	355	400	-0.38727378	2676518	1.06710729	2592063	0.91180997		experimental	Microsource	1503614	Ciprofloxacin
2093 I04	X	354	360	-0.39926343	432	440	-0.32690486	2606986	1.01415553	2328075	0.72095403		experimental	Microsource	1505024	Olanzapine
2093 I05	X	834	840	0.47284782	1235	1240	0.98326378	2615763	1.02083961	2746420	1.02358868		experimental	Microsource	1503650	Nabumetone
2093 I06	X	434	440	-0.25391156	313	320	-0.52106435	2370037	0.83370816	2751417	0.8598546		experimental	Microsource	1505111	Tiostrepton
2093 I07	X	395	400	-0.32477059	515	520	-0.1914827	2593449	1.00384649	3906437	1.86362318		experimental	Microsource	1503678	Celecoxib
2093 I08	X	515	520	-0.10674278	393	400	-0.39053696	2571315	0.98699045	3315653	1.43580278		experimental	Microsource	1505112	Timilcosin
2093 I09	X	392	400	-0.33022129	513	520	-0.19474588	2341147	0.81170712	3132539	1.30319948		experimental	Microsource	1503705	Anethole
2093 I10	X	1033	1040	0.8344106	874	880	0.39425895	2650519	1.04730787	2747676	1.02449822		experimental	Microsource	1505113	Flunixin meglumine
2093 I11	X	553	560	-0.03770064	473	480	-0.26000957	2429721	0.87916023	1944633	0.44296897		experimental	Microsource	1503708	Terfenadine
2093 I12	X	675	680	0.18396097	394	400	-0.38890537	2690335	1.07762956	2273021	0.68077345		experimental	Microsource	1505114	Cloiquinol
2093 I13	X	353	360	-0.40108033	595	600	-0.06095531	2593973	1.00424554	2251843	0.88268437		experimental	Microsource	1503710	Clopidogrel sulfate
2093 I14	X	475	480	-0.17941872	473	480	-0.26000957	2638555	1.03819675	2743280	1.02131483		experimental	Microsource	1505115	Clorsolan
2093 I15	X	314	320	-0.47193937	551	560	-0.13274537	2723493	1.10288087	2870490	1.11343485		experimental	Microsource	1503712	Loratadine
2093 I16	X	555	560	-0.03406685	794	800	0.26373156	2809309	1.16823363	2947450	1.16916598		experimental	Microsource	1505116	Estradiol
2093 I17	X	512	520	-0.11219348	591	600	-0.06748168	2472800	0.91196683	3042059	1.23767775		experimental	Microsource	1503720	Selamectin
2093 I18	X	474	480	-0.18123562	473	560	-0.12948219	2811902	1.17020832	2860196	1.10598038		experimental	Microsource	1505124	Clavulanate lithium
2093 I19	X	513	520	-0.11037658	629	640	-0.00848117	2729837	1.10771211	3375973	1.47948393		experimental	Microsource	1503722	Atorvastatin calcium
2093 I20	X	554	560	-0.03589374	743	750	-0.18052037	2817304	1.17432219	2821704	1.03519745		experimental	Microsource	1505166	Acetaminofen sodium
2093 I21	X	513	520	-0.11037658	792	800	0.26046838	2615516	0.20261511	3516212	1.581038915		experimental	Microsource	1503721	Enrofloxacin
2093 I22	X	632	640	0.10583433	591	600	-0.06748168	2606032	1.01342902	2631900	0.94065822		experimental	Microsource	1505120	Acarbose
2093 I23	E	473	720	-0.18305252	714	1000	0.13320418	82523	-0.90833706	87547	-0.90185297		empty			
2093 I24	P	82045	82760	148.024986	95728	96320	155.157317	2257637	0.74811049	2791145	1.05597661		empty			
2093 J01	N	477	480	-0.17578492	477	480	-0.2534832	2121121	0.64414739	2587523	0.9085223		empty			
2093 J02	E	356	360	-0.39562963	315	320	-0.51780116	80032	-0.91023407	90223	-0.89991513		empty			
2093 J03	X	595	600	0.03860909	795	800	0.26536315	2631696	1.03297331	2718227	1.00172421		experimental	Microsource	1505426	Ethoxzolamide
2093 J04	X	394	400	-0.39744653	395	400	-0.58145621	2120414	0.6496657	2648657	0.90490415		experimental	Microsource	1505371	D-lactitol monohydrate
2093 J05	X	474	480	-0.18123562	629	400	-0.39216855	2659262	1.05396606	2597203	0.91553214		experimental	Microsource	1505429	Flucytosine
2093 J06	X	555	560	-0.03406685	395	400	-0.38727378	2636335	1.03650612	3175673	1.33443527		experimental	Microsource	1505972	Bromperidol
2093 J07	X	314	320	-0.47193937	394	400	-0.38890537	2869910	1.21438403	2966859	1.18322114		experimental	Microsource	1505432	Fomepizole hydrochloride
2093 J08	X	435	440	-0.25209466	555	560	-0.126219	2417355	0.86974296	2439290	0.80117832		experimental	Microsource	1505973	Cyproheptadine hydrochloride
2093 J09	X	435	440	-0.25209466	474	480	-0.25837798	2844205	1.19480851	2815565	1.07366052		experimental	Microsource	1505433	Glipizide
2093 J10	X	553	560	-0.03770064	474	480	-0.25837798	2479844	0.91733115	2833585	1.08670983		experimental	Microsource	1505974	Clofazimine
2093 J11	X	394	400	-0.39744653	594	600	-0.06095531	2755285	1.11901381	2105780	1.06378564		experimental	Microsource	1505382	Amiclonide
2093 J12	X	474	480	-0.18123562	474	480	-0.25837798	2992039	1.30739870	3037892	1.23466019		experimental	Microsource	1505975	Benzydamin hydrochloride
2093 J13	X	594	600	0.03679219	472	480	-0.26164117	2784631	1.14944022	2782904	1.05000883		experimental	Microsource	1505437	Levocarnitine
2093 J14	X	514	520	-0.1085968	793	800	0.26209997	2631693	1.03297103	2954856	1.17452908		experimental	Microsource	1505976	Doxazosin mesylate
2093 J15	X	473	480	-0.18305252	1033	1040	0.65368213	2738131	1.11402837	3012160	1.21602618		experimental	Microsource	1505438	Hydrocortisone valerate
2093 J16	X	353	360	-0.40108033	471	480	-0.26327276	2804462	1.16454242	2730163	1.01181606		experimental	Microsource	1505977	Isoetharine mesylate
2093 J17	X	834	840	0.47284782	833	840	0.32736366	2799417	1.16070043	2943827	1.16654236		experimental	Microsource	1505440	Lobenzazole
2093 J18	X	709	710	0.00195754	709	720	0.12504621	2821748	1.1770649	2817304	1.14951742		experimental	Microsource	1505978	Flefenidol
2093 J19	X	874	880	0.54007306	1951	1960	0.25148388	7425261	1.1740202	2690317	0.98329611		experimental	Microsource	1505444	Methylenblue
2093 J20	X	593	600	0.03497529	587	600	-0.07400805	2605192	1.01278932	2889184	1.12697224		experimental	Microsource	1505979	Ethynodiol diacetate
2093 J21	X	591	600	0.0313415	833	840	0.32736366	2598416	1.00762909	2622084	0.93354989		experimental	Microsource	1505445	Methylatropine nitrate
2093 J22	X	592	600	0.0331584	592	600	-0.06585009	2496915	0.93033149	2596147	0.91476743		experimental	Microsource	1505981	Ornidazole
2093 J23	E	573	960	-0.00136267	600	920	-0.05279735	81730	-0.90894097	85674	-0.90320932		empty			
2093 J24	P	130918	131400	236.822263	107521	108000	174.398686	2473860	0.91277407	2502467	0.84692824		empty			
2093 K01	N	437	440	-0.24846086	396	400	-0.38564218	2116788	0.64084761	2185380	0.61730761		empty			
2093 K02	E	235	240	-0.61547434	276	280	-0.58145326	82105	-0.90865539	82524	-0.90549041		empty			
2093 K03	X	555	560	-0.03406685	554	560	-0.1278506	2592393	1.03030423	2419270	0.7866807		experimental	Microsource	1503801	Naproxol
2093 K04	X	355	360	-0.39744653	433	440	-0.32527327	2599803	1.00868535	2152883	0.59377467		experimental	Microsource	1505178	Ropinorel
2093 K05	X	435	440	-0.25209466	634	640	0.00267679	2675138	1.06605636	2868313	1.11185836		experimental	Microsource	1503804	Colforsin
2093 K06	X	434	440	-0.25391156	514	520	-0.19311429	2558373	0.97713453	2366575	0.74852124		experimental	Microsource	1505187	Quetiapine
2093 K07	X	795	800	0.40198878	474	480	-0.25837798	3372312	1.59698584	2986271	1.19727848		experimental	Microsource	1503807	Isoorbide mononitrate
2093 K08	X	514	520	-0.1085968	514	520	-0.19311429	2619234	1.02348293	3052117	1.24496132		experimental	Microsource	1505189	Rizatriptan benzoate
2093 K09	X	352	360	-0.40289723	595	600	-0.06095531	2595887	1.00646468	2801901	1.06378564		experimental	Microsource	1503816	Amiclonide
2093 K10	X	475	480	-0.17941872	274	280	-0.58469645	2336072	0.80784228	2482719	0.83262774		experimental	Microsource	1505200	Benzpiperidol hydrochloride
2093 K11	X	315	320	-0.47012247	515	520	-0.1914827	2670657	1.06264387	2801827	1.06371205		experimental	Microsource	1503818	Bupivacaine hydrochloride
2093 K12	X	474	480	-0.18123562	433	440	-0.32527327	2682114	1.07136889	2716892	1.00220577		experimental	Microsource	1505201	Famciclovir
2093 K13	X	634	640	0.10946813	755	760	0.20009946	2502066	0.93425421	2922688	1.1512344		experimental	Microsource	1503903	Albendazole
2093 K14	X	432	440	-0.25754535	352	360	-0.45743225	2510427	0.94062149	2723238	1.00680127		experimental	Microsource	1505203	Ezetimibe
2093 K15	X	1155	1160	1.05607221	673	680	0.06630889	2581007	0.99437135	2278217	0.68453617		experimental	Microsource	1503908	Pacitaxel
2093 K16	X	433	440	-0.25728453	313	320	-0.52106435	2738085	1.11399334	2738948	1.01817778		experimental	Microsource	1505205	Olimetasan medoxomil
2093 K17	X	632	640	0.10583433	753	760	0.19883628	1318170	1.10746714	2914383	1.14521883		experimental	Microsource	1503941	Butacaine
2																

2093 L13	X		434	440	-0.25391156	553	560	-0.12948219	2240416	0.73499592	2666937	0.96603051	experimental	Microsource	1505463	Taurine
2093 L14	X		514	520	-0.1085968	594	600	-0.0625869	2921389	1.25358761	3075022	1.26154814	experimental	Microsource	1505993	Mesalamine
2093 L15	X		512	520	-0.11219348	634	640	0.00267679	2486629	0.92249824	2859481	1.1054626	experimental	Microsource	1505464	Thiamine
2093 L16	X		514	560	-0.39926343	833	840	0.19474588	1897621	0.47394204	2184995	0.62423038	experimental	Microsource	2300691	Clomipramine hydrochloride
2093 L17	X		752	760	0.3238614	833	840	0.32763666	1722223	0.34036854	1636913	0.22013136	experimental	Microsource	1505465	Triclosan
2093 L18	X		593	600	0.03497529	552	560	-0.13111378	1920018	0.49099837	2302469	0.70209843	experimental	Microsource	2300094	Astemizole
2093 L19	X		551	560	-0.04133444	512	520	-0.19637747	2567590	0.9841537	2634770	0.94273655	experimental	Microsource	1505467	Zinc undecylenate
2093 L20	X		594	400	-0.32658749	472	480	-0.26164117	2516197	0.94501561	3236193	1.37826126	experimental	Microsource	2300154	Acecaidine hydrochloride
2093 L21	X		311	520	-0.11401038	831	840	0.32410048	2732608	1.10982236	2567041	0.89369011	experimental	Microsource	1505468	Undecylenic acid
2093 L22	X		112	1120	0.97794558	831	840	0.32410048	2655922	1.0514225	3378275	1.48115094	experimental	Microsource	2300173	Bupropione hydrochloride
2093 L23	E		501	800	-0.13217936	642	920	0.01572953	83186	-0.90783216	86824	-0.90237654	empty			
2093 L24	P	99846	100440	180.367595	64	93169	93640	150.982073	2526757	0.95305752	2764192	0.74864218	empty			
2093 M01	N		477	480	-0.17578492	636	640	0.00593998	2276125	0.76218993	2094274	0.55133255	empty			
2093 M02	E		356	360	-0.39562963	356	360	-0.45090588	80970	-0.90951974	82070	-0.90581918	empty			
2093 M03	X		475	480	-0.17941872	315	320	-0.51780116	2738782	1.11452414	1972852	0.46340395	experimental	Microsource	1503923	Iopanic acid
2093 M04	X		434	440	-0.25391156	474	480	-0.25837798	2819624	1.17608897	2174634	0.60952581	experimental	Microsource	1505210	Sibutramine hydrochloride
2093 M05	X		635	640	0.11182503	474	480	-0.25837798	2465922	0.90672892	2434064	0.79739388	experimental	Microsource	1503925	Ketorolac tromethamine
2093 M06	X		433	440	-0.25572845	433	440	-0.32527327	2792741	1.15561635	2435348	0.7983237	experimental	Microsource	1505212	Perindopril erbumine
2093 M07	X		1115	1120	0.98339627	1114	1120	0.78584111	2616219	1.02118688	2764192	1.0364584	experimental	Microsource	1503926	Lansoprazole
2093 M08	X		513	520	-0.11037658	433	440	-0.32527327	2807805	1.16708827	2409970	0.77994604	experimental	Microsource	1505213	Rosuvastatin calcium
2093 M09	X		352	360	-0.40289723	514	520	-0.19311429	2656102	1.05159558	2385179	0.76199346	experimental	Microsource	1503929	Mexiletine hydrochloride
2093 M10	X		594	600	0.03679219	595	600	-0.06095531	2708758	1.0916595	2261688	0.67256658	experimental	Microsource	1505214	Ramipril
2093 M11	X		746	760	0.31296075	422	440	-0.34322078	2501381	0.93373255	2049046	0.51858038	experimental	Microsource	1505231	Morantil citrate
2093 M12	X		513	520	-0.11037658	394	400	-0.38890537	2882081	1.2236528	1323458	0.57898377	experimental	Microsource	1505222	Deracoxib
2093 M13	X		514	520	-0.1085968	435	440	-0.32201008	2545041	0.96698161	2284500	0.68904985	experimental	Microsource	1503932	Oxyphencyclimine hydrochloride
2093 M14	X		633	640	0.107675123	394	400	-0.38890537	28089037	1.16140257	2284500	0.68904985	experimental	Microsource	2300230	Perphenazine
2093 M15	X		794	800	0.40011968	434	440	-0.32364657	1744538	0.35736242	1760035	0.30929102	experimental	Microsource	1503935	Perphenazine
2093 M16	X		514	520	-0.11219348	514	520	-0.19311429	2780517	1.14630722	2642651	0.94844363	experimental	Microsource	1505244	Citicoline
2093 M17	X		1114	1120	0.98157938	471	480	-0.26327276	2240098	0.73475375	2620200	0.93218558	experimental	Microsource	1503935	Propafenone hydrochloride
2093 M18	X		431	440	-0.25936225	1034	1040	0.65531372	2415361	0.86822444	2491934	0.83930085	experimental	Microsource	1505248	Canrenone
2093 M19	X		714	720	0.25482	632	640	-0.00058639	2616183	1.02115946	2611177	0.92565151	experimental	Microsource	1503968	Tacrolimus
2093 M20	X		554	560	-0.03588374	472	480	-0.26164117	2765042	1.13452231	2740963	1.01963696	experimental	Microsource	1505249	Acpramycin
2093 M21	X		433	440	-0.25572845	1193	1200	0.9147369	2345155	0.8147594	2890611	1.12800561	experimental	Microsource	1503975	Fluconazole
2093 M22	X		720	720	0.2475524	670	720	0.06141411	2324444	0.64885602	7998974	0.77848417	experimental	Microsource	1505261	Telmisartan
2093 M23	E		560	920	-0.02498235	562	840	-0.11479786	91841	-0.90124099	85790	-0.90312532	empty			
2093 M24	P	121207	121800	219.178362	93009	93560	150.721018	2246142	0.73935653	2857243	1.10384194	empty				
2093 N01	N		356	360	-0.39562963	596	600	-0.05932372	2012318	0.56128899	2203915	0.63072986	empty			
2093 N02	E		276	280	-0.54098151	195	200	-0.71359224	77896	-0.91186073	80603	-0.90688152	empty			
2093 N03	X		555	560	-0.03406685	435	440	-0.32201008	2421034	0.87254468	2531792	0.8681643	experimental	Microsource	1505470	Clindamycin palmitate hydrochloride
2093 N04	X		474	480	-0.18123562	595	600	-0.06095531	2151989	0.66765476	2579273	0.9025248	experimental	Microsource	2300205	Levodopa
2093 N05	X		440	440	-0.25391156	394	400	-0.38890537	2643821	1.0420705	10992613	0.62423038	experimental	Microsource	1505474	Felicitinid sodium
2093 N06	X		435	440	-0.25209466	474	480	-0.25674639	2134201	0.65541084	2754695	1.02598108	experimental	Microsource	2300104	Taurine hydrochloride
2093 N07	X		313	320	-0.47375626	432	440	-0.32690486	2602424	1.01068136	2664760	0.96445402	experimental	Microsource	1505480	Ifosfamide
2093 N08	X		315	320	-0.47012247	474	480	-0.25837798	2152138	0.66776823	2422942	0.78933981	experimental	Microsource	2300161	Amoxapine
2093 N09	X		275	280	-0.54279841	554	560	-0.1278506	2731265	1.1087996	2699916	0.98991248	experimental	Microsource	1505482	Nelmiclin sulfate
2093 N10	X		387	400	-0.33930578	501	520	-0.21432499	2104774	0.63169841	2274081	0.68154106	experimental	Microsource	2300165	Amiodarone hydrochloride
2093 N11	X		3274	3280	4.90607998	4914	4920	0.98589195	1948791	0.51291031	1926048	0.42951051	experimental	Microsource	1505483	Doxorubicin
2093 N12	X		706	720	0.24028482	670	720	0.34322078	2127304	0.64885602	7998974	0.77848417	experimental	Microsource	2300206	Diazoxide
2093 N13	X		593	600	0.03497529	315	320	-0.51780116	2692760	1.08290326	2814602	0.7296329	experimental	Microsource	1505492	Methysergide maleate
2093 N14	X		474	480	-0.18123562	434	440	-0.32364167	2486673	0.741284	2191190	0.62151496	experimental	Microsource	2300214	Diltiazem hydrochloride
2093 N15	X		274	280	-0.5446153	635	640	0.00430838	2153778	0.66901717	2548761	0.88045252	experimental	Microsource	1505498	Acepromazine maleate
2093 N16	X		435	440	-0.25209466	593	600	-0.0642185	2075058	0.60906833	2848435	1.09746357	experimental	Microsource	2300219	Ederophonium chloride
2093 N17	X		472	480	-0.18486941	594	600	-0.0625869	2582989	0.99588073	2626303	0.93660511	experimental	Microsource	1505514	Biperiden
2093 N18	X		594	600	0.03679219	390	400	-0.39543174	2277203	0.76301088	2821198	1.0777397	experimental	Microsource	2300176	Phenoxybenzamine hydrochloride
2093 N19	X		632	640	0.10583433	834	840	0.32899526	2700206	1.08514677	2871319	1.11403518	experimental	Microsource	1505530	Dexchlorpheniramine maleate
2093 N20	X		593	600	0.03497529	593	600	-0.0642185	2141141	0.65939352	2958126	1.17689708	experimental	Microsource	2300242	Loxapine succinate
2093 N21	X		553	560	-0.03770064	511	520	-0.19809007	2360047	0.82610033	2436417	0.79909782	experimental	Microsource	1505532	Diloxanate furoate
2093 N22	X		832	840	0.46921402	592	600	-0.06585009	2055490	0.59416642	2201714	0.62913599	experimental	Microsource	2300212	Domperidone
2093 N23	E		613	920	0.07131326	715	1000	0.13483577	78270	-0.91157592	80996	-0.90659693	empty			
2093 N24	P	102702	103440	185.556657	95206	95800	154.305626	2184157	0.69215215	2292676	0.69500676	empty				
2093 O01	N		557	560	-0.03043305	514	520	-0.19311429	2037456	0.58043271	1908245	0.41661834	empty			
2093 O02	E		196	200	-0.6863338	275	280	-0.58036485	75883	-0.91393372	79752	-0.90749778	empty			
2093 O03	X		395	400	-0.32477059	716	720	0.13646736	2486174	0.92215173	2067764	0.53213515	experimental	Microsource	1503977	Lovastatin
2093 O04	X		554	560	-0.03588374	311	320	-0.52437253	2103677	0.63086299	1621266	0.20880047	experimental	Microsource	1505262	Sertraline hydrochloride
2093 O05	X		434	440	-0.25391156	394	400	-0.38890537	2358459	0.82489099	2386837	0.76319411	experimental	Microsource	1503978	Hydroxychloroquine sulfate
2093 O06	X		514	520	-0.1085968	474	480	-0.25837798	2463703	0.90503905	2228305	0.64839205	experimental	Microsource	1505263	Alfuzosin
2093 O07	X		595	600	0.03860909	554	560	-0.1278506	2668049	1.06065776	2572816	0.89787212	experimental	Microsource	1503985	Brompheniramine maleate
2093 O08	X		474	480	-0.18123562	554	560	-0.1278506	2448791	0.89386289	2554432	0.88455922	experimental	Microsource	1505267	Oxapropin
2093 O09	X		515	520	-0.10674278	512	520	-0.19637747	1790964	0.39271792	1996916	0.48083007	experimental	Microsource	1504008	Sirolimus
2093 O10	X		395	400	-0.32477059	634	640	0.00267679	2194707	0.70018645	1982329	0.47070128	experimental	Microsource	1505270	Proparanolol hydrochloride (+/-)
2093 O11	X		360	360	0.41198172	501	520	-0.21432499	1444378	0.66185864	1917635	0.42349187	experimental	Microsource	1504985	Paroxetine hydrochloride

2094 D01	N	436	440	-0.58814244	237	240	-1.6154876	1960093	-1.29036079	2309609	-0.82892723								empty
2094 D02	E	317	320	-1.03696938	277	280	-1.36595531	84195	-7.73235677	85845	-9.71106041								empty
2094 D03	E	435	440	-0.5919141	356	360	-0.87312905	2564495	0.78520795	2702889	0.74190733								empty
2094 D04	E	394	400	-0.74655195	392	400	-0.64855	24455675	0.3771698	276252	0.97210441								empty
2094 D05	E	395	400	-0.7427803	434	440	-0.3865411	7527472	0.65806777	2602371	0.34281598								empty
2094 D06	E	315	320	-1.04451269	675	680	-1.1168909	2709577	1.28343209	2657864	0.56206898								empty
2094 D07	E	432	440	-0.60322906	275	280	-1.37843193	2745199	1.40576112	2845264	1.31057996								empty
2094 D08	E	475	480	-0.4410479	275	280	-1.37843193	2665954	1.13362693	2866681	1.3961235								empty
2094 D09	E	394	400	-0.74655195	315	320	-1.12889964	2789684	1.55852646	2638569	0.48500111								empty
2094 D10	E	435	440	-0.5919141	356	360	-0.87312905	2785065	1.54266441	3126472	2.43377779								empty
2094 D11	E	555	560	-0.1393155	275	280	-1.37843193	2815059	1.6456664	2950841	1.73227442								empty
2094 D12	E	298	320	-1.10863083	275	280	-1.37843193	2700462	1.25213039	2540272	0.11778738								empty
2094 D13	E	1352	1360	2.8666935	395	400	-0.62983508	2501117	0.56756242	2792528	1.09994242								empty
2094 D14	E	513	520	-0.29772501	395	400	-0.62983508	2662340	1.12121615	2806662	1.15639628								empty
2094 D15	E	315	320	-1.04451269	395	440	-0.38030279	2889406	1.90098043	3062005	2.17628442								empty
2094 D16	E	396	400	-0.73900864	395	400	-0.62983508	2856274	1.78720227	2723392	0.82380018								empty
2094 D17	E	355	360	-0.8936465	514	520	0.11252346	2488473	0.52414183	2461079	-0.22392745								empty
2094 D18	E	474	480	-0.44481956	594	600	0.61158803	2386071	0.1724845	2807329	1.15906041								empty
2094 D19	E	634	640	0.15864524	434	440	-0.3865411	2574318	0.81894098	2628018	0.442285842								empty
2094 D20	E	473	480	-0.44859121	514	520	0.11252346	2927409	2.03148602	2803784	1.14490101								empty
2094 D21	E	794	800	0.76211003	474	480	-0.13700882	2283062	-0.18125731	2658101	0.56301556								empty
2094 D22	E	511	520	-0.30526832	712	720	1.34770826	2354358	0.06357932	2570490	0.21380873								empty
2094 D23	E	789	1160	0.74325175	661	1040	1.0295546	88031	-7.71918362	88474	-9.70055969								empty
2094 D24	P	125562	126080	471.343956	127777	128320	794.018197	2178999	-0.53861865	2390209	-0.50699561								empty
2094 E01	N	477	480	-0.43350459	398	400	-0.61112016	2114359	-0.760598	2235787	-1.12378623								empty
2094 E02	X	112	120	-1.79884369	157	157	2.8455116	84031	-7.73291996	85281	-9.71331314								empty
2094 E03	X	475	480	-0.4410479	276	280	-1.37219362	2616331	0.96321466	2704861	0.74893387								experimental
2094 E04	E	835	840	0.91674788	434	440	-0.37406449	2579862	0.83797956	2593952	0.30679239		Microsource	1506082					Pentetic acid
2094 E05	X	394	400	-0.74655195	435	440	-0.38030279	2627065	1.00007874	2879854	1.44873895		Microsource	1506043					Sotalol hydrochloride
2094 E06	E	392	400	-0.75409526	555	560	0.36829405	2581437	0.84338825	2659405	0.56822403								empty
2094 E07	X	1355	1360	2.87800846	435	440	-0.38030279	2564265	0.78441811	2814240	1.18666424		Microsource	1506029					Pepstatin a
2094 E08	E	432	440	-0.60322906	594	600	0.61158803	2450623	0.39416166	2669736	0.60948799								empty
2094 E09	X	595	600	0.01155069	675	680	-1.1168909	2602352	0.91521216	2657609	0.56105046		Microsource	1505420					Diexpanthenol
2094 E10	X	474	480	-0.44481956	674	680	-0.44481956	2407705	0.46454399	2471116	0.29261302								empty
2094 E11	X	554	560	-0.14308716	355	360	-0.87936736	2736390	1.37551025	2832471	1.2594823		Microsource	1601020					Diethyltoluamide
2094 E12	E	433	440	-0.59945741	475	480	-0.13077051	2825892	1.68286786	2523727	0.02630048								empty
2094 E13	X	872	880	1.05629912	675	680	-1.1168909	2508530	0.5930193	2400392	-0.46632279		Microsource	1505202					Amlodipine besylate
2094 E14	E	394	400	-0.74655195	354	360	-0.88560567	2376804	1.04066802	2462233	-0.21931816								empty
2094 E15	X	435	440	-0.5919141	475	480	-0.13077051	2286211	-0.17044337	2656693	0.55739179		Microsource	1503692					Bleomycin (bleomycin b2 shown)
2094 E16	E	395	400	-0.7427803	434	440	-0.3865411	2382118	0.15899056	2531189	0.05610512								empty
2094 E17	X	435	440	-0.5919141	674	680	-1.065226	2287371	1.17694882	2440725	-0.4406057		Microsource	1505022					Propofol
2094 E18	E	595	600	0.01155069	514	520	0.11252346	2652665	0.95268835	2434133	-0.33155487								empty
2094 E19	X	473	480	-0.44859121	475	480	-0.13077051	2474488	0.47611613	2695003	0.71040916		Microsource	1503216					Filipin
2094 E20	E	593	600	0.00400738	514	520	0.11252346	2646383	1.06641843	2449586	-0.26983267								empty
2094 E21	X	592	600	0.00023573	433	440	-0.39277941	2197544	-0.47493352	2661892	0.57815757		Microsource	1900006					Pentobarbital
2094 E22	E	593	600	0.00400738	592	600	0.59911142	2422991	0.29927098	2284444	-0.92944099								empty
2094 E23	E	594	840	0.00777904	687	920	1.19175059	85202	-7.72889865	86803	-9.70723398								empty
2094 E24	P	815206	822000	305.247814	77081	77760	477.769981	2844786	-0.86215424	238706	-0.5050105								empty
2094 F01	N	476	480	-0.43727625	317	320	-1.1642033	2328603	0.21164209	2515657	-0.00593262								empty
2094 F02	E	317	320	-1.03696938	197	200	-1.86501988	87345	-7.7215394	86568	-9.70817261								empty
2094 F03	E	355	360	-0.8936465	276	280	-1.37219362	2584667	0.85448035	2649345	0.52804249								empty
2094 F04	E	434	440	-0.59568575	395	400	-0.62983508	2880220	1.86943491	2959173	1.765554								empty
2094 F05	E	434	440	-0.59568575	396	400	-0.62359677	2809674	1.62717384	2719729	0.80916947								empty
2094 F06	E	834	840	0.91297623	275	280	-1.37843193	2808071	1.621669	2957884	1.76040549								empty
2094 F07	E	351	360	-0.90873312	435	440	-0.38030279	2818085	1.65605795	2709695	0.76099178								empty
2094 F08	E	355	360	-0.8936465	555	560	0.36829405	2840012	1.73135716	2851181	1.33421357								empty
2094 F09	E	434	440	-0.59568575	314	320	-1.13513795	2501490	0.56884333	2597571	0.32124736								empty
2094 F10	E	434	440	-0.59568575	395	400	-0.62983508	3224011	0.05004294	2891916	1.49691685								empty
2094 F11	E	554	560	-0.14308716	475	480	-0.13077051	2757750	1.44886234	2734630	0.86868688								empty
2094 F12	E	554	560	-0.14308716	355	360	-0.87936736	3210789	3.00463745	2928627	1.64354751								empty
2094 F13	E	473	480	-0.44859121	513	520	0.10628516	2722465	1.3276906	2454673	-0.24951423								empty
2094 F14	E	314	320	-1.04828435	434	440	-0.3865411	2863855	1.81323608	2718666	0.80492365								empty
2094 F15	E	474	480	-0.4410479	595	600	0.61782634	2468845	0.45673758	2490725	-0.10551573								empty
2094 F16	E	435	440	-0.5919141	394	400	-0.6307338	3096559	2.61236175	2613925	0.38856832								empty
2094 F17	E	435	440	-0.5919141	635	640	0.86735862	2439918	0.35739976	2467196	-0.199495								empty
2094 F18	E	354	360	-0.89741815	314	320	-1.13513795	2458645	0.4217099	2413674	-0.41327197								empty
2094 F19	E	474	480	-0.44481956	354	360	-0.88560567	2403191	0.23127607	2489988	-0.10845945								empty
2094 F20	E	713	720	0.45660598	674	680	1.11065226	2640310	1.04556322	2785580	1.07219079								empty
2094 F21	E	673	680	0.30573978	673	680	1.10441429	2315537	-0.06973535	2664834	0.58990848								empty
2094 F22	E	600	600	0.00023573	582	582	0.34957913	2430444	0.32486522	2436380	-0.32425792								empty
2094 F23	E	605	920	0.04928724	607	920	0.69286802	87280	-7.72176262	87279	-9.70532275								empty
2094 F24	P	105912																	

2094 K13	X	1074	1080	1.81817342	315	320	-1.12889964	2832321	1.7049456	2858564	1.36370267	experimental	Microsource	1501196	Flumethasone
2094 K14	E	433	440	-0.59945741	635	640	0.86735862	2278009	-0.19860975	2534434	0.06906626	empty			
2094 K15	X	394	400	-0.7465195	314	320	-1.13513795	2369416	0.11528979	2399700	-0.46908677	experimental	Microsource	1500261	Disopyramide phosphate
2094 K16	E	594	600	0.00777904	554	560	0.36205575	2787144	1.54980388	2602098	0.33932905	empty			
2094 K17	X	433	440	-0.59945741	393	400	-0.64231169	2942043	0.08174040	2632524	2.2223488	experimental	Microsource	1505434	Halothane
2094 K18	E	435	440	-0.5919141	674	680	-1.1106526	2452824	0.40172008	2613011	0.38291763	empty			
2094 K19	X	433	440	-0.59945741	713	720	1.35394657	2636795	1.03349241	2990343	1.89005287	experimental	Microsource	1300030	Omega-3-acid esters (epa shown)
2094 K20	E	473	480	-0.44859121	553	560	0.35581744	2407006	0.24437711	2391653	-0.501228	empty			
2094 K21	X	794	800	0.76211003	509	520	0.08133193	2730445	1.35509461	2444217	-0.29127747	experimental	Microsource	1300028	Mannitol
2094 K22	E	694	600	-0.00353593	592	600	0.59911142	2260795	-0.25772411	2501151	-0.06387232	empty			
2094 K23	E	684	960	0.34722798	696	960	1.24789535	87663	-7.72044736	87706	-9.70362723	empty			
2094 K24	P	92098	92640	345.125294	88350	88840	548.060464	2207168	-0.44188387	2639415	-0.44406317	empty			
2094 L01	N	357	360	-0.88610319	316	320	-1.12266134	2319488	-0.05616728	2457033	-0.24008794	empty			
2094 L02	E	236	240	-1.34247344	317	320	-1.11642303	78284	-7.75265566	83845	-9.71904879	empty			
2094 L03	E	355	360	-0.8936465	396	400	-0.62359677	2329670	-0.02120141	2545965	0.11512325	empty			
2094 L04	E	395	400	-0.7427803	396	400	-0.62359677	2934081	2.05439824	2732191	0.85894505	empty			
2094 L05	E	475	480	-0.4410479	395	360	-0.87936736	2472096	0.46790179	2690549	0.69261904	empty			
2094 L06	E	475	480	-0.4410479	355	400	-0.62983508	2959793	2.14269547	2780104	1.05031862	empty			
2094 L07	E	475	480	-0.4410479	356	360	-0.87312905	2423058	0.32010558	2639411	0.48836422	empty			
2094 L08	E	515	520	-0.2901817	316	320	-1.12266134	2889804	1.90234719	3072168	2.21687736	empty			
2094 L09	E	395	400	-0.7427803	355	360	-0.87936736	2532414	0.67503902	2508175	-0.03581714	empty			
2094 L10	E	474	480	-0.44481956	436	440	-0.37406449	3073580	2.53344987	2944195	1.70572904	empty			
2094 L11	E	634	640	0.15864524	394	400	-0.63607338	2472884	0.47060785	2947640	1.71948902	empty			
2094 L12	E	473	480	-0.44859121	436	440	-0.37406449	2717000	1.30892331	2905488	1.55112598	empty			
2094 L13	E	433	440	-0.59945741	355	360	-0.87936736	2267602	-0.23434829	2234684	-1.12819182	empty			
2094 L14	E	440	440	0.5919141	594	440	0.61150896	2964880	2.16105468	2431191	1.29431403	empty			
2094 L15	E	515	520	-0.2901817	395	400	-0.62983508	2454750	0.40833413	2574361	0.22854284	empty			
2094 L16	E	513	520	-0.29772501	514	520	0.11252346	2837812	1.72380217	2647291	0.51983842	empty			
2094 L17	E	674	680	0.30951143	554	560	0.36205575	2444136	0.37188474	2528186	0.04411057	empty			
2094 L18	E	393	400	-0.75032361	433	440	-0.39277941	2540550	0.70297875	2713083	0.78262409	empty			
2094 L19	E	914	920	1.21470862	512	520	0.10004685	2341642	0.10911148	2342548	-0.69736264	empty			
2094 L20	E	713	720	0.45660598	510	520	0.08757024	2488441	0.52403194	2847884	1.32104473	empty			
2094 L21	E	552	560	-0.15063047	1594	1600	6.8498951	2531401	0.67156029	2364798	-0.60849194	empty			
2094 L22	E	629	600	0.00023573	629	600	0.09819964	2684574	0.3684028	2846044	0.5852848	empty			
2094 L23	E	728	1000	0.5131808	706	1000	1.31027842	84312	-7.73195498	85031	-9.71431168	empty			
2094 L24	P	90979	91520	340.908812	98530	99080	611.56643	2180640	-0.53298332	2420361	-0.38656283	empty			
2094 M01	N	437	440	-0.58437079	477	480	-0.1182939	2118234	-0.74729092	2247510	-1.07696236	empty			
2094 M02	E	196	200	-1.49333963	236	240	-1.6217259	82695	-7.7375079	85426	-9.71273398	empty			
2094 M03	X	476	480	-0.43727625	275	280	-1.37843193	2071101	-0.90914972	2440265	-0.3070625	experimental	Microsource	1505426	Ethoxzolamide
2094 M04	E	435	440	-0.5919141	356	360	-0.87312905	2332436	-0.01170272	2677193	0.63927266	empty			
2094 M05	X	435	440	-0.5919141	595	600	0.37453236	2393013	0.19632393	2560620	0.17365809	experimental	Microsource	1504231	Clarithromycin
2094 M06	E	435	440	-0.5919141	394	560	0.36829405	2053364	0.10467031	2837174	1.27826697	empty			
2094 M07	X	355	360	-0.8936465	394	400	-0.63607338	2357283	0.07362402	2628436	0.44452799	experimental	Microsource	1500368	Lincomycin hydrochloride
2094 M08	E	355	360	-0.8936465	395	400	-0.62983508	2648535	1.07380858	2623451	0.42461696	empty			
2094 M09	X	554	560	-0.14308716	596	600	0.62406464	2070673	-0.91061951	2370811	-0.58447489	experimental	Microsource	1503373	Oxibendazole
2094 M10	E	554	560	-0.14308716	354	360	-0.88560567	2413221	0.26571995	2571069	0.21539337	empty			
2094 M11	X	273	280	-1.2029222	475	480	-0.13077051	1929493	-1.39544384	1996349	-2.0801468	experimental	Microsource	1503679	Azithromycin
2094 M12	E	594	600	0.01155086	315	320	-1.12889964	2559532	0.76164558	2378386	0.55114048	empty			
2094 M13	X	434	440	-0.59568575	395	400	-0.62983508	2274146	-0.30459598	2271001	-0.98313487	experimental	Microsource	1505447	Octodrine
2094 M14	E	395	400	-0.7427803	635	640	0.86735862	2500059	0.56392916	2448485	-0.27423027	empty			
2094 M15	X	514	520	-0.29395336	394	400	-0.63607338	1895739	-1.51135799	2225367	-1.16540568	empty			
2094 M16	E	674	680	0.30951143	673	680	1.10441429	2477083	0.48502758	2522756	0.02242213	empty			
2094 M17	X	633	640	0.15487358	553	560	0.35581744	1912396	-1.45415641	2421428	-0.38230103	experimental	Microsource	1505265	Telithromycin
2094 M18	E	394	400	-0.7465195	713	720	1.35394657	2206617	-0.44377605	2573435	0.22484362	empty			
2094 M19	X	434	440	-0.59568575	953	960	2.85114027	1949547	-1.32657667	2224699	-1.16807328	experimental	Microsource	1300039	Sodium phenylacetate
2094 M20	E	553	560	-0.14685881	672	680	1.09817598	2383845	0.16484023	2662524	0.58068819	empty			
2094 M21	X	673	680	0.30573978	429	440	-0.41773264	1925333	-1.40972964	2407490	-0.43797204	experimental	Microsource	1502036	Vigabatrin
2094 M22	E	632	640	0.15110193	632	640	0.8486437	2388588	0.1811281	2409723	-0.42905301	empty			
2094 M23	E	682	960	0.33968467	702	1000	1.28532519	84112	-7.7326418	87475	-9.70454988	empty			
2094 M24	P	92616	93200	347.083011	99534	100160	617.82969	1926643	-1.40523098	2279887	-0.94764251	empty			
2094 N01	N	397	400	-0.73523699	476	480	-0.1245322	1885794	-1.54550998	2078705	-1.75120139	empty			
2094 N02	E	237	240	-1.33870178	275	280	-1.37843193	79803	-7.74743928	79828	-9.73509345	empty			
2094 N03	E	315	320	-1.04451269	556	560	0.37453236	2393013	0.19632393	2560620	0.17365809	empty			
2094 N04	E	435	440	-0.5919141	394	400	-0.63607338	2234148	-0.34923222	2348861	-0.67214733	empty			
2094 N05	E	435	440	-0.5919141	595	600	0.61782634	2722037	1.32622081	2689811	0.68967133	empty			
2094 N06	E	395	400	-0.7427803	593	600	0.60534972	2210642	-0.42995385	2499481	-0.07054262	empty			
2094 N07	E	435	440	-0.5919141	714	720	1.36018488	2481636	0.50066298	2521108	0.0158397	empty			
2094 N08	E	434	440	-0.59568575	474	480	-0.13700882	2239028	-0.33247388	2550771	0.13431932	empty			
2094 N09	E	589	600	-0.01107924	394	400	-0.63607338	2495213	0.52478757	2474240	-0.17135994	empty			
2094 N10	E	574	600	0.30951143	574	580	1.11876177	2245094	-0.31164271	2433381	-0.39047114	empty			
2094 N11	E	473	480	-0.44859121	514	520	0.11252346	2555942	0.70545973	2663558	0.58481189	empty			
2094 N12	E	634	640	0.15864524	435	440	-0.38030279	2203292	-0.45519439	2241393	-1.10139481	empty			
2094 N13	E	634	640	0.15864524	515	520	0.11876177	2214335	-0.41727177	2512611	-0.01809892	empty			
2094 N14	E	434	440	-0.59568575	393	400	-0.64231169	2104296	-0.79515522	2364154	-0.6110642	empty			
2094 N15	E	355	360	-0.8936465	473	480	-0.14324713	2238384	-0.33648543	2440693	-0.30535299	empty			
2094 N16	E	434	440	-0.59568575	953	960	2.85114027	2131121	-0.70303585	2229320	-1.14961665	empty			
2094 N17	E	554	560	-0.14308716	593	600	0.60534972	2482027	0.50200571	2502906	-0.05868252	empty			
2094 N18	E	475	480	-0.4410479	473	480	-0.14324713	2011723	-1.1305589	240427	-1.1305589	empty			

2094 007	X	514	520	-0.29395336	434	440	-0.3865411	2107642	-0.78366476	2397762	-0.4768275	experimental	Microsource	1504183	Trifluridine
2094 008	E	750	760	0.59615721	395	400	-0.62983508	2152214	-0.63060066	2490809	-0.10518022	empty			
2094 009	X	1993	2000	5.28432432	475	480	-0.13077051	2065748	-0.92753238	2194408	-1.28906177	experimental	Microsource	1503938	Ribavirin
2094 010	X	548	560	-0.16571709	434	440	-0.3865411	2095781	-0.82439646	2425311	-0.3667916	empty			
2094 011	X	835	840	0.91674788	635	640	0.86735862	2144914	-0.6556694	2503625	-0.0839907	experimental	Microsource	1505705	Fludarabine phosphate
2094 012	E	473	480	-0.44859121	474	480	-0.13700882	1972873	-1.24647317	2180920	-1.34293539	empty			
2094 013	X	632	640	0.15110193	513	520	0.10628516	1976068	-1.23550126	2251314	-1.06176846	experimental	Microsource	1504263	Rosiglitazone
2094 014	E	714	720	0.46037763	814	880	2.35831401	2047359	-0.9906818	2316723	-0.80051257	empty			
2094 015	X	433	440	-0.59945741	573	520	0.10628516	1972674	-1.24715655	2400754	-0.46487689	experimental	Microsource	1505684	Rolitetracycline
2094 016	E	394	400	-0.74655195	553	560	0.35581744	2010187	-1.11833366	2467901	-0.1966791	empty			
2094 017	X	514	520	-0.29395336	434	440	-0.3865411	2306957	-0.09919981	2519323	0.00871008	experimental	Microsource	1505703	Altrenogest
2094 018	E	434	440	-0.59568575	554	560	0.36205575	2279155	-0.19467429	2791712	0.73728605	empty			
2094 019	X	594	600	0.00777904	634	640	0.86112031	2167943	-0.57658591	2359552	-0.62944546	experimental	Microsource	1505704	Bisoprolol fumarate
2094 020	E	474	480	-0.44481956	552	560	0.34957913	2103629	-0.79744575	2372816	-0.57646654	empty			
2094 021	X	513	520	-0.29772501	632	640	0.8486437	2063197	-0.93629274	2433670	-0.33340417	experimental	Microsource	1503432	Mepartricin
2094 022	E	591	600	-0.00353593	551	560	0.34334083	1948787	-1.32918657	2287972	-0.91534949	empty			
2094 023	E	834	1200	0.91297623	697	1120	1.25413366	77961	-7.75376487	82248	-9.72542751	empty			
2094 024	P	121232	122960	458.407179	142406	143240	885.278391	1914603	-1.44657739	2244785	-1.08784652	empty			
2094 P01	N	558	560	-0.12800054	758	760	1.63467039	1445369	-3.05796753	1708434	-3.23013366	empty			
2094 P02	E	237	240	-1.33870178	315	320	-1.12889964	73515	-7.76903282	75780	-9.75126192	empty			
2094 P03	E	396	400	-0.73900864	556	560	0.37453236	1908186	-1.46861392	2062126	-1.81742105	empty			
2094 P04	E	475	480	-0.4410479	476	480	-0.1245322	2070446	-0.91139904	2284263	-0.93016394	empty			
2094 P05	E	755	760	0.61501549	396	400	-0.62359677	1994058	-1.17372204	2152705	-1.45563142	empty			
2094 P06	E	555	560	-0.1393155	476	480	-0.1245322	2230951	-0.36021099	2213344	-1.21342781	empty			
2094 P07	E	475	480	-0.4410479	436	460	-0.37406449	2080442	-0.87707192	2075957	-1.76217742	empty			
2094 P08	E	635	640	0.91674788	476	480	-0.1245322	2254608	-0.27897081	2519323	-0.79784545	empty			
2094 P09	E	471	480	-0.45613452	636	640	0.87359693	2167320	-0.57882535	2241207	-1.0213773	empty			
2094 P10	E	596	600	0.01532235	516	520	0.12500008	2253452	-0.28294061	2250766	-1.06395728	empty			
2094 P11	E	355	360	-0.8936465	396	400	-0.62359677	1971532	-1.25107828	2283540	-0.93305173	empty			
2094 P12	E	434	440	-0.59568575	356	360	-0.87312905	1769895	-1.94351717	2098627	-1.67162916	empty			
2094 P13	E	1075	1080	1.82194507	516	520	0.12500008	1967675	-1.26432355	2065146	-1.80535886	empty			
2094 P14	E	552	560	-0.15063047	555	560	0.36829405	2058646	-0.95192127	2156045	-1.44229083	empty			
2094 P15	E	955	960	1.36934648	475	480	-0.13077051	1931676	-1.38794723	2087775	-1.71494741	empty			
2094 P16	E	1640	1640	2.01429948	820	820	72.44543	72.2578	-7.72725055	1774742	-1.4649577	empty			
2094 P17	E	595	600	0.01155069	435	440	-0.38030279	2015967	-1.09848464	2137919	-1.5146895	empty			
2094 P18	E	555	560	-0.1393155	676	680	1.12312921	1947743	-1.33277176	2172932	-1.37484097	empty			
2094 P19	E	635	640	0.16241689	515	520	0.11876177	2106786	-0.78660434	2160201	-1.42569098	empty			
2094 P20	E	435	440	-0.5919141	475	480	-0.13077051	1978735	-1.22634255	2321854	-0.78001839	empty			
2094 P21	E	755	760	0.61501549	755	760	1.61595547	1941425	-1.35446832	2210388	-1.22523463	empty			
2094 P22	E	791	800	0.75079506	712	720	1.34770826	1873897	-1.58636531	2329654	-0.74886371	empty			
2094 P23	P	175319	175680	659.010191	170541	170960	1060.793116	1681626	-2.24664655	1736780	-3.11691438	empty			
2095 A01	N	477	480	-0.0555226	558	560	-0.21963478	1069816	-0.88746142	1112605	-0.98541242	empty			
2095 A02	E	116	120	-1.97931998	116	120	-2.24355551	74953	-3.00795158	81357	-3.13425676	empty			
2095 A03	X	716	720	1.21812718	796	800	0.87016869	986113	-1.06586929	1003840	-1.21204952	experimental	Prestick	1	Azaguanine-8
2095 A04	X	875	880	2.06545068	675	680	0.31610894	1285512	-0.42771848	1241109	-0.71764454	experimental	Prestick	81	Metronidazole
2095 A05	X	675	680	0.99963496	435	440	-0.78285254	1346631	-0.29744704	1492522	-0.19376725	experimental	Prestick	2	Allantoin
2095 A06	X	440	440	-0.27934391	814	820	0.67785043	1484662	-0.003320972	1810032	0.46695045	experimental	Prestick	82	Cotinine (-)
2095 A07	X	635	640	0.78647181	833	840	0.03959192	1474861	-0.03787867	197576	0.23351033	experimental	Prestick	3	Acetazolamide
2095 A08	X	715	720	1.2127981	993	1000	1.77223291	1594167	0.23016093	1810237	0.46826563	experimental	Prestick	83	Edrophonium chloride
2095 A09	X	555	560	0.36014553	794	800	0.86101068	1415196	-0.1513049	1681780	0.20059568	experimental	Metformin	4	Metformin hydrochloride
2095 A10	X	756	760	1.43129032	755	760	0.68242944	1440639	-0.09707469	1560888	-0.05131084	experimental	Prestick	84	Moroxidine hydrochloride
2095 A11	X	475	480	-0.06618076	475	480	-0.59969229	1371485	-0.24447224	1444196	-0.29446568	experimental	Atracurium	5	Atracurium besylate
2095 A12	X	555	560	0.36014553	475	480	-0.59511328	1592778	0.22720036	1387308	-0.41300502	experimental	Prestick	85	Baclofen (R,S)
2095 A13	X	676	680	1.00496404	356	360	-1.14917303	1470618	-0.03317627	1335015	-0.52196961	experimental	Prestick	6	Isoflupredone acetate
2095 A14	X	514	520	-0.14165333	555	560	-0.23373718	1347372	-0.29586764	1487760	-0.20368998	experimental	Prestick	86	Acyclovir
2095 A15	X	913	920	2.26795566	794	800	0.86101068	1400331	-0.18298875	1813612	0.47529822	experimental	Prestick	7	Amiloride hydrochloride dihydrate
2095 A16	X	513	520	0.13632423	432	440	-0.79658956	1463218	-0.04894892	1897320	0.64972325	experimental	Prestick	87	Diazoxide
2095 A17	X	516	520	0.15231146	834	840	1.04417093	1547668	0.13105114	1708512	0.256298	experimental	Prestick	8	Amprolium hydrochloride
2095 A18	X	436	440	-0.27401483	873	880	1.22275217	1549422	-0.13478968	1803510	0.45424836	experimental	Prestick	88	Acetylpyrine
2095 A19	X	515	520	0.14698238	953	960	1.58907266	1439839	-0.09877984	1975493	0.81261482	experimental	Prestick	9	Hydrochlorothiazide
2095 A20	X	516	520	0.15231146	952	960	-1.58449365	1329018	-0.33498808	2103997	1.08038271	experimental	Prestick	89	Ursolic acid
2095 A21	X	555	560	0.36014553	952	960	1.58449365	1466107	-0.04279119	2001471	0.86574601	experimental	Prestick	10	Sulfaguanidine
2095 A22	X	513	520	0.13632423	1031	1040	1.94623514	1264065	-0.47343146	1927107	0.71179137	experimental	Prestick	90	Pindolol
2095 A23	E	624	1240	0.72785195	597	1400	-0.04105354	78199	-3.00103292	83175	-3.13046854	empty			
2095 A24	P	210934	211360	1121.48637	274635	275280	1254.78064	1118123	-0.78449798	1065755	-1.08303526	empty			
2095 B01	N	757	760	1.4366194	477	480	-0.59053428	1175492	-0.66221944	1264370	-0.66917485	empty			
2095 B02	E	116	120	-1.97931998	117	120	-2.2389765	81016	-2.99502866	83869	-3.12902243	empty			
2095 B03	X	515	520	0.14698238	554	560	-0.2379508	1521798	0.0759108	1548193	-0.07776381	experimental	Prestick	161	Isoniazid
2095 B04	X	474	480	-0.07150984	474	480	-0.24710883	1566279	0.17711367	1597488	0.02495375	experimental	Prestick	58	Penicillietine hydrochloride
2095 B05	X	434	440	-0.28467298	433	440	-0.79201055	1599674	0.24189877	1607502	0.18217549	experimental	Prestick	162	Penflutendazole
2095 B06	X	435	440	-0.27934391	953	960	1.58907266	1540729	0.11626108	1621622	0.07524254	experimental	Prestick	242	Flavoxate hydrochloride
2095 B07	X	435	440	-0.27934391	550	560	-0.25626683	1638933	0.32557695	1745988	0.33438794	experimental	Prestick	163	Chlorzoxazone
2095 B08	X	435	440	-0.27934391	832	840	1.03501291	1425563	-0.12920827	1623304	0.07874737	experimental	Prestick	243	Bufexamac
2095 B09	X	235	240	-1.34515962	471	480	-0.61800832	1563533	0.16486642	2031457	0.92922879	experimental	Prestick	164	Ornidazole
2095 B10	X	435	440	-0.27934391	553	560	-0.24252981	1629446	0.30535598	1779646	0.40452218	experimental	Prestick	244	Glutethimide, para-amino
2095 B11	X	354	360	-0.17109927	534	560	-0.2379508	1848073	0.77134617	2213131	1.30777887	experimental	Prestick	165	Ethosux

2095 C01	N	516	520	0.15231146	317	320	-1.32317527	1291459	-0.41504281	1374978	-0.43869743	empty				
2095 C02	E	77	80	-2.18715404	37	40	-2.60529699	86789	-2.98272386	86038	-3.12450282	empty				
2095 C03	X	436	440	-0.27401483	434	440	-0.78743154	1298869	-0.39924884	1388311	-0.41091504	experimental	Prestwick	11	Metricrane	
2095 C04	X	315	320	-0.91883334	994	1000	-1.77681191	1585460	0.21160249	1554754	-0.06490245	experimental	Prestwick	91	Khellin	
2095 C05	X	395	400	-0.49252705	552	560	-0.24710882	1468288	-0.03814252	1498540	-0.18122735	experimental	Prestwick	12	Benzonate	
2095 C06	X	475	480	-0.06618076	549	560	-0.26084583	1537431	0.10923159	1771848	0.38827324	experimental	Prestwick	92	Zimeldine dihydrochloride monohydrate	
2095 C07	X	354	360	-0.71099927	832	840	1.03501291	1556225	0.14928986	1683550	0.20428388	experimental	Prestwick	13	Hydroflumethiazide	
2095 C08	X	396	400	-0.48717797	711	720	0.48095317	1655223	0.36232981	1728879	0.29873737	experimental	Prestwick	93	Azacyclonol	
2095 C09	X	275	280	-1.13199648	753	760	0.67327143	1590969	0.22334459	1734075	0.30956444	experimental	Prestwick	14	Sulfacetamide sodic hydrate	
2095 C10	X	516	520	0.15231146	553	560	-0.24252981	1606453	0.2563478	1589078	0.00742956	experimental	Prestwick	94	Azathioprine	
2095 C11	X	475	480	-0.06618076	554	560	-0.23795008	1628992	0.30438831	1583669	-0.00384134	experimental	Prestwick	15	Heptaminol hydrochloride	
2095 C12	X	433	440	-0.29000206	632	640	-0.79201055	1728662	0.51562887	1467590	-0.24509374	experimental	Prestwick	95	Lynestrol	
2095 C13	X	435	440	-0.27934391	634	640	0.12836969	1533049	0.09989162	1565810	-0.04105471	experimental	Prestwick	16	Sulfathiazole	
2095 C14	X	434	440	-0.28467298	592	600	-0.06394857	1503013	0.03587171	1483120	-0.2133585	experimental	Prestwick	96	Guanabenz acetate	
2095 C15	X	392	400	-0.50849428	792	800	0.85185267	1602778	0.24851476	1715759	0.2713988	experimental	Prestwick	17	Levodopa	
2095 C16	X	671	680	0.97831864	549	560	-0.26084583	1538549	0.11161454	1928029	0.71371257	experimental	Prestwick	97	Dulifiram	
2095 C17	X	674	680	0.99430588	753	680	0.30695093	1633298	0.31356629	1704312	0.24754633	experimental	Prestwick	18	Iodouridine	
2095 C18	X	594	600	0.56797959	673	760	0.67327143	1765874	0.59614399	1932675	0.72339359	experimental	Prestwick	98	Acetylsalicylic acid	
2095 C19	X	274	280	-1.13732556	632	640	0.11921168	1552718	0.14181449	1943245	0.74541864	experimental	Prestwick	19	Captopril	
2095 C20	X	396	400	-0.48717797	712	720	0.48553217	1802800	0.67484952	2117902	1.109357	experimental	Prestwick	99	Mianserin hydrochloride	
2095 C21	X	511	520	0.12566607	550	560	-0.25626683	1629926	0.30637907	1688734	0.21508595	experimental	Prestwick	20	Minoxidil	
2095 C22	X	1193	1200	3.76009767	1391	1400	3.59467736	1614260	0.27298794	1703963	0.2468191	W	experimental	Prestwick	100	Nocodazole
2095 C23	E	336	760	-0.80692269	552	1080	-0.24710882	85328	-2.98583789	89503	-3.11728268	empty				
2095 C24	P	142600	757	329115	177846	178960	811.583212	1394744	-0.1948971	1504340	-0.16977933	empty				
2095 D01	N	397	400	-0.48184889	637	640	0.14210671	1060048	-0.90828132	1381059	-0.42602626	empty				
2095 D02	E	77	80	-2.18715404	37	40	-2.42671572	86789	-2.98272386	86038	-3.12450282	empty				
2095 D03	X	396	400	-0.48717797	476	480	-0.59511328	1658841	0.36800964	1786368	-0.1852903	experimental	Prestwick	171	Tranexamic acid	
2095 D04	X	396	400	-0.48717797	553	360	-1.15833104	1491162	0.01061202	1479979	-0.2199035	experimental	Prestwick	251	Chlorothiazide	
2095 D05	X	315	320	-0.91883334	632	640	0.11921168	1912127	0.90787339	1861575	0.57561949	experimental	Prestwick	172	Etofylline	
2095 D06	X	354	360	-0.71099927	1512	1520	4.14873711	1481761	-0.00942564	1531713	-0.11210372	experimental	Prestwick	252	Diphenidol hydrochloride	
2095 D07	X	876	880	2.07077976	990	1000	1.75849589	1630051	0.3066455	1683699	0.20459436	experimental	Prestwick	173	Tranlycypromine hydrochloride	
2095 D08	X	354	360	-0.71099927	512	520	-0.43026906	1600705	0.24409628	1683275	0.20371086	experimental	Prestwick	253	Norethindrone	
2095 D09	X	476	480	-0.06085168	514	520	-0.42111105	1829179	0.73107476	1889753	0.63395565	experimental	Prestwick	174	Alverine citrate salt	
2095 D10	X	274	280	-1.13732556	632	640	0.11921168	1552718	0.14181449	1943245	0.74541864	experimental	Prestwick	254	Proprietyline hydrochloride	
2095 D11	X	434	440	-0.28467298	514	520	-0.42111105	1765088	0.59446868	2043412	0.95413981	experimental	Prestwick	175	Acedofenac	
2095 D12	X	834	840	1.84695846	714	720	0.49469018	1832084	0.73726659	1669190	0.17436149	experimental	Prestwick	255	Niflumic acid	
2095 D13	X	433	440	-0.29000206	472	480	-0.61342931	2012906	1.12267772	1496171	-0.18616371	experimental	Prestwick	176	Iproniazide phosphate	
2095 D14	X	875	880	2.06545068	834	840	1.04417093	1543163	0.121449	1717573	0.27517869	experimental	Prestwick	256	Isotretinoin	
2095 D15	X	433	440	-0.29000206	551	560	-0.25168782	1781415	0.62926869	2021518	0.90851858	experimental	Prestwick	177	Sulfamethoxazole	
2095 D16	X	755	760	1.42596125	1034	1040	1.95997216	1929209	0.94389898	1624424	0.08108115	experimental	Prestwick	257	Retinoic acid	
2095 D17	X	354	360	-0.72161042	592	600	-0.05394857	1708727	0.47647007	1708727	0.47647007	experimental	Prestwick	178	Mephlofenacin	
2095 D18	X	714	720	0.74699202	593	600	-0.05936956	1515869	0.20532735	1507414	-0.16273632	experimental	Prestwick	258	Antizoline hydrochloride	
2095 D19	X	515	520	0.14698238	433	440	-0.79201055	1741446	0.54407719	1833698	0.51715206	experimental	Prestwick	179	Phenformin hydrochloride	
2095 D20	X	314	320	-0.92416242	472	480	-0.61342931	1546718	0.12902627	1540558	-0.09367311	experimental	Prestwick	259	Ethacrynic acid	
2095 D21	X	674	680	0.99430588	793	800	0.85643167	1597786	0.23787461	1827193	0.50359738	experimental	Prestwick	180	Flutamide	
2095 D22	X	630	640	0.75982642	588	600	-0.08226459	1531459	0.09650263	1579770	-0.01196581	experimental	Prestwick	260	Praziquantel	
2095 D23	E	419	880	-0.36460916	482	960	-0.56763925	87281	-2.98167519	91495	-3.11313189	empty				
2095 D24	E	156591	157360	831.888253	161487	162560	736.675252	1482139	-0.00086195	1658860	-3.12580424	empty				
2095 E01	N	675	680	-0.06618076	677	680	0.32526696	1342027	-0.30786019	1435483	-0.32621213	empty				
2095 E02	E	157	160	-1.76082776	76	80	-2.42671575	92131	-2.97133771	94425	-3.10702656	empty				
2095 E03	X	356	360	-0.70034111	396	400	-0.96143378	1394852	-0.1946669	1263812	-0.67033757	experimental	Prestwick	21	Sulfaphenazole	
2095 E04	X	475	480	-0.06618076	355	360	-1.14917303	1266688	-0.46784069	999068	-1.22199309	experimental	Prestwick	101	R(-) Apomorphine hydrochloride hemihydrate	
2095 E05	X	396	400	-0.48717797	394	400	-0.97059179	1548762	0.13338293	1525810	-0.12440398	experimental	Prestwick	22	Panthenol (D)	
2095 E06	X	276	280	-1.1266674	511	520	-0.43484807	1312411	-0.37038489	1480965	-0.21784894	experimental	Prestwick	102	Amoxapine	
2095 E07	X	395	400	-0.49250705	473	480	-0.6088503	1519615	0.07125787	1888622	0.62805561	experimental	Prestwick	253	Sulfadiazine	
2095 E08	X	276	280	-1.1266674	395	400	-0.96501278	1387656	-0.21000474	1627665	0.08783453	experimental	Prestwick	103	Cyproheptadine hydrochloride	
2095 E09	X	395	400	-0.49250705	474	480	-0.6042713	1514009	0.05930902	1509887	-0.15758325	experimental	Prestwick	24	Norethynodrel	
2095 E10	X	355	360	-0.70567019	475	480	-0.59969229	1529048	0.09136373	1495476	-0.18761191	experimental	Prestwick	104	Fenpropion	
2095 E11	X	475	480	-0.06618076	354	360	-1.15375204	1827285	0.72703701	1519471	-0.13761276	experimental	Prestwick	25	Thiamphenicol	
2095 E12	X	674	680	0.99430588	474	480	-0.6042713	1576711	0.19295453	1268809	-0.65992516	experimental	Prestwick	105	Danzol	
2095 E13	X	354	360	-0.71099927	474	480	-0.6042713	1695164	0.44542991	1264050	-0.66984164	experimental	Prestwick	26	Cimetidine	
2095 E14	X	475	480	-0.06618076	474	480	-0.6042713	1627708	0.30165154	1264161	-0.66961035	experimental	Prestwick	106_2009	Nicorandil	
2095 E15	X	316	320	-0.91350426	316	480	-0.59969229	1657895	0.3659933	1506466	-0.16471169	experimental	Prestwick	27	Doxylamine succinate	
2095 E16	X	194	200	-1.56365185	353	360	-1.15833104	812232	-1.4364861	841594	-1.55012668	experimental	Prestwick	107_2009	Tomatine	
2095 E17	X	475	480	-0.06618076	594	600	-0.05479056	1971762	1.03498178	1606287	0.04328851	experimental	Prestwick	28	Ethambutol dihydrochloride	
2095 E18	X	554	560	0.35481645	633	640	0.12379068	1879696	0.83874868	1783284	0.4121028	experimental	Prestwick	108	Nomifensine maleate	
2095 E19	X	474	480	-0.07150984	673	680	0.30695093	1713165	0.48379795	1837063	0.52416382	experimental	Prestwick	29	Antipyrene	
2095 E20	X	433	440	-0.29000206	712	720	0.48553217	1827923	0.72839767	2086805	1.04455919	experimental	Prestwick	30	Dizocilpine maleate	
2095 E21	X	633	640	0.77581366	912	920	1.40133341	1612297	0.26880393	2005567	0.87628098	experimental	Prestwick	109	Antipyrene, 4-hydroxy	
2095 E22	X	632	640	0.77048458	870	880	1.20901515	1519354	0.07112785	2053330	0.98105746	experimental	Prestwick	110	Acenocoumarol	
2095 E23	X	603	600	-1.302527	400	960	-0.94311275	89070	-2.97786205	99804	-3.09581816	empty				
2095 E24	P	120409	121160	639.071532	189616	190560	865.478114	2266807	1.6638523	1563798	-0.04524718	empty				
2095 F01	N	997	1000	2.71559827	436	440	-0.77827353	1111255	-0.79913671	1548458	-0.07721162	empty				
2095 F02	E	75	80	-2.1978122	77	80	-2.42213675	87729	-2.98072031	85105	-3.12644694	empty				
2095 F03	X	316	320	-0.91350426	316	320	-1.327									

2095 F19	X		593	600	0.56265051	712	720	0.48553217	1596053	0.23418083	1864795	0.58194987	experimental					
2095 F20	X		833	840	1.84162938	512	520	-0.43026906	1156069	-0.70361838	1280867	-0.63479952	experimental	Prestwick	189		Aminopurine, 6-benzyl	
2095 F21	X		511	520	0.12566607	510	520	-0.43942707	1607777	0.25916982	1821835	0.49243275	experimental	Prestwick	269		Clomipramine hydrochloride	
2095 F22	X		713	720	1.20213994	830	840	0.10258549	962091	-1.11707073	1067345	-1.07972213	experimental	Prestwick	270		Tolbutamide	
2095 F23	E		300	600	-0.99876952	521	1000	-0.38958801	88902	-0.97822013	867007	-3.1211088	empty				Fendiline hydrochloride	
2095 F24	P	100855	101600	534.866729	161449	162600	736.501247	1493583	0.01577224	1698611	0.23566697		empty					
2095 G01	N		395	400	-0.49250705	558	560	-0.21963478	1325965	-0.34149536	1487145	-0.20497148	empty					
2095 G02	E		117	120	-1.9739909	36	40	-2.609876	86105	-2.98418176	94253	-3.10738496	empty					
2095 G03	X		397	400	-0.48184889	516	520	-0.41195304	1374529	-0.23798414	1241677	-0.71646098	experimental	Prestwick	31		Chloramphenicol	
2095 G04	X		355	360	-0.70567019	514	520	-0.42111105	1558549	0.15424333	1518264	-0.14012783	experimental	Prestwick	311		Naloxone hydrochloride	
2095 G05	X		475	480	-0.06618076	553	560	-0.24252981	1396312	-0.18729212	1488988	-0.20113116	experimental	Prestwick	322		Epirizole	
2095 G06	X		475	480	-0.06618076	553	560	-0.06618076	122733117	1583662	0.20777916	1567402	0.54964577	experimental	Prestwick	312		Metolazone
2095 G07	X		275	280	-1.13199648	434	440	-0.78743154	1481486	-0.01001178	1618513	0.06876421	experimental	Prestwick	33		Diprophylline	
2095 G08	X		355	360	-0.70567019	435	440	-0.78285254	1780999	0.62838201	1936741	0.73186605	experimental	Prestwick	113		Ciprofloxacin hydrochloride	
2095 G09	X		634	640	0.78114274	514	520	-0.42111105	7341970	12.4812545	7456374	12.2333014	experimental	Prestwick	34		Triamterene	
2095 G10	X		434	440	-0.28467298	394	400	-0.97059179	1571461	0.18176447	1457166	-0.26743968	experimental	Prestwick	114		Ampicillin trihydrate	
2095 G11	X		355	360	-0.70567019	315	320	-1.33233328	1450226	-0.07664058	1371547	-0.44584672	experimental	Prestwick	35		Dapsone	
2095 G12	X		316	320	-0.91350426	355	360	-1.14917303	1384050	-0.21769071	1393849	-0.39937533	experimental	Prestwick	115		Haloperidol	
2095 G13	X		435	440	-0.27934391	515	520	-0.41653204	1333024	-0.32644953	1341462	-0.50853579	experimental	Prestwick	36		Troisandamycin	
2095 G14	X		355	360	-0.70567019	394	400	-0.97059179	1361086	-0.26663708	1304207	-0.58616522	experimental	Prestwick	116		Nalrexone hydrochloride dihydrate	
2095 G15	X		515	520	0.14698238	515	520	-0.41653204	1303457	-0.3894698	1330362	-0.53166521	experimental	Prestwick	37		Pyrimethamine	
2095 G16	X		475	480	-0.06618076	474	480	-0.6042713	1584970	0.21055809	1636432	0.1061026	experimental	Prestwick	117		Chlorpheniramine maleate	
2095 G17	X		313	320	-0.92949149	474	480	-0.6042713	1396491	-0.19117347	1500955	-0.17619514	experimental	Prestwick	38		Hexamethonium dibromide dihydrate	
2095 G18	X		675	680	0.99963496	553	560	-0.24252981	1556578	0.15004226	1800478	0.44793049	experimental	Prestwick	118		Nalbufine hydrochloride	
2095 G19	X		713	720	1.20213994	953	960	1.58907266	1637808	0.32317908	1642561	0.1188738	experimental	Prestwick	39		Diflunisal	
2095 G20	X		751	760	1.404646203	874	880	0.476537416	1755541	0.24179646	1572863	0.76294749	experimental	Prestwick	49		Tolazamide monohydrate	
2095 G21	X		1070	1080	3.1104621	1149	1160	2.4865787	879556	-1.07584513	1267043	-0.66360503	experimental	Prestwick	119		Niclosamide	
2095 G22	X		791	800	1.61780808	1029	1040	1.93707713	1658280	0.36681391	1997744	0.85897994	experimental	Prestwick	120		Triamcinolone	
2095 G23	E		402	800	-0.45252035	354	960	-1.15375204	87425	-2.98136826	89949	-3.11635334	empty					
2095 G24	P	134677	135440	715.106825	204941	206040	935.651384	1435888	-0.10720116	1435888	-0.10720116	1573801	-0.02440361	empty				
2095 H01	N		477	480	-0.0555226	317	320	-1.32317527	1290272	-0.41757283	1384523	-0.41880821	empty					
2095 H02	E		117	120	-1.9739909	77	80	-2.42213675	87087	-2.98208869	83116	-3.13059148	empty					
2095 H03	X		396	400	-0.48717797	434	440	-0.78743154	1630971	0.30860664	1710209	0.25983409	experimental	Prestwick	191		Midodrine hydrochloride	
2095 H04	X		395	400	-0.49250705	394	400	-0.97059179	1519891	0.07184705	1697337	0.05017075	experimental	Prestwick	271		Vincamine	
2095 H05	X		395	400	-0.49250705	394	400	-0.97059179	1833667	0.74064066	1768650	0.38160947	experimental	Prestwick	192		Thalidomide	
2095 H06	X		555	560	0.36014553	474	480	-0.6042713	1619896	0.28500074	1737364	0.31641783	experimental	Prestwick	272		Indomethacin	
2095 H07	X		475	480	-0.06618076	434	440	-1.33691228	1701176	0.45824413	1806300	0.46006197	experimental	Prestwick	193		Oxolinic acid	
2095 H08	X		435	440	-0.27934391	434	440	-0.78743154	1754534	0.57197347	1710374	0.26017791	experimental	Prestwick	273		Cortisone	
2095 H09	X		593	600	0.56265051	434	440	-0.78743154	1784903	0.63670315	1827754	0.50476636	experimental	Prestwick	194		Nimesulide	
2095 H10	X		792	800	1.62313715	554	560	-0.2379508	1639160	0.32606078	1729188	0.29938124	experimental	Prestwick	274		Prednisolone	
2095 H11	X		440	440	-0.27934391	435	440	-0.27934391	4786504	0.0308453	4567264	-0.34497899	experimental	Prestwick	195		Hydrastinine hydrochloride	
2095 H12	X		355	360	-0.70567019	515	520	-0.41653204	1507437	0.0453012	1716701	-0.27336168	experimental	Prestwick	275		Fenofibrate	
2095 H13	X		514	520	0.1416533	435	440	-0.78285254	1755617	0.6169106	1802098	0.45130613	experimental	Prestwick	196		Pentoxifylline	
2095 H14	X		436	440	-0.27401483	515	520	-0.41653204	1566640	0.1714888	1673978	0.1843384	experimental	Prestwick	276		Bumetamide	
2095 H15	X		354	360	-0.71099927	514	520	-0.42111105	1763277	0.59060064	1752947	0.34888863	experimental	Prestwick	197		Metaraminol bitartrate	
2095 H16	X		555	560	0.36014553	674	680	0.31152994	1248561	-0.5064773	1546039	-0.08225217	experimental	Prestwick	277		Labeltalol hydrochloride	
2095 H17	X		595	600	0.57330867	594	600	-0.05479056	1720249	0.49889707	1878595	0.61070537	experimental	Prestwick	198		Salbutamol	
2095 H18	X		434	440	-0.29006206	432	440	-0.29006206	1598626	0.24179646	1567385	0.18249538	experimental	Prestwick	278		Hexiprone	
2095 H19	X		474	480	-0.07150984	472	480	-0.61342937	8190585	1.879552	787257	0.42038147	experimental	Prestwick	199		Procaine hydrochloride	
2095 H20	X		591	600	0.55199236	710	720	0.47637416	1501775	0.03323299	1651909	0.13835252	experimental	Prestwick	279		Methylprednisolone, 6-alpha	
2095 H21	X		1512	1520	5.46007374	1429	1440	3.7686796	3801290	4.93450976	3475174	3.93754795 W	experimental	Prestwick	200		Camptothecin (S, +)	
2095 H22	X		628	640	0.74916826	947	960	1.56159862	1505590	0.04136443	1475855	-0.22849681	experimental	Prestwick	280		Quinidine hydrochloride monohydrate	
2095 H23	E		327	800	-0.85488439	447	1080	-0.72790446	87597	-2.98100166	89304	-3.11769735	empty					
2095 H24	P	160478	161240	852.602382	214786	215880	980.7317	1521065	0.07434845	1876777	0.60691715	empty						
2095 I01	N		437	440	-0.26868575	357	360	-1.14001502	1367281	-0.25343282	1309159	-0.57584658	empty					
2095 I02	E		117	120	-1.9739909	116	120	-2.24355551	86122	-2.98414553	87599	-3.12125011	empty					
2095 I03	X		356	360	-0.70034111	955	960	1.59823067	1332229	-0.32814403	1201875	-0.79939767	experimental	Prestwick	41		Procaine hydrochloride	
2095 I04	X		435	440	-0.27934391	633	640	0.12379068	1473518	-0.02699509	1345021	-0.50111979	experimental	Prestwick	121		Bromocryptine mesylate	
2095 I05	X		394	400	-0.49783613	473	480	-0.6088503	1485690	-0.00105121	1582141	-0.00720258	experimental	Prestwick	42		Moxisylyte hydrochloride	
2095 I06	X		514	520	0.1416533	554	560	-0.2379508	1405793	-0.17134682	1598405	0.02686453	experimental	Prestwick	122		Metanephron hydrochloride DL	
2095 I07	X		434	440	-0.28467298	674	680	0.31152994	1503876	0.03771114	1587873	0.00491867	experimental	Prestwick	43		Metazole hydrochloride	
2095 I08	X		436	440	-0.27401483	753	760	0.67327143	1683304	0.42015104	2038631	0.94417749	experimental	Prestwick	123		Dehydrocholic acid	
2095 I09	X		392	400	-0.50849428	432	440	-0.6042713	1465896	0.38304695	1567268	-0.03801663	experimental	Prestwick	44		Isoxicam	
2095 I10	X		1154	1160	3.55226361	874	880	1.22733117	1607490	0.2585581	1553037	-0.06767022	experimental	Prestwick	124		Hesperadin	
2095 I11	X		353	360	-0.71632835	394	400	-0.97059179	1503051	0.03595271	1285460	-0.62522894	experimental	Prestwick	45		Naproxen	
2095 I12	X		355	360	-0.70567019	515	520	-0.41653204	1168018	-0.67814982	999830	-1.22040528	experimental	Prestwick	125		Perphenazine	
2095 I13	X		716	720	1.21812718	315	320	-1.33233328	1543492	0.12215024	1333431	-0.52527024	experimental	Prestwick	46		Naphazoline hydrochloride	
2095 I14	X		114	120	-1.98997813	235	240	-1.69865377	654263	-1.77318744	734465	-1.7733548	experimental	Prestwick	126		Mefloquine hydrochloride	
2095 I15	X		516	520	0.15231146	394	400	-0.97059179	1615603	0.27585047	1378525	-0.43130644	experimental	Prestwick	47		Ticlopidine hydrochloride	
2095 I16	X		395	400	-0.49250705	474	480	-0.49250705	1149613	-0.71737896	1065325	-1.08705838	experimental	Prestwick	127		Eticoxacin	
2095 I17	X		314	320	-0.92416242	352	360	-1.16291005	1151055	-0.7								

2095 J13	X	515	520	0.14698238	675	680	0.31610894	1571873	0.18264262	1653615	0.14190737	experimental	Prestwick	206	Meclofenamic acid sodium salt monohydrate
2095 J14	X	395	400	-0.49250705	394	400	-0.97059179	1179667	-0.65332068	1373840	-0.44106872	experimental	Prestwick	286	Perhexiline maleate
2095 J15	X	435	440	-0.27934391	793	800	0.85643167	1637988	0.32356274	1741619	0.32528411	experimental	Prestwick	207	Kawain
2095 J16	X	355	360	-0.70567019	593	600	-0.05936856	1214749	-0.57854552	1272326	-0.79864545	experimental	Prestwick	208	Oxybutynin chloride
2095 J17	X	435	440	-0.27934391	672	680	0.30237193	1702915	0.4702915	1870348	0.59352083	experimental	Prestwick	207	Trimethoprim
2095 I18	X	514	520	0.1416533	631	640	0.11463267	1351614	-0.28682608	1214907	-0.77224248	experimental	Prestwick	288	Sipiperone
2095 I19	X	515	520	0.14698238	472	480	-0.61342931	1663306	0.37752652	1701978	0.2426829	experimental	Prestwick	209	Meclofenamic acid sodium salt monohydrate
2095 J20	X	391	400	-0.51382336	750	760	0.65953441	1385832	-0.21389248	1549264	-0.07553214	experimental	Prestwick	289	Pyrimilamine maleate
2095 J21	X	1434	1440	0.50440561	1351	1360	3.41151712	1533326	0.10048203	1674561	0.18555322	experimental	Prestwick	210	Fenbendazole
2095 J22	X	628	640	0.74916826	669	680	0.28863491	1421338	-0.1382136	1419370	-0.34619641	experimental	Prestwick	290	Sulfipyrizone
2095 J23	E	392	392	880	880	880	-1.58875762	86288	-2.98379171	86865	-3.11898718	empty			
2095 J24	P	165758	164880	880.739917	141945	142880	647.169416	1584785	0.21016577	1508590	-0.16028585	empty			
2095 K01	N	517	520	0.15764054	397	400	-0.95685477	1247212	-0.50935261	1354072	-0.48225993	empty			
2095 K02	E	77	80	-2.18715404	157	160	-2.05581625	84411	-2.98779242	90100	-3.1160387	empty			
2095 K03	X	355	360	-0.70567019	475	480	-0.59969229	1378273	-0.23000403	1296098	-0.6030622	experimental	Prestwick	51	Trichlorfon
2095 K04	X	516	520	0.15231146	394	400	-0.97059179	1422130	-0.1365255	1357268	-0.47560032	experimental	Prestwick	131	Glipizide
2095 K05	X	434	440	-0.28467298	554	560	-0.2379508	1498975	0.02726494	1663630	0.10589006	experimental	Prestwick	52	Carbamazepine
2095 K06	X	315	320	-0.91883334	354	360	-1.15375204	1408881	-0.16476494	1569343	-0.03369288	experimental	Prestwick	132	Loxapine succinate
2095 K07	X	275	280	-1.13199648	715	720	0.49926919	1220661	-0.56594445	1508590	-0.16028585	experimental	Prestwick	53	Triflupromazine hydrochloride
2095 K08	X	396	400	-0.48717797	434	440	-0.78743154	1510918	0.05272074	1798969	0.44478614	experimental	Prestwick	133	Hydroxyzine dihydrochloride
2095 K09	X	395	400	-0.49250705	393	400	-0.9751708	1503948	0.03786461	1524419	-0.12730246	experimental	Prestwick	54	Mefenamic acid
2095 K10	X	516	520	0.15231146	635	640	0.1329487	1549385	0.13471082	1476417	-0.22732575	experimental	Prestwick	134	Diltiazem hydrochloride
2095 K11	X	275	280	-1.13199648	354	360	-1.15375204	1460369	-0.05502139	1372025	-0.44485069	experimental	Prestwick	55	Acetohexamide
2095 K12	X	476	480	-0.06085168	435	440	-0.7825254	1499843	0.02911505	1475439	-0.22936364	experimental	Prestwick	135	Methotrexate
2095 K13	X	434	440	-0.28467298	474	480	-0.6042713	1603556	0.25017302	1533296	-0.10880517	experimental	Prestwick	56	Sulpiride
2095 K14	X	375	380	-0.36014553	474	480	-0.6042713	874171	-1.30446688	1470325	-1.03162856	experimental	Prestwick	296	Acetaminophen
2095 K15	X	475	480	-0.06618076	873	880	1.22275217	1539587	-1.13826987	1744499	-0.33128526	experimental	Prestwick	57	Benoxinate hydrochloride
2095 K16	X	395	400	-0.49250705	391	400	-0.98432881	1517456	0.06665609	1720147	-0.28054222	experimental	Prestwick	137	Clindamycin hydrochloride
2095 K17	X	395	400	-0.49250705	1072	1080	2.13397439	1602425	0.24776236	1781210	0.40778114	experimental	Prestwick	58	Oxethazaine
2095 K18	X	395	400	-0.49250705	752	760	0.66869242	1410960	-0.16033368	1660645	-0.15655601	experimental	Prestwick	138	Terfenadine
2095 K19	X	515	520	0.14698238	673	680	0.30695093	1613297	0.27093537	1775523	0.39593096	experimental	Prestwick	59	Pheniramine maleate
2095 K20	X	474	480	-0.07150984	832	840	1.03501291	1775542	0.61675075	1796196	0.43900795	experimental	Prestwick	139	Cefotaxime sodium salt
2095 K21	X	591	600	0.55192326	789	800	0.83811565	1618691	0.28243235	1741498	0.32503198	experimental	Prestwick	60	Tolazoline hydrochloride
2095 K22	X	375	380	-0.49250705	409	416	-0.41530309	1663592	-0.37818173	1378181	-0.63149865	experimental	Prestwick	140	Tetracycline hydrochloride
2095 K23	E	361	720	-0.67369572	496	920	-0.62716633	88673	-2.97870823	89500	-3.11728894	empty			
2095 K24	P	120860	121720	641.474946	152325	153280	694.722395	1378167	-0.23022997	1581283	-0.00881313	empty			
2095 L01	N	477	480	-0.0555226	357	360	-1.14001502	1214753	-0.578537	1205716	-0.79139406	empty			
2095 L02	E	76	80	-2.19248312	75	80	-2.43129476	80070	-2.997045	81335	-3.13430261	empty			
2095 L03	X	637	640	0.79712997	916	920	1.41964943	1424463	-0.13155285	1597612	0.02521213	experimental	Prestwick	211	Piroxicam
2095 L04	X	275	280	-1.13199648	394	400	-0.97059179	1329125	-0.33476002	1266637	-0.66467503	experimental	Prestwick	291	Dantrolene sodium salt
2095 L05	X	440	440	-0.27401483	476	480	-0.27401483	1602020	0.24689913	1122327	-0.13123367	experimental	Prestwick	292	Glipizide tartrate
2095 L06	X	435	440	-0.27934391	476	480	-0.59511328	1588099	0.21722736	1553499	-0.06670753	experimental	Prestwick	212	Trazodone hydrochloride
2095 L07	X	475	480	-0.06618076	353	360	-1.15833104	1526803	0.08657865	1492819	-0.19314838	experimental	Prestwick	213	Fenfluramine hydrochloride
2095 L08	X	475	480	-0.06618076	474	480	-0.6042713	1399913	-0.18387969	1605319	0.04127145	experimental	Prestwick	293	Glaucine hydrochloride
2095 L09	X	436	440	-0.27401483	315	320	-1.33233328	1595172	0.23230303	1766551	0.18990822	experimental	Prestwick	214	Gemfibrozil
2095 L10	X	235	240	-1.34515962	355	360	-1.14917303	1132260	-0.75436582	1140484	-0.92732006	experimental	Prestwick	294	Pimethixene maleate
2095 L11	X	395	400	-0.49250705	514	520	-0.42111105	1726651	0.51254255	1776214	0.39737082	experimental	Prestwick	215	Mefenamic acid hydrochloride
2095 L12	X	375	380	-0.49250705	409	416	-0.41530309	1305415	-0.38259644	1470323	-2.40002462	experimental	Prestwick	295	Tergipride mesylate
2095 L13	X	475	480	-0.06618076	435	440	-0.7825254	1578497	0.1916128	148438	-0.19363185	experimental	Prestwick	216	Tripelennamine hydrochloride
2095 L14	X	394	400	-0.49783613	474	480	-0.6042713	1426756	-0.12666546	1525629	-0.12478114	experimental	Prestwick	296	Acemetacin
2095 L15	X	475	480	-0.06618076	633	640	0.12379068	1603945	0.25100215	1856258	0.56416105	experimental	Prestwick	217	Mefenamic acid
2095 L16	X	394	400	-0.49783613	433	440	-0.79201055	1413552	-0.15480899	1531265	-0.11303723	experimental	Prestwick	297	Benzydamine hydrochloride
2095 L17	X	556	560	0.36547461	912	920	1.40133341	1606943	0.2573922	1557115	-0.05917276	experimental	Prestwick	218	Fenbufen
2095 L18	X	275	280	-1.13199648	472	480	-0.61342931	1486411	0.00048555	1539683	-0.09549637	experimental	Prestwick	298	Fluprednide hydrochloride
2095 L19	X	435	440	-0.27934391	474	480	-0.6042713	1529174	0.09163323	1265942	-0.66589922	experimental	Prestwick	219	Ketoprofen
2095 L20	X	395	400	-0.49250705	352	360	-1.16291005	1445961	-0.08573117	1328709	-0.53510962	experimental	Prestwick	299	Mifepristone
2095 L21	X	353	360	-0.71632835	790	800	0.84269465	1433377	-0.1125532	1639581	0.11266428	experimental	Prestwick	220	Indanaprine
2095 L22	X	553	560	0.34948737	630	640	0.11005367	1193291	-0.62428195	1366140	-0.45711346	experimental	Prestwick	300	Diperodon hydrochloride
2095 L23	E	299	680	-1.00409859	455	1000	-0.69127241	87450	-2.98131498	87964	-3.12048955	empty			
2095 L24	P	128870	129680	684.160866	185364	186160	846.00818	1357346	-0.27460867	1512442	-0.15225931	empty			
2095 M01	N	517	520	0.15764054	557	560	-0.22421378	1242082	-0.52028689	1366723	-0.45589864	empty			
2095 M02	E	77	80	-2.18715404	117	120	-2.2389765	83241	-2.99028621	86040	-3.124449865	empty			
2095 M03	X	436	440	-0.27401483	314	320	-1.33591228	1185767	-0.6403189	1023425	-1.17123363	experimental	Prestwick	61	Morantel tartrate
2095 M04	X	196	200	-1.55299369	355	360	-1.14917303	1190119	-0.63104287	1100036	-0.101160285	experimental	Prestwick	141	Verapamil hydrochloride
2095 M05	X	314	320	-0.92416242	315	320	-1.33233328	1307067	-0.38177531	1307054	-0.58023284	experimental	Prestwick	62	Homatropine hydrobromide (R,S)
2095 M06	X	396	400	-0.48717797	354	360	-1.15375204	2003353	1.10231608	2160931	1.1990179	experimental	Prestwick	142	Dipyridamole
2095 M07	X	395	400	-0.49250705	714	720	0.49469018	1321538	-0.35093125	1469322	-0.24210983	experimental	Prestwick	63	Nifedipine
2095 M08	X	516	520	0.15231146	833	840	1.03959192	1299920	-0.3970087	1541847	-0.09098718	experimental	Prestwick	143	Chlorhexidine
2095 M09	X	275	280	-1.13199648	554	560	-0.2379508	948817	-1.14536345	990245	-1.24037785	experimental	Prestwick	64	Chlorpromazine hydrochloride
2095 M10	X	434	440	-0.28467298	352	360	-1.16291005	1183080	-0.64646608	1267540	-0.66256492	experimental	Prestwick	144	Isoperamide hydrochloride
2095 M11	X	875	880	-0.06545068	1035	1040	0.96455117	1022858	-0.98754955	1459513	-1.2438067	experimental	Prestwick	65	Diphenhydramine hydrochloride
2095 M12	X	474	480	-0.07150984	353	360	-1.15833104	1522790	-0.07802519	1938554	-0.38957137	experimental	Prestwick	145	Chlorzacycline hydrochloride
2095 M13	X	435	440	-0.27934391	435	440	-0.7825254	1269847	-0.46110748	1186211	-0.83203725	experimental	Prestwick	66	Minaprine dihydrochloride
2095 M14	X	434	440	-0.28467298	515	520	-0.41653204	944437	-1.15469916	1101158	-1.0092649	experimental	Prestwick	146	Tamoxifen citrate
2095 M															

2095 N07	X	316	320	-0.91350426	474	480	-0.6042713	1384246	-0.2127295	1580976	-0.00945283	experimental	Prestwick	223	Xylometazoline hydrochloride
2095 N08	X	355	360	-0.70567019	593	600	-0.05936956	1377569	-0.23150457	1400115	-0.38631866	experimental	Prestwick	303	Telenzepine dihydrochloride
2095 N09	X	276	280	-1.1266674	513	520	-0.42569006	1480425	-0.01227324	1708154	0.25555202	experimental	Prestwick	224	Oxymetazoline hydrochloride
2095 N10	X	516	520	0.15231146	715	720	0.4926919	929902	-1.1866796	1139891	-0.9285571	experimental	Prestwick	304	Econazole nitrate
2095 N11	X	274	280	-1.13732556	592	600	-0.0639487	1378877	-0.23297952	1642191	0.11810282	experimental	Prestwick	225	Nifenazone
2095 N12	X	355	360	-0.70567019	554	560	-0.2379508	1273861	-0.45255188	1382727	-0.42255059	experimental	Prestwick	305	Bupivacaine hydrochloride
2095 N13	X	354	360	-0.71099927	475	480	-0.59969229	1388896	-0.20736175	1576554	-0.01866709	experimental	Prestwick	226	Griseofulvin
2095 N14	X	796	800	1.64445347	395	400	-0.96601278	1106341	-1.00144014	1280633	-0.63528712	experimental	Prestwick	306	Clemastine fumarate
2095 N15	X	314	320	-0.92416242	354	360	-1.15375204	1353211	-0.28342217	1525690	-0.12465403	experimental	Prestwick	227	Clemizole hydrochloride
2095 N16	X	475	480	-0.06618076	514	520	-0.42111105	1246048	-0.5118336	1431688	-0.320529	experimental	Prestwick	307	Oxytetracycline dihydrate
2095 N17	X	435	440	-0.27934391	554	560	-0.2379508	1441888	-0.09441252	1531691	-0.11214956	experimental	Prestwick	228	Tropicamide
2095 N18	X	395	400	-0.49250705	432	440	-0.79589556	1174318	-0.57927215	1304253	-0.5835861	experimental	Prestwick	308	Pimozide
2095 N19	X	395	400	-0.49250705	873	880	1.22275217	1435450	-0.10813473	1716671	0.27329917	experimental	Prestwick	229	Nefopam hydrochloride
2095 N20	X	475	480	-0.06618076	551	560	-0.25168782	793305	-1.47682785	894336	-1.4402265	experimental	Prestwick	309	Amodiaquin dihydrochloride dihydrate
2095 N21	X	513	520	0.13632423	749	760	0.6549554	1256857	-0.48879488	1416922	-0.35129738	experimental	Prestwick	230	Phentolamine hydrochloride
2095 N22	X	673	680	0.9889768	911	920	1.3967544	1214074	-0.57998425	1338074	-0.51559547	experimental	Prestwick	310	Mebeverine hydrochloride
2095 N23	E	291	720	-1.04673122	329	960	-1.26822719	86509	-2.98332066	84937	-3.126797	empty			
2095 N24	P	144718	145680	768.616103	214266	215160	978.350616	1363524	-0.26144063	1558051	-0.05722238	empty			
2095 O01	N	518	520	0.16299662	636	640	0.1375277	1107318	-0.80752818	1233356	-0.73379971	empty			
2095 O02	E	76	80	-2.19248312	76	80	-2.42671575	82640	-2.9915672	84301	-3.12812226	empty			
2095 O03	X	596	600	0.57863775	515	520	-0.41653204	1133972	-0.7507168	953870	-1.3161736	experimental	Prestwick	71	Todralazine hydrochloride
2095 O04	X	393	400	-0.50316521	594	600	-0.05479056	1154151	-0.70770649	1027446	-1.16286094	experimental	Prestwick	151	Erythromycin
2095 O05	X	634	640	0.78114274	473	480	-0.6088503	955727	-1.13063521	1004993	-1.20964698	experimental	Prestwick	72	Imipramine hydrochloride
2095 O06	X	235	240	-1.34515962	474	480	-0.6042713	1143558	-0.73028482	1433055	-0.31768054	experimental	Prestwick	152	Oleandomycin phosphate
2095 O07	X	395	400	-0.49250705	514	520	-0.42111105	1240716	-0.52319844	1438321	-0.3067076	experimental	Prestwick	73	Sulindac
2095 O08	X	435	440	-0.27934391	554	560	-0.2379508	1217858	-0.5220298	1602316	-0.03833393	experimental	Prestwick	153_2009	Idanosone
2095 O09	X	355	360	-0.70567019	474	480	-0.6042713	1046526	-0.37010265	133580	-0.96254346	experimental	Prestwick	74	Amtryptiline hydrochloride
2095 O10	X	355	360	-0.70567019	353	360	-1.15833104	1203650	-0.60202037	1094986	-1.02212569	experimental	Prestwick	154	Josamycin
2095 O11	X	435	440	-0.27934391	513	520	-0.42569006	1269756	-0.46130144	1129648	-0.94989938	experimental	Prestwick	75	Adiphenine hydrochloride
2095 O12	X	595	600	0.57330867	554	560	-0.2379508	1059736	-0.90894633	1004173	-1.21135564	experimental	Prestwick	155	Paclitaxel
2095 O13	X	516	520	0.15231146	394	400	-0.97059179	1030630	-0.97098041	1019958	-1.17846393	experimental	Prestwick	76	Dibucaine
2095 O14	X	114	120	-1.98997813	235	240	-1.69865377	558059	-1.97824043	640293	-1.969584	experimental	Prestwick	156	Ivermectin
2095 O15	X	357	360	-0.69501204	755	760	0.68242944	1341665	-0.30803177	1230763	-0.73920283	experimental	Prestwick	77	Prednisone
2095 O16	X	516	520	-0.41789995	529	530	-0.242490	80772	-0.99154873	1233769	-0.12602602	experimental	Prestwick	157	Gallamine triethiodide
2095 O17	X	555	560	0.36014553	473	480	-0.6088503	868477	-1.31660329	1016098	-1.18650713	experimental	Prestwick	78	Thioridazine hydrochloride
2095 O18	X	474	480	-0.07150984	552	560	-0.24710882	1400754	-0.18208715	1161671	0.06500933	experimental	Prestwick	158	Neomycin sulfate
2095 O19	X	395	400	-0.49250705	752	760	0.66869242	1309383	-0.37683889	1693540	0.22510037	experimental	Prestwick	79	Diphenamil methylsulfate
2095 O20	X	555	560	0.36014553	872	880	1.21817316	1344722	-0.30151596	1548211	-0.07772631	experimental	Prestwick	159	Dihydrostreptomycin sulfate
2095 O21	X	394	400	-0.49783613	631	640	0.11463267	1254043	-0.49479275	1393639	-0.39981291	experimental	Prestwick	80	Trimethobenzamide hydrochloride
2095 O22	X	592	600	0.55732143	750	760	0.65953441	1252028	-0.4990786	1401010	-0.38445372	experimental	Prestwick	160	Gentamicin sulfate
2095 O23	E	519	520	-0.41789995	529	530	-0.242490	80772	-0.99154873	1233769	-0.12602602	empty			
2095 O24	P	173298	174160	920.921117	185869	187200	848.320578	1177515	-0.65790754	1308817	-0.57505322	empty			
2095 P01	N	358	360	-0.68968296	718	720	0.51300621	844747	-1.36718235	952670	-1.31867408	empty			
2095 P02	E	117	120	-1.9739909	116	120	-2.24355551	74887	-3.00809225	73512	-3.15060364	empty			
2095 P03	X	556	560	0.36547461	677	680	0.32526696	1164303	-0.68606811	1225553	-0.75005907	experimental	Prestwick	231	Etodolac
2095 P04	X	596	600	0.57863775	554	560	-0.2379508	994177	-1.04868137	1066786	-1.08088693	experimental	Prestwick	311	Ifenprodil tartrate
2095 P05	X	435	440	-0.27934391	755	760	0.68242944	1138129	-0.74185641	1239870	-0.72022628	experimental	Prestwick	232	Scopolamin-N-oxide dihydrobromide
2095 P06	X	595	600	0.36547461	795	800	0.86558968	917527	-1.21205619	1063372	-1.08365764	experimental	Prestwick	312	Alfuzosin hydrochloride
2095 P07	X	635	640	0.79180089	635	640	0.1394887	1214413	-0.297555	297555	-6.00033243	experimental	Prestwick	313	Hydrocortisone (L)
2095 P08	X	436	440	-0.27401483	355	360	-1.14917303	908528	-1.23123701	988327	-1.24437445	experimental	Prestwick	313	Trifluoperazine dihydrochloride
2095 P09	X	437	440	-0.26868575	515	520	-0.41653204	1214927	-0.57816613	1238264	-0.72357275	experimental	Prestwick	234	Chlorthalidone
2095 P10	X	396	400	-0.48717797	715	720	0.49926919	1105863	-0.81062943	1237564	-0.72503137	experimental	Prestwick	314	Enalapril maleate
2095 P11	X	477	480	-0.0555226	755	760	0.68242944	1218709	-0.57010250	1321882	-0.54933526	experimental	Prestwick	235	Metampicillin sodium salt
2095 P12	X	356	360	-0.70034111	474	480	-0.6042713	1004307	-1.02708988	1130875	-0.94734264	experimental	Prestwick	315	Minocycline hydrochloride
2095 P13	X	397	400	-0.48184889	797	800	0.8747477	1207911	-0.59312031	1267407	-0.66284656	experimental	Prestwick	236	Dilazep dihydrochloride
2095 P14	X	317	320	-0.90817518	316	320	-1.32775427	1138281	-0.74153243	1323769	-0.54503216	experimental	Prestwick	316	Gilbenclamide
2095 P15	X	357	360	-0.69501204	435	440	-0.78285254	1207912	-0.59311817	1354519	-0.4813285	experimental	Prestwick	237	Oxofloxacin
2095 P16	X	277	280	-1.12133832	635	640	0.1329487	1086145	-0.85265715	1163829	-0.87867534	experimental	Prestwick	317	Guaethidine sulfate
2095 P17	X	475	480	-0.06618076	634	640	0.12836969	1201994	-0.60573203	1402637	-0.38106349	experimental	Prestwick	238	Lomefloxacin hydrochloride
2095 P18	X	716	720	1.21812718	1115	1120	2.33087166	853891	-1.34769247	869426	-1.49213226	experimental	Prestwick	318	Quinacrine dihydrochloride dihydrate
2095 P19	X	396	400	-0.48717797	393	400	-0.9751708	1151878	-0.71255125	1219745	-0.76216139	experimental	Prestwick	239	Orphenadrine hydrochloride
2095 P20	X	396	400	-0.48717797	674	680	0.31152994	969890	-1.1002558	1130952	-0.94718219	experimental	Prestwick	319	Clofium tosylate
2095 P21	X	516	520	0.15231146	674	680	0.31152994	1146662	-0.72366883	1292740	-0.61005938	experimental	Prestwick	240	Progildium
2095 P22	X	634	640	0.78114274	912	920	1.40133341	856392	-1.34236174	1033096	-1.15108786	experimental	Prestwick	320	Fluphenazine dihydrochloride
2095 P23	E	477	920	-0.0555226	649	1360	0.19705478	76802	-3.00401054	78657	-3.13988284	empty			
2095 P24	P	150773	151280	800.883674	242934	243480	1109.62157	947393	-1.14839862	1212300	-0.77767477	empty			
2096 A01	N	718	720	0.63932902	678	680	0.02327644	1094118	-0.68641359	1016750	-0.78909314	empty			
2096 A02	X	316	320	-0.93061877	436	440	-1.7004483	1297618	-0.37183014	1279028	-0.39240175	experimental	Prestwick	321	Streptomycin sulfate
2096 A03	X	876	880	1.25637317	595	600	-0.04302796	1540362	0.00341923	1449281	-1.13489674	experimental	Prestwick	401	Testosterone propionate
2096 A04	X	554	560	-0.00112457	674	680	0.12445573	1420083	-0.18127913	1449689	-0.08557641	experimental	Prestwick	322	Alfuzosin hydrochloride
2096 A05	X	556	560	0.00666349	634	640	-0.01187288	1485820	-0.08089532	1504677	-0.05111115	experimental	Prestwick	402	Chlorpropamide
2096 A06	X	475	480	-0.30966927	833	840	0.14709791	1488441	-0.07684361	1443546	-0.14357084	experimental	Prestwick	323	Chlorpropamide
2096 A08	X	835	840	1.09625412	1075	1080	0.34041918	1553055	0.02304089	1671102	0.20060407	experimental	Prestwick	403	Thiroxine (L)
2096 A09	X	635	640	0.31518557	514	520	-0.10773467	1498528	-0.06125048	1583302	0.06780794	experimental	Prestwick	324	Phenylpropanolamine hydrochloride</

2096 B04	X	513	520	-0.16126625	354	360	-0.23555038	1634277	0.1485991	1613332	0.11322785	experimental	Prestwick	561	Tubocurarine chloride pentahydrate (+)
2096 B05	X	515	520	-0.15345556	353	360	-0.23634923	1683749	0.22507612	1598073	0.09014885	experimental	Prestwick	482	Cefotiam hydrochloride
2096 B06	X	394	400	-0.62600204	314	320	-0.26750431	1446482	-0.14170655	1420342	-0.17866652	experimental	Prestwick	562	Dihydroergocristine mesylate
2096 B07	X	475	480	-0.30966927	554	560	-0.07578074	1705616	0.25887954	1818452	0.42346665	experimental	Prestwick	475	Azathioprine, 6
2096 B08	X	473	480	-0.31747996	432	440	-0.17324022	3140887	-0.34687129	1810152	-0.25373265	experimental	Prestwick	563	Nescapine
2096 B09	X	314	320	-0.93842946	514	520	-0.10773467	1558877	0.03204091	1625931	0.13228364	experimental	Prestwick	484	Benperidol
2096 B10	X	392	400	-0.63381272	592	600	-0.04542451	1804860	0.41229733	1699667	0.24426193	experimental	Prestwick	564	Syringopipone
2096 B11	X	474	480	-0.31357461	633	640	-0.17244137	1697007	0.24557119	1941120	0.60900209	experimental	Prestwick	485	Cefaclor
2096 B12	X	434	440	-0.46978833	474	480	0.02008105	1716271	0.27535073	1872979	0.50593989	experimental	Prestwick	565	Atropine sulfate monohydrate
2096 B13	X	590	600	0.13944514	514	520	-0.10773467	1725060	0.28893733	1753840	0.32574401	experimental	Prestwick	486	Colistin sulfate
2096 B14	X	594	600	0.15506652	473	480	-0.14048744	1688471	0.22928396	1720040	0.27462203	experimental	Prestwick	566	Eserine sulfate, physostigmine sulfate
2096 B15	X	753	760	0.77601601	952	960	0.24215685	1258576	-0.43218379	1266418	-0.41138343	experimental	Prestwick	487	Daunorubicin hydrochloride
2096 B16	X	592	600	0.14725583	392	400	-0.20519415	1862474	0.50136077	1552575	0.02541754	experimental	Prestwick	567	Acotinine
2096 B17	X	552	560	-0.00895788	591	600	-0.04622335	1619222	0.12532611	1301696	-0.35811675	experimental	Prestwick	488	Dosulepin hydrochloride
2096 B18	X	434	440	-0.46978833	992	1000	0.27411478	1551686	0.0209246	1398404	-0.21184741	experimental	Prestwick	568	Rescinamin
2096 B19	X	474	480	-0.31357461	712	720	0.05043728	1685404	0.22763452	1840479	0.45678415	experimental	Prestwick	489	Ceftazidime pentahydrate
2096 B20	X	473	480	-0.31747996	512	520	-0.10933236	1497573	-0.06272678	1650542	0.16950739	experimental	Prestwick	569	Dihydroergotamine mesylate
2096 B21	X	513	520	-0.16126625	450	520	-0.15886095	1950518	0.63746488	1817743	0.42233963	experimental	Prestwick	490	Iobenguane sulfate
2096 B22	X	672	680	0.45968325	1113	1120	0.37077541	1147685	-0.60360626	1158495	-0.57470604	experimental	Prestwick	570	Emetine dihydrochloride
2096 B24	P	175366	176320	682.699631	133396	134320	106.044813	1396422	-0.21909523	1354675	-0.27798684	empty			
2096 C01	N	516	520	-0.14955022	477	480	-0.13729205	1413352	-0.19292104	1357095	-0.27432663	empty			
2096 C03	X	556	560	0.00666349	755	760	0.08478775	1414961	-0.19043375	1496366	-0.06368141	experimental	Prestwick	331	Tremorin dihydrochloride
2096 C04	X	594	600	0.15506652	672	680	0.01848335	1695059	0.24255985	1870718	0.50252016	experimental	Prestwick	411	Androsterone
2096 C05	X	353	360	-0.78612109	594	760	0.08398889	1457179	-0.12517403	1517146	-0.03225198	experimental	Prestwick	332	Practolol
2096 C06	X	515	520	-0.15345556	754	600	-0.04382681	1112554	-0.65791403	1124995	-0.62537426	experimental	Prestwick	412	Amisomycin
2096 C07	X	515	520	-0.16907693	635	640	-0.01748008	1539953	0.00278697	1580811	0.03461334	experimental	Prestwick	333	Acetabuvine, AZT
2096 C08	X	674	680	0.46748194	635	640	-0.01107403	1755605	-0.08122118	1899841	0.54656825	experimental	Prestwick	413	Carpazone
2096 C09	X	511	520	-0.16907693	591	600	-0.04622335	1779455	0.37302464	1721951	0.27751239	experimental	Prestwick	334	Sulfisoxazole
2096 C10	X	1434	1440	3.43555443	1273	1280	0.49859113	1315478	-0.344221	1309360	-0.34652507	experimental	Prestwick	414	Apigenin
2096 C11	X	472	480	-0.3213853	673	680	0.0192822	1631356	0.14408363	1719777	0.27422425	experimental	Prestwick	335	Zaprinasat
2096 C12	X	475	480	-0.3096927	513	520	-0.10853352	1622788	0.13083866	1818001	0.42278652	experimental	Prestwick	415	Aspartic acid, N-acetyl (R,S)
2096 C13	X	391	400	-0.63771806	592	600	-0.04542451	1456139	-0.12677813	1659631	0.18325436	experimental	Prestwick	336	Chlormezanone
2096 C14	X	515	520	-0.15345556	473	480	-0.14048744	1668512	0.20152178	1788313	0.37788388	experimental	Prestwick	416	Bacampicillin hydrochloride
2096 C15	X	515	520	-0.15345556	672	680	0.01848335	1748212	-0.06498008	1759802	0.34347208	experimental	Prestwick	337	Acetaminophen hydrochloride
2096 C16	X	673	680	0.46358859	833	840	0.14709791	1859815	0.49725032	1815642	0.41921857	experimental	Prestwick	417	Betulic acid
2096 C17	X	873	880	1.24465714	672	680	0.01848335	1897153	0.55496981	1579545	0.06212553	experimental	Prestwick	338	N6-methyladenosine
2096 C18	X	513	520	-0.16126625	912	920	0.21020692	1674893	0.21138594	1888003	0.52866346	experimental	Prestwick	418	Biotin
2096 C19	X	593	600	0.15116117	512	520	-0.10933236	1623102	0.13132406	1573242	0.05259234	experimental	Prestwick	339	Guafacine hydrochloride
2096 C20	X	554	560	-0.00114719	634	640	-0.01187288	1803980	0.41093697	1894937	0.53915102	experimental	Prestwick	419	Bisacodyl
2096 C21	X	513	520	-0.16126625	513	520	-0.10853352	1294480	-0.37668106	1366642	-0.25988694	experimental	Prestwick	340_2009	Domperidone
2096 C22	X	672	680	0.76820533	710	720	0.04883958	1693864	0.24071254	1742722	0.11668044	experimental	Prestwick	420	Calciferol
2096 C24	P	143866	144880	559.681334	127522	128440	101.385237	1285161	-0.39108697	1438926	-0.15055851	empty			
2096 D01	N	557	560	0.01056883	357	360	-0.23315384	1280626	-0.39809747	1245621	-0.44229232	empty			
2096 D02	E	117	120	-1.70778198	117	120	-0.42487741	87536	-2.2424531	89009	-2.19228696	empty			
2096 D03	X	313	320	-0.9423348	754	360	-0.23555038	1056901	-0.74394603	1008706	-0.80125957	experimental	Prestwick	491	Metixene hydrochloride
2096 D04	X	515	520	-0.15345556	315	720	0.05283382	1569466	0.04841007	1509063	-0.04447739	experimental	Prestwick	571	Tetracaine hydrochloride
2096 D05	X	835	840	1.09625412	593	600	-0.04462566	1492077	-0.07122285	1415377	-0.18617601	experimental	Prestwick	492	Nitrofurantoin
2096 D06	X	551	560	-0.01286333	594	600	-0.01347958	1294480	-0.29475024	1347480	-0.03463316	experimental	Prestwick	572	Clometasone furate
2096 D07	X	1514	1520	3.74789895	954	960	0.24375895	1845634	-0.08118285	1858745	-0.18188405	experimental	Prestwick	493	Omeprazole
2096 D08	X	510	520	-0.17298228	433	440	-0.17244137	1756311	0.33724715	1627474	0.1346714	experimental	Prestwick	573	Tomatidine
2096 D09	X	512	520	-0.16517159	512	520	-0.10933236	1769441	0.35754435	1823248	0.43072253	experimental	Prestwick	494	Propylthiouracil
2096 D10	X	671	680	0.45577791	432	440	-0.17324022	1575275	0.05739	1564921	0.04000696	experimental	Prestwick	574	Dacarbazine
2096 D11	X	434	440	-0.46978833	314	320	-0.26750431	1825211	0.44375722	1520749	-0.0268025	experimental	Prestwick	495	Terconazole
2096 D12	X	352	360	-0.79002643	433	440	-0.17244137	1650829	0.17418625	1627914	0.13528289	experimental	Prestwick	575	Ipratropium bromide
2096 D13	X	1395	1400	3.28324606	1155	1160	0.40432704	1725164	0.2890981	1925040	0.58468134	experimental	Prestwick	496	Tiaprofenic acid
2096 D14	X	432	440	-0.47369367	512	520	-0.10933236	1415312	-0.18899115	1450375	-0.13324208	experimental	Prestwick	576	Acetopromazine maleate salt
2096 D15	X	555	560	0.00275815	634	640	-0.01187288	1978180	0.68022659	1973620	0.65815784	experimental	Prestwick	497	Vancomycin hydrochloride
2096 D16	X	514	520	-0.1573609	433	440	-0.17244137	1825295	0.44388707	1610417	0.10881895	experimental	Prestwick	577	Rauwolficine hydrochloride
2096 D17	X	553	560	-0.00505254	514	520	-0.10773467	1654606	0.18002498	1698035	0.24133981	experimental	Prestwick	498	Artemisinin
2096 D18	X	433	440	-0.47369367	673	680	0.0192822	1503059	-0.05424616	2066966	0.79934221	experimental	Prestwick	578	Corynanthine hydrochloride
2096 D19	X	834	840	1.09234878	353	360	-0.23634923	1484266	-0.0832976	1621068	0.12492842	experimental	Prestwick	499	Profenone hydrochloride
2096 D20	X	392	400	-0.63381272	673	680	0.0192822	1418628	-0.18476506	1752664	0.32396533	experimental	Prestwick	579	Palmitate chloride
2096 D21	X	634	640	0.31128023	74	80	-0.0192822	1711080	0.26732614	1730145	0.28990569	experimental	Prestwick	500	Ethivanol
2096 D22	X	871	880	1.25684646	791	800	0.11354629	1877330	0.21515321	1569961	0.04762988	experimental	Prestwick	580	Trimethylchloridic acid
2096 D23	E	452	960	-0.39949216	466	1000	-0.14607938	88452	-2.24103709	87269	-2.19491868	empty			
2096 D24	P	172101	172880	669.948687	180899	181760	143.9925	1482448	-0.08610798	1706608	0.2534896	empty			
2096 E01	N	477	480	-0.30185859	477	480	-0.13729205	1366651	-0.26511447	1406069	-0.20025422	empty			
2096 E02	E	115	120	-1.71559266	156	160	-0.39372233	86287	-2.24438389	85667	-2.19734166	empty			
2096 E03	X	1117	1120	2.19756078	597	600	-0.04143027	1548018	0.01525436	1495214	-0.06542379	experimental	Prestwick	341	Furosemide
2096 E04	X	113	120	-1.72340335	74	80	-0.4592786	546846	-1.5324202	546024	-1.50408386	experimental	Prestwick	421	Sulcitol
2096 E05	X	355	360	-0.77839504	395	400	-0.20279796	1537291	-0.08112812	1483655	-0.0829066	experimental	Prestwick	342	Acrylamide hydrochloride
2096 E06	X	394	400	-0.62600204	554	560	-0.07578074	1578684	0.06265985	1578417	0.06041945	experimental	Prestwick	422	Carboline
2096 E07	X	431	440	-0.48150435	473	480	-0.14048744	1379330	-0.24551445	1318103	-0.33330142	experimental	Prestwick	343	Desipramine hydrochloride
2096 E08	X	713	720	0.6198023	431	440	-0.17403907	1901079							

2096 F01	N	436	440	-0.46197764	397	400	-0.20119991	1496000	-0.06515842	1358836	-0.27169339	empty							
2096 F02	E	77	80	-1.86399569	117	120	-0.42487741	87584	-2.2423789	84369	-2.19930489	empty							
2096 F03	X	434	440	-0.46978833	395	400	-0.2027976	1670560	0.20468771	1644423	0.1602525	experimental	Prestwick	501					Vigabatrin
2096 F04	X	516	520	-0.14955022	515	520	-0.10693582	14550051	-0.13618936	1414486	-0.18752363	experimental	Prestwick	501					Hydralazine hydrochloride
2096 F05	X	354	360	-0.78221575	635	640	-0.01107403	1552987	0.02293573	1644350	0.16104343	experimental	Prestwick	502					Biperiden hydrochloride
2096 F06	X	595	600	-0.15897186	554	560	-0.07578074	1579338	0.06367085	1654846	0.17601712	experimental	Prestwick	582					Leboline alpha hydrochloride
2096 F07	X	513	520	-0.16126625	473	480	-0.14048744	1645056	0.16526198	1755137	0.3277057	experimental	Prestwick	503					Cetirizine dihydrochloride
2096 F08	X	593	600	0.15116117	474	480	0.17985069	1495717	-0.0655959	1548667	-0.126448	experimental	Prestwick	583					Papaverine hydrochloride
2096 F09	X	433	440	-0.47369367	871	880	-0.14208514	1760661	0.34397166	1692634	0.23317089	experimental	Prestwick	504					Etifenine
2096 F10	X	474	480	-0.31357461	434	440	-0.17164252	1559169	0.0324923	1644249	0.15998933	experimental	Prestwick	584					Yohimbine hydrochloride
2096 F11	X	554	560	-0.00114719	554	560	-0.07578074	1848307	0.47946051	1944505	0.61412185	experimental	Prestwick	505					Metaprotérenol sulfate, orciprenaline sulfate
2096 F12	X	555	560	0.00275815	433	440	-0.17244137	1535599	-0.00394373	1644350	-0.03713428	experimental	Prestwick	585					Leboline alpha (-) hydrochloride
2096 F13	X	434	440	-0.46978833	635	640	-0.01107403	1844549	0.47365115	1632439	0.14212689	experimental	Prestwick	506					Sisomicin sulfate
2096 F14	X	431	440	-0.48150435	592	600	-0.04542451	1604607	0.1027333	1559626	0.03199836	experimental	Prestwick	586					Berberine chloride
2096 F15	X	1635	1640	4.22052833	1035	1040	0.30846525	1731046	0.29819088	1632078	0.14158088	experimental	Prestwick	507					Quercetine dihydrate
2096 F16	X	387	400	-0.65333943	471	480	-0.14208514	1534836	-0.00512322	1569957	0.04762383	experimental	Prestwick	587_2009					Clostrazol
2096 F17	X	1834	1834	4.99769153	1474	1480	0.65915962	1640314	0.15793149	1481693	-0.08587409	experimental	Prestwick	508					Resveratrol
2096 F18	X	589	600	0.1355398	747	760	0.07839697	1719752	0.28073188	1552669	0.021476	experimental	Prestwick	588					Galanthamine hydrobromide
2096 F19	X	394	400	-0.6260204	432	440	-0.17324022	1484237	-0.08334243	1538218	-0.00038091	experimental	Prestwick	509					Bromperidol
2096 F20	X	433	440	-0.47369367	754	760	0.0839889	1502890	-0.05450741	1648273	0.16607556	experimental	Prestwick	589					Bicycluciline (+)
2096 F21	X	714	720	0.62370765	352	360	-0.23714808	1534491	-0.00556555	1641767	0.15623534	experimental	Prestwick	510					Cilicizine hydrochloride
2096 F22	X	672	680	0.45968325	752	760	0.08239121	1459929	-0.1209193	1563068	0.03720433	experimental	Prestwick	590					Yohimbic acid monohydrate
2096 F23	E	324	760	-0.89937603	233	640	-0.33221101	88679	-2.24068618	86569	-2.19597742	empty							
2096 F24	P	147709	148480	574.689566	137081	138000	108.988569	1421816	-0.17983684	1487317	-0.07736788	empty							
2096 G01	N	757	760	0.79167339	357	360	-0.23315384	1516106	-0.03407727	1361861	-0.26711813	empty							
2096 G02	E	116	120	-1.71168751	433	440	-0.42487741	87794	-2.24205427	152424	-2.17961949	empty							
2096 G03	X	396	400	-0.61819135	556	560	-0.07418304	1500575	0.05808609	1455242	-0.12588082	experimental	Prestwick	351					Chlorthalidone
2096 G04	X	395	480	-0.30966927	514	520	-0.10773467	2423357	1.36840996	2224373	1.03741784	experimental	Prestwick	431					Carolyne chloride hydrate
2096 G05	X	435	440	-0.46588298	394	400	-0.20359645	1369564	-0.26061136	1222782	-0.47747295	experimental	Prestwick	352					Dobutamine hydrochloride
2096 G06	X	433	440	-0.47369367	474	480	-0.1396886	1810247	0.4206249	1670349	0.19946517	experimental	Prestwick	432					Corticosterone
2096 G07	X	755	760	0.7838267	634	640	-0.01187288	1642982	0.16205585	1473878	-0.09769416	experimental	Prestwick	353_2009					Moclobemide
2096 G08	X	593	600	0.15116117	532	560	-0.07737843	1688754	0.23281317	1507767	-0.04643757	experimental	Prestwick	433					Cyanocobalamin
2096 G09	X	474	480	-0.31357461	354	360	-0.23555038	1800072	0.40489573	1416971	-0.18376511	experimental	Prestwick	354					Clopidamide
2096 G10	X	434	440	-0.46588298	434	440	-0.17164252	1777514	0.3790411	1395810	0.16786149	experimental	Prestwick	434					Clopidoxil
2096 G11	X	435	440	-0.46588298	674	680	0.02080105	802677	-1.13694192	734013	-1.21672845	experimental	Prestwick	355					Yohanthone
2096 G12	X	394	400	-0.6260204	554	560	-0.07578074	1599486	0.09481693	1393455	-0.21933269	experimental	Prestwick	435					Cyclosporin A
2096 G13	X	515	520	-0.15345556	513	520	-0.10853352	1335152	-0.01380766	1650062	0.1687814	experimental	Prestwick	356					Adenosine 5'-monophosphate monohydrate
2096 G14	X	475	480	-0.30966927	555	560	-0.07498189	1261104	-0.42827584	1726296	-0.39653386	experimental	Prestwick	436					Digitoxigenin
2096 G15	X	391	400	-0.63771806	353	360	-0.23634923	1337186	-0.31066337	1440342	-0.14841684	experimental	Prestwick	357					Amoxicillin
2096 G16	X	634	640	0.31128023	354	360	-0.23555038	1368123	-0.26283895	1350399	-0.2774363	experimental	Prestwick	437					Digoxin
2096 G17	X	434	480	-0.3331308511	548	560	-0.08057383	1796101	0.35867571	1483272	0.17137621	experimental	Prestwick	358					Cephalexin monohydrate
2096 G18	X	914	920	1.4407762	1714	1720	0.85088319	3314896	-0.34512069	1307859	-0.34879531	experimental	Prestwick	438					Doxorubicin hydrochloride
2096 G19	X	553	560	-0.00505254	590	600	-0.0470222	1540104	0.00302039	1847488	0.46738515	experimental	Prestwick	359					Dextromethorphan hydrobromide monohydrate
2096 G20	X	514	520	-0.1573609	632	640	-0.01347058	1756134	0.33697353	1758254	0.33242011	experimental	Prestwick	439					Carbimazole
2096 G21	X	593	600	0.15116117	793	800	0.11514398	1360153	-0.27515949	1363666	-0.26438809	experimental	Prestwick	360					Droperidol
2096 G22	X	672	680	0.45968325	831	840	0.14550022	1641836	0.16028429	1802652	0.3995714	experimental	Prestwick	440					Epiandrosterone
2096 G23	E	381	800	-0.67677149	482	920	-0.13329781	86709	-2.24373153	84347	-2.19933816	empty							
2096 G24	P	141466	142320	550.308511	147834	148760	117.6559469	1445594	-0.14308082	1430305	-0.17860149	empty							
2096 H01	N	396	400	-0.61819135	597	600	0.04143027	1370084	-0.25980751	1286175	-0.38159202	experimental	Prestwick	397					
2096 H02	E	77	80	-1.86399569	157	160	-0.39292348	85192	-2.24607661	87727	-2.19422596	empty							
2096 H03	X	355	360	-0.7783104	275	280	-0.29865939	1303059	-0.36341909	1384218	-0.23303351	experimental	Prestwick	511					Fluoxetine hydrochloride
2096 H04	X	515	520	-0.15345556	515	520	-0.10693582	1654602	0.1800188	1590766	0.07909712	experimental	Prestwick	591					Laudanosine (R,S)
2096 H05	X	354	360	-0.78221575	354	360	-0.23555038	1850385	0.48267282	1576989	0.05825962	experimental	Prestwick	512					Iohexol
2096 H06	X	476	480	-0.30576393	635	640	-0.01107403	1534925	-0.00498564	1534702	-0.00569881	experimental	Prestwick	592					Ajmalicine hydrochloride
2096 H07	X	313	320	-0.9423348	430	440	-0.17483792	1380545	-0.24363622	1453945	-0.12784251	experimental	Prestwick	513					Norcyclohexaprine
2096 H08	X	434	440	-0.46978833	714	720	0.05203498	1583019	0.06936117	1296760	-0.3657185	experimental	Prestwick	593_2009					Trigonelline
2096 H09	X	555	560	0.00275815	474	480	-0.1396886	1795960	0.34226966	1832660	0.44495803	experimental	Prestwick	514					Pyrazinamide
2096 H10	X	354	360	-0.78221575	435	440	-0.17084368	1530215	-0.01226666	1795839	0.38926684	experimental	Prestwick	594					Diclofenac sodium
2096 H11	X	475	480	-0.30966927	434	440	-0.17164252	1812248	0.42371818	1751032	0.32149695	experimental	Prestwick	515					Trimethadione
2096 H12	X	396	400	-0.61819135	515	520	-0.10693582	1416106	-0.18866373	1512497	-0.03928352	experimental	Prestwick	595					Calycanthine
2096 H13	X	395	400	-0.62209669	515	520	-0.10693582	1930363	0.06306798	1836494	0.45075699	experimental	Prestwick	516					Loxastatin
2096 H14	X	435	440	-0.46588298	394	400	-0.20359645	1600760	0.09678636	1669920	0.19881631	experimental	Prestwick	596					Convallamine hydrochloride
2096 H15	X	474	480	-0.31357461	474	480	-0.1396886	1735730	0.30543171	1803226	0.40043956	experimental	Prestwick	517					Nystatine
2096 H16	X	674	680	1.46493934	715	720	0.05283382	1689035	0.23324756	1581895	0.06567987	experimental	Prestwick	597					Isocorydine (+)
2096 H17	X	474	480	-0.31357461	594	600	-0.04382681	1642929	0.16197392	1733971	0.29569245	experimental	Prestwick	518					Budesonide
2096 H18	X	433	440	-0.47369367	309	320	-0.27149855	1522186	-0.02467841	1617616	0.11970733	experimental	Prestwick	598					Xylazine
2096 H19	X	514	520	-0.1573609	672	680	0.01848335	1774354	0.36513918	1822057	0.42892116	experimental	Prestwick	519					Impipenem
2096 H20	X	554	560	-0.00114719	752														

2096 I19	X	674	680	0.46749394	953	960	0.2429597	1496151	-0.064925	1539570	0.001666397	experimental	Prestwick	369_2009	Meloxicam
2096 I20	X	594	600	0.15506652	431	440	-0.17403907	1841587	0.4690723	1668469	0.1966217	experimental	Prestwick	449	Pilocarpine nitrate
2096 I21	X	553	560	-0.00505254	634	640	-0.01187288	1199196	-0.52397723	1169973	-0.55734574	experimental	Prestwick	370	Benzbromarone
2096 I22	X	890	1.24075168	712	720	0.05043728	1603135	0.10045779	1650436	0.23579051	empty	Prestwick	450	Dicloxacillin sodium salt	
2096 I23	E	464	840	-0.2562804	686	720	-0.20998724	85572	-2.24548918	86928	-2.19543444	empty			
2096 I24	P	126424	127240	491.564346	112059	112840	88.9997891	1465844	-0.11177552	1350737	-0.283943	empty			
2096 J01	N	476	480	-0.30576393	557	560	-0.07338419	1371991	-0.25685955	1229491	-0.46732569	empty			
2096 J02	E	117	120	-1.70778198	156	160	-0.39372233	85756	-2.24520474	85834	-2.1970891	empty			
2096 J03	X	315	320	-0.93452411	516	520	-0.10613697	1538961	0.00125347	1631518	0.14073389	experimental	Prestwick	521	Glycocholic acid
2096 J04	X	515	520	-0.15345556	513	520	-0.10853352	1408254	-0.20080186	1496803	-0.06302045	experimental	Prestwick	521	Scoulerine
2096 J05	X	389	400	-0.64552875	394	400	-0.20359645	1262824	-0.42561695	1285467	-0.38266286	experimental	Prestwick	602	Thiostrepton
2096 J06	X	2355	2360	7.03237511	554	560	-0.07578074	1231517	-0.47401334	1417303	-0.18323994	experimental	Prestwick	602	Almaline
2096 J07	X	469	480	-0.33310133	551	560	-0.07817728	1800881	0.40614633	1754657	0.32697971	experimental	Prestwick	523	Methionine sulfoximine (L)
2096 J08	X	312	320	-0.94624014	429	440	-0.17563676	1638425	0.15501135	1491189	-0.07151154	experimental	Prestwick	603	Monocrotaline
2096 J09	X	1195	1200	2.50217751	2114	2120	1.17042247	1863898	0.50356208	1827447	0.43707345	experimental	Prestwick	524	Tiabendazole
2096 J10	X	512	520	-0.16517159	389	400	-0.20759069	1146122	-0.60602245	1161697	-0.56986306	experimental	Prestwick	604	Piperlongumine
2096 J11	X	474	480	-0.31357461	714	720	0.05203498	1586201	0.07428011	1743333	0.30985233	experimental	Prestwick	525	Rifampicin
2096 J12	X	756	760	0.78773204	474	480	-0.1396886	1510353	-0.04297063	1580301	0.06326897	experimental	Prestwick	605	Hydrocotarnine hydrobromide
2096 J13	X	434	440	-0.46978833	555	560	-0.07498189	1736435	0.30652154	1704291	0.25080192	experimental	Prestwick	526	Ethionamide
2096 J14	X	675	680	0.47139928	394	400	-0.20359645	1446201	-0.14214093	1514226	-0.03666844	experimental	Prestwick	606	(-)-Cinchonidine
2096 J15	X	393	400	-0.62990738	555	560	-0.07498189	1683459	0.22462782	1785918	0.37426148	experimental	Prestwick	527	Tenoxicam
2096 J16	X	474	480	-0.31357461	434	440	-0.17164252	1638309	0.15483203	1503764	-0.05249205	experimental	Prestwick	607	Eburnamnone (-)
2096 J17	X	515	520	-0.15345556	554	560	-0.07578074	1716999	0.27647612	1616609	0.11818426	experimental	Prestwick	528	Trifusal
2096 J18	X	394	400	-0.62600204	674	680	0.02008105	1448221	-0.13901829	1613742	0.11384796	experimental	Prestwick	608	Cinchonine
2096 J19	X	434	440	-0.46978833	512	520	-0.10933236	1343124	-0.30148402	1621477	0.12554703	experimental	Prestwick	529	Mesoridazine besylate
2096 J20	X	434	440	-0.46978833	594	600	-0.04382681	1515148	-0.03092061	1491421	0.13017174	experimental	Prestwick	609	Anavarine sulfate monohydrate (L, +)
2096 J21	X	434	440	-0.46978833	512	520	-0.10933236	732919	0.30108628	1545575	0.01025249	experimental	Prestwick	530	Timoxine
2096 J22	X	672	680	0.45968325	833	840	0.14709791	10068563	13.1868635	10334561	13.3039509	experimental	Prestwick	610	Harmaline hydrochloride dihydrate
2096 J23	E	361	760	-0.75487835	278	640	-0.29626284	88797	-2.24050376	85397	-2.19775005	empty			
2096 J24	P	134544	135320	523.275729	121891	122560	96.8540647	1506943	-0.04824202	1441910	-0.14604526	empty			
2096 K01	N	797	800	0.9478511	637	640	-0.00947634	1397749	-0.21704117	1263653	-0.4156662	empty			
2096 K02	E	75	80	-1.87180637	76	80	-0.45763018	85126	-2.24617863	87076	-2.19521059	empty			
2096 K03	X	596	600	0.1628772	355	360	-0.23475153	1417914	-0.18586881	1275702	-0.39743227	experimental	Prestwick	371	Ketotifen fumarate
2096 K04	X	474	480	-0.31357461	394	400	-0.20359645	1643626	0.14703789	1543232	0.11101925	experimental	Prestwick	371_2009	Alizaprine HCl
2096 K05	X	395	400	-0.62099669	595	600	-0.2027976	1403231	-0.20856674	1392487	-0.22079678	experimental	Prestwick	372	Debrisoquin sulfate
2096 K06	X	469	480	-0.33310133	394	400	-0.20359645	1547853	0.0149993	1519954	-0.02800493	experimental	Prestwick	452	Lactobionic acid
2096 K07	X	434	440	-0.46978833	433	440	-0.17244137	1482219	-0.08646198	1636020	0.14754309	experimental	Prestwick	373	Amethopterin (R,S)
2096 K08	X	471	480	-0.32529064	592	600	-0.04542451	1611360	0.11317252	1750275	0.320352	experimental	Prestwick	453	Lumicolchicine gamma
2096 K09	X	472	480	-0.3213853	389	400	-0.20759069	1517306	-0.03222223	1572041	0.05077585	experimental	Prestwick	374	Methylergometrine maleate
2096 K10	X	516	520	-0.14955022	421	440	-0.18202755	1665540	0.19383574	1716238	0.26887157	experimental	Prestwick	454	Lysergol
2096 K11	X	275	280	-1.09073762	474	480	-0.05396645	1127812	-0.63037223	1282397	-0.77495295	experimental	Prestwick	375	Methiothepin maleate
2096 K12	X	274	280	-1.09465117	474	480	-0.1396886	1407306	-0.10487787	1331083	-0.31366937	experimental	Prestwick	455	Methiodoline 1,5-naphthalenedisulfonate
2096 K13	X	435	440	-0.46588298	434	440	-0.17164252	1496440	-0.06447824	1500005	-0.05817748	experimental	Prestwick	376	Clofazimine
2096 K14	X	434	440	-0.46978833	435	440	-0.17084368	1735744	0.30545335	1672182	0.20223755	experimental	Prestwick	456	Mefloquine sulfosalicylate
2096 K15	X	555	560	0.00275815	474	480	-0.1396886	1669104	0.20243693	1469932	-0.10366242	experimental	Prestwick	377	Nafrolyl oxalate
2096 K16	X	434	440	-0.46978833	435	440	-0.17084368	1758341	0.34038525	1808048	0.40773276	experimental	Prestwick	457	Meclozine dihydrochloride
2096 K17	X	515	520	-0.15345556	495	540	-0.17084368	1604406	0.10242258	1555566	0.02585767	experimental	Prestwick	378	Bezafibrate
2096 K18	X	474	480	-0.31357461	394	400	-0.20359645	1695552	0.24327867	1743921	0.26687963	experimental	Prestwick	458	Melastatin
2096 K19	X	515	520	-0.15345556	435	600	-0.04302796	1514508	0.05775018	1651255	0.02018556	experimental	Prestwick	379	Mimosine
2096 K20	X	274	280	-1.09464317	433	440	-0.17244137	1272619	-0.41047521	1255332	-0.42824158	experimental	Prestwick	459	Menadione
2096 K21	X	474	480	-0.31357461	631	640	-0.01187288	1461045	-0.11919412	1399921	-0.20955297	experimental	Prestwick	380	Cleboprine maleate
2096 K22	X	791	800	0.92441904	631	640	-0.01426943	1641923	0.16041878	1502311	-0.05468969	experimental	Prestwick	460	Dinoprost trometamol
2096 K23	E	588	1000	0.13163446	493	840	-0.12451048	89030	-2.24014358	84101	-2.19971023	empty			
2096 K24	P	139124	139880	541.162199	116875	117640	92.8470421	1409923	-0.19822181	1313049	-0.34094552	empty			
2096 L01	N	476	480	-0.30576393	556	560	-0.07418304	1184103	-0.54730896	1162769	-0.56824168	empty			
2096 L02	E	76	80	-1.86790103	76	80	-0.45763018	83050	-2.24938785	83632	-2.20041959	empty			
2096 L03	X	595	600	0.15897186	515	520	-0.10693582	1422905	-0.1781534	1548817	0.01564991	experimental	Prestwick	531	Prenperone
2096 L04	X	554	560	-0.00114719	554	560	-0.07578074	7789525	9.66377927	7755492	9.40314921	experimental	Prestwick	611	Harmalol hydrochloride dihydrate
2096 L05	X	474	480	-0.31357461	393	400	-0.2043953	1589449	0.07930108	1606999	0.10364928	experimental	Prestwick	532	Isquinoline, 6,7-dimethoxy-1-methyl-1,2,3,4-tetrahyr
2096 L06	X	594	600	0.15506652	794	800	0.11594283	1851510	0.48441191	2032128	0.74665027	experimental	Prestwick	612	Harmol hydrochloride monohydrate
2096 L07	X	511	520	-0.16907693	790	800	0.11274744	1448264	-0.13895182	1677377	0.21009491	experimental	Prestwick	533	Phenacetin
2096 L08	X	1874	1880	5.15390524	1553	1560	0.72226863	1649236	0.17172369	1626679	0.13341498	experimental	Prestwick	613	Harmine hydrochloride
2096 L09	X	591	600	0.14335049	639	600	-0.05580953	1330567	-0.32089544	1208134	-0.49962762	experimental	Prestwick	534	Atovagoune
2096 L10	X	235	240	-1.24695153	5075	5080	3.53581203	621937	-1.4163415	947335	-0.89408225	experimental	Prestwick	614	Ellipticine
2096 L11	X	314	320	-0.93842946	419	440	-0.18362525	1520495	-0.02729247	1606806	0.10335737	experimental	Prestwick	535	Methoxamine hydrochloride
2096 L12	X	676	680	0.47530462	515	520	-0.10693582	1453999	-0.13008628	1520626	-0.05506663	experimental	Prestwick	615	Chrysen-1,4-quinone
2096 L13	X	394	400	-0.62600204	475	480	-0.13888975	1633557	0.14748608	1634523	0.1452789	experimental	Prestwick	953	(S)-(-)-Atenolol
2096 L14	X	354	360	-0.78221575	314	320	-0.26750431	1492494	-0.00957822	1528213	-0.01551332	experimental	Prestwick	536	Demecarium bromide
2096 L15	X	354	360	-0.78221575	515	520	-0.10693582	1544443	0.07077279	1682226	0.21742895	experimental	Prestwick	617	Piracetam
2096 L16	X	435	440	-0.46588298	395	400	-0.2027976	1350027	-0.29081282	1454841	-0.27775357	experimental	Prestwick	537	Piizupazine dimaleate salt
2096 L17	X	383	400	-0.62980388	395	400	-0.2027976	1574508	0.05775018	1478812	-0.09203156	experimental	Prestwick	538	Reminodin
2096 L18	X	675	680	0.47139928	315	320	-0.26670546	1552408	0.02204071	1408889	-0.19598901	experimental	Prestwick	618	Sparteine (-)
2096 L19	X	554	560	-0.00114719	434	440	-0.17164252	1449682	-0.13675978	1642178	0.15685697	experimental	Prestwick	539	Thiocolchicoside
2096 L20	X	554	560	-0.00114719	715	720	0.05283382	1377727	-0.24799247	1562716	0.03667193				

2096 M13	X	634	640	0.31128023	474	480	-0.1396886	984185	-0.85635513	945049	-0.89753979	experimental	Prestwick	386	GBR 12909 dihydrochloride
2096 M14	X	834	840	1.09234878	795	800	0.11674168	1597077	0.09109294	1660770	0.10330292	experimental	Prestwick	466	Naringenine
2096 M15	X	594	600	0.15506628	474	480	-0.1396886	1444019	-0.14551401	1419116	-0.18052083	experimental	Prestwick	387	Carbetapentane citrate
2096 M16	X	453	440	-0.47362767	514	480	-0.1073467	1578600	0.062523	1733895	0.29555751	experimental	Prestwick	467	Naringin hydrate
2096 M17	X	675	680	0.7139928	435	640	-0.01077403	6307699	-0.35624628	1150221	-0.58722033	experimental	Prestwick	388	Equilinium dichloride
2096 M18	X	434	440	-0.46978833	434	440	-0.17164252	1716863	0.27626588	1592641	0.08193303	experimental	Prestwick	468	Neostigmine bromide
2096 M19	X	474	480	-0.31357461	554	560	-0.07578074	1316572	-0.34252982	1377126	-0.24403005	experimental	Prestwick	389	Ketoconazole
2096 M20	X	513	520	-0.16126625	513	520	-0.10853352	1450624	-0.13530357	1380388	-0.23096333	experimental	Prestwick	469	Niridazole
2096 M21	X	713	720	0.61980023	512	520	-0.10933236	1373349	-0.25476026	1343761	-0.29449409	experimental	Prestwick	390	Fusidic acid sodium salt
2096 M22	X	591	600	0.14335049	572	760	0.08239121	1421175	-0.18082774	1385913	-0.23073985	experimental	Prestwick	470	Ceforanide
2096 M23	E	570	960	0.06133829	750	1080	-0.1133266	86597	-2.24390467	83866	-2.20065667	empty			
2096 M24	P	131785	132520	512.500888	194620	195480	-54.953496	1271931	-0.41153876	124261	-0.47131865	empty			
2096 N01	N	315	320	-0.93452411	276	280	-0.29786054	1003072	-0.82715838	1079324	-0.69445094	empty			
2096 N02	E	77	80	-1.86399569	117	120	-0.42487741	83118	-2.24928273	77213	-2.21012822	empty			
2096 N03	X	435	440	-0.46588298	435	440	-0.17084368	1453303	-0.1311622	1311950	-0.34260774	experimental	Prestwick	541	Ciclopirox ethanalamine
2096 N04	X	474	480	-0.31357461	434	440	-0.17164252	1225454	-0.48338591	1143839	-0.59687301	experimental	Prestwick	621	Methoxy-6-harmaline
2096 N05	X	555	560	0.00275815	475	480	-0.13888975	1450686	-0.13520773	1426890	-0.16876278	experimental	Prestwick	542	Probencid
2096 N06	X	314	320	-0.93842946	475	480	-0.13888975	1220556	-0.49095756	1333828	-0.3095176	experimental	Prestwick	622	Stachyridine hydrochloride
2096 N07	X	315	320	-0.93452411	435	440	-0.17084368	1550818	0.01958279	1523880	-0.02206691	experimental	Prestwick	543	Betahistine mesylate
2096 N08	X	474	480	-0.31357461	435	440	-0.17084368	1357161	-0.27978472	1331268	-0.31338956	experimental	Prestwick	623	Pyridoxine hydrochloride
2096 N09	X	595	600	0.15897186	315	320	-0.26670546	1517486	-0.03194397	1512076	-0.03992028	experimental	Prestwick	544	Troxarycin
2096 N10	X	473	480	-0.31747996	473	480	-0.14048744	1319618	-0.33782112	1306837	-0.35034107	experimental	Prestwick	624	Cytisine (-)
2096 N11	X	474	480	-0.31357461	433	440	-0.17244137	1567839	0.04589495	1662876	0.18816237	experimental	Prestwick	545	Tetramisole hydrochloride
2096 N12	X	354	360	-0.78221575	555	560	-0.07498189	1400110	-0.21339138	1308024	-0.34854575	experimental	Prestwick	625	Pseudopelletierine hydrochloride
2096 N13	X	714	720	0.62370765	314	320	-0.26750431	1522497	-0.02419765	1488016	-0.07631065	experimental	Prestwick	546	Progrenolone
2096 N14	X	354	360	-0.78221575	395	400	-0.2027976	1346439	-0.3059467	1307875	-0.45533598	experimental	Prestwick	626	Acetazolil
2096 N15	X	474	480	-0.31357461	275	280	-0.29865939	1492489	-0.07058895	1440412	-0.14831096	experimental	Prestwick	547	Molodomin
2096 N16	X	594	600	0.15506652	476	480	-0.1380909	1561917	0.03674034	1491643	-0.07082487	experimental	Prestwick	627	Folic acid
2096 N17	X	434	440	-0.46978833	314	320	-0.26750431	1441129	-0.14998156	1368299	-0.25738075	experimental	Prestwick	548	Chloroquine diphosphate
2096 N18	X	395	400	-0.62209669	395	400	-0.2027976	1358949	-0.27702071	1199644	-0.51246881	experimental	Prestwick	628	Salsolinol hydrochloride
2096 N19	X	394	400	-0.62600204	595	600	-0.04302796	1459824	-0.12108162	1473820	-0.09778188	experimental	Prestwick	549	Trimetazidine dihydrochloride
2096 N20	X	554	560	-0.00114719	472	480	-0.14128629	1326559	-0.32709127	1229051	-0.46799118	experimental	Prestwick	629	Gramine
2096 N21	X	674	680	0.46749394	874	880	0.17985069	1222204	-0.48840997	1188511	-0.52393073	experimental	Prestwick	550	Parthenolide
2096 N22	X	434	440	-0.46978833	474	480	-0.16126625	1271149	-0.8749826	1368986	-0.86609347	experimental	Prestwick	630	Dimethisoquin hydrochloride
2096 N23	E	303	680	-0.98138823	463	920	-0.14847593	83603	-2.24853299	146218	-2.10575924	empty			
2096 N24	P	127336	128160	495.126018	154238	155280	122.694408	1351223	-0.28896406	1395154	-0.21676298	empty			
2096 O01	N	917	920	1.41649223	437	440	-0.16924598	1254583	-0.43835642	1133313	-0.61279342	empty			
2096 O02	E	115	120	-1.71559266	77	80	-0.45683134	79571	-2.25476591	82254	-2.20250379	empty			
2096 O03	X	715	720	0.62761299	394	400	-0.20359645	1211490	-0.50497237	1206624	-0.50191167	experimental	Prestwick	391	Terbutaline hemisulfate
2096 O04	X	754	760	0.77992136	795	800	0.11674168	1112997	-0.65722921	999092	-0.81580059	experimental	Prestwick	471	Strophantine octahydrate
2096 O05	X	435	440	-0.46978833	714	720	-0.26750431	1240103	-0.46107054	1233357	-0.75278426	experimental	Prestwick	392	Chlorazepate dihydrochloride
2096 O06	X	555	560	0.00275815	355	360	-0.23164252	1238121	-0.46380445	1183501	-0.55888485	experimental	Prestwick	472	Pantothenic acid calcium salt monohydrate
2096 O07	X	473	480	-0.31747996	395	400	-0.2027976	1343773	-0.30048076	1264411	-0.41450973	experimental	Prestwick	393	Heximicholium bromide
2096 O08	X	635	640	0.31518557	555	560	-0.07498189	1534849	-0.00510313	1443426	-0.14375233	experimental	Prestwick	473	Cefotaxim
2096 O09	X	432	440	-0.47759901	432	440	-0.17324022	1294138	-0.37720975	1151882	-0.58470809	experimental	Prestwick	394	Kanamycin A sulfate
2096 O10	X	1114	1120	2.18584475	1475	1480	0.65995846	1280803	-0.39782385	1233350	-0.46148901	experimental	Prestwick	474	Piperine
2096 O11	X	474	480	-0.31357461	392	400	-0.20519415	1258700	-0.4319921	1239727	-0.45184349	experimental	Prestwick	395	Amikacin hydrate
2096 O12	X	474	480	-0.31357461	554	560	-0.1396886	1221149	-0.49004086	1188086	-0.61798426	experimental	Prestwick	475	Riboflavin
2096 O13	X	632	640	0.30347804	554	560	-0.07578074	1167557	-0.45195667	1744004	-0.55064392	experimental	Prestwick	396	Etoposide
2096 O14	X	235	240	-1.24695153	194	200	-0.36336609	564669	-1.50487007	489720	-1.58621781	experimental	Prestwick	476	Primaquine diphosphate
2096 O15	X	475	480	-0.30966927	516	520	-0.10613697	1145158	-0.60751266	975092	-0.85210022	experimental	Prestwick	397	Clomiphene citrate (Z,E)
2096 O16	X	593	600	0.15116117	353	360	-0.23634923	1397306	-0.21772599	1327732	-0.31873771	experimental	Prestwick	477	Progesterone
2096 O17	X	474	480	-0.31357461	595	600	-0.04302796	1323648	-0.33159128	1523199	-0.02309691	experimental	Prestwick	398	Oxantel pamoate
2096 O18	X	595	600	0.15897186	315	320	-0.26670546	1470157	-0.1051082	1457530	-0.12242025	experimental	Prestwick	478	Felodipin
2096 O19	X	554	560	-0.00114719	435	440	-0.17084368	1064663	-0.73194703	995496	-0.82123949	experimental	Prestwick	399	Prochlorperazine dimaleate
2096 O20	X	554	560	-0.00114719	634	640	-0.01187288	1504110	-0.05262146	1381886	-0.23683063	experimental	Prestwick	479	Methoxy- β -psoralen
2096 O21	X	434	440	-0.46978833	552	560	-0.07737843	1253325	-0.44030112	1235231	-0.45864403	experimental	Prestwick	400	Hesperidin
2096 O22	X	394	400	-0.62600204	432	440	-0.17324022	649414	-1.37386577	574537	-1.45793342	experimental	Prestwick	480	Puromycin dihydrochloride
2096 O23	E	236	680	-1.24304619	520	1000	-0.10294158	82238	-2.25064309	95467	-2.18251933	empty			
2096 O24	P	150463	151360	585.44488	162484	163440	129.28171	1235401	-0.46800092	1099799	-0.66348282	empty			
2096 P01	N	517	520	-0.14564488	518	520	-0.10453927	751292	-1.21637618	893861	-0.97496084	empty			
2096 P02	E	117	120	-1.70778198	196	200	-0.3617684	75030	-2.26178568	89367	-2.19174549	empty			
2096 P03	X	436	440	-0.46197764	677	680	0.02247759	1138298	-0.61011729	1153351	-0.58248626	experimental	Prestwick	551	Hexetidine
2096 P04	X	515	520	-0.15345556	434	440	-0.17164252	1105742	-0.68844446	1095324	-0.67025119	experimental	Prestwick	631	Thiamine hydrochloride
2096 P05	X	596	600	0.1628772	437	440	-0.16924598	1227610	-0.48005303	1287056	-0.38025952	experimental	Prestwick	552	Selegrin hydrochloride
2096 P06	X	514	520	-0.15713609	356	360	-0.23935268	1092456	-0.68898282	1111557	-0.64569903	experimental	Prestwick	632	Dipivefrin hydrochloride
2096 P07	X	916	920	1.41258688	516	520	-0.10613697	1163781	-0.57872402	1083375	-0.68832387	experimental	Prestwick	553	Pentamidine isethionate
2096 P08	X	474	480	-0.31357461	475	480	-0.10693582	1175512	-0.56058948	1152156	-0.58429367	experimental	Prestwick	633	Thiorphan
2096 P09	X	555	560	0.00275815	516	520	-0.1380909	1277501	-0.40292893	1190392	-0.52646232	experimental	Prestwick	554	Tolazamide
2096 P10	X	474	480	-0.31357461	474	480	-0.1396886	2164147	-0.96770639	2958977	-0.83283235	experimental	Prestwick	634	Riboflavin
2096 P11	X	115	120	-1.71559266	196	200	-0.3617684	598898	-1.45195667	550043	-1.49489021	experimental	Prestwick	555	Nifuroxazide
2096 P12	X	434	440	-0.46978833	515	520	-0.10693582	1115715	-0.65302755	1073478	-0.70329292	experimental	Prestwick	635	Hydroquinone hydrobromide hydrate
2096 P13	X	1516	1520	3.75579254	1195	1200	0.43628097	1221954	-0.48879644	1195716	-0.51840985	experimental	Prestwick	556	Myophenolic acid
2096 P14	X	354	360	-0.78221575	714	720	0.05203498	1062890	-0.73468785	1126367	-0.62329914	experimental	Prestwick		

2097 A07	X	995	1000	2.07610866	674	680	-0.0622339	1816201	-0.25461035	1871876	-0.52660028	experimental	Prestwick	643	Flunisolide
2097 A08	X	513	520	0.04832807	554	560	-0.06929265	1726605	-0.37437983	1987655	-0.37944001	experimental	Prestwick	723	Phenethicillin potassium salt
2097 A09	X	635	640	0.56158374	715	720	-0.05982216	1817248	-0.25231075	1900685	-0.48998276	experimental	Prestwick	644	N-Acetyl-DL-homocysteine Thiolactone
2097 A10	X	515	520	0.0567421	635	640	-0.06452799	1844950	-0.21617948	2003193	-0.35969052	experimental	Prestwick	724	Sulfamethoxyypyridazine
2097 A11	X	474	480	-0.11574546	553	560	-0.06935747	1900327	-0.14705302	1941701	-0.06924662	experimental	Prestwick	645	Flurandrenolide
2097 A12	X	676	680	0.7340713	954	960	-0.04576348	1753600	-0.33829365	2096916	-0.24056441	experimental	Prestwick	725	Deferoxamine mesylate
2097 A13	X	555	560	0.22502264	954	960	-0.04576348	1654257	-0.47109265	1708218	-0.7346169	experimental	Prestwick	646	Helveticoside
2097 A14	X	515	520	0.0567421	634	640	-0.07399848	1820817	-0.24843981	2100105	-0.35101945	experimental	Prestwick	726	Mephentermine hemisulfate
2097 A15	X	596	600	0.39751021	474	640	-0.06458681	1858523	-0.19803546	1980506	-0.38852671	experimental	Prestwick	647	Myosmine
2097 A16	X	474	480	-0.11574546	670	680	-0.06246919	1896496	-0.14727242	2282289	-0.00494706	experimental	Prestwick	727	Ergocryptine-alpha
2097 A17	X	596	600	0.39751021	1194	1200	-0.03164599	1878156	-0.17179061	1989483	-0.37711654	experimental	Prestwick	648	Betonicine
2097 A18	X	515	520	0.0567421	553	560	-0.06935147	1868675	-0.18448455	1992705	-0.38613842	experimental	Prestwick	728	Sulfadiazinone
2097 A19	X	556	560	0.22922966	675	680	-0.06217507	1865708	-0.18843075	1961833	-0.41226092	experimental	Prestwick	649	Etanidazole
2097 A20	X	509	520	0.03150001	0	440	-0.10188053	1659649	-0.46388478	2242624	-0.05536304	experimental	Prestwick	729	Sulfanilamide
2097 A21	X	755	760	1.06642538	1154	1160	-0.0339989	1683132	-0.43249334	1926737	-0.45686951	experimental	Prestwick	650	Butirosin disulfate salt
2097 A22	X	396	400	-0.44389253	553	560	-0.06935147	1845903	-0.21490553	1710536	-0.73167062	experimental	Prestwick	730_2009	Balsalazide Sodium
2097 A23	E	142	400	-1.51247401	238	600	-0.08788068	1577449	-0.57376748	1816228	-0.59733137	empty			
2097 A24	P	88341	88480	369.541926	123794	124080	7.18004203	1538784	-0.62545379	1545678	-0.94121249	empty			
2097 B01	N	434	440	-0.28402601	594	600	-0.06693973	1666135	-0.45521447	1805435	-0.61104976	empty			
2097 B02	E	116	120	-1.62185636	236	240	-0.08799833	1892118	-0.15312659	2270760	-0.01960093	empty			
2097 B03	X	595	600	0.39330319	513	520	-0.07170438	1797460	-0.27966281	2090363	-0.24889356	experimental	Prestwick	801	Carbinoxamine maleate salt
2097 B04	X	554	560	0.22081563	552	560	-0.06941029	2018633	0.01599519	2285716	-0.00059119	experimental	Prestwick	881	Niacin
2097 B05	X	514	520	0.05253508	634	640	-0.06458681	1960722	-0.06141864	2228552	-0.07324918	experimental	Prestwick	802	Methazolamide
2097 B06	X	354	360	-0.62058711	512	520	-0.07176321	2072596	0.08813145	2318580	0.04152326	experimental	Prestwick	882	Bemegride
2097 B07	X	712	720	0.88552379	794	800	-0.05517515	2067133	0.08082866	2366035	0.10149784	experimental	Prestwick	803	Pyritihedione
2097 B08	X	713	720	0.88552379	593	600	-0.06699855	1707455	-0.4018006	1995844	-0.23695504	experimental	Prestwick	883	Xyloxygennin
2097 B09	X	674	680	0.72565727	473	480	-0.07405725	1039857	0.04436411	2276477	-0.01233457	experimental	Prestwick	804	Spesoxanone dihydrochloride
2097 B10	X	473	480	-0.11995248	353	360	-0.08111605	2055954	0.06588488	2318892	0.04157699	experimental	Prestwick	884	Meglumine
2097 B11	X	714	720	0.89393782	714	720	-0.05988098	1992767	-0.01858177	2232406	-0.06835057	experimental	Prestwick	805	Promidic acid
2097 B12	X	273	280	-0.96135521	632	640	-0.06470446	1416653	-0.78871517	1617560	-0.84984726	experimental	Prestwick	885	Cantharidin
2097 B13	X	395	400	-0.44809954	472	480	-0.07411612	1731683	-0.3675917	1980133	-0.38900081	experimental	Prestwick	806	Trimipramine maleate salt
2097 B14	X	395	400	-0.44809954	433	440	-0.07641022	2176159	0.22657163	1777103	-0.13864315	experimental	Prestwick	886	Clioquinol
2097 B15	X	472	480	-0.12415949	750	760	-0.05776336	2267508	0.34866447	2035017	-0.13192408	experimental	Prestwick	807	Chloropyramine hydrochloride
2097 B16	X	395	400	-0.44809954	674	680	-0.06458681	1901259	-0.14697322	2251091	-0.27210358	experimental	Prestwick	887	Proxiphetone
2097 B17	X	393	400	-0.45651357	708	720	-0.06023392	1976336	-0.04054628	2262002	-0.03073274	experimental	Prestwick	808	Furazolidone
2097 B18	X	395	400	-0.44809954	393	400	-0.07876313	1740062	-0.35639088	2003390	-0.35944012	experimental	Prestwick	888	Promethazine hydrochloride
2097 B19	X	430	440	-0.30085407	0	800	-0.10188053	1725206	-0.37624998	2476642	0.24208427	experimental	Prestwick	809	Dichlorphenamide
2097 B20	X	2314	2320	7.62515971	304832	304840	17.82922229	1885358	-0.16216317	1814949	-0.59895704	experimental	Prestwick	889	Chrysin
2097 B21	X	869	880	1.54602494	71	960	-0.09770411	1603631	-0.53876811	1677163	-0.77408919	experimental	Prestwick	810	Sulconazole nitrate
2097 B22	X	354	360	-0.62058711	591	600	-0.0671162	1766459	-0.3211041	2003374	-0.35946046	experimental	Prestwick	890	Proxiphetone
2097 B23	E	138	400	-1.5293206	271	280	-0.07641022	1564888	-0.01705918	1871097	-0.27210358	empty			
2097 B24	P	4732	47760	197.016502	97458	98080	5.63088204	1655022	-0.47007002	1834823	-0.57384758	empty			
2097 C01	N	517	520	0.06515612	517	520	-0.07146909	1770698	-0.31543752	1853202	-0.55033577	empty			
2097 C02	E	76	80	-1.79013691	35	40	-0.09982173	1954682	-0.06949275	1957621	-0.41761456	empty			
2097 C03	X	635	640	0.56158374	674	680	-0.0622339	1964089	-0.05691773	2091624	-0.24729078	experimental	Prestwick	651	Glimepiride
2097 C04	X	594	600	0.38909618	674	680	-0.0622339	1781749	-0.30066484	2213356	-0.09256397	experimental	Prestwick	731	Sulfaxoquinoline sodium salt
2097 C05	X	474	480	-0.11574546	354	360	-0.08105723	2080187	0.09927889	2142553	-0.18255774	experimental	Prestwick	652	Picrotoxinin
2097 C06	X	440	440	-0.28402601	433	440	-0.07641022	1993906	-0.01705918	2145162	-0.18375328	experimental	Prestwick	732	Treprozolinol
2097 C07	X	554	560	0.22081563	394	400	-0.07870431	102899107	0.0889107	2122260	-0.20842732	experimental	Prestwick	653	Meprozolate bromide
2097 C08	X	473	480	-0.11995248	434	440	-0.07635139	2113559	0.14288967	2232306	-0.08004418	experimental	Prestwick	733	Metoprolol-(+,-)-tartrate salt
2097 C09	X	354	360	-0.62058711	634	640	-0.06458681	1998046	-0.01152494	2212436	-0.09373334	experimental	Prestwick	654	Betnamine
2097 C10	X	432	440	-0.29244004	474	480	-0.07399848	1971017	-0.04765657	2277220	-0.01138998	experimental	Prestwick	734	Flumethasone
2097 C11	X	754	760	1.06221837	474	480	-0.07399848	2102073	0.1275355	2331372	0.05743963	experimental	Prestwick	655	Halcinonide
2097 C12	X	515	520	0.0567421	633	640	-0.07641022	2047754	0.05492335	2146125	-0.17801757	experimental	Prestwick	735	Flonaidic acetate
2097 C13	X	395	400	-0.44809954	474	680	-0.0622339	1851554	-0.20735143	1869652	-0.52947209	experimental	Prestwick	656	Lanatoside C
2097 C14	X	354	360	-0.62058711	674	680	-0.0622339	1901434	-0.14067322	2510892	0.28561755	experimental	Prestwick	736	Cefazolin sodium salt
2097 C15	X	915	920	1.73954757	674	680	-0.0622339	1830315	-0.23574315	2030740	-0.32467705	experimental	Prestwick	657	Benzamil hydrochloride
2097 C16	X	512	520	0.04412106	350	360	-0.08129252	1947619	-0.07893437	2329882	0.05554577	experimental	Prestwick	737	Attractyliside potassium salt
2097 C17	X	355	360	-0.61638009	474	720	-0.05988098	1875899	-0.1748077	2163211	-0.15630051	experimental	Prestwick	658	Sulixibuzone
2097 C18	X	395	400	-0.44809954	714	480	-0.07399848	2021364	0.01964592	2235460	-0.0644688	experimental	Prestwick	738	Folic acid calcium salt
2097 C19	X	316	320	-0.78045363	433	440	-0.07641022	1901089	-0.1411344	2396438	0.14014141	experimental	Prestwick	659	Levononandrin
2097 C20	X	310	320	-0.80569571	0	640	-0.10188053	2196586	0.25387789	2365130	0.10034755	experimental	Prestwick	739	Levononandrin
2097 C21	X	394	400	-0.45230656	349	360	-0.08135134	1734455	-0.36386117	1871097	-0.52759043	experimental	Prestwick	660	Avermectin B1
2097 C22	X	635	640	0.56158374	1113	1120	-0.03641064	1680083	-0.43656916	1816525	-0.59695387	experimental	Prestwick	740	Ebisenel
2097 C23	E	185	360	-1.33157242	173	440	-0.09170417	1756196	-0.33482339	2098389	-0.23869216	empty			
2097 C24	P	58689	59000	244.795556	89518	90040	5.16382818	1826841	-0.24038709	1994992	-0.3712583	empty			
2097 D01	N	437	440	-0.27140497	557	560	-0.06911618	1759607	-0.33026366	2013973	-0.34598866	empty			
2097 D02	E	157	160	-1.4493688	115	120	-0.0951159	2173953	0.23622271	2311997	0.03281314	empty			
2097 D03	X	436	440	-0.27561198	835	840	-0.06276341	1931745	-0.1001543	2269299	-0.02145793	experimental	Prestwick	811	Bergenin monohydrate
2097 D04	X	440	440	-0.28402601	553	560	-0.06935147	2147643	0.18457262	21436150	0.19061714	experimental	Prestwick	891	7-Acetyloumarin
2097 D05	X	474	480	-0.11574546	353	360	-0.08111605	2125571	0.16028322	2343015	0.0722384	experimental	Prestwick	812	Chromolone disodium salt
2097 D06	X	515	520	0.0567421	1195	1200	-0.03158716	11642497	12.8809127	11706164	11.9732184	experimental	Prestwick	892	Esculin Hydrate
2097 D07	X	474	480	-0.11574546	553	560	-0.06935147	2137176	0.17446023	2297024	0.01378179	experimental	Prestwick	813	Bucadesine sodium salt
2097 D08	X	634	640	0.55737673	474	480	-0.07399848	2272656	0.35556618	2437638	0.19250845				

2097 H19	X	475	480	-0.11153845	831	840	-0.0529987	2067538	0.08137006	2354261	0.08653256	experimental	Prestwick	839	Ganciclovir
2097 H20	X	474	480	-0.11574546	710	720	-0.06011627	1997155	-0.01271601	2377428	0.11597886	experimental	Prestwick	919	Bacitracin
2097 H21	X	515	520	0.0567421	871	880	-0.05064578	1735089	-0.36303865	2352816	0.08469591	experimental	Prestwick	840	Etifopazine hydrochloride
2097 H22	X	475	480	-0.11153845	790	800	-0.05541044	2010087	0.00457114	2493961	0.01243066	experimental	Prestwick	920	L(-)-vesamicol hydrochloride
2097 H23	E	258	480	-1.02446042	465	720	-0.07452788	1781800	-0.30059667	2042979	-0.30912074	empty			
2097 H24	P	74951	75240	313.210012	85435	85960	4.92365426	1922038	-0.11313035	2137135	-0.18944426	empty			
2097 I01	N	557	560	0.23343667	994	1000	-0.04341057	1921108	-0.11437355	1967343	-0.40525747	empty			
2097 I02	E	117	120	-1.61764935	392	400	-0.07882196	1899784	-0.14287889	2172586	-0.14438446	empty			
2097 I03	X	434	440	-0.28402601	789	800	-0.05546926	2007097	0.00057419	2203320	-0.10532018	experimental	Prestwick	681	Austricrine hydrate
2097 I04	X	1115	1120	2.58095031	1671	1680	-0.00358746	2033768	0.03622725	2286562	0.00048412	experimental	Prestwick	762	Butamben
2097 I05	X	393	400	-0.45651357	670	680	-0.06246919	2201391	0.26030108	2364102	0.09904091	experimental	Prestwick	681	beta-Belladonnine dichloroethylate
2097 I06	X	433	440	-0.28823302	588	600	-0.06729267	2155036	0.19833498	2473266	0.23703006	experimental	Prestwick	762	Sulfapyridine
2097 I07	X	355	360	-0.61638009	752	760	-0.05764571	2103349	0.12942122	2231582	-0.06939792	experimental	Prestwick	683	Pempidine tartrate
2097 I08	X	594	600	0.38909618	712	720	-0.05998663	2121586	0.15361994	2500438	0.27233005	experimental	Prestwick	763	Meclofenoxate hydrochloride
2097 I09	X	434	440	-0.28402601	752	760	-0.05764571	2104654	0.13098571	2256166	-0.03815055	experimental	Prestwick	684	Heliotrine
2097 I10	X	476	480	-0.10733144	752	760	-0.05764571	1951359	-0.07393484	2258376	-0.03534155	experimental	Prestwick	764	Furaltadone hydrochloride
2097 I11	X	355	360	-0.61638009	913	920	-0.04817522	2569132	0.75188716	2812694	0.66922135	experimental	Prestwick	685	Nitratine dihydrochloride
2097 I12	X	315	320	-0.78466064	629	640	-0.06488093	2215527	0.27919769	2328055	0.05322357	experimental	Prestwick	765	Ethoxyquin
2097 I13	X	633	640	0.55316971	1151	1160	-0.03417537	1669148	-0.4518677	1841387	-0.56535316	experimental	Prestwick	686	Lycorine hydrochloride
2097 I14	X	514	520	0.05253508	791	800	-0.05535162	2124300	0.15724794	2271972	-0.01806042	experimental	Prestwick	766	Tinidazole
2097 I15	X	395	400	-0.44809954	792	800	-0.05529279	2105535	0.1321634	2346207	0.07629557	experimental	Prestwick	687	Karakolone
2097 I16	X	434	440	-0.28402601	591	600	-0.0671162	2033528	0.03590642	2276184	-0.01270678	experimental	Prestwick	767	Guanadrel sulfate
2097 I17	X	356	360	-0.61217308	910	920	-0.04835169	2014137	0.00998506	2365326	0.10059667	experimental	Prestwick	688	Estropipate
2097 I18	X	395	400	-0.44809954	791	1160	-0.03417537	2000025	-0.00887947	2637065	0.44598906	experimental	Prestwick	768	Vidarabine
2097 I19	X	474	480	-0.11574546	750	760	-0.05776336	2067085	0.0807645	2306779	0.02618083	experimental	Prestwick	689	Ungerine nitrate
2097 I20	X	475	480	-0.11574546	831	840	-0.05249987	2099864	0.12294927	2249382	0.04767544	experimental	Prestwick	769	Sulfamerazine
2097 I21	X	313	320	-0.79307467	909	920	-0.04841051	1940756	-0.08810864	2408524	0.15550326	experimental	Prestwick	690	Napellacine
2097 I22	X	395	400	-0.44809954	712	720	-0.05998663	1963002	-0.05837008	2089341	-0.25019257	experimental	Prestwick	770	Isopropamide iodide
2097 I23	E	161	320	-1.43254075	316	560	-0.0832925	1962403	-0.05917153	2078046	-0.26454902	empty			
2097 I24	P	53361	53720	222.380587	81385	81960	4.6854215	1913383	-0.12470012	2064353	-0.28195343	empty			
2097 J01	N	396	400	-0.44389253	834	840	-0.05282223	1571082	-0.58227871	2079454	-0.26275939	empty			
2097 J02	E	117	120	-1.61764935	433	440	-0.07641022	1860362	-0.19557714	2572696	0.36417319	empty			
2097 J03	X	316	320	-0.78045363	712	720	-0.05998663	1866007	-0.18803106	2209685	-0.09722998	experimental	Prestwick	841	Securinine
2097 J04	X	314	320	-0.78045363	709	720	-0.06017537	1860175	-0.18803106	2209685	-0.09722998	experimental	Prestwick	842	Nitrazidone
2097 J05	X	355	360	-0.61638009	511	520	-0.07182203	1797679	-0.27937006	2201585	-0.10752544	experimental	Prestwick	922	Trimiprazine tartrate
2097 J06	X	392	400	-0.46072059	950	960	-0.04599878	1947702	-0.07882342	2427691	0.17986537	experimental	Prestwick	922	Thiopromazine maleate
2097 J07	X	435	440	-0.2798119	711	720	-0.06005745	2260401	0.33918403	2482651	0.24972198	experimental	Prestwick	843	Nafclillin sodium salt monohydrate
2097 J08	X	475	480	-0.11153845	471	480	-0.07417495	2263593	0.34345101	2759389	0.60146832	experimental	Prestwick	923	Xamoterol hemifumarate
2097 J09	X	436	440	-0.27561198	673	680	-0.06229272	1995469	-0.01496891	2158519	-0.16226425	experimental	Prestwick	844	Procyclidine hydrochloride
2097 J10	X	355	360	-0.61638009	593	600	-0.06698955	2034041	0.03659219	2449717	0.2078614	experimental	Prestwick	924	Rolipram
2097 J11	X	394	400	-0.45230656	430	440	-0.28402601	22155915	0.15940683	2445212	0.26252545	experimental	Prestwick	845	Altiprosone hydrochloride
2097 J12	X	435	440	-0.2798119	753	760	-0.05758689	1700517	-0.40925355	1926661	-0.45696611	experimental	Prestwick	925	Nitrazidone bromide
2097 J13	X	394	400	-0.45230656	709	720	-0.06017537	2042278	0.04760318	2261258	-0.0316784	experimental	Prestwick	846	Ethinylestradiol 3-methyl ether
2097 J14	X	395	400	-0.44809954	632	640	-0.06470446	2076376	0.09318445	2446523	0.20380168	experimental	Prestwick	926	Idoxazon hydrochloride
2097 J15	X	395	400	-0.44809954	671	680	-0.06241037	2043779	0.04960968	2168330	-0.14979403	experimental	Prestwick	847	(-)-Levonulolol hydrochloride
2097 J16	X	516	520	0.06094911	793	800	-0.05523397	2126551	0.16025702	2501687	0.27391759	experimental	Prestwick	927_2009	Quinapril HCl
2097 J17	X	355	360	-0.61638009	831	840	-0.0529987	2124168	0.15707149	2456400	0.21635579	experimental	Prestwick	848	Idoxianol
2097 J18	X	356	360	-0.61217308	710	720	-0.06011627	2107032	0.08059163	2308551	0.20075743	experimental	Prestwick	928	Nitrazidone
2097 J19	X	435	440	-0.2798119	711	720	-0.06005745	2145007	0.18495523	2135308	-0.10547186	experimental	Prestwick	849	Rolisticycline
2097 J20	X	553	560	0.21660862	869	880	-0.05076343	2107373	0.13462039	2429552	0.18223078	experimental	Prestwick	929	Ketorolac tromethamine
2097 J21	X	915	920	1.73954757	1350	1360	-0.02246961	1970469	-0.04838912	2117048	-0.21497574	experimental	Prestwick	850	Equilin
2097 J22	X	473	480	-0.11995248	630	640	-0.0648221	1753727	-0.33812388	1964423	-0.40896892	experimental	Prestwick	930	Protriptyline hydrochloride
2097 J23	E	216	360	-1.20115499	429	760	-0.07664551	1920553	-0.11511546	2123687	-0.20653727	empty			
2097 J24	P	48174	48480	200.558807	111594	112160	6.46240261	1881811	-0.1669047	2333323	0.05991943	empty			
2097 K01	N	677	680	0.73827831	794	800	-0.05517515	1893755	-0.15093829	1894185	-0.49824445	empty			
2097 K02	E	36	40	-1.95841746	352	360	-0.08117487	2101834	0.12721601	2117154	-0.21484101	empty			
2097 K03	X	397	400	-0.43968552	831	840	-0.0529987	2008436	0.00236412	2169273	-0.14859543	experimental	Prestwick	691	Fillalbin
2097 K04	X	395	400	-0.44809954	711	720	-0.06005745	2051087	0.05937881	2494481	0.26475844	experimental	Prestwick	771	Alclometasone dipropionate
2097 K05	X	432	440	-0.29244004	749	760	-0.05782218	1981443	-0.03371938	2308716	-0.3145392	experimental	Prestwick	692_2009	Citalopram Hydrobromide
2097 K06	X	1595	1600	4.60031687	1630	1640	-0.0059992	2043668	0.0494613	2325846	0.05041583	experimental	Prestwick	772	Leflunomide
2097 K07	X	512	520	0.04412106	868	880	-0.05082225	1764650	-0.32352232	1830763	-0.57885674	experimental	Prestwick	693	Promazine hydrochloride
2097 K08	X	355	360	-0.61638009	872	880	-0.05058696	2157278	0.20133203	2508065	0.28202431	experimental	Prestwick	773	Norgestrel-(1-)-D
2097 K09	X	196	200	-1.28529527	630	640	-0.06470446	2001172	-0.00734619	2148550	-0.17493529	experimental	Prestwick	694	Sulfamerazine
2097 K10	X	275	280	-0.95294119	631	640	-0.06476328	2129477	0.16416841	2433559	0.18745096	experimental	Prestwick	774	Fluocinonide
2097 K11	X	875	880	1.57126702	1192	1200	-0.03176363	1988235	-0.02464002	2200268	-0.36073913	experimental	Prestwick	695	Acacetin
2097 K12	X	474	480	-0.11574546	628	640	-0.06493975	2021278	0.01953096	2453407	0.21255155	experimental	Prestwick	775	Sulfamethazine sodium salt
2097 K13	X	475	480	-0.11153845	1112	1120	-0.03646947	1945274	-0.08206911	2130489	-0.19789163	experimental	Prestwick	696	Ethotoin
2097 K14	X	354	360	-0.62058711	589	600	-0.06723384	2060956	0.07257142	2331214	0.0572388	experimental	Prestwick	776	Guaifenesin
2097 K15	X	356	360	-0.61217308	750	760	-0.05764571	1801328	-0.27449217	2283647	-0.00322098	experimental	Prestwick	697	3-alpha-Hydroxy-5-beta-androstan-17-one
2097 K16	X	155	160	-0.45778283	391	400	-0.0788007	1102023	-1.21173685	1914022	-1.54452143	experimental	Prestwick	777	Hexidine dihydrochloride
2097 K17	X	357	360	-0.60796606	632	640	-0.06470446	2064072	0.18495523	2203240	-0.10547186	experimental	Prestwick	698	Tetracycline hydrochloride
2097 K18	X	276	280	-0.94873417	791	800	-0.05535162	1926317	-0.1074103	2056620	-0.29178242	experimental	Prestwick	778	Proadifen hydrochloride
2097 K19	X	276	280	-0.94873417	711	720	-0.06005745	1573730	-0.57873894	1743415	-0.68987994	experimental	Prestwick	699	Hexestrol
2097 K20	X	315	320	-0.78466064	749	760	-0.05782218	1891829	-0.15351292						

2097 L13	X	595	600	0.39330319	948	960	-0.04611642	2135104	0.17169043	2420296	0.17046599	experimental	Prestwick	856	Tolmetin sodium salt dihydrate
2097 L14	X	675	680	0.72986429	1230	1240	-0.02952836	2085124	0.10487854	2420503	0.1707291	experimental	Prestwick	856	Benphenium hydroxynaphthoate
2097 L15	X	435	440	-0.279819	989	1000	-0.04370468	2005949	-0.00156866	2118257	-0.21343904	experimental	Prestwick	857	(+)-Levobunolol hydrochloride
2097 L16	X	356	360	-0.61217308	750	760	-0.05776339	2085705	-0.10585576	2289896	0.00346345	experimental	Prestwick	857	Denhydroacetonacetone 3-acetate
2097 316	P	4633	4720	-0.78043963	790	800	-0.05541105	1951363	-0.07383593	2245533	-0.05166555	experimental	Prestwick	858	Hexoxazin mesylate
2097 L18	X	357	360	-0.60796606	1030	1040	-0.04129294	2023374	0.02233283	2438844	0.19404133	experimental	Prestwick	938	Benserazide hydrochloride
2097 L19	X	276	280	-0.94873417	748	760	-0.057881	2212158	0.27469411	2332731	0.05916697	experimental	Prestwick	859	Fluvastatin sodium salt
2097 L20	X	275	280	-0.95294119	1030	1040	-0.04129294	1948641	-0.07756819	2288133	0.00248093	experimental	Prestwick	939	Iodipamide
2097 L21	X	475	480	-0.11153845	786	800	-0.05564573	2030506	0.03186669	2444554	0.20129899	experimental	Prestwick	860	Methylhydantoin-5-(L)
2097 L22	X	512	520	0.04412106	1346	1360	-0.02270491	8866291	0.16975667	9872543	0.64260429	experimental	Prestwick	940	Esculetin
2097 L23	E	218	360	-1.19274097	516	800	-0.07152792	1960747	-0.06138522	2392060	0.13457678	empty			
2097 L24	P	47633	47920	198.282815	94419	95040	5.4520604	1819605	-0.25005998	1993438	-0.3714032	empty			
2097 M01	N	437	440	-0.27140497	1073	1080	-0.03876356	1826161	-0.2412961	1905072	-0.48440669	empty			
2097 M02	E	117	120	-1.61764935	470	480	-0.07423377	1934740	-0.09615067	2006533	-0.35544523	empty			
2097 M03	X	276	280	-0.94873417	870	880	-0.05070461	1860226	-0.19575894	2096395	-0.24122662	experimental	Prestwick	701	Trihexyphenidyl-D,L Hydrochloride
2097 M04	X	475	480	-0.11153845	910	920	-0.04835169	1594220	-0.55134847	2184981	-0.12862986	experimental	Prestwick	781	Clobetasol propionate
2097 M05	X	555	560	0.22502264	748	760	-0.057881	2031992	0.03385314	2294525	0.01060544	experimental	Prestwick	702	Succinylsulfathiazole
2097 M06	X	395	400	-0.44809954	1070	1080	-0.03894003	1862701	-0.19245043	1988815	-0.37795656	experimental	Prestwick	782	Podophyllotoxin
2097 M07	X	275	280	-0.95294119	869	880	-0.05076343	2083127	0.102209	2288469	0.0023908	experimental	Prestwick	703	Famprofazone
2097 M08	X	315	320	-0.78466064	1070	1080	-0.03894003	1922586	-0.1123978	2067906	-0.27743741	experimental	Prestwick	783	Clofibrate
2097 M09	X	396	400	-0.44389253	910	920	-0.04835169	2053870	0.06309905	2239395	-0.05878088	experimental	Prestwick	704	Bromopride
2097 M10	X	276	280	-0.94873417	830	840	-0.05305752	1841982	-0.22014702	2288681	0.00317746	experimental	Prestwick	784	Bendroflumethiazide
2097 M11	X	316	320	-0.78045363	830	840	-0.05305752	1335914	-0.89664485	1531241	-0.95956256	experimental	Prestwick	705	Methyl benzethonium chloride
2097 M12	X	316	320	-0.78045363	869	1000	-0.04370468	1863089	-0.19193176	2068305	-0.27693026	experimental	Prestwick	785	Dicumarol
2097 M13	X	435	440	-0.279819	989	880	-0.05076343	1610339	-0.52980103	1801059	-0.61661185	experimental	Prestwick	706_2009	Chlorcyclizine hydrochloride
2097 M14	X	280	440	-0.95714465	939	820	-0.05113105	1955160	-0.06885377	2242422	-0.07948639	experimental	Prestwick	786	Salmeterol
2097 M15	X	395	400	-0.44809954	909	920	-0.04811051	1912222	-0.12678111	2243881	-0.08172832	experimental	Prestwick	707	Diphenhydraline hydrochloride
2097 M16	X	436	440	-0.27561198	1109	1120	-0.03664593	1785472	-0.29568804	1997768	-0.36658594	experimental	Prestwick	787	Merbromin
2097 M17	X	356	360	-0.61217308	989	1000	-0.04370468	1552407	-0.60724294	1576852	-0.90158894	experimental	Prestwick	708	Benzethonium chloride
2097 M18	X	275	280	-0.95294119	988	1000	-0.04376351	1887445	-0.15937333	2428563	0.18097372	experimental	Prestwick	788	Hexylcaine hydrochloride
2097 M19	X	475	480	-0.11153845	1230	1240	-0.02952836	2075761	0.09236234	2329947	0.05562839	experimental	Prestwick	709	Trioxsalen
2097 M20	X	475	480	-0.11153845	987	1000	-0.04382233	1795733	-0.28197142	2165308	-0.15363512	experimental	Prestwick	789	Drofenine hydrochloride
2097 M21	X	589	600	0.36806111	1262	1280	-0.02764603	1613023	-0.52621313	1916313	-0.47011887	experimental	Prestwick	710	Strophantidin
2097 M22	E	1240	1240	3.08571466	2347	2400	-0.05076343	2499072	-0.07805283	2301438	-0.70868435	experimental	Prestwick	790	Cycloheximide
2097 M23	E	218	360	-1.19274097	535	840	-0.07041028	1963676	-0.05746982	2212187	-0.09404983	empty			
2097 M24	P	46673	46960	194.24408	100668	101240	5.81970356	1861599	-0.19392355	2172934	-0.14394214	empty			
2097 N01	N	597	600	0.40171722	871	880	-0.05064578	1405380	-0.8037846	1923517	-0.46096227	empty			
2097 N02	E	156	160	-1.45357581	712	720	-0.05999863	1668884	-0.45153968	2202869	-0.10589342	empty			
2097 N03	X	517	520	0.06515612	909	920	-0.04841051	1837301	-0.22640445	2150301	-0.17270969	experimental	Prestwick	861	Gabapentin
2097 N04	X	313	320	-0.79307467	828	840	-0.05317517	1799375	-0.27710289	2178683	-0.1366349	experimental	Prestwick	941	Pentetic acid
2097 N05	X	480	480	0.72565727	1149	1149	0.04382233	1489585	-0.6912167	1821811	-0.02740466	experimental	Prestwick	862	Salicylic acid hydrochloride
2097 N06	X	674	680	-0.1153845	908	920	-0.04846934	2025223	0.02480453	2180588	-0.13421356	experimental	Prestwick	863	Bretylium mesylate
2097 N07	X	435	440	-0.279819	870	880	-0.05070461	2001451	-0.00697323	2305170	0.02413571	experimental	Prestwick	863	Etidronic acid, disodium salt
2097 N08	X	435	440	-0.279819	989	1000	-0.04370468	2037144	0.04074019	2252902	-0.04229924	experimental	Prestwick	943	Priloxime chloride
2097 N09	X	475	480	-0.11153845	909	920	-0.04841051	2088116	0.10887816	2193587	-0.11769125	experimental	Prestwick	864	Methylhydantoin-5-(D)
2097 N10	X	395	400	-0.44809954	950	960	-0.04599878	1989565	-0.02286211	2269494	-0.02121007	experimental	Prestwick	944	Phenoxybenzamine hydrochloride
2097 N11	X	475	480	-0.11153845	709	720	-0.0601751	1966730	-0.0538731	2134770	-0.19245003	experimental	Prestwick	865	Simvastatin
2097 N12	X	475	480	-0.11153845	987	1000	-0.04382233	1671659	-0.44783014	1941467	-0.40864353	experimental	Prestwick	945_2009	Salmeterol
2097 N13	X	514	520	0.05253508	1069	1080	-0.03899885	4922515	-0.68730492	1604254	-0.86675977	experimental	Prestwick	866	Acetylcysteine-5
2097 N14	X	475	480	-0.11153845	790	800	-0.05541044	2071633	0.08684414	2346893	0.07716751	experimental	Prestwick	946	Altretamine
2097 N15	X	395	400	-0.44809954	829	840	-0.05311635	1975434	-0.04175205	2092839	-0.24574646	experimental	Prestwick	867	Paromomycin sulfate
2097 N16	X	315	320	-0.78466064	989	1000	-0.04370468	2092487	-0.1147212	2375487	0.11351176	experimental	Prestwick	947	Prazosin hydrochloride
2097 N17	X	435	440	-0.279819	1028	1040	-0.04141059	1910618	-0.1283963	2518909	-0.29580752	experimental	Prestwick	868	Acetaminophen
2097 N18	X	475	480	-0.11153845	890	1000	-0.04364586	1924738	-0.10952107	2336424	0.06386094	experimental	Prestwick	948	Timolol maleate salt
2097 N19	X	555	560	0.22502264	927	840	-0.05323399	1896003	-0.14793323	2209274	-0.09775238	experimental	Prestwick	869	Phthalylsulfathiazole
2097 N20	X	231	240	-1.13804979	946	960	-0.04623407	2027687	0.02808933	2301438	0.01939218	experimental	Prestwick	949	(+)-Octopamine hydrochloride
2097 N21	X	1475	1480	0.09547523	2029	2040	0.01747114	1564900	-0.59054264	1698528	-0.74693332	experimental	Prestwick	870	Luteolin
2097 N22	X	350	360	-0.63741516	902	920	-0.04882227	1971920	-0.04644946	2150525	-0.17242498	experimental	Prestwick	950	(S)-Nipeptic acid
2097 N23	E	209	360	-1.23060409	617	920	-0.06558668	1716701	-0.38761923	2031155	-0.32414957	empty			
2097 N24	P	50614	50960	210.82392	101147	101760	5.84787973	1852258	-0.20641034	2091454	-0.24750685	empty			
2097 O01	N	596	600	0.39751021	1433	1440	-0.01758731	1674090	-0.44458044	1757994	-0.67134938	empty			
2097 O02	E	116	120	-1.62185636	549	560	-0.06958676	1792564	-0.28620765	1795357	-0.62385934	empty			
2097 O03	X	435	440	-0.279819	989	1240	-0.02952836	1835015	-0.22946031	1817983	-0.59510069	experimental	Prestwick	711	Sulfabenzamide
2097 O04	X	674	680	0.72565727	988	1000	-0.04376351	1790424	-0.28906834	2192740	-0.11876783	experimental	Prestwick	791	(R)-Naproxen sodium salt
2097 O05	X	673	680	0.72145026	1227	1240	-0.02970483	1797713	-0.27932461	2153497	-0.16864743	experimental	Prestwick	712	Benzocaine
2097 O06	X	434	440	-0.28402601	1108	1120	-0.03670476	1885126	-0.1624733	2004978	-0.35742171	experimental	Prestwick	792	Propidium iodide
2097 O07	X	353	360	-0.61638009	749	760	-0.05782218	1783746	-0.29799531	2026981	-0.32945491	experimental	Prestwick	713	Dipyron
2097 O08	X	353	360	-0.62479412	829	840	-0.05311635	1642242	-0.48715398	2027466	-0.32883845	experimental	Prestwick	793	Cloperastine hydrochloride
2097 O09	X	554	560	0.22081563	1030	1040	-0.04129294	1522167	-0.64766694	2062112	-0.28480184	experimental	Prestwick	714	Isosorbide dinitrate
2097 O10	X	594	600	0.38909618	908	920	-0.04846934	1762855	-0.32592182	2202402	-0.33425319	experimental	Prestwick	794	Eucastropine hydrochloride
2097 O11	X	434	440	-0.28402601	909	920	-0.04841051	1672812	-0.44088884	1954555	-0.42151159	experimental	Prestwick	715	Sulfachloropyridazine
2097 O12	X	594	600	0.38909618	1508	1520	-0.01317556	1759756	-0.33066448	2189352	-0.12307411	experimental	Prestwick	795	Isocarboxazid
2097 O13	X	594	600	0.38909618	1106	1120	-0.03682224	1691159	-0.42176307	2092855	-0.2460693	experimental	Prestwick	716	Pramoxine hydrochloride
2097 O14	X	354	360	-0.62058711	829										

2098 G19	X	873	880	0.47435536	552	560	-0.60852832	2290661	0.07393589	2172109	-0.31929506	experimental	Prestwick	999	Proguanil hydrochloride
2098 G20	X	673	680	0.04906758	512	520	-0.81212397	2188440	-0.0421734	2388521	-0.06114921	empty			
2098 G21	X	671	680	0.0448147	991	1000	1.62593396	2009056	-0.24592946	2347963	-0.1095286	experimental		1000	Lymecycline
2098 G22	X	792	800	0.30211381	752	760	0.40944994	2144943	-0.09158013	2272324	-0.1515116	empty			
2098 G23	E	320	600	-0.70156536	368	640	-1.54506832	2160102	-0.07436155	2304765	-0.16105709	empty			
2098 G24	P	94318	94840	199.179439	91537	92120	462.495231	2141724	-0.09523648	2347664	-0.10988526	empty			
2098 H01	N	593	600	-0.12104753	913	920	1.22892244	2021656	-0.23161756	2200383	-0.28556858	empty			
2098 H02	E	275	280	-0.79725511	233	240	-2.23220364	2264459	0.04417395	2432592	-0.00857936	empty			
2098 H03	E	634	640	-0.03386354	792	800	0.61304559	2200543	-0.02842602	2633792	0.23142094	experimental	Prestwick	1071	Imidurea
2098 H04	E	587	600	-0.13380617	828	840	0.79628168	2254439	0.03279258	2514942	0.08965138	empty			
2098 H05	E	2712	2720	4.38487651	2192	2200	7.73889341	2245654	0.022814	2584827	0.17301331	experimental	Prestwick	1072	Lansoprazole
2098 H06	E	507	520	-0.30392124	707	720	0.18044983	2322508	0.1101099	2370817	-0.08228733	empty			
2098 H07	E	633	640	-0.03598998	911	920	1.21874266	2352845	0.14456854	2575605	0.1620129	experimental	Prestwick	1073	Bethanechol chloride
2098 H08	E	354	360	-0.62926643	511	520	-0.81721386	2385096	0.18120134	2439952	0.00019997	empty			
2098 H09	E	554	560	-0.20397865	552	560	-0.60852832	2346098	0.13690486	2702096	0.31289699	experimental	Prestwick	1074	Cyproterone acetate
2098 H10	E	554	560	-0.20397865	594	600	-0.39475288	2320031	0.10729626	2772621	0.39702234	empty			
2098 H11	E	434	440	-0.45915132	472	480	-1.01571962	2179937	-0.05183166	2456345	0.01975427	experimental	Prestwick	1075	(R)-Propranolol hydrochloride
2098 H12	E	473	480	-0.3762202	672	680	0.00225864	2366203	0.15974143	2614549	0.20846704	empty			
2098 H13	E	834	840	0.39142424	554	560	-0.59834853	2215704	-0.01120516	2370817	-0.08228733	empty			
2098 H14	E	512	520	-0.29328909	393	400	-1.41782103	2350002	0.14133928	2668307	0.27259197	empty			
2098 H15	E	634	640	-0.03386354	591	600	-0.41002256	2191222	-0.03901342	2387878	-0.06191621	experimental	Prestwick	1076	Tropine
2098 H16	E	593	600	-0.12104753	1513	1520	4.28285722	2340076	0.13006468	2362530	-0.09215243	empty			
2098 H17	E	552	560	-0.20823153	711	720	0.2007644	2300074	0.0846278	2292039	-0.17623723	experimental	Prestwick	1078	Benzylpenicillin sodium
2098 H18	E	473	480	-0.3762202	811	820	-1.83519212	2259802	0.03800664	2360460	-0.09462162	empty			
2098 H19	E	673	680	0.04906758	334	340	0.82682103	2292770	0.07633143	2552220	0.13411823	experimental	Prestwick	1079	Chlorambucil
2098 H20	E	440	440	-0.46553064	954	960	-0.91361821	2157160	0.1040237	2453839	-0.07680907	empty			
2098 H21	E	993	1000	0.72952803	1031	1040	1.82952962	2296862	-0.07483861	2252458	-0.2234512	experimental	Prestwick	1080	Methiazole
2098 H22	E	671	680	0.0448147	751	760	0.40436005	2197742	-0.03160758	2314465	-0.1494865	empty			
2098 H23	E	248	480	-0.8546896	270	600	-2.04387766	2068896	-0.17795928	2104333	-0.40014129	empty			
2098 H24	P	77787	78360	164.027278	111237	111760	562.76609	2100804	-0.14171609	2202374	-0.28319363	empty			
2098 I01	N	1236	1240	1.24625268	1553	1560	4.48645287	1883870	-0.3881239	2794876	0.4235691	empty			
2098 I02	E	193	200	-0.9716231	311	320	-1.83519212	2182785	-0.04859671	2873306	0.51712389	empty			
2098 I03	X	634	640	-0.03386354	832	840	0.81664125	2029524	-0.22268057	2629872	0.22674499	experimental	Prestwick	1001	Alfadolone acetate
2098 I04	X	730	740	0.13199887	551	560	-0.91361821	2147339	0.0888829	2506029	0.08228733	empty			
2098 I05	X	745	760	0.20217118	508	520	-0.83248353	2306241	0.09163268	2581705	0.16928925	experimental	Prestwick	1002	Alfaxalone
2098 I06	X	791	800	0.2998737	791	800	0.6079557	2184174	-0.047019	2459091	0.02302982	empty			
2098 I07	X	1033	1040	0.81458558	1111	1120	2.23672092	2261406	0.04070615	2527303	0.10439613	experimental	Prestwick	1003	Azapropazone
2098 I08	X	552	560	-0.20823153	830	840	0.80646146	2176082	-0.05621042	2382310	-0.06855797	empty			
2098 I09	X	633	640	-0.03598998	873	880	1.02532679	2166527	-0.06706361	2370892	-0.08217786	experimental	Prestwick	1004	Meptazinol hydrochloride
2098 I10	X	553	560	-0.20610509	592	600	-0.40493266	2281633	0.06368113	2276601	-0.19465236	empty			
2098 I11	X	634	640	-0.03386354	673	680	0.07348523	21413036	0.21293741	2640364	0.19840003	experimental	Prestwick	1005	Apramycin
2098 I12	X	514	520	-0.28903621	712	720	0.20585429	2260531	0.03971227	2598950	0.18985986	empty			
2098 I13	X	434	440	-0.45915132	593	600	-0.39984277	2245008	0.02208023	2454682	0.01777057	experimental	Prestwick	1006	Epitiostanol
2098 I14	X	394	400	-0.54420888	593	600	-0.39984277	2208314	-0.01959921	2522224	0.09833767	empty			
2098 I15	X	554	560	-0.20397865	673	680	0.00734853	2300769	0.08541722	2735016	0.37363663	experimental	Prestwick	1007	Fursultiamine Hydrochloride
2098 I16	X	672	680	0.04694114	590	600	-0.41511245	2502258	0.31428159	2521217	0.09713648	empty			
2098 I17	X	673	680	0.04906758	632	640	-0.20133701	2393511	0.19035073	2364737	-0.08951982	experimental	Prestwick	1008	Gabaxete mesilate
2098 I18	X	792	800	0.30424025	954	960	-0.91361821	2235292	0.0040679	2228831	-0.25163456	empty			
2098 I19	X	513	520	-0.29116265	631	640	-0.19624712	2289818	0.07297836	2451651	0.01415506	experimental	Prestwick	1009	Flivampicillin
2098 I20	X	634	640	-0.03386354	713	720	0.21094418	2164910	-0.06890031	2572797	0.15866339	empty			
2098 I21	X	552	560	-0.20823153	711	720	0.2007644	2322168	0.1097236	2562424	0.14629002	experimental	Prestwick	1010	Talampicillin hydrochloride
2098 I22	X	713	720	0.13412513	752	760	0.40944994	2287794	0.07067937	2397343	-0.05062594	empty			
2098 I23	E	177	480	-1.00564612	420	680	-1.28039397	2151235	-0.08443326	2201601	-0.28411569	empty			
2098 I24	P	102196	102680	215.931525	87414	88000	441.50961	2226675	0.00125642	2483367	0.05198732	empty			
2098 J01	N	594	600	-0.1189211	1032	1040	1.83461951	1937982	-0.32665995	2223829	-0.25760115	empty			
2098 J02	E	235	240	-0.88231266	312	320	-1.83010223	2403224	0.2017923	2506029	0.07901956	empty			
2098 J03	E	674	680	0.05119402	1072	1080	2.03821516	2113324	-0.12749506	2372589	-0.08015361	experimental	Prestwick	1081	(S)-propranolol hydrochloride
2098 J04	E	711	720	0.12987226	872	880	1.0202369	2399510	0.1975737	2464320	0.02926721	empty			
2098 J05	E	872	880	0.47222892	512	520	-0.81212397	2008112	-0.24700172	2265450	-0.20795377	experimental	Prestwick	1082	(-)-Eseroline fumarate salt
2098 J06	E	672	680	0.04694114	592	600	-0.40493266	2535903	0.35249778	2332084	-0.12846977	empty			
2098 J07	E	432	440	-0.4634042	671	680	-0.00283125	2203279	-0.02531829	2670166	0.27480947	experimental	Prestwick	1083	Condolphine
2098 J08	E	553	560	-0.20610509	792	800	0.61304559	2588535	0.41228064	2662906	0.26614942	empty			
2098 J09	E	793	800	0.30424025	954	960	-0.91361821	2235292	0.0040679	2228831	-0.25163456	experimental	Prestwick	1084	Leucamisine
2098 J10	E	552	560	-0.20823153	513	520	-0.80703408	2508531	0.32140687	2374081	-0.07837388	empty			
2098 J11	E	633	640	-0.03598998	633	640	-0.19624712	2305977	0.09133281	2577927	0.16478269	experimental	Prestwick	1085	Dubininine
2098 J12	E	554	560	-0.20397865	632	640	-0.20133701	2579123	0.40158988	2563214	0.14723237	empty			
2098 J13	E	474	480	-0.37409376	673	680	0.00734853	2188897	-0.0416543	2338364	-0.12097871	experimental	Prestwick	1086	D-cycloserine
2098 J14	E	515	520	-0.28690977	633	640	-0.19624712	2328540	0.11696134	2419661	-0.02400403	empty			
2098 J15	E	433	440	-0.46127776	512	520	-0.81212397	2355808	0.14793411	2402277	-0.04474044	experimental	Prestwick	1087	2-Chloropyrazine
2098 J16	E	754	760	0.22130613	834	840	1.19115723	2365684	0.1515192	2755661	-0.19589411	empty			
2098 J17	E	513	520	-0.29116265	632	640	-0.20133701	2258637	0.03756094	2329390	-0.12571907	experimental	Prestwick	1088	(+,-)-Synephrine
2098 J18	E	554	560	-0.20397865	711	720	0.2007644	2368536	0.16239141	2510057	0.08382433	empty			
2098 J19	E	474	480	-0.37409376	712	720	0.20585429	1981620	-0.27709306	2466166	0.0314692	experimental	Prestwick	1089	(S)-(-)-Cycloserine
2098 J20	E	474	480	-0.37409376	632	640	-0.20133701	2363953	0.15718574	2399131	-0.04849313	empty			
2098 J21	E	554	560	-0.20397865	512	520	-0.81212397	2308372	0.09405321	2378938	-0.07258024	experimental	Prestwick	1090	Homosalate
2098 J22	E	633	640	-0.03598998	713	720	0.21094418	2219655	-0.00671736	2369671	-0.08363433	empty			
2098 J23	E	419	680	-0.49147											

2098 K13	X	394	400	-0.54420888	632	640	-0.20133701	2287481	0.07032384	2341316	-0.11745743	experimental	Prestwick	1016	Moxonidine
2098 K14	X	555	560	-0.20185221	552	560	-0.60852832	2426728	0.22848968	2312939	-0.15130678	empty			
2098 K15	X	434	440	-0.45915132	634	640	-0.19115723	2063193	-0.18443712	2267037	-0.20606073	experimental	Prestwick	1017	Etilefrine hydrochloride
2098 K16	X	514	520	-0.28903621	432	440	-1.21031527	2443343	0.24736209	2428522	-0.01343424	empty			
2098 K17	X	551	560	-0.21035797	630	640	-0.21153568	2120260	-0.10761348	2282472	-0.18764917	experimental	Prestwick	1018	Alprostadiol
2098 K18	X	514	520	-0.28903621	752	760	0.40944994	2385864	0.18207368	2686869	0.29473355	empty			
2098 K19	X	634	640	-0.03386354	712	720	0.20585429	2188742	-0.04183036	2310850	-0.15379863	experimental	Prestwick	1019	Trifenoside
2098 K20	X	394	400	-0.54420888	633	640	-0.19624712	2310220	0.09615228	2368796	-0.08467807	experimental			
2098 K21	X	513	520	-0.29116265	553	560	-0.60343843	2407296	0.20641755	2251146	-0.22501622	experimental	Prestwick	1020	Rimexolone
2098 K22	X	573	600	-0.12104753	673	680	0.00734853	2676695	0.51241853	2383315	-0.06735916	empty			
2098 K23	E	292	600	-0.80363442	312	600	-1.83010223	2007386	-0.24782636	2156002	-0.33850821	empty			
2098 K24	P	111000	111480	234.652693	96817	97360	489.369857	2366225	0.15976642	229463	-0.17346506	empty			
2098 L01	N	555	560	-0.20185221	833	840	0.82173114	2170359	-0.06271098	2245964	-0.23119754	empty			
2098 L02	E	275	280	-0.79725511	233	240	-2.23220364	2143913	-0.09275007	2207630	-0.27692404	empty			
2098 L03	E	794	800	0.30636669	911	920	1.21874266	2209456	-0.01830205	2427055	-0.01518414	experimental	Prestwick	1091	Spaglumic acid
2098 L04	E	671	680	0.0448147	912	920	1.22383255	2173158	-0.05953169	2282291	-0.18786508	empty			
2098 L05	E	913	920	0.55941292	549	560	-0.62379799	2180306	-0.05141252	2381274	-0.06979375	experimental	Prestwick	1092_2009	Ranolazine
2098 L06	E	552	560	-0.20823153	632	640	-0.20133701	2260300	0.03944989	2446104	0.00753835	empty			
2098 L07	E	714	720	0.13621557	631	640	-0.2064269	2233759	0.00930289	2774426	0.39917543	experimental	Prestwick	1093	(-)-Quinpirole hydrochloride
2098 L08	E	553	560	-0.20610509	713	720	0.21094418	2351935	0.14353491	2466476	0.03183898	empty			
2098 L09	E	593	600	-0.12104753	631	640	-0.2064269	2383475	0.1793601	2457836	0.0215328	experimental	Prestwick	1094	Sulfadoxine
2098 L10	E	673	680	0.04906758	593	600	-0.39984277	2244941	0.02200413	2456876	0.02038767	empty			
2098 L11	E	394	400	-0.54420888	792	800	0.61304559	2547106	0.36522288	2356263	-0.09962799	experimental	Prestwick	1095	Cyclopentolate hydrochloride
2098 L12	E	394	400	-0.54420888	672	680	0.00225864	2167262	-0.06622875	2482494	0.05094596	empty			
2098 L13	E	555	560	-0.20185221	790	800	0.60286581	2335933	0.12535879	2487395	0.05679299	experimental	Prestwick	1096	Estriol
2098 L14	E	473	480	-0.37622061	631	640	-0.21094418	2107440	0.07198886	2416735	0.04579077	empty			
2098 L15	E	514	520	-0.28903621	672	680	0.00225864	1981137	-0.07641669	2464469	0.02944494	experimental	Prestwick	1097	(-)-Isoproterenol hydrochloride
2098 L16	E	470	480	-0.38259952	751	760	0.40436005	2263070	0.04259623	2501842	0.07402512	empty			
2098 L17	E	1714	1720	2.26269048	1552	1560	4.48136298	2243345	0.02019129	2446370	0.00785565	experimental	Prestwick	1098	Kaempferol
2098 L18	E	470	480	-0.38259952	550	560	-0.6187081	2262777	0.04226343	2280669	-0.18979987	empty			
2098 L19	E	634	640	-0.03386354	714	720	0.21603407	2248234	0.02574454	2618151	0.21319309	experimental	Prestwick	1099	Nialamide
2098 L20	E	514	520	-0.28903621	512	520	-0.81212397	2175945	-0.05636603	2317585	-0.14576482	empty			
2098 L21	E	753	760	0.21918269	673	680	0.00734853	2090407	-0.15352568	2119125	-0.38249673	experimental	Prestwick	1100	Vitamin K2
2098 L22	E	394	400	-0.54420888	632	640	-0.21094418	2107440	0.07198886	2167896	0.05661617	empty			
2098 L23	E	372	600	-0.59099053	595	880	-0.38966299	2431404	0.23380099	2163886	-0.32910382	empty			
2098 L24	P	76405	77000	161.088539	96382	96840	487.155755	2038197	-0.21282921	2170617	-0.32107479	empty			
2098 M01	N	716	720	0.14050445	1234	1240	2.86277755	1685559	-0.61337849	2638352	0.23686031	empty			
2098 M02	E	235	240	-0.88231266	272	280	-2.03369788	2132489	-0.1057262	2824779	0.45923873	empty			
2098 M03	X	593	600	-0.12104753	1112	1120	2.24181081	2039564	-0.21127648	2518293	0.0936486	experimental	Prestwick	1021	Isradipine
2098 M04	X	433	440	-0.46127776	627	640	-0.22678647	2229514	0.00448114	2559754	0.14310512	empty			
2098 M05	X	480	480	-0.37834664	630	640	-0.37834664	2209584	-0.01815566	2413765	-0.1304727	experimental	Prestwick	1022	Tiletamine hydrochloride
2098 M06	X	674	680	0.05119402	670	680	-0.00792114	2215535	-0.01139712	2401498	-0.04566697	empty			
2098 M07	X	393	400	-0.54633532	832	840	0.81664125	2197599	-0.03177	2438068	-0.00204735	experimental	Prestwick	1023	Isometheptene mucate
2098 M08	X	554	560	-0.20397865	551	560	-0.61361821	2158697	-0.07595744	2335482	-0.12441649	empty			
2098 M09	X	591	600	-0.12530041	831	840	0.81155136	2108610	-0.13284952	2208169	-0.27628109	experimental	Prestwick	1024	Nifurtimox
2098 M10	X	554	560	-0.20397865	312	320	-1.83010223	2154825	-0.08035551	2415660	-0.0287766	empty			
2098 M11	X	355	360	-0.62713999	834	840	0.826682103	2152551	-0.08293847	2248432	-0.2282536	empty			
2098 M12	X	393	400	-0.20185221	430	440	-1.22949055	2102307	-0.14000888	2416265	-0.14652378	empty			
2098 M13	X	393	400	-0.54633532	1274	1280	3.0663732	2227384	-0.00202737	2434207	-0.06337417	experimental	Prestwick	1026_2009	Arbutin
2098 M14	X	634	640	-0.03386354	391	400	-1.42800082	2271782	0.05249189	2466819	0.03224813	empty			
2098 M15	X	673	680	0.04906758	714	720	0.21603407	2299619	0.08411098	2426381	-0.01598812	experimental	Prestwick	1027	Tocainide hydrochloride
2098 M16	X	714	720	0.13621557	511	520	-0.81721386	2176295	-0.05596848	2342427	-0.11613218	empty			
2098 M17	X	470	480	-0.38259952	710	720	0.19567451	2256415	0.03503705	2541883	0.1217878	experimental	Prestwick	1028	Benzathine benzylpenicillin
2098 M18	X	554	560	-0.20397865	553	560	-0.60343843	2312072	0.09825591	2414647	-0.02783784	empty			
2098 M19	X	594	600	-0.1189211	392	400	-1.42291092	2501960	0.3139431	2320419	-0.1423843	experimental	Prestwick	1029	Risperidone
2098 M20	X	433	440	-0.46127776	632	640	-0.20133701	2296256	0.19387759	2492029	0.06231973	empty			
2098 M21	X	552	560	-0.20823153	832	840	0.81664125	2247678	0.025113	2331644	-0.12899462	experimental	Prestwick	1030	Torseamide
2098 M22	X	473	480	-0.3762202	553	560	-0.60343843	2110447	-0.13076294	2198118	-0.28827037	empty			
2098 M23	E	204	480	-0.94823227	381	560	-1.47889973	2100211	-0.14238966	2225885	-0.25514866	empty			
2098 M24	P	93067	93600	196.519264	59298	59800	298.402226	2046836	-0.20301647	2159164	-0.33473643	empty			
2098 N01	N	475	480	-0.37196733	833	840	0.82173114	1858129	-0.41736221	2068286	-0.44313975	empty			
2098 N02	E	235	240	-0.88231266	273	280	-2.02860799	2018706	-0.23496836	2219508	-0.26275543	empty			
2098 N03	E	874	880	0.4764818	951	960	1.42233831	2123646	-0.12712931	2548443	0.12661286	experimental	Prestwick	1101_2009	Perindopril
2098 N04	E	713	720	0.13412513	1076	1080	2.02803538	2122679	-0.11686903	2236324	-0.24269656	empty			
2098 N05	E	633	640	-0.03598998	866	880	0.98969755	2074785	-0.17127017	2322013	-0.14048291	experimental	Prestwick	1102_2009	Fexofenadine HCl
2098 N06	E	513	520	-0.29116265	711	720	0.2007644	2247206	0.02457687	2296004	-0.1715076	empty			
2098 N07	E	434	440	-0.45915132	792	800	0.61304559	2003507	-0.25223238	2357788	-0.0978089	experimental	Prestwick	1103	Quinic acid
2098 N08	E	472	480	-0.37834664	549	560	-0.62379799	2227198	0.00185047	2345955	-0.11192383	empty			
2098 N09	E	1353	1360	1.49504604	1592	1600	4.68495863	2223346	-0.00252488	2426172	-0.01623742	experimental	Prestwick	1104_2009	Clonixin Lysinate
2098 N10	E	472	480	-0.12317397	482	480	-1.01571962	2277097	0.05852302	24121235	-0.03214639	empty			
2098 N11	E	314	320	-0.7143399	352	360	-0.6605658	1998024	-0.00202737	2202932	-1.47537247	experimental	Prestwick	1105	Verteporfin
2098 N12	E	470	480	-0.37409376	714	720	0.21603407	2114279	-0.1264103	2326357	-0.13530119	empty			
2098 N13	E	555	560	-0.20185221	470	480	-1.0258994	2036671	-0.21456254	2335005	-0.12498547	experimental	Prestwick	1106	Meropenem
2098 N14	E	594	600	-0.1189211	433	440	-1.21422538	2337702	0.12736814	2483330	0.05194318	empty			
2098 N15	E	593	600	-0.12104753	593	600	-0.39984277	2203692	-0.02484918	2286244	-0.18314976	experimental	Prestwick	1107	Ramipril
2098 N16	E	472	480	-0.37834664	793	800	0.61813549	2427636	0.22952105	2343320	-0.11506697	empty			
2098 N17	E	594	600												

3229 C01	D	1543	1560	-1.12867135	1744	1760	-1.00510337	2715465	0.08874007	2462002	-0.88235517	DMSO		
3229 C02	D	1977	2000	-0.61011758	1900	1920	-0.80579772	3023071	0.7528757	2799391	-0.26922571	DMSO		
3229 C03	X	2532	2560	0.05300994	1933	1960	-0.76363691	2768442	0.20311987	2604597	-0.62322048	experimental	EMD Bioscienc 203297	Bisindolylmaleimide IV
3229 C04	X	3540	3560	1.25739289	2618	2640	0.11159193	2930442	0.56288539	2785270	-0.29498749	experimental	EMD Bioscienc 189406	Aurora Kinase/Cdk Inhibitor
3229 C05	X	1610	1640	-0.04861812	1493	1520	-1.25781005	2792852	0.25582219	2850375	-0.75765736	experimental	EMD Bioscienc 203696	BPD-1
3229 C06	X	3700	3720	1.44856478	3220	3240	0.8806347	2373825	-0.64887655	2727682	-0.39954087	experimental	EMD Bioscienc 402085	Indirubin-3'-monoxide
3229 C07	X	1447	1480	-1.24337449	1208	1240	-1.68989715	1811507	-1.86294722	2159501	-1.43208345	experimental	EMD Bioscienc 220285	Chelerythrine Chloride
3229 C08	X	1981	2000	-0.60533828	2780	2800	0.31849056	2656125	-0.03937775	3047672	0.18196978	experimental	EMD Bioscienc 196870	BAY 11-7082
3229 C09	X	1857	1880	-0.75349665	1977	2000	-0.7074225	2471707	-0.43754477	2760342	-0.34018858	experimental	EMD Bioscienc 234505	Compound 56
3229 C10	X	2220	2240	-0.31977526	2058	2080	-0.60393687	2840318	0.35830349	3418212	0.8553438	experimental	EMD Bioscienc 203600	Bohemine
3229 C11	X	1814	1840	-0.80487395	1853	1880	-0.86584494	2820997	0.31658856	2866574	-0.11079	experimental	EMD Bioscienc 260951	DNA-PK Inhibitor II
3229 C12	X	2376	2400	-0.13338266	3088	3120	0.71199145	2331044	-0.74124272	2159505	-0.79537941	experimental	EMD Bioscienc 217695	Cdk1 Inhibitor
3229 C13	X	2208	2240	-0.33411316	5320	5360	3.57637137	2505991	-0.36352402	3042886	0.17327228	experimental	EMD Bioscienc 260962	DNA-PK Inhibitor III
3229 C14	X	2977	3000	0.58470677	2738	2760	0.25205534	2257459	-0.90011215	2675005	-0.4952696	experimental	EMD Bioscienc 217696	Cdk1 Inhibitor, CGP74514A
3229 C15	X	2049	2080	-0.52409023	2169	2200	-0.46212324	2625036	-0.10650034	3113436	0.30148122	experimental	EMD Bioscienc 528100	PI-103
3229 C16	X	2975	3000	0.58231713	2613	2640	0.1051313	2438416	-0.50942158	2985808	0.06954572	experimental	EMD Bioscienc 217714	Cdk1/2 Inhibitor III
3229 C17	X	2731	2760	0.29077998	2690	2720	0.20350653	2502575	-0.37089932	2891222	-0.1023433	experimental	EMD Bioscienc 266788	Diacylglycerol Kinase Inhibitor II
3229 C18	X	2125	2160	-0.43283858	2491	2520	-0.05073594	3009336	0.7232212	3364211	0.7572309	experimental	EMD Bioscienc 217720	Cdk1/5 Inhibitor
3229 C19	X	5012	5040	3.01617434	3893	3920	1.74045971	2845326	0.3691116	3128786	0.32937643	experimental	EMD Bioscienc 317200	DMB1
3229 C20	X	2328	2360	-0.19073423	1972	2000	-0.71381005	3072681	0.85989859	4103913	2.10145284	experimental	EMD Bioscienc 218696	Casein Kinase I Inhibitor, D4476
3229 C21	X	1891	1920	-0.71287248	2134	2160	-0.50683925	2332845	-0.73735427	3729423	1.42090057	experimental	EMD Bioscienc 324673	EGFR/ErbB-2 Inhibitor
3229 C22	X	3011	3040	0.62533008	2090	2120	-0.56305366	2844882	0.36815738	3235354	0.52304006	experimental	EMD Bioscienc 218710	Casein Kinase II Inhibitor III, TBCA
3229 C23	N	3332	3880	1.00886942	2654	3040	0.15751292	2488650	-0.40096405	2983039	0.06451367	empty		
3229 C24	P	177948	178920	209.644319	124356	125080	185.644027	2577253	-0.20966606	3035511	0.15986986	empty		
3229 D01	X	2026	2040	-0.55157119	1867	1880	-0.84795854	2710412	0.07783041	2468147	-0.871188	experimental	EMD Bioscienc 218697	Casein Kinase II Inhibitor I
3229 D02	E	2996	2980	-0.94586323	2492	2480	-1.47270937	3621444	0.3621444	2842097	-0.74809494	empty		
3229 D03	X	2295	2320	-0.23016524	2492	2520	-0.04945834	2858943	0.39851573	2757567	-0.34523153	experimental	EMD Bioscienc 218713	Keratinocyte Differentiation Inducer
3229 D04	E	1332	1360	-1.38077929	2173	2200	-0.45701284	3018846	0.74375373	2950114	0.40647981	experimental	EMD Bioscienc 218714	Keratinocyte Differentiation Inducer
3229 D05	X	1461	1480	-1.22664695	1897	1920	-0.80963053	3231161	1.20215167	3038354	0.15685863	experimental	EMD Bioscienc 218714	Keratinocyte Differentiation Inducer
3229 D06	E	1815	1840	-0.80367913	2414	2440	-0.14911116	3183275	1.09876357	3434938	0.88573958	empty		
3229 D07	X	1816	1840	-0.8024843	2093	2120	-0.55922086	3254464	1.25246393	3528385	1.05555872	experimental	EMD Bioscienc 219445	Cdk2 Inhibitor II
3229 D08	E	1542	1560	-1.12986618	1738	1760	-1.01276898	3019977	0.74619561	3443002	0.90039411	empty		
3229 D09	X	1652	1680	-0.9984355	1653	1680	-1.121365	2916502	0.52278828	3410161	0.8407129	experimental	EMD Bioscienc 219448	Cdk2/5 Inhibitor
3229 D10	E	1640	1640	-0.04149217	1893	1880	-0.86070782	3479275	1.7378492	2857423	0.28406944	experimental	EMD Bioscienc 219457	Cdk2 Inhibitor, p35
3229 D11	X	2575	2600	0.10438738	1657	1680	-1.1162546	3307227	1.3663817	3095934	0.2696752	experimental	EMD Bioscienc 219457	Chk2 Inhibitor
3229 D12	E	2088	2120	-0.47749208	1650	1680	-1.1251978	3128778	0.98110202	3325613	0.68706572	empty		
3229 D13	X	2575	2600	0.10438738	2049	2080	-0.61543528	3249219	1.24113973	3439254	0.89358295	experimental	EMD Bioscienc 220485	Chk2 Inhibitor
3229 D14	E	2250	2280	-0.28393053	1691	1720	-1.07281619	3025545	0.75821718	3358498	0.74682689	empty		
3229 D15	X	2094	2120	-0.47032313	2658	2680	0.16262332	3062071	0.83707851	2926055	0.63335063	experimental	EMD Bioscienc 234501	Compound 401
3229 D16	E	1968	2000	-0.6208701	2085	2120	-0.56944187	3183919	1.1001554	3616706	1.21606429	empty		
3229 D17	X	2480	2480	0.045736894	2884	2880	-0.57138094	2938324	0.5703344	2947273	0.0948622	experimental	EMD Bioscienc 238806	Cdk2/9 Inhibitor
3229 D18	E	2451	2480	-0.43770884	1570	1600	-1.22740583	2982096	0.66440877	3094711	0.26745269	empty		
3229 D19	X	2207	2240	-0.33530798	2453	2480	-0.0928475	2729038	1.11804481	3193291	0.44659992	experimental	EMD Bioscienc 238811	Cdk9 Inhibitor II
3229 D20	E	2089	2120	-0.47629725	1772	1800	-0.96933057	3069048	0.85214218	3110996	0.29704706	empty		
3229 D21	X	2247	2280	-0.28751501	2212	2240	-0.40718643	2733601	0.12789653	2905830	-0.07579651	experimental	EMD Bioscienc 238900	4-Cyano-3-methylisoquinoline
3229 D22	E	2086	2120	-0.47988173	2172	2200	-0.45829044	2543044	-0.28352488	3524704	1.04886932	empty		
3229 D23	N	3516	4000	1.2787171	3060	3480	0.67621865	3011738	0.72840723	3161890	0.38953558	empty		
3229 D24	P	156674	157600	184.225626	136116	136800	170.668607	2351053	0.6942236	2869804	0.24840944	empty		
3229 E01	D	1464	1480	-1.22306208	1225	1240	-0.69187794	24691126	-0.38698206	2724181	-0.40599316	DMSO		
3229 E02	D	1737	1760	-0.89687543	1376	1400	-1.47526029	2911443	0.51186657	3379744	0.78543677	DMSO		
3229 E03	X	3096	3120	0.72689087	3938	3960	1.79795173	2866173	0.41412564	3914523	-0.05999891	experimental	EMD Bioscienc 324674	EGFR Inhibitor
3229 E04	X	2296	2320	-0.22896861	2170	2200	-0.46084564	2477290	-0.42549081	2743529	-0.37074247	experimental	EMD Bioscienc 219476	Cdk4 Inhibitor
3229 E05	X	1538	1560	-1.13464547	1738	1760	-1.01276898	2684277	0.02140373	3189071	0.438931	experimental	EMD Bioscienc 324840	EGFR/ErbB-2/ErbB-4 Inhibitor
3229 E06	X	1735	1760	-0.89926508	1811	1840	-0.91950415	2519061	-0.33530529	3033319	0.15588639	experimental	EMD Bioscienc 219477	Cdk4 Inhibitor II, 625987
3229 E07	X	3221	3240	0.87624392	3701	3720	1.49516045	3173429	-0.10755056	3372387	0.77206706	experimental	EMD Bioscienc 343020	Flt-3 Inhibitor
3229 E08	X	768	800	-2.05465023	1009	1040	-1.94413961	1431162	-2.68412973	1605756	-2.43839181	experimental	EMD Bioscienc 219478	Cdk4 Inhibitor III
3229 E09	X	4502	4520	2.40681392	3621	3640	1.39295242	2712829	0.08304882	2570051	-0.68600015	experimental	EMD Bioscienc 343021	Flt-3 Inhibitor II
3229 E10	X	1809	1840	-0.81084807	2373	2400	-0.20149277	2875162	0.4335333	3340682	0.71445027	experimental	EMD Bioscienc 219479	Cdc2-Like Kinase Inhibitor, TG003
3229 E11	X	2889	2920	0.47956223	2370	2400	-0.20532557	3038929	0.78711386	3023825	0.13863316	experimental	EMD Bioscienc 344036	cFMS Receptor Tyrosine Kinase Inhibitor
3229 E12	X	3535	3560	1.25141876	3416	3440	1.13104436	2661359	-0.02800773	3128266	0.32843144	experimental	EMD Bioscienc 220486	Chk2 Inhibitor II
3229 E13	X	1928	1960	-0.66866397	1972	2000	-0.71381005	2475828	-0.42864734	2829357	-0.21476917	experimental	EMD Bioscienc 365250	G7 6976
3229 E14	X	2775	2800	0.34335225	2500	2520	-0.03923753	4312499	3.53681061	3368142	0.76435271	experimental	EMD Bioscienc 234503	Compound 52
3229 E15	X	2449	2480	-0.04616049	1849	1880	-1.1264754	3110523	0.94168863	2561486	-0.70156513	experimental	EMD Bioscienc 365251	G7 6983
3229 E16	E	2885	2920	0.47478293	3846	3880	1.6804125	3503613	1.79038819	3562560	1.11766418	experimental	EMD Bioscienc 238803	Cdk2 Inhibitor III
3229 E17	X	5329	5360	3.39493366	5889	5920	4.29054995	3549325	1.88908252	3799713	1.5486317	experimental	EMD Bioscienc 371806	GTP-14564
3229 E18	X	2606	2640	0.14142694	2327	2360	-0.26026239	3381862	1.52752213	4520293	2.85813087	experimental	EMD Bioscienc 238804	Cdk2 Inhibitor IV, NU6140
3229 E19	X	1847	1880	-0.76544475	2052	2080	-0.61160248	2795127	0.26073402	3231098	0.51530573	experimental	EMD Bioscienc 375670	Herbimycin A, Streptomyces sp.
3229 E20	X	3927	3960	1.71978991	2894	2920	0.46413699	2647456	-0.05809452	3442632	0.89972172	experimental	EMD Bioscienc 219491	Cdk/Crk Inhibitor
3229 E21	X	5088	5120	3.10698099	3333	3360	1.02500353	2456551	-0.47026728	2462524	-0.88140655	experimental	EMD Bioscienc 343022	Flt-3 Inhibitor III
3229 E22	X	2464	2520	-0.00434163	2374	2400	-0.87095534	2800172	0.27162641	3858768	1.65559533	experimental	EMD Bioscienc 328009	ERK Inhibitor III
3229 E23	X	3134	3560	0.7729242	2504	2920	-0.03412713	2500365	-0.37349782	282216	-0.22229452	DMSO		
3229 E24	P	136106	137080	159.650478	134783	135400	168.965565	2604890	-0.14999649	3186232	0			

3229 F19	X	2376	2400	-0.13338266	1857	1880	-0.86073454	3146771	1.01994974	3055258	0.19575564	experimental	EMD Bioscienc 401488	IKK-3 Inhibitor IX
3229 F20	E	2122	2160	-0.43686805	1688	1720	-1.07664899	3070310	0.8548669	2927130	-0.0370885	empty		
3229 F21	X	2168	2200	-0.38190613	2212	2240	-0.40718643	2777151	0.22192301	3125270	0.32298688	experimental	EMD Bioscienc 401489	IKK Inhibitor X
3229 F22	E	1567	1600	-0.09999557	2133	2160	-0.50811685	2514760	-0.34459134	2843922	-0.18830053	empty		
3229 F23	X	3026	3260	0.64325317	2565	2800	0.3800649	2531698	-0.30802142	3142707	0.35467475	empty		
3229 F24	P	174419	175360	205.427784	72510	73240	89.4055608	2765342	0.19642683	2369492	-1.05047152	empty		
3229 G01	D	1705	1720	-0.93510981	1623	1640	-1.15969301	2791656	0.25323997	2521113	-0.77493408	DMSO		
3229 G02	D	1620	1640	-1.03666988	1899	1920	-0.80707533	3058999	0.83044592	2929074	-0.03355571	DMSO		
3229 G03	X	1936	1960	-0.65910538	2457	2480	-0.09417435	2533599	-0.30391707	2326845	-1.12797295	experimental	EMD Bioscienc 407248	IGF-1R Inhibitor II
3229 G04	X	1498	1520	-1.18243845	1213	1240	-1.68350914	3086413	0.88963402	2981861	0.06237292	W	EMD Bioscienc 688000	ROCK Inhibitor, Y-27632
3229 G05	X	1699	1720	-0.94227875	2381	2400	-0.19127157	2675481	0.00241276	3056460	0.19794001	experimental	EMD Bioscienc 407651	IRAK-1/4 Inhibitor
3229 G06	X	2019	2040	-0.55993496	1815	1840	-0.91439755	2292562	0.68700535	3041657	0.17254719	experimental	EMD Bioscienc 328007	ERK Inhibitor II, FR180204
3229 G07	X	1813	1840	-0.80606878	2497	2520	-0.04307033	2740942	0.14374609	2805225	-0.25862372	experimental	EMD Bioscienc 420099	JAK Inhibitor I
3229 G08	X	2098	2120	-0.46554383	1735	1760	-1.01660178	2908938	0.50645262	2876172	-0.12969333	experimental	EMD Bioscienc 328008	ERK Inhibitor II, Negative Control
3229 G09	X	1940	1960	-0.65432608	2742	2760	0.26994174	2493381	-0.3907496	3469956	0.94937701	experimental	EMD Bioscienc 420104	JAK3 Inhibitor II
3229 G10	X	897	920	-1.90052789	855	880	-2.14089006	1336039	-2.8895047	1312295	-2.9716919	experimental	EMD Bioscienc 341251	Fascapslysin, synthetic
3229 G11	X	2539	2560	0.06137371	2099	2120	-0.55155526	2545981	-0.27718376	3762360	1.48075624	experimental	EMD Bioscienc 420121	JAK3 Inhibitor I
3229 G12	X	1814	1840	-0.80487395	1411	1440	-1.43054428	2724289	0.10779149	3147410	0.3632214	experimental	EMD Bioscienc 361540	GSK-3b Inhibitor I
3229 G13	X	2736	2760	0.2967541	3219	3240	0.8793571	2788746	0.24695715	2661600	-0.51963021	experimental	EMD Bioscienc 420126	JAK3 Inhibitor VI
3229 G14	X	1694	1720	-0.94825287	2133	2160	-0.50811685	2867592	0.41718932	3317776	0.67282371	experimental	EMD Bioscienc 361541	GSK-3b Inhibitor II
3229 G15	X	2247	2280	-0.28751501	2047	2080	-0.61799048	2941675	0.57713796	3371009	0.76956285	experimental	EMD Bioscienc 428205	Lck Inhibitor
3229 G16	X	4536	4560	2.44743794	4576	4600	2.61306073	2642390	-0.06903225	3160406	0.38683874	experimental	EMD Bioscienc 361549	GSK-3b Inhibitor VIII
3229 G17	X	2043	2080	-0.53125917	2045	2080	-0.62054568	2739924	0.14154818	3110303	0.29578769	experimental	EMD Bioscienc 442002	LY 294002
3229 G18	X	3616	3640	1.34819954	3376	3400	1.07994035	2161356	-1.10760699	3214439	0.4850137	experimental	EMD Bioscienc 361550	GSK-3 Inhibitor IX
3229 G19	X	2402	2440	-0.10231723	2486	2520	-0.05712394	2776451	0.22041167	3110679	0.29647098	experimental	EMD Bioscienc 442003	LY 303511
3229 G20	X	4640	4640	2.54064024	3975	4000	1.82523206	2678472	0.00887046	3144441	0.56508057	experimental	EMD Bioscienc 361551	GSK-3 Inhibitor X
3229 G21	X	2004	2040	-0.57785732	2288	2320	-0.3100888	239542	-0.60220445	2659826	-0.52285406	experimental	EMD Bioscienc 448181	Met Kinase Inhibitor
3229 G22	X	3052	3080	0.6743186	2492	2520	-0.04945834	2636719	-0.0812762	3044890	0.17691411	experimental	EMD Bioscienc 361553	GSK-3b Inhibitor XI
3229 G23	N	3397	3960	1.086533	2487	2840	-0.05584634	2747651	0.15823114	2913124	-0.06254219	empty		
3229 G24	P	183467	184320	216.238555	113329	113800	141.555928	2871477	0.42557722	3244101	0.53893579	empty		
3229 H01	X	1786	1800	-0.83832903	2265	2280	-0.33947361	2527729	-0.31659067	2635251	-0.56751365	experimental	EMD Bioscienc 401490	IKK-2 Inhibitor XI
3229 H02	E	1375	1400	-1.32940184	1612	1640	-1.17374662	2796636	0.26399203	2941274	-0.01138492	empty		
3229 H03	X	3417	3440	1.11042949	3376	3400	1.07994035	2697403	0.04974337	3078531	0.23804914	experimental	EMD Bioscienc 402086	Indirubin-3′-monoxime, 5-Iodo-
3229 H04	X	1840	1840	-0.80965325	2044	2080	-0.61799048	2941675	0.57713796	3371009	0.76956285	experimental	EMD Bioscienc 406170	IP3K Inhibitor
3229 H05	X	1779	1800	-0.8466928	1976	2000	-0.7087001	3339644	1.43637151	3282442	0.60861203	empty		
3229 H06	E	1973	2000	-0.61489688	1813	1840	-0.91694895	3089502	0.89630331	3327648	0.69076388	experimental	EMD Bioscienc 406170	IP3K Inhibitor
3229 H07	X	2973	3000	0.57992748	3012	3040	0.61489383	2838209	0.35375006	2787748	-0.29038428	experimental	EMD Bioscienc 407900	5-Iodotubercidin
3229 H08	E	1853	1880	-0.7582758	1934	1960	-0.76235931	3265013	1.27523971	3393938	0.8112312	experimental	EMD Bioscienc 402320	KT5720
3229 H09	X	2016	2040	-0.56351943	2053	2080	-0.61032488	2701182	0.05790241	3427967	0.87307134	experimental	EMD Bioscienc 402320	KT5720
3229 H10	E	1938	1960	-0.65671573	2098	2120	-0.55283286	3403926	1.57515933	3603759	1.19253442	empty		
3229 H11	X	1561	1580	-1.14300924	2217	2240	-0.61160234	27726367	0.71263867	2428296	-0.11261342	experimental	EMD Bioscienc 422709	KN-92
3229 H12	E	1936	1960	-0.65910538	2416	2440	-0.45555996	2962813	0.62278588	3208312	0.43897274	experimental	EMD Bioscienc 442006	LY 294002, 4′-NH2
3229 H13	X	2452	2480	-0.04257601	1891	1920	-0.81729613	3175350	1.08165313	3101039	0.11448881	empty		
3229 H14	E	2089	2120	-0.47629725	2292	2320	-0.3049784	3268250	1.28222854	3523599	1.04686123	empty		
3229 H15	X	2052	2080	-0.52050575	2852	2880	0.41047778	2428006	-0.53189726	2702432	-0.44542713	experimental	EMD Bioscienc 444965	MEK1/2 Inhibitor II
3229 H16	E	1766	1800	-0.86222552	2002	2040	-0.67548249	2906226	0.50060192	3131307	0.33395778	empty		
3229 H17	X	2294	2320	-0.23135826	2614	2640	-0.1064089	2978705	0.65708745	3144936	0.35872546	experimental	EMD Bioscienc 475864	MK-2 Inhibitor III
3229 H18	E	1765	1780	-0.86342034	2044	2080	-0.61799048	2941675	0.57713796	3371009	0.76956285	experimental	EMD Bioscienc 475880	ML-7, Hydrochloride
3229 H19	X	2332	2360	-0.18595494	2408	2440	-0.15677676	2782828	0.118642552	3128285	0.18745492	experimental	EMD Bioscienc 475880	ML-7, Hydrochloride
3229 H20	E	2243	2280	-0.2922943	2088	2240	-0.41229683	2957543	0.61139771	2940379	-0.01301139	empty		
3229 H21	X	2653	2680	-0.19758368	2208	2120	-0.56560886	2692811	0.03982903	3195856	0.45126123	experimental	EMD Bioscienc 480065	Necrostatin-1
3229 H22	E	1881	1920	-0.72482072	2207	2240	-0.41357443	2852731	0.38510373	3229025	0.51153851	empty		
3229 H23	N	3036	3400	0.65520141	2606	2880	0.0961881	2806230	0.28470592	3088860	0.2568198	empty		
3229 H24	P	114308	115400	133.605697	85955	86600	106.582897	2623178	-0.11051185	2665781	-0.51203217	empty		
3229 I01	D	1584	1600	-1.07968355	1781	1800	-0.95783216	2535296	-0.30025317	2444472	-0.19566388	DMSO		
3229 I02	D	1897	1920	-0.70570353	2217	2240	-0.40709842	2838758	0.35493538	3097411	0.27235934	empty		
3229 I03	X	2687	2720	0.23820771	2204	2240	-0.41740723	2371903	-0.65302624	2365538	-1.05765703	experimental	EMD Bioscienc 513035	PD 158780
3229 I04	X	3455	3480	1.15583282	3655	3680	1.43639084	3100636	0.92034214	3311577	0.66155841	experimental	EMD Bioscienc 572635	SU6656
3229 I05	X	1810	1840	-0.80965325	1890	1920	-0.81857373	2932380	0.55706962	3021910	0.13515307	experimental	EMD Bioscienc 513040	PD 174265
3229 I06	X	2572	2600	0.10080291	2372	2400	-0.20277037	3019177	0.74446838	3273995	0.59326148	experimental	EMD Bioscienc 361555	GSK-3 Inhibitor XIII
3229 I07	X	3608	3640	1.33864094	3290	3320	0.97006672	2930749	0.55354822	2954509	0.01266675	experimental	EMD Bioscienc 521231	PDGF Receptor Tyrosine Kinase Inhibitor II
3229 I08	X	2291	2320	-0.23494273	2091	2120	-0.56177606	3462618	1.70187808	3147250	0.36293064	experimental	EMD Bioscienc 371957	Isogranulamide
3229 I09	X	2533	2560	0.05420476	2413	2640	0.1051313	2376806	-0.64244043	2426096	-0.94760534	experimental	EMD Bioscienc 521232	PDGF Receptor Tyrosine Kinase Inhibitor III
3229 I10	X	2888	2920	0.47836741	2411	2440	-0.15294396	3088899	0.89500141	3133349	0.33766866	experimental	EMD Bioscienc 400090	IC261
3229 I11	X	3573	3600	1.29682209	3011	3040	0.61361623	2704163	0.06433853	2924032	-0.04271842	experimental	EMD Bioscienc 521233	PDGF Receptor Tyrosine Kinase Inhibitor IV
3229 I12	X	2529	2560	0.04942546	2852	2880	0.41047778	2734479	0.12979218	2836915	-0.20103419	experimental	EMD Bioscienc 401481	IKK-2 Inhibitor I
3229 I13	X	2885	2920	0.47478293	1849	1880	-0.87095534	3177889	1.08713945	3084064	0.24810414	experimental	EMD Bioscienc 521234	PDGF RTK Inhibitor
3229 I14	X	4409	4420	2.29596525	2851	2880	0.40920018	2842608	0.3632471	2647051	-0.54606978	experimental	EMD Bioscienc 402081	Indirubin Derivative E804
3229 I15	X	3407	3440	1.09848125	3325	3360	1.01478273	2431225	-0.52494729	2242256	-1.28169464	experimental	EMD Bioscienc 527450	PKR Inhibitor
3229 I16	X	2889	2920	0.47956223	2090	2120	-0.71454666	3200360	1.13565088	3583236	1.15523021	experimental	EMD Bioscienc 420119	PKR Inhibitor
3229 I17	X	3169	3200	0.81411305	2685	2720	0.19711853	2418116	-0.43882077	3050660	0.18745492	experimental	EMD Bioscienc 527455	PKR Inhibitor, Negative Control
3229 I18	X	3850	3880	1.62778844	3848	3880	1.6829677	3555933	1.9033495	3594009	1.17481574	experimental	EMD Bioscienc 420123	JMK

3229 J13	X	2492	2520	0.00521696	2973	3000	0.56506742	2979554	0.65892048	3806497	1.56096542	experimental	EMD Bioscienc 506163	p38 MAP Kinase Inhibitor VIII
3229 J14	X	2206	2240	-0.3365028	2406	2440	-0.15933196	3113573	0.94827372	3466406	0.94292567	empty		
3229 J15	X	1810	1840	-0.80965325	3049	3080	0.66216504	2978063	0.65570134	4478431	2.78205599	experimental	EMD Bioscienc 524611	PIKfyve Inhibitor
3229 J16	E	2094	2120	-0.47032313	2368	2400	-0.20780078	3161731	1.05224908	3465373	0.88634738	empty		
3229 J17	X	1691	1720	-0.55183739	2332	2360	-0.25387439	2935624	0.35648125	1728965	0.02985092	experimental	EMD Bioscienc 526520	PIM1 Kinase Inhibitor II
3229 J18	E	2209	2240	-0.33291833	1847	1880	-0.87351054	3034869	0.77834813	3170023	0.4043155	empty		
3229 J19	X	2932	2960	0.53093968	2327	2360	-0.26026239	3030151	0.76816175	2895027	-0.09542856	experimental	EMD Bioscienc 526522	PIM1 Kinase Inhibitor IV
3229 J20	E	2045	2080	-0.52886953	2171	2200	-0.45956804	3029773	0.76734563	3093994	0.26614971	empty		
3229 J21	X	3693	3720	1.44020101	3210	3240	0.86785869	2696661	0.04814136	3648823	1.27442799	experimental	EMD Bioscienc 526523	PIM1/2 Kinase Inhibitor V
3229 J22	E	2870	2920	0.45686057	2521	2560	-0.01240793	2780259	0.22863332	3170231	0.40469349	empty		
3229 J23	N	3162	3480	0.80574928	3209	3480	0.86658109	2649322	-0.05406574	2966412	0.0342978	empty		
3229 J24	P	97731	98680	113.799094	87993	84400	103.820725	2679333	0.01072594	2324474	0.68499584	empty		
3229 K01	D	2263	2280	-0.26839782	2342	2360	-0.24109838	2457803	-0.46756415	3063905	0.21146964	DMSO		
3229 K02	D	1932	1960	-0.66388468	1972	2000	-0.7138105	2981298	0.66268586	3418186	0.85529655	DMSO		
3229 K03	X	2612	2640	0.14859588	2730	2760	0.25461054	2950473	0.59613325	3741719	1.44324581	experimental	EMD Bioscienc 529574	PP3
3229 K04	X	1374	1400	-1.33059667	1414	1440	-1.42671148	2708795	0.07433923	3352846	0.73655564	experimental	EMD Bioscienc 475863	MK2a Inhibitor
3229 K05	X	1816	1840	-0.8024843	1974	2000	-0.7112553	2907345	0.50301079	3345424	0.7230678	experimental	EMD Bioscienc 529581	PP1 Analog II, 1NM-PP1
3229 K06	X	2335	2360	-0.18237046	2573	2600	0.05402729	3037346	0.78369609	3325229	0.68636788	experimental	EMD Bioscienc 420135	JNK Inhibitor VIII
3229 K07	X	2967	3000	0.57275853	2927	2960	0.5062978	2988317	0.6778402	3324474	0.68499584	experimental	EMD Bioscienc 539652	PKCII/JEGFR Inhibitor
3229 K08	X	2453	2480	-0.04138119	2532	2560	0.00164568	2165807	-1.09799707	1994796	-1.73139815	experimental	EMD Bioscienc 420298	K-252a, Nocardiopsis sp.
3229 K09	X	2167	2200	-0.38310095	2326	2360	-0.26153999	2967695	0.63331635	3389788	0.8036895	experimental	EMD Bioscienc 539654	PKCb Inhibitor
3229 K10	X	4572	4600	2.49045162	4212	4240	2.14801421	2925326	0.54183971	3006779	0.10765584	experimental	EMD Bioscienc 422000	Kenpaullone
3229 K11	X	2478	2520	-0.01151058	2800	2840	0.34404256	2171736	-1.08519608	2741222	-0.37493493	experimental	EMD Bioscienc 553210	Rapamycin
3229 K12	X	2214	2240	-0.32694421	2531	2560	0.00036808	2373836	-0.6488528	3247111	0.5444079	experimental	EMD Bioscienc 422708	KM-93
3229 K13	X	2251	2280	-0.28273571	2687	2720	0.19967373	2678262	0.00841706	3501636	1.00694836	experimental	EMD Bioscienc 555553	Rho Kinase Inhibitor III, Rockout
3229 K14	X	2854	2880	-0.43774338	2609	2640	-0.1000209	2444669	-0.49160297	3032600	0.72345308	experimental	EMD Bioscienc 444937	Rho Kinase Inhibitor IV
3229 K15	X	2453	2480	-0.04138119	2609	2640	0.1000209	2846539	0.37173492	3032600	0.72345308	experimental	EMD Bioscienc 555554	Rho Kinase Inhibitor IV
3229 K16	X	2613	2640	0.14979071	2291	2320	-0.306256	3318765	1.39129277	3036704	0.16203787	experimental	EMD Bioscienc 444938	MEK Inhibitor II
3229 K17	X	2375	2400	-0.13457749	2571	2600	0.05147209	2746754	0.15629447	3187206	0.43554178	experimental	EMD Bioscienc 539648	Staurosporine, N-benzoyl-
3229 K18	X	2254	2280	-0.27915124	2812	2840	0.35937377	3127944	0.97930138	3901640	1.73386665	experimental	EMD Bioscienc 444939	MEK 1/2 Inhibitor
3229 K19	X	2213	2240	-0.32813903	2853	2880	0.41175538	2617006	-0.12383748	2824129	-0.2242699	experimental	EMD Bioscienc 567805	Src Kinase Inhibitor I
3229 K20	X	2137	2160	-0.41894568	1894	1920	-0.81346333	2927563	0.5466695	3421350	0.86104642	experimental	EMD Bioscienc 454861	MNK1 Inhibitor
3229 K21	X	1400	1440	-1.29953123	1569	1600	-1.22868343	1272296	-3.0271288	1373209	-2.86099425	experimental	EMD Bioscienc 572660	SU16152
3229 K22	P	5869	5900	0.92065637	2002	2040	-0.67542049	2741877	0.09015219	2915029	0.73238066	experimental	EMD Bioscienc 481406	NF-KB Activation Inhibitor
3229 K23	N	3373	3800	1.05785722	3001	3360	0.60084023	2550077	-0.2683403	2982755	0.06399757	empty		
3229 K24	P	134112	134720	157.267999	113319	114040	141.543152	2635828	-0.08319991	4151165	2.18732284	empty		
3229 L01	D	2181	2200	-0.36637341	2179	2200	-0.44934724	2795944	0.26249797	3177907	0.41864292	DMSO		
3229 L02	E	2491	2520	0.00402214	2248	2280	-0.36119281	3257747	1.25955208	3124404	0.32141312	empty		
3229 L03	X	3812	3840	1.58238511	3692	3720	1.48366205	2821276	0.31719093	2906542	-0.07450261	experimental	EMD Bioscienc 526524	PIM1/2 Kinase Inhibitor VI
3229 L04	E	2013	2040	-0.56713079	1890	1920	-0.81857373	3205766	1.14732269	3028441	1.47027121	empty		
3229 L05	X	1976	2000	-0.61131244	2034	2060	-0.61131244	2808429	0.28032527	3682029	0.47386433	experimental	EMD Bioscienc 528111	PI 3-Kα Inhibitor IV
3229 L06	E	1770	1800	-0.85744622	2007	2040	-0.66909449	3001286	0.70584088	3299124	0.63892785	experimental	EMD Bioscienc 528112	PI 3-Kγ Inhibitor
3229 L07	X	3372	3400	1.05666239	3492	3520	1.22814198	3773407	2.37288596	3603384	1.19185272	experimental	EMD Bioscienc 528112	PI 3-Kγ Inhibitor
3229 L08	E	2326	2360	-0.19312388	2325	2360	-0.26281759	3337251	1.43120491	3674534	1.32115202	empty		
3229 L09	X	2094	2120	-0.47032313	2293	2320	-0.3037008	3045667	0.80166151	3721500	1.40650228	experimental	EMD Bioscienc 528113	PI 3-Kβ Inhibitor VI, TGX-221
3229 L10	E	2121	2160	-0.43806287	2242	2280	-0.36885842	2935176	0.56310632	3180416	0.42320247	experimental	EMD Bioscienc 528114	PI 3-Kβ Inhibitor VII
3229 L11	X	5175	5200	3.21093071	4133	4160	2.04708379	2948586	0.59202027	3217926	0.49136855	experimental	EMD Bioscienc 528114	PI 3-Kγ Inhibitor VIII
3229 L12	X	2005	2040	0.5766625	2002	2040	-0.67542049	3086553	0.09015219	2915029	0.73238066	experimental	EMD Bioscienc 528116	PI 3-Kα Inhibitor VIII
3229 L13	X	2414	2440	-0.08797934	2447	2480	0.65960984	2417777	-0.55398214	2934669	-0.02338800	experimental	EMD Bioscienc 528116	PI 3-Kα Inhibitor VIII
3229 L14	E	1931	1960	-0.6650795	3005	3040	0.60595063	3172641	1.07580428	3523604	1.04687032	empty		
3229 L15	X	1894	1920	-0.709288	2648	2680	0.14984731	2896828	0.4803112	3779377	1.51168085	experimental	EMD Bioscienc 528282	Polo-like Kinase Inhibitor I
3229 L16	E	2135	2160	-0.42133533	2450	2480	-0.10311755	3015400	0.73631366	3393623	0.81065876	empty		
3229 L17	X	1896	1920	-0.70689835	2490	2520	-0.05201354	2765789	0.19739192	3443837	0.90191154	experimental	EMD Bioscienc 528283	Polo-like Kinase Inhibitor II, BTO-1
3229 L18	E	1936	1960	-0.65910538	2320	2320	-0.306256	2703403	0.06269765	3040691	0.16928336	empty		
3229 L19	X	1929	1960	-0.66746915	2296	2360	-0.26153999	2110136	-1.28189334	2331299	-1.1198788	experimental	EMD Bioscienc 539644	UCN-01
3229 L20	E	2016	2040	-0.56351943	2212	2240	-0.40718643	2715860	0.08959289	3040009	0.16804398	empty		
3229 L21	X	1967	2000	-0.62065883	2528	2560	-0.00346472	2770658	0.20790432	3228225	0.51008469	experimental	EMD Bioscienc 551590	Quercetagenin
3229 L22	E	2440	2480	-0.0569139	2247	2280	-0.36247041	2735376	0.13172884	3177439	0.41779243	empty		
3229 L23	N	3300	3640	0.97063504	3026	3520	0.63278023	2930488	0.55298471	2777798	-0.30846619	empty		
3229 L24	P	106973	107680	124.84166	160580	161400	201.923821	2579944	-0.20385606	3422133	0.86246935	empty		
3229 M01	D	1823	1840	-0.79412053	2578	2600	0.06041529	2393320	-0.60678594	2923016	-0.04456478	DMSO		
3229 M02	D	1855	1880	-0.75588615	2932	2960	0.5126858	2579387	-0.20505865	3874378	1.68432403	empty		
3229 M03	X	2332	2360	-0.18595494	2646	2680	0.14729211	2554627	-0.25851664	2764166	-0.33323933	experimental	EMD Bioscienc 574711	Syk Inhibitor
3229 M04	X	1893	1920	-0.71048283	2771	2800	0.30699215	2846160	0.37091664	3031902	0.15331131	experimental	EMD Bioscienc 506121	p38 MAP Kinase Inhibitor III
3229 M05	X	2736	2760	0.2967541	3089	3120	0.71326905	2339128	-0.72378899	2773495	-0.31628593	experimental	EMD Bioscienc 574712	Syk Inhibitor II
3229 M06	X	2415	2440	-0.08678451	2852	2880	0.41047778	3206488	1.14888152	3484975	0.9766707	experimental	EMD Bioscienc 506126	p38 MAP Kinase Inhibitor
3229 M07	X	2326	2360	-0.19312388	2365	2400	-0.21171358	3220575	1.17929601	3048576	0.18361259	experimental	EMD Bioscienc 574713	Syk Inhibitor III
3229 M08	X	3693	3720	1.44020101	3652	3680	1.43255803	2816399	0.30666126	3007560	0.10907514	experimental	EMD Bioscienc 513000	PD98059
3229 M09	X	2093	2120	-0.47151796	2209	2240	-0.41101923	2405761	-0.57992525	3281958	0.60773246	experimental	EMD Bioscienc 616451	TGF- β RI Kinase Inhibitor
3229 M10	X	1736	1760	-0.13702312	2374	2400	-0.2021517	285741	-0.41819293	3031143	0.93881318	experimental	EMD Bioscienc 513030	PD 169316
3229 M11	X	1925	1960	-0.67223812	2343	2380	-0.36758082	2364952	-0.68803377	3228850	0.51232042	experimental	EMD Bioscienc 616453	TGF- β RI Inhibitor III
3229 M12	X	2294	2320	-0.23135826	3132	3160	0.76820587	2524038	-0.32455971	2771930	-0.31912997	experimental	EMD Bioscienc 559396	SB 220025
3229 M13	X	2812	2840	0.38756076										

3229 N07	X	2171	2200	-0.37832166	1849	1880	-0.87095534	3246635	1.23556076	3422869	0.86380686	experimental	EMD Bioscienc	555550	Rho Kinase Inhibitor
3229 N08	X	2492	2520	-0.00521696	2491	2520	-0.05073594	2962444	0.62197919	3238439	0.52864636	empty			
3229 N09	X	1813	1840	-0.80668878	2373	2400	-0.20149277	3037540	0.78411494	3232368	0.51761367	experimental	EMD Bioscienc	555551	Rho Kinase Inhibitor II
3229 N10	X	2175	2200	-0.37354236	2051	2200	-0.61288008	2925338	0.54186568	3545968	1.08751139	empty			
3229 N11	X	1150	1160	0.76870972	2302	3120	0.71710186	3117762	0.95731797	3306973	0.65319166	experimental	EMD Bioscienc	555555	Rho Kinase Inhibitor V
3229 N12	E	2213	2240	-0.32813903	1647	1680	-1.12903061	2619704	-0.11801238	3128669	0.32916381	empty			
3229 N13	X	2290	2320	-0.23613756	2649	2680	0.15112491	3002461	0.70837776	3175301	0.41390709	experimental	EMD Bioscienc	557360	Roscovitine
3229 N14	E	2002	2040	-0.58024697	2283	2320	-0.31647688	2950042	0.5952027	3258861	0.56575888	empty			
3229 N15	X	2894	2920	0.48553635	2765	2800	0.29932655	2714757	0.08721146	3498199	1.00070238	experimental	EMD Bioscienc	557362	Roscovitine, (S)-Isomer
3229 N16	E	1971	2000	-0.61728653	2468	2440	-0.15677676	2720310	0.09920065	3072983	0.22796689	empty			
3229 N17	X	2693	2720	0.24537666	2650	2680	0.15240251	1610279	-2.29740781	1515010	-2.60330248	experimental	EMD Bioscienc	557520	Ro-31-8220
3229 N18	X	2414	2440	-0.08797934	2053	2080	-0.61032488	2886871	0.45881358	3349449	0.34519583	empty			
3229 N19	X	2125	2160	-0.43328358	2008	2040	-0.66781689	3352872	1.46493137	3246942	0.54409867	experimental	EMD Bioscienc	559285	RSK Inhibitor, SL0101
3229 N20	E	2332	2360	-0.18595494	1804	1840	-0.92844736	2886857	0.45878335	3192421	0.44501888	empty			
3229 N21	X	1966	2000	-0.62326065	2127	2160	-0.51578245	3241481	1.02443303	3523373	1.04645053	experimental	EMD Bioscienc	559399	SB 203580, Sulfone
3229 N22	E	2207	2240	-0.33530798	2485	2520	-0.05840154	2786916	0.24300609	2755873	-0.34831	empty			
3229 N23	N	4166	4600	2.00535293	4442	4960	2.44186229	2835529	0.34796382	3063532	0.21079118	empty			
3229 N24	P	139714	140488	163.961405	167816	168760	211.168537	2477479	-0.42508275	3351871	0.73478379	empty			
3229 O01	D	2021	2040	-0.55754531	2380	2400	-0.19254957	2237580	-0.94303583	2548850	-0.72452825	DMSO			
3229 O02	D	2535	2560	0.05659441	2253	2280	-0.35480481	2663809	-0.02278763	2994531	0.08539783	DMSO			
3229 O03	X	2216	2240	-0.32455456	2171	2200	-0.45956804	2349481	-0.70143638	2608285	-0.61651836	experimental	EMD Bioscienc	658552	AG 1478
3229 O04	X	1773	1800	-0.85386175	2290	2320	-0.30753326	3085765	0.88823496	3300903	0.64216079	experimental	EMD Bioscienc	559389	SB 203580
3229 O05	X	3097	3120	0.7280857	3694	3720	1.48621725	2375636	-0.64496652	2711894	-0.42823205	experimental	EMD Bioscienc	676480	VEGF Receptor 2 Kinase Inhibitor I
3229 O06	X	2091	2120	-0.47309076	2006	2040	-0.67037209	2390039	-0.61386977	2738252	-0.38033225	experimental	EMD Bioscienc	6731970	HA 1077, Dihydrochloride Fasudil
3229 O07	X	3376	3400	1.06144169	3694	3720	1.48621725	2569439	-0.22653684	2874265	-0.13315887	experimental	EMD Bioscienc	676481	VEGF Receptor Tyrosine Kinase Inhibitor II
3229 O08	X	2069	2100	-0.61967618	2127	2160	-0.51578245	3241481	-0.41295322	3128669	0.33156268	experimental	EMD Bioscienc	559402	SB 218078
3229 O09	X	2332	2360	-0.18595494	2493	2520	-0.46180774	8333024	0.45881358	2086774	0.56424132	experimental	EMD Bioscienc	676483	VEGR Tyrosine Kinase Inhibitor IV
3229 O10	X	2131	2160	-0.42611463	2170	2200	-0.46084564	2980795	0.66159986	3202057	0.46253017	experimental	EMD Bioscienc	565625	SC-68376
3229 O11	X	3731	3760	1.48560434	3611	3640	1.38017642	2286154	-0.83816231	2857648	-0.16335658	experimental	EMD Bioscienc	676485	VEGF Receptor 2 Kinase Inhibitor II
3229 O12	X	1647	1680	-1.00440962	2368	2400	-0.20788078	3157716	1.04358051	2662496	-0.51800192	experimental	EMD Bioscienc	567305	SKF-86002
3229 O13	X	3168	3200	0.81291823	3209	3240	0.86658109	2049237	-1.34967711	2451680	-0.90111311	experimental	EMD Bioscienc	676487	VEGF Receptor 2 Kinase Inhibitor III
3229 O14	X	5170	5200	0.20495659	3645	3680	1.42361483	2345624	-0.70976382	2941180	-0.01155575	experimental	EMD Bioscienc	569413	Sphingosine Kinase Inhibitor
3229 O15	X	2564	2600	0.09124432	4446	4480	2.44697269	2485617	-0.40751243	2995093	0.08641914	experimental	EMD Bioscienc	676489	VEGF Receptor 2 Kinase Inhibitor IV
3229 O16	X	3133	3160	0.77109937	3009	3120	0.24698074	1517845	-0.01370787	2724	-0.47217078	experimental	EMD Bioscienc	569397	Staurosporine, Streptomycetes sp.
3229 O18	X	1890	1920	-0.7140673	2370	2400	-0.20532557	3209296	1.15494412	2750436	-0.35819054	experimental	EMD Bioscienc	570250	DNA-PK Inhibitor V
3229 O19	X	3011	3040	0.62533008	2964	3000	0.55356901	2051029	-1.34580801	2259791	-1.24982868	experimental	EMD Bioscienc	189405	STO-609
3229 O20	X	3333	3360	1.01006424	5453	5480	3.73351621	2448565	-0.48750942	2859959	-0.15099142	experimental	EMD Bioscienc	572650	Aurora Kinase Inhibitor III
3229 O21	X	1966	2000	-0.62326065	2004	2040	-0.67292729	1304913	-2.95670718	1177133	-3.21731877	experimental	EMD Bioscienc	569397	SU9516
3229 O22	X	2651	2680	0.19519403	2689	2720	0.20222893	1315077	-1.16434457	2461466	-0.96568825	experimental	EMD Bioscienc	616373	Staurosporine, Streptomycetes sp.
3229 O23	N	3324	3600	0.999931083	3315	3310	1.00200673	2457316	-0.4661562	2457316	-0.62991363	empty			Tp12 Kinase Inhibitor
3229 O24	P	153182	153920	180.053299	154447	155440	194.088328	3412494	1.59365804	4067193	2.03472241	empty			
3229 P01	D	2347	2360	-0.16803257	2345	2360	-0.23726558	2487221	-0.40404932	2454739	-0.89555406	DMSO			
3229 P02	E	2380	2400	-0.12860337	2658	2680	0.16262332	2578960	-0.20598056	2729171	-0.39683494	empty			
3229 P03	X	1941	1960	-0.65313126	2899	2920	0.47052499	2555559	-0.25650441	3000847	0.09687575	experimental	EMD Bioscienc	559404	SB 239063
3229 P04	E	1903	1920	-0.69853458	2378	2400	-0.19510477	2523079	-0.32663024	2698869	-0.45190209	empty			
3229 P05	X	2100	2120	-0.46315419	2176	2200	-0.45318004	2507342	-0.36060715	2350730	-1.08456728	experimental	EMD Bioscienc	565715	Scytonein, Lyngbya sp.
3229 P06	E	1982	1800	-0.84310833	2300	2320	-0.9475776	2392747	-0.17621379	2970065	-0.04093632	empty			
3229 P07	X	1978	2000	-0.60892276	2775	2800	0.31210253	2475856	-0.42858689	2762876	-0.3355836	experimental	EMD Bioscienc	569615	Stem-Cell Factor/c-Kit Inhibitor, ISCK03
3229 P08	E	2298	2320	-0.22657896	2498	2520	-0.04179273	2712641	0.08264292	3083523	0.24712099	empty			
3229 P09	E	3501	3520	0.21079474	2500	2520	-0.03923753	2884901	0.45456026	2673157	-0.49862793	empty			
3229 P10	E	1775	1800	-0.8514721	2220	2040	-0.65248569	2533140	-0.30490807	2670815	-0.50288399	empty			
3229 P11	X	3078	3080	0.68148755	2056	2280	-0.35097201	2194159	-1.03678379	2307950	-1.16231041	experimental	EMD Bioscienc	616404	Tp12 Kinase Inhibitor II
3229 P12	E	2181	2200	-0.36637341	2541	2560	0.01314408	2476044	-0.42818099	3007383	0.10875348	empty			
3229 P13	X	1857	1880	-0.7534965	1977	2000	-0.7074225	2086205	-1.26986148	1957590	-1.79901178	experimental	EMD Bioscienc	655203	TX-1918
3229 P14	E	2453	2480	-0.04138119	2096	2120	-0.55388006	2456613	-0.47011342	2639682	-0.55946129	empty			
3229 P15	X	2180	2200	-0.36756824	2534	2560	0.00420088	2308470	-0.78998013	2831390	-0.21107465	experimental	EMD Bioscienc	681500	WHI-P180, Hydrochloride
3229 P16	E	1900	1920	-0.70211906	2336	2360	-0.24876399	2530100	-0.31147157	2517619	-0.78128364	empty			
3229 P17	X	2580	2600	0.1103615	2818	2840	0.36703937	2006888	-1.44111057	2251135	-1.26555904	experimental	EMD Bioscienc	681637	Weel/Chk1 Inhibitor
3229 P18	E	1700	1720	-0.94108393	2337	2360	-0.24748639	2505523	-0.36453446	2640197	-0.5585254	empty			
3229 P19	X	2460	2480	-0.03301742	2537	2560	0.00803368	1941170	-1.58299878	2130080	-1.48554957	experimental	EMD Bioscienc	681640	Weel1 Inhibitor
3229 P20	E	1972	2000	-0.6160917	2451	2480	-0.10183995	2429808	-0.52800666	2656025	-0.52976153	empty			
3229 P21	X	3663	3680	1.40435628	2300	2120	-0.55027765	2114396	-1.20899581	2126881	-1.49136304	experimental	EMD Bioscienc	681641	Weel1 Inhibitor II
3229 P22	E	1933	1960	-0.66268985	2214	2240	-0.40463128	2303625	-0.80044161	2527522	-0.76328715	empty			
3229 P23	N	2743	3080	0.30511787	3769	4280	1.58203727	2323116	-0.75835964	2802179	-0.26415914	empty			
3229 P24	P	110065	110520	128.536057	170018	170480	213.981813	2110290	-1.21786085	2496411	-0.81982447	empty			
3244 A01	E	2229	2240	-0.7539853	2866	2880	-0.78473463	2073081	-1.12946068	1883425	-1.28555041	empty			
3244 A02	E	1867	1880	-1.17434607	2260	2280	-1.25133897	2328223	-0.70703164	2254035	-0.76676109	empty			
3244 A03	X	706	720	-2.52252008	1222	1240	-2.05057213	1123589	-2.70149896	1181052	-2.26875002	experimental	SYNthesis	SYN-1025	Bosutinib (10 mM)
3244 A04	X	1181	1200	-1.97094157	1293	1320	-1.99590767	1242388	-2.50331782	1223357	-2.20950325	experimental	SYNthesis	SYN-1025	Bosutinib (3.33 mM)
3244 A05	X	2320	2320	-0.67153871	3301	3320	-0.44979588	1706199	-0.74823494	1592682	-1.69253986	experimental	SYNthesis	SYN-1035	Dasatinib (3.33 mM)
3244 A06	X	3181	3200	0.35149428	2576	2600	-1.00802713	1898685	-1.41820159	1756185	-1.46366642	experimental	SYNthesis	SYN-1036	Dasatinib (3.33 mM)
3244 A07	X	2059	2080	-0.95139223	218										

3244 E19	X	3647	3680	0.89262183	4446	4480	0.43182453	2668950	-0.14290273	2779488	-0.0312186	experimental	SYNthesis	SYN-1113	SMI-4a (10 mM)
3244 E20	X	3647	3680	0.89262183	3926	3960	0.03143797	3250014	0.81914314	3835258	1.44667514	experimental	SYNthesis	SYN-1113	SMI-4a (3.33 mM)
3244 E21	X	2331	2360	-0.63554096	2205	2240	-1.29368754	1728208	-1.70045397	1638869	-1.62788612	experimental	SYNthesis	SYN-1021	Bisindolylmaleimide X, HCl salt (10 mM)
3244 E22	X	2130	2160	-0.86894576	2928	2960	-0.73698623	2372837	-0.63116591	3110955	0.43011208	experimental	SYNthesis	SYN-1021	Bisindolylmaleimide X, HCl salt (3.33 mM)
3244 E23	N	3294	3260	0.4827119	3204	3560	-0.52448263	28270471	0.19074803	2822477	0.0289585	empty			
3244 E24	P	150463	151440	171.377992	112896	113320	83.9355211	2937233	0.30128337	2973305	0.24009138	empty			
3244 F01	E	1541	1560	-1.55290311	2450	2480	-1.10504388	2948921	0.32063475	3254312	0.63345213	empty			
3244 F02	E	1780	1800	-1.27537203	2449	2480	-1.10581385	2997816	0.40158837	2887379	0.11980997	empty			
3244 F03	X	1775	1800	-1.28117812	2451	2480	-1.1042739	2833190	0.12902328	2736799	-0.09097575	W	SYNthesis	SYN-1115	GNE-493 (1.11 mM)
3244 F04	X	2458	2480	-0.48806628	2491	2520	-1.07347494	2723731	-0.05220388	2702334	-0.13922073	experimental	SYNthesis	SYN-1114	GNE-490 (10 mM)
3244 F05	X	1655	1680	-1.42052427	2690	2720	-0.92025008	2968277	0.35268176	3198555	0.55542026	experimental	SYNthesis	SYN-1045	IC87114 (1.11 mM)
3244 F06	X	1696	1720	-1.37291434	2365	2400	-1.17049168	1686034	-1.77027988	1761416	-1.42189201	experimental	SYNthesis	SYN-1019	BI-2536 (R-) (10 mM)
3244 F07	X	2096	2120	-0.90842717	2726	2760	-0.89253101	2424269	-0.54801188	2340580	-0.64561319	experimental	SYNthesis	SYN-1067	PIK-75 (1.11 mM)
3244 F08	X	1975	2000	-1.04893454	2645	2680	-0.95489892	2859927	0.17329073	3122308	0.44866957	experimental	SYNthesis	SYN-1114	GNE-490 (3.33 mM)
3244 F09	X	1898	1920	-1.13834832	2532	2560	-1.041906	3261751	0.83857565	3523245	1.00991139	W	SYNthesis	SYN-1068	PIK-90 (1.11 mM)
3244 F10	X	1976	2000	-1.04777332	2448	2480	-1.10658383	2583603	-0.28420856	2654744	-0.20583843	W	SYNthesis	SYN-1019	BI-2536 (R-) (3.33 mM)
3244 F11	X	2095	2120	-0.90958839	2407	2440	-1.13815277	3187048	0.71489269	3155663	0.49536075	experimental	SYNthesis	SYN-1065	PI-103 (1.11 mM)
3244 F12	X	2576	2600	-0.35104256	1932	1960	-1.50389049	3350751	0.98592961	3231616	0.60168169	W	SYNthesis	SYN-1114	GNE-490 (1.11 mM)
3244 F13	X	2015	2040	-1.00248582	2171	2200	-1.31986667	3309510	0.91764843	3450960	0.90872501	experimental	SYNthesis	SYN-1098	PIK-294 (1.11 mM)
3244 F14	X	1935	1960	-1.09538325	2692	2720	-0.91871013	3115612	0.59661879	3112736	0.43527044	experimental	SYNthesis	SYN-1019	BI-2536 (R-) (1.11 mM)
3244 F15	X	2459	2480	-0.48690506	2334	2360	-1.19436088	3987890	2.04081675	3300425	0.69800228	experimental	SYNthesis	SYN-1089	TGX221 (1.11 mM)
3244 F16	E	1936	1960	-1.09422204	2212	2240	-1.28829772	3587226	1.37745239	3355611	0.77525305	empty			
3244 F17	X	2129	2160	-0.87010698	2565	2600	-1.01649685	4130595	2.27708806	3783777	1.37461072	experimental	SYNthesis	SYN-1094	YM201636 (1.11 mM)
3244 F18	X	2247	2280	-0.73308326	2445	2480	-1.10889375	3081606	0.54031633	2917113	0.23758289	empty			
3244 F19	X	2884	2920	0.00661256	2680	2720	-0.92794982	3434215	1.12411782	2917895	0.16252705	experimental	SYNthesis	SYN-1113	SMI-4a (1.11 mM)
3244 F20	E	2086	2120	-0.92003835	2522	2560	-1.04966754	28974232	0.28973352	34081362	0.13492557	empty			
3244 F21	X	1759	1760	-1.37626894	2648	2680	-0.952589	2655990	-0.16278022	2874433	0.10169482	experimental	SYNthesis	SYN-1021	Bisindolylmaleimide X, HCl salt (1.11 mM)
3244 F22	E	1728	1760	-1.33575536	2483	2520	-1.07963473	2795203	0.06612963	3277613	0.66606947	empty			
3244 F23	N	3379	3880	0.58141543	3340	3600	-0.41976688	3268814	0.85026959	2767358	-0.04819848	empty			
3244 F24	P	161932	162920	184.696001	78623	79160	57.546197	2687394	-0.11236569	2647352	-0.21618594	empty			
3244 G01	E	1703	1720	-1.36478581	4374	4400	0.37638639	2557719	-0.32706372	3043847	0.33883786	empty			
3244 G02	E	1738	1760	-1.32414318	2763	2800	-0.86404197	2758953	0.06611186	3123434	0.45024577	empty			
3244 G03	X	1736	1760	-1.32646562	2168	2200	-1.32217659	2538112	-0.3595263	2526784	-0.38496009	W	SYNthesis	SYN-1016	AZD6244 (10 mM)
3244 G04	X	2264	2280	-0.72495474	2171	2200	-0.81781521	416514850	0.36976317	48481961	0.24848196	experimental	SYNthesis	SYN-1066	AZD6244 (3.33 mM)
3244 G05	X	1855	1880	-1.18828069	3126	3160	-0.58454135	2332276	-0.70032124	2715325	-0.12103556	experimental	SYNthesis	SYN-1031	CI-1040 (10 mM)
3244 G06	X	2577	2600	-0.34988135	3124	3160	-0.5860813	2800720	0.07526392	2899244	0.1364189	experimental	SYNthesis	SYN-1031	CI-1040 (3.33 mM)
3244 G07	X	1892	1920	-1.14531562	2725	2760	-0.89330099	2540771	-0.35512389	2318129	-0.67704068	experimental	SYNthesis	SYN-1059	PD0325901 (10 mM)
3244 G08	X	2214	2240	-0.77140345	2607	2640	-0.98415794	3151158	0.65547097	3413057	0.85566743	experimental	SYNthesis	SYN-1059	PD0325901 (3.33 mM)
3244 G09	X	1815	1840	-1.2347294	2328	2360	-1.19898072	2725580	-0.04914256	2616034	-0.26002567	W	SYNthesis	SYN-1047	JN33877605 (10 mM)
3244 G10	X	2015	2040	-1.00248582	2287	2320	-1.23054966	3500671	1.23414653	2970456	0.23610327	experimental	SYNthesis	SYN-1047	JN33877605 (3.33 mM)
3244 G11	X	2174	2200	-0.81781521	2487	2520	-0.81781521	416514850	0.36976317	48481961	0.24848196	W	SYNthesis	SYN-1060	PF04217903 (1.11 mM)
3244 G12	X	1972	2000	-0.5241819	2487	2520	-1.07655483	3116304	0.68054763	3999028	1.67592456	experimental	SYNthesis	SYN-1040	PF04217903 (3.33 mM)
3244 G13	X	1973	2000	-1.05125697	2727	2760	-0.89176104	4056433	2.15430082	4297829	2.09419381	experimental	SYNthesis	SYN-1050	KU0063794 (10 mM)
3244 G14	X	2179	2200	-0.81204608	2888	2920	-0.7677952	3367379	1.01345996	3863668	1.48644418	experimental	SYNthesis	SYN-1050	KU0063794 (3.33 mM)
3244 G15	X	894	920	-2.30421111	1648	1680	-1.72256315	1314217	-2.38858333	1388499	-1.97836043	experimental	SYNthesis	SYN-1026	BX795 (10 mM)
3244 G16	X	1373	1400	-1.47498773	2044	2080	-1.41765338	1415420	-2.21832532	1409206	-1.94937424	experimental	SYNthesis	SYN-1026	BX795 (3.33 mM)
3244 G17	X	4130	4160	1.45349009	4442	4480	-0.42874463	1810681	-1.56390651	1792552	-1.41275675	experimental	SYNthesis	SYN-1027	BX912 (10 mM)
3244 G18	X	3760	3800	1.02383966	4568	4600	0.21007197	2470037	-0.47223552	3188283	0.61103321	experimental	SYNthesis	SYN-1027	BX912 (3.33 mM)
3244 G19	X	4359	4400	0.19408999	4156	4200	0.20853202	3368732	0.71940885	3188283	0.61103322	experimental	SYNthesis	SYN-1009	AS-252424 (10 mM)
3244 G20	X	3327	3360	0.5210321	3839	3880	-0.03554978	3083102	0.5427932	2863530	0.08642554	experimental	SYNthesis	SYN-1009	AS-252424 (3.33 mM)
3244 G21	X	2526	2560	-0.40910346	3640	3680	-0.18877464	2358436	-0.65700911	2223865	-0.80899382	experimental	SYNthesis	SYN-1018	BEZ-235 (10 mM)
3244 G22	X	3245	3280	0.42581223	3360	3400	-0.4043674	2504640	-0.41494463	2311608	-0.68616894	experimental	SYNthesis	SYN-1018	BEZ-235 (3.33 mM)
3244 G23	N	4145	4720	1.47090836	4327	4560	0.3401976	2830273	0.12419371	3011315	0.29329874	empty			
3244 G24	P	184575	185840	210.989458	68092	68640	49.43755993	2899132	0.23820097	2878500	0.10787086	empty			
3244 H01	E	2460	2480	-0.48574384	3645	3680	-0.18492477	2938545	0.30340556	3117411	0.44181463	empty			
3244 H02	E	2332	2360	-0.63437974	3720	3760	-0.12717671	2734871	-0.0337598	2850740	0.06852177	empty			
3244 H03	X	2488	2520	-0.45322974	3480	3520	-0.3119705	2669554	-0.14190271	2849907	0.06735571	experimental	SYNthesis	SYN-1016	AZD6244 (1.11 mM)
3244 H04	X	2771	2800	-0.12460507	3681	3720	-0.1572057	3060873	0.50598948	2756986	-0.06271747	experimental	SYNthesis	SYN-1093	VX-702 (10 mM)
3244 H05	X	2208	2240	-0.77837076	3477	3520	-0.31428043	2975967	0.3654138	2780743	-0.02946182	experimental	SYNthesis	SYN-1031	CI-1040 (1.11 mM)
3244 H06	X	2487	2520	-0.45439096	4195	4240	0.23856101	2965902	0.34874956	2957063	0.21735541	experimental	SYNthesis	SYN-1041	GDC-0941 (10 mM)
3244 H07	X	2848	2880	-0.03519129	3598	3640	-0.22111355	2987662	0.38477677	3056880	0.35708179	experimental	SYNthesis	SYN-1059	PD0325901 (1.11 mM)
3244 H08	X	3051	3080	0.20053595	3480	3520	-0.3119705	3193834	0.72612802	3611480	1.1334225	experimental	SYNthesis	SYN-1093	VX-702 (3.33 mM)
3244 H09	X	2490	2520	-0.45090731	3528	3600	-0.25114255	3122156	0.60745344	3380672	0.81033408	experimental	SYNthesis	SYN-1047	JN33877605 (1.11 mM)
3244 H10	X	2411	2440	-0.54264352	3363	3400	-0.40205748	3343420	0.97379195	3532801	1.02338813	experimental	SYNthesis	SYN-1041	GDC-0941 (3.33 mM)
3244 H11	X	2771	2800	-0.12460507	3520	3560	-0.28117154	3697479	1.55999415	3399758	0.83705115	experimental	SYNthesis	SYN-1060	PF04217903 (1.11 mM)
3244 H12	X	2768	2800	-0.12808872	3321	3360	-0.43439639	3244789	0.8104423	3200808	0.58855587	experimental	SYNthesis	SYN-1093	VX-702 (1.11 mM)
3244 H13	X	2768	3000	0.10763851	3880	3920	-0.00398084	3194019	0.72643432	3359913	0.7812751	experimental	SYNthesis	SYN-1050	KU0063794 (1.11 mM)
3244 H14	X	2327	2360	-0.64018583	3797	3840	-0.0678887	3307840	0.91488348	3530284	1.01976477	experimental	SYNthesis	SYN-1041	GDC-0941 (1.11 mM)
3244 H15	X	2855	2880	-0.02706276	3641	3680	-0.18800467	2558086	-0.32645609	2668272	-0.18690159	experimental	SYNthesis	SY	

3244 I13	X	2805	2840	-0.08512366	3915	3960	0.02296825	3284580	0.87637277	3917887	1.56234132	experimental	SYNthesis	SYN-1073	SB202190 (10 mM)
3244 I14	X	3288	3320	0.4757446	4274	4320	0.29938897	3423836	1.1069337	3580673	1.09030057	experimental	SYNthesis	SYN-1073	SB202190 (3.33 mM)
3244 I15	X	2765	2800	-0.13157238	3834	3880	-0.03939965	3222344	0.77333096	3224968	0.59237565	experimental	SYNthesis	SYN-1074	SB203580 (10 mM)
3244 I16	X	2807	2840	-0.08280122	3355	3400	-0.40817177	3671835	1.51753634	3991962	1.66603339	experimental	SYNthesis	SYN-1074	SB203580 (3.33 mM)
3244 I17	X	3005	3040	0.14711992	3674	3720	-0.16256562	3207856	3.10449041	3104262	0.42427463	experimental	SYNthesis	SYN-1076	SB242235 (10 mM)
3244 I18	X	3085	3120	0.24001736	3877	3920	-0.00629077	3652544	1.48559696	3943345	1.59797807	experimental	SYNthesis	SYN-1076	SB242235 (3.33 mM)
3244 I19	X	2685	2720	-0.22446981	3752	3800	-0.10253753	3362369	1.0051651	3387721	0.82020145	experimental	SYNthesis	SYN-1078	SD-06 (10 mM)
3244 I20	X	2686	2720	-0.22330859	3912	3960	0.02065833	3514487	1.25702116	3506660	0.98669529	experimental	SYNthesis	SYN-1078	SD-06 (3.33 mM)
3244 I21	X	4043	4080	1.35246413	4507	4560	0.47879295	2787721	0.05374196	3013496	0.29635176	experimental	SYNthesis	SYN-1079	SD169 (10 mM)
3244 I22	X	3757	3800	1.0203558	4992	5040	0.85223041	3113516	0.59314852	3350079	0.76750922	experimental	SYNthesis	SYN-1079	SD169 (3.33 mM)
3244 I23	N	4314	4960	1.66715418	4510	4880	0.48110287	2758495	0.00535357	3086381	0.39637804	empty			
3244 I24	P	208214	209440	238.493989	111950	112520	83.2071255	2899744	0.23921424	2342164	0.2494968	empty			
3244 J01	E	2696	2720	-0.21169641	4762	4800	0.67513636	3060625	0.50557887	2842600	0.05637128	empty			
3244 J02	E	2687	2720	-0.22214738	3910	3960	0.01911838	3028691	0.45270695	3108655	0.42955775	empty			
3244 J03	X	3199	3240	0.3723962	4303	4360	0.32171822	3464110	1.17361385	3233626	0.60449534	experimental	SYNthesis	SYN-1084	SU-5402 (1.11 mM)
3244 J04	X	4485	4520	1.86572245	7750	7800	2.97581912	1377249	-2.28152362	1417888	-1.93722096	experimental	SYNthesis	SYN-1053	Masatinib (10 mM)
3244 J05	X	2633	2680	-0.28485314	4138	4200	0.19467249	2841874	0.14340105	3307175	0.70745111	experimental	SYNthesis	SYN-1007	AMG-47a (1.11 mM)
3244 J06	X	3200	3240	0.37355742	5062	5120	0.9061286	2594310	-0.26648138	3068455	0.37328471	experimental	SYNthesis	SYN-1087	TAK-715 (10 mM)
3244 J07	X	2356	2400	-0.60651051	4184	4240	0.2300913	3183666	0.70929324	3342164	0.7564296	experimental	SYNthesis	SYN-1024	BMS-5 (1.11 mM)
3244 J08	X	4241	4280	1.58238528	5310	5360	1.09708219	2958102	0.33583539	2922759	0.1693358	experimental	SYNthesis	SYN-1053	Masatinib (3.33 mM)
3244 J09	X	3002	3040	0.14363627	4305	4360	0.32325817	4011032	2.07913209	3694342	1.24941733	experimental	SYNthesis	SYN-1101	R1487 (1.11 mM)
3244 J10	X	3327	3360	0.51203211	4516	4560	0.48572272	3721952	1.60051318	3486154	0.95799047	experimental	SYNthesis	SYN-1087	TAK-715 (3.33 mM)
3244 J11	X	2641	2680	-0.2755634	3574	3640	-0.22804332	3150767	0.6548236	2984981	0.25643574	experimental	SYNthesis	SYN-1072	RWJ-67657 (1.11 mM)
3244 J12	X	4485	4520	1.86572245	5469	5520	1.21950808	3168794	0.68467023	3276422	0.66440227	experimental	SYNthesis	SYN-1053	Masatinib (1.11 mM)
3244 J13	X	2319	2360	-0.64947597	3865	3920	-0.01553046	3369178	0.10164385	3855973	1.47567252	experimental	SYNthesis	SYN-1073	SB202190 (1.11 mM)
3244 J14	X	3040	3080	0.19472996	4230	4280	0.19472996	3312508	0.92261211	3236132	0.71261678	experimental	SYNthesis	SYN-1087	TAK-715 (1.11 mM)
3244 J15	X	2965	3000	0.09711855	4586	4640	0.53962091	3307335	1.58498241	3535071	1.02645483	experimental	SYNthesis	SYN-1074	SB203580 (1.11 mM)
3244 J16	E	3085	3120	0.24001736	3870	3920	-0.01168058	3266911	0.84711887	3601742	1.11979349	empty			
3244 J17	X	3004	3040	0.14595871	4432	4480	0.42104489	3446125	1.14383676	3085014	0.39646448	experimental	SYNthesis	SYN-1076	SB242235 (1.11 mM)
3244 J18	E	3288	3320	0.4757446	4230	4280	0.26551011	3125988	0.61379794	3173173	0.51987169	empty			
3244 J19	X	2363	2400	-0.59838198	4030	4080	0.11151528	3054066	0.49471938	3478885	0.94781514	experimental	SYNthesis	SYN-1078	SD-06 (1.11 mM)
3244 J20	E	2645	2680	-0.27091853	4183	4240	0.22932132	3349673	0.9841448	3454052	0.91305327	empty			
3244 J21	X	2962	3000	0.09718755	5550	5600	1.28187599	3391189	1.05288129	3302775	0.70129187	experimental	SYNthesis	SYN-1079	SD169 (1.11 mM)
3244 J22	X	2962	3000	0.09493275	4108	4200	0.04493275	2790023	0.41785421	2917225	0.05061606	empty			
3244 J23	N	3967	4440	1.26421157	5228	5520	1.03394431	2916805	0.2674615	3212015	0.57424371	empty			
3244 J24	P	148113	149440	168.64913	85952	86560	63.1893376	2680397	-0.12395036	2670230	-0.18416073	empty			
3244 K01	E	2537	2560	-0.39633006	5040	5080	0.88918917	2925256	0.2814535	2844121	0.05925632	empty			
3244 K02	E	2568	2600	-0.36033231	4269	4320	0.2955391	2849039	0.15526387	3140557	0.47421499	empty			
3244 K03	X	2884	2920	0.00661256	3903	3960	0.01372856	1488068	-2.09804476	1471713	-1.86187535	experimental	SYNthesis	SYN-1090	Vandetanib (10 mM)
3244 K04	X	3279	3320	0.46529363	4503	4560	0.47571305	2748109	-0.45887101	2072499	-1.02087981	experimental	SYNthesis	SYN-1090	Vandetanib (3.33 mM)
3244 K05	X	4560	4600	0.13005297	4450	4500	0.1265617	2277440	-1.2265525	2120525	-0.48292619	experimental	SYNthesis	SYN-1033	CP-724714 (10 mM)
3244 K06	X	4876	4920	0.13975866	6303	6360	1.86166652	3082505	0.54180477	2397123	-0.56646286	experimental	SYNthesis	SYN-1033	CP-724714 (3.33 mM)
3244 K07	X	4273	4320	1.61954425	4702	4760	0.62893791	2815628	0.09994653	2115042	-0.96132703	experimental	SYNthesis	SYN-1064	PF562271 (10 mM)
3244 K08	X	5398	5440	0.292591441	4745	4800	0.6620468	2680446	-0.12386923	2146226	-0.91767487	experimental	SYNthesis	SYN-1064	PF562271 (3.33 mM)
3244 K09	X	2640	2680	-0.27672462	4348	4400	0.3563706	2764972	0.01607729	1786872	-1.42070776	experimental	SYNthesis	SYN-1003	AC220 (10 mM)
3244 K10	X	2725	2760	-0.17802109	3831	3880	-0.04170958	3332227	0.95526012	1746490	-1.47723551	experimental	SYNthesis	SYN-1003	AC220 (3.33 mM)
3244 K11	X	2884	2920	0.00661256	3667	3720	-0.16798534	2716136	-0.06477864	1838257	-1.34877772	experimental	SYNthesis	SYN-1049	K20227 (10 mM)
3244 K12	X	3557	3600	0.78811222	6545	6600	2.04800027	3277440	0.8642202	3277440	5.60801210	experimental	SYNthesis	SYN-1049	K20227 (3.33 mM)
3244 K13	X	3680	3720	0.89029929	5183	5240	0.99929547	3253384	0.8240702	2547402	1.02645483	experimental	SYNthesis	SYN-1075	SB-216763 (10 mM)
3244 K14	X	2958	3000	0.09254268	4421	4480	0.41257517	3453400	1.15588171	4306534	2.10637929	experimental	SYNthesis	SYN-1075	SB-216763 (3.33 mM)
3244 K15	X	4044	4080	1.35362535	6346	6400	1.89477541	2177141	-0.95717244	2474669	-0.457912	experimental	SYNthesis	SYN-1015	AZ-960 (10 mM)
3244 K16	X	3201	3240	0.37471864	4863	4920	0.75290375	2988555	0.4028119	2733690	-0.0953278	experimental	SYNthesis	SYN-1015	AZ-960 (3.33 mM)
3244 K17	X	3085	3120	0.24001736	4628	4680	0.57195982	3180333	0.70377492	3242131	0.61640086	experimental	SYNthesis	SYN-1032	CP690550 (Tasocitinib) (10 mM)
3244 K18	X	2601	2640	-0.32201212	4788	4840	0.69515568	3551072	1.31759357	3615905	1.13835938	experimental	SYNthesis	SYN-1032	CP690550 (Tasocitinib) (3.33 mM)
3244 K19	X	4165	4200	1.49413271	4864	4920	0.75367372	3100216	0.57112821	2741825	-0.08394022	experimental	SYNthesis	SYN-1035	CT111387 (10 mM)
3244 K20	X	3920	3960	1.20963432	6108	6160	1.71152156	3799469	1.72885517	4013925	1.69677776	experimental	SYNthesis	SYN-1035	CT111387 (3.33 mM)
3244 K21	X	3320	3360	0.51290357	4339	4400	0.34943729	2982871	0.37684449	2824345	0.03157337	experimental	SYNthesis	SYN-1054	Merck-5 (10 mM)
3244 K22	X	3555	3600	0.78578978	4587	4640	0.54039088	3095390	0.56313798	2795467	-0.00885079	experimental	SYNthesis	SYN-1054	Merck-5 (3.33 mM)
3244 K23	N	5176	5920	2.66812403	4888	5200	0.7721531	3013696	0.42788029	2919453	0.16470797	empty			
3244 K24	P	243604	244440	279.534991	91163	91840	67.2016729	3695949	1.55746099	3086446	0.39846903	empty			
3244 L01	E	2616	2640	-0.30459385	4637	4680	0.57888959	2973056	0.36059417	3303191	0.70247333	empty			
3244 L02	E	2807	2840	-0.08280122	4462	4520	0.44414411	2892144	0.2266312	3109324	0.43049424	empty			
3244 L03	X	3281	3320	0.46761607	6431	6480	1.96023221	2438287	-0.5248028	3191694	0.54579786	experimental	SYNthesis	SYN-1090	Vandetanib (1.11 mM)
3244 L04	X	1996	2040	-1.02454896	3298	3360	-0.4521058	1195516	-2.58241213	1234237	-2.1943003	experimental	SYNthesis	SYN-1100	TOVOK (10 mM)
3244 L05	X	4600	4640	1.99926251	5382	5440	1.15252033	2707417	-0.07921436	2468767	-0.46617377	experimental	SYNthesis	SYN-1033	CP-724714 (1.11 mM)
3244 L06	X	3191	3240	0.36310646	5011	5080	0.86685992	2316400	-0.72660654	2439494	-0.50715086	experimental	SYNthesis	SYN-1028	CC-401 (10 mM)
3244 L07	X	3593	3640	0.82991606	5541	4600	0.50497207	3792728	1.71769435	3535187	1.02662811	experimental	SYNthesis	SYN-1064	PF562271 (1.11 mM)
3244 L08	X	3272	3320	0.45716511	4417	4480	0.40949528	2006941	-1.23896619	1687599	-1.55967263	experimental	SYNthesis	SYN-1100	TOVOK (3.33 mM)
3244 L09	X	2644	2680	-0.27207975	4906	4960	0.78601263	3493333	1.22199728	3089403	0.40260831	experimental	SYNthesis	SYN-1003	AC220 (1.11 mM)
3244 L10	X	3003	3040	0.124756											

3244 M07	X	5396	5440	2.92359198	6049	6120	1.66609309	2769621	0.02377447	2604333	-0.27640503	experimental	SYNthesis	SYN-1070	Purvalanol B (10 mM)
3244 M08	X	4754	4800	2.17809007	7379	7440	2.69015871	3683898	1.5375086	3063468	0.36630384	experimental	SYNthesis	SYN-1070	Purvalanol B (3.33 mM)
3244 M09	X	3358	3400	0.55702985	5216	5280	1.02470462	2056977	-1.15612347	2092079	-0.99347122	experimental	SYNthesis	SYN-1080	SNS-032 (10 mM)
3244 M10	X	3801	3840	1.07144939	4980	5040	0.84298072	2837031	0.13538268	2655034	-0.33141677	experimental	SYNthesis	SYN-1080	SNS-032 (3.33 mM)
3244 M11	X	3919	3960	0.0847311	6142	6200	1.37770068	2034870	-1.11927255	2262817	-0.75446782	experimental	SYNthesis	SYN-1070	AZD7762 (10 mM)
3244 M12	X	3159	3200	0.32594748	5178	5240	0.99544556	2455315	-0.49661018	2754660	-0.06597346	experimental	SYNthesis	SYN-1017	AZD7762 (3.33 mM)
3244 M13	X	2803	2840	-0.0874461	5582	5640	1.30651516	2502117	-0.41912187	2890635	0.1243678	experimental	SYNthesis	SYN-1109	CX-4945 (10 mM)
3244 M14	X	3646	3680	0.89146061	5267	5320	1.06397333	3473326	1.18887244	2922676	0.16921961	experimental	SYNthesis	SYN-1109	CX-4945 (3.33 mM)
3244 M15	X	1962	2000	-1.06403037	3585	3640	-0.23112322	1400253	-2.24343676	1419352	-1.93517161	experimental	SYNthesis	SYN-1012	AV-412 (10 mM)
3244 M16	X	3406	3440	0.61276831	4228	4280	0.26397016	2137406	-1.02269019	1932768	-1.21647882	experimental	SYNthesis	SYN-1012	AV-412 (3.33 mM)
3244 M17	X	3762	3800	1.02616189	4911	4960	0.78986625	1823705	-1.54234317	1630766	-1.63922891	experimental	SYNthesis	SYN-1030	CI-1033 (Canertinib) (10 mM)
3244 M18	X	3362	3400	0.56167472	4508	4560	0.47055292	2182947	-0.94755966	1803799	-1.39785228	experimental	SYNthesis	SYN-1030	CI-1033 (Canertinib) (3.33 mM)
3244 M19	X	3282	3320	0.46877729	4187	4240	0.23240122	2701993	-0.08819467	2732619	-0.09682702	experimental	SYNthesis	SYN-1039	Erlotinib (10 mM)
3244 M20	X	3284	3320	0.47109972	5030	5080	0.88148943	3152366	0.65747101	3234117	0.60518266	experimental	SYNthesis	SYN-1039	Erlotinib (3.33 mM)
3244 M21	X	2484	2520	-0.45787461	4147	4200	0.20160225	1563126	-1.97377404	1493220	-1.8317693	experimental	SYNthesis	SYN-1042	Gefitinib (10 mM)
3244 M22	X	2876	2920	-0.00267719	4385	4440	0.3848561	2077256	-1.12254829	2433518	-0.51551621	experimental	SYNthesis	SYN-1042	Gefitinib (3.33 mM)
3244 M23	N	5284	5284	2.79353557	5242	5560	1.04472395	2860439	0.17413842	2699947	-0.14256211	empty			
3244 M24	P	288685	289680	331.883856	93231	93960	68.7939794	3080971	0.53926498	2988091	0.26218902	empty			
3244 N01	E	3174	3200	0.34336575	4436	4480	0.42412478	2649237	-0.1755408	2689712	-0.15688933	empty			
3244 N02	E	2964	3000	0.09590999	4864	4920	0.75367372	2957682	0.33514001	2755361	-0.06499219	empty			
3244 N03	X	3517	3560	0.7416635	5261	5320	1.05935346	2482228	-0.45205134	3147470	0.48389198	experimental	SYNthesis	SYN-1040	Flavopipridol (1.11 mM)
3244 N04	X	3398	3440	0.60347857	5775	5840	1.45512017	1970181	-1.29982835	2028287	-1.00703833	experimental	SYNthesis	SYN-1010	AT-7519 (10 mM)
3244 N05	X	4482	4520	1.86223888	6813	6880	2.25435334	2764737	0.01568821	3087816	0.40038679	experimental	SYNthesis	SYN-1097	PHA690509 (1.11 mM)
3244 N06	X	2398	2440	-0.55773935	3640	3720	-0.18877464	1736977	-1.68593546	1679095	-1.57157674	experimental	SYNthesis	SYN-1052	Lapatinib (10 mM)
3244 N07	X	2957	3000	0.09138148	5141	5200	0.96695656	2858618	0.17112346	2910518	0.15220053	experimental	SYNthesis	SYN-1070	Purvalanol B (1.11 mM)
3244 N08	X	3679	3720	0.5297808	4798	4860	0.92974226	2495515	-0.43005255	2679	0.43411266	experimental	SYNthesis	SYN-1043	GSK690693 (3.33 mM)
3244 N09	X	3159	3200	0.32478627	4701	4760	0.62818793	256953783	-0.30750207	3723493	-0.10960182	experimental	SYNthesis	SYN-1080	SNS-032 (10 mM)
3244 N10	X	3158	3200	0.32594748	4662	4720	0.59813894	2179343	-0.95352667	2154214	-0.90649307	experimental	SYNthesis	SYN-1052	Lapatinib (3.33 mM)
3244 N11	X	3475	3520	0.69289235	5374	5440	1.14636054	2886273	0.21691081	3018848	0.30384363	experimental	SYNthesis	SYN-1017	AZD7762 (1.11 mM)
3244 N12	X	3520	3560	0.74514715	4816	4880	0.71671496	2244505	-0.84564039	2373990	-0.59884503	experimental	SYNthesis	SYN-1010	AT-7519 (1.11 mM)
3244 N13	X	2841	2880	-0.04331982	4900	4960	0.78139279	2707986	-0.07827229	2145325	-0.91893612	experimental	SYNthesis	SYN-1109	Lapatinib (1.11 mM)
3244 N14	X	3284	3320	0.47109972	4623	4680	0.56810995	2634801	-0.19944195	2790802	-0.01538097	experimental	SYNthesis	SYN-1052	Lapatinib (1.11 mM)
3244 N15	X	2805	2840	-0.08512366	4626	4680	0.57041987	2682017	-0.12126819	2686977	-0.16071785	experimental	SYNthesis	SYN-1012	AV-412 (1.11 mM)
3244 N16	X	3040	3080	0.14247505	4798	4860	0.59659899	2876089	0.14560199	2616272	0.48389198	experimental	SYNthesis	SYN-1039	Erlotinib (1.11 mM)
3244 N17	X	3084	3120	0.23885614	4186	4240	0.23163125	2536449	-0.36227966	2265609	-0.75055951	experimental	SYNthesis	SYN-1030	CI-1033 (Canertinib) (1.11 mM)
3244 N18	X	3364	3400	0.56399716	4829	4880	0.72672462	3294664	0.89306847	3104896	0.42429581	empty			
3244 N19	X	3162	3200	0.32943114	4187	4240	0.23240122	3100724	0.57196928	3278691	0.66757848	experimental	SYNthesis	SYN-1039	Erlotinib (1.11 mM)
3244 N20	E	2924	2960	0.05306127	4588	4640	0.54116085	2685383	-0.11569523	2802158	0.00051545	empty			
3244 N21	X	2888	2920	0.01125743	4350	4400	0.35790701	2504875	-0.41455555	2637433	-0.2300708	experimental	SYNthesis	SYN-1042	Gefitinib (1.11 mM)
3244 N22	E	3039	3080	0.18660133	4546	4600	0.50882194	2659321	-0.15888451	2932163	0.18249976	empty			
3244 N23	N	2890	2920	2.33601571	6172	5520	0.92057426	2923084	-0.2828807	2686370	-0.22696807	empty			
3244 N24	P	202774	20280	332.122463	103604	104240	76.7809213	2450962	-0.50381728	2638704	-0.22829316	empty			
3244 O01	E	3173	3200	0.34220454	4719	4760	0.64202747	2682704	-0.12013075	2594124	-0.29069585	empty			
3244 O02	E	2726	2760	-0.17685988	4825	4880	0.72364473	2800221	0.07443774	2986124	0.25803574	empty			
3244 O03	X	2926	2960	0.05538371	4222	4280	0.25935032	1956879	-1.321851975	1645763	-1.61823573	experimental	SYNthesis	SYN-1006	Akt-1-1,2 (10 mM)
3244 O04	X	2519	2560	-0.41723199	3938	5015	0.86993982	2584620	-0.28252475	2140381	-0.92585685	experimental	SYNthesis	SYN-1006	Akt-1-1,2 (3.33 mM)
3244 O05	X	3400	3440	0.37355742	6448	6520	1.97331272	2206731	-0.90818139	2298635	-0.70442966	experimental	SYNthesis	SYN-1043	GSK690693 (10 mM)
3244 O06	X	3200	3240	0.60928466	7938	8000	1.20574226	2689619	-0.10068188	2465122	-0.47629475	experimental	SYNthesis	SYN-1043	GSK690693 (3.33 mM)
3244 O07	X	3204	3240	0.37820229	6332	6400	1.11402168	2682967	-0.11969531	2803091	0.05895938	experimental	SYNthesis	SYN-1051	KU55933 (10 mM)
3244 O08	X	2999	3040	0.14015262	5140	5200	0.96618659	2977683	0.36825492	3296307	0.6922378	experimental	SYNthesis	SYN-1051	KU55933 (3.33 mM)
3244 O09	X	4002	4040	1.30485419	5223	5280	1.03009444	2459528	-0.48963488	2164637	-0.89190269	experimental	SYNthesis	SYN-1011	AT9283 (10 mM)
3244 O10	X	3395	3440	0.59999491	4895	4960	0.77754292	2448857	-0.50730245	2098253	-0.9848287	experimental	SYNthesis	SYN-1011	AT9283 (3.33 mM)
3244 O11	X	4798	4840	2.22918366	7092	7160	2.46917613	2829920	0.12360926	3009531	0.29080145	experimental	SYNthesis	SYN-1034	CYC-116 (10 mM)
3244 O12	X	4154	4200	1.48135932	6536	6600	2.0410705	3160941	0.67166831	2863493	0.08637374	experimental	SYNthesis	SYN-1034	CYC-116 (3.33 mM)
3244 O13	X	3600	3640	0.83804459	5379	5440	1.15021041	2998332	0.40244269	2846705	0.06287347	experimental	SYNthesis	SYN-1095	Danusertib (10 mM)
3244 O14	X	3079	3120	0.23305005	4660	4720	0.59659899	2878083	0.20335093	3169674	0.5149737	experimental	SYNthesis	SYN-1095	Danusertib (3.33 mM)
3244 O15	X	3721	3760	0.97851596	5384	5440	1.15406028	2426200	-0.54481148	2782322	-0.02725149	experimental	SYNthesis	SYN-1048	JNJ706621 (10 mM)
3244 O16	X	3964	4000	1.26072791	5066	5120	0.9092085	2915252	0.26489025	2714672	-0.12194968	experimental	SYNthesis	SYN-1048	JNJ706621 (3.33 mM)
3244 O17	X	2163	2200	-0.83062557	3786	3840	-0.07635841	1603408	-1.90780864	1601339	-1.68014161	experimental	SYNthesis	SYN-1081	SNS-314 (10 mM)
3244 O18	X	2562	2600	-0.36729962	4548	4600	0.51036189	1767860	-1.63480364	1763851	-1.45293314	experimental	SYNthesis	SYN-1081	SNS-314 (3.33 mM)
3244 O19	X	3405	3440	0.61160709	4588	4640	0.54116085	3019498	0.43748644	2718511	-0.11657575	experimental	SYNthesis	SYN-1092	VX-680 (10 mM)
3244 O20	X	3045	3080	0.19356864	4348	4400	0.35636706	2927971	0.28594862	2975272	0.24284483	experimental	SYNthesis	SYN-1092	VX-680 (3.33 mM)
3244 O21	X	2447	2480	-0.50083968	4798	4860	-0.04247955	1886170	-1.43892221	1712312	-1.51248031	experimental	SYNthesis	SYN-1001	ABT-737 (10 mM)
3244 O22	X	2601	2640	-0.32201212	4265	4320	0.2924592	1787668	-1.60200828	1845463	-1.338869058	experimental	SYNthesis	SYN-1001	ABT-737 (3.33 mM)
3244 O23	N	3869	4400	1.15041221	5484	5880	1.23105769	2822958	0.11208254	2760472	-0.05783768	empty			
3244 O24	P	168325	169640	192.119667	119253	120120	88.8302467	2893459	0.2288084	2836379	0.04841887	empty			
3244 P01	E	3303	3320	0.49316286	4932	4960	0.80603196	2746800	-0.0140094	2664177	-0.19263387	empty			
3244 P02	E	2694	2720	-0.21401885	4877	4920	0.76368338	2384893	-0.61320525	2393092	-0.57210556	empty			
3244 P03	X	2931	2960	0.0611898	4797	4840	0.70208545	2353507	-0.66516987	2611167	-0.26683862	experimental	SYNthesis	SYN-1006	Akt-1-1,2 (1.11 mM)
3244 P04	X	437													

3259 A01	N	598	600	0.65959198	519	520	0.01611436	1004605	-0.44089765	empty			
3259 A02	E	76	80	-1.81496609	117	120	-2.05713366	80277	-1.89973641	empty			
3259 A03	X	518	520	0.28034937	398	400	-0.60792298	927623	-0.562396	experimental	NIH	SAM002264608	DOXEPIH HYDROCHLORIDE
3259 A04	X	396	400	-0.29799562	516	520	0.00064236	1455973	0.27148274	experimental	NIH	SAM002554930	Novocain
3259 A05	X	435	440	-0.11311485	432	440	-0.43257365	1468364	0.29103908	experimental	NIH	SAM002264616	Folic acid
3259 A06	X	356	360	-0.48761693	597	600	0.41838636	1318949	0.05522193	experimental	NIH	SAM002554928	Pronestyl
3259 A07	X	475	480	0.07650646	434	440	-0.42225898	1348308	0.10155834	experimental	NIH	SAM002264625	NORFLOXACIN
3259 A08	X	836	840	1.78783877	636	640	0.61952236	1559376	0.43468055	experimental	NIH	SAM002554936	Tolbutamide
3259 A09	X	475	480	0.07650646	516	520	0.00064236	1048344	-0.37186571	experimental	NIH	SAM002264636	Phenergan
3259 A10	X	756	760	1.40859615	516	520	0.00064236	1387014	0.16264685	experimental	NIH	SAM002564250	CLOBETASOL PROPIONATE
3259 A11	X	551	560	0.43678695	394	400	-0.62855232	1342066	0.09170679	experimental	NIH	SAM002264645	Ranitidine hydrochloride
3259 A12	X	477	480	0.08598753	636	640	0.61952236	1065554	-0.34312542	experimental	NIH	SAM002564205	DIGOXIN
3259 A13	X	275	280	-0.87160008	675	680	0.82065836	1226155	-0.09123202	experimental	NIH	SAM002264653	URSODEOXYCHOLIC ACID
3259 A14	X	514	520	0.26138724	594	600	0.40291436	1372894	0.14036168	experimental	NIH	SAM002564213	HYDROCORTISONE HEMISUCCINATE
3259 A15	X	996	1000	2.546324	915	920	2.05841837	1484213	0.31605307	experimental	NIH	SAM003107539	3,5,3'-TRIIODOTHYRONINE
3259 A16	X	474	480	0.07176593	754	760	1.2280877	1583444	0.47266634	experimental	NIH	SAM002564222	19-NORETHINDRONE ACETATE
3259 A17	X	756	760	1.40859615	754	760	1.2280877	1393606	0.17305008	experimental	NIH	SAM002554899	Chlorpropamide
3259 A18	X	515	520	0.26612777	753	760	1.22293037	1655780	0.58683205	experimental	NIH	SAM002564229	Pfizerpen
3259 A19	X	675	680	1.024613	874	880	1.84696771	1164901	-0.181790735	experimental	NIH	SAM002554902	Vistaril Pamoate
3259 A20	X	710	720	1.19053165	794	800	1.43438104	1255252	-0.04530911	experimental	NIH	SAM002564237	TRIAMCINOLONE ACETONIDE
3259 A21	X	2275	2280	8.60946533	754	760	1.2280877	1061750	-0.35070743	experimental	NIH	SAM002554911	Maxolon
3259 A22	X	749	760	1.37541242	634	640	0.60920769	1269568	-0.0227146	experimental	NIH	SAM002564258	6ALPHA-METHYL-11BETA-HYDROXYPROGESTERONE
3259 A23	E	420	920	-0.18422284	441	840	-0.38615765	82226	-1.89666037	empty			
3259 A24	P	170843	171200	807.711582	136117	136560	699.340206	855953	-0.67551058	empty			
3259 B01	N	557	560	0.46523014	356	360	-0.82453098	1169610	-0.18047527	empty			
3259 B02	E	115	120	-1.62060425	158	160	-1.84566299	85748	-1.8911017	empty			
3259 B03	X	646	640	-1.62153478	196	200	-0.64970433	528957	-1.18159842	experimental	NIH	SAM002589929	Primaquine Diphosphate
3259 B04	X	355	360	-0.49235746	472	480	-0.22628031	1153193	-0.20638573	experimental	NIH	SAM002699889	Inderal
3259 B05	X	875	880	1.97271954	1555	1560	5.35911174	1400581	0.18405923	experimental	NIH	SAM002589939	Albendazole
3259 B06	X	434	440	-0.11785538	310	320	-1.06176832	1314654	0.04844326	experimental	NIH	SAM002589988	Ethambutol
3259 B07	X	515	520	0.26612777	795	800	1.43953837	1431960	0.23358375	experimental	NIH	SAM002589947	Floxuridine
3259 B08	X	394	400	-0.30747669	514	520	-0.00967231	1550415	0.42053767	experimental	NIH	SAM002589956	clidogrel
3259 B09	X	116	120	-1.62534478	114	120	-2.07260566	525375	-1.19725178	experimental	NIH	SAM002699904	Clomid
3259 B10	X	281	280	-0.89056221	515	520	-0.00967231	1192133	1.24987198	experimental	NIH	SAM002554902	Triamteram
3259 B11	X	1796	1800	6.33875016	1075	1080	2.88359172	1530181	0.38860297	experimental	NIH	SAM002548959	Mebendazole
3259 B12	X	230	240	-1.08492405	232	240	-1.46404032	1084849	-0.31425098	experimental	NIH	SAM002589969	Simvastatin
3259 B13	X	556	560	0.46048961	554	560	0.19662102	1821500	0.84838288	experimental	NIH	SAM002548936	Ganciclovir
3259 B14	X	635	640	0.83499169	594	600	0.40291436	1496399	0.33528587	experimental	NIH	SAM002703129	CARBIDOPA
3259 B15	X	233	240	-1.07070245	193	200	-1.66517633	686813	-0.94245909	experimental	NIH	SAM002548935	Paroxetine
3259 B16	E	315	320	-0.68197877	434	440	-0.42225898	1663570	0.59912677	empty			
3259 B17	X	315	320	-0.68197877	553	560	0.19146369	1645867	0.57118656	experimental	NIH	SAM002548982	Eszopiclone
3259 B18	X	314	320	0.6887193	633	640	0.60405036	6524972	0.53820872	empty			
3259 B19	X	595	600	0.64537039	433	440	-0.42741631	1559450	0.43479734	experimental	NIH	SAM002699891	(+/-)-Epinephrine hydrochloride
3259 B20	E	394	400	-0.30747669	553	560	0.19146369	1382975	0.15627222	empty			
3259 B21	X	389	400	-0.33117935	472	480	-0.22628031	1400988	0.18470159	experimental	NIH	SAM002264603	Carbamazepine
3259 B22	E	513	520	0.2566467	632	640	0.59889303	1303397	0.03067668	empty			
3259 B23	E	320	680	-0.65827611	233	680	-1.45888299	88590	-1.88661626	empty			
3259 B24	P	121407	122240	573.358607	151510	152240	573.727039	1133216	-1.23791482	empty			
3259 C01	N	317	320	-0.67249771	557	560	0.209302	1221324	-0.09885664	empty			
3259 C02	E	117	120	-1.62060425	116	120	-2.062291	86023	-1.89066768	empty			
3259 C03	X	437	440	-0.10363378	436	440	-0.41194431	6377014	8.03821207	experimental	NIH	SAM002264609	DIPYRIDAMOLE
3259 C04	X	395	400	-0.30273615	554	560	0.19662102	1443657	0.25204477	experimental	NIH	SAM002554921	Pyrimethamine
3259 C05	X	554	560	0.45100855	551	560	0.18114902	1370305	0.13627554	experimental	NIH	SAM002264617	HYDROCORTISONE
3259 C06	X	435	440	-0.11311485	595	600	0.40807169	1515682	0.36571964	experimental	NIH	SAM002554929	Sulfisoxazole
3259 C07	X	354	360	-0.497098	433	440	-0.42741631	1130573	-0.24208618	experimental	NIH	SAM002264627	NADLOL
3259 C08	X	476	480	0.08124699	635	640	0.61436503	9544643	13.0375846	experimental	NIH	SAM002554937	Triamterene
3259 C09	X	276	280	-0.86685955	395	400	-0.62339498	525421	-1.19717918	experimental	NIH	SAM002264637	PERPHENAZINE
3259 C10	X	316	320	-0.67723824	354	360	-0.83484565	767882	-0.81451036	experimental	NIH	SAM002564196	Sonazine
3259 C11	X	351	360	-0.51131959	593	600	0.39775703	871771	-0.65054551	experimental	NIH	SAM002264646	RIFAMPICIN
3259 C12	X	596	600	0.65011092	435	440	-0.41710165	1301185	0.02718555	experimental	NIH	SAM002564206	17-BETA-ESTRADIOL 17-VALERATE
3259 C13	X	274	280	-0.87634061	514	520	-0.00967231	1271876	-0.01907196	experimental	NIH	SAM002554879	Dapsone
3259 C14	X	396	400	-0.29799562	594	600	0.40291436	1505112	0.34903733	experimental	NIH	SAM002564214	INDAPAMIDE
3259 C15	X	355	360	-0.49235746	515	520	-0.00451498	1348239	0.10144984	experimental	NIH	SAM002703134	HYDROFLUMETHIAZIDE
3259 C16	X	757	760	1.41333668	474	480	-0.21596565	1694262	0.64756702	experimental	NIH	SAM002564238	19-Norethindrone
3259 C17	X	274	280	-0.87634061	434	440	-0.42225898	1027497	-0.4047679	experimental	NIH	SAM002554894	Bentyl
3259 C18	X	556	560	0.46048961	554	560	0.19662102	1515406	0.36528404	experimental	NIH	SAM002564230	Valproic Acid
3259 C19	X	153	160	-1.44994507	272	280	-1.25774699	687503	-0.94137009	experimental	NIH	SAM002554903	Hexachlorophene
3259 C20	X	515	520	0.26612777	794	800	1.43438104	1445379	0.25476255	experimental	NIH	SAM002564238	S(-)-Timolol maleate
3259 C21	X	515	520	0.26612777	632	640	0.59889303	1186694	-0.15351212	experimental	NIH	SAM002554912	Methyldopa
3259 C22	X	511	520	0.2566467	833	840	1.63551704	1302139	0.02869122	experimental	NIH	SAM002564245	Thalidomide
3259 C23	E	459	800	0.00065794	381	720	0.48059765	86133	-1.89049407	empty			
3259 C24	P	115039	115800	543.170895	114226	115000	586.441021	1085990	-0.31245018	empty			
3259 D01	N	318	320	-0.66775717	477	480	-0.20049365	1141018	-0.22560116	empty			
3259 D02	E	118	120	-1.61586371	156	160	-1.85599766	92010	-1.88121858	empty			
3259 D03	X	276	280	-0.86685955	515	520	-0.00451498	1389239	0.1661585	experimental	NIH	SAM002589930	Microphenin
3259 D04	X	396	400	-0.29799562	514	520	-0.00967231	1293392	0.01488609	experimental	NIH	SAM002589951	Ribavirin
3259 D05	X	355	360	-0.49235746	474	480	-0.21596565	1448447	0.25960468	experimental	NIH	SAM002589948	Griseofulvin
3259 D06	X	480	480	0.07650646	315	320	-1.04113893	1288419	0.0070373	experimental	NIH	SAM002589949	Cefazolin
3259 D07	X	596	600	0.65011092	515	520	-0.00451498	1028691	-0.40288344	experimental	NIH	SAM002699896	MITOXANTRONE
3259 D08	X	195	200	-1.2508427	434	440	-0.42225898	1295967	0.01895014	experimental	NIH	SAM002643511	CEFOTAXIME SODIUM SALT
3259 D09	X	436	440	-0.10837431	515	520	-0.00451498	1432984	0.2351999	experimental	NIH	SAM003107541	PHENTOLAMINE HCL
3259 D10	X	435	440	-0.11311485	395	400	-0.62339498	1129119	-0.24438099	experimental	NIH	SAM002589961	Azithromycin
3259 D11	X	474	480	0.07176593	434	440	-0.42225898	1308004	0.03794777	experimental	NIH	SAM002548969	Duremesin
3259 D12	X	354	360	-0.497098	555	360	-0.82968832	905143	-0.5978755	experimental	NIH	SAM002589970	Rifabutin
3259 D13	X	440	440	-0.10363378	315	320	-0.20177836	1562940	0.44030055	experimental	NIH	SAM002554937	Mesna
3259 D14	E	235	240										

3259 D19	X	674	680	1.01987247	794	800	1.43438104	1123107	-0.25386954	experimental	NIH	SAM002264595	5-Azacytidine
3259 D20	E	632	640	0.8207701	669	680	0.78971436	1271318	-0.01995263	empty			
3259 D21	X	434	440	-0.11785538	512	520	-0.01998698	1365167	0.12816639	experimental	NIH	SAM002699890	Memantine hydrochloride
3259 D22	E	474	480	0.07176593	512	520	-0.01998698	1246347	-0.05936366	empty			
3259 D23	E	310	320	-0.70566843	383	400	-0.68528298	90459	-1.88366647	empty			
3259 D24	P	139038	139640	656.93894	113596	114280	583.191901	1394479	0.17442863	empty			
3259 E01	N	398	400	-0.28851456	437	440	-0.40678698	1285511	0.00244775	empty			
3259 E02	E	37	40	-1.99984686	116	120	-2.062291	93041	-1.87959138	empty			
3259 E03	X	356	360	-0.48761693	635	640	0.61436503	1308057	0.03803142	experimental	NIH	SAM002264610	Propofol
3259 E04	X	475	480	0.07650646	473	480	-0.22112298	1420003	0.21471238	experimental	NIH	SAM002554922	Pro-Banthine
3259 E05	X	396	400	-0.29799562	635	640	0.61436503	1431303	0.23254683	experimental	NIH	SAM002264618	Cortell
3259 E06	X	275	280	-0.87160008	394	400	-0.62855232	1313747	0.04701177	experimental	NIH	SAM002554930	Sulfamethoxazole
3259 E07	X	356	360	-0.48761693	475	480	-0.21080831	1303238	0.03042573	experimental	NIH	SAM002264628	Disipal
3259 E08	X	236	240	-1.05648085	434	440	-0.42225898	1410300	0.19939843	experimental	NIH	SAM002554938	Intropin
3259 E09	X	476	480	0.08124699	514	520	-0.00967231	1331004	0.07424797	experimental	NIH	SAM002264639	Prednisolone
3259 E10	X	394	400	-0.30747669	354	360	-0.83484565	1307570	0.03726228	experimental	NIH	SAM002564200	CEFAZOLIN SODIUM SALT
3259 E11	X	795	800	1.59347693	836	840	1.65098904	1207047	-0.1213896	experimental	NIH	SAM002264647	Retinoic acid
3259 E12	X	395	400	-0.30273615	354	360	-0.83484565	1368566	0.13353093	experimental	NIH	SAM002564207	EDROPHONIUM CHLORIDE
3259 E13	X	314	320	-0.6867193	434	440	-0.42225898	1098451	-0.29278336	experimental	NIH	SAM002554881	Symmetrel
3259 E14	X	315	320	-0.68197877	475	480	-0.21080831	1361440	0.12228418	experimental	NIH	SAM002564215	IPRATROPIUM BROMIDE MONOHYDRATE
3259 E15	X	315	320	-0.68197877	274	280	-1.24743232	996117	-0.454294	experimental	NIH	SAM002554886	Annolytin
3259 E16	X	316	320	-0.67723824	474	480	-0.21596565	1523240	0.3776482	experimental	NIH	SAM002564224	NICOTINE
3259 E17	X	556	560	0.46048961	634	640	0.60920769	1276657	-0.01152625	experimental	NIH	SAM002554895	Chloroxine
3259 E18	X	314	320	-0.6867193	713	720	1.01663703	1340351	0.08900005	experimental	NIH	SAM002564231	Kemadrin
3259 E19	X	592	600	0.63114879	710	720	1.00116503	1440170	0.24654134	experimental	NIH	SAM002554904	Isoniazid
3259 E20	X	1194	1200	0.48494948	1561	1600	5.338482	1555665	-0.42882359	experimental	NIH	SAM002554913	Sulfamethoxazole
3259 E21	X	492	400	-0.31695775	1070	1080	2.85780505	1582880	-0.1985707	experimental	NIH	SAM002554919	NITROFURANTOIN
3259 E22	X	314	320	0.26138724	631	640	0.59373569	1359997	0.12000674	experimental	NIH	SAM002558919	Aminolevulinic Acid
3259 E23	E	450	720	-0.04200686	524	880	0.04190102	99210	-1.86985504	empty			
3259 E24	P	90796	91520	428.246161	119920	120680	615.806877	1108068	-0.27760514	empty			
3259 F01	N	237	240	-1.05174032	397	400	-0.61308032	1208828	-0.1185787	empty			
3259 F02	E	157	160	-1.43098294	37	40	-2.46972033	92296	-1.88076719	empty			
3259 F03	X	436	440	-0.10837431	476	480	-0.20565098	1881788	0.9435336	experimental	NIH	SAM002589932	DOXYCYCLINE
3259 F04	X	355	360	-0.49235746	474	480	-0.00451498	1319339	0.0581815	experimental	NIH	SAM002589936	Tecumidate
3259 F05	X	355	360	-0.49235746	434	440	-0.42225898	1538381	0.40154478	experimental	NIH	SAM002589936	Lincomycin hydrochloride
3259 F06	X	436	440	-0.10837431	515	520	-0.00451498	1395018	0.17527932	experimental	NIH	SAM002589990	DICLOXACILLIN SODIUM
3259 F07	X	275	280	-0.87160008	514	520	-0.00967231	1598672	0.49670023	experimental	NIH	SAM002699897	ENALAPRIL MALEATE
3259 F08	X	356	360	-0.48761693	554	560	0.19662102	1452927	0.26667533	experimental	NIH	SAM002589994	LAMIVUDINE
3259 F09	X	436	440	-0.10837431	675	680	0.82065836	1361280	0.12203166	experimental	NIH	SAM002548956	FLUDARABINE
3259 F10	X	235	240	-1.06122139	315	320	-1.03598165	1457244	0.27348872	experimental	NIH	SAM002589963	Lovastatin
3259 F11	X	275	280	-0.87160008	274	280	-1.24227499	807493	-0.75189252	experimental	NIH	SAM002548968	Felodipin Acetate
3259 F12	X	234	240	-1.06596192	274	280	-1.24743232	1283618	-0.00053991	experimental	NIH	SAM002589971	Felodipin
3259 F13	X	955	960	2.35196216	715	720	1.0269517	1348866	0.10243902	experimental	NIH	SAM002548942	Mectomen
3259 F14	E	714	720	1.20949378	393	400	-0.63370965	1386503	0.16184035	empty			
3259 F15	X	555	560	0.45574908	715	720	1.0269517	1531125	0.39009285	experimental	NIH	SAM002548930	Etomidate
3259 F16	E	355	360	-0.49235746	475	480	-0.21080831	1277513	-0.01017525	empty			
3259 F17	X	195	200	-1.2508427	234	240	-1.45372566	564031	-1.13624219	experimental	NIH	SAM002548975	Evista
3259 F18	E	276	280	-0.86685955	474	480	-0.21596565	1424147	0.22125227	empty			
3259 F19	X	395	400	-0.30273615	473	480	-0.21122998	407581	0.19510712	experimental	NIH	SAM002264597	Buspar
3259 F20	E	394	400	-0.30747669	591	600	0.38744236	1331350	0.07479405	empty			
3259 F21	X	435	440	-0.11311485	713	720	1.01663703	921438	-0.57215759	experimental	NIH	SAM002264605	Norpramin
3259 F22	E	474	480	0.07176593	512	520	-0.01998698	1255577	-0.04479617	empty			
3259 F23	E	317	640	-0.67249771	407	840	-0.56150698	92825	-1.87993229	empty			
3259 F24	P	109155	109680	515.277601	146524	147280	753.012574	1364234	0.12669387	empty			
3259 G01	N	358	360	-0.47813586	517	520	0.00579969	1253711	-0.064774122	empty			
3259 G02	E	157	160	-1.43098294	117	120	-2.05713366	90388	-1.88377853	empty			
3259 G03	X	316	320	-0.67723824	275	280	-1.24227499	1126968	-0.24777585	experimental	NIH	SAM002264611	ETHACRYNIC ACID
3259 G04	X	396	400	-0.29799562	434	440	-0.42225898	1394916	0.17511833	experimental	NIH	SAM002554923	Probencid
3259 G05	X	315	320	-0.68197877	475	480	-0.21080831	1200648	-0.13148894	experimental	NIH	SAM002264619	IBUPROFEN
3259 G06	X	355	360	-0.49235746	472	480	-0.22628031	1453390	0.26740607	experimental	NIH	SAM002554931	Sulfacetamide
3259 G07	X	516	520	0.2708683	674	680	0.81550103	1500643	0.34198404	experimental	NIH	SAM002264629	OFLOXACIN
3259 G08	X	315	320	-0.68197877	514	520	-0.00967231	1019475	-0.41742878	experimental	NIH	SAM002564189	AMOXAPINE
3259 G09	X	435	440	-0.11311485	435	440	-0.41710165	1197772	-0.13602805	experimental	NIH	SAM002264640	PRILCICLAINE HYDROCHLORIDE
3259 G10	X	436	440	-0.10837431	235	240	-1.44856832	1413657	0.20469668	experimental	NIH	SAM002564201	CAPTROPIL
3259 G11	X	355	360	-0.49235746	356	360	-0.82453098	1118216	-0.26158886	experimental	NIH	SAM002264648	Spirolactone
3259 G12	X	515	520	0.26612777	556	560	0.20693569	1333708	0.07851561	experimental	NIH	SAM002564208	FLUCICINOLONE ACETONIDE
3259 G13	X	353	360	-0.50183853	434	440	-0.42225898	1127524	-0.24689833	experimental	NIH	SAM002554882	WARFARIN SODIUM
3259 G14	X	315	320	-0.68197877	394	400	-0.62855232	1017925	-0.4198751	experimental	NIH	SAM002564216	Tofranil
3259 G15	X	434	440	-0.11785538	634	640	0.60920769	1325780	0.06600309	experimental	NIH	SAM002554887	Busulfan
3259 G16	X	594	600	0.6062985	434	440	-0.42225898	717919	-0.89136544	experimental	NIH	SAM002564254	Gardene
3259 G17	X	555	560	0.45574908	635	640	0.61436503	1244302	-0.05959403	experimental	NIH	SAM002554896	Diffusal
3259 G18	X	475	480	0.07650646	634	640	0.60920769	1392553	0.17138888	experimental	NIH	SAM002564232	Proxymetacaine
3259 G19	X	355	360	-0.49235746	554	560	0.19662102	1348928	0.10253687	experimental	NIH	SAM002554905	Duvaldin
3259 G20	X	115	120	-1.63008531	274	280	-1.24743232	505231	-1.22904444	experimental	NIH	SAM002564240	THIORIDAZINE HYDROCHLORIDE
3259 G21	X	596	600	0.65011092	354	360	-0.83484565	773916	-0.80498708	experimental	NIH	SAM002554915	Pamelor
3259 G22	X	393	400	-0.31221722	634	640	0.60920769	1219957	-0.10101413	experimental	NIH	SAM002589920	Carbinoxamine Maleate
3259 G23	E	417	680	-0.19844444	429	840	-0.44804565	90194	-1.88408471	empty			
3259 G24	P	88529	89120	417.499373	138769	139310	713.017454	1082275	0.31811345	empty			
3259 H01	N	397	400	-0.29325509	357	360	-0.81937365	1121964	-0.25567351	empty			
3259 H02	E	196	200	-1.24610216	157	160	-1.85084033	87955	-1.88761846	empty			
3259 H03	X	517	520	0.27560884	516	520	0.00064236	1460249	0.27823142	experimental	NIH	SAM002699895	Beclomethasone dipropionate
3259 H04	X	355	360	-0.49235746	714	720	1.02179437	1250327	-0.05308209	experimental	NIH	SAM002589983	Chlorthalidone
3259 H05	X	556	560	0.46048961	392	400	-0.63886698	1402741	0.18746829	experimental	NIH	SAM002589943	Methazolamide
3259 H06	X	395	400	-0.30273615	955	960	2.26471771	1152760	-0.20706912	experimental	NIH	SAM002589991	Meloxicam
3259 H07	X	475	480	0.07650646	473	480	-0.22628031	1440665	0.24731259	experimental	NIH	SAM002699898	EDISONIDE
3259 H08	X	395	400	-0.30273615	514	520	-0.00967231	1292869	0.01406066	experimental	NIH	SAM002589958	Ondansetron

3259 H13	X	514	520	0.26138724	395	400	-0.62339498	1549336	0.41883472	experimental	NIH	SAM002589905	Fluconazole
3259 H14	E	275	280	-0.87160008	435	440	-0.41710165	1219537	-0.10167701	empty			
3259 H15	X	595	600	0.64537039	475	480	-0.21080831	1527566	0.38447579	experimental	NIH	SAM002548933	Moban
3259 H16	E	640	640	0.81602956	351	360	-0.85031765	1432731	0.23480066	empty			
3259 H17	X	555	560	0.45574908	475	480	-0.21080831	1545160	0.4065621	experimental	NIH	SAM002548971	zidovudine
3259 H18	E	432	440	-0.12733644	354	360	-0.83484565	1277363	-0.01041199	empty			
3259 H19	X	595	600	0.64537039	554	560	0.19662102	1340711	0.08956823	experimental	NIH	SAM002264596	Flumadine
3259 H20	E	515	520	0.26612777	395	400	-0.62339498	1247706	-0.05721873	empty			
3259 H21	X	513	520	0.2566467	515	520	-0.00451498	1244970	-0.06153688	experimental	NIH	SAM002264606	Mexitil
3259 H22	E	514	520	0.26138724	512	520	-0.01998698	1172584	-0.1757815	empty			
3259 H23	E	243	520	-1.02329713	472	800	-0.22628031	88928	-1.8860828	empty			
3259 H24	P	93363	93920	440.415108	110399	111120	566.703906	1271812	-0.01917297	empty			
3259 I01	N	357	360	-0.4828764	357	360	-0.81937365	1233910	-0.07899254	empty			
3259 I02	E	157	160	-1.43098294	157	160	-1.85084033	83979	-1.89389366	empty			
3259 I03	X	276	280	-0.86685955	315	320	-1.03598165	1177636	-0.16780808	experimental	NIH	SAM002264612	FLUTAMIDE
3259 I04	X	396	400	-0.29799562	554	560	0.19662102	1488445	0.32273231	experimental	NIH	SAM002554924	PYRIDINE-2-ALDOXIME METHOCHLORIDE
3259 I05	X	395	400	-0.30273615	435	440	-0.41710165	1245188	-0.06119282	experimental	NIH	SAM002264620	KETOPROFEN
3259 I06	X	395	400	-0.30273615	393	400	-0.63370965	1402079	0.18642348	experimental	NIH	SAM002554932	Sulfipyrazone
3259 I07	X	475	480	0.07650646	474	480	-0.21598565	1397722	0.17954696	experimental	NIH	SAM002264631	PINDOLOL
3259 I08	X	515	520	0.26612777	754	760	1.2280877	1481604	0.31193537	experimental	NIH	SAM002564191	Adenine 9-beta;-D-arabinofuranoside
3259 I09	X	434	440	-0.11785538	473	480	-0.22112298	1326882	0.06774234	experimental	NIH	SAM002264641	Prednisone
3259 I10	X	436	440	-0.10837431	515	520	-0.00451498	1401053	0.18480417	experimental	NIH	SAM002564202	CHLORAMBUCIL
3259 I11	X	395	400	-0.30273615	354	360	-0.83484565	1221291	-0.09890872	experimental	NIH	SAM002264649	Trimethoprim
3259 I12	X	394	400	-0.30747669	396	440	-0.41194431	1336045	0.08220402	experimental	NIH	SAM002564209	Flurbiprofen
3259 I13	X	555	560	0.45574908	436	400	-0.61823765	1106938	-0.27938858	experimental	NIH	SAM002554883	Acetazolamide
3259 I14	X	315	320	-0.69197877	365	360	-0.82968832	1169948	-0.17994182	experimental	NIH	SAM002564217	LABELALOL HYDROCHLORIDE
3259 I15	X	313	320	-0.69145984	432	440	-0.43257365	1537328	-0.20554135	experimental	NIH	SAM002554888	Chlorzaxatone
3259 I16	X	1195	1200	3.48969001	1635	1640	5.77169841	1416437	0.20908427	experimental	NIH	SAM002564225	NABUMETONE
3259 I17	X	230	240	-1.08492405	311	320	-1.05661099	572945	-1.121217349	experimental	NIH	SAM002554898	Econazole Nitrate
3259 I18	X	1235	1240	3.67931132	515	520	-0.00451498	1470373	0.29420982	experimental	NIH	SAM002703137	NALOXONE HYDROCHLORIDE
3259 I19	X	472	480	0.06228486	632	640	0.59889303	1149401	-0.21237052	experimental	NIH	SAM002554906	Isuprel
3259 I20	X	474	480	0.07176593	514	520	-0.00967231	1408599	0.1967138	experimental	NIH	SAM002564241	Alitretamine
3259 I21	X	634	640	0.83025116	433	440	-0.42741631	1266927	-0.02688281	experimental	NIH	SAM002554916	Albalon
3259 I22	E	640	640	0.82551063	634	640	0.60920769	1662272	0.59707818	experimental	NIH	SAM002589921	Demeclocycline
3259 I23	E	297	600	-0.76730836	359	680	-0.80905898	84397	-1.89323394	empty			
3259 I24	P	102222	102800	482.411488	107963	108600	554.140642	1028144	-0.40374676	empty			
3259 J01	N	477	480	0.08598753	397	400	-0.61308032	995596	-0.45511628	empty			
3259 J02	E	157	160	-1.43098294	197	200	-1.64454699	88026	-1.8875064	empty			
3259 J03	X	397	400	-0.29325509	355	360	-0.82968832	1369208	0.13454418	experimental	NIH	SAM002589934	Cromolyn Sodium
3259 J04	X	435	440	-0.11311485	555	560	0.20177836	1264356	-0.03094054	experimental	NIH	SAM002589984	METHYLPREDNISOLONE
3259 J05	X	276	280	-0.86685955	435	440	-0.41710165	1470395	0.29424544	experimental	NIH	SAM002589944	TABETALOL Sulfate
3259 J06	X	315	320	-0.68197877	394	400	-0.62855232	509510	-1.22229103	experimental	NIH	SAM002589992	DAUNORUBICIN HYDROCHLORIDE
3259 J07	X	355	360	-0.49235746	475	480	-0.21080831	1379897	0.1514143	experimental	NIH	SAM002699899	RAMIPRIL
3259 J08	X	434	440	-0.11785538	432	440	-0.43257365	1395403	0.17588695	experimental	NIH	SAM002589959	Betamethasone
3259 J09	X	796	800	1.59821746	835	840	1.6458317	1378130	0.1486255	experimental	NIH	SAM002548955	Isotretinoin
3259 J10	X	194	200	-1.25558323	313	320	-1.04629632	620411	-1.04725935	experimental	NIH	SAM002589965	Prozac
3259 J11	X	316	320	-0.67723824	716	720	1.03210903	1379063	0.15009803	experimental	NIH	SAM002548945	Miochol
3259 J12	X	320	320	-0.67723824	324	320	-1.04113899	931767	-0.55585565	experimental	NIH	SAM002589973	Acetretin
3259 J13	X	355	360	-0.49235746	314	320	-1.03598165	1453518	0.26760809	experimental	NIH	SAM002548965	Metaproterenol
3259 J14	E	396	400	-0.29799562	476	480	-0.20565098	1320587	0.05780713	empty			
3259 J15	X	315	320	-0.68197877	314	320	-1.04113899	1349980	0.10419721	experimental	NIH	SAM002548940	fluvastatin
3259 J16	E	434	440	-0.11785538	512	520	-0.01998698	1264598	-0.0305586	empty			
3259 J17	X	356	360	-0.48761693	435	440	-0.41710165	1117143	-0.26328234	experimental	NIH	SAM002548976	Clozapine
3259 J18	E	392	400	-0.31695775	432	440	-0.43257365	1278384	-0.00880058	empty			
3259 J19	X	595	600	0.64537039	1114	1120	3.08472772	1176338	-0.16985668	experimental	NIH	SAM002548978	Podoflox
3259 J20	E	354	360	-0.497098	632	640	0.59889303	1251082	-0.05189049	empty			
3259 J21	X	474	480	0.07176593	594	600	0.40291436	1262173	-0.03438591	experimental	NIH	SAM002264607	Norpace
3259 J22	E	633	640	0.82551063	552	560	0.18630636	1213717	-0.11086254	empty			
3259 J23	E	370	680	-0.42124947	521	840	0.02642902	89263	-1.88555408	empty			
3259 J24	P	104625	105200	493.802988	107505	108120	551.778583	1306080	0.03491118	empty			
3259 K01	N	357	360	-0.4828764	398	400	-0.60792298	1286179	0.00350203	empty			
3259 K02	E	157	160	-1.43098294	156	160	-1.85599766	88291	-1.88708816	empty			
3259 K03	X	276	280	-0.86685955	556	560	0.20693569	1282338	-0.0025601	experimental	NIH	SAM002264613	FENOFIBRATE
3259 K04	X	475	480	0.07650646	353	360	-0.84000298	1387841	0.16395208	experimental	NIH	SAM002554925	Primidone
3259 K05	X	435	440	-0.11311485	434	440	-0.42225898	1161006	-0.19405471	experimental	NIH	SAM002264621	MINOCYCLINE HYDROCHLORIDE
3259 K06	X	356	360	-0.48761693	675	680	0.82065836	1245128	-0.06128751	experimental	NIH	SAM002554933	Sulindac
3259 K07	X	395	400	-0.30273615	514	520	-0.00967231	1194645	-0.14096329	experimental	NIH	SAM002264632	PRAZQUANTEL
3259 K08	X	315	320	-0.68197877	554	560	0.19662102	1463812	0.28385479	experimental	NIH	SAM002564193	ATENOLOL
3259 K09	X	314	320	-0.6867193	353	360	-0.84000298	1222535	-0.09694536	experimental	NIH	SAM002264642	DL-PENICILLAMINE
3259 K10	X	396	400	-0.29799562	409	400	-0.61823765	1291474	0.01185897	experimental	NIH	SAM002564251	CFCIXOTIN SODIUM SALT
3259 K11	X	395	400	-0.30273615	314	320	-1.04113899	1207292	-0.12100292	experimental	NIH	SAM002264650	Tyzine
3259 K12	X	436	440	-0.10837431	555	560	0.20177836	1322524	0.06086424	experimental	NIH	SAM002564210	GLIPIZIDE
3259 K13	X	275	280	-0.87160008	395	400	-0.62339498	1160923	-0.1941857	experimental	NIH	SAM002554884	Allopurinol
3259 K14	X	395	400	-0.30273615	355	360	-0.82968832	934063	-0.55223194	experimental	NIH	SAM002564218	Imodium
3259 K15	X	516	520	0.27086683	596	600	0.41322903	1226879	-0.09008935	experimental	NIH	SAM002554891	Chlorothiazide
3259 K16	X	354	360	-0.497098	274	280	-1.24743232	941069	-0.54117458	experimental	NIH	SAM002564226	OXYBUTYMIN CHLORIDE
3259 K17	X	395	400	-0.30273615	474	480	-0.21596565	1189677	-0.14880414	experimental	NIH	SAM002554899	Ethionamide
3259 K18	X	157	160	-1.43098294	635	640	0.61436505	1384495	-1.89393309	experimental	NIH	SAM002564233	SPECTINOMYCIN DIHYDROCHLORIDE PENTAHYDRATE
3259 K19	X	314	320	-0.6867193	512	520	-0.01998698	748440	-0.84519507	experimental	NIH	SAM002554907	Triclosan
3259 K20	X	475	480	0.07650646	514	520	-0.00967231	1344796	0.09601546	experimental	NIH	SAM002564257	Phylloquinone
3259 K21	X	513	520	0.2566467	433	440	-0.42741631	1297594	0.02151798	experimental	NIH	SAM002554917	Nicotinic Acid
3259 K22	X	753	760	1.39437455	593	600	0.39775703	1270723	-0.0208917	experimental	NIH	SAM002589925	Westcort
3259 K23	E	478	760	0.09072806	455	760	-0.31395498	90977	-1.88284893	empty			
3259 K24	P	94426	95040	445.454295	102175	102960	524.289996	1137730	-0.23079051	empty			
3259 L01	N	237	240	-1.05174032	277	280	-1.21196032	1086790	-0.31125069	empty			
3259 L02	E	157	160	-1.43098294	277	280	-1.21196032	83916	-1.89393309	empty			
3259 L03	X	316	320										

3259 L07	X	515	520	0.26612777	514	520	-0.00967231	1468973	0.29200024	experimental	NIH	SAM002699893	DEPO-MEDROL
3259 L08	X	715	720	1.21423431	594	600	0.40291436	1354738	0.11170662	experimental	NIH	SAM002589995	Celecoxib
3259 L09	X	395	400	-0.30273615	475	480	-0.21080831	1496271	0.33508385	experimental	NIH	SAM002548951	Methimazole
3259 L10	X	395	400	-0.30273615	475	480	-0.21080831	1232057	-0.08191707	experimental	NIH	SAM002589966	Famotidine
3259 L11	X	396	400	-0.29793652	514	520	-0.00967231	16161843	-0.19273369	experimental	NIH	SAM002703131	Dantrolene sodium salt
3259 L12	X	275	280	-0.87160008	515	520	-0.00451498	1227039	-0.08983683	experimental	NIH	SAM002700173	Allegra
3259 L13	X	476	480	0.08124699	435	440	-0.41710165	1279880	-0.00643949	experimental	NIH	SAM002548974	Methoxsalen
3259 L14	E	596	600	0.65011092	394	400	-0.62855232	1316828	0.05187442	empty			
3259 L15	X	354	360	-0.497098	555	560	0.20177836	1324862	0.06455424	experimental	NIH	SAM002548931	Urecholine
3259 L16	E	555	560	0.45574908	394	400	-0.62855232	1348524	0.10189925	empty			
3259 L17	X	555	560	0.45574908	715	720	-0.0269517	1367149	0.13129452	experimental	NIH	SAM002264590	Ampicillin Sodium
3259 L18	E	314	320	-0.6867193	432	440	-0.43257365	1210969	-0.11519962	empty			
3259 L19	X	636	640	0.83973223	554	560	0.19662102	1311935	0.04415194	experimental	NIH	SAM002264599	D-CYCLOSERINE
3259 L20	E	353	360	-0.50183853	633	640	0.60405036	1181416	-0.16184222	empty			
3259 L21	X	635	640	0.83499169	673	680	0.8103437	1379455	0.15071671	experimental	NIH	SAM002589948	STAVUDINE
3259 L22	E	512	520	0.25190617	711	720	1.00632237	1219733	-0.10136767	empty			
3259 L23	E	447	760	-0.05622845	483	960	-0.16954965	90527	-1.88355915	empty			
3259 L24	P	105627	106280	498.553001	161652	162400	831.032714	1209617	-0.11733344	empty			
3259 M01	N	398	400	-0.28851456	398	400	-0.60792298	1134898	-0.23526017	empty			
3259 M02	E	157	160	-1.43098294	157	160	-1.85084033	91241	-1.88243227	empty			
3259 M03	X	397	400	-0.29325509	355	360	-0.82968832	1119224	-0.25999796	experimental	NIH	SAM002264614	FUROSEMIDE
3259 M04	X	315	320	-0.68197877	675	680	0.82065836	1404616	0.19042755	experimental	NIH	SAM002554926	Propylthiouracil
3259 M05	X	195	200	-1.2508427	154	160	-1.86631233	455022	-1.30828778	experimental	NIH	SAM002264623	MICONAZOLE NITRATE
3259 M06	X	516	520	0.2708683	435	440	-0.41710165	1400303	0.18362047	experimental	NIH	SAM002554934	TETRACYCLINE
3259 M07	X	354	360	-0.497098	435	440	-0.41710165	1183322	-0.15883404	experimental	NIH	SAM002264634	Benzenebutanoic Acid
3259 M08	X	395	400	-0.30273615	515	520	-0.00451498	1391791	0.17176461	experimental	NIH	SAM002703131	Tamoxifen
3259 M09	X	396	400	-0.6239498	395	400	-0.6239498	1226389	-0.0908627	experimental	NIH	SAM002264643	PIPERACILLIN SODIUM SALT
3259 M10	X	356	360	-0.48761693	435	440	-0.41710165	1247969	-0.05680365	experimental	NIH	SAM002564203	DANAZOL
3259 M11	X	435	440	-0.11311485	755	760	1.23324503	965011	-0.50338765	experimental	NIH	SAM002264651	L-THYROXINE
3259 M12	X	315	320	-0.68197877	354	360	-0.83484565	1323612	0.0625814	experimental	NIH	SAM002564211	GEMFIBROZIL
3259 M13	X	316	320	-0.67723824	515	520	-0.00451498	1083728	-0.31602022	experimental	NIH	SAM002554885	ATROPINE
3259 M14	X	275	280	-0.87160008	635	640	0.61436503	1203083	-0.12764586	experimental	NIH	SAM002564219	Pro-Amatine
3259 M15	X	316	320	-0.67723824	314	320	-1.04113899	1163432	-0.19022582	experimental	NIH	SAM002554892	Cimetidine
3259 M16	X	440	440	0.00311485	395	400	-0.6239498	1280718	-0.05619469	experimental	NIH	SAM002564227	Mestlinon
3259 M17	X	435	440	-0.11311485	513	520	-0.01482964	1113638	-0.26881418	experimental	NIH	SAM002554900	Methocarbamol
3259 M18	X	355	360	-0.49235746	674	680	0.81550103	1354221	0.11089065	experimental	NIH	SAM002564235	TROPICAMIDE
3259 M19	X	514	520	0.26138724	633	640	0.60405036	1331090	0.0743837	experimental	NIH	SAM002554908	Mefenamic Acid
3259 M20	X	635	640	0.83499169	633	640	0.60405036	1999558	1.12940641	experimental	NIH	SAM002564242	Eryped
3259 M21	X	474	480	0.07176593	632	640	0.59889303	1168801	-0.18175209	experimental	NIH	SAM002554918	Norflex
3259 M22	X	433	440	-0.12259591	952	960	2.24923971	1219021	-0.1024914	experimental	NIH	SAM002589926	DEPRENALIN
3259 M23	E	720	720	0.57294652	466	520	-0.57294652	87497	-1.88834131	empty			
3259 M24	P	129196	129840	610.282617	153534	154320	789.165481	1189393	-0.14925237	empty			
3259 N01	N	397	400	-0.29325509	357	360	-0.81937365	958655	-0.51341913	empty			
3259 N02	E	197	200	-1.24136163	157	160	-1.85084033	83460	-1.89471278	empty			
3259 N03	X	355	360	-0.49235746	556	560	0.20693569	1191033	-0.146664	experimental	NIH	SAM002589937	Mercaptopurine
3259 N04	X	556	560	0.46048961	274	280	-1.24743232	1004870	-0.4404794	experimental	NIH	SAM002589986	NALTREXONE HYDROCHLORIDE
3259 N05	X	316	320	-0.67723824	556	560	0.20693569	1274092	-0.01557451	experimental	NIH	SAM002589945	FLUOCINOLONE ACETONIDE 21-ACETATE
3259 N06	X	395	400	-0.30273615	515	520	-0.00451498	1117139	-0.28759401	experimental	NIH	SAM002589954	Famotidin V
3259 N07	X	595	600	0.64537039	315	320	-1.03598165	1316048	0.05064337	experimental	NIH	SAM002699901	(+/-)-NOREPINEPHRINE HYDROCHLORIDE
3259 N08	X	354	360	-0.497098	354	360	-0.83484565	1180602	-0.16312693	experimental	NIH	SAM002589996	4-(AMINOMETHYL)BENZENESULFONAMIDE ACETATE
3259 N09	X	356	360	-0.48761693	436	440	-0.41194431	1336332	0.08265699	experimental	NIH	SAM002548957	Zonisamide
3259 N10	X	315	320	-0.68197877	355	360	-0.82968832	1165291	-0.18729182	experimental	NIH	SAM002589967	Acyclovir
3259 N11	X	475	480	0.07650646	554	560	0.19662102	1309003	0.03952446	experimental	NIH	SAM002548948	Dexamethasone
3259 N12	X	675	680	1.024613	395	400	-0.6239498	1285819	0.00293386	experimental	NIH	SAM002700174	Fluorometholone
3259 N13	X	394	400	-0.30747669	435	440	-0.41710165	1355338	0.11265358	experimental	NIH	SAM002548963	Chloramphenicol
3259 N14	E	596	600	0.65011092	474	480	-0.21596565	1186115	-0.15442593	empty			
3259 N15	X	395	400	-0.30273615	395	400	-0.6239498	1264475	-0.03075273	experimental	NIH	SAM002589901	Cefuroxime
3259 N16	E	315	320	-0.68197877	434	440	-0.42225898	1200809	-0.13123484	empty			
3259 N17	X	436	440	-0.10837431	674	680	0.81550103	1281327	-0.00415573	experimental	NIH	SAM002264591	ACEBUTOLOL HYDROCHLORIDE
3259 N18	E	355	360	-0.49235746	473	480	-0.22112298	1148036	-0.21452486	empty			
3259 N19	X	554	560	0.45100855	553	560	0.19146369	1366443	0.13018026	experimental	NIH	SAM002264600	CORTISONE ACETATE
3259 N20	E	433	440	-0.12259591	473	480	-0.22112298	1021915	-0.4135778	empty			
3259 N21	X	394	400	-0.30747669	593	600	0.39775703	976324	-0.48552269	experimental	NIH	SAM002554927	Pyrazinamide
3259 N22	E	554	560	0.45100855	632	640	0.59889303	1041877	-0.38207238	experimental	NIH	SAM002589981	Doxazosin
3259 N23	E	420	760	-0.18422284	400	720	-0.59760832	83744	-1.89426455	empty			
3259 N24	P	114548	115280	540.843294	107142	108000	549.906471	1173425	-0.17445418	empty			
3259 O01	N	397	400	-0.29325509	477	480	-0.20049365	1071015	-0.33608476	empty			
3259 O02	E	156	160	-1.43572347	116	120	-2.062291	81429	-1.89791825	empty			
3259 O03	X	436	440	-0.10837431	475	480	-0.21080831	1033311	-0.39559184	experimental	NIH	SAM002264615	5-FLUOROURACIL
3259 O04	X	395	400	-0.30273615	435	440	-0.41710165	1228909	-0.08686547	experimental	NIH	SAM002554928	Pyrazinamide
3259 O05	X	316	320	-0.67723824	476	480	-0.20565098	1011440	-0.43011017	experimental	NIH	SAM002297829	METYPARONE
3259 O06	X	355	360	-0.49235746	274	280	-1.24743232	1112098	-0.27124471	experimental	NIH	SAM002554935	Theophylline
3259 O07	X	594	600	0.64062985	475	480	-0.21080831	1242939	-0.06474234	experimental	NIH	SAM002264635	PREDNISOLONE ACETATE
3259 O08	X	595	600	0.64537039	755	760	1.23324503	1333453	0.07811315	experimental	NIH	SAM002564195	BUMETANIDE
3259 O09	X	355	360	-0.49235746	394	400	-0.62855232	1099616	-0.29094467	experimental	NIH	SAM002264644	Quinidine hydrochloride monohydrate
3259 O10	X	435	440	-0.11311485	275	280	-1.24227499	1056847	-0.35844569	experimental	NIH	SAM002564204	(+)-CIS-DILTIAZEM HYDROCHLORIDE
3259 O11	X	435	440	-0.11311485	515	520	-0.00451498	840020	-0.70065715	experimental	NIH	SAM002264652	Artane
3259 O12	X	394	400	-0.30747669	394	400	-0.6182376	1107036	-0.2792338	experimental	NIH	SAM002564212	Nibyracil
3259 O13	X	515	520	0.26612777	274	280	-1.24743232	1095732	-0.29707467	experimental	NIH	SAM002254914	Nalidixic Acid
3259 O14	X	434	440	-0.11785538	435	440	-0.41710165	983431	-0.47431593	experimental	NIH	SAM002564220	Medroxyprogesterone 17-acetate
3259 O15	X	355	360	-0.49235746	355	360	-0.82968832	1116629	-0.26409357	experimental	NIH	SAM002554889	Carisoprodol
3259 O16	X	316	320	-0.67723824	475	480	-0.21080831	1017200	-0.42101934	experimental	NIH	SAM002564228	Rythmol
3259 O17	X	275	280	-0.87160008	554	560	0.19662102	1066273	-0.34356892	experimental	NIH	SAM002554901	Hydrochlorothiazide
3259 O18	X	515	520	0.26612777	513	520	-0.01482964	1188686	-0.1503682	experimental	NIH	SAM002564236	TOLAZAMIDE
3259 O19	X	600	600	0.63588932	713	720	1.01663703	1105394	-0.28182543	experimental	NIH	SAM002554911	Cantil
3259 O20	X	834	840	1.7783577	753	760	-1.22293037						

3259 P01	N	638	640	0.84921329	478	480	-0.19533631	800074	-0.7637027	empty			
3259 P02	E	196	200	-1.24610216	277	280	-1.23196032	76978	-1.90494312	empty			
3259 P03	X	437	440	-0.10363378	517	520	0.00579969	1061483	-0.35112883	experimental	NIH	SAM002589938	Azathioprine
3259 P04	X	517	520	0.27560884	357	360	-0.81937365	951652	-0.52447176	experimental	NIH	SAM002589937	Glycyrrhizic acid
3259 P05	X	196	200	-1.24610216	116	120	-2.062291	436941	-0.35682497	experimental	NIH	SAM002698984	Mesifenine hydrochloride
3259 P06	X	396	400	-0.29799562	437	440	-0.40678698	1045391	-0.37652634	experimental	NIH	SAM002589955	Gatifloxacin
3259 P07	X	676	680	1.02935354	476	480	-0.20565098	1114946	-0.2667498	experimental	NIH	SAM002699903	AMCINONIDE
3259 P08	X	515	520	0.26612777	435	440	-0.41710165	507290	-1.22579478	experimental	NIH	SAM002589997	THIOTHIXENE
3259 P09	X	436	440	-0.10837431	476	480	-0.20565098	1046077	-0.37544365	experimental	NIH	SAM002548958	Brimonidine
3259 P10	X	516	520	0.2708683	516	520	0.00064236	1055117	-0.36117609	experimental	NIH	SAM002589968	Etodolac
3259 P11	X	397	400	-0.29325509	516	520	0.00064236	854535	-0.67774856	experimental	NIH	SAM002548938	Cogentin Mesylate
3259 P12	X	236	240	-1.05648085	235	240	-1.44855832	421840	-1.36065792	experimental	NIH	SAM002700175	Sertraline
3259 P13	X	557	560	0.46523014	637	640	0.6246797	1134012	-0.23665851	experimental	NIH	SAM002548961	Tizanidine hydrochloride
3259 P14	E	435	440	-0.11311485	556	560	0.20693569	982958	-0.47506245	empty			
3259 P15	X	717	720	1.22371538	436	440	-0.41194431	1139684	-0.22770657	experimental	NIH	SAM002548983	Cytosax
3259 P16	E	355	360	-0.49235746	476	480	-0.20565098	877874	-0.64091333	empty			
3259 P17	X	597	600	0.65485145	355	360	-0.82968832	1110932	-0.27308498	experimental	NIH	SAM002264592	AMOXICILLIN CRYSTALLINE
3259 P18	E	515	520	0.26612777	756	760	1.23840237	952954	-0.52241685	empty			
3259 P19	X	475	480	0.07050646	434	440	-0.42225898	621615	-1.04535911	experimental	NIH	SAM002264601	Anafanil
3259 P20	E	435	440	-0.11311485	475	480	-0.21080831	968534	-0.49782741	empty			
3259 P21	X	556	560	0.46048961	635	640	0.61436503	1068455	-0.34012513	experimental	NIH	SAM002589949	Minoxidil
3259 P22	E	554	560	0.45100855	634	640	0.60920769	897032	-0.61067684	empty			
3259 P23	E	431	1000	-0.13207698	345	800	-0.88126165	81081	-1.89846748	empty			
3259 P24	X	194723	195080	920.915503	155229	155640	797.907161	812324	-0.74436889	empty			
3260 A01	N	1237	1240	0.99603778	1157	1160	0.37277492	2445588	-0.01683321	2141142	-1.49218396		
3260 A02	E	240	240	-1.80264779	232	240	-1.89757414	1102459	-5.118393	95127	-5.29587326		
3260 A03	X	1234	1240	0.98768336	1474	1480	-1.15011233	2352502	-2.1954098	241663	-0.98003006		
3260 A04	X	833	840	-0.12902366	1232	1240	0.55631506	2145712	-0.66985511	2931556	-0.02274738		
3260 A05	X	953	960	0.205153	1192	1200	0.45816032	1998216	-0.99104826	2396507	-1.01744202		
3260 A06	X	672	680	-0.57737735	869	880	-0.33443921	2236080	-0.47306616	2786141	-0.29308434		
3260 A07	X	913	920	0.09376078	1432	1440	1.04708875	2041075	-0.8977168	2898245	-0.08467493		
3260 A08	X	952	960	0.2023682	1070	1080	0.15878836	2345216	-0.23540727	3101716	0.29359232		
3260 A09	X	754	760	-0.3490233	1071	1080	0.16124223	1950610	-1.09471698	2949918	0.0113889		
3260 A10	X	840	840	-0.31618104	1282	1282	0.6544606	1764606	-1.49976568	2482331	-0.85788902		
3260 A11	X	553	560	-0.90876921	832	840	-0.42523234	2321452	-0.2871567	2949820	0.01120671		
3260 A12	X	873	880	-0.01763144	789	800	-0.53074869	2181104	-0.59278408	2965878	0.04105969		
3260 A13	X	714	720	-0.46041552	871	880	-0.32953147	2086777	-0.79819431	2394199	-1.02173276		
3260 A14	X	473	480	-1.13155366	913	920	-0.226469	2326622	-0.47188888	2585115	-0.66680616		
3260 A15	X	994	1000	0.31933003	912	920	-0.22892286	2195944	-0.56046791	2535325	-0.75936936		
3260 A16	X	912	920	0.09097598	870	880	-0.33198534	2406058	-0.10291531	2780947	-0.30274036		
3260 A17	X	1000	1000	0.31376042	1282	1272	0.6544606	1764606	-1.49976568	2482331	-0.85788902		
3260 A18	X	1112	1120	0.07937309	990	1000	-0.03752112	2663783	0.4583169	3042572	0.18363937		
3260 A19	X	910	920	0.08540637	1228	1240	0.54649958	2255887	-0.42993365	2641381	-0.56220361		
3260 A20	X	831	840	-0.13459327	1109	1120	0.25448923	2151186	-0.65793471	2968989	0.04684327		
3260 A21	X	1270	1280	1.08793636	1548	1560	1.3317375	1508778	-2.05668791	1957260	-1.83403384		
3260 A22	X	1451	1480	1.59198617	1570	1600	1.38572261	2210092	-0.5295866	3027741	0.15606747		
3260 A23	E	4342	7000	9.64285899	4310	7200	8.1093223	1022554	-5.11911719	1808031	-5.2718838		
3260 A24	X	910478	912160	2533.055442	9914	9920	2430.57814	1606408	-1.8474694	2897688	-1.66921267		
3260 B01	N	793	800	-0.20041588	793	800	-0.32462374	2085939	-8.0001917	2573537	-0.6883305		
3260 B02	E	194	200	-1.9085144	194	200	-1.99080045	106098	-5.12315889	114361	-5.26011587		
3260 B03	X	952	960	0.2023682	671	680	-0.82030517	2404168	-0.10703105	2988325	0.08279028		3-Bromo-7-nitroindazole
3260 B04	X	191	200	-1.91686882	229	240	-1.90491505	818559	-3.55991624	901700	-3.79639594		Chelerythrine chloride; 1,2-Dimethoxy-N-methyl(1,3)be-
3260 B05	X	832	840	-0.13180847	709	720	-0.72705817	2540047	0.18886446	3399708	0.84758092		Bumetanide; 3-(Aminosulfonyl-5)-(butylamino)-4-phenc
3260 B06	X	831	840	-0.13459327	1310	1320	0.7477168	1632600	-1.7872282	2042346	-1.67585284		Cyclosporin A; Antibiotic C 3662
3260 B07	X	790	800	-0.2487703	827	840	-0.43750169	2420497	-0.07147237	3379445	0.80991054		(4)-Baclofen; Lioreal
3260 B08	X	952	960	0.2023682	949	960	-0.13812973	2379731	-0.16024603	3393075	0.8352497		Carbachol; Carbamylcholine chloride
3260 B09	X	431	440	-1.24851549	949	960	-0.13812973	1706440	-1.62643128	2709490	-0.43558407		Brefeldin A from Penicillium brefeldianum; BFA; Ascotoci
3260 B10	X	592	600	-0.8001618	910	920	-0.23383006	2390699	-0.13636168	3199469	0.47532219		Cephalexin hydrate
3260 B11	X	792	800	-0.24320069	787	800	-0.53565643	2553003	0.21707796	3020036	0.14174332		BP 897; N-[4-(2-methoxyphenyl)piperazinyl]butyl]-2
3260 B12	X	1032	1040	0.42515264	1949	1960	2.31573877	1829085	-1.35935465	2211794	-1.3608368		Roscovitine; (R)-2-(1-Ethyl-2-hydroxyethylamino)-6-ber
3260 B13	X	632	640	-0.68876958	7467	1480	1.13297415	2699942	0.53705817	3449848	0.94079479		Bupropion hydrochloride; (4)-1-(3-Chlorophenyl)-2-[(1,
3260 B14	X	552	560	-0.91155402	1067	720	-0.73441978	2103725	-0.76128767	2792440	-0.28137405		Cyproheptadine hydrochloride
3260 B15	X	831	840	-0.13459327	870	1080	0.15878836	2822086	0.8038438	3627438	1.2709474		BL224 hydrochloride; 2-(4,5-Dihydroimidazol-2-yl)-quin
3260 B16	X	750	760	-0.36016252	1110	1120	0.2569431	2814827	0.78723631	3632722	1.28077074		Sigma-Aldrich M5793
3260 B17	X	747	760	-0.35737772	747	760	-0.63381117	2485108	0.06922711	3796041	1.58439252		Sigma-Aldrich C 0330
3260 B18	X	788	800	-0.25433991	1027	1040	0.05327201	1334111	-2.43722971	1576961	-2.54103709		Sigma-Aldrich C 7632
3260 B19	X	1429	1440	1.53072044	1866	1880	2.11206768	2442070	-0.02449415	3331432	0.72065092		Sigma-Aldrich C 0862
3260 B20	X	987	1000	0.29983639	1064	1080	0.14406515	1475830	-2.12861678	1803172	-2.12049454		Sigma-Aldrich C 8138
3260 B21	X	1105	1120	0.62844345	1304	1320	0.73299339	1738876	-1.55579735	2489233	-0.84505771		Sigma-Aldrich C 1671
3260 B22	X	1816	1840	2.60840419	1656	1800	1.5627553	2557644	-1.22718449	2976288	0.06041263		Sigma-Aldrich C 8773
3260 B23	E	2619	4320	8.44639604	2294	3720	2.1592320	109533	-5.10391944	1780226	-5.25330237		
3260 B24	P	569465	573960	1583.40052	473750	478560	1160.05335	2034951	-0.91105266	2756721	-0.34778724		empty
3260 C01	N	1114	1120	0.6535067	1073	1080	0.16614996	3227349	1.68556062	2853549	-0.16776801		empty
3260 C02	E	192	200	-1.91408401	272	280	-1.7993987	101547	-5.12131007	99080	-5.28852435		empty
3260 C03	X	1153	1160	0.76211411	1192	1200	0.45816032	2477547	0.05276198	2876832	-0.12448324		experimental
3260 C04	X	512	520	-0.102294624	991	1000	-0.03506725	2817540	0.79314425	3372314	0.7966535		Sigma-Aldrich 144509
3260 C05	X	752	760	-0.35459291	870	880	-0.33198534	2720270	-0.39861266	2717696	-0.42032853		Sigma-Aldrich 861669
3260 C06	X	804	800	-0.33688030	868	880	-0.43570645	2627166	0.10825074	2878474	0.03638176		Sigma-Aldrich A 7845
3260 C07	X	712	720	-0.46598513	830	840	-0.43014008	2449519	-0.00827291	2878506	-0.12137115		Sigma-Aldrich O7639
3260 C08	X	511	520	-0.102573105	911	920	-0.23137673	3221340	1.67247518	3571873	1.16764806		experimental
3260 C09	X	794	800	-0.23763108	790	800	-0.52829482	2630617	0.3860933	3129910	0.346007		Sigma-Aldrich A 1755
3260 C10	X	592	600	-0.8001618	590	600	-0.10968652	2679217	0.49192659	3485708	1.00746112		experimental
3260 C11	X	632	640	-0.68876958	831	840							

3260 K07	X	790	800	-0.2487703	752	760	-0.62154182	2447798	-0.01202063	2546289	-0.73898649	experimental	Sigma-Aldrich A 0937	(Φ)-Norepinephrine (+)bitartrate; (Φ)-Arterenol (+)bita
3260 K08	X	672	680	-0.57737735	471	480	-1.31107887	3241710	1.7168337	3704152	1.41356425	experimental	Sigma-Aldrich A 9256	L-Aspartic acid
3260 K09	X	553	560	-0.90876921	753	760	-0.61908796	2260708	-0.42080716	2771838	-0.31967465	experimental	Sigma-Aldrich A 1895	Aurintricarboxylic acid; ATA
3260 K10	X	513	520	-1.02016144	591	600	-1.01661465	3256012	1.74787831	3445382	0.93294218	experimental	Sigma-Aldrich A 9639	(Φ)-HA-966; (Φ)-3-Amino-1-hydroxy-2-pyrrolidone
3260 K11	X	554	560	-0.90589441	593	600	-1.0170692	2258978	-0.49448978	2662215	-0.5234717	experimental	3-Aminopropionitrile fumarate	3-Aminopropionitrile fumarate
3260 K12	X	552	560	-0.91155402	791	800	-0.52584095	1325430	1.46361775	3756379	1.51065801	experimental	Sigma-Aldrich A-013	8-(p-Sulfophenyl)theophylline
3260 K13	X	752	760	-0.35459291	792	800	-0.5238708	2203478	-0.54406157	2847304	-0.17937792	experimental	Sigma-Aldrich A 3940	1-Aminobenzotriazole; A8T; 1-Benzotriazolamine
3260 K14	X	792	800	-0.24320069	707	680	-0.82275904	2379725	-0.62369121	3593018	1.20695814	experimental	Sigma-Aldrich A-140	Arcaidine propargyl ester hydrobromide; APE
3260 K15	X	520	520	-1.02851585	609	720	-0.72705817	2173944	-0.60837598	2718454	-0.41891935	experimental	Sigma-Aldrich S 9318	Sandoz 58-035; 3-[Decyldimethylsilyl]-N-[2-(4-methylp
3260 K16	X	951	960	0.19958339	1071	1080	0.16124223	3277045	1.79378061	3782834	1.45833443	experimental	Sigma-Aldrich P 9872	Psora-4; 5-(4-Phenylbutoxy)psoralen
3260 K17	X	790	800	0.2487703	870	880	-0.33198534	2436626	-0.03634922	3061908	0.21958638	experimental	Sigma-Aldrich A 5626	Acetylthiocholine chloride
3260 K18	X	870	880	-0.02598586	668	680	-0.82766678	2828389	0.81676946	3478414	0.98981109	experimental	Sigma-Aldrich A-230	gamma-Acetylnicotinic GABA; A-3-Amino-5-hexynoic acid
3260 K19	X	949	960	0.19401378	1228	1240	0.54649958	2301374	-0.33087935	2458801	-0.90163299	experimental	Sigma-Aldrich A 6351	A-315456; N-[3-(cyclohexylidene)-1H-imidazol-4-yl]meth
3260 K20	X	947	960	0.18844417	1026	1040	0.05081814	2964203	1.11252343	3743391	1.48651238	experimental	Sigma-Aldrich A-263	ATPA; (RS)-2-Amino-3-(3-hydroxy-5-tert-butylisoxazol-
3260 K21	X	1225	1240	0.96262011	1305	1320	0.73544746	2067333	-0.84053633	2545341	-0.74074889	experimental	Sigma-Aldrich A 7127	Agmatine sulfate; (4-Aminobutyl)guanadine sulfate
3260 K22	X	1776	1800	2.49704797	1576	1600	1.40044582	2639108	0.40458363	2554601	-0.72353388	experimental	Sigma-Aldrich T6951	TBBz; 4,5,6,7-Tetrabromobenzimidazole
3260 K23	E	2832	4280	4.3780262	2956	4400	4.78678435	100918	-5.12267981	117427	-5.25441595	empty		
3260 K24	P	487329	490240	1354.66773	486162	489120	1190.51077	1939445	-1.11903033	2181340	-1.41745298	empty		
3260 L01	N	714	720	-0.46041552	794	800	-0.51847935	1703538	-1.62878748	2483634	-0.85548665	empty		
3260 L02	E	312	320	-1.57990735	313	320	-1.6987901	91989	-5.14212395	107590	-5.27270365	empty		
3260 L03	X	1193	1200	0.87350633	993	1000	-0.03015952	2601073	0.32157111	2973243	0.05475176	experimental	Sigma-Aldrich B 2417	Benzamil hydrochloride; N-(Benzylamino)-3,5-diamino
3260 L04	X	590	600	-0.80573141	471	480	-1.31107887	991904	-3.18243327	1232955	-3.18056903	experimental	Sigma-Aldrich C 3353	CGP-74514A hydrochloride; N2-(cis-2-Aminocyclohexyl)
3260 L05	X	912	920	0.09097598	671	680	-0.82030517	2938184	1.05586342	3196821	0.47033937	experimental	Sigma-Aldrich B 5002	5-Bromo-2'-deoxyuridine; Br-dU; 5-Bromo-1-(2-deoxy-1
3260 L06	X	828	840	-0.14294769	869	880	-0.33443921	2276587	-0.28485651	3257544	0.58328276	experimental	Sigma-Aldrich C 4024	Carbamazepine; 5H-Dibenz[b,f]azepine-5-carboxamide
3260 L07	X	872	880	-0.02041624	791	800	-0.52584095	3468975	2.211735	3265244	0.59760268	experimental	Sigma-Aldrich B 7005	Betamethasone; 9alpha-Fluoro-16beta-methylprednisol
3260 L08	X	689	690	-0.58731177	791	800	-0.52584095	2379286	-0.16151508	2484577	0.52923334	experimental	Sigma-Aldrich C 9398	Cytidine; SKF-92334; Tagamet
3260 L09	X	553	560	-0.90876921	631	640	-0.9485991	2018569	-0.69074952	2334907	-1.13196086	experimental	Sigma-Aldrich B 8385	Bestatin hydrochloride; N-[(2S,3R)-3-Amino-2-hydroxy-
3260 L10	X	714	720	-0.46041552	794	800	-0.51847935	1911710	-1.17942716	2840866	-0.19134662	experimental	Sigma-Aldrich C 5134	2-Chloroadenosine; 2-CADO
3260 L11	X	347	360	-1.48243916	387	400	-1.51720383	1017807	-3.12602587	1109816	-3.57680978	experimental	Sigma-Aldrich B-015	Bromoacetyl alprenolol methane
3260 L12	X	794	800	-0.23763108	793	800	-0.52093322	2171780	-0.61308839	2867979	-0.1409416	experimental	Sigma-Aldrich C 5976	Cl 316,243; Disodium 5-(2R)-2-[[[(2R)-2-(3-Chlorophe
3260 L13	X	591	600	-0.8029466	551	560	-1.11476939	2821932	0.80270844	3261968	0.59151234	experimental	Sigma-Aldrich B-135	R(+)-6-Bromo-APB hydrobromide; R(+)-6-Bromo-7,8-d
3260 L14	X	787	800	-0.25712472	864	880	-0.34670855	1904074	-1.19605562	2112690	-1.54507827	experimental	Sigma-Aldrich C 6628	Chloroquine diphosphate
3260 L15	X	871	880	-0.02320105	830	840	-0.43014008	2724893	0.59139246	3296367	0.65546256	experimental	Sigma-Aldrich B 5311	Biperiden hydrochloride; 1-(5-Bicyclo[2.2.1]hept-2-enyl
3260 L16	X	400	400	4.84181623	737	740	-0.95018911	992729	-1.2525902	2292913	-1.04186787	experimental	Sigma-Aldrich C 7255	Cyproheptadine hydrochloride; Decarboxycystidine dihydro
3260 L17	X	830	840	-0.13737808	870	880	-0.33198534	2935288	1.04955698	3786878	1.56735785	experimental	Sigma-Aldrich C 0737	Clotazolol; OPC 13013; OPC 21; Pletaal
3260 L18	X	910	920	0.08540637	949	960	-0.13812973	2191865	-0.5693505	2730139	-0.39719609	experimental	Sigma-Aldrich C 8011	Chelidamide; 4-Hydroxypyridine-2,6-dicarboxylic acid
3260 L19	X	789	800	-0.25155511	1146	1160	0.34528236	2805047	0.765939	3648231	1.30960308	experimental	Sigma-Aldrich C 1251	(+)-Catechin Hydrate; (+)-Cyanidol-3
3260 L20	X	909	920	0.08262156	1107	1120	0.24958149	2080780	-0.81125361	2934132	-0.10795841	experimental	Sigma-Aldrich A9361	Artemether; Dihydroartemisinin methyl ether, Dihydroq
3260 L21	X	1187	1200	0.8567975	1186	1200	0.44343771	2964596	1.11337924	3358801	0.77153186	experimental	Sigma-Aldrich C 2505	Corticosterone; Kendall's Compound B; 4-Pregnene-11b
3260 L22	X	1495	1520	1.71451761	1377	1400	0.91212599	2087284	-0.79709024	2576988	-0.68191484	empty		
3260 L23	E	2619	4000	4.84181623	737	740	-0.95018911	992729	-1.2525902	2292913	-1.04186787	empty		
3260 L24	P	464747	467640	1291.78126	472213	475040	1156.28175	797877	0.74141872	3066922	0.22880777	empty		
3260 M01	N	915	920	0.09933039	955	960	-0.12340652	3112535	1.43535709	3241768	0.55395908	empty		
3260 M02	E	434	440	-1.24016107	353	360	-1.60063536	293954	-4.70231694	100920	-5.28510366	empty		
3260 M03	X	551	560	-0.91433882	791	800	-0.52584095	2078200	-0.81687111	2330244	-1.14062971	experimental	Sigma-Aldrich 246557	Tryptamine hydrochloride; 3-(2-Aminoethyl)indole hydr
3260 M04	X	673	680	-0.57459255	752	760	-0.62154182	2939325	1.05834921	3617839	1.25310217	experimental	Sigma-Aldrich A 7762	L-allylglycine; L-2-Amino-4-pentenoic acid
3260 M05	X	629	640	-0.69712399	909	920	-0.23628447	1879018	-1.25061856	2456016	-0.9068105	experimental	Sigma-Aldrich A 0384	Arcaine sulfate; N,N'-1,4-Butanedithiylbis(guanidine) sulfat
3260 M06	X	1472	1480	-0.65046708	1351	1360	-0.33909911	2905945	0.98165849	2651905	0.51552648	experimental	Sigma-Aldrich A 8598	Anticabine hydrochloride; Cyclocytidine hydrochloride; C
3260 M07	X	543	560	-0.92826285	3428	640	0.92582152	22963625	0.25678152	2614445	0.18629682	experimental	Sigma-Aldrich A 0966	4-Amino-1,8-naphthalimide
3260 M08	X	1593	1600	-1.98742855	1071	1080	0.16124223	2925203	1.02795448	3582627	1.18764052	experimental	Sigma-Aldrich A 9335	Astaxanthin; 3,3'-Dihydroxy-beta,beta-carotene-4,4'-dic
3260 M09	X	509	520	-1.03130066	671	680	-0.32953147	2176578	-0.60264008	2622228	-0.59781042	experimental	Sigma-Aldrich A 1910	(Φ)-2-Amino-4-phosponobutyric acid; (Φ)-AP-4
3260 M10	X	748	760	-0.36573213	586	600	-1.028884	2742939	0.63069015	3027656	0.15590945	experimental	Sigma-Aldrich L 6668	Lercanidipine hydrochloride hemihydrate
3260 M11	X	2272	2280	3.87831152	2192	2200	2.91202881	2048379	-0.88181132	2013226	-1.72998902	experimental	Sigma-Aldrich A 3145	Agipenin; 4',5,7-Trihydroxyflavone
3260 M12	X	707	720	-0.47990916	587	600	-1.02643013	2931840	1.04204847	3707671	1.42010633	experimental	Sigma-Aldrich A-022	1,3-Dipropyl-8-p-sulfophenylxanthine
3260 M13	X	668	680	-0.58851658	704	720	-0.73932751	1759392	-1.5111209	2278354	-1.23709696	experimental	Sigma-Aldrich A 4147	3-Amino-1-propanesulfonic acid sodium
3260 M14	X	2152	2160	3.54413485	3471	3480	6.05052662	2043436	-0.89257539	2272013	-1.24888534	experimental	Sigma-Aldrich 10404	Indinibin-3'-oxime
3260 M15	X	782	800	-0.27104874	895	920	-0.27063863	2126876	-0.71087313	2685867	-0.47950093	experimental	Sigma-Aldrich A 4910	(Φ)-2-Amino-3-phosponopropionic acid; (Φ)-AP-3
3260 M16	X	1431	1440	-1.53629005	2670	2680	0.408497796	2645734	0.41901268	3055112	1.04353455	experimental	Sigma-Aldrich S 0568	SB 200646 hydrochloride; N-(1-Methyl-1H-indol-5-yl)-N
3260 M17	X	828	840	-0.14294769	864	880	-0.34670855	1734466	-1.56540075	2262720	-1.25770292	experimental	Sigma-Aldrich T3955	TNP
3260 M18	X	869	880	-0.02877066	1067	1080	0.15142675	2693084	0.52212392	3847863	1.68073336	experimental	Sigma-Aldrich A-236	AB-MECA; N6-(4-Aminobenzyl)-9-[5-(methylcarbonyl)-b
3260 M19	X	990	1000	0.30819081	1548	1560	1.3317375	1721645	-1.59332062	2396184	-1.0180425	experimental	Sigma-Aldrich G 8543	Sigma-Aldrich A 2654
3260 M20	X	949	960	0.19401378	1026	1040	0.05081814	2874631	0.91746788	3704313	1.41386356	experimental	Sigma-Aldrich A-265	ARL 67156 trisodium salt; FPL 67156
3260 M21	X	946	960	0.18565937	1105	1120	0.24467375	1852121	-1.30919054	2524906	-0.77873903	experimental	Sigma-Aldrich A 7200	4-Aminobenzamide hydrochloride
3260 M22	X	1615	1640	2.04869427	1416	1440	1.00782686	2884369	0.93867374	3223807	0.52056829	experimental	Sigma-Aldrich A P20005	Vericizone
3260 M23	E	2547	4040	4.64413304	2452	3880	3.55003462	124157	-5.07207364	109973	-5.26827348	empty		
3260 M24	P	501816	504920	1395.01121	480646	483520	1176.97523	1896407	-1.21275159	2138659	-1.49680003	empty		
3260 N01	N	713	720	-0.46320033	553	560	-1.10986166	1807253	-1.40689688	2413369	-0.98609435	empty		
3260 N02	E	313	320	-1.57712254	474	480	-1.30371727	93047	-5.13982001	107376	-5.27310149	empty		
3260 N03	X	753	760	-0.3518081	831	840	-0.42768621	2711176	0.56152178	3173646	0.42731537	experimental	Sigma-Aldrich B 2515	L-Buthionine-sulfoximine
3260 N04	X	511	520	-1.02573105	591	600	-1.01661465	1984010	-0.2198381	2594227	-0.65789694			

3260 001	N	1193	1200	0.87350633	834	840	-0.42032461	2824095	0.80741868	2857452	-0.16051205		empty
3260 002	E	352	360	-1.46851513	352	360	-1.60308922	100049	-5.12457217	96831	-5.2927054		empty
3260 003	X	1111	1120	0.64515228	1192	1200	0.45816032	2600205	0.31986692	2751911	-0.35672038		experimental
3260 004	X	870	880	-0.33198534	870	880	-0.33198534	2926807	1.03108841	3108899	0.30659404		experimental
3260 005	X	671	680	-0.58011616	671	680	-0.82030517	2954888	1.12593296	2798940	-0.26929008		experimental
3260 006	X	751	760	-0.35737772	549	560	-1.11967713	2486808	0.0729291	2709095	-0.43631841		experimental
3260 007	X	1191	1200	0.86793672	1391	1400	0.94648015	2365762	-0.19066548	2831846	-0.20811545		experimental
3260 008	X	711	720	-0.46876994	790	800	-0.52829482	2728459	0.59915792	3261221	0.59012361		experimental
3260 009	X	672	680	-0.57737735	631	640	-0.91845991	2462190	0.01931997	2814391	-0.24056556		experimental
3260 010	X	351	360	-1.47129993	349	360	-1.61045083	850461	-3.49404517	909563	-3.78177805		experimental
3260 011	X	792	800	-0.24232069	831	840	-0.42768621	2249684	-0.44344155	2623921	-0.59466301		experimental
3260 012	X	630	640	-0.69433919	714	720	-0.72215043	2704724	0.54747164	3088010	0.25455924		experimental
3260 013	X	951	960	0.19589339	870	880	-0.33198534	1944181	-1.10871702	2317083	-1.16509696		experimental
3260 014	X	589	600	-0.80851621	1108	1120	0.25203536	2511019	0.12565194	3011243	0.29271298		experimental
3260 015	X	1025	1040	0.405659	821	840	-0.4522249	2321943	-0.28608748	3073857	0.24180043		experimental
3260 016	X	2111	2120	3.42995782	2670	2680	4.08497796	2296059	-0.3424535	2925588	-0.03384232	W	experimental
3260 017	X	945	960	0.18287456	824	840	-0.44486329	2266251	-0.40736459	3127581	0.34167722		experimental
3260 018	X	1029	1040	0.41679823	948	960	-0.1405836	2447804	-0.01200756	3122231	0.33173118		experimental
3260 019	X	909	920	0.08262156	1148	1160	0.3501901	2399394	-0.1174271	3132035	0.349995753		experimental
3260 020	X	1022	1040	0.39730459	1179	1200	0.42626002	2574282	0.26341596	3296802	0.65493272		experimental
3260 021	X	1225	1240	0.96262011	1104	1120	0.24221989	2271847	-0.39517852	2861024	-0.15387145		experimental
3260 022	X	1493	1520	1.708948	1493	1520	1.19677473	2314755	-0.30174035	2903927	-0.07411168		experimental
3260 023	E	3189	4960	6.4319782	2972	4840	4.82604624	97614	-5.12987473	108734	-5.27057687		empty
3260 024	P	592338	597160	1647.09738	629131	632960	1541.33789	1899083	-1.20535632	2352795	-1.09870578		empty
3260 N1	N	1276	1280	1.10464519	997	1000	-0.02034404	1568383	-1.92706969	2092950	-1.58177636		empty
3260 P12	E	272	280	-1.69129497	314	320	-1.69129497	280	-1.69129497	280	-1.69129497		empty
3260 P03	X	1034	1040	0.43072225	833	840	-0.42277848	2261018	-0.9616018	2638404	-0.56773063		experimental
3260 P04	X	792	800	-0.24320069	953	960	-0.12831426	2194622	-0.56334675	2688748	-0.47414495		experimental
3260 P05	X	834	840	-0.12623886	793	800	-0.52093322	173222	-0.60994824	2562991	-0.70793627		experimental
3260 P06	X	753	760	-0.3518081	793	800	-0.52093322	1704813	-0.62997473	2109141	-1.55167612		experimental
3260 P07	X	872	880	-0.02041624	912	920	-0.22892286	2513232	0.13047105	2928369	-0.02867224		experimental
3260 P08	X	633	640	-0.68598477	632	640	-0.91600604	1796507	-1.4302978	2245259	-1.29862295		experimental
3260 P09	X	834	840	-0.12623886	912	920	-0.22892286	2409289	-0.09587936	2887692	-0.10429377		experimental
3260 P10	X	834	840	-0.12623886	912	920	-0.22892286	2409289	-0.09587936	2887692	-0.10429377		experimental
3260 P11	X	633	640	-0.68598477	792	800	-0.52387808	2168997	-0.61914877	2568420	-0.69784337		experimental
3260 P12	X	714	720	-0.46041552	554	560	-1.10740779	1377489	-2.34276805	1517189	-2.65215754		experimental
3260 P13	X	912	920	0.09097598	714	720	-0.72215043	1818511	-1.38238101	2341764	-1.1192132		experimental
3260 P14	X	1113	1120	0.65072189	1671	1680	1.63356333	2143873	-0.67385799	2667025	-0.51452957		experimental
3260 P15	X	792	800	-0.24320069	1111	1120	0.25939697	2481396	0.06114379	2803451	-0.26090398		experimental
3260 P16	X	549	560	-0.91990844	746	760	-0.63626504	1122112	-2.89988716	1354334	-2.95491672		experimental
3260 P17	X	1040	1040	0.42793761	982	1000	-0.42793761	2052367	-0.2062367	2538404	-0.2062367		experimental
3260 P18	X	951	960	0.19589339	1111	1120	0.25939697	1125473	-2.89158611	1410137	-2.85117492		experimental
3260 P19	X	866	880	-0.03712508	982	1000	-0.05715207	2268624	-0.40219705	2787232	-0.29942192		experimental
3260 P20	X	3031	3040	5.99197892	3910	3920	7.1277749	1951597	-1.09256765	2158865	-1.45923562		experimental
3260 P21	X	1304	1320	1.18261975	1261	1280	0.62747724	2472064	0.04082198	2850072	-0.17423201		experimental
3260 P22	X	1289	1320	1.14084767	1494	1520	1.19922886	2017751	-0.94850807	2588053	-0.66134421		experimental
3260 P23	E	4712	7800	10.673237	3934	6280	7.18666774	91974	-5.14215662	100339	-5.28618378		empty
3260 A01	N	1058460	10660	2945.01448	801989	802840	1965.50869	193291	-1.1165568	228373	-1.12466214		empty
3261 A01	N	838	840	-0.92449044	1038	1040	-0.99741324	1979257	-0.84506796	1582012	-1.6940338		empty
3261 A02	E	274	280	-1.70196035	592	600	-2.18048004	80974	-3.44811905	87488	-3.99744822		empty
3261 A03	X	874	880	-0.8748647	1112	1120	-0.79490631	1857898	-1.01148344	1823786	-1.32140298		experimental
3261 A04	X	1074	1080	-0.59916615	1070	1080	-0.90681804	2202625	-0.538771	2270150	-0.63345064		experimental
3261 A05	X	672	680	-1.15332024	1351	1360	-0.15807311	2417659	-0.24390217	1491491	-1.83354804		experimental
3261 A06	X	993	1000	-0.71082406	1188	1200	-0.59239938	2609730	0.01947828	2245878	-0.67089593		experimental
3261 A07	X	1072	1080	-0.60192314	1468	1480	0.15367878	2526740	-0.09432309	2498311	-0.28180066		experimental
3261 A08	X	791	800	-0.9892796	1986	2000	1.53392337	2566354	-0.04000176	2669482	-0.01798573		experimental
3261 A09	X	1394	1400	-0.15804847	2148	2160	1.96558288	1973955	-0.85233841	2079276	-0.92763255		experimental
3261 A10	X	750	760	-1.0457978	1306	1320	-0.27798073	2358437	-0.32511129	2968150	0.44233219		experimental
3261 A11	X	1153	1160	-0.49026522	1549	1560	0.36950853	1580327	-1.39210714	2386933	-0.45346046		experimental
3261 A12	X	792	800	-0.98790111	1348	1360	-0.166069	2513548	-0.11241283	3271301	0.90955947		experimental
3261 A13	X	753	760	-1.04166232	1309	1320	-0.26998703	2257483	-0.46354608	3068023	0.95626007		experimental
3261 A14	X	713	720	-1.09680203	1068	1080	-0.91214716	1784530	-1.11209049	2582408	-0.15218733		experimental
3261 A15	X	914	920	-0.81972499	1127	1140	0.15900791	1650384	-1.29604037	3009586	0.50619485		experimental
3261 A16	X	912	920	-0.82241898	1109	1120	-0.80290001	1934130	-0.90694908	3305931	0.96293248		experimental
3261 A17	X	753	760	-1.04310348	1110	1120	-0.80023544	2147865	-0.61386153	2283865	-0.61231259		experimental
3261 A18	X	912	920	-0.82241898	1230	1240	-0.48048766	2100123	-0.67932851	2099530	-0.89641635		experimental
3261 A19	X	1192	1200	-0.436504	1108	1120	-0.80556457	2347712	-0.33981811	2440156	-0.37143125		experimental
3261 A20	X	1149	1160	-0.49577919	1628	1640	0.58000916	2525374	-0.09619624	3290845	0.93968139		experimental
3261 A21	X	1508	1520	-0.00090029	1745	1760	0.89176324	2420362	-0.24019563	3070664	0.60033047		experimental
3261 A22	X	1800	1800	0.37125275	1935	1940	1.39800257	2319455	-0.37855998	2581742	0.35538144		experimental
3261 A23	X	2578	2680	1.40929778	3023	5160	0.92707713	87831	-3.48571628	86931	-3.99830669		experimental
3261 A24	P	735762	737280	1012.16292	730691	732240	1943.21566	1723153	-1.19625469	1948330	-1.12945126		empty
3261 B01	N	555	560	-1.31460389	712	720	-1.86073225	2329691	-0.3645297	2403432	-0.42803161		empty
3261 B02	E	314	320	-1.64682064	591	600	-2.1831446	88037	-3.4384338	82971	-4.00440998		empty
3261 B03	X	873	880	-0.87624319	1229	1240	-0.48315222	2434605	-0.22066469	2745722	0.09951811		experimental
3261 B04	X	550	560	-1.32149635	908	920	-1.33847554	2865783	0.3705908	3236980	0.85666227	W	experimental
3261 B05	X	512	520	-1.37387908	826	840	-1.55697186	1861359	-1.00673749	1880175	-1.23366194		experimental
3261 B06	X	1304	1320	-0.82380948	1225	1240	-0.28309898	2947245	-0.34517405	2645811	-0.04646833		experimental
3261 B07	X	791	800	-0.9892796	1026	1040	-1.02405889	2680828	0.11697256	2977999	0.17978017		experimental
3261 B08	X	590	600	-0.26635664	1145	1160	-0.70697567	2559625	-0.049229	2823412	0.21925675		experimental
3261 B09	X	589	600	-1.26773514	944	960	-1.24255321	2720440	0.17129115	2435910	-0.37797534	W	experimental
3261 B10	X	751	760	-1.04441931	1026	1040	-1.02405889	2840250	0.33582554	2777435	0.14839534	W	experimental
3261 B11	X	790	800	-0.99065809	1026	1040							

3261 B19	X		788	800	-0.99341508	1306	1320	-0.27798073	2824552	0.3140564	2575254	-0.16321333		experimental	Sigma-Aldrich D 8816	N-(3,3-Diphenylpropyl)glycinamide; N2OC
3261 B20	X		1028	1040	-0.66257682	1183	1200	-0.60572221	2809177	0.29297319	2554265	-0.19556233		experimental	Sigma-Aldrich H-168	R-(+)-7-Hydroxy-DPAT hydrobromide; R(+)-7-Hydroxy-L-Canavanine; L-alpha-Amino-gamma-(guanidinoxy)-n-Iodacetamide
3261 B21	X		1105	1120	-0.55643287	1662	1680	-0.67060436	2709005	0.15561072	2582578	-0.15192532		experimental	Sigma-Aldrich C 1625	
3261 B22	X		1440	1440	-0.12634313	1851	1880	-1.17420712	2044834	-0.7551444	2432379	-0.3831092		experimental	Sigma-Aldrich I 1149	
3261 B23	X		1708	3240	0.27479826	2476	4040	2.83956015	93635	-3.43075745	89299	-3.99589986		empty		
3261 B24	P	516079	519760	709.331496	526735	529960	1399.76167	2434386	-0.220965		2274795	-0.6262916		empty		
3261 C01	N		435	440	-1.48002302	953	960	-1.21857212	2403006	-0.26399533	1917635	-1.1767595		empty		
3261 C02	E		275	280	-1.70058186	630	640	-2.07922657	90397	-3.43519761	96112	-3.9841566		empty		
3261 C03	X		592	600	-1.26359966	1109	1120	-0.80290001	2187156	-0.55998311	2268697	-0.63569006		experimental	Sigma-Aldrich C 9901	N6-Cyclohexyladenosine; CHA
3261 C04	X		872	880	-0.87762169	947	960	-1.23455951	2500353	-0.13050669	2331455	-0.53896516		experimental	Sigma-Aldrich D 6035	Disopyramide phosphate
3261 C05	X		866	880	-0.88589264	1145	1160	-0.70697567	2208482	-0.53073949	1182300	-2.31008439		experimental	Sigma-Aldrich C-106	CGS-12066A maleate; 7-Trifluoromethyl-4(4-methyl-1-p-Daldetone; 7-Hydroxy-3-(4-hydroxyphenyl)-4H-1-benzop
3261 C06	X		2791	2800	-1.76770592	2387	2400	-1.620421388	3457760	-1.18235306	2779081	-0.07275327		experimental	Sigma-Aldrich D 780	Y-27632 dihydrochloride; (R)-(+)-trans-4-(1-Aminoethyl
3261 C07	X		703	720	-1.11058696	903	920	-1.35180037	2984157	0.53291733	2851048	0.26185035		experimental	Sigma-Aldrich Y 0503	Imperatorin; 9-((3-Methyl-2-buten-1-yl)oxy)-7H-furo[3,
3261 C08	X		1311	1320	-0.27246337	1106	1120	-0.8108937	3065703	0.64473859	3121432	0.67857595		experimental	Sigma-Aldrich D 16659	2-Chloro-2-deoxy-D-glucose; 2-Chloro-DG
3261 C09	X		949	960	-0.77147774	1227	1240	-0.48848135	2721928	0.17333159	3364936	1.05387311		experimental	Sigma-Aldrich C-203	3,4-Dihydroxyphenylacetic acid; DOPAC
3261 C10	X		906	920	-0.83075293	1463	1480	-0.14035595	2611126	0.02139257	2955974	0.42356661		experimental	Sigma-Aldrich D 9128	WB-4101 hydrochloride; 2-(2,6-Dimethoxyphenoxyethyl
3261 C11	X		870	880	-0.88037867	1266	1280	-0.38456332	2450348	-0.19907685	3262274	0.89564673		experimental	Sigma-Aldrich D 0411	6,7-ADTN hydrobromide; (♣)-2-Amino-6,7-dihydroxy-1,
3261 C12	X		951	960	-0.76872076	1346	1360	-0.17139813	2799745	0.28003941	2934598	0.39062063		experimental	Sigma-Aldrich D-002	2,3-didehydro-3'-deoxythymidine; 2'-3'-Amhydrothymid
3261 C13	X		670	680	-1.15607722	1425	1440	-0.03910249	2449659	-0.20002165	2779081	0.15093232		experimental	Sigma-Aldrich D 1413	Mephetryl tetrazole; 1-[2-(4-Methoxyphenyl)ethyl]-5-(1-
3261 C14	X		751	760	-1.04441931	1146	1160	-0.70431111	2740690	0.19059529	2873803	0.29692118		experimental	Sigma-Aldrich M 7945	Dextromethorphan hydrobromide monohydrate; d-3-Me-
3261 C15	X		552	560	-1.31873937	1186	1200	-0.59772851	2076339	-0.7119427	2648499	-0.05032549		experimental	Sigma-Aldrich D 2531	1,3-Dipropyl-7-methylxanthine
3261 C16	X		508	520	-1.37939305	1226	1240	-0.49114592	2327947	-0.36692219	2791258	0.16969984		experimental	Sigma-Aldrich D-108	Dequalinium chloride hydrobromide; 1,1'-Decamethylenebis(4-
3261 C17	X		1031	1040	-0.65844134	1307	1320	-0.27531616	2070881	-0.71942708	1986404	-1.07077024		experimental	Sigma-Aldrich D 3768	Doxepin hydrochloride
3261 C18	X		1109	1120	-0.5509189	1146	1160	-0.70431111	2976458	0.52259995	2927827	0.38018492		experimental	Sigma-Aldrich A 8054	4-Diamino-6-pyrimidinone; DAHP; 2,4-Diamino-6-hydr
3261 C19	X		948	960	-0.77285624	1305	1320	-0.28064529	2964445	-0.12215294	2330106	-0.54104429		experimental	Sigma-Aldrich D 4526	DM 235
3261 C20	X		907	916	-0.82937464	1384	1390	-0.70114467	3241385	0.88156536	2641385	0.18932128		experimental	Sigma-Aldrich H-108-6	Etoposide; Lastet
3261 C21	X		1186	1200	-0.44747496	1500	1520	-0.23984485	2880098	0.38022475	2585279	-0.2478444		experimental	Sigma-Aldrich D 5689	
3261 C22	X		1818	1840	0.42643246	2336	2360	2.4652107	2872991	0.38047916	2514989	-0.25609593		experimental	Sigma-Aldrich E 1383	
3261 C23	E		1638	3200	0.17830376	1999	3120	1.56856272	90361	-3.43524698	92351	-3.98995319		empty		
3261 C24	P	528068	531040	725.858245	374987	377680	995.41928	2633249	0.05172909		2316319	-0.56229331		empty		
3261 D01	N		795	800	-0.98376563	1332	1040	-1.0080715	2292531	-0.41548595	2517835	-0.25170957		empty		
3261 D02	E		274	280	-1.70196035	790	800	-1.6528962	219259	-3.25849352	86801	-3.99850705		empty		
3261 D03	X		832	840	-0.9327614	1025	1040	-1.02672345	2823888	0.31314588	3308313	0.9666037		experimental	Sigma-Aldrich E 3149	S-Ethylisothiourea hydrobromide; 2-Ethyl-2-thiopseudoi
3261 D04	X		680	690	-0.80822137	1107	1120	-1.15607722	2449659	-0.20002165	2779081	0.15093232		experimental	Sigma-Aldrich T 22	G-108
3261 D05	X		751	760	-1.04441931	1108	1120	-0.80556457	3075648	0.65837583	3399741	1.10751584		experimental	Sigma-Aldrich E 3876	N-Ethylmaleimide; NEM
3261 D06	X		624	640	-1.21948789	982	1000	-1.14129974	2564519	-0.04251803	3011401	0.50899219		experimental	Sigma-Aldrich G-133	GR-89696 fumarate; 4-[(3,4-Dichlorophenyl)acetyl]-3-
3261 D07	X		994	1000	-0.71358105	1186	1200	-0.59772851	3263930	0.91656055	3255140	0.88465155		experimental	Sigma-Aldrich N 3911	NBI 27914; 5-Chloro-4-(N-(cyclopropyl)methyl-N-propyl
3261 D08	X		788	800	-0.99341508	1425	1440	-0.03910249	2973599	0.5184395	2915953	0.36188429		experimental	Sigma-Aldrich H 1384	Hypotaurine; 2-Aminoethanesulfonic acid
3261 D09	X		826	840	-0.94103235	1062	1080	-0.92813455	2980042	0.52727457	2816072	0.20794408		experimental	Sigma-Aldrich T 5648	Tamoxifen; (Z)-1-(p-Dimethylaminoethoxyphenyl)-1,2-d
3261 D10	X		2270	2280	1.04951119	2185	2200	2.06417178	2774456	0.24536146	2968988	0.44362374		experimental	Sigma-Aldrich H 3132	Ciprofloxacin hydrochloride; Cyclopropyl[4-[3-(1H-imidazol
3261 D11	X		706	710	-0.10549524	1105	1120	-0.8108937	3011401	0.50899219	289397	0.22274544		experimental	Sigma-Aldrich F 2802	Fluvoxamine maleate; (♣)-2-Amino-1-[4-(trifluoromet
3261 D12	X		711	720	-1.09595902	1106	1120	-0.81355827	1659541	-1.28348367	1743044	-1.44584546		experimental	Sigma-Aldrich H 6036	1,3,5-Tris(4-hydroxyphenyl)-4-propyl-1H-pyrazole; PPT
3261 D13	X		711	720	-1.09595902	1105	1280	-0.38722789	3207089	0.83861642	3171936	0.75641454		experimental	Sigma-Aldrich F 6145	Fensipride hydrochloride; 8-(2-Phenylethyl)-1-oxa-3,8-d
3261 D14	X		990	1000	-0.71495954	1265	1120	-0.81355827	2537735	-0.07924602	2843211	0.24977169		experimental	Sigma-Aldrich H 8250	(♣)-8-Hydroxy-DPAT hydrobromide; (♣)-8-Hydroxy-dip
3261 D15	X		1109	1120	-0.5509189	1347	1360	-0.16873357	3188939	0.81372794	3175541	0.76197069		experimental	Sigma-Aldrich F 6889	Famotidine; N-(Aminosulfonyl)-3-[[2-(diaminomethylen
3261 D16	X		1710	1720	-0.27755524	1105	1120	-0.81355827	2782566	0.25648243	2731743	0.07797317		experimental	Sigma-Aldrich H 9003	Hydroquinone; 1,4-Benzenediol
3261 D17	X		827	840	-0.93965386	1106	1120	-0.8108937	2911186	0.43285467	2809145	0.19276793		experimental	Sigma-Aldrich F 9552	Formoterol; (R*,R*)-N-[2-hydroxy-5-[1-hydroxy-2-[[2-(
3261 D18	X		948	960	-0.77285624	985	1000	-1.13330505	2535945	0.81700529	2959376	0.42227454		experimental	Sigma-Aldrich H-108	Hemicholinium-3
3261 D19	X		1148	1160	-0.49715769	1266	1280	-0.38456332	2091128	0.60960303	3004522	0.49840082		experimental	Sigma-Aldrich D 0639	Doxylamine succinate; Glycerol
3261 D20	X		1107	1120	-0.55367589	1303	1320	-0.28597442	2840065	0.33532886	3138579	0.70500352		experimental	Sigma-Aldrich S0323	Sematiide monohydrochloride monohydrate; N-[2-(Diet
3261 D21	X		945	960	-0.77699172	1543	1560	0.35352114	3074049	0.65518318	2671586	-0.01474297		experimental	Sigma-Aldrich B 7273	Bezafibrate
3261 D22	X		1657	1680	0.20449513	1694	1720	0.75587044	2546695	-0.06695948	2700175	0.02931943		experimental	Sigma-Aldrich I 1392	HA-100; 1-(5-Isouquinolinesulfonyl)piperazine hydrochlor
3261 D23	E		1838	3320	0.45400232	2105	3280	1.85100659	94694	-3.42930528	91745	-3.99088718		empty		
3261 D24	P	500245	503400	687.504441	394712	397200	1047.97782	2953924	0.49145984		2621268	-0.09172463		empty		
3261 E01	N		875	880	-0.87348621	1152	1160	-0.68832372	2724732	0.17717662	2265386	-0.64079309		empty		
3261 E02	E		232	240	-1.75985705	666	680	-1.98300224	97818	-3.42502145	96403	-3.9837081		empty		
3261 E03	X		1273	1280	-0.32484609	2268	2280	-2.8533066	3315480	0.98724932	4239196	2.40131423		experimental	Sigma-Aldrich C 9911	(S)-(+)-Camptothecin
3261 E04	X		870	880	-0.88037867	1184	1200	-0.60305764	2689442	0.12878464	2490310	-0.29413209		experimental	Sigma-Aldrich D 6140	Demeclocycline hydrochloride; 7-chloro-6-demethyltetra
3261 E05	X		790	800	-0.99065809	907	920	-1.34114211	2780151	0.25317082	1434870	-1.92081437		experimental	Sigma-Aldrich C-108	2-Cyclooctyl-2-hydroxyethylamine hydrochloride; CONH
3261 E06	X		1031	1040	-0.65844134	1307	1360	-0.16873357	2343610	-0.34544305	1971275	-1.09408746		experimental	Sigma-Aldrich I1493	Clinidine; 1,4-Dihydro-2,6-dimethyl-4-(3-nitrophenyl)-
3261 E07	X		989	1000	-0.71633803	1505	1520	0.25226768	3316890	0.9891828	3543052	1.32908549		experimental	Sigma-Aldrich C-144	1-(m-Chlorophenyl)-biguanide hydrochloride; m-CPBG
3261 E08	X		991	1000	-0.71358105	1624	1640	0.5693509	3223694	0.86138629	3404215	1.11441133		experimental	Sigma-Aldrich D 8296	3-deazaadenosine; 4-Amino-1-(beta-D-ribofuranosyl)-11
3261 E09	X		750	760	-1.0457978	1343	1440	-0.03377339	2784356	0.25893699	3329434	0.99915515		experimental	Sigma-Aldrich T0202	Tocainide hydrochloride; 2'-5-Methoxy-1-[4-(trifluoromet
3261 E10	X		827	840	-0.93965386	1343	1360	-0.17939183	2518662	-0.10540018	2786630	0.1625656		experimental	Sigma-Aldrich D 9175	Dantrolene sodium; 1-[(5-(p-Nitrophenyl)furfurylidene)]
3261 E11	X		785	800	-0.99755056	1343	1360	-0.17939183	2669808	0.10186121	2789256	0.16661429		experimental	Sigma-Aldrich D 0540	DNQX; 6,7-Dinitroquinoxaline-2,3-dione
3261 E12	X		872	880	-0.87762169	1265	1280	-0.38722789	2898514	0.41547799	2975349	0.4				

3261 J07	X	1622	1640	0.15624788	2022	2040	1.62984771	2100235	-0.67917493	2879381	0.3055182	experimental	Sigma-Aldrich P0111	Phenserine; (-)-N-Phenylcarbamoyleseroline
3261 J08	X	2343	2360	1.15014116	2542	2560	3.01542144	2667637	0.09888419	3106545	0.65563157	experimental	Sigma-Aldrich H 1877	4-Imidazolemethanol hydrochloride; 4-(Hydroxymethyl)
3261 J09	X	1460	1480	-0.06706795	1222	1240	-0.50180418	2645928	0.06911537	3167350	0.74934643	experimental	Sigma-Aldrich F 0778	Felbamate; 2-Phenyl-1,3-propanediol dicarbamate
3261 J10	X	1505	1520	0.10524365	947	960	-1.23455951	3005502	0.562187	3348817	1.02803093	experimental	Sigma-Aldrich L 4408	Lithium Chloride
3261 J11	X	1504	1520	-0.00641426	1107	1120	-0.80822914	1469238	-1.5443971	1903961	-1.19783437	experimental	Sigma-Aldrich F 4303	Fidusoxin hydrochloride;
3261 J12	X	1464	1480	-0.06155397	1226	1280	-0.38456332	2876268	0.3849728	3295094	0.9462301	experimental	Sigma-Aldrich H 7258	Harmane; Aribine
3261 J13	X	1502	1520	-0.00917125	1265	1240	-0.49381048	2612051	0.02266099	3000435	0.492091	experimental	Sigma-Aldrich F 6513	Fusaric acid; 5-Butyl-2-pyridinecarboxylic acid
3261 J14	X	1504	1520	-0.00641426	1066	1080	-0.91747629	2836407	0.33031276	3374990	1.0693867	experimental	Sigma-Aldrich H 8645	(+)-Hydrastine; (+)-beta-Hydrastine 1(5S),9(R)
3261 J15	X	1662	1680	0.21138759	1346	1360	-0.17139813	1974389	-0.85174328	2468131	-0.32831517	experimental	Sigma-Aldrich F 8257	Flunarizine dihydrochloride; 1-bis(4-fluorophenyl)meth
3261 J16	X	1664	1680	0.21414458	1146	1160	-0.70431111	3173872	0.79306707	3291992	0.94144919	experimental	Sigma-Aldrich H 9523	Serotonin hydrochloride; 5-HT hydrochloride
3261 J17	X	1463	1480	-0.06293247	1287	1280	-0.38189876	2026323	-0.78052795	2170251	-0.78741859	experimental	Sigma-Aldrich F 1194	cis-(2)-Flupenthixol dihydrochloride; (Z)-4-[3-[2-(Triflu
3261 J18	X	1263	1280	-0.33863102	1186	1200	-0.59772851	2172228	-0.58045337	2658645	-0.1028351	experimental	Sigma-Aldrich H 1127	Hexyldro-silica-difenidol dihydrochloride, p-fluoro analog;
3261 J19	X	1464	1480	-0.06155397	1343	1360	-0.17939183	3292329	0.95550314	3066084	0.93237161	experimental	Sigma-Aldrich G 2128	L-Glutamic acid hydrochloride; (S(+)-1-Amino-propane-1,
3261 J20	X	1501	1520	-0.101054974	1463	1480	0.14035595	2309774	-0.39184121	3111135	0.66270584	experimental	Sigma-Aldrich I 0375	Imidazole-4-acetic acid hydrochloride; 14AA
3261 J21	X	1299	1320	-0.28900528	1300	1320	-0.29396812	1101303	-2.0489765	1051005	-2.51244099	experimental	Sigma-Aldrich G 6793	GW7647; 2-(4-(2-(1-Cyclohexanebutyl)-3-cyclohexylure
3261 J22	X	1649	1680	0.19346718	1603	1640	0.54004068	2974133	0.51917176	2936695	0.39385261	experimental	Sigma-Aldrich M 1195	Metolazone; 7-Chloro-1,2,3,4-tetrahydro-2-methyl-3-(2
3261 J23	E	2337	3840	1.1418702	2489	3800	2.8741995	92212	-3.43270076	90472	-3.99284917	empty		
3261 J24	P	509662	509840	696.763777	440733	443480	1170.60376	3210534	0.84336785	2980600	0.46068831	empty		
3261 K01	N	1507	1520	-0.00227879	1071	1080	-0.90415347	2479717	-0.15800414	2576335	-0.16154725	empty		
3261 K02	E	863	880	-0.89002812	668	680	-1.97797311	90917	-3.43448455	95895	-3.98449105	empty		
3261 K03	X	1659	1680	0.20725211	864	880	-1.4557184	2125897	-0.6439855	2062564	-0.95338969	experimental	Sigma-Aldrich P2014	CP-91149
3261 K04	X	1458	1480	-0.06982493	946	960	-1.23722408	2645712	0.06688198	2586535	-0.14582664	experimental	Sigma-Aldrich D 6908	DL-erythro-Dihydrospingosine; DL-Sphinganine
3261 K05	X	1742	1760	0.32166701	1226	1240	-0.49114592	2910759	0.43226914	1213105	-2.26260661	experimental	Sigma-Aldrich C 1255	(-)-CGP-12177A hydrochloride; 4-[4-[[[1,1-Dimethyleth
3261 K06	X	1420	1440	-0.12220766	1146	1160	-0.70431111	3284208	0.94436709	3494395	1.25340001	experimental	Sigma-Aldrich D 7938	D80-83; 3-(6-Chloro-3-pyridazinyl)-3,8-diazabicyclo[3.1.
3261 K07	X	1538	1560	0.04045449	1261	1280	-0.39788615	2431479	-0.22495127	3072685	0.60344531	experimental	Sigma-Aldrich C 191	Capsazepine; N-[2-(4-Chlorophenyl)ethyl]-1,3,4,5-tetra
3261 K08	X	1738	1760	0.31615304	1226	1280	-0.50180418	3055395	0.6167670	3243508	0.81740406	experimental	Sigma-Aldrich H 8555	N,N-Diethyl-2-(4-fluorophenyl)indole-3-acetamide; FGII
3261 K09	X	1720	1760	0.49114592	1126	1240	-0.49114592	2830236	0.32185068	3298233	0.16122166	experimental	Sigma-Aldrich C 237	5,1'S,2'S-carboxycyclopropylglycine; L-CGCS-1
3261 K10	X	1461	1480	-0.06568945	1206	1120	-0.8108937	2888617	0.40190657	2904260	0.34386261	experimental	Sigma-Aldrich D 9628	L-3,4-Dihydroxyphenylalanine; L-DOPA; Levodopa
3261 K11	X	1381	1400	-0.17596887	1187	1200	-0.59506395	2671677	0.1044241	2526007	-0.23911459	experimental	Sigma-Aldrich D 1064	Dihydrokainic acid; 2-Carboxy-4-isopropyl-3-pyrrolidine
3261 K12	X	1500	1520	-0.01192824	904	920	-1.3491358	2468976	-0.7135329	2272037	-0.63054233	experimental	Sigma-Aldrich D-030	RC(-)-2,10,11-Trihydroxy-N-propylnoraporphine hydrobro
3261 K13	X	2300	2320	0.190806597	1506	1520	0.25493224	2656525	0.08364668	2341286	-0.52381327	experimental	Sigma-Aldrich K3519	KRM-III
3261 K14	X	1458	1480	-0.06982493	946	960	-1.23722408	2128067	-0.64100985	1765754	-1.41084399	experimental	Sigma-Aldrich D 1054	RC(+)-SCH-23390 hydrochloride; R(+)-7-Chloro-8-hydro:
3261 K15	X	1860	1880	0.48432916	1026	1040	-1.02405889	2428725	-0.22872774	1871430	-1.24797232	experimental	Sigma-Aldrich D 3630	Diphenhydramine hydrochloride
3261 K16	X	1560	1580	0.18329508	847	860	-1.34573079	2482507	0.38984413	2575903	0.79996579	experimental	Sigma-Aldrich H 0627	R(+)-7-Hydroxy-DPAT hydrobromide; (S)-DIOXA
3261 K17	X	1580	1600	0.09835118	947	960	-1.23455951	2791648	0.26893627	1244869	-2.21365078	experimental	Sigma-Aldrich D 4007	5,5-Diphenylhydantoin; Phenytoin
3261 K18	X	1821	1840	0.43056794	984	1000	-1.13597061	3348966	1.03316754	1579424	-1.69802252	experimental	Sigma-Aldrich D14204	1,10-Diaminododecane; DA10; Decamethylenediamine
3261 K19	X	1778	1800	0.37129275	1743	1760	0.88643411	3352448	1.03794228	3534562	1.31530684	experimental	Sigma-Aldrich G 7795	Ganaxalone; 3a-Hydroxy-3beta-Hydroxy-5a-pregnan-20-
3261 K20	X	2096	2120	0.80965345	2069	1880	-1.1981882	3197563	0.85553474	4279757	2.46382831	experimental	Sigma-Aldrich E 0137	Vanillic acid diethylamide; Ethivan
3261 K21	X	2454	2480	1.30315385	1850	2080	1.72843661	2999103	0.52531227	3532649	1.31235845	experimental	Sigma-Aldrich C0494	Cambinol; NSC-1125476; Tetrahydro-5-[(2-hydroxy-1-n
3261 K22	X	2969	3000	2.01307762	2373	2400	2.56510997	2109745	-0.66613419	2177750	-0.77586086	experimental	Sigma-Aldrich E 2375	Emetine dihydrochloride hydrate
3261 K23	E	4040	4150	35054494	3250	3280	1.65053405	94111	-4.3010473	90904	-3.79919644	empty		
3261 K24	P	446523	449440	613.449054	445337	448560	1183.40433	2799913	0.28026978	2974194	0.65164742	empty		
3261 L01	N	1824	1840	0.43470342	1390	1400	-0.05415728	4018472	1.95123841	1280655	-0.77138357	empty		
3261 L02	E	1698	1720	0.26101333	1184	1200	-0.60305764	86233	-3.44090756	88491	-3.99590236	empty		
3261 L03	X	3216	3240	2.35356533	2586	2600	3.13266229	99635	-3.42252986	2872569	0.2950193	experimental	Sigma-Aldrich E 3380	Ellipticine; 5,11-Dimethyl-6H-pyrrolo[4,3-b]carbazole
3261 L04	X	2655	2680	1.58023009	1702	1720	0.77718695	3745944	1.577553	2327666	-0.54480409	experimental	Sigma-Aldrich 34829	JFD00244; 1,4-Bis[(p-hydroxyphenethyl)amino]-anthrac
3261 L05	X	1693	1720	0.25412087	1344	1360	-0.17672726	93129	-3.43145131	3250917	0.87814291	experimental	Sigma-Aldrich E 7138	Ethosuximide; 2-Ethyl-2-methylsuccinimide
3261 L06	X	1896	1920	0.53895499	1261	1280	-0.39788615	3446332	1.16668223	3126780	0.79996579	experimental	Sigma-Aldrich H 0627	6-Hydroxydopamine; 3-(N-Acetylaminoethyl)-6-hydroxy
3261 L07	X	2766	2780	0.25639588	2264	2280	-0.27487591	5197676	0.36614089	3232229	0.84934029	experimental	Sigma-Aldrich E-006	N-Methyl-beta-carboline-3-carboxamide; FC7; F142
3261 L08	X	1935	1960	0.58771611	1221	1240	-0.50446874	94616	-3.42941224	3370587	1.06258264	experimental	Sigma-Aldrich H 2138	Hexamethonium iodide; N,N,N,N,N'-Hexamethyl-
3261 L09	X	2217	2240	0.97645107	1224	1240	-0.49647505	5007559	3.30753986	2867256	0.28683071	experimental	Sigma-Aldrich F 0881	Fusaric acid sodium; Fusidin
3261 L10	X	1777	1800	0.36991426	1545	1560	0.35885027	87361	-3.43936708	3066459	0.59384957	experimental	Sigma-Aldrich H 4759	Hydrochlorothiazide; 6-Chloro-3,4-dihydro-2H-1,2,4-ber
3261 L11	X	1899	1920	0.53809037	1384	1400	-0.07014467	2738520	0.19608364	3139062	0.70574794	experimental	Sigma-Aldrich F 4381	Furosemide
3261 L12	X	1776	1800	0.36853576	1345	1360	-0.1740627	3402096	1.1060229	2467755	-0.32889467	experimental	Sigma-Aldrich J 4137	3S-K; O2-(2,4-Dinitrophenyl)-1-[(4-ethoxycarbonyl)pipe
3261 L13	X	2335	2360	1.13911322	1704	1720	0.78251608	3453052	1.17589714	2848830	0.25843189	experimental	Sigma-Aldrich F 6627	5-Fluorouracil; 5-FU
3261 L14	X	2016	2040	0.69937403	1384	1360	-0.17672726	398055	-0.10331663	2675003	-0.00947656	experimental	Sigma-Aldrich H 8653	(-)-7-Hydroxy-DPAT hydrobromide; (S)-7-OH-DPAT HB
3261 L15	X	2137	2160	0.86617165	1546	1560	0.36151484	2525797	-0.09561619	3031435	0.53986932	experimental	Sigma-Aldrich F 8791	5-Fluoro-5'-deoxyuridine; 5'FdUrd
3261 L16	X	2057	2080	0.75589223	1345	1360	-0.1740627	3842326	1.70969537	3293487	0.94375333	experimental	Sigma-Aldrich L 2167	L-165,041; 4-{3-[4-Acetyl-3-hydroxy-2-propylphenoxy]}-
3261 L17	X	1897	1920	0.53533339	1505	1520	0.25226768	1880997	-0.97980856	3469821	1.21552657	experimental	Sigma-Aldrich F-124	Furafylline; 3-(2-Furanyl-methyl)-3,7-dihydro-1,8-dimet
3261 L18	X	1896	1920	0.5339549	1464	1480	0.14302052	3217370	0.8527144	2872049	0.29421785	experimental	Sigma-Aldrich H-128	Histamine, R(-)-alpha-methyl-, dihydrochloride; R(-)-al-
3261 L19	X	2294	2320	1.08259501	1540	1560	0.34552745	2535169	-0.08276469	3089205	0.62890639	experimental	Sigma-Aldrich G 2536	Ganciclovir
3261 L20	X	2332	2360	1.13497774	1500	1520	0.23894485	3126465	0.72805946	2934932	0.39113541	experimental	Sigma-Aldrich C 3118	CPWG; 5-(4-(4-Chlorobenzyloxy)-1-piperazinyl)-8-nitroqui
3261 L21	X	2652	2680	1.57609542	1384	1720	0.76386413	2209798	-0.5289349	3274870	0.91506014	experimental	Sigma-Aldrich G 7748	alpha-Guanidinoglutaric acid; GGA
3261 L22	X	2322	2360	1.12119281	2091	2120	1.81370268	2696155	0.13798995	2336680	-0.53183694	experimental	Sigma-Aldrich G 0719	GR 55562 dihydrochloride; 3-(3-(Dimethylamino)propyl
3261 L23	E	3020	4480	2.08338075	2723	4080	3.49770767	94865	-3.42907079	90385	-3.99298326	empty		
3261 L24	P	490820	493480	674.512147	463558	459120	1212.23759	2491479	-0.1426753	3034867	0.54515884	empty		
3261 M01	N	2143	2160	0.87444261	1229	1240	-0.48315222	3052441	0.62655286	2488363	-0.29713288	empty		
3261 M02	E	1737	1760	0.31477455	946	960	-1.23722408	88436	-3.43788666	97432	-3.98212217	empty		
3261 M03	X	2173	2200	0.91579739										

3261 N01	N	2340	2360	1.14600568	1470	1480	0.15900791	86553	-3.44046876	1990275	-1.06480411	empty		
3261 N02	E	1937	1960	0.5904731	1105	1120	-0.81355827	84144	-3.44377214	137667	-3.92011053	empty		
3261 N03	X	2216	2240	0.97507258	1745	1760	0.89176324	3780607	1.6250622	3207488	0.81120857	experimental	Sigma-Aldrich R0158	RepSox
3261 N04	X	2084	2080	0.75175675	1301	1320	-0.29130355	87312	-3.4394787	2449909	-0.35639567	experimental	Sigma-Aldrich G-117	Glipizide
3261 N05	X	2092	2120	0.80413948	1943	1960	0.41934709	4163800	2.15052176	2612705	-0.10529249	experimental	Sigma-Aldrich J4774	JK401; 1-[2-Methoxy-4-(methylthio)benzoyl]-4-benzylpi
3261 N06	X	2094	2120	0.80689646	1741	1760	0.88110498	84972	-3.44263673	2652514	-0.04413742	experimental	Sigma-Aldrich H 0879	Hexamethonium bromide; Hexane-1,6-bis(trimethylamn
3261 N07	X	2094	2120	0.80689646	1342	1360	-0.18205639	4716661	2.9086413	3256944	1.04155556	experimental	Sigma-Aldrich D7443	DPO-1; Diphenyl phosphine oxide-1
3261 N08	X	2291	2320	1.07845953	1459	1480	0.12969769	88361	-3.43798951	2332453	-0.53742701	experimental	Sigma-Aldrich B 5437	Bendamustine hydrochloride; Treadna, 1H-Benzimidaz
3261 N09	X	2522	2560	1.41067629	1622	1640	0.56402177	2312333	-0.38833214	3152967	0.72717883	experimental	Sigma-Aldrich F 1016	Fenoterol hydrobromide; 2-(3,5-Dihydroxyphenyl)-2-hy
3261 N10	X	2132	2160	0.85927919	1301	1320	-0.29130355	2676407	0.11091019	2260191	-0.73229196	experimental	Sigma-Aldrich S 8817	SB 218795; (-)-(R)-N-(alpha-methoxycarbonylbenzyl)-2
3261 N11	X	2334	2360	1.13773472	1543	1560	0.35352114	2426239	-0.2321367	3155005	0.73031987	experimental	Sigma-Aldrich F 4646	p-Fluoro-L-phenylalanine; 4-Fluoro-L-phenylalanine
3261 N12	X	2093	2120	0.80591794	1580	1600	0.45211004	1295222	-1.78306195	173257	-1.46071377	experimental	Sigma-Aldrich H 7779	Retinoic acid p-hydroxyamide; N-(4-Hydroxyphenyl)eth
3261 N13	X	2373	2400	1.19149594	3022	3040	0.429441257	2324697	-0.3713778	3217572	0.826575039	experimental	Sigma-Aldrich E 7906	Esomeprazole magnesium dihydrate; (S)-Omeprazole m
3261 N14	X	1894	1920	0.53119791	1778	1800	0.44678091	3506657	1.24940386	2278543	-0.62051505	experimental	Sigma-Aldrich H 8759	MHPG sulfate potassium; 4-Hydroxy-3-methoxyphenylgl
3261 N15	X	2175	2200	0.91855437	1903	1920	1.31276449	1820986	-1.06209961	3382012	1.08019126	experimental	Sigma-Aldrich F 8927	Flupirtine maleate; 2-amino-6-[[[4-fluorophenyl]methyl
3261 N16	X	2452	2480	1.30039687	1501	1520	0.24160942	2700783	0.14433617	2608311	-0.11226469	experimental	Sigma-Aldrich H 9772	5-Hydroxy-L-tryptophan; S(+)-1-alpha-Amino-5-hydrox
3261 N17	X	2652	2680	1.57609542	1904	1920	1.31542906	2528582	-0.09179722	3516192	1.28699343	experimental	Sigma-Aldrich F-131	FPL 64176; 2,5-Dimethyl-4-[2-(phenylmethyl)benzoyl]-
3261 N18	X	2453	2480	1.30177536	1617	1640	0.55069894	3013502	0.57315713	2197180	-0.74591465	experimental	Sigma-Aldrich H-135	5-Hydroxydecanoic acid sodium
3261 N19	X	2292	2320	1.07983803	2061	2080	1.73376574	2120336	-0.05161111	3333455	1.00535346	experimental	Sigma-Aldrich G 3126	L-Glutamine; S(+)-L-Glutamic acid 5-amide
3261 N20	X	2291	2320	1.07845953	1458	1480	0.12703313	1291872	-1.78765569	906281	-2.73549485	experimental	Sigma-Aldrich N 1786	NSC 95397; 2,3-bis[(2-Hydroxyethyl)thio]-1,4-naphtho
3261 N21	X	2528	2560	1.40516232	1777	1800	0.97702932	2114726	-0.65930391	3174937	0.76103979	experimental	Sigma-Aldrich G 8134	Gallamine triethiodide
3261 N22	X	3039	3080	2.10957212	2130	2160	1.91762071	3107387	0.70189485	2184854	-0.76491192	experimental	Sigma-Aldrich I 2279	IMID-4F hydrochloride; 2-[N-(2,6-dichlorophenyl)-N-(4
3261 N23	E	3949	3949	3.36400052	2873	4520	3.8973924	86682	-3.44029186	84287	-4.00238171	empty		
3261 N24	P	540337	543640	742.770973	554684	558080	1474.23359	2231472	-0.49921408	3161454	0.74025929	empty		
3261 O01	N	2621	2640	1.53336214	1148	1160	-0.69898198	2791468	0.26688944	2111935	-0.87729732	empty		
3261 O02	E	1640	1640	1.43219194	1105	1160	0.1809337	87236	-3.4395218	87236	-3.4395218	empty		
3261 O03	X	2014	2040	0.69661704	1543	1560	0.35352114	2549272	0.6232572	2287441	-0.60680113	experimental	Sigma-Aldrich C-102	8-Cyclopentyl-1,3-dimethylxanthine; CPT; 8-Cyclopentyl
3261 O04	X	2374	2400	1.19287443	1343	1360	-0.17939183	2683972	0.11228382	2299368	-0.58841881	experimental	Sigma-Aldrich D 7505	2,2'-Bipyridyl; alpha, alpha'-Bipyridyl
3261 O05	X	2453	2480	1.30177536	1420	1440	0.02577967	2798867	0.27883544	1587680	-1.68529808	experimental	Sigma-Aldrich C-130	(*)-Chloro-APB hydrobromide; (*)-SKF-82958 hydrobrn
3261 O06	X	2413	2440	1.24663565	1382	1400	-0.0754738	3089794	0.67777376	2613150	-0.10480664	experimental	Sigma-Aldrich D 8040	(*)-trans-U-50488 methanesulfonate; trans-(*)-3,4-Di
3261 O07	X	2370	2400	1.18736046	1460	1480	0.13236226	3184787	0.80803444	3023539	0.52769972	experimental	Sigma-Aldrich C-197	8-(3-Chlorostyryl)caffeine; CSC
3261 O08	X	3452	3480	2.67888962	2582	2600	3.12200403	4237616	2.25174314	4253697	2.4236637	experimental	Sigma-Aldrich S 5567	SP600125; Anthrapyrazolone; 9-Pyrazoloanthrone
3261 O09	X	2490	2520	1.35277959	1738	1760	0.87311129	2822027	0.31059396	2996582	0.48656875	experimental	Sigma-Aldrich C-271	CK 546; 1-(1,4-Benzodioxan-6-ylcarbamoyl)piperidine
3261 O10	X	2490	2520	1.35277959	1738	1760	0.87311129	2822027	0.31059396	2996582	0.48656875	experimental	Sigma-Aldrich C-271	CK 546; 1-(1,4-Benzodioxan-6-ylcarbamoyl)piperidine
3261 O11	X	2413	2440	1.24663565	1422	1440	0.03110879	2729836	0.18417557	2725089	0.06771179	experimental	Sigma-Aldrich D 1262	PI, P4-D(adenosine-5')tetraphosphate triammonium; Ac
3261 O12	X	2252	2280	1.02469832	1182	1200	-0.60838677	864309	-2.37395833	798187	-2.90209323	experimental	Sigma-Aldrich A9605	Ac-93253 iodide; 2-[3-{1,3-Dihydro-1,3,3-trimethyl-2H-
3261 O13	X	2753	2760	1.68775333	1459	1480	0.12969769	2733811	0.18962635	2062010	-0.95424354	experimental	Sigma-Aldrich S4572	SANT-1; (4-Benzyl)piperazin-1-yl]-3-(5-dimethyl-1-pher
3261 O14	X	2252	2280	1.02469832	1341	1360	-0.18472096	2673035	0.10628628	1837950	-1.29957291	experimental	Sigma-Aldrich D-103	(*)-2,3-Dichloro-alpha-methylbenzylamine hydrochlorid
3261 O15	X	2172	2200	0.9144189	1540	1560	0.34552745	2509159	-0.11843132	1579333	-1.69816278	experimental	Sigma-Aldrich D 3648	N,N,N'-Tetramethylazodicarboxamide; Azodicarbonyloxyl
3261 O16	X	2753	2760	1.68775333	1583	1600	0.46010374	2638329	0.05869512	1321261	-2.09591267	experimental	Sigma-Aldrich D-131	3,5-Dinitrocatatechol; OR-486
3261 O17	X	2212	2240	1.02313982	1624	1640	0.32231952	2082121	0.40032012	14407001	-2.25175375	experimental	Sigma-Aldrich C 2444	Idronomic acid; ClzMDI; Clodronic acid disodium magne
3261 O18	X	2212	2240	0.96955861	2624	2640	3.23391574	2338626	0.88186216	3791068	1.7064314	experimental	Sigma-Aldrich A 3846	AG-8810; (5Z, 13E)-(9S, 15S, 15R)-9,15-Dihydroxy-11-fl
3261 O19	X	2132	2160	0.85927919	1295	1320	-0.30729094	955741	-2.24858073	1013878	-2.56966246	experimental	Sigma-Aldrich D 5439	2,3-Dimethoxy-1,4-naphthoquinone; DMNQ
3261 O20	X	2252	2280	1.02469832	1182	1200	-0.60838677	864309	-2.37395833	798187	-2.90209323	experimental	Sigma-Aldrich E 0516	Etodolac; 1,8-Diethyl-1,3,4,9-tetrahydropyran[3,4-b]in
3261 O21	X	2928	2960	1.95655942	2217	2240	2.14943786	2951701	0.48841152	3114259	0.66752066	experimental	Sigma-Aldrich D 5891	1,1-Dimethyl-4-phenyl-piperazinone iodide; DMPPP
3261 O22	X	3117	3160	2.21709455	2207	2240	2.12279221	2709455	0.15622799	2533714	-0.22723628	experimental	Sigma-Aldrich E 3132	E-64; L-trans-3-Carboxyoxiran-2-carbonyl-L-leucylgama
3261 O23	E	3334	3320	2.51627248	2752	4720	3.57498006	88777	-3.43741906	87346	-4.00321552	empty		
3261 O24	E	666361	670480	916.494144	662641	666720	1761.89202	2630859	0.05942189	2630859	-0.05155848	empty		
3261 P01	N	2626	2640	1.5025461	1254	1520	2.7624876	1418847	-1.51353918	1964063	1.05202099	empty		
3261 P02	E	2260	2280	1.03572626	1028	1040	-0.101872976	84845	-3.44281088	75261	-0.41629291	empty		
3261 P03	X	2781	2800	1.75392098	1620	1640	0.58000916	2025618	-0.78149469	2576718	-0.16095696	experimental	Sigma-Aldrich G 9797	GW9508; 4-(3-Phenoxybenzylamino)phenylpropionic aci
3261 P04	X	2218	2240	0.97782956	1425	1440	0.03910249	1804787	-1.08431275	2510476	-0.26305152	experimental	Sigma-Aldrich G-119	GYKI 52466 hydrochloride; 1-(4-Aminophenyl)-4-methy
3261 P05	X	2027	2040	1.14462719	2027	2040	1.64317053	2351542	-0.33456617	2649914	-0.04814464	experimental	Sigma-Aldrich E 7881	Emodin
3261 P06	X	2460	2480	1.31142481	1545	1560	0.35885027	2079678	-0.70736405	2582983	-0.15130112	experimental	Sigma-Aldrich H 1252	4-Hydroxy-3-methoxyphenylacetic acid; Homovanillic ac
3261 P07	X	2219	2240	0.97928086	1627	1640	0.57734459	2139815	-0.62490022	2495205	-0.28658774	experimental	Sigma-Aldrich H 1050	(-)-Eseroline fumarate
3261 P08	X	2338	2360	1.14324869	1464	1480	0.14302052	1837925	-1.03887174	2516478	-0.25380103	experimental	Sigma-Aldrich H 2380	5-Hydroxy-DL-DOPA; 2,5-Dihydroxy-DL-tyrosine
3261 P09	X	1979	2000	0.64836979	1385	1400	-0.06748011	1355912	-1.69983981	1717497	-1.48521942	experimental	Sigma-Aldrich F 1553	S-(+)-Fluoxetine hydrochloride
3261 P10	X	2381	2400	1.20252388	2026	2040	1.64050597	1901423	-0.95179908	2306241	-0.57782598	experimental	Sigma-Aldrich H 5257	HSPD-1; 6-(3,4-dihydroxyethyl)-4-hydroxy-2-pyrone
3261 P11	X	2259	2280	1.03434777	1465	1480	0.14568508	1344562	-1.71540368	1587686	-1.68528883	experimental	Sigma-Aldrich F 4765	Fluphenazine dihydrochloride
3261 P12	X	2342	2360	1.14600568	1547	1560	0.3641794	901951	-2.32234114	1052883	-2.50954655	experimental	Sigma-Aldrich P20013	Nelfinavir mesylate hydrate; AG-1343; Nelfinavir metha
3261 P13	X	2377	2400	1.19700991	1666	1680	0.68126262	1994186	-0.82459633	2413945	-0.41182859	experimental	Sigma-Aldrich F 6800	Fenoldopam bromide; SKF-82526
3261 P14	X	2860	2880	1.86282191	1746	1760	0.89442781	2068447	-0.72276474	2340807	-0.52455152	experimental	Sigma-Aldrich H 8876	5-Hydroxyindoleacetic acid; 5-HIAA
3261 P15	X	2378	2400	1.13983884	1656	1880	1.21417559	2107382	-0.66937449	2681641	0.00075916	experimental	Sigma-Aldrich F 9397	Flutamide; 2-Methyl-N-(4-nitro-3-(trifluoromethyl)phenyl
3261 P16	X	2338	2360	1.14324869	1625	1640	0.57201546	2161342	-0.59538097	2474068	-0.31916485	experimental	Sigma-Aldrich H 9876	Hydroxyflavone hydrochloride
3261 P17	X	2459	2480	1.31004632	1548	1560	0.36684397	1552094	-1.43082209	1830957	-1.31035077	experimental	Sigma-Aldrich F-132	Fluoxetine hydrochloride; Prozac; LY-1100, 140 hydrochl
3261 P18	X	2658	2680	1.58436638	1382	1400	-0.0754738	1920746	-0.92530211	2431616	-0.38459341	experimental	Sigma-Aldrich H-140	R-(+)-8-Hydroxy-DPAT hydrobromide; (+)-8-Hydroxy-2
3261 P19	X	2898	2920	1.91520464	1946	1960	1.42734078	2356615	-0.32760973	2549185	-0.20339181	experimental	Sigma-Aldrich G 3416	Guandinyl-naltrindole dihydrochloride; GNTI di-triflu
3261 P20	X	2656	2680	1.58160939	1943	1960	1.14934709	2161444	-0.59					

3262 A19	X	2032	2040	3.80623254	2274	2280	4.55095841	3574129	0.81259029	3889445	0.96971277	W	experimental	Sigma-Aldrich L 5025	Leflunomide; 5-Methylisoxazole-4-(4-(trifluoromethyl)car
3262 A20	X	1029	1040	0.70508249	708	720	-0.33069425	3353553	0.47147564	3745925	0.75532849		experimental	Sigma-Aldrich P20139	SC-58125 ; 5-(4-Fluorophenyl)-1-[4-(methylsulfonyl)]p
3262 A21	X	1032	1040	0.71435811	1192	1200	1.17806685	2432954	-0.95220513	3239248	-0.00152482		experimental	Sigma-Aldrich P20100	CP-154526 hydrochloride; N-Butyl-N-ethyl-2,5-dimeth
3262 A22	X	908	920	0.33096568	1065	1080	0.78217293	2613966	-0.67227511	3374859	0.20104533		experimental	Sigma-Aldrich M 6690	MDL 28170; Z-val-Phe-CHO
3262 A23	E	1202	1040	-2.39976796	2265	3280	4.52902923	604660	-4.2395	72250	-2.56792545		empty		
3262 A24	P	286259	286920	882.600426	346443	347240	1077.42038	1122687	-1.43202442	2683661	-0.83143788		empty		
3262 B01	N	515	520	-0.88414097	595	600	-0.68294632	2526432	-0.807644	2966587	-0.40881463		empty		
3262 B02	E	155	160	-1.99721577	196	200	-1.92673905	63595	-4.61635297	70746	-4.73450307		empty		
3262 B03	X	712	720	-0.27504171	394	400	-1.3095186	2623442	-0.65762073	3099711	-0.209995946		experimental	Sigma-Aldrich M 8046	Mifepristone; RU-486
3262 B04	X	711	720	-0.27813358	633	640	-0.56448987	2649729	-0.61696861	3333604	0.1394203		experimental	Sigma-Aldrich N-144	Nitrendipine; 1,4-Dihydro-2,6-dimethyl-4-(3-nitrophen
3262 B05	X	630	640	-0.52857541	712	720	-0.31822515	2728826	-0.4946473	3282775	0.06349403		experimental	Sigma-Aldrich M 9511	Minoxidil hydrochloride
3262 B06	X	831	840	0.09289135	632	640	-0.56760715	2812461	-0.3653081	356458	0.52958118		experimental	Sigma-Aldrich P20135	PhA-543613 ; N-(3R)-1-Azabicyclo[2.2.2]oct-3-yl)furo
3262 B07	X	832	840	0.09598322	471	480	-1.06948842	3117152	0.10588806	3616858	0.5625335		experimental	Sigma-Aldrich M-108	(-)-MK-801 hydrogen maleate; (5S,10R)-(4)-5-Methyl-
3262 B08	X	550	560	-0.77592537	829	840	0.04649603	2839885	-0.32289765	3380179	0.20899212		experimental	Sigma-Aldrich O 0886	Olumocine; 2-[[9-Methyl-6-[[phenylmethyl]amino]-9H
3262 B09	X	672	680	-0.39871669	869	880	0.17118703	2448492	-0.92817604	2724802	-0.76998314		experimental	Sigma-Aldrich M-149	Methiothepin mesylate; 1-[10,11-Dihydro-8-(methylthi
3262 B10	X	672	600	-0.64915852	631	640	-0.57072442	3634734	0.90631424	3379003	0.20723546		experimental	Sigma-Aldrich O 3752	Orphenadrine hydrochloride; beta-Dimethylaminoethyl 2
3262 B11	X	1152	1160	1.08538304	1074	1080	0.8102284	3936795	1.37344318	4007523	1.14609284		experimental	Sigma-Aldrich M-216	MDL 105,519; (Z)-2-Carboxy-4,6-dichloroindole-3-(2'-pi
3262 B12	X	629	640	-0.53166729	592	600	-0.69229815	2041749	-1.55719279	2280334	-1.43391122		experimental	Sigma-Aldrich O-111	(4)-Octoclotheptin maleate; 1-(8-Chloro-10,11-dihydro
3262 B13	X	913	920	0.34642505	632	640	-0.56760715	3968018	1.42172868	3762392	0.77992622		experimental	Sigma-Aldrich N 1771	nor-Binaltorphimine dihydrochloride; nor-BNI dihydroc
3262 B14	X	590	600	-0.65225039	994	1000	0.5680464	2933953	-0.1774241	3664408	0.63356174		experimental	Sigma-Aldrich P 0878	O-Phospho-L-serine; L-Phosphoserine
3262 B15	X	1110	1120	0.95552431	548	560	-0.82945825	1686821	-2.10660797	2346863	-1.33453291		experimental	Sigma-Aldrich .	PD-407824
3262 B16	X	669	680	-0.40799231	1191	1200	1.17494958	3582724	0.78807098	3585811	0.47537715		experimental	Sigma-Aldrich P 1918	Pancuronium bromide; 1,1'-(2beta,3alpha,5alpha,16beta'
3262 B17	X	869	880	-0.21038258	587	600	-0.70788452	3491503	0.68481148	3351587	0.16628257		experimental	Sigma-Aldrich E 2515	Eprosartan mesylate
3262 B18	X	588	600	-0.65843414	787	800	-0.08442952	3147469	0.15277246	3289600	0.07288223		experimental	Sigma-Aldrich P 3520	Pentolinum di(L(+)-tartrate); 1,1'-Pentamethylenebis(1
3262 B19	X	627	640	-0.53785104	707	720	-0.33381152	2520636	-0.81660735	3285527	-1.27677821		experimental	Sigma-Aldrich N 7510	Nicardipine hydrochloride; YC-93 hydrochloride
3262 B20	X	859	870	-0.21688755	835	840	-0.33381152	3257016	0.80159024	3874958	0.55552568		experimental	Sigma-Aldrich M 5433	Sulpiric acid sodium; 2-Propylpentanoic acid sodium
3262 B21	X	871	880	0.21655215	831	840	0.05273058	2676701	0.64597647	3828994	0.87810056		experimental	Sigma-Aldrich N 8652	NF 023; 8,8'-[carboxylate]-3,1-phenylene carbonyl
3262 B22	X	988	1000	0.57831563	825	840	0.03402693	2755096	-0.45402148	3575195	0.50029902		experimental	Sigma-Aldrich P 5514	Pyrimilamine maleate; Mepyramine maleate
3262 B23	E	1011	1680	0.64942875	1554	2360	2.3065204	65997	-4.61263834	73322	-4.73065514		empty		
3262 B24	P	224911	226400	692.920114	270126	271840	839.519302	2278774	-1.19064021	2899011	-0.50975689		empty		
3262 C01	N	756	760	-0.13899923	876	880	0.19300795	3051848	0.00489724	3309869	0.10396593		empty		
3262 C02	E	193	200	-1.87972454	154	160	-2.0576646	62281	-4.61838503	78776	-4.72250818		empty		
3262 C03	X	1152	1160	1.08538304	755	760	-0.18418232	3314939	0.41176016	3296269	0.08365081		experimental	Sigma-Aldrich I 2765	(4)-Ibotenic acid; (4)-alpha-Amino-3-hydroxy-5-isoxaz
3262 C04	X	959	960	-0.46082442	712	720	-0.69853232	3434342	0.3234548	3874958	0.74837959		experimental	Sigma-Aldrich L 1498	4-(3-Phenylpropyl)-1-piperazine dihydrochloride
3262 C05	X	751	760	-0.15445861	912	920	0.30522985	2898855	-0.23170218	3323680	0.12459624		experimental	Sigma-Aldrich I 6138	Idoxazon hydrochloride; RX 781094
3262 C06	X	912	920	0.34333318	791	800	-0.07196042	3814755	1.18471171	4384477	1.70917126		experimental	Sigma-Aldrich L-134	Linopirdine; DuP 996
3262 C07	X	547	560	-0.78520099	670	680	-0.4491507	3070222	0.03331212	3497705	0.38454764		experimental	Sigma-Aldrich I 8005	S(+)-Isoproterenol (+)-bitartrate
3262 C08	X	1392	1400	1.8274329	1352	1360	1.67683085	3633530	0.90445529	3763018	0.78086613		experimental	Sigma-Aldrich M 1404	Nocodazole; R 17934
3262 C09	X	910	920	0.33714943	709	720	-0.32757697	3685953	0.985523	3361455	0.18102298		experimental	Sigma-Aldrich I-106	S(+)-Ibuprofen; S-(+)-2-(4-Isobutylphenyl)propionic ac
3262 C10	X	792	800	-0.02769175	713	720	-0.31510787	3707343	1.01860204	3820711	0.86704074		experimental	Sigma-Aldrich M 2398	Metaprotrenolol hemisulfate
3262 C11	X	1547	1560	-0.64915852	735	740	-0.32913548	3258084	0.3234548	3874958	0.74837959		experimental	Sigma-Aldrich L 138	1,5-Isosquinolinediol; 1,5-Dihydroxyisoguinoline
3262 C12	X	392	400	-1.26444153	312	400	-1.30648202	2444551	-0.61817022	2414451	-1.23357273		experimental	Sigma-Aldrich B7936	BMBP; 5-(Benzyloxyethyl)-4-bromo-2-methyl-3-(2H)-pyrid
3262 C13	X	632	640	-0.52239166	473	480	-1.06325387	3566466	0.80073968	3381362	0.21075924		experimental	Sigma-Aldrich K 0250	Kainic acid; 2-Carboxy-3-carboxymethyl-4-isopropenylp
3262 C14	X	714	720	-0.27813358	632	640	-0.56760715	3468470	0.64919159	3541603	0.45012067		experimental	Sigma-Aldrich U-106	(-)-cis-(1S,2R)-U-50488 tartrate; (-)-(1S,2R)-cis-3,4-Di
3262 C15	X	909	900	1.000.58449938	1072	1080	-1.06637115	2491955	-0.80696172	2133082	-1.65387019		experimental	Sigma-Aldrich U 6881	U-73343; 1-[6-((17)-3-Methoxyestra-1,3,5[10]-trien
3262 C16	X	990	1020	0.33405755	431	1040	0.67618558	4256843	1.86838852	3261084	0.0310929		experimental	Sigma-Aldrich M 4659	Milrinone; 1,6-Dihydro-2-methyl-6-oxo-[3,4'-bipyridin
3262 C17	X	1468	1480	2.06241536	1066	1080	0.7852902	3298433	0.38623409	3051697	0.186218081		experimental	Sigma-Aldrich L 2536	2,5-Dihydroxy-1-methylpyrrolidine hydrochloride
3262 C18	X	1569	2.30667364	2347	2360	4.77851948	106332782	3166546	1.60332782	31067381	0.78137958		experimental	Sigma-Aldrich P 20135	Methyl-2-(phenylethynyl)pyridine hydrochloride; MPF
3262 C19	X	1068	1080	0.82566559	846	800	-0.0875468	3446339	0.57917647	3092329	-0.20007875		experimental	Sigma-Aldrich V 11829	VER-332-L-arginine; (S)-1-(6-Bromo-2,3-dihy
3262 C20	X	911	920	0.3402413	952	960	0.42992085	3501296	0.69995680	3626204	0.57649417		experimental	Sigma-Aldrich M 6383	DNC 2-methoxyestradiol; 2-Hydroxyestradiol-2-methyl et
3262 C21	X	391	400	-1.2675334	390	400	-1.3219877	928695	-3.27849896	1093634	-3.20655495		experimental	Sigma-Aldrich N 0287	Sigma-Aldrich N 0287
3262 C22	X	668	680	-0.41108418	827	840	0.04026148	3260589	0.3277094	3600817	0.53857211		experimental	Sigma-Aldrich M 6760	Myricetin; Cannabiscetin
3262 C23	E	936	1600	0.41753816	1682	2400	2.7055316	66033	-4.61258267	74329	-4.72915093		empty		
3262 C24	P	224501	225800	691.652445	240721	242240	747.855831	2532297	-0.79857394	2968252	-0.40632752		empty		
3262 D01	N	635	640	-0.51311604	595	600	-0.68294632	2848398	-0.30973253	2952462	-0.42991398		empty		
3262 D02	E	195	200	-1.87354079	156	160	-2.05143005	64467	-4.61500444	74580	-4.72877599		empty		
3262 D03	X	873	880	0.22275007	554	560	-0.8107546	3547011	0.77065306	3609642	0.55175454		experimental	Sigma-Aldrich M 8131	L-alpha-Methyl-p-tyrosine; (S)-alpha-Methyltyrosine
3262 D04	X	706	720	-0.29359296	931	1000	0.55149458	2983566	-0.10069897	3192716	-0.07103241		experimental	Sigma-Aldrich N-149	Nitrodipine; 1,4-Dihydro-2,6-dimethyl-4-(3-nitrophenyl)
3262 D05	X	711	720	-0.27813358	633	640	-0.57072442	2980282	-0.10577759	2766367	-0.70789505		experimental	Sigma-Aldrich M 9651	Maprotiline hydrochloride; 9-(gamma-Methylaminoprop
3262 D06	X	750	760	-0.15755048	752	760	-0.19353415	3159783	0.17181572	3515738	0.41148459		experimental	Sigma-Aldrich N-170	NS-1619; 1,3-Dihydro-1-[2-hydroxy-5-(trifluoromethyl)
3262 D07	X	1273	1280	1.45949985	752	760	-0.19353415	3419475	0.57342218	3802593	0.83997682		experimental	Sigma-Aldrich M-109	2-Methyl-5-hydroxytryptamine maleate; 2-Methylseroto
3262 D08	X	628	640	-0.53475916	549	560	-0.82634097	3256681	0.32166578	3712848	0.70591942		experimental	Sigma-Aldrich O 1008	Oleic acid; Elaicic acid
3262 D09	X	711	720	-0.27813358	633	640	-0.57072442	2980282	-0.10577759	2766367	-0.70789505		experimental	Sigma-Aldrich N4163	Nemadipine-A; 1,4-Dihydro-2,6-dimethyl-4-(pentafluorc
3262 D10	X	792	800	-0.02769175	713	720	-0.31510787	3707343	1.01860204	3820711	0.86704074		experimental	Sigma-Aldrich T 5575	TC003; (Z)-1-(3-Ethyl-5-methoxy-2,3-dihydrobenzothia
3262 D11	X	672	680	-0.39871669	869	880	0.17118703	2448492	-0.92817604	2724802	-0.76998314		experimental	Sigma-Aldrich S 7198	Sivilestat sodium salt hydrate ; EI 546, Etaspol, LY 544
3262 D12	X	714	720	-0.26885796	614	320	-1.56201787	3571846	0.8090597	3421503	0.27072022		experimental	Sigma-Aldrich P 0130	Progesterone; 4-Pregnone-3,20-dione
3262 D13	X	593	600	-0.64297477	873	880	0.1867734	3792141	1.14973979	3989084	1.11854942		experimental	Sigma-Aldrich N2001	Neostigmine bromide
3262 D14															

3262 E13	X	472	480	-1.01709157	670	680	-0.4491507	2326204	-1.11729103	2818640	-0.62981179	experimental	Sigma-Aldrich K 1003	Ketoconazole; cis-1-Acetyl-4-[[4-(2-(2-(4-Chlorophenyl)hydrochloride; N-Methyl-N-propargyl-3-(2,4-t
3262 E14	X	914	920	0.34951693	1353	1360	1.67994813	3170128	0.18781398	3566548	0.48738249	experimental	Sigma-Aldrich M 3778	Clorgyline hydrochloride; N-Methyl-N-propargyl-3-(2,4-t
3262 E15	X	512	520	-0.8934166	710	720	-0.3244597	3179711	0.20263382	3670681	0.64293209	experimental	Sigma-Aldrich L 0258	alpha-Methyl-4-carboxyphenylglycine; (S)-MCPG
3262 E16	X	840	850	0.0990751	832	840	0.05584785	3306926	0.39356828	3591820	0.52513276	experimental	Sigma-Aldrich M 4796	Osivamils; N-Vanillyloxyethylamine
3262 E17	X	750	760	-0.15755048	832	840	0.05584785	3306926	0.39356828	3591820	0.52513276	experimental	Sigma-Aldrich O 0287	Mibefradil dihydrochloride; Ro 40-5967; (1S,2S)-2-[2-[3
3262 E18	X	629	640	-0.53166729	908	920	-0.95414925	1846901	-1.8585198	1792475	-2.16265495	experimental	Sigma-Aldrich M 5441	LiDocaine hydrochloride
3262 E19	X	911	920	0.3402413	511	520	0.30211258	3581480	0.82395841	3715097	0.70927889	experimental	Sigma-Aldrich L 5647	Cysteamine hydrochloride; Mercaptamine; MEA hydroch
3262 E20	X	868	880	0.2072907	1028	1040	0.66683375	3378495	1.06677774	4076382	1.24895159	experimental	Sigma-Aldrich M 6500	Ro 90-7501; 2'-(4-Aminophenyl)-[2,5'-bi-1H-benzimidaz
3262 E21	X	1548	1560	2.30976531	1058	1070	2.16312575	3387574	0.52408817	3360853	0.18012374	experimental	Sigma-Aldrich R 0529	NG-Monomethyl-L-arginine acetate; L-NMMA
3262 E22	X	1106	1120	0.94315682	1182	1200	1.1468941	3670729	0.96197951	3931138	1.03199207	experimental	Sigma-Aldrich M 7033	
3262 E23	E	711	720	-0.27813358	1767	1780	-0.27813358	1767	1780	67548	-4.61023976	empty		
3262 E24	P	191374	192560	589.227921	265918	267520	826.401809	2659088	-0.61526904	3242650	0.00542415	empty		
3262 F01	N	636	640	-0.51002417	635	640	-0.55825532	3027667	-0.032498	2963027	-0.41413241	empty		
3262 F02	E	116	120	-2.11779887	115	120	-2.17923833	64681	-4.6146735	74618	-4.72871923	empty		
3262 F03	X	475	480	-1.00781595	755	760	-0.18418232	3237467	0.29195187	3461490	0.33045116	experimental	Sigma-Aldrich S 1068	SB-215505; 6-Chloro-5-methyl-1-5-quinolincarbonyl-ir
3262 F04	X	509	520	-0.90269222	470	480	-1.0726057	2915284	-0.20629519	3454402	0.31986639	experimental	Sigma-Aldrich N-151	Nisoxetine hydrochloride; LY-94,939
3262 F05	X	713	720	-0.27194983	712	720	-0.31510787	3583221	0.82665082	3426396	0.27802819	experimental	Sigma-Aldrich M 9656	H-8 dihydrochloride; N-[2-(Methylamino)ethyl]-5-isouqui
3262 F06	X	553	560	-0.76664974	752	760	-0.19353415	3232146	0.28372309	3628563	0.58001795	experimental	Sigma-Aldrich P20124	CP-66713 ; 8-chloro-N-phenyl-1,2,4-triazolo[4,3-a]qui
3262 F07	X	713	720	-0.27194983	712	720	-0.31510787	3583221	0.82665082	3426396	0.27802819	experimental	Sigma-Aldrich M-110	alpha-Methyl-5-hydroxytryptamine maleate; alpha-Meth
3262 F08	X	671	680	-0.40180856	630	640	-0.5738417	3171332	0.19245958	3680214	0.65717209	experimental	Sigma-Aldrich O 2378	Oxymetazoline hydrochloride; 3-(4,5-Dihydro
3262 F09	X	1032	1040	0.71435811	1192	1200	1.17806685	3293837	0.37912651	3921856	1.01812699	experimental	Sigma-Aldrich M3071	Moclobemide; 4-Chloro-N-[2-(4-morpholinyl)ethyl]benz
3262 F10	X	751	760	-0.15445861	911	920	0.30211258	3093307	0.06659489	3821266	0.86786978	experimental	Sigma-Aldrich O 8757	Ofloxacin; Ofloxacin; DL-8280; HOE-280
3262 F11	X	868	880	0.2072907	827	840	0.04026148	3707989	1.01960106	3566975	0.48802032	experimental	Sigma-Aldrich M-226	p-MPPF dihydrochloride; 4-Fluoro-N-(2-[4-(2-methoxyp
3262 F12	X	2152	2160	4.17725477	1992	2000	3.67188868	7907191	7.51355025	8653469	8.08601615	experimental	Sigma-Aldrich T2705	Topotecan hydrochloride hydrate
3262 F13	X	629	640	-0.53166729	829	840	0.04649603	3177941	0.19989565	4051878	1.21234852	experimental	Sigma-Aldrich M 9656	R, 24c; Nebostol
3262 F14	X	311	320	-1.51488336	310	320	-0.92479147	3165911	1.1812925	3827207	0.65629345	experimental	Sigma-Aldrich P 1061	NC-525A hydrochloride; Proadifen hydrochloride
3262 F15	X	593	600	-0.29749877	552	560	-0.481698915	3044820	-0.78650369	3986721	1.11418018	experimental	Sigma-Aldrich N 4159	NCS-3919; 4,4-dihydro-7-methyl-4-oxo-1,8-nap
3262 F16	X	711	720	-0.27813358	752	760	-0.19353415	3536438	0.75430221	3299324	0.08821424	experimental	Sigma-Aldrich P 2116	Pirfenidone; 5-Methyl-1-phenyl-2-(1H)-pyridine
3262 F17	X	993	1000	0.59377501	671	680	-0.44603342	3711964	1.02574829	3546022	0.45672159	experimental	Sigma-Aldrich N 5504	Naphazoline hydrochloride; 2-(1-Naphthylmethyl)imidaz
3262 F18	X	510	520	-0.89960034	591	600	-0.69541542	3573908	0.81224852	3525260	0.42570817	experimental	Sigma-Aldrich T 9567	Thiolactomycin; [R-(E)]-4-hydroxy-3,5-dimethyl-5-(2-m
3262 F19	X	711	720	-0.27813358	671	680	-0.44603342	3522710	0.73307224	3621676	0.56973043	experimental	Sigma-Aldrich N 7758	Naloxone hydrochloride
3262 F20	X	869	880	0.21038258	709	720	-0.32757697	3696390	1.00166353	3743653	0.75193467	experimental	Sigma-Aldrich P 4668	Praziquantel; 2-(Cyclohexylcarbonyl)-1,2,3,6,7,11b-hex
3262 F21	X	1309	1320	1.57080733	947	960	0.41433448	3427078	0.58518001	3505327	0.39593307	experimental	Sigma-Aldrich M 8784	Norcantharidin
3262 F22	E	840	850	0.07434801	1812	1820	-0.07434801	3175779	0.29695342	3296537	0.18541682	experimental	Sigma-Aldrich P 5679	3-n-Propylxanthine; Enprofylline
3262 F23	E	1125	1160	1.00190243	1762	1680	2.79904985	64862	-4.61439359	76710	-4.72559429	empty		
3262 F24	P	186799	187920	575.082595	298976	300440	929.452686	2826704	-0.3432817	3628648	0.58014492	empty		
3262 G01	N	636	640	-0.51002417	836	840	0.06831695	3008528	-0.06209593	3292203	0.07757719	empty		
3262 G02	E	236	240	-1.74677394	155	160	-2.05454732	66989	-4.61110424	80234	-4.72033028	empty		
3262 G03	X	554	560	-0.76355787	753	760	-0.19041687	3251036	0.31293595	3174824	-0.09775875	experimental	Sigma-Aldrich I 3639	Isotharaine mesylate; 4-[1-Hydroxy-2-((1-methylethyl)ar
3262 G04	X	554	560	-0.76355787	552	560	-0.81698915	3309418	0.40322209	2978149	-0.39453131	experimental	Sigma-Aldrich P 0618	cis-(+)-8-OH-P821 hydrobromide; cis-8-Hydroxy-3-(n-j
3262 G05	X	553	560	-0.76664974	512	520	-0.92479147	3165911	1.1812925	3827207	0.65629345	experimental	Sigma-Aldrich I 6504	(-)-Isoproterenol hydrochloride; (-)-Isoprenaline hydroc
3262 G06	X	312	320	-1.51719148	512	520	-0.94168015	1893469	-1.78650369	2246321	-0.48471842	experimental	Sigma-Aldrich L119	L-701,606 oxalate salt hydrate; cis-2-(Diphenylmethyl)-
3262 G07	X	713	720	-0.27194983	669	680	-0.45226797	3201601	0.2364861	3597118	0.5330467	experimental	Sigma-Aldrich I 8250	3-Iodo-L-tyrosine; S(-)-3-Iodo-4-hydroxyphenylalanine
3262 G08	X	713	720	-0.27194983	673	680	-0.43979887	3722480	1.04201099	3812471	0.85473217	experimental	Sigma-Aldrich M 1559	Moxonidine hydrochloride; BDF-5895
3262 G09	X	471	480	-1.02018345	590	600	-0.6985327	3331593	0.43751511	3396902	0.23276231	experimental	Sigma-Aldrich I-117	R(+)-IAA-94; R(+)-Methylindazole; Indanyloxyacetic ac
3262 G10	X	673	680	-0.39562481	751	760	-0.19665142	3264086	0.33311271	3529909	0.43265265	experimental	Sigma-Aldrich M 2537	Mevastatin; Compactin
3262 G11	X	551	560	-0.77283349	871	880	0.17742158	3329550	0.43435567	3320586	0.11997455	experimental	Sigma-Aldrich I-146	IB-MECA; 1-Deoxy-1-[6-[[[3-iodophenyl]amino]oxy]methyl
3262 G12	X	673	680	-0.07123249	626	640	-0.07123249	3617686	0.8794998	3620446	0.26155302	experimental	Sigma-Aldrich M 3127	S-Methylisothiourea hemisulfate; Carbamimidohthioic ac
3262 G13	X	547	560	-0.39871669	672	680	-0.19353415	3542865	0.04280685	3269339	0.04350452	experimental	Sigma-Aldrich K 1136	Ketorolac tris salt; Toradol
3262 G14	X	792	800	-0.02769175	672	680	-0.44291615	3185000	0.21081311	3520069	0.41795046	experimental	Sigma-Aldrich M 3808	MRS 2179; 2'-Deoxy-N6-methyl adenosine 3',5'-diphosp
3262 G15	X	712	720	-0.27504171	713	720	-0.31510787	3799436	1.16102131	3554005	0.46864627	experimental	Sigma-Aldrich L 0664	loprofen; Kolox
3262 G16	X	792	800	-0.02769175	711	720	-0.32134242	3468089	0.64860238	3961453	1.07727537	experimental	Sigma-Aldrich M 4910	1-Methylhistamine dihydrochloride
3262 G17	X	469	480	-1.0263672	790	800	-0.0750777	3842348	1.22738352	3686676	0.66682476	experimental	Sigma-Aldrich L 2906	Lomefloxacin hydrochloride
3262 G18	X	1152	1160	1.08538304	1351	1360	1.67371358	3855726	1.24807223	4090991	1.27017641	experimental	Sigma-Aldrich M 5501	N6-Methyladenosine; 6-Methylaminopurine-9-ribofurano
3262 G19	X	950	960	0.46082441	828	840	0.04337875	3684843	0.98380642	3582384	0.51103765	experimental	Sigma-Aldrich L 5783	LiDocaine N-ethyl bromide quaternary salt; QX-314
3262 G20	X	790	800	-0.0338755	1071	1080	0.80087658	3843880	1.22975272	4258048	1.52031681	experimental	Sigma-Aldrich M 6517	alpha,beta-Methylene adenosine 5'-triphosphate dithiue
3262 G21	X	588	600	-0.65843414	908	920	0.29276075	3075209	0.04102438	3466946	0.33860111	experimental	Sigma-Aldrich L 9664	Loratadine; 4-(8-chloro-5,6-dihydro-11H-benzo[5,6]cycl
3262 G22	X	987	1000	0.57522376	1083	1200	1.15001138	3438575	0.6029598	3676252	0.65125382	experimental	Sigma-Aldrich M 7065	MK-912; L-657,743 hydrochloride
3262 G23	E	1028	1600	0.70199061	1701	2400	2.76475983	70116	-4.60626842	75812	-4.72693568	empty		
3262 G24	P	191657	192880	590.102921	233959	235480	726.776817	2803168	-0.37967947	3075002	-0.24686875	empty		
3262 H01	N	595	600	-0.63679102	595	600	-0.68294632	2810462	-0.3683995	3277930	0.05625676	empty		
3262 H02	E	195	200	-1.87354079	75	80	-2.30392933	64768	-4.61453896	71998	-4.73263288	experimental	Sigma-Aldrich M 8878	1-Methylimidazole; Methimazole
3262 H03	X	712	720	-0.27504171	791	800	-0.07196504	3526186	0.73844778	3876970	0.95107813	experimental	Sigma-Aldrich N-153	Nylidrin hydrochloride
3262 H04	X	592	600	-0.64606664	952	960								

3262 107	X	709	720	-0.28431733	546	560	-0.8356928	3060979	0.01901808	3590807	0.52361959	experimental	Sigma-Aldrich C1618	Cibenzoline succinate; 2-(2,2-diphenylcyclopropyl)-4,5-c
3262 108	X	913	920	0.34642505	752	760	-0.19353415	3420513	0.57502742	3785713	0.81476217	experimental	Sigma-Aldrich P20107	CP-101537
3262 109	X	391	400	-1.2675334	872	880	0.18053885	2045560	-1.55129918	2284013	-1.42841566	experimental	Sigma-Aldrich L-119	Indatralin hydrochloride; Lu 19-005
3262 110	X	713	720	-0.27194983	632	640	-0.56760715	3635934	-0.90817001	3611311	-0.55428080	experimental	Sigma-Aldrich M 2547	8-Methoxy methyl-3-isobutyl-1-methylxanthine; 8-Meth
3262 111	X	831	840	0.09289135	871	680	-0.44603345	3005748	-0.06639513	2801338	-0.65565681	experimental	Sigma-Aldrich A0660	Autrothiogluccose; 1-Thio-D-glucopyranose gold salt
3262 112	X	586	600	-0.66461789	710	720	-0.3244597	3266570	0.33695885	3163765	-0.11427823	experimental	Sigma-Aldrich M 3184	MG 624; N,N,N-Triethyl-2-(4-trans-stibutyl)ethylam
3262 113	X	952	960	0.46700815	792	800	-0.06884315	3232081	0.28362257	3241479	0.00180776	experimental	Sigma-Aldrich K 1751	Ketoprofen; 2-(3-Benzoyloxyphenyl)propionic acid
3262 114	X	831	840	0.09289135	872	680	-0.44291615	3290578	0.37408655	3429982	0.2833858	experimental	Sigma-Aldrich M 3935	Meloxicam sodium; 4-Hydroxy-2-methyl-N-(5-methyl-2
3262 115	X	873	680	-0.39562481	673	880	0.18365613	2871416	-0.27413583	2978185	-0.39149002	experimental	Sigma-Aldrich L 1011	Labetalol hydrochloride; 2-Hydroxy-5-(1-hydroxy-2-[(1-
3262 116	X	710	920	-0.28122546	1010	920	-0.28122546	3791049	1.14805104	3214827	-0.03800391	experimental	Sigma-Aldrich M 5154	Moxisylyte hydrochloride; 4-Dimethylaminoethoxy-5-iso
3262 117	X	991	1000	0.58759126	1029	1040	0.66995103	3172436	0.19138323	3470483	0.34888453	experimental	Sigma-Aldrich L 3791	Lantrolin; GI 267119X; 6-(2,3-dichlorophenyl)-1,2,4-
3262 118	X	869	880	0.21038258	1066	1080	0.7852902	3802791	1.16620972	3815258	0.94422178	experimental	Sigma-Aldrich M 5560	(S)-2-Amino-2-methyl-4-phos
3262 119	X	789	800	-0.03696738	1105	1120	0.90686393	3304440	0.39552375	3460010	0.32824039	experimental	Sigma-Aldrich A 6664	4-Aminodiphenylmethanesulfonyl fluoride hydrochloride;
3262 120	X	749	760	-0.16064236	1399	1400	1.79217003	3529207	0.74311967	3866983	0.93615996	experimental	Sigma-Aldrich M 6524	Methoxamine hydrochloride
3262 121	X	1269	1280	1.44713235	1027	1040	0.66371648	3433537	0.59516867	3454421	0.31989178	experimental	Sigma-Aldrich L 9756	(-)-Tetramisole hydrochloride; Levamisole hydrochloride
3262 122	X	1064	1080	0.81329809	1183	1200	1.15001138	3342049	0.45368502	3770203	0.79159397	experimental	Sigma-Aldrich M 7277	(-)-3-(3,4-dihydroxyphenyl)-2-methyl-DL-alanine; DL-a
3262 123	E	1152	1800	1.08538304	1662	2440	2.6431861	66138	-4.61242029	77874	-4.72385555	empty		
3262 124	P	217700	219080	670.624607	260844	262400	810.584756	3090308	0.0639570	3431999	0.28639871	empty		
3262 101	N	875	880	0.22893382	595	600	-0.68294632	2706758	-0.52877485	2980056	-0.38869519	empty		
3262 102	E	234	240	-1.75295769	156	160	-2.05143005	65843	-4.6128765	72236	-4.73227736	empty		
3262 103	X	671	680	-0.40180856	472	480	-1.06371115	3165883	0.1812492	3319585	0.11847929	experimental	Sigma-Aldrich M 9020	Mecamylamine hydrochloride
3262 104	X	910	920	0.33714943	631	680	-0.44603342	226842	-1.30188105	2462872	-1.16124342	experimental	Sigma-Aldrich S 8061	SB 242084 dihydrochloride hydrate; 6-Chloro-2,3-dihyd
3262 105	X	1190	1200	1.20287427	1711	1320	1.54902258	3410741	0.55991529	3605040	0.54488922	experimental	Sigma-Aldrich F 0030	Fenobam; N-(3-Chlorophenyl)-N'-(4,5-dihydro-1-methyl
3262 106	X	668	680	-0.41108418	818	880	0.16806975	3031336	-0.02682399	3515514	0.41114999	experimental	Sigma-Aldrich N-211	NS 2028; 4H-8-Bromo-1,2,4-oxadiazolo[3,4-b]benz(b)
3262 107	X	1154	1160	1.09156679	1164	1120	0.9349194	3354174	0.472436	3651242	0.61389491	experimental	Sigma-Aldrich D 0943	DFB; 3,3'-Difluorobenzalazine
3262 108	X	713	720	-0.27194983	632	640	-0.56760715	3635934	-0.90817001	3611311	-0.55428080	experimental	Sigma-Aldrich M 2851	Rxylbutynin Chloride; alpha-Phenylcyclohexanecylocl
3262 109	X	594	600	-0.39258234	512	520	-0.94168015	1091851	0.06677685	3038191	0.30185558	experimental	Sigma-Aldrich Z 4626	SN 39023 dihydrochloride; 3-(N-Benzyl-N'-N'-amin
3262 110	X	672	680	-0.64066664	506	560	-0.81387187	3007823	-0.0631862	3670824	0.6431457	experimental	Sigma-Aldrich T1	Netrolapril; (2S,3aR,7aS)-1-[(2S)-2-[[[(1S)-1-(ethoxy
3262 111	X	1231	1240	1.32964112	952	960	0.42992085	3594559	0.84418472	3679053	0.65543708	experimental	Sigma-Aldrich N 0630	Niflumic acid; 2-(3-Trifluoromethyl)anilino]nicotinic ac
3262 112	X	831	840	0.09289135	872	800	-0.06884315	2643410	-0.62674077	3800159	-0.34671684	experimental	Sigma-Aldrich P 0547	Pentamidine isethionate; 4'-[4-[[1,5-Pentanediyloxy]]b
3262 113	X	751	760	-0.15445861	672	680	-0.44291615	3005815	-0.06629151	3346944	0.15934704	experimental	Sigma-Aldrich N 3136	Naltrexone hydrochloride; 17'-(Cyclopropylmethyl)-4,5-e
3262 114	X	673	680	-0.39562481	473	480	-1.06325387	1742266	-2.02033492	1868639	-2.04888429	experimental	Sigma-Aldrich L 9793	LP44; 4-[2-(Methylthio)phenyl]-N-(1,2,3,4-tetrahydrop
3262 115	X	232	240	-1.75914144	153	160	-2.06078187	1240901	-2.79568196	1170545	-3.09166846	experimental	Sigma-Aldrich G6761	Gossypol; 2,2'-bis(8-Formyl-1,6,7-trihydroxy-5-isoprop
3262 116	X	713	720	-0.27194983	632	640	-0.56760715	3635934	-0.90817001	3611311	-0.55428080	experimental	Sigma-Aldrich P 2607	Phenethane
3262 117	X	750	760	-0.15755048	827	840	0.04026148	3386321	0.52215044	3627725	0.57876618	experimental	Sigma-Aldrich N 5751	NG-Nitro-L-arginine methyl ester hydrochloride; L-NAME
3262 118	X	1189	1200	1.19978239	1668	1680	2.66188975	2724531	-0.5012894	3198217	-0.06281524	experimental	Sigma-Aldrich P 4405	Podophyllotoxin
3262 119	X	1550	1560	2.31594906	1507	1520	2.16000848	3373266	0.50196125	3636056	0.59121068	experimental	Sigma-Aldrich M2199	PMEE hydrate
3262 120	X	708	720	-0.28740921	824	840	0.03090965	3297157	0.38426079	3152725	-0.13076933	experimental	Sigma-Aldrich P 5052	Salpha-Pregnan-3alpha-ol-11,20-dione; Alfalanox
3262 121	X	829	840	0.0867076	1322	1120	0.91621575	2938764	-0.16998402	3048717	-0.28613121	experimental	Sigma-Aldrich T 8703	To070907; 2-Chloro-5-nitro-N-4-pyridinyl-benzamide, B
3262 122	X	947	960	0.45154878	1102	1120	0.8975121	1905710	-1.76757332	1886100	-0.20280711	experimental	Sigma-Aldrich P 6402	Perphenazine
3262 123	E	1600	1600	0.26803622	1999	1999	0.69370776	67857	0.609761	1470	0.73008306	empty		
3262 124	E	240655	241920	741.598985	310848	312280	966.460975	3370074	0.49707242	3769000	0.78979698	empty		
3262 K01	N	755	760	-0.14209111	676	680	-0.43044705	3031803	-0.02610179	3305026	0.09673166	empty		
3262 K02	E	155	160	-1.99721577	195	200	-1.92985632	64387	-4.61512816	80261	-4.72028995	empty		
3262 K03	X	673	680	-0.39562481	594	600	-0.6860636	3065053	0.02531841	2886306	-0.52873509	experimental	Sigma-Aldrich I 4883	(-)-Ibuprofen; alpha-Methyl-4-(isobutyl)phenylacetate ac
3262 K04	X	791	800	-0.3078363	633	640	-0.56448987	3149885	0.156500874	2895324	-0.51526438	experimental	Sigma-Aldrich L-121	Levallorphan tartrate; 17'-(2-Propenyl)morphinan-3-ol t
3262 K05	X	1070	1080	0.83184934	711	720	-0.32134242	2859774	-0.29213986	3125421	-0.17155492	experimental	Sigma-Aldrich I 7378	Indomethacin
3262 K06	X	640	650	-0.5129979	564	560	-0.81075046	3373633	0.5025268	3795248	0.82455238	experimental	Sigma-Aldrich M 0814	R(-)-MeS; 1-(2,6-Dimethylphenoxy)-3-methyl-2-butana
3262 K07	X	113	120	-0.30161337	111	120	-2.10170761	1093801	-3.02316800	1168297	-3.10955461	experimental	Sigma-Aldrich M 8897	Imverectin; MK-933
3262 K08	X	595	600	-0.63679102	714	720	-0.3119906	1540524	-2.33232332	1681950	-2.32775266	experimental	Sigma-Aldrich B 1686	BIO; (2Z,3E)-6-Bromindirubin-3'-oxime
3262 K09	X	554	560	-0.76355787	713	720	-0.31510787	2949662	-0.15313057	3349353	0.16294551	experimental	Sigma-Aldrich I-120	Iofetamine hydrochloride; N-Isopropyl-p-iodoamphetam
3262 K10	X	113	120	-0.212707449	153	160	-2.06078187	956609	-3.23533164	960969	-3.35225471	experimental	Sigma-Aldrich M 2692	MK-886; 3-[3-tert-Butylthio-1-(4-chlorobenzyl)-5-isop
3262 K11	X	672	680	-0.39871669	594	600	-0.6860636	2763577	-0.44090585	2679547	-0.8375832	experimental	Sigma-Aldrich I-160	3-(1H-Imidazol-4-yl)propyl (p-fluorophenyl)methyl etf
3262 K12	X	592	600	-0.64066664	672	480	-1.06637115	3416055	0.56813325	3312065	0.10724623	experimental	Sigma-Aldrich M 3262	N-Methyl-D-aspartate acid; NMDA
3262 K13	X	672	680	-0.39871669	432	640	-0.56760715	2940303	-0.167604	3152426	-0.13121596	experimental	Sigma-Aldrich K 1888	K 185; N-Butanoyl-2-(5,6,7-trihydro-11-methoxybenzo[
3262 K14	X	512	520	-0.8934166	914	920	0.3114644	3074123	0.03934491	3120159	-0.17941504	experimental	Sigma-Aldrich M 4008	Morin; 2,3,4,5,7-Pentahydroxyflavone
3262 K15	X	593	600	-0.64297477	391	400	-1.31887042	1456383	-2.46244504	1297423	-2.90214331	experimental	Sigma-Aldrich L 1415	L-162,313; (5,7-dimethyl-2-ethyl-3-[4-[2-(n-butyl)oxca
3262 K16	X	752	760	-0.15136673	952	960	0.42992085	3831937	1.2112832	3535474	0.440696542	experimental	Sigma-Aldrich M 5171	S-Methyl-L-thiocitrulline acetate; N5-[Imino(methylthio
3262 K17	X	552	560	-0.76974162	591	800	-0.07196042	3296364	0.38033404	3800405	0.83670848	experimental	Sigma-Aldrich L 4376	Methoxy-Lobeline hydrochloride; (-)-Lobeline hydrochloride
3262 K18	X	671	680	-0.40180856	588	600	-0.70476725	3101265	0.08131926	3446244	0.30767731	experimental	Sigma-Aldrich M 5644	(-)-Methoxyverapamil hydrochloride; D606; Gallopamil
3262 K19	X	830	840	0.08979947	988	1000	0.54214275	3358531	0.47917398	3477981	0.35580874	experimental	Sigma-Aldrich L 8401	LE 300; 7-(Methyl-6,7,8,9,14,15-hexahydro-5H-benz[d]i
3262 K20	X	911	920	0.3402413	1350	1360	1.6705963	2201459	-1.31020571	2613825	-0.93575603	experimental	Sigma-Aldrich M 6545	Mitoxantrone; 1,4-Dihydroxy-5,8-bis[2-[[(-2-hydroxyeth
3262 K21	X	750	760	-0.15755048	827	1040	0.66683375	2554131	-0.76480826	2954291	-0.42781819	experimental	Sigma-Aldrich L 0878	L-655,708; Ethyl (5)-11,12,13,13a-Tetrahydro-7-metho
3262 K22	X	1027	1040	0.69889874	1104	1120	0.903746675	3141136	0.14297865	3417529	0.26478402	experimental	Sigma-Aldrich M 7684	MRS 2159
3262 K23	E	921	1560	0.37116005	1719	2400	2.82087078	65733	-4.61304661	76477	-4.72594233	empty		
3262 K24	P	214836	216200	661.769479	227557	229120	706.820023	2799534	-0.38529935	3051602	-0.28182271	empty		
3262 L01	N	635	640	-0.51311604	635	640	-0.55825532	2666013	-0.59178586	3025349	-0.32103387	empty		
3262 L02	E	155	160	-1.99721577	195	240	-1.80516532	61417	-4.61972118	68654	-4.73672801	empty		
3262 L03	X	793	800	-0.02										

3262 M01	N	715	720	-0.26576609	756	760	-0.18106505	2958036	-0.14018041	3101882	-0.20671651	empty		
3262 M02	E	194	200	-1.87663266	154	160	-2.0576664	59338	-4.6229363	81945	-4.71777446	empty		
3262 M03	X	1073	1080	0.84112496	875	880	0.18989068	2342359	-1.09230778	2477083	-1.14001562	experimental	Sigma-Aldrich S0572	
3262 M04	X	720	720	-0.27504171	512	520	-0.94168015	3651292	-0.91492073	3518201	0.41516372	experimental	Sigma-Aldrich A 2355	
3262 M05	X	512	520	0.89341666	952	960	0.42992087	22017753	-1.40872527	2202051	-1.37159009	experimental	Sigma-Aldrich I 73719	
3262 M06	X	512	520	-0.8934166	632	640	-0.56760715	3167599	0.18390295	3844009	0.90184234	experimental	Sigma-Aldrich M 1022	
3262 M07	X	993	1000	0.59377501	751	760	-0.19665142	2493569	-0.85846571	2967500	-0.40745083	experimental	Sigma-Aldrich I 9531	
3262 M08	X	753	760	-0.14827486	1033	1040	0.68242013	3321586	0.42203956	4073551	1.24472276	experimental	Sigma-Aldrich M 1809	
3262 M09	X	552	560	-0.76974162	670	680	-0.4491507	2602004	-0.690774	2929892	-0.46362812	experimental	Sigma-Aldrich I-122	
3262 M10	X	793	800	-0.02459888	872	880	0.18053885	3713765	1.02853349	3578400	0.50508652	experimental	Sigma-Aldrich M 2727	
3262 M11	X	832	840	0.09598322	712	720	-0.31822515	2355546	-0.79354945	2871668	-0.505060074	experimental	Sigma-Aldrich I18008	
3262 M12	X	713	720	-0.27194983	593	600	-0.68918087	3431899	0.59263595	3049586	0.48088762	experimental	Sigma-Aldrich M 3281	
3262 M13	X	591	600	-0.64915852	472	480	-1.06637115	2325567	-1.11827614	2404111	-1.24901819	experimental	Sigma-Aldrich K 2628	
3262 M14	X	594	600	-0.63988289	475	480	-1.05701932	3444780	0.61255566	3458692	0.32627162	experimental	Sigma-Aldrich M 4145	
3262 M15	X	792	800	-0.02769175	510	520	-0.9479147	2670714	-0.5845159	2530773	-1.0598157	experimental	Sigma-Aldrich C5493	
3262 M16	X	789	800	-0.03696738	1351	1360	1.67371358	3436715	0.60008336	3725088	0.72420303	experimental	Sigma-Aldrich M 5250	
3262 M17	X	670	680	-0.40490044	548	560	-0.82945825	2007659	-1.60991202	2143451	-1.6383814	experimental	Sigma-Aldrich L 4762	
3262 M18	X	1467	1480	2.05932349	1627	1640	2.53408148	3268616	0.34012293	3613235	0.55712161	experimental	Sigma-Aldrich M 5685	
3262 M19	X	2187	2200	4.28547308	1946	1960	3.52849221	2690527	-0.99387564	3049586	-0.28483413	W	experimental	Sigma-Aldrich L 8533
3262 M20	X	867	880	0.20419883	1108	1120	0.91621575	3362951	0.48600939	4212672	1.4525356	experimental	Sigma-Aldrich M 6628	
3262 M21	X	831	840	0.09289135	830	840	0.0496133	2373770	-1.04373154	2853307	-0.57843096	experimental	Sigma-Aldrich L 9908	
3262 M22	X	1106	1120	0.94315682	1146	1160	1.0346722	1901420	-1.77420768	1993653	-1.86214351	experimental	Sigma-Aldrich G 5793	
3262 M23	E	1170	1800	1.14103678	1217	1880	1.25599873	64653	-4.6147168	75107	-4.72798878	empty		
3262 M24	P	211586	212920	651.720887	221991	223400	689.466227	2494332	-0.85728576	27222078	-0.77405214	empty		
3262 N01	N	955	960	0.47628378	635	640	-0.55825532	2342099	-1.09270986	2381483	-1.28281897	empty		
3262 N02	E	74	80	-2.2476576	155	160	-0.94547337	59982	-4.62194037	81998	-4.73711166	empty		
3262 N03	X	713	720	-0.27194983	593	600	-0.81387187	3157020	-1.6754282	3436511	-2.0931505	experimental	Sigma-Aldrich M 9292	
3262 N04	X	632	640	-0.52239166	592	600	-0.69229815	2025354	-1.5825472	2136899	-1.64816851	experimental	Sigma-Aldrich N-158	
3262 N05	X	753	760	-0.14827486	992	1000	0.55461185	3377020	0.5077667	3845526	0.90370506	experimental	Sigma-Aldrich M-105	
3262 N06	X	593	600	-0.64297477	551	560	-0.82010642	2788544	-0.40229507	2741526	-0.74500152	experimental	Sigma-Aldrich O 0383	
3262 N07	X	513	520	-0.89032472	713	720	-0.31510787	3636500	0.90904531	3696570	0.68160401	experimental	Sigma-Aldrich M-137	
3262 N08	X	232	240	-1.75914144	511	520	-0.94479742	2007757	-1.60976047	2121769	-1.67076909	experimental	Sigma-Aldrich O 3125	
3262 N09	X	554	560	-0.76355787	592	600	-0.69229815	2719754	-0.5086769	2924747	-0.47133293	experimental	Sigma-Aldrich P20117	
3262 N10	X	792	800	-0.03696738	1351	1360	1.67371358	3436715	0.60008336	3725088	0.72420303	experimental	Sigma-Aldrich Q 9637	
3262 N11	X	592	600	-0.64606664	712	720	-0.31822515	3437901	0.60191748	3702977	0.60191745	experimental	Sigma-Aldrich N 1392	
3262 N12	X	671	680	-0.40180856	671	680	-0.44603342	2311460	-1.14009222	2617212	-0.93069667	experimental	Sigma-Aldrich P 0667	
3262 N13	X	1074	1080	0.84421683	1114	1120	0.9349194	2275354	-1.19592915	2326918	-1.36432593	experimental	Sigma-Aldrich N 3510	
3262 N14	X	152	160	-0.200649139	271	280	-1.69294342	826082	-3.43718801	1028694	-3.30355966	experimental	Sigma-Aldrich P 1793	
3262 N15	X	512	520	-0.8934166	832	840	0.05584785	2750009	-0.46188838	3263499	0.03470033	experimental	Sigma-Aldrich A 6605	
3262 N16	X	1672	1680	2.69315774	1474	1480	2.04466665	2110286	-1.45122022	2500884	-1.10446266	experimental	Sigma-Aldrich A 0233	
3262 N17	X	540	560	-0.90578409	592	600	-0.95414932	2950510	-0.151291916	3087591	-0.24767545	experimental	Sigma-Aldrich B 7261	
3262 N18	X	1023	1040	0.68853124	980	1000	0.52967665	1712156	-1.35553745	2272758	-1.38066479	experimental	Sigma-Aldrich P 4509	
3262 N19	X	1786	1800	3.04563143	1627	1640	2.53408148	3798900	1.1601924	3550906	0.46401711	experimental	Sigma-Aldrich N 8403	
3262 N20	X	867	880	0.20419883	826	840	0.0371442	2669845	-0.58585978	2957665	-0.42214195	experimental	Sigma-Aldrich P 5295	
3262 N21	X	550	560	-0.77592537	669	680	-0.45226797	2340718	-1.09484504	2110863	-1.68706002	experimental	Sigma-Aldrich S 6319	
3262 N22	X	1025	1040	0.69271499	864	880	0.15560065	2554181	-0.76473354	2612904	-0.93713178	experimental	Sigma-Aldrich P 6503	
3262 N23	E	1157	1840	1.10084241	1633	2400	2.55278513	63273	-4.61685093	73007	-4.73112568	empty		
3262 N24	P	230195	231480	709.257578	258359	259800	802.638328	2629478	0.34145599	3497366	0.38404125	empty		
3262 O01	N	1075	1080	0.84733982	675	680	-0.4335862	2464984	-0.90267162	2960751	-0.72532261	empty		
3262 O02	E	114	120	-12.398262	195	200	-1.92985632	58926	-4.62357345	79054	-4.72209292	empty		
3262 O03	X	714	720	-0.26885796	634	640	-0.5613726	2356349	-1.07067263	2545896	-1.03722558	experimental	Sigma-Aldrich I 5627	
3262 O04	X	712	720	-0.27504171	713	720	-0.31510787	2760069	-0.44633087	2823945	-0.6218874	experimental	Sigma-Aldrich L-131	
3262 O05	X	632	640	-0.52239166	551	560	-0.82010642	2964098	-1.13080569	3168560	-1.01711565	experimental	Sigma-Aldrich I 7388	
3262 O06	X	632	640	-0.52239166	832	840	0.05584785	2720293	-0.50784335	3474869	0.35043616	experimental	Sigma-Aldrich M 1275	
3262 O07	X	672	680	-0.39871669	711	720	-0.32134242	2794384	-0.39326368	3200596	-0.05926159	experimental	Sigma-Aldrich S5572	
3262 O08	X	872	880	0.2196582	752	760	-0.19333415	2984047	-0.09995512	3229415	-0.01621295	experimental	Sigma-Aldrich F7932	
3262 O09	X	872	880	0.2196582	871	880	0.17421258	2504301	-0.84186897	2763360	-0.71238678	experimental	Sigma-Aldrich S 8822	
3262 O10	X	552	560	-0.76974162	631	640	-0.57072442	2893807	-0.23950877	2908706	-0.49527489	experimental	Sigma-Aldrich M 2776	
3262 O11	X	550	560	-0.77592537	432	440	-1.19106215	2440479	-0.94056792	2460493	-1.16479708	experimental	Sigma-Aldrich P20137	
3262 O12	X	632	640	-0.52239166	793	800	-0.06572587	2737546	-0.48116206	2912060	-0.49026483	experimental	Sigma-Aldrich M 7319	
3262 O13	X	712	720	-0.27504171	710	720	-0.3244597	2701756	-0.5365103	2771219	-0.70064733	experimental	Sigma-Aldrich K 3375	
3262 O14	X	556	560	-0.75737412	834	840	0.0620824	2783774	-0.40967175	3004775	-0.35177096	experimental	Sigma-Aldrich R 8404	
3262 O15	X	112	120	-2.13016637	311	320	-1.56825242	848700	-3.40209991	971599	-3.3888518	experimental	Sigma-Aldrich L 2037	
3262 O16	X	830	840	0.08979947	670	680	-0.4491507	2882234	-0.25740609	3417225	0.26432992	experimental	Sigma-Aldrich M 5379	
3262 O17	X	668	680	-0.41108418	1026	1040	0.6605992	2977256	-0.11045721	3727663	0.72804946	experimental	Sigma-Aldrich L 4900	
3262 O18	X	2029	2040	3.79695692	1869	1880	3.28846203	2993054	-0.08602604	3511617	0.40532881	W	experimental	Sigma-Aldrich M 6191
3262 O19	X	861	880	0.18564758	803	720	-0.34628062	2693424	-0.54939551	3066897	-0.25897567	experimental	Sigma-Aldrich L 8539	
3262 O20	X	1391	1400	1.82434103	1430	1440	1.9199783	2895758	-0.2364916	3526300	0.42685836	experimental	Sigma-Aldrich E4660	
3262 O21	X	667	680	-0.41417605	1187	1200	1.16248048	2401213	-1.0012917	3121973	-0.1767054	experimental	Sigma-Aldrich L-106	
3262 O22	X	1600	1620	4.30034842	1583	1600	1.55001138	3235073	2.28824961	3425517	0.27731367	experimental	Sigma-Aldrich D 8941	
3262 O23	X	1047	1060	0.74218498	674	2480	2.6805934	62364	-4.61819489	74188	-4.7293155	empty		
3262 O24	P	227415	229080	700.662167	270377	272080	840.301739	2509324	-0.83410104	2929328	-0.4644706	empty		
3262 P01	N	796	800	-0.01532426	878	880	0.1992425	2003567	-1.61624210	2698860	-0.80873424	empty		
3262 P02	E	196	200	-1.87044892	155	160	-2.05454732	57878	-4.62519415	66892	-4.74026001	empty		
3262 P03	X	596	600	-0.63699114	676	680	-0.43044705	2475803	-0.88594034	2839093	-0.59925994	experimental	Sigma-Aldrich M 9440	
3262 P04	X	594	600	-0.63988289	554	560	-0.8107546	2606158	-0.68434995	2912394	-0.48976591	experimental	Sigma-Aldrich B 2185	
3262 P05	X	674	680	-0.39253294	634	640	-0.5613726	2729492	-0.49361735	3405922	-0.29474596	experimental	Sigma-Aldrich M-107	
3262 P06	X	954	960	0.09598322	954	960	0.43615505	2356149	-0.59166849	2672316	-0.84835833	experimental	Sigma-Aldrich O 0877	
3262 P07	X	832	840	0.09598322	712	720</								

3262 P19	X	1432	1440	1.95110788	753	760	-0.19041687	2948947	-0.15423629	3158910	-0.12153043	experimental	Sigma-Aldrich N 8534	Nilotamide; Anandron
3262 P20	X	749	760	-0.16064236	590	600	-0.6985327	2887154	-0.24979745	3190855	-0.07381213	experimental	Sigma-Aldrich P 5396	Phosphomycin disodium; Fosfomycin; Phosphonomycin;
3262 P21	X	872	880	0.2196582	1191	1200	1.17494958	2854676	-0.30002377	3261736	0.03206683	experimental	Sigma-Aldrich N-142	NO-711 hydrochloride; 1-(2-(((Diphenylmethylene)imin
3262 P22	X	1147	1160	1.06892367	1225	1240	1.28093663	2685504	-0.56164357	3112126	-0.11807068	experimental	Sigma-Aldrich P 6628	Pilocarpine nitrate
3262 P23	E	1862	2160	1.11630178	1868	2840	3.1445571	61371	6879232	empty	empty	empty	empty	empty
3262 P24	P	341251	341920	1052.62878	324964	325760	1010.46443	2616298	-0.66866873	2829325	-0.61385097	empty	empty	empty
3263 A01	N	998	1000	0.137622	1278	1280	0.72596522	2558055	-0.81993735	4414834	2.04538558	empty	empty	empty
3263 A02	E	154	160	-1.0874187	193	200	-1.19723885	67545	-4.59586897	78638	-4.48552597	empty	empty	empty
3263 A03	X	828	840	-0.1091279	911	920	0.07544366	2279563	-1.24216683	2739775	-0.47748519	experimental	Sigma-Aldrich P 6656	Promazine hydrochloride; 10-(3-[Dimethylamino]propyl
3263 A04	X	1697	1720	1.15219955	1135	1160	0.47249224	2921121	-0.26948286	3359197	0.4554501	experimental	Sigma-Aldrich R 0758	Ritodrine hydrochloride; and N-(p-Hydroxyphenyl)-4-hydi
3263 A05	X	1351	1360	0.64999092	1313	1320	0.78800406	2953785	-0.21996006	3531313	0.71468063	experimental	Sigma-Aldrich P 7412	Prezempine dihydrochloride; 5,11-Dihydro-11-
3263 A06	X	753	760	-0.21798816	1074	1080	0.36436741	2956656	-0.21560726	4197652	1.62250408	experimental	Sigma-Aldrich P20102	CP-93129 dihydrochloride hydrate
3263 A07	X	512	520	-0.56779243	874	880	0.00985974	1484881	-2.44700636	2002616	-1.58774871	experimental	Sigma-Aldrich P20112	PD-184161
3263 A08	X	1275	1280	0.5396792	954	960	0.15166281	3182460	0.12674048	3992258	1.40892762	experimental	Sigma-Aldrich R 8900	Ro 8-4304; [4-[3-(4-fluorophenyl)-3,6-dihydro-2H-p
3263 A09	X	831	840	-0.10477349	1032	1040	0.2899208	3314717	0.327259	3856958	1.20514709	experimental	Sigma-Aldrich P 8782	(Φ)-cis-Piperidine-2,3-dicarboxylic acid
3263 A10	X	1112	1120	0.30308958	1071	1080	0.35904979	2746950	-0.53354837	3217067	0.24138264	experimental	Sigma-Aldrich R 108	Ro 41-0960; 2'-Fluoro-3,4-dihydroxy-5-nitrobenzophenc
3263 A11	X	912	920	0.01279558	991	1000	0.21724673	3169755	0.10747807	3374824	0.47898653	experimental	Sigma-Aldrich P 9233	Piribedil maleate; 2-(4-[1,3-Benzodioxol-5-ylmethyl]-1-)
3263 A12	X	633	640	-0.39216456	951	960	0.14634519	3116405	0.02659265	3634477	0.8700599	experimental	Sigma-Aldrich R-140	Ro 04-6790 dihydrochloride; 4-Amino-N-[2,6-bis(methy
3263 A13	X	755	760	-0.21508522	1074	1080	0.36436741	2956656	-0.21560726	4197658	0.121215	experimental	Sigma-Aldrich P 9879	Procaine hydrochloride; Novocaine hydrochloride
3263 A14	X	195	200	-1.02790843	153	160	-1.26814038	795940	-3.49152901	848497	-3.32601172	experimental	Sigma-Aldrich A 6733	Auranofin; SKF 39162; 1-Thio-Φ-D-glucopyranosatriet
3263 A15	X	515	520	-0.56343802	716	720	-0.27020131	3113726	0.02252304	3081681	0.03747258	experimental	Sigma-Aldrich P-118	Phlofenin; 3-Amino-2-(4-dihydroxy(1)propyl)phosphonic
3263 A16	X	915	920	0.01714999	553	560	-0.55912505	3171815	0.1106103	3505098	0.67519721	experimental	Sigma-Aldrich S 2501	Spermidine trihydrochloride; N-(3-Aminopropyl)-1,4-but
3263 A17	X	1025	1040	0.17681169	1105	1120	0.41931609	3226232	0.19310443	3443251	0.58204706	experimental	Sigma-Aldrich P-162	Pregnenolone sulfate sodium; 5-Pregnen-3βeta-ol-20-or
3263 A18	X	3672	3680	0.418885285	4350	4360	6.17120292	1877468	-1.85179426	1883394	-1.76731355	experimental	Sigma-Aldrich S7947	Stattic; 6-Nitrobenzo[1]thiophene-1,1-dioxide
3263 A19	X	824	840	-0.11493378	1141	1160	0.48312747	3293838	0.29560737	3716621	0.99578013	experimental	Sigma-Aldrich P-233	PD 168,077 maleate; N-[1-(2-Cyanophenyl)-1-piperazi
3263 A20	X	1260	1270	0.46777626	1572	1520	1.14079712	3209392	0.16839156	4493129	1.48929109	experimental	Sigma-Aldrich V 8409	Nitro-1,4-inhibitor 7-1; 2-(4-Morpholinyl)ethyl)-2-(3-nit
3263 A21	X	550	560	0.51263657	710	720	-0.28083654	1489079	0.45629238	1605286	2.1864827	experimental	Sigma-Aldrich Q 3251	Quinacrine dihydrochloride
3263 A22	X	1150	1160	0.35824545	987	1000	0.21015657	3076927	-0.03261320	3841138	1.18131998	experimental	Sigma-Aldrich S 8010	(Φ)-Sulpiride; (Φ)-5-(Aminosulfonyl)-N-[[1-ethyl-2-pyr
3263 A23	E	1371	2160	0.67902032	1689	2720	1.45447847	70037	-4.59209078	73837	-4.49275694	empty	empty	empty
3263 A24	P	268008	268840	387.694634	351356	352440	621.252632	2275833	-1.24782198	2139971	-1.38087306	empty	empty	empty
3263 B01	N	674	680	-0.33265429	593	600	-0.48822352	3075464	-0.03547914	2247271	-1.21926441	empty	empty	empty
3263 B02	E	150	160	-1.09322458	152	160	-1.26991292	76849	-4.58176291	78351	-4.48595823	empty	empty	empty
3263 B03	X	2378	2400	2.14065064	1856	1880	1.75049237	2903885	-0.29561484	2955124	-0.15313978	experimental	Sigma-Aldrich S 8567	SU 4312; 3-(4-Dimethylaminobenzylidene)-2-indolinon
3263 B04	X	600	620	-0.19739948	627	640	-0.79496395	1797195	-0.0766905	1954259	-1.13532307	experimental	Sigma-Aldrich P20141	PD-156; 2-(4-(4-Methoxyphenyl)-2-oxo-1-(3,4,5-1
3263 B05	X	736	760	-0.24266315	655	680	-0.37832615	3378320	0.42368928	3699499	0.96799203	experimental	Sigma-Aldrich S-008	1-(2-Methoxyphenyl)piperazine hydrochloride; 2-MPP hy
3263 B06	X	632	640	-0.39361603	632	640	-0.41909453	3168674	0.10583914	3029429	-0.04122616	experimental	Sigma-Aldrich T 7947	Tomoxetine; (R)-N-methyl-gamma-(2-methylphenoxy)-1
3263 B07	X	593	600	-0.45022336	592	600	-0.48999606	3761709	1.00495603	4057893	1.50778302	experimental	Sigma-Aldrich S-154	Sepiapterin; S(-)-2-Amino-7,8-dihydro-6-(2-hydroxy-1-
3263 B08	X	191	200	-1.03371431	311	320	-0.98807933	970969	-3.22616266	1269622	-2.65062158	experimental	Sigma-Aldrich T 9262	Tamoxifen citrate; (Z)-2-[4-(1,2-Diphenyl-1-butenyl)ph
3263 B09	X	593	600	-0.45022336	871	880	0.00454213	3563502	0.70444887	4039983	1.48080808	experimental	Sigma-Aldrich T 0410	Triapiride hydrochloride; N-(2-[[Diethylamino]ethyl]-5-(m
3263 B10	X	911	920	0.01134411	1110	1120	0.42817879	3240747	0.21511102	3193672	0.20614654	experimental	Sigma-Aldrich T-122	Telenzepine dihydrochloride; 4,9-Dihydro-3-methyl-4-(1-
3263 B11	X	900	910	0.04671463	1170	1180	0.07367111	3240746	0.38643196	447429	1.13532307	experimental	Sigma-Aldrich T 1516	Tiluxiphenil hydrochloride
3263 B12	X	591	600	-0.4531263	870	880	0.00276959	3325059	0.33093388	3108991	0.07860522	experimental	Sigma-Aldrich U 4125	Uridine 5'-diphosphate sodium; UDP
3263 B13	X	902	1000	1.2891318	911	920	0.07544366	3554672	0.69106146	4222151	1.75517831	experimental	Sigma-Aldrich T 2528	Terbutaline hemisulfate; 2-T-Butylamino-1-(3,5-dihydro
3263 B14	X	432	440	-0.68391003	593	600	-0.48822352	3295103	0.29752167	3569957	0.77288384	experimental	Sigma-Aldrich U-103	U-69593; (+)-[Salpha,7alpha,beta)-N-Methyl-N-[7-(1-
3263 B15	X	593	600	-0.45022336	590	600	-0.49354114	3119109	0.03069226	2968911	-0.13237465	experimental	Sigma-Aldrich T 4182	Uprhospin AG 1478; N-(3-Chlorophenyl)-6,7-dimethoxy
3263 B16	X	312	320	-0.85808644	553	560	-0.55912505	3198259	0.15069978	3704182	0.97504528	experimental	Sigma-Aldrich U-116	U-99194A maleate; 5-(6-Dimethoxy-2-(di-n-propylamino
3263 B17	X	440	440	-0.8653615	230	240	-1.13165493	1005327	-3.17407154	1160751	-2.85571396	experimental	Sigma-Aldrich B9311	BIX 01294 trihydrochloride hydrate; 2-(Hexahydro-4-m
3263 B18	X	631	640	-0.00118392	826	840	0.11399948	3042282	0.0766905	3435305	0.13139237	experimental	Sigma-Aldrich V 8879	Vincristine sulfate; VCR
3263 B19	X	668	680	-0.4313621	836	840	-0.07522209	318130	0.48404633	3435305	0.57007922	experimental	(Φ)-alpha-Lipic acid; (Φ)-1, 2-Dithiolane-3-pentanoic a	
3263 B20	X	949	960	0.06649997	868	880	-0.00077549	3383581	0.43166563	3451129	0.59391242	experimental	Sigma-Aldrich W-104	WIN 62,577; 17-beta-Hydroxy-17-alpha-ethyl-17-delta-4
3263 B21	X	950	960	0.06795144	788	800	-0.14257855	2974894	-0.18795612	3120150	0.09541222	experimental	Sigma-Aldrich T 6764	Triprolidine hydrochloride; (E)-2-[3-(1-Pyrrolidinyl)-1-p
3263 B22	X	825	840	-0.11348231	985	1000	0.2066115	3358265	0.39328334	3261168	0.30780486	experimental	Sigma-Aldrich Y 3125	Yohimbine hydrochloride; 17-Hydroxyyohimban-16-carb
3263 B23	E	1680	2520	1.12752456	1627	2720	1.34458109	72743	-4.58798813	82054	-4.480381	empty	empty	empty
3263 B24	P	283758	285160	410.555287	369848	371680	654.030411	2805024	-0.44550076	2678283	-0.57010066	empty	empty	empty
3263 C01	N	876	880	-0.03945734	1116	1120	0.43881402	3126796	0.04234674	4840834	2.68700057	empty	empty	empty
3263 C02	E	154	160	-1.0874187	193	200	-1.19723885	77464	-4.58083049	84523	-4.47666234	empty	empty	empty
3263 C03	X	950	960	0.06795144	791	800	-0.13726094	3081344	-0.02656431	3804701	1.12549194	experimental	Sigma-Aldrich P 6777	Phenolazine sulfate
3263 C04	X	578	600	-0.47199541	612	640	-0.44745514	1269039	-2.77425043	1521882	-2.31180067	experimental	Sigma-Aldrich R 1402	Ranolazine hydrochloride; LY 139481
3263 C05	X	633	640	-0.39216456	512	520	-0.63179912	3122318	0.03555571	3828660	1.16252638	experimental	Sigma-Aldrich P 7505	Putrescine dihydrochloride; Putrescine dihydrochloride
3263 C06	X	591	600	-0.4531263	832	840	-0.06458686	2020843	-1.63441943	2697689	-0.54087253	experimental	Sigma-Aldrich R 5648	Rottlerin; Mollitoxin
3263 C07	X	993	1000	0.13036465	992	1000	0.21901927	2988111	-0.16791746	3370609	0.47182484	experimental	Sigma-Aldrich P 8293	Protoporphylin IX disodium; Kammerer's porphyrin
3263 C08	X	633	640	-0.39216456	553	560	-0.55912505	3524270	0.64496814	4155312	1.65450952	experimental	Sigma-Aldrich R 9525	RK 821002 hydrochloride; 2-[2-(2-Methoxy-1,4-benzodi
3263 C09	X	593	600	-0.45022336	552	560	-0.56089759	2232042	-1.31421474	2725305	-0.49968567	experimental	Sigma-Aldrich P 9813	Protriptyline hydrochloride
3263 C10	X	432	440	-0.68391003	632	640	-0.41909453	3139514	0.06162885	2898663	-0.23772602	experimental	Sigma-Aldrich R 1115	Reactive Blue 2; Basilen blue E-3G
3263 C11	X	672	680	-0.33555723	472	480	-0.70270066	3366143	0.40522739	3164407	0.16206939	experimental	Sigma-Aldrich P 9297	Paromomycin sulfate
3263 C12	X	752	760	-0.21943963	593	600	-0.48822352	3530609	0.65457888	3645461	0.88660332	experimental	Sigma-Aldrich S 0278	(Φ)-Sotalol hydrochloride; N-(4-[1-Hydroxy-2-(isoprop
3263 C13	X	880	880	-0.04816616	511	520	-0.63357166	3612369	0.77853749	3054714	-0.00314345	experimental	Sigma-Aldrich P-101	2-Phenylaminoadenosine; CV-1808
3263 C14	X	910	920	0.00989264	751	760	-0.20816247	3845234	1.13159661	3647931	0.89032348	experimental	Sigma-Aldrich S 1563	SKF 86466; 6-Chloro-2,3,4,5-tetrahydro-3-methyl-1H-3
3263 C15	X	1271	1280	0.53387332	1551	1560	1.20986818	3085482	-0.02029057	3147832	0.13710515	experimental		

3263 H07	X	832	840	-0.10332202	352	360	-0.91540525	4125318	1.55623377	3867202	1.22057597	experimental	Sigma-Aldrich S-174	SDZ-205,557 hydrochloride; 4-Amino-5-chloro-2-metho	
3263 H08	X	671	680	-0.3370087	632	640	-0.41909453	3527186	0.64938917	3095796	0.05873173	experimental	Sigma-Aldrich T-101	THIP hydrochloride; Gaboxadol hydrochloride	
3263 H09	X	711	720	-0.2789499	750	760	-0.20993501	3870808	1.17036406	3692814	0.9575235	experimental	Sigma-Aldrich T 0891	Tolbutamide	
3263 H10	X	951	960	0.06940291	913	920	0.07898874	3138511	1.06010817	2703506	-0.5311113	experimental	Sigma-Aldrich A 8852	A-68930 hydrochloride; cis-(*)-1-(Aminomethyl)-3,4-di	
3263 H11	X	750	760	-0.22234257	432	440	-0.77560219	3660476	0.85147386	3301015	0.78050189	experimental	Sigma-Aldrich T 1698	Tetradecylthioacetic acid; TTA	
3263 H12	X	832	840	-0.10332202	554	560	-0.55735252	3640777	0.82160765	3105409	0.07321024	experimental	Sigma-Aldrich U 6756	U-73122; 1-[(6-[[17beta]-3-Methoxyestra-1,3,5(10)-tri	
3263 H13	X	466	480	-0.63456005	433	440	-0.77182965	3204495	0.16014835	2871977	-0.27837068	experimental	Sigma-Aldrich T 3146	Trimipramine maleate	
3263 H14	X	2753	2760	0.26849519	872	880	0.00631467	3436354	0.51167625	3200665	0.21577528	experimental	Sigma-Aldrich U-108	SC-)-UH-301 hydrochloride; (S)-)-5-Fluoro-8-hydroxy-DP	
3263 H15	X	466	480	-0.63456005	711	720	-0.279064	2087210	-1.53379857	2010229	-1.57628248	experimental	Sigma-Aldrich T 4376	N-p-Tosyl-L-phenylalanine chloromethyl ketone; TPCK	
3263 H16	X	631	640	-0.3950675	552	560	-0.56089759	2928507	-0.25828474	2690116	-0.55227852	experimental	Sigma-Aldrich V 4629	(*)-Verapamil hydrochloride	
3263 H17	X	748	760	-0.22524551	707	720	-0.28615415	3570448	0.7149799	3370913	0.473059602	experimental	Sigma-Aldrich P20138	SC-51089 hydrate ; 8-Chloro-dibenz[b,f][1,4]oxazepine	
3263 H18	X	751	760	-0.2208917	830	840	-0.06813194	3382257	0.42965828	3350119	0.49200406	experimental	Sigma-Aldrich M0253	L-Himosine from Koa hoale seeds; Leucenol, (S)-)-Amin	
3263 H19	X	749	760	-0.22379404	668	680	-0.35528315	3576240	0.72376131	3302379	0.36987433	experimental	Sigma-Aldrich T 6154	Trazodone hydrochloride; 2-[3-[4-(3-Chlorophenyl)-1-pi	
3263 H20	X	389	400	-0.74632324	389	400	-0.84982134	3257309	0.24022113	2973231	-0.12586813	experimental	Sigma-Aldrich A9480	AC-55649; 4'-Octyl-4-biphenylcarboxylic acid, 4'-n-octyl	
3263 H21	X	1071	1080	0.24357931	990	1000	0.21547419	3458146	0.54471571	3413083	0.53660988	experimental	Sigma-Aldrich T 7165	Tyrphostin 23; 3,4-(Dihydroxybenzylidene)malononitrile	
3263 H22	X	975	1000	0.10423819	974	1000	0.18711358	3468806	0.56087763	3125036	0.10277122	experimental	Sigma-Aldrich Z 0878	Zaprinast; 1,4-Dihydro-5-(2-propoxyphenyl)-7H-1,2,3-t	
3263 H23	E	1301	1960	0.57741742	1421	2040	0.9794382	76075	-4.5829364	77934	-4.48658629	empty			
3263 H24	P	221268	222520	0.31982925	207162	208760	0.365663243	3488341	0.58746293	3484306	0.64388158	empty			
3263 I01	N	1235	1240	0.4816204	836	840	-0.05749671	3365888	0.40484078	4492973	2.46430143	empty			
3263 I02	E	193	200	-1.03081137	234	240	-1.12456478	76897	-4.58169014	82472	-4.47975143	empty			
3263 I03	X	627	640	-0.40087338	669	680	-0.35351061	3362524	0.39974053	3638110	0.87555137	experimental	Sigma-Aldrich 218359	(-)-Perillic acid; 4-Isopropenyl-1-cyclohexene-1-carboxy	
3263 I04	X	1710	1720	1.17106866	1109	1120	0.42640625	3273908	0.26538734	3159277	0.1543429	experimental	Sigma-Aldrich R 3255	15-cis-retinoic acid; Isotretinoin	
3263 I05	X	789	800	-0.16573523	1071	1080	0.35904979	2994388	-0.15840072	3066746	0.01497841	experimental	Sigma-Aldrich P 6791	Prazosin hydrochloride	
3263 I06	X	551	560	-0.5111851	511	520	-0.63357166	3475157	0.57050656	3520228	0.69798508	experimental	Sigma-Aldrich R 7150	Ro 25-6981 hydrochloride; (R-[R*,S*])-alpha-(4-Hydrox	
3263 I07	X	1028	1040	0.1811661	831	840	-0.06635994	3372501	0.41486693	3299361	0.3653288	experimental	Sigma-Aldrich P 8477	Picotamide; 4-Methoxy-N,N'-bis(3-pyridinylmethyl)-1,3-	
3263 I08	X	663	670	-0.1531265	720	730	-0.9094954	3210917	-1.19493138	3019717	-1.22676488	experimental	Sigma-Aldrich R-1043	Salphar; 6-[2-[4-bis(4-Fluorophenyl)methylene]-1-pi]	
3263 I09	X	912	920	0.01279558	753	760	-0.20461739	2407571	0.46803759	3251387	0.29388393	experimental	Sigma-Aldrich P 8887	Salphar; 6-[2-[4-bis(4-Fluorophenyl)methylene]-1-pi]	
3263 I10	X	831	840	-0.10477349	512	520	-0.63179912	3667008	0.8613772	3201908	0.21855109	experimental	Sigma-Aldrich R-121	Salphar; 6-[2-[4-bis(4-Fluorophenyl)methylene]-1-pi]	
3263 I11	X	673	680	-0.33410576	514	520	-0.62825405	3184827	0.10330215	2763327	-0.44201262	experimental	Sigma-Aldrich P 9547	Prilocaine hydrochloride; N-(2-Methylphenyl)-2-(propyl	
3263 I12	X	551	560	-0.5111851	473	480	-0.70092812	3587099	0.74022494	3122524	0.0989878	experimental	Sigma-Aldrich S 0752	(*)-Synephrine; 4-hydroxy-alpha-(methylamino)methyl	
3263 I13	X	711	720	-0.2789499	473	480	-0.70092812	2624575	-0.71908452	2313971	-1.11880497	experimental	Sigma-Aldrich P-105	(*)-PPHT hydrochloride; (*)-2-(N-Phenylethyl)-N-prop	
3263 I14	X	666	680	-0.34426605	713	720	-0.27551892	3576298	0.72384925	3276706	0.33120724	experimental	Sigma-Aldrich T2952	Tetrabenazine; 9,10-Dimethoxy-1,3,4,6,7,11b-hexahydr	
3263 I15	X	592	600	-0.45167483	592	600	-0.48999606	3159983	0.08811409	2614587	-0.66603565	experimental	Sigma-Aldrich P-126	Piprenone; R-47,465	
3263 I16	X	948	960	-0.45984835	744	750	-0.36497394	3464964	0.70374387	3019319	0.49201764	experimental	Sigma-Aldrich P20108	Phenylbenzene-omega-phosphono-alpha-amino acid; PM	
3263 I17	X	708	720	-0.28330431	592	600	-0.45984835	3159983	0.08811409	2614587	-0.66603565	experimental	Sigma-Aldrich P-126	Piprenone; R-47,465	
3263 I18	X	991	1000	0.12746171	1431	1440	0.99716358	3457846	0.54426087	3492971	0.56099125	experimental	Sigma-Aldrich S 4250	D-Serine; R(-)-2-Amino-3-hydroxypropionic acid	
3263 I19	X	789	800	-0.16573523	709	720	-0.28260908	3231581	0.20121419	3096080	0.05915947	experimental	Sigma-Aldrich Q 0875	Quinidine sulfate	
3263 I20	X	911	920	0.01134411	852	960	0.14811773	3243456	0.49212123	3426810	0.55728464	experimental	Sigma-Aldrich S 7771	(-)-Sulpiride; (-)-5-Aminosulfonyl-N-[(1-ethyl-2-pyrrolid	
3263 I21	X	1018	1040	0.1666514	957	880	-0.02027341	2843630	-0.38696913	2715862	-0.51350148	experimental	Sigma-Aldrich Q-109	Quipazine, 6-nitro-, maleate; 6-Nitro-2-(1-piperziny)-q	
3263 I22	X	4426	4440	5.11326125	5025	5040	7.36766628	2345414	-1.14232829	2671563	-0.58022191	experimental	Sigma-Aldrich I 7160	IMS2186; 3-[1-(3-Hydroxy-4-methoxyphenyl)-meth-(E	
3263 I23	E	1760	1760	0.45984835	744	750	-0.36497394	3464964	0.70374387	3019319	0.49201764	empty			
3263 I24	P	17722	17840	255.921476	268340	269680	474.103592	13616227	0.10212819	3076805	0.03012865	empty			
3263 J01	N	633	640	-0.39216456	715	720	-0.27197385	2991754	-0.1623942	2899034	-0.23761909	empty			
3263 J02	E	192	200	-1.03226284	192	200	-1.19901138	77985	-4.58004059	80434	-4.48282094	empty			
3263 J03	X	1713	1720	1.17542307	1631	1640	1.35167125	3419673	0.48638572	3301165	0.36804588	experimental	Sigma-Aldrich S 9186	SIB 1757; 6-Methyl-2-(phenylazo)-3-pyridinol	
3263 J04	X	542	560	-0.52424833	1343	1360	0.84118021	2621432	-0.72384971	2485088	-0.86107908	experimental	Sigma-Aldrich P0115	PAC-1; (4-Benzylpiperazino)acetic acid (3-allyl-2-hydrox	
3263 J05	X	870	880	-0.04816616	507	520	-0.64066182	3226144	0.19297101	3049786	0.10105657	experimental	Sigma-Aldrich S-143	(*)-6-Chloro-P8 hydrobromide; (*)-SKF-81297 hydrobri	
3263 J06	X	948	960	-0.45984835	744	750	-0.36497394	3464964	0.70374387	3019319	0.49201764	experimental	Sigma-Aldrich P20108	Phenylbenzene-omega-phosphono-alpha-amino acid; PM	
3263 J07	X	2189	2200	0.16663228	1591	1600	1.28859771	3913628	1.23184666	3749695	1.043597117	experimental	Sigma-Aldrich S-1807	SIB 20653; 3-(1-(3-Hydroxy-4-methoxyphenyl)-N-(3-pyridinyl	
3263 J08	X	588	600	-0.45748071	669	680	-0.35351061	2917908	-0.27435418	2827755	-0.34497513	experimental	Sigma-Aldrich T-103	Trifluoperidol hydrochloride; R 2498 hydrochloride; Triper	
3263 J09	X	712	720	-0.27749843	552	560	-0.56089759	3675936	0.87491319	3519515	0.69691121	experimental	Sigma-Aldrich T 1132	Tetraethylthiuram disulfide; Disulfur	
3263 J10	X	632	640	-0.39361603	594	600	-0.48645098	3195360	0.14629853	2822369	-0.35308719	experimental	Sigma-Aldrich H 9415	SHPP-33 ; 5-Hydroxy-(2,6-disiropropylphenyl)-1H-isoind	
3263 J11	X	312	320	-0.85808644	473	480	-0.70092812	3218045	-0.18069189	3459651	0.60674774	experimental	Sigma-Aldrich T 2057	Trequinsin hydrochloride; HL 725	
3263 J12	X	912	920	0.01279558	773	880	0.00808721	2887398	-0.32061124	2629901	-0.64419062	experimental	Sigma-Aldrich S 5317	SKF 95282 dimaleate; N-[3-[3-(1-Piperidinylmethyl)ph	
3263 J13	X	1232	1240	0.47726599	853	760	-0.20461739	3564048	0.70527668	3535455	0.71954847	experimental	Sigma-Aldrich P20123	Avridine; CP 20961, N,N-Dioctadecyl-N,N'-bis(2-hydroxy	
3263 J14	X	589	600	-0.45602924	552	560	-0.56089759	3563037	0.70374387	3013169	-0.06571597	experimental	Sigma-Aldrich N3288	(+)-Norfluramine hydrochloride; JP 92, NSC 43036, t	
3263 J15	X	912	920	0.01279558	593	600	-0.48822352	3920718	1.24603401	3727057	1.10949482	experimental	Sigma-Aldrich T 4425	Trifluoperidol hydrochloride; R 2498 hydrochloride; Triper	
3263 J16	X	589	600	-0.45602924	547	560	-0.56976028	3306064	0.31413995	3043635	-0.01982996	experimental	Sigma-Aldrich P20130	CP-64434 hydrate ; N'-Desmethylazithromycin hydrate	
3263 J17	X	1512	1520	0.8836776	2552	2560	2.98417903	2916299	-0.27679363	2772000	-0.42894988	experimental	Sigma-Aldrich T 5193	Tyrphostin A6 698; Tyrphostin B5	
3263 J18	X	708	720	-0.28330431	784	800	-0.1496687	2895573	-0.3082169	2686464	-0.55777894	experimental	Sigma-Aldrich W 1628	Wortmannin from Penicillium funiculosum	
3263 J19	X	989	1000	0.12455877	791	800	-0.13726094	3221319	0.18565569	2941453	-0.1737302	experimental	Sigma-Aldrich .	Bay 61-3606 hydrochloride hydrochloride; 2-[[7-(3,4-Dimeth	
3263 J20	X	989	1000	0.12455877	629	640	-0.42441214	3263515	0.24963022	3075555	0.02824598	experimental	Sigma-Aldrich X 1251	Xylazine hydrochloride; N-(2,6-Dimethylphenyl)-5,5-dih	
3263 J21	X	988	1000	0.1231073	869	880	0.00999705	2174927	-1.40080838	2079944	-1.47128204	experimental	Sigma-Aldrich P0122	Pifflitrin-mu; PFTmu; 2-Propenyl-1-sulfonamide	
3263 J22	X	857	880	-0.06703527	975	1000	0.18888611	3105408	0.00991979	2987687	-0.10409539	experimental	Sigma-Aldrich Z 2001	Zonisamide sodium; 1,2-Benzisoxazole-3-methanesulfon	
3263 J23	E	1059	1640	0.22616167	1215	1960	0.61429531	75693	-4.58351556	80212	-4.48315553	empty			
3263 J24	P	195281	196360	282.133573	250440	252040	442.375156	3482425	0.58152577	3441508	0.57942187	empty			
3263 K01	N	1074	1080	0.24793372	716	720	-0.27020131	3060839	-0.05765251	4569179	2.27785052	empty			
3263 K02	E	192	200	-1.03226284	114	120	-1.33726937	78457	-4.57932498	87689	-4.47189391	empty			
3263 K03	X	1143	1160	0.34808816	904	92									

3263 O19	X	910	920	0.00989264	667	680	-0.35705569	3457417	0.54361045	3293637	0.35670767	experimental	Sigma-Aldrich Q 2128	(+)-Quisqualic acid; L(+)-alpha-Amino-3,5-dioxo-1,2,4-
3263 O20	X	991	1000	0.12746171	1750	1760	1.56260331	3079806	-0.02889611	3569253	0.77182352	experimental	Sigma-Aldrich S 7936	SB 205384; 4-Amino-7-hydroxy-2-methyl-5,6,7,8-tetra
3263 O21	X	909	920	0.00844117	1387	1400	0.9191719	3048098	-0.0769695	3087599	0.04638591	experimental	Sigma-Aldrich R 0500	Cortexolone; 11-Deoxyoxycort
3263 O22	X	1160	1160	0.35243957	1186	1200	0.5628917	3014860	-0.12736255	3159787	0.15511103	experimental	Sigma-Aldrich S 8502	(-)-Scopolamine methyl bromide; Hyoscine methyl brom
3263 O23	E	955	1680	0.07520879	1985	1640	0.08253382	76874	-4.98172501	1147860	-4.43108207	empty		
3263 O24	P	243254	244800	351.764945	243506	245080	0.304.084375	2746720	-0.53389708	2842446	-0.32284845	empty		
3263 P01	N	837	840	-0.09606467	718	720	-0.26665623	2594649	-0.76445616	2438437	-0.93134194	empty		
3263 P02	E	73	80	-1.20498777	115	120	-1.33549683	72142	-4.58889933	69729	-4.49894415	empty		
3263 P03	X	1411	1440	0.73707912	675	680	-0.34287538	2947558	-0.22940099	2728811	-0.49399849	experimental	Sigma-Aldrich S-006	Ketanserin tartrate; R 41468
3263 P04	X	8986	9000	11.7319646	990	1000	0.21547419	3092972	-0.00893477	2918374	-0.20849037	experimental	Sigma-Aldrich T 7883	Trimethoprim
3263 P05	X	1010	1040	0.15503964	1074	1080	0.36436741	3095639	-0.00489126	3022305	-0.05195589	experimental	Sigma-Aldrich S-153	SQ 22536; 9-(Tetrahydro-2-furanyl)-9H-purin-6-amine
3263 P06	X	834	840	-0.10041908	754	760	-0.20284485	2690468	-0.61918231	2589612	-0.71027847	experimental	Sigma-Aldrich I 2285	IPA-3; 1,1-Diethyl-2-methylpiperazine-2-ol
3263 P07	X	591	600	0.4531263	711	720	-0.279064	3130058	0.04729234	3140938	0.12672183	experimental	Sigma-Aldrich T 0318	Tranilast; SB-252218
3263 P08	X	1634	1640	1.06075694	1834	1840	1.71149652	3188102	0.13529447	2880471	-0.26557754	experimental	Sigma-Aldrich T-113	3-Tropanylindole-3-carboxylate methiodide
3263 P09	X	787	800	-0.16863817	788	800	-0.14257855	2966034	-0.20138901	3026515	-0.04561505	experimental	Sigma-Aldrich T 1512	Tetramisole hydrochloride; (±)-2,3,5,6-Tetrahydro-6-ph
3263 P10	X	2113	2120	1.75601108	1673	1680	1.42611786	1445713	-2.50639005	1439730	-2.43553296	experimental	Sigma-Aldrich .	CP-31398 dihydrochloride hydrate ; N'-2-[2-(4-Methox
3263 P11	X	749	760	-0.22379404	751	760	-0.20816247	3044436	-0.08252156	3178015	0.18256493	experimental	Sigma-Aldrich T 2408	Zalamide
3263 P12	X	553	560	-0.50828216	873	880	0.00808721	2520511	-0.87685885	2654268	-0.60627057	experimental	Sigma-Aldrich U-101	Urapidil, 5-Methyl-, 5-Methyl-6[[3-[4-(o-Methoxyphenyl
3263 P13	X	794	800	-0.15847888	914	920	0.08076128	5950924	-4.3240859	5934692	4.33450217	experimental	Sigma-Aldrich T 4143	Triamterene
3263 P14	X	754	760	-0.21653669	555	560	-0.55557998	2816435	-0.42820023	2869200	-0.28282433	experimental	Sigma-Aldrich U-115	U-101958 maleate; 1-Benzyl-4-aminomethyl-N-[(3'-isop
3263 P15	X	674	680	-0.33265429	554	560	-0.55735252	3088870	-0.01515393	2958552	-0.14797674	experimental	Sigma-Aldrich T 4512	(±)-Taxifolin; Dihydroquercetin
3263 P16	X	554	560	-0.50683069	673	680	-0.34642046	2837640	-0.39605073	2617304	-0.66194347	experimental	Sigma-Aldrich V 8261	(±)-gamma-Vinyl GABA; Vigabatrin
3263 P17	X	914	920	0.01569852	1233	1240	0.646201	2858102	-0.36502773	2681252	-0.56562893	experimental	Sigma-Aldrich T 5568	Tyrphostin AG 835; Tyrphostin B50
3263 P18	X	954	960	0.07375732	1111	1120	-0.279064	2452526	-0.9799328	2168621	-1.33772297	experimental	Sigma-Aldrich P20121	CP-135807 ;
3263 P19	X	672	680	-0.33555723	713	720	-0.4334964	2950501	-0.22493903	3185760	0.194229927	experimental	Sigma-Aldrich P20140	EBPC ; 2,5-Dihydro-4-hydroxy-5-oxo-1-(phenylmethyl)
3263 P20	X	852	860	-0.10322678	859	860	-0.10322678	2477877	-0.9401261	3159787	0.15511103	experimental	Sigma-Aldrich P20143	PCO-008671 ; 2-((4-(5-Ethylpiperidin-4-yl)piiperazin-1-
3263 P21	X	1071	1080	-0.35793931	1070	1080	0.35797725	2821489	-0.42053772	3058177	0.00202702	experimental	Sigma-Aldrich T 7314	1-[2-(Trifluoromethyl)phenyl]imidazole; TRIM
3263 P22	X	1307	1320	0.58612624	987	1000	0.21015657	2740579	-0.54320762	2575870	-0.72434882	experimental	Sigma-Aldrich Z-101	Zimeldine dihydrochloride; (Z)-3-(4-Bromophenyl)-N,N-
3263 P23	E	1517	2400	0.89093495	1225	2080	0.63202069	70091	-4.59200889	76593	-4.48860602	empty		
3263 P24	P	301164	301880	435.819574	292084	292800	516.190742	2476520	-0.94355483	2864122	-0.29020139	empty		
3264 A01	N	518	520	-0.40380193	878	880	0.05514541	2927214	-1.39038573	3606833	0.40517785	empty		
3264 A02	E	116	120	-0.80057641	34	40	-1.40067961	91895	-4.34426024	2083513	-0.98889242	empty		
3264 A03	X	916	920	-0.01097545	1113	1120	0.46049953	2937633	-0.52479443	3654202	0.44852771	experimental	MicroSource	ALLYLTHIOUREA
3264 A04	X	709	720	-0.11527678	1550	1560	-0.21428575	2976865	-0.87895037	3986637	0.63302807	experimental	MicroSource	MALATHION
3264 A05	X	2332	2240	1.28791812	1190	1200	0.59331769	2784934	-0.72974253	2734735	-0.39292491	experimental	MicroSource	TIRATRICOL
3264 A06	X	1470	1480	0.53582321	631	640	-0.37090765	2719254	-0.8178963	3387814	0.20474204	experimental	MicroSource	ITOPRIDE HYDROCHLORIDE
3264 A07	X	709	720	-0.2152847	793	800	-0.09147204	3300985	-0.03711406	99352	-2.80470253	experimental	MicroSource	PIPERONYL BUTOXIDE
3264 A08	X	1833	1840	0.89410464	712	720	-0.23118984	2673851	-0.87883487	3291234	0.1163566	experimental	MicroSource	DIMETRIDAZOLE
3264 A09	X	951	960	0.02356959	1233	1240	0.66748887	3247889	-0.10837795	3453777	0.26510825	experimental	MicroSource	CARGLUMIC ACID
3264 A10	X	713	720	-0.21133667	830	840	-0.02765033	2843549	-0.6510712	95365	-2.80835124	experimental	MicroSource	NICOPHOLINE
3264 A11	X	1000	1000	0.06997678	830	840	-0.02765033	3174443	-0.56565981	3292231	0.08428522	experimental	MicroSource	DIFLOXALIN HYDROCHLORIDE
3264 A12	X	834	840	-0.09190955	632	640	-0.36493274	2944232	-0.51593744	3990206	0.75785259	experimental	MicroSource	SORBITOL
3264 A13	X	1034	1040	0.10549069	832	840	-0.0242005	3052807	-0.37021127	3450739	0.26232802	experimental	MicroSource	DEXFOSFOSERINE
3264 A14	X	633	640	-0.29029679	1034	1040	0.32423155	2936716	-0.5260252	3382753	0.200111045	experimental	MicroSource	PAROXYPROPRIONE
3264 A15	X	954	960	0.02653059	672	680	-0.30018629	3163061	-0.2222316	3502387	0.30959382	experimental	MicroSource	THYMOPENTIN
3264 A16	X	952	960	0.02455659	911	920	0.11206748	3289406	-0.05265506	3435386	0.24827768	experimental	MicroSource	OXINIAIC ACID
3264 A17	X	1231	1240	0.29992992	1592	1600	1.28673198	3315668	-0.01740697	3415096	0.22970923	experimental	MicroSource	BENZOCICLINE
3264 A18	X	1112	1120	0.18247678	830	840	-0.02765033	3174443	-0.56565981	3292231	0.08428522	experimental	MicroSource	PROCOXAZOLE
3264 A19	X	832	840	-0.09387855	1153	1160	0.52495998	2201992	-0.16592354	3950866	0.17758036	experimental	MicroSource	DARIFENACIN HYDROBROMIDE
3264 A20	X	711	720	-0.2133107	752	760	-0.1621934	3208239	-0.16159502	4239607	0.98426262	experimental	MicroSource	NITARSONE
3264 A21	X	1153	1160	0.22294383	913	920	0.1155173	3420925	0.12386588	3093400	-0.0646917	experimental	MicroSource	MEPARYLON
3264 A22	X	1031	1040	0.10252968	952	960	0.18278884	2874083	-0.01608937	3712464	0.50184633	experimental	MicroSource	PICOLAMINE
3264 A23	E	641	1000	-0.28240078	782	1160	-0.11044606	94765	-4.34040821	91008	-2.81233856	empty		
3264 A24	P	121959	122240	119.45861	128321	128720	219.882999	2860049	-0.62892539	4047987	0.80890108	empty		
3264 B01	N	476	480	-0.44525598	714	720	-0.22774002	2594128	-0.98583673	2972653	-0.17519363	empty		
3264 B02	E	76	80	-0.84005646	36	40	-1.39722979	98567	-4.33530528	2980637	-0.16788705	empty		
3264 B03	X	634	640	-0.28930979	671	680	0.3019112	2486280	-1.13058714	2202666	-0.87984924	experimental	MicroSource	ISOWALERAMIDE
3264 B04	X	513	520	-0.40873693	1267	1280	0.72613585	3133048	-0.26251416	3968194	0.73587831	experimental	MicroSource	QUINAPRILAT
3264 B05	X	427	440	-0.49361904	1348	1360	0.86585366	2716665	-0.82137118	3824810	0.60466007	experimental	MicroSource	IMEXON
3264 B06	X	631	640	-0.29227079	989	1000	0.24661055	3789432	0.61846513	4371869	1.10530254	experimental	MicroSource	BETAXALOL HYDROCHLORIDE
3264 B07	X	628	640	-0.2952318	1069	1080	0.38460344	2817229	-0.68639713	3805657	0.58713215	experimental	MicroSource	CINOCITRAMIDE
3264 B08	X	830	840	-0.09585756	591	600	-0.43990409	2602865	-0.97411019	4024242	0.78717078	experimental	MicroSource	ERYTHROMYCIN STEARATE
3264 B09	X	511	520	-0.41071094	708	720	-0.23808949	3322310	-0.00849228	3234112	0.064081263	experimental	MicroSource	MELGLUTOL
3264 B10	X	314	320	-0.60515017	832	840	-0.0242005	2000704	-1.78231296	3400953	0.21676623	experimental	MicroSource	FENOLDIPAM MESYLATE
3264 B11	X	194	200	-0.72359032	630	640	-0.37263256	1822259	-0.02181659	97677	-2.80623541	experimental	MicroSource	TIOPRONIN
3264 B12	X	193	200	-0.72457732	512	520	-0.57617208	1993385	-1.79213631	4446721	1.21040964	experimental	MicroSource	TERPENE HYDRATE
3264 B13	X	433	440	-0.48769703	1153	1160	0.52949598	1647270	-2.25668168	2999973	-0.15019166	experimental	MicroSource	TOLONIUM CHLORIDE
3264 B14	X	392	400	-0.52816408	629	640	-0.37435747	2736556	-0.79467406	91248	-2.81211892	experimental	MicroSource	SODIUM MONOFLUOROPHOSPHATE
3264 B15	X	426	440	-0.49460604	705	720	-0.24326422	2709757	-0.83064289	2971512	-0.17623789	experimental	MicroSource	TRICLOSENE POTASSIUM
3264 B16	X	591	600	-0.31750678	830	840	-0.02765033	3174443	-0.56565981	3292231	0.08428522	experimental	MicroSource	BENZYL ALCOHOL
3264 B17	X	871	880	-0.05539051	1108	1120	0.45187498	3688320	-0.48275558	3716130	0.50520102	experimental	MicroSource	TRICLOSENE
3264 B18	X	670	680	-0.25377775	790	800	-0.09664677	3846683	0.69530574	3313999	0.13719005	experimental	MicroSource	GUANIDINE HYDROCHLORIDE
3264 B19	X	829	840	-0.09684456	790	800	-0.09664677	3963952	0.85270074	3563352	0.3653863	experimental	MicroSource	ETHANOLAMINE OLEATE
3264 B20	X	1266	1280	0.33447496	785	800	-0.10527133							

3264 C13	X	711	720	-0.2133107	472	480	-0.64516852	3523850	0.26200878	3353166	0.17303383	experimental	MicroSource	01502345	URACIL
3264 C14	X	1267	1280	0.33546197	707	720	-0.2398144	3247208	-0.10929197	3260613	0.08833371	experimental	MicroSource	01301024	D-(+)-MALTOSE
3264 C15	X	2790	2800	1.83866478	2831	2840	3.42389692	3840443	0.68693059	97882	-2.8060478	experimental	MicroSource	01506199	MEXENONE
3264 C16	X	826	840	-0.09805556	624	640	-0.38298203	3355270	0.0362253	3653799	0.36579517	experimental	MicroSource	01506556	TRILLOSTANE
3264 C17	X	748	760	-0.17879165	910	920	0.11034257	3855851	0.70761076	3304386	0.12839269	experimental	MicroSource	01502551	DOBROBUTANOL
3264 C18	X	711	720	-0.2133107	671	680	-0.3019112	3529056	0.26899612	93391	-2.81015775	experimental	MicroSource	01503320	TIMONACIC
3264 C19	X	986	1000	0.05811463	705	720	-0.24326422	3858840	0.7116225	3588369	0.38828047	experimental	MicroSource	01506176	PIMAGEDINE HYDROCHLORIDE
3264 C20	X	2431	2480	1.48433136	2118	2840	3.40147307	3394029	0.08776686	3820994	0.60116785	experimental	MicroSource	01504286	FEBUXOSTAT
3264 C21	X	865	880	-0.06131251	2805	1120	0.44670024	5275377	2.61285679	3648699	0.44349163	experimental	MicroSource	01504305	PROFLAVINE HEMISULFATE
3264 C22	X	1231	1240	0.29992992	629	640	-0.37435747	3144443	-0.24722013	3700561	0.49095327	experimental	MicroSource	01505497	SOLIFENACIN SUCCINATE
3264 C23	E	379	600	-0.54099509	635	920	-0.364008	99110	-4.33457648	2681273	-0.4418508	empty			
3264 C24	P	73050	73560	71.1853667	95794	96400	163.775814	3450607	0.16370418	4040405	0.80180224	empty			
3264 D01	N	277	280	-0.64166922	1273	1280	0.73648532	1545029	-2.39390654	3377019	0.19486297	empty			
3264 D02	E	38	40	-0.8775625	73	80	-1.33340808	96215	-4.33846207	2717100	-0.40906362	empty			
3264 D03	X	355	360	-0.56468312	913	920	0.1155173	2082804	-1.67212076	3970787	0.7382513	experimental	MicroSource	01503870	VALGANICLOVIR HYDROCHLORIDE
3264 D04	X	314	320	-0.60515017	868	880	0.0378963	2434287	-1.20037062	3796362	0.57862581	experimental	MicroSource	01506164	IDRAMANTONE
3264 D05	X	471	480	-0.45019098	1350	1360	0.86930348	2932915	-0.53112679	31116737	-0.04333478	experimental	MicroSource	01503875	PROCTONE OLAMINE
3264 D06	X	835	840	-0.09092255	788	800	-0.1009966	3115501	-0.28606523	3352543	0.17246369	experimental	MicroSource	01506103	ALLYLSIOTHIOCYANATE
3264 D07	X	386	400	-0.53408609	1148	1160	0.52087143	3093807	-0.31518228	2410757	-0.68941422	experimental	MicroSource	01503831	DROSPIRONONE
3264 D08	X	1192	1200	0.26143688	1032	1040	0.32078173	3584334	0.34318863	3556036	0.35869084	experimental	MicroSource	01506196	ISOBUTAMBEN
3264 D09	X	749	760	-0.17580465	549	560	-0.51235036	3443149	0.15369427	2865210	-0.27352037	experimental	MicroSource	01503832	ECAMSULE TRIETHANOLAMINE
3264 D10	X	792	800	-0.1333636	673	680	-0.29846138	3868781	0.72496502	3978472	0.74528425	experimental	MicroSource	01506162	FLURXENE
3264 D11	X	593	600	-0.32977684	433	440	-0.71244006	3530894	0.27146303	3692799	0.48384986	experimental	MicroSource	01503834	GADOTERICIDOL
3264 D12	X	469	480	-0.45216499	510	520	-0.5796219	3415658	0.11679666	4004665	0.76925484	experimental	MicroSource	01505462	SULISALBENZONE
3264 D13	X	472	480	-0.44920398	594	600	-0.43472936	3515008	0.25014131	3907960	0.68050792	experimental	MicroSource	01503836	IOTHALMIC ACID
3264 D14	X	711	720	-0.2133107	671	680	-0.50899053	3404364	0.95967878	3892156	0.66157084	experimental	MicroSource	01506154	ALLYLSIOTHIOCYANATE
3264 E15	X	746	760	-0.17876566	986	1000	0.24143582	3597354	0.36066369	3405459	0.25658086	experimental	MicroSource	01503838	IODINE
3264 D16	X	827	840	-0.09881856	831	840	-0.02592541	3669535	0.4575429	4208504	0.95579863	experimental	MicroSource	01506123	MODALINE SULFATE
3264 D17	X	1550	1560	0.6147833	1030	1040	0.31733191	3062195	-0.35761098	3629070	0.4255281	experimental	MicroSource	01503840	MANGAFODIPIR TRISODIUM
3264 D18	X	589	600	-0.33372484	631	640	-0.37090765	3857271	0.70951664	4244559	0.98870294	experimental	MicroSource	01506157	NKETHAMIDE
3264 D19	X	753	800	-0.17185665	699	720	-0.25361369	4162232	1.11882632	100095	-2.80402257	experimental	MicroSource	01503841	METHYLCLOTHIAZIDE
3264 D20	X	13746	13760	12.6522499	5105	5120	7.34634491	2671802	-0.88158497	4652944	1.36252906	experimental	MicroSource	01502267	VORINOSTAT
3264 D21	X	633	680	-0.29029679	858	880	0.02064719	3309853	-0.02521169	3243539	0.07270884	experimental	MicroSource	01503842	NEVIRAPINE
3264 D22	E	824	840	-0.09684454	832	840	-0.09684454	3375004	0.06301808	3643098	0.06301808	experimental	MicroSource	01502341	TAZOBACTAM
3264 D23	E	483	720	-0.43834697	345	560	-0.86423224	101903	-4.3308278	2461425	-0.64304527	empty			
3264 D24	P	78984	79480	77.0422338	71309	71840	121.542364	3270498	-0.07803282	3589840	0.38962666	empty			
3264 E01	N	516	520	-0.40577593	1192	1200	0.59676752	2805499	-0.70214079	3588038	0.38797756	empty			
3264 E02	E	76	80	-0.84005646	74	80	-1.33168317	96369	-4.33825537	2749636	-0.37928822	empty			
3264 E03	X	755	760	-0.16988265	792	800	-0.09319695	4480326	1.54576273	3863830	0.64036932	experimental	MicroSource	01506166	PICONOL
3264 E04	X	633	640	-0.29029679	990	1000	0.24833546	9185287	7.86062295	3593249	0.39274642	experimental	MicroSource	01506174	HYMECHROME
3264 E05	X	840	840	-0.09190955	758	840	-0.09190955	3991553	0.89156233	3161051	0.61577088	experimental	MicroSource	03070854	LIMONENE
3264 E06	X	510	520	-0.41169794	950	760	-0.16564322	3478466	0.20109571	3507470	0.31424554	experimental	MicroSource	01506178	LEVYCLOSERINE
3264 E07	X	833	840	-0.09289655	591	600	-0.43990409	3787804	0.61628008	3478535	0.28776556	experimental	MicroSource	1502400	ESTRADIOL DIPROPIONATE
3264 E08	X	950	960	0.02258259	511	520	-0.57789699	3385863	0.07680669	3587561	0.38754103	experimental	MicroSource	1505458	PHENISUCCIMIDE
3264 E09	X	711	720	-0.2133107	752	760	-0.16046849	4350797	1.37191272	3882152	0.65713675	experimental	MicroSource	300047	ANISODAMINE HYDROBROMIDE
3264 E10	X	713	720	-0.2113367	753	760	-0.1621934	3409805	0.10894904	3639208	0.43480591	experimental	MicroSource	1504815	MILNACIPRAN HYDROCHLORIDE
3264 E11	X	430	440	-0.49065803	471	480	-0.64689343	3747049	0.56157991	3502520	0.30971554	experimental	MicroSource	1505808	OXDRINE
3264 E12	X	1920	1920	0.32104983	1954	1960	1.91114983	3559390	0.30979953	3746742	0.30168023	experimental	MicroSource	1504282	DEXLANISOPROZOLE
3264 E13	X	989	1000	0.06107563	508	520	-0.58307172	4213547	1.18769988	3760223	0.54555311	experimental	MicroSource	1301027	LACTUL
3264 E14	X	711	720	-0.2133107	673	680	-0.29846138	1957834	-1.83985182	3304702	0.12868188	experimental	MicroSource	1504140	BUTOXANAZOLE
3264 E15	X	550	560	-0.37221789	511	520	-0.57789699	4426332	1.47329357	2638756	-0.48076034	experimental	MicroSource	1506107	SULFACARBAMIDE
3264 E16	X	1150	1160	0.21998283	511	520	-0.57789699	3414518	0.11526569	3536641	0.34094146	experimental	MicroSource	1503084	INAMINONE
3264 E17	X	1188	1200	0.25748887	1192	1200	0.59676752	4041387	0.95663172	3511577	0.31800407	experimental	MicroSource	1506106	SULBENTINE
3264 E18	X	670	680	-0.25377775	631	640	-0.37090765	3625610	0.39858806	3563674	0.36568078	experimental	MicroSource	1506104	HYDROXYTOLUIC ACID
3264 E19	X	830	840	-0.09585756	671	680	-0.3019112	4045932	0.96273188	3418865	0.23315844	experimental	MicroSource	1508161	HEXYLENE GLYCOL
3264 E20	X	673	720	-0.25081674	858	880	0.02064719	3445769	0.15721076	3464381	0.27481253	experimental	MicroSource	1506185	PIDOLIC ACID
3264 E21	X	871	880	-0.0539051	631	640	-0.37090765	3436746	0.14510036	3433420	0.24647849	experimental	MicroSource	1506124	ADRENOLONE HYDROCHLORIDE
3264 E22	X	1070	1080	0.14102273	631	640	-0.37090765	3309068	-0.0262653	3234380	0.06432652	experimental	MicroSource	1505125	ALLCLOMETAZONE DIPROPIONATE
3264 E23	E	551	840	-0.37123089	265	520	-1.00222514	100521	-4.33268268	2811774	-0.32242247	empty			
3264 E24	P	96630	97200	94.4588569	85789	86280	146.519078	3682803	0.47535082	4095282	0.5218322	empty			
3264 F01	N	1156	1160	0.22590483	1274	1280	0.73821023	3719910	0.52515475	3882173	0.65715599	empty			
3264 F02	E	114	120	-0.80255041	33	40	-1.40240453	94656	-4.34055451	2679067	-0.44388962	empty			
3264 F03	X	713	720	-0.2113367	874	880	0.04824577	3188355	-0.18828274	3114525	-2.79081692	experimental	MicroSource	1503869	ACETOPHENAZINE MALEATE
3264 F04	X	553	560	-0.36925689	631	640	-0.37090765	4005812	0.908884	3457238	0.26827556	experimental	MicroSource	1503425	ESZOPICLONE
3264 F05	X	592	600	-0.33076384	590	600	-0.44162901	3414215	0.11485991	3542209	0.34603703	experimental	MicroSource	1503862	AZATADINE MALEATE
3264 F06	X	874	880	-0.0524295	872	880	0.04479594	3707567	0.50879013	93838	-2.80974868	experimental	MicroSource	1505727	MELENGESTROL ACETATE
3264 F07	X	554	560	-0.37123089	672	680	-0.30018629	3414706	0.11551892	3860790	0.63758726	experimental	MicroSource	1503863	BEMOTRIZINOL
3264 F08	X	550	560	-0.37221789	593	600	-0.43645427	4132651	1.07912357	3964471	0.7324712	experimental	MicroSource	1505740	LIPOMIDE
3264 F09	X	752	760	-0.17284365	592	600	-0.43817918	3605650	0.37179834	3916936	0.68896942	experimental	MicroSource	1503866	BISACOTRIZOLE
3264 F10	X	553	560	-0.36925689	754	760	-0.18741357	4150976	1.10371885	3746746	0.53118063	experimental	MicroSource	1401414	CRESOPRINE
3264 F11	X	73	80	-0.84301746	73	80	-1.3340808	1161691	-2.98894176	3914365	0.68661656	experimental	MicroSource	1503887	CANDICIDIN
3264 F12	X	749	760	-0.17580465	668	680	-0.30708594	3807101	0.6458217994	3405842	0.22124041	experimental	MicroSource	1	

3264 K01	N	596	600	-0.32681584	874	880	0.04824577	3241752	-0.11661485	4005294	0.76983047	empty		
3264 K02	E	36	40	-0.8795365	72	80	-1.33513299	94190	-4.34117996	3639621	0.43518387	empty		
3264 K03	X	554	560	-0.36826989	1630	1640	1.35227861	3968398	0.85861434	3242091	0.07138326	experimental	MicroSource	1301015 CYCLAMIC ACID
3264 K04	X	954	960	0.02552359	1306	1320	0.79340739	2655672	-0.90323419	3571547	0.37289577	experimental	MicroSource	1502034 NEFAZODONE HYDROCHLORIDE
3264 K05	X	432	440	-0.48868403	585	600	-0.45025356	4064649	0.92074476	3454389	0.26566833	experimental	MicroSource	1301016 DEHYDROACETIC ACID
3264 K06	X	635	640	-0.28832279	872	880	0.04479594	3165380	-0.2191191	3207777	0.03998071	experimental	MicroSource	1502325 PRASUGREL
3264 K07	X	393	400	-0.52717708	591	600	-0.43990409	5066720	2.3328035	1829314	-1.22152329	experimental	MicroSource	1505082 CYCLANDLATE
3264 K08	X	714	720	-0.21034969	792	800	-0.09319695	3971427	0.86273346	3244609	0.07368761	experimental	MicroSource	1502330 QUINESTROL
3264 K09	X	433	440	-0.48769703	591	600	-0.43990409	4183359	1.14718236	3318152	0.14099068	experimental	MicroSource	1505903 CYROMAZINE
3264 K10	X	675	680	-0.24884274	1034	1040	0.32423155	3485166	0.21008826	3484489	0.29321442	experimental	MicroSource	1502332 RACTOPAMINE HYDROCHLORIDE
3264 K11	X	592	600	-0.33076384	552	560	-0.50717563	3412715	0.11284666	3199324	0.03224493	experimental	MicroSource	1502382 CYCLANDLATE
3264 K12	X	512	520	-0.40972394	551	560	-0.50890054	3306763	-0.029359	1769165	-1.27605632	experimental	MicroSource	1502333 RASAGILINE
3264 K13	X	1194	1200	0.26341088	952	960	0.18278884	3790844	0.62306207	3310448	0.13394034	experimental	MicroSource	1503871 TRAVOPROST
3264 K14	X	833	840	-0.09289655	631	640	-0.37090765	3309548	-0.02562106	3975341	0.74241891	experimental	MicroSource	1502334 ROXATIDINE ACETATE HYDROCHLORIDE
3264 K15	X	552	560	-0.37024389	712	720	-0.23118984	2614621	-0.95833163	3340676	0.16160358	experimental	MicroSource	1502275 DASATINIB
3264 K16	X	832	840	-0.09388355	514	520	-0.57272225	3630995	0.40581565	2999198	-0.15090009	experimental	MicroSource	1502336 SERATODAST
3264 K17	X	710	720	-0.2142977	513	520	-0.57444717	2819639	-0.6831625	1737402	-1.3056368	experimental	MicroSource	1504143 ARTENIMOL
3264 K18	X	1751	1760	0.81317054	830	840	-0.02765033	3590710	0.35174631	3391613	0.20821871	experimental	MicroSource	1502350 IDOXURIDINE
3264 K19	X	867	880	-0.05933851	672	680	-0.30018629	4401122	-1.43945745	92377	-2.81108572	experimental	MicroSource	1504525 CROTIC ACID
3264 K20	X	829	840	-0.09684456	512	520	-0.57617208	3639018	0.41658388	1605198	-1.42662364	experimental	MicroSource	1502357 LOFEXIDINE HYDROCHLORIDE
3264 K21	X	1067	1080	0.13806173	671	680	-0.3019112	3862496	0.71652948	3003079	-0.1473492	experimental	MicroSource	1500819 BERGENIN
3264 K22	X	1548	1560	0.6128093	1112	1120	0.45877462	3648033	0.42868355	87576	-2.81547936	experimental	MicroSource	1502373 RAMOPLANIN [A2 shown; 2mM]
3264 K23	E	634	1040	-0.28930979	451	720	-0.68139166	100408	-4.33283435	3798493	0.580576	experimental	MicroSource	
3264 K24	P	136648	137120	133.956671	89831	90400	153.491168	3886630	0.74919523	3682191	0.47414192	empty		
3264 L01	N	997	1000	0.06897164	1234	1240	0.66921379	3036867	-0.39160547	4166715	0.91755532	empty		
3264 L02	E	76	80	-0.84005656	33	33	-1.40246453	92464	-4.34349555	376748	0.39959844	empty		
3264 L03	X	353	360	-0.56665713	1149	1160	0.52596334	1979967	-1.81014555	2991617	-0.15783868	experimental	MicroSource	1505751 ERYTHROSINE SODIUM
3264 L04	E	785	800	-0.14027261	1260	1280	0.71406148	3241074	-0.11752484	4294410	0.10344173	empty		
3264 L05	X	434	440	-0.48671003	1190	1200	0.59331769	2861791	-0.62568733	3789199	0.57207057	experimental	MicroSource	1505679 TETRAMIZOLE HYDROCHLORIDE
3264 L06	E	433	440	-0.48769703	830	840	-0.02765033	2867461	-0.61897722	2905723	-0.23644479	experimental	MicroSource	
3264 L07	X	674	680	-0.24982974	632	640	-0.36918274	2850906	-0.64119685	3359900	0.17919647	experimental	MicroSource	1300019 OXIGLUTATION DISODIUM SALT
3264 L08	E	474	480	-0.44722998	673	680	-0.29846138	3067044	-0.35110279	3865369	0.64177774	empty		
3264 L09	X	354	360	-0.56567012	513	520	-0.57444717	2654056	-0.90540313	3752708	0.53867574	experimental	MicroSource	1505678 TICARCILLIN DISODIUM
3264 L10	X	474	480	-0.44722998	513	520	-0.57444717	2848467	-0.64374592	480	-0.26292978	experimental	MicroSource	
3264 L11	X	355	360	-0.56468312	593	600	-0.43645427	1682490	-2.20941043	3270549	0.09742667	experimental	MicroSource	1505682 TOCAMPHEPINE CITRATE
3264 L12	E	515	520	-0.40676293	1032	1040	0.32078173	3141163	-0.25162245	3979386	0.7461207	empty		
3264 L13	X	152	160	-0.76504437	711	720	-0.23291475	1306258	-2.71437795	3455656	0.26682782	experimental	MicroSource	1505691 PENFLURIDOL
3264 L14	E	232	240	-0.68608427	552	560	-0.50717563	1846303	-1.98954544	2757532	-0.37206217	experimental	MicroSource	
3264 L15	X	314	320	-0.60515017	593	600	-0.43645427	1833935	-2.00614541	3398065	0.21412327	experimental	MicroSource	1505850 AMPYZINE SULFATE
3264 L16	E	551	560	-0.37123089	553	560	-0.50545072	2359390	-1.30089517	93545	-2.81001682	empty		
3264 L17	X	120	120	-0.86469856	349	360	-0.65733238	1102944	-3.98726002	3812509	0.4953144	experimental	MicroSource	1505902 DORAMECTIN
3264 L18	E	669	680	-0.25476475	913	920	0.1155173	2757184	-0.76698777	3604742	0.40326427	empty		
3264 L19	X	1030	1040	0.10154268	710	720	-0.23463967	3085839	-0.32587669	3047364	-0.10682166	experimental	MicroSource	1504914 LEVOCETIRIZINE DIHYDROCHLORIDE
3264 L20	E	866	880	-0.06032551	913	920	0.1155173	3677151	0.46776487	3384031	0.20128002	experimental	MicroSource	
3264 L21	X	1305	1320	0.37296801	591	600	-0.43990409	3054059	-0.36853088	2932911	-0.21156362	experimental	MicroSource	1504912 OSELTAMIVIR PHOSPHATE
3264 L22	E	1067	1080	0.13806173	791	800	-0.09492186	4203036	1.17359225	3251595	0.08008087	empty		
3264 L23	E	383	600	-0.53704709	458	760	-0.66931728	99685	-4.33804073	3391770	0.20836238	empty		
3264 L24	P	71327	72000	69.4847356	101709	102160	173.976653	3221542	-0.14374012	2319111	-0.92629781	empty		
3264 M01	N	435	440	-0.48572303	1113	1120	0.46409953	3088546	-0.32244344	98163	4.40879064	empty		
3264 M02	E	115	120	-0.80156341	74	80	-1.33168317	93036	-4.34272883	2493290	-0.61388393	empty		
3264 M03	X	907	920	-0.01985846	705	720	-0.24326422	2078496	-1.67790283	3534191	0.33869933	experimental	MicroSource	1300042 SODIUM TETRADECYL SULFATE
3264 M04	X	3431	3440	2.47133255	3067	3080	3.83097595	3412204	0.11216081	3459628	0.27046281	experimental	MicroSource	1502410 ABACAVIR SULFATE
3264 M05	X	560	560	-0.3771529	782	800	-0.11044606	3040278	-0.38702733	3247587	0.07641294	experimental	MicroSource	1505774 OXELAININ CITRATE
3264 M06	X	514	520	-0.40774993	591	600	-0.43990409	3412338	0.11234066	3909550	0.6822101	experimental	MicroSource	1502414 BAL SALAZIDE DISODIUM
3264 M07	X	633	640	-0.29029679	593	600	-0.43645427	3729457	0.53796845	33754072	0.539924	experimental	MicroSource	1505785 CAMLYOFINE DIHYDROCHLORIDE
3264 M08	X	473	480	-0.44821698	593	600	-0.43645427	3302421	-0.03518671	3812509	0.59340278	experimental	MicroSource	1502422 CEFMENOXIME HYDROCHLORIDE
3264 M09	X	714	720	-0.21034969	472	480	-0.64516852	3253134	-0.10133827	4026593	0.78932231	experimental	MicroSource	1504623 FTALIDEX
3264 M10	X	795	800	-0.1304026	715	720	-0.22601511	3499565	0.22941417	4040317	0.80188186	experimental	MicroSource	1502366 FASUDIL HYDROCHLORIDE
3264 M11	X	153	160	-0.76405736	152	160	-1.1971401	1758931	-2.10681357	3932491	0.70320462	experimental	MicroSource	1504502 BITOSCANATE
3264 M12	X	714	720	-0.21034969	713	720	-0.22946493	3374019	0.06091002	4229822	0.97530786	experimental	MicroSource	1502368 ACEGLUTAMIDE
3264 M13	X	712	720	-0.2123237	511	520	-0.57789699	3837763	0.68333358	90540	-2.81276685	experimental	MicroSource	1503711 ORBIFLOXACIN
3264 M14	X	1434	1440	0.50029117	633	640	-0.36745783	3183459	-0.194854	5078008	1.75152748	experimental	MicroSource	1502328 PRULIFLOXACIN
3264 M15	X	543	560	-0.3791269	633	640	-0.36745783	3183459	-0.194854	5078008	1.75152748	experimental	MicroSource	1505762 PRRITINOL
3264 M16	X	1671	1680	0.73421045	870	880	0.04134612	1817862	-2.02771812	86382	-2.81657206	experimental	MicroSource	1502329 PYRONARIDINE TETRAPHTHOSPHATE
3264 M17	X	1551	1560	0.61577031	719	720	-0.23118984	3169299	-0.21385914	3391752	0.20834591	experimental	MicroSource	1504510 CHINIOFON
3264 M18	X	789	800	-0.1363246	586	600	-0.44852865	4123178	0.106640919	2094783	-0.97857865	experimental	MicroSource	1502335 RUFLOXACIN HYDROCHLORIDE
3264 M19	X	868	880	-0.05835151	1032	1040	0.32078173	3681426	0.47350265	3722160	0.51071965	experimental	MicroSource	1504616 METOPROLOL
3264 M20	X	1547	1560	0.6118223	719	720	-0.23118984	3169299	-0.21385914	3391752	0.20834591	experimental	MicroSource	1502344 TROPISERON HYDROCHLORIDE
3264 M21	X	2104	2120	1.16158197	462	480	-0.64516852	3253134	-0.10133827	4026593	0.78932231	experimental	MicroSource	1505083 PRASTERONE
3264 M22	X	1026	1040	0.09759468	510	520	-0.57789699	3837763	0.68333358	90540	-2.81276685	experimental	MicroSource	1502349 DIMINAZENE ACETURATE
3264 M23	E	558	840	-0.36432188	486	680	-0.61101977	97751	-4.33640049	3610553	0.40858222	empty		
3264 M24	P	94114	94760	91.9755619	64138	64760	109.173026	3658187	0.44231195	4142992	0.89584516	empty		
3264 N01	N	556	560	-0.36629588	1192	1200	0.59676752	2796897	-0.71368615	4464241	1.17336427	empty		
3264 N02	E	116	120	-0.80057641	33	40	-1.40240453	91427	-4.34488838	3458035	0.26900497	empty		
3264 N03	X	552	560	-0.37024389	910	920	0.11034257	2800930	-0.70827317	3589409	0.38923223			

3264 N19	X	871	880	-0.05539051	789	800	-0.09837168	2500782	-1.11112299	3750290	0.5364629	experimental	MicroSource	1504506	CHLORAMINE-T
3264 N20	E	741	760	-0.18370066	1031	1040	0.31905682	2961451	-0.49282661	3477441	0.28676442	empty			
3264 N21	X	1504	1520	0.56938125	1068	1080	0.38287853	3006140	-0.43284635	3235530	0.06537894	experimental	MicroSource	1503680	SEVOFLURANE
3264 N22	E	744	760	-0.18073966	1390	1400	0.01829993	3105428	-0.24958491	3184965	0.02825788	empty			
3264 N23	X	597	1040	-0.32582883	508	840	-0.58307172	98822	-0.33496303	3292191	0.11723204	empty			
3264 N24	P	149428	150240	146.570546	111421	111920	190.732001	3271898	-0.07615378	3148234	-0.01451022	empty			
3264 O01	N	715	720	-0.20936269	1552	1560	1.21773554	2790463	-0.72232167	3172957	0.00811151	empty			
3264 O02	E	35	40	-0.88052351	70	80	-1.33858281	90918	-4.34557154	4981253	1.66298189	empty			
3264 O03	X	753	760	-0.17185665	1073	1080	0.39150309	3657934	0.44197238	3802672	0.58440042	experimental	MicroSource	330058	CHLORPYRIFOS
3264 O04	X	1511	1520	0.57629026	743	760	-0.1777176	2548623	-1.0469122	3503168	0.31030855	experimental	MicroSource	1502303	LOMERIZINE HYDROCHLORIDE
3264 O05	X	909	920	-0.01788446	705	720	-0.24326422	3688996	0.48366288	2973109	-0.17477632	experimental	MicroSource	1504507	CHLORINDIONE
3264 O06	X	752	760	-0.17284365	1269	1280	0.72958568	3109816	-0.29369547	3066201	-0.08949142	experimental	MicroSource	1506027	OXOLAMINE CITRATE
3264 O07	X	551	560	-0.37123089	550	560	-0.51062545	3491756	0.21893316	90155	-2.81311918	experimental	MicroSource	1504505	CARZENIDE
3264 O08	X	789	800	-0.1363246	671	680	-0.3019112	3276601	-0.06984155	3112837	-0.04690388	experimental	MicroSource	330068	PYRTHRINS
3264 O09	X	2231	2240	1.28693112	872	880	0.04479594	3711784	0.51424827	2348301	-0.74657099	experimental	MicroSource	1504518	EFLOXATE
3264 O10	X	1165	1200	0.23478784	614	640	-0.40023114	2991240	-0.45284469	83382	-2.81931751	experimental	MicroSource	1506049	meta-CRESYL ACETATE
3264 O11	X	8507	8520	7.48135061	6993	7000	10.6029772	5183369	2.48936636	2735343	-0.39236849	experimental	MicroSource	1505168	ETHALRIDINE LACTATE
3264 O12	X	1648	1680	0.71150942	694	720	-0.26223824	3184828	-0.19301657	3730333	0.5181992	experimental	MicroSource	1506085	CLORGRILINE HYDROCHLORIDE
3264 O13	X	829	840	-0.09684456	791	800	-0.09492185	3921788	0.79610946	3239021	0.06857374	experimental	MicroSource	1504617	ISAXONINE
3264 O14	X	830	840	-0.09585756	632	640	-0.36918274	2932651	-0.53148112	3498048	0.30562297	experimental	MicroSource	1506078	MOROXYDINE HYDROCHLORIDE
3264 O15	X	946	960	0.01863458	590	600	-0.44162901	3568410	0.3218159	2462393	-0.6421594	experimental	MicroSource	1504515	DIACETAMATE
3264 O16	X	1232	1240	0.30091692	812	520	-0.57617208	3006585	-0.43224908	3189118	0.02290488	experimental	MicroSource	1506100	PENTAGASTRIN
3264 O17	X	1071	1080	0.14200973	532	840	-0.0242005	3936357	0.81566354	2607051	-0.50977525	experimental	MicroSource	1503606	CYPERMETHRIN
3264 O18	X	511	520	-0.11071094	629	640	-0.37435747	3371724	0.05782974	3284329	0.11003747	experimental	MicroSource	1506101	PROTIRELIN
3264 O19	X	825	840	-0.10079256	831	840	-0.02592541	3927516	0.80379741	2650155	-0.47032851	experimental	MicroSource	1701060	HYDROXYPROGESTERONE
3264 O20	X	254	256	-0.59684949	589	590	-0.44339392	3484828	0.2096346	3422163	0.23615762	experimental	MicroSource	1506033	EPIDIDISATE DISODIUM
3264 O21	X	1799	1760	-0.76184648	829	840	-0.02937524	2990904	-0.45329563	2951326	1.74527056	experimental	MicroSource	1502318	NIFURSOL
3264 O22	X	1786	1800	0.84771559	989	1000	0.24661055	3557699	0.30743991	3135763	-0.02592309	experimental	MicroSource	1502371	AMOROLFINE HYDROCHLORIDE
3264 O23	E	694	1240	-0.23008972	322	640	-0.9039052	95225	-4.33979082	3085544	-0.07188114	empty			
3264 O24	P	183543	184520	180.242092	105960	106840	181.312261	3663112	0.44892214	4032266	0.79451397	empty			
3264 P01	N	1118	1120	0.18839879	713	1520	1.150464	2762504	-0.75984742	93908	-2.80968462	empty			
3264 P02	E	115	120	-0.80156341	153	760	-0.16046849	75059	-4.36685703	95973	-2.80779483	empty			
3264 P03	X	435	440	-0.48572303	668	680	-0.30708594	2355047	-1.30672422	2985058	-0.16384116	experimental	MicroSource	1300017	EVANS BLUE
3264 P04	X	752	760	-0.17284365	952	960	-0.17284365	2487919	-0.2378256	7218402	0.04982186	experimental	MicroSource	1506202	AMMONIUM LACTATE
3264 P05	X	752	760	-0.17284365	1666	1680	1.41437541	2626580	-0.94228061	3365725	0.18452723	experimental	MicroSource	1506100	AMMONIUM LACTATE
3264 P06	E	1033	1040	0.10450369	1909	1920	1.83352882	3150774	-0.23872285	3470288	0.28021834	empty			
3264 P07	X	754	760	-0.17086965	911	920	0.11206748	2516223	-1.09039853	3309963	0.1334965	experimental	MicroSource	1506184	DOCUSATE SODIUM
3264 P08	E	473	480	-0.44821698	794	800	-0.08974713	2725002	-0.8101815	96136	-2.80764566	empty			
3264 P09	X	790	800	-0.1353376	434	440	-0.71071515	2450124	-1.17911466	3740309	0.52732876	experimental	MicroSource	1502510	BORNLYN ACETATE
3264 P10	E	872	880	-0.05440351	555	560	-0.5020009	2888342	-0.59699112	3197051	0.03016478	empty			
3264 P11	X	930	940	-0.03563491	537	560	-0.3048921	27465613	-0.78117583	3192502	0.19393236	experimental	MicroSource	1502500	SAXAGLIPTIN
3264 P12	E	670	680	-0.25377775	434	440	-0.71071515	2660734	-0.89644012	3691126	0.48231881	empty			
3264 P13	X	913	920	-0.01393646	835	840	-0.01902577	2340848	-1.3257817	3338945	0.16001945	experimental	MicroSource	212037	MEQUINOL
3264 P14	E	874	880	-0.0524295	514	520	-0.57272225	2158770	-1.57016143	3595165	0.39449985	empty			
3264 P15	X	393	400	-0.52717708	534	560	-0.50372581	1554644	-2.38100157	3363674	0.18265026	experimental	MicroSource	1504511	CHLORALOSE
3264 P16	E	514	520	-0.40774993	834	840	-0.02075068	1557039	-2.37787807	3465262	0.27561878	experimental	MicroSource	1504511	CHLORALOSE
3264 P17	X	594	600	-0.32878984	872	880	0.04479594	1814528	-2.03219291	3760488	0.54579562	experimental	MicroSource	1504512	DEFERIPRONE
3264 P18	E	563	560	-0.09259889	952	960	-0.09259889	2189532	-1.52887358	3450015	0.26166545	empty			
3264 P19	X	1191	1200	0.26044988	1112	1120	0.45877462	24587745	0.89297915	88620	1.14523994	experimental	MicroSource	1505448	NITHIAMIDE
3264 P20	E	1865	1880	0.92568868	1031	1040	0.31905682	2691024	-0.85578577	3245864	0.07483613	empty			
3264 P21	X	1346	1360	0.41343506	1232	1240	0.66576396	2753449	-0.77200077	4489303	1.21277257	experimental	MicroSource	1505443	METHSUXIMIDE
3264 P22	E	1187	1200	0.25650187	950	960	0.17933901	3202829	-0.16885616	3127633	-0.03336328	empty			
3264 P23	E	655	1200	-0.26858276	602	1160	-0.42093007	94157	-4.34122425	3350700	0.17077707	empty			
3264 P24	P	185342	185880	182.017707	190967	191280	327.941784	3055292	-0.36687598	3625836	0.42256849	empty			
3266 A01	N	318	320	-0.761464	638	640	0.41624237	2455382	-0.73715915	2177268	-0.93828049	empty			
3266 A02	E	157	160	-1.53287004	196	200	-1.03426815	67219	-4.71217418	68409	-4.70581436	empty			
3266 A03	X	477	480	0.00035935	517	520	0.01915691	2588142	-0.51345959	2602819	-0.17802207	experimental	Tocris	109	(-)-Bicuculline methobromide
3266 A04	X	597	600	0.57532037	397	400	-0.37464685	2722529	-0.28963179	2391413	-0.55570463	experimental	Tocris	440	m-Chlorophenylguanidine hydrochloride
3266 A05	X	355	360	-0.58418436	337	440	-0.24337893	2871136	-0.04211991	2968541	-0.47535201	experimental	Tocris	114	NMDA
3266 A06	X	477	480	0.00035935	416	320	-0.64046439	2777811	-0.19755704	2535490	-0.29830716	experimental	Tocris	442	4-Chlorophenylguanidine hydrochloride
3266 A07	X	396	400	-0.38773934	797	800	0.93803235	3206776	0.51690413	3077702	0.67036993	experimental	Tocris	130	(+)-Bicuculline
3266 A08	X	436	440	-0.19608567	435	440	-0.24994232	3312712	0.69334547	2710280	0.01395992	experimental	Tocris	443	6-Chloromestolonin
3266 A09	X	477	480	0.00035935	516	520	0.01587521	3085205	0.31442197	2950718	0.44350894	experimental	Tocris	131	(-)-Bicuculline methochloride
3266 A10	X	436	440	-0.19608567	476	480	-0.11539271	2252524	-1.07244699	2029967	-1.20143773	experimental	Tocris	444	Clozapine
3266 A11	X	396	400	-0.38773934	395	400	-0.38121024	3086998	0.31740829	2924770	0.39715213	experimental	Tocris	162	S-Sulfo-L-cysteine sodium salt
3266 A12	X	397	400	-0.382948	557	560	0.15042483	2460871	-0.72543537	2394715	-0.54980552	experimental	Tocris	448	Calpeptin
3266 A13	X	515	520	0.18243034	315	320	-0.64374608	2928962	0.05419198	2459990	-0.43318996	experimental	Tocris	169	(RS)-AMPA
3266 A14	X	675	680	0.94904504	435	440	-0.24994232	2556473	-0.56620579	2443931	-0.4618798	experimental	Tocris	452	CCCP
3266 A15	X	315	320	-0.77583803	795	800	0.93146896	3065248	0.28118266	2594791	-0.19236431	experimental	Tocris	180	ZAPA sulphate
3266 A16	X	477	480	0.00035935	395	476	0.93146896	2643921	-0.42055707	4500173	0.42681384	experimental	Tocris	453	FCCP
3266 A17	X	355	360	-0.58418436	474	480	-0.12185761	3520309	1.03909627	2804226	0.181797	experimental	Tocris	186	cis-ACPD
3266 A18	X	596	600	0.57052903	356	360	-0.50919647	3097928	0.33561272	2666142	-0.06489381	experimental	Tocris	454	Carbetapentane citrate
3266 A19	X	514	520	0.177639	393	400	-0.38773934	3221462	0.54136435	3137671	0.77750555	experimental	Tocris	1435	SD 22536
3266 A20	X	554	560	0.36929267	753	760	0								

3266 F07	X	435	440	-0.20087701	435	440	-0.24994232	3042896	0.24395436	2606861	-0.17080093	experimental	Tocris	645 2-(1-Thienyl)ethyl 3,4-dihydroxybenzylideneacyanoacetate
3266 F08	X	395	400	-0.39253068	513	520	0.00603012	3297083	0.66731464	3063942	0.64578669	experimental	Tocris	788 3-Aminobenzamide
3266 F09	X	315	320	-0.77583803	555	560	0.14386144	3408257	0.85248011	3137961	0.77802364	experimental	Tocris	646 HTMT dimaleate
3266 F10	X	476	480	-0.00443199	435	440	-0.24994232	3383410	0.81109628	3082348	0.67686951	experimental	Tocris	750 Rilmenidine hemifumarate
3266 F11	X	395	400	-0.39253068	435	440	-0.24994232	3341855	0.74188449	3011023	0.55124466	experimental	Tocris	649 (S)-Timocil maleate
3266 F12	X	394	400	-0.39732202	314	320	-0.64702778	3267023	0.61724831	2750115	0.08512623	experimental	Tocris	791 Antazolone hydrochloride
3266 F13	X	596	600	0.57052903	435	440	-0.24994232	3191858	0.49205751	2820833	0.21146586	experimental	Tocris	652 Thallidomide
3266 F14	X	394	400	-0.39732202	435	440	-0.24994232	3294362	0.66278269	2817677	0.20582758	experimental	Tocris	792 Efaroxan hydrochloride
3266 F15	X	435	440	-0.20087701	475	480	-0.11867444	3418124	0.86891406	3089261	0.69101977	experimental	Tocris	653 (R)-Vesamicol hydrochloride
3266 F16	X	434	440	-0.20566835	395	400	-0.38121024	3015502	0.19832838	2686647	-0.02826107	experimental	Tocris	793 Idazoxan hydrochloride
3266 F17	X	515	520	0.18243034	395	400	-0.38121024	2516539	-0.63271772	2248795	-0.10494956	experimental	Tocris	654 Verapamil hydrochloride
3266 F18	X	393	400	-0.40211337	435	440	-0.24994232	2240526	-1.09243022	2232925	-0.82528846	experimental	Tocris	797 8-Hydroxy-PIPAT oxalate
3266 F19	X	633	640	0.74780868	555	560	0.14386144	3075930	0.29897403	2902216	0.35685888	experimental	Tocris	658 FGIN-1-27
3266 F20	X	554	560	0.36929267	554	560	0.14057974	3428560	0.8862957	2923019	0.39402392	experimental	Tocris	800 7-NINA
3266 F21	X	553	560	0.36450133	632	640	0.39655218	3197378	0.50125132	2880023	0.3172104	experimental	Tocris	659 FGIN-1-43
3266 F22	X	711	720	1.12153334	712	720	0.65908802	3115557	0.36497464	2771641	0.12358302	experimental	Tocris	805 (S)-3,5-DHPG
3266 F23	E	853	1240	1.80190389	816	1160	1.00038462	78913	-4.69269728	79107	-4.68670209	empty		
3266 F24	P	129986	130600	620.522251	115007	115680	375.740761	2905292	0.01476849	2880038	0.3172372	empty		
3266 G01	N	517	520	0.19201302	437	440	-0.24337893	2984626	0.14690296	2916138	0.38173083	empty		
3266 G02	E	157	160	-1.53287004	116	120	-1.29680399	75969	-4.69760065	76662	-4.69107015	empty		
3266 G03	X	357	360	-0.57460167	436	440	-0.24666063	3438990	0.90366735	2879745	0.31671375	experimental	Tocris	289 Muscimol
3266 G04	X	355	360	-0.58418436	555	560	0.14386144	3179191	0.47096003	3135194	0.77308032	experimental	Tocris	497 AC 99
3266 G05	X	436	440	-0.19608567	355	360	-0.51247816	3305404	0.68117365	2900479	0.35375556	experimental	Tocris	310 (RIS)-4-Carboxy-3-hydroxyphenylglycine
3266 G06	X	315	320	-0.77583803	395	360	-0.50919647	3452506	0.92617888	3035728	0.59538161	experimental	Tocris	498 U-54494A hydrochloride
3266 G07	X	434	440	-0.20566835	356	400	-0.38777364	3120390	0.37302422	2918019	0.38509129	experimental	Tocris	312 (RIS)-Tetraol-5-ylglycine
3266 G08	X	635	640	0.75739136	355	360	-0.11288034	1551511	-2.30095522	1465268	-2.21694933	experimental	Tocris	3050 Dorsomorphin dihydrochloride
3266 G09	X	434	440	-0.20566835	392	400	-0.39105344	3325541	0.71471277	2856206	0.48666068	experimental	Tocris	652 (S)-Carboxy-3-hydroxyphenylglycine
3266 G10	X	675	680	-0.00922333	435	440	-0.24994232	2158776	-1.22858865	2097218	-1.08129199	experimental	Tocris	504 Diphenyletidonum chloride
3266 G11	X	395	400	-0.39253068	394	400	-0.38449194	3461988	0.94197159	3188903	0.86903291	experimental	Tocris	328 (R)-3-Carboxy-4-hydroxyphenylglycine
3266 G12	X	435	440	-0.20087701	436	440	-0.24666063	3082616	0.31010987	2892916	0.3402441	experimental	Tocris	506 Dimaprit dihydrochloride
3266 G13	X	354	360	-0.5889757	554	360	-0.51575986	3330132	0.72235929	2779899	0.13833616	experimental	Tocris	329 (S)-3-Carboxy-4-hydroxyphenylglycine
3266 G14	X	395	400	-0.39253068	315	520	0.01259352	2523441	-0.62122212	2424961	-0.49577022	experimental	Tocris	507 Dantrolene, sodium salt
3266 G15	X	355	360	-0.58418436	474	480	-0.1219561	3196498	0.49978564	2782216	0.14229689	experimental	Tocris	342 (RS)-3,5-DHPG
3266 G16	X	434	440	-0.20566835	436	440	-0.24994232	3482402	0.10349729	2954686	0.45059788	experimental	Tocris	508 Tolipin hydrochloride
3266 G17	X	513	520	0.17284766	473	480	-0.12523778	3286132	0.64907524	2701851	-0.00109871	experimental	Tocris	347 <i>rac</i> -Binaltorphimine dihydrochloride
3266 G18	X	394	400	-0.39732202	395	400	-0.38121024	3101303	0.34123394	2854739	0.27203985	experimental	Tocris	511 BD 1008 dihydrobromide
3266 G19	X	671	680	0.92987967	433	440	-0.25650572	3343925	0.74533217	2999372	0.53043063	experimental	Tocris	348 2-BFI hydrochloride
3266 G20	X	474	480	-0.10401467	634	640	0.40311558	3299043	0.67057911	3075512	0.66645681	experimental	Tocris	512 SKF 91488 dihydrochloride
3266 G21	X	474	480	-0.10401467	634	640	0.40311558	3056280	0.26624604	2883984	0.32428684	experimental	Tocris	351 1-Acetyl-4-methylpiperazine hydrochloride
3266 G22	X	232	240	-1.1735194	230	240	-0.92269041	1178629	-2.8610691	1171887	-2.73442095	experimental	Tocris	513 BGR 12783 dihydrochloride
3266 G23	P	1040	1040	0.36581009	831	831	0.36581009	75418	-4.6981837	75418	-4.68667478	empty		
3266 G24	P	92945	93640	443.046158	123807	124520	404.619704	2764697	-0.12939902	2667186	-0.06302868	empty		
3266 H01	N	437	440	-0.19129432	397	400	-0.37464685	2780480	-0.1931117	2635536	-0.11957226	empty		
3266 H02	E	157	160	-1.53287004	157	160	-1.16225437	79013	-4.69253073	77307	-4.68991784	empty		
3266 H03	X	276	280	-0.96270036	435	440	-0.24994232	3084604	0.31342098	3014832	0.55805034	experimental	Tocris	660 Mepyramine maleate
3266 H04	X	397	400	-0.382948	594	600	0.27184766	3367135	0.78398951	3203525	0.89515551	experimental	Tocris	807 THIP hydrochloride
3266 H05	X	355	360	-0.58418436	595	600	0.27512936	2908940	0.02084441	3144487	0.79037927	experimental	Tocris	861 2-[4-(2-Methoxyphenyl)piperazin-1-yl]methyl-6-methyl-2,3 dihydro
3266 H06	X	436	440	-0.19608567	631	640	-0.51247816	2250317	-1.07612285	1884950	-1.46521953	experimental	Tocris	2777 Melafazone hydrochloride
3266 H07	X	513	520	0.18243034	395	320	-0.64734608	3161677	0.186269	2903869	0.15870971	experimental	Tocris	862 <i>trans</i> -Triprolidine hydrochloride
3266 H08	X	394	400	-0.39732202	433	440	-0.25650572	3010402	0.18983409	2525553	-0.31605988	experimental	Tocris	821 ICI-118,551 hydrochloride
3266 H09	X	475	480	-0.00922333	475	480	-0.11867444	3361087	0.77391628	3094827	0.70096358	experimental	Tocris	665 L-NAME hydrochloride
3266 H10	X	475	480	-0.00922333	314	320	-0.64702778	3172497	0.45981086	2921153	0.39069026	experimental	Tocris	822 ICI 204,448 hydrochloride
3266 H11	X	435	440	-0.20087701	636	640	0.40967897	3476811	0.96665999	2940960	0.42607601	experimental	Tocris	666 3-(4-Allylpiperazin-1-yl)-2-quinoxalinecarboxylic acid maleate
3266 H12	X	395	400	-0.39253068	394	400	-0.38449194	3394221	0.8291025	3003328	0.53749813	experimental	Tocris	825 Clofluric acid
3266 H13	X	475	480	-0.00922333	515	520	0.01259352	3451053	0.92375884	3054245	0.62846274	experimental	Tocris	668 Arthamine dihydrobromide
3266 H14	X	394	400	-0.39253068	394	400	-0.38449194	2958520	0.10342221	2954686	0.45059788	experimental	Tocris	826 Tolidine
3266 H15	X	315	320	-0.77583803	594	600	0.27184766	3001727	0.17538548	3017760	0.56328129	experimental	Tocris	670 PK 11915
3266 H16	X	314	320	-0.78062937	592	600	0.26528426	2972641	0.12694139	2705369	0.00518629	experimental	Tocris	629 Pronethalol hydrochloride
3266 H17	X	1034	1040	2.66913676	1154	1160	2.10959854	3208219	0.51930751	2913024	0.37616758	experimental	Tocris	671 AH 6809
3266 H18	X	550	560	0.35012731	429	440	-0.26963251	3498775	1.00324205	2833030	0.23325613	experimental	Tocris	801 Primidone
3266 H19	X	1514	1520	4.96898085	955	960	1.45654064	3509038	1.02033556	3040538	0.60397481	experimental	Tocris	675 NPC 15199
3266 H20	X	311	320	-0.7950034	392	400	-0.39105344	1672036	-2.03927677	1549393	-2.05999623	experimental	Tocris	2908 EO 1428
3266 H21	X	715	720	1.14069871	674	680	0.5343835	2989153	0.15444289	2797614	0.16998449	experimental	Tocris	677 Naltrexone hydrochloride
3266 H22	X	592	600	0.55136366	751	760	0.78707424	2916073	0.03272475	2505360	-0.35213522	experimental	Tocris	832 ICI-89406
3266 H23	E	598	920	0.58011171	1057	1440	1.79127383	76865	-4.69610832	76989	-4.69408596	empty		
3266 H24	P	107698	108320	513.732824	128687	129320	420.63439	2923871	0.04571268	2967098	0.47277225	empty		
3266 I01	N	397	400	-0.382948	557	560	0.15042483	3444321	0.91254638	3314139	1.09277042	empty		
3266 I02	E	116	120	-1.72931506	156	160	-1.16553607	75474	-4.69842509	77246	-4.69002622	empty		
3266 I03	X	477	480	0.00035935	436	440	-0.24666063	3200997	0.50727894	3022440	0.57164244	experimental	Tocris	352 4-Acetyl-1,1-dimethylpiperazinium iodide
3266 I04	X	155	160	-1.54245273	495	440	-0.38121024	1686879	-2.01455507	1672580	-1.83991931	experimental	Tocris	514 BGR 12935 dihydrochloride
3266 I05	X	435	440	-0.19608567	395	400	-0.38121024	2556020	0.8959223	2903869	0.35841844	experimental	Tocris	808 N-Acetyltyramine
3266 I06	X	316	320	-0.77104669	356	360	-0.50919647	3211860	0.52537177	3133366	0.76981812	experimental	Tocris	515 Dobutamine hydrochloride
3266 I07	X	315	320	-0.77583803	435	440	-0.24994232	3198397	0.50294851	2920887	0.39021505	experimental	Tocris	660 (R)-1-(1,2-Diphenylethyl)piperidine maleate
3266 I08	X	556	560	0.37887536	475	480	-0.11867444	3528785	1.05322511	3399175	1.24468955	experimental	Tocris	518 EBPC
3266 I09	X	235	240	-1.15914538	395									

3266 J01	N	516	520	0.18722168	396	400	-0.37792855	2632237	-0.44001732	2547635	-0.27660979	empty		
3266 J02	E	197	200	-1.34121637	157	160	-1.16225437	76899	-4.69605169	81319	-4.68275029	empty		
3266 J03	X	356	360	-0.57939301	316	320	-0.64046439	3113665	0.36182342	3032251	0.58916986	experimental	Tocris	678 (+)-AJ 76 hydrochloride
3266 J04	X	435	440	-0.20087701	395	400	-0.38121024	3231679	0.55838122	2815019	0.20107899	experimental	Tocris	833 ICI-162,846
3266 J05	X	515	520	-0.58243034	436	440	-0.24666063	1217571	0.38498451	2758375	0.099886295	experimental	Tocris	660 2-Phenylmelatonin
3266 J06	X	275	280	-0.9674917	315	320	-0.64374608	2745981	-0.25057139	2599527	-0.18390332	experimental	Tocris	834 (S)-(-)-Propranolol hydrochloride
3266 J07	X	476	480	-0.00443199	435	440	-0.24994232	3212057	0.52569988	3005435	0.54126235	experimental	Tocris	681 L-690,330
3266 J08	X	435	440	-0.20087701	395	400	-0.38121024	2710176	-0.31020628	2671248	-0.0557718	experimental	Tocris	835 (R)-(+)-Propranolol hydrochloride
3266 J09	X	356	360	-0.57939301	315	320	-0.64374608	3107606	0.35173188	3047619	0.61662521	experimental	Tocris	685 Diltiazem hydrochloride
3266 J10	X	396	400	-0.38773934	376	380	-0.77173231	3372066	0.79220232	2690428	-0.02150621	experimental	Tocris	836 ICI-185,282
3266 J11	X	315	320	-0.77583803	436	440	-0.24666063	3349537	0.75467922	3328294	1.11805872	experimental	Tocris	686 Galanthamine hydrobromide
3266 J12	X	395	400	-0.39253068	312	320	-0.65359118	3279780	0.63949569	2850592	0.30847607	experimental	Tocris	837 ICI 192,605
3266 J13	X	675	680	0.94904504	595	600	0.27512936	2725246	-0.23963708	2661639	-0.07293854	experimental	Tocris	687 Danazol
3266 J14	X	435	440	-0.20087701	475	480	-0.1186744	3106001	0.34905868	2909567	0.36999156	experimental	Tocris	838 DHPB dibromide
3266 J15	X	314	320	-0.78062937	395	400	-0.38121024	3372182	0.79239552	3163435	0.82353364	experimental	Tocris	690 Clonidine hydrochloride
3266 J16	X	475	480	-0.00922333	395	400	-0.38121024	2263432	-1.05427921	1951284	-1.34200704	experimental	Tocris	840 Loperamide hydrochloride
3266 J17	X	395	400	-0.39253068	475	480	-0.1186744	6974399	6.79205559	7737744	8.99566088	experimental	Tocris	691 Dipyridamole
3266 J18	X	393	400	-0.40211337	470	480	-0.13508289	3389995	0.8220639	2781371	0.14096593	experimental	Tocris	841 DTG
3266 J19	X	635	640	0.75739136	473	480	-0.1252378	3005962	0.18243907	3000299	0.53208674	experimental	Tocris	692 Ipratropium bromide
3266 J20	X	594	600	0.56094635	633	640	0.39983388	3048503	0.25329308	2801098	0.17620875	experimental	Tocris	843 Oxotremorine sesquifumarate
3266 J21	X	474	480	-0.10401467	994	1000	1.58452686	3005225	0.18121156	3103996	0.71734425	experimental	Tocris	694 Picotamide hydrochloride
3266 J22	X	630	640	0.73343465	710	720	0.65252463	2925385	0.04823432	2782146	0.14235048	experimental	Tocris	847 Statal
3266 J23	E	1057	1400	2.77933763	715	1040	0.66893312	78081	-4.69408301	77453	-4.68965701	empty		
3266 J24	P	114401	115120	545.849189	108675	109240	354.96105	3102821	0.34376224	3032191	0.58906267	empty		
3266 K01	N	676	680	0.95383638	517	520	0.01915691	2868158	-0.04707991	3048503	0.6182045	empty		
3266 K02	E	156	160	-1.53766139	156	160	-1.16553607	78262	-4.6937875	78500	-4.68778761	empty		
3266 K03	X	554	560	-0.57243034	435	440	-0.24994232	1320412	0.47892291	2478898	1.03994103	experimental	Tocris	2768 PD 401
3266 K04	X	596	600	0.57052903	515	520	0.01259352	2822713	-0.12277067	2628202	-0.13267465	experimental	Tocris	542 H-9 dihydrochloride
3266 K05	X	395	400	-0.39253068	395	400	-0.38121024	3103654	0.34514964	2960144	0.46034874	experimental	Tocris	382 Arcaidine but-2-ynyl ester tosylate
3266 K06	X	356	360	-0.57939301	436	440	-0.24666063	3200993	0.50727227	2784688	0.14689184	experimental	Tocris	543 C-1
3266 K07	X	276	280	-0.96270036	376	380	-0.11539271	3153051	0.42742264	2904037	0.36011207	experimental	Tocris	383 Arcaidine propargyl ester tosylate
3266 K08	X	315	320	-0.77583803	435	360	-0.51247816	1940433	-1.59224908	1956012	-1.33356034	experimental	Tocris	544 IPAG
3266 K09	X	356	360	-0.57939301	436	440	-0.24666063	3255623	0.59826108	3134592	0.77200483	experimental	Tocris	385 N-[2-(Acetoxy)ethyl]-3-pyridinecarboxamide
3266 K10	X	515	520	-0.01880602	473	480	-0.00724842	3245915	0.58378415	3150322	0.47626594	experimental	Tocris	391 Pyrogallol hemitartrate
3266 K11	X	396	400	-0.38773934	473	480	-0.1252378	3202989	0.5105967	3016735	0.5614501	experimental	Tocris	386 3-Methyl-GABA (2:1 salt with naphthalene-1,5-disulphonic acid)
3266 K12	X	315	320	-0.77583803	615	1120	1.98161232	3159665	0.43843857	3183154	0.85876127	experimental	Tocris	545 Methylergometrine maleate
3266 K13	X	395	400	-0.39253068	473	480	-0.1252378	3232799	0.56024665	2710889	0.01504792	experimental	Tocris	387 (RS)-Atenolol
3266 K14	X	395	400	-0.39253068	395	400	-0.38121024	3243399	0.57790144	3035462	0.5949064	experimental	Tocris	552 MPMX
3266 K15	X	436	440	-0.19608567	395	400	-0.38121024	3319299	0.70431642	3068560	0.65403687	experimental	Tocris	388 Ambenonium dichloride
3266 K16	X	435	440	-0.20087701	355	360	-0.51247816	3165754	0.44885080	3409354	1.26287461	experimental	Tocris	553 NAN-190 hydrobromide
3266 K17	X	480	490	-0.01880602	473	480	-0.00724842	3245915	0.58378415	3150322	0.47626594	experimental	Tocris	391 Pyrogallol hemitartrate
3266 K18	X	1115	1120	3.05723545	1233	1240	2.36885268	3333498	0.69465459	3258644	0.93936271	experimental	Tocris	554 FS 142
3266 K19	X	312	320	-0.79021206	592	600	0.26528426	3077878	0.30221851	2858064	0.27798005	experimental	Tocris	393 S(-)-Atenolol
3266 K20	X	474	480	-0.10401467	473	480	-0.1252378	3270124	0.62241317	2919832	0.38833026	experimental	Tocris	556 BP 554 maleate
3266 K21	X	474	480	-0.10401467	433	440	-0.25650572	3046429	0.24983874	2950412	0.44296226	experimental	Tocris	395 N-Acetylglycyl-D-glutamic acid
3266 K22	P	671	680	0.92987967	539	560	0.09135427	2925722	0.04879561	2746718	0.0790574	experimental	Tocris	557 ?-Methyl-5-hydroxytryptamine maleate
3266 K23	E	943	1320	2.23312465	978	1280	1.53201969	74968	-4.69926786	75942	-4.69235645	empty		
3266 K24	P	126275	126920	602.741582	100861	101520	329.383495	2863917	-0.05411018	2491716	-0.37640341	empty		
3266 L01	N	556	560	0.37887536	397	400	-0.37464685	2737699	-0.26435656	2620955	0.56621611	empty		
3266 L02	E	274	280	-0.97228305	236	240	-0.90300023	76107	-4.6973708	75426	-4.6932783	empty		
3266 L03	X	990	1000	2.45831772	674	680	0.5343835	2893959	-0.00410714	2728971	0.0473519	experimental	Tocris	695 Retinoic acid
3266 L04	X	313	320	-0.78542071	353	360	-0.51904156	3065439	0.28150078	2999230	0.53017694	experimental	Tocris	855 MTPG
3266 L05	X	395	400	-0.39253068	395	400	-0.37792855	3006283	0.18297371	2968422	0.47513762	experimental	Tocris	699 BRL 52537 hydrochloride
3266 L06	X	395	400	-0.39253068	276	280	-0.77173231	2822692	-0.12280565	2577228	-0.22374109	experimental	Tocris	864 GR 46611
3266 L07	X	195	200	-1.35079905	156	160	-1.16553607	1107059	-2.98027226	1067015	-2.92177762	experimental	Tocris	701 3'-Fluorobenzylspiperone maleate
3266 L08	X	517	520	0.19201302	276	280	-0.77173231	3145497	0.4148411	3050997	0.6226601	experimental	Tocris	867 Antiprilocam
3266 L09	X	235	240	-1.15914538	395	400	-0.38121024	2833329	-0.10508923	2698387	-0.00728724	experimental	Tocris	702 BTCP maleate
3266 L10	X	436	440	-0.19608567	435	440	-0.24994232	3026165	0.2160881	2834522	0.23592163	experimental	Tocris	868 L-732,138
3266 L11	X	355	360	-0.58418436	594	600	0.27184766	3190973	0.4905835	3106571	0.72194456	experimental	Tocris	703 Aniprilocam hydrochloride
3266 L12	X	355	360	-0.58418436	392	400	-0.39105534	3000179	0.17280721	3059895	0.63855661	experimental	Tocris	869 Felbamate
3266 L13	X	395	400	-0.39253068	395	360	-0.51247816	3066626	0.28347778	3233177	0.94812961	experimental	Tocris	705 L-701,252
3266 L14	X	395	400	-0.39253068	395	400	-0.38121024	3119685	0.37185001	2782918	0.14372968	experimental	Tocris	870 MDL 11,939
3266 L15	X	355	360	-0.58418436	395	400	-0.38121024	3037565	0.23057533	3050968	0.62260829	experimental	Tocris	706 7-Hydroxy-DPAT hydrobromide
3266 L16	X	395	400	-0.39253068	475	480	-0.1186744	3004403	0.17984248	2567355	-0.24137947	experimental	Tocris	871 AMT hydrochloride
3266 L17	X	475	480	-0.00922333	514	520	0.00931182	3206636	0.51667095	2766789	0.11491479	experimental	Tocris	713 Cyclothiazide
3266 L18	X	513	520	0.17284766	752	760	0.79035594	3042949	0.24404264	2733531	0.05549847	experimental	Tocris	873 ET hydrobromide
3266 L19	X	475	480	-0.00922333	474	480	-0.1219561	2657144	-0.39853355	2353744	-0.62300132	experimental	Tocris	719 7-Hydroxy-PIPAT maleate
3266 L20	X	554	560	0.36929267	635	640	0.40639728	2981217	0.14122512	2834763	0.23635218	experimental	Tocris	875 m-CPP hydrochloride
3266 L21	X	273	280	-0.97707439	221	240	-0.9522257	948678	-3.24406319	1003092	-3.0359778	experimental	Tocris	723 Tetrindole mesylate
3266 L22	X	672	680	0.93467101	4671	4680	0.93467101	2026143	-1.44494508	1799109	-1.61387181	experimental	Tocris	876 AM 92016 hydrochloride
3266 L23	X	1003	1320	5.20605167	1020	1360	1.66989101	77975	-0.69425956	78942	-0.79171552	empty		
3266 L24	P	105520	106240	503.297282	109647	110280	358.15086	2991506	0.15836192	2808794	0.18995786	empty		
3266 M01	N	556	560	0.37887536	357	360	-0.50591477	3136515	0.39988116	3052331	0.62504332	empty		
3266 M02	E	189	200	-1.3795471	195	200	-1.03754984	76487	-4.6967379	77835	-4.68897455	empty		
3266 M03	X	2714	2720	10.7185911	954	960	1.45325894	2473564	-0.70429458	2491556	-0.37679644	experimental	Tocris	396 H-9 dihydrochloride
3266 M04	X	388	400	-0.42607007	754									

3266 M19	X	193	200	-1.36038174	234	240	-0.90956362	884005	-3.35177908	971587	-3.09226234	experimental	Tocris	421 GBR 12909 dihydrochloride
3266 M20	X	795	800	1.52400606	553	560	0.13729804	2575870	-0.53389918	2913731	0.37743066	experimental	Tocris	579 Tyrphostin B44, (+) enantiomer
3266 M21	X	553	560	0.36450133	633	640	0.39983388	2798519	-0.16306691	2262658	-0.78572894	experimental	Tocris	424 Benzothiazine dibromide
3266 M22	X	551	560	0.35491865	899	920	1.27276555	2939615	0.07193505	3113389	0.73502551	experimental	Tocris	581 3-[2-(4-{2-Methoxyphenyl}piperazin-1-yl)-ethyl]pyrimido[5,4-b] imidazole
3266 M23	E	1042	1400	2.70746275	976	1320	1.52455633	76397	-4.69688779	76887	-6.6946426	empty		
3266 M24	P	119588	120280	570.701879	114978	115600	375.645592	2343934	-0.92019938	2502282	-0.35763415	empty		
3266 N01	N	476	480	-0.00443199	317	320	-0.63718269	2282072	-1.02323342	2190444	-0.91474121	empty		
3266 N02	E	157	160	-1.53287004	175	160	-1.16225437	73955	-4.70095506	72891	-4.69780715	empty		
3266 N03	X	389	400	-0.42127873	257	280	-0.775014	2791016	-0.1755635	2802655	0.17899037	experimental	Tocris	724 Pirlindole mesylate
3266 N04	X	556	560	0.37887536	356	360	-0.50919647	2680077	-0.36033757	2492443	-0.37521179	experimental	Tocris	877 Luzindole
3266 N05	X	394	400	-0.39732202	276	280	-0.77173231	3625629	-1.2145233	3142277	0.78573429	experimental	Tocris	725 BU 224 hydrochloride
3266 N06	X	394	400	-0.39732202	395	400	-0.38210224	2481540	-0.69101018	2452070	-0.46407723	experimental	Tocris	878 Oxleamide
3266 N07	X	354	360	-0.5889757	595	600	0.27512936	3341152	0.74071361	3293689	1.05623594	experimental	Tocris	726 BU 239 hydrochloride
3266 N08	X	394	400	-0.39732202	435	440	-0.24994232	2662285	-0.38997097	2451213	-0.44887031	experimental	Tocris	879 Palmitylolethanolamide
3266 N09	X	716	720	1.14549005	355	360	-0.51247816	3483194	0.97729117	3421127	1.28390739	experimental	Tocris	727 Pyrolidinedithiocarbamate ammonium
3266 N10	X	435	440	-0.20087701	475	480	-0.1186744	2421612	-1.27082306	2407601	-0.52678433	experimental	Tocris	880 ODO
3266 N11	X	394	400	-0.39732202	274	280	-0.7782957	3573194	-1.12719036	3149846	0.79925652	experimental	Tocris	728 RS 23597-190 hydrochloride
3266 N12	X	355	360	-0.58418436	395	400	-0.38121024	2534237	-0.60324088	2477498	-0.40191144	experimental	Tocris	881 Chlormethiazole hydrochloride
3266 N13	X	435	440	-0.20087701	475	480	-0.1186744	3121721	0.37524107	3145208	0.79097061	experimental	Tocris	729 Imetit dihydrobromide
3266 N14	X	475	480	-0.00922333	315	320	-0.64374608	2841902	-0.0908105	2456124	-0.44009667	experimental	Tocris	882 ZM 226600
3266 N15	X	355	360	-0.58418436	395	400	-0.38121024	3136922	-0.40055904	3047771	0.61689676	experimental	Tocris	730 4-Phenyl-1,2,3,4-tetrahydroisoquinoline hydrochloride
3266 N16	X	434	440	-0.20566835	495	600	0.27512936	2275266	-1.03456913	2186844	-0.92117271	experimental	Tocris	883 BU 1063 dihydrochloride
3266 N17	X	395	400	-0.39253068	575	480	-0.1186744	3192970	0.49390959	3265691	1.00621676	experimental	Tocris	731 Sulfoxazole
3266 N18	X	474	480	-0.01401467	374	480	0.5343835	2640271	-0.42663632	2373704	-0.58734224	experimental	Tocris	884 Dihydroxymethylene hydrochloride
3266 N19	X	515	520	0.18243034	553	560	0.13729804	3279187	0.63750802	3109886	0.72786689	experimental	Tocris	735 3-Bromo-7-nitroindazole
3266 N20	X	803	800	0.16805632	1053	1030	1.72251308	1995936	-1.49980625	1830161	-1.37501385	experimental	Tocris	885 Guanabenz acetate
3266 N21	X	873	880	-0.89773072	791	800	-0.91842416	2835011	-1.02287768	2692871	-0.60994181	experimental	Tocris	736 2-(1-(4-Piperonyl)piperazinyl)benzothiazole
3266 N22	X	590	600	0.54178098	500	560	0.12745295	2721859	-0.2907477	2310058	-0.70104755	experimental	Tocris	888 Cirazoline hydrochloride
3266 N23	E	930	1320	2.17083721	692	1000	0.59345406	75080	-4.69980132	73517	-4.69668878	empty		
3266 N24	P	130770	131480	624.278663	102667	103320	335.244608	3146666	0.41678813	2994744	0.52216258	empty		
3266 O01	N	556	560	0.37887536	477	480	-0.11211101	2763177	-0.22193065	2780358	0.13915617	empty		
3266 O02	E	116	120	-1.72931506	197	200	-1.03098645	78759	-4.69295377	76338	-4.69164899	empty		
3266 O03	X	475	480	-0.00922333	317	320	-0.63718269	2898052	0.00270994	2758093	0.09937915	experimental	Tocris	425 UK 14,304
3266 O04	X	514	520	0.94904504	515	520	0.96919334	2104131	-0.79514827	2194	-0.37158913	experimental	Tocris	582 Methyl dihydroin maleate
3266 O05	X	436	440	-0.19608567	356	360	-0.50919647	2527452	-0.61454161	2591295	-0.19861001	experimental	Tocris	426 L-693,403 maleate
3266 O06	X	435	440	-0.20087701	395	400	-0.38121024	3070112	0.28928388	3042945	0.60827498	experimental	Tocris	583 Minoxidil
3266 O07	X	554	560	0.36929267	473	480	-0.1252378	2215390	-1.1342954	2352845	-0.62460741	experimental	Tocris	427 Bromocriptin mesylate
3266 O08	X	435	440	-0.20087701	355	360	-0.51247816	2963499	0.11171496	3027650	0.58095005	experimental	Tocris	584 L(-)-7-Methylopa
3266 O09	X	234	240	-1.16393672	354	360	-0.51575986	2046464	-1.41564951	2113045	-1.05301662	experimental	Tocris	430 SC-10
3266 O10	X	355	360	-0.58418436	315	320	-0.64374608	2789368	-0.17830832	2868532	0.29668142	experimental	Tocris	588 S-Methylfurmethiodide
3266 O11	X	600	600	0.94904504	514	520	1.5247816	2400701	-0.8255513	1870265	-0.97158913	experimental	Tocris	431 M1 9 hydrochloride
3266 O12	X	435	440	-0.20087701	314	520	0.00913182	2922730	0.0438123	2952428	0.44656329	experimental	Tocris	589 PDE-084 hydrochloride
3266 O13	X	395	400	-0.39253068	753	760	0.79363764	1960160	-1.55939284	1979480	-1.29163412	experimental	Tocris	432 MY-5445
3266 O14	X	275	280	-0.9674917	434	440	-0.25322402	1176875	-2.86399047	1585573	-1.99535967	experimental	Tocris	590 Methylgoline
3266 O15	X	355	360	-0.58418436	432	480	-0.1285195	2358964	-0.89516622	2163423	-0.96301496	experimental	Tocris	433 SC-9
3266 O16	X	754	760	1.32756104	673	640	0.39983388	2530879	-0.60883378	2511732	-0.34075147	experimental	Tocris	593 NPPB
3266 O17	X	554	560	0.36929267	353	360	-0.51904156	2967950	0.11912831	2878955	0.31530239	experimental	Tocris	435 Cimeterol
3266 O18	X	510	520	0.177639	754	760	0.79691934	2039909	-1.42656717	1870265	-1.48708913	experimental	Tocris	597 Nalfopadol hydrochloride
3266 O19	X	514	520	0.177639	473	480	-0.1252378	2877448	-0.03160698	2692651	-0.01753476	experimental	Tocris	589 Etazolate hydrochloride
3266 O20	X	475	480	-0.00922333	553	560	0.13729804	2832283	-0.10683139	2883510	0.32344002	experimental	Tocris	599 Naloxone hydrochloride
3266 O21	X	592	600	0.55136366	711	720	0.65580632	2869950	-0.04409525	2820160	0.21026353	experimental	Tocris	438 DPCPX
3266 O22	X	592	600	0.55136366	831	840	1.04961009	2757516	-0.23135931	2710490	0.01433509	experimental	Tocris	600 Nimodipine
3266 O23	E	753	1120	1.3227697	954	1280	1.45325894	74506	-4.70003734	75547	-4.69306213	empty		
3266 O24	P	122837	123680	586.268949	108044	108920	352.890298	2749297	-0.24504844	2557325	-0.25929834	empty		
3266 P01	N	718	720	1.15507274	358	360	-0.50265307	2292297	-1.00620321	2346079	-0.63669505	empty		
3266 P02	E	195	200	-1.35079905	237	240	-0.89971853	71329	-4.70532878	70812	-4.70152134	empty		
3266 P03	X	837	840	1.72524242	557	560	0.15042483	2758000	-0.28418379	2714894	0.02220296	experimental	Tocris	737 2-Iodometolatin
3266 P04	X	516	520	0.18722168	356	360	-0.50919647	2438189	-0.76321329	2444915	-0.46012186	experimental	Tocris	889 RS 45041-190 hydrochloride
3266 P05	X	236	240	-1.15435404	636	640	0.40967897	2096083	-1.33300676	2145199	-0.99557263	experimental	Tocris	740 Naltrindole hydrochloride
3266 P06	X	435	440	-0.20087701	634	640	0.40311558	2585929	-0.51714545	2478049	-0.40092706	experimental	Tocris	890 Amiloride hydrochloride
3266 P07	X	916	920	2.10375842	956	960	1.45982234	1241483	-2.75638283	1316700	-2.47570859	experimental	Tocris	741 GF 109203X
3266 P08	X	475	480	-0.00922333	313	320	-0.65030948	2601346	-0.49146772	2699444	-0.00539889	experimental	Tocris	891 Rauwolfoscine hydrochloride
3266 P09	X	477	480	0.00035935	1037	1040	1.72563987	2726466	-0.28307453	2806890	0.18655631	experimental	Tocris	742 L-695,580
3266 P10	X	316	320	-0.77104669	474	480	-0.1219561	2268638	-1.04560837	2209032	-0.88153324	experimental	Tocris	892 Naltriben mesylate
3266 P11	X	596	600	0.57052903	555	560	0.14714313	2618460	-0.46296355	2511578	-0.34102566	experimental	Tocris	743 DPPE fumarate
3266 P12	X	396	400	-0.38773934	594	600	0.27184766	2624048	-0.45365648	2667165	-0.06306662	experimental	Tocris	894 (RS)-(-)-Sulpiride
3266 P13	X	436	440	-0.19129432	914	920	1.32199102	1715120	-1.96751837	1740997	-1.71769048	experimental	Tocris	744 Ceramide
3266 P14	X	437	440	-0.19129432	1234	1240	0.39655218	2638260	-0.42998573	2526648	-0.31410363	experimental	Tocris	895 (S)-(-)-Sulpiride
3266 P15	X	396	400	-0.38773934	634	1240	2.37213438	2526247	-0.61654886	2504767	-0.35319463	experimental	Tocris	748 4-IBP
3266 P16	X	515	520	0.177639	515	520	0.177639	2738077	-1.26373587	2602950	-0.17788804	experimental	Tocris	896 GR 135531
3266 P17	X	515	520	0.18243034	515	520	0.18243034	580134	-0.52109729	2452666	-0.44418425	experimental	Tocris	750 PG-9 maleate
3266 P18	X	595	600	0.56573769	555	560	0.14386144	2728157	-0.28025809	2545269	-0.28083671	experimental	Tocris	897 S-Isopropylisothiourea hydrobromide
3266 P19	X	636	640	0.76218271	436	440	-0.24666063	2532319	-0.6064354	2281558	-0.75196357	experimental	Tocris	751 SM-21 maleate
3266 P20	X	195	200	-1.35079905	195	200	-1.03754984	1354831	-2.56759647	1263391	-2.57094657	experimental	Tocris	899 BNTX maleate
3266 P21	X	677	680	0.95862772	756	760	0.80348273	1965628	-1.55028563	2097745	-1.08035049	experimental	Tocris	752 Clobenpropit dihydrobromide
3266 P22														

3267 A13	X		553	560	-0.27245068	751	760	-0.13316531	3055719	-0.06299995	3730336	0.12122497	experimental	Tocris	909 Tropicamide	
3267 A14	X		1154	1160	1.51118034	1472	1480	1.77990438	2822617	-0.35367158	3497933	-0.15859433	experimental	Tocris	1036 ZN 241385	
3267 A15	X		634	640	-0.03206114	673	680	-0.34012707	3154313	0.05994399	4036390	0.48972201	experimental	Tocris	911 Gibencilamide	
3267 A16	X		554	560	-0.26948939	514	520	-0.76201068	1996742	-1.38102049	2431869	-1.444216334	experimental	Tocris	1038 WIN 55,212-2 mesylate	
3267 A17	X		873	880	0.67723639	792	800	-0.02437771	3587037	0.59953862	3481438	-0.17845475	experimental	Tocris	912 RU 24989 hemisuccinate	
3267 A18	X		1432	1440	2.33622098	1111	1120	0.82204286	4178267	1.33678578	3909270	0.3366662	experimental	Tocris	1041 L-EBIO	
3267 A19	X		1151	1160	1.50227702	1073	1080	0.72121533	4222651	1.39213137	4094239	0.55937372	experimental	Tocris	914 (R)-Bisoprolol hemifumarate	
3267 A20	X		750	760	0.31220042	592	600	-0.55504891	4133150	1.28052615	3584264	-0.05464955	experimental	Tocris	1042 N-Methylglucosamine iodide	
3267 A21	X		1351	1360	2.09583144	868	880	0.17727735	3880761	0.96580418	4161294	0.6401097	experimental	Tocris	915 Clotamide	
3267 A22	X		628	640	-0.04986777	1227	1240	1.12983216	3785293	0.84675827	4043211	0.49793467	experimental	Tocris	1043 QX 222	
3267 A23	E		1487	2080	2.49944844	1692	2440	2.36364271	67954	-3.78865872	68359	-4.28789134	empty			
3267 A24	P	201934	202440	597.380457	254601	252000	673.42126	2561573	-0.67918609		5108402	1.78045256	empty			
3267 B01	N		675	680	0.08961752	675	680	-0.33482036	2460592	-0.80510655	3445449	-0.22178645	empty			
3267 B02	E		195	200	-1.33491308	234	240	-1.50495037	72157	-3.7834177	72206	-4.28325945	empty			
3267 B03	X		634	640	-0.03206114	471	880	0.18523742	2545510	-0.6992162	2608003	-1.23009338	experimental	Tocris	1147 SKF 96365 hydrochloride	
3267 B04	X		594	600	-0.15077202	872	480	-0.87345163	2948278	-0.19697585	3579625	-0.06023502	experimental	Tocris	1355 P1075	
3267 B05	X		434	440	-0.62561555	554	560	-0.65587644	3359340	0.31560688	4020854	0.47101626	experimental	Tocris	1148 Siguazodan	
3267 B06	X		431	440	-0.63451887	548	560	-0.67179658	3031364	-0.09336995	3931407	0.36331973	experimental	Tocris	1356 MG 624	
3267 B07	X		474	480	-0.50690467	1673	1680	2.31322894	3922595	1.01797	5108402	1.78045256	experimental	Tocris	1202 SB 203580	
3267 B08	X		353	360	-0.86600509	750	760	-0.13581866	3032765	-0.09162294	3842285	0.2560145	experimental	Tocris	1357 U 99194 maleate	
3267 B09	X		313	320	-0.98471597	431	440	-0.98223923	3327837	0.27632353	4149762	0.62622487	experimental	Tocris	1205 SR 57227 hydrochloride	
3267 B10	X		434	440	-0.62561555	513	1120	0.82734957	3268179	0.20193168	3941303	0.37523477	experimental	Tocris	3861 PO 123319 difluorocetate	
3267 B11	X		393	400	-0.74729421	1151	560	-0.66383651	3689503	0.72731084	4100052	0.56637273	experimental	Tocris	1206 SC 19220	
3267 B12	X		674	680	0.08664974	672	680	-0.34278043	3431427	0.40549734	3568441	-0.07370085	experimental	Tocris	1363 PO 81723	
3267 B13	X		392	400	-0.75026198	790	800	-0.02968442	2622143	-0.60365701	3293393	-0.40486586	experimental	Tocris	2207 BRL 15572 hydrochloride	
3267 B14	X		640	650	-0.58582555	430	440	-0.17451799	3015144	-0.10860795	3015144	-0.10860795	experimental	Tocris	849 3-((1S)-1-phenylethoxy)propane	
3267 B15	X		312	320	-0.98768375	552	560	-0.66118315	3371793	0.33113542	3934205	0.36668859	experimental	Tocris	1209 LU 341495	
3267 B16	X		594	600	-0.15077202	1151	520	-0.76997075	1699418	-1.75426908	2216071	-1.70198979	experimental	Tocris	1387 ZN 38923 hydrochloride	
3267 B17	X		472	480	-0.51284021	1151	1160	0.9281771	3231435	0.15611295	4061054	0.51941811	experimental	Tocris	1210 FR 139317	
3267 B18	X		790	800	0.4309113	1310	1320	1.35006071	3233592	0.15880267	3956719	0.39379604	experimental	Tocris	1371 SB 200646 hydrochloride	
3267 B19	X		750	760	0.31220042	629	640	-0.45687474	2786418	-0.39881071	3083161	-0.65799069	experimental	Tocris	1211 ZD 7155 hydrochloride	
3267 B20	X		789	800	0.42794353	947	960	0.38689247	3173208	0.08350552	3609730	-0.02398781	experimental	Tocris	1375 SB 228357	
3267 B21	X		1551	1560	2.68938585	2230	2240	3.79114825	4024983	1.14564495	3805047	0.21117897	experimental	Tocris	1212 MPEP hydrochloride	
3267 B22	E		686	690	-0.17445104	974	980	-0.14979192	3423692	0.14609593	3423692	0.14609593	experimental	Tocris	1376 SB 218795	
3267 B23	E		1288	1800	1.9088618	1153	1760	0.93348381	71584	-3.78413221	74038	-4.28105367	empty			
3267 B24	P	171640	172720	507.47477	203242	204480	537.147548	2829595	-0.34497021	3117310	-0.6168744		empty			
3267 C01	N		517	520	-0.37929047	596	600	-0.54443549	3366406	0.32441798	3854904	0.27120811	empty			
3267 C02	E		156	160	-1.45065619	235	240	-1.50229701	74256	-3.78800083	75022	-4.27986891	empty			
3267 C03	X		554	560	-0.26948929	790	800	-0.02968442	2706789	-0.49810583	3880784	0.30236831	experimental	Tocris	916 Remoxipride hydrochloride	
3267 C04	X		435	440	-0.62624778	753	760	-0.12785859	2867641	-0.29752792	4162625	0.64171226	experimental	Tocris	1044 NBQX disodium salt	
3267 C05	X		916	920	-0.46252728	712	720	-0.98489245	13313916	-2.23497921	3641460	-2.5558024	experimental	Tocris	917 3-(4-(4-chlorophenyl)phenylmethoxy)tropane hydrochloride	
3267 C06	X		916	920	0.80485059	712	720	-0.23664619	4124582	1.26984209	3985137	0.428011206	experimental	Tocris	1045 CNQX disodium salt	
3267 C07	X		472	480	-0.51284021	466	480	-0.88937177	2541443	-0.70428763	2003569	-1.95784776	experimental	Tocris	918 3'-Bis-(4-fluorophenyl) methoxytropane hydrochloride	
3267 C08	X		794	800	0.44278239	792	800	-0.02437771	4020987	1.14066205	4505234	1.05422248	experimental	Tocris	1046 Zardaverine	
3267 C09	X		713	720	0.20239286	671	680	-0.34543379	3966400	1.07259336	4063451	0.52230416	experimental	Tocris	919 TRIM	
3267 C10	X		715	720	0.20832884	751	760	-0.13316531	4200094	1.36400343	4781170	1.38645666	experimental	Tocris	1047 ICI 182,780	
3267 C11	X		354	360	-0.86303732	552	560	-0.66118315	2253090	-1.0638557	2859641	-0.92711463	experimental	Tocris	921 SB 205607 dihydrobromide	
3267 C12	X		674	680	-0.78704625	434	440	-0.17451799	3015144	-0.10860795	3015144	-0.10860795	experimental	Tocris	1048 1-6CP	
3267 C13	X		514	520	-0.38819379	672	680	-0.34278043	3454316	0.43403925	4057289	0.51488495	experimental	Tocris	922 SKF 38393 hydrobromide	
3267 C14	X		633	640	-0.03502891	711	720	-0.23929955	3533637	0.53295033	4543618	1.10043782	experimental	Tocris	1049 CHPG	
3267 C15	X		634	640	-0.03206114	512	520	-0.76731739	3527220	0.52494851	4159020	0.63737175	experimental	Tocris	924 (+)-MK 801 maleate	
3267 C16	X		673	680	0.08368197	834	840	0.08706324	3565197	0.52730476	4334548	0.84871206	experimental	Tocris	1050 RS 102221 hydrochloride	
3267 C17	X		633	640	-0.03502891	630	640	-0.45422138	3060715	-0.05677008	3078335	-0.66380133	experimental	Tocris	925 SCH 23390 hydrochloride	
3267 C18	X		712	720	0.19942508	631	640	-0.45156803	4195835	1.35869258	4247975	0.74447559	experimental	Tocris	1052 A 81603 hydrobromide	
3267 C19	X		632	640	-0.03799668	511	520	-0.76997075	3211243	0.1309341	3492646	-0.16496002	experimental	Tocris	926 7-Funaltrexamine hydrochloride	
3267 C20	X		674	680	0.08664974	872	880	0.18789077	3223402	0.14609603	3447016	-0.21389974	experimental	Tocris	1054 GR 5562 dihydrochloride	
3267 C21	X		387	400	-0.76510084	505	520	-0.78589089	1559228	-1.92908206	1448630	-2.62600887	experimental	Tocris	927 Fluoxetine hydrochloride	
3267 C22	X		831	840	0.55258996	828	840	0.07114311	2912316	-0.24181945	3233133	-0.47742047	experimental	Tocris	1057 WIN 64338 hydrochloride	
3267 C23	E		979	1480	0.99182023	1293	1800	1.30495366	72717	-3.78271939	70771	-4.28498723	empty			
3267 C24	P	167936	168840	496.482142	169322	170520	447.145712	3077338	-0.03604167	3077338	-0.03604167	3059443	-0.68654779	empty		
3267 D01	N		316	320	-0.97581266	556	560	-0.65056973	2880172	-0.28190211	3397898	-0.2790391	empty			
3267 D02	E		236	240	-1.21323442	192	200	-1.61639132	76326	-3.77821907	73730	-4.28142451	empty			
3267 D03	X		835	840	0.56446105	843	1680	2.31322894	2793585	-0.38987366	3641401	0.01414449	experimental	Tocris	1213 PD 98059	
3267 D04	X		552	560	-0.27541845	706	720	-0.25256633	3431697	0.40583402	4112035	0.58080057	experimental	Tocris	1377 Cromakalim	
3267 D05	X		1075	1080	1.27672635	1471	1480	1.77725103	3645439	0.67236427	4182710	0.66589513	experimental	Tocris	1214 SB 1893	
3267 D06	X		350	360	-0.87490841	1227	1240	1.12983216	3251922	0.18165966	3902843	0.32892792	experimental	Tocris	1378 Levromakalim	
3267 D07	X		715	720	0.20832884	1671	1680	2.30792223	3737770	0.78749843	4521671	1.07401306	experimental	Tocris	1215 SB 1757	
3267 D08	X		432	440	-0.63155111	668	680	-0.35339385	3430474	0.40430988	4110000	0.57835038	experimental	Tocris	1379 SB 221284	
3267 D09	X		514	520	-0.38819379	1072	1080	1.71856198	3664665	0.69633855	4300505	0.80772339	experimental	Tocris	1217 MRS 1220	
3267 D10	X		320	360	-0.98471597	640	640	-0.45422138	3728180	0.77553997	4846600	1.02937786	experimental	Tocris	1380 PMPA (MAALADase inhibitor)	
3267 D11	X		516	520	-0.38225824	993	1000	0.50894685	3502836	0.49459235	4315042	0.82523532	experimental	Tocris	1218 DH 97	
3267 D12	X		234	240	-1.21916997	312	320	-1.2979886	1219076	-1.20602794	2235456	-1.67864974	experimental	Tocris	1381 GW 5074	
3267 D13	X		514	520	-0.38819379	634	640	-0.4436079								

3267 E07	X	592	600	-0.15670757	710	720	-0.2419529	3876127	0.96002571	3703009	0.08832255	experimental	Tocris	930 ZD 7114 hydrochloride
3267 E08	X	594	600	-0.15077202	673	680	-0.34012707	4456923	1.68426196	4241714	0.73693749	experimental	Tocris	1061 (-)-Quinpirole hydrochloride
3267 E09	X	635	640	-0.02909337	631	640	-0.45156803	3666647	0.69881005	3882345	0.30424779	experimental	Tocris	931 Haloperidol hydrochloride
3267 E10	X	515	520	-0.38522662	713	720	-0.23399283	4105345	1.2458541	4702361	1.29129097	experimental	Tocris	1063 CGS 21680 hydrochloride
3267 E11	X	831	840	-0.38819379	831	840	0.07910318	3534475	0.53399529	3956071	0.59301583	experimental	Tocris	932 Imipenem dihydrobromide
3267 E12	X	474	480	-0.50690467	673	680	-0.34012707	3077170	-0.03625116	4023046	0.47365548	experimental	Tocris	1064 Mefesrigide maleate
3267 E13	X	751	760	0.31516819	669	680	-0.3507405	2793721	-0.38970407	3988031	0.43149651	experimental	Tocris	933 MM 77 dihydrochloride
3267 E14	X	592	600	-0.15670757	831	840	0.07910318	3474720	0.45948249	4159116	0.63748733	experimental	Tocris	1065 PD 168077 maleate
3267 E15	X	634	640	-0.03206114	632	640	-0.44891467	2379545	-0.90616988	3619060	-0.10275425	experimental	Tocris	934 Olanol
3267 E16	X	553	560	-0.27245068	793	800	0.19054413	3842745	0.9183993	4263291	0.76291676	experimental	Tocris	1066 IB-MECA
3267 E17	X	834	840	0.56149328	871	800	-0.02703106	2713116	-0.494021624	3212422	-0.50235706	experimental	Tocris	935 Maprotiline hydrochloride
3267 E18	X	674	680	0.08664974	672	680	-0.34278043	4321884	1.51587213	4515813	1.06730904	experimental	Tocris	1067 Quaxeterone M
3267 E19	X	273	280	-1.10342686	431	440	-0.98223923	1032891	-2.58540947	1123947	-3.01693571	experimental	Tocris	937 Pimozide
3267 E20	X	594	600	-0.15077202	832	840	0.08175653	3647301	0.67468613	3440289	-0.22799922	experimental	Tocris	1070 Zolantidine dimaleate
3267 E21	X	1031	1040	1.14614437	870	880	0.18258406	3911291	1.00387423	3960688	0.39857482	experimental	Tocris	940 4-Aminopyridine
3267 E22	X	788	800	0.42497576	867	880	0.17462399	4066970	1.19800155	4045301	0.50045109	experimental	Tocris	1072 AGN 192403 hydrochloride
3267 E23	E	1081	1520	1.29453298	1269	1840	1.24127311	71201	-3.7846098	73888	-4.28123428	empty		
3267 E24	P	147343	148080	435.366812	191084	192240	504.888046	3409061	0.37760757	3595638	-0.04095495	empty		
3267 F01	N	515	520	-0.38522662	875	880	0.19585084	2800377	-0.38140423	3704920	0.09062344	empty		
3267 F02	E	194	200	-1.33788085	154	160	-1.71721885	75465	-3.77929272	74486	-4.28051427	empty		
3267 F03	X	1396	1400	2.22938118	955	960	0.40811932	3320128	0.26671062	3897401	0.32237561	experimental	Tocris	1228 Nocodazole
3267 F04	X	391	400	-0.75322975	510	520	-0.77262411	3168071	0.07709983	3890474	0.31403532	experimental	Tocris	1393 SB 222000
3267 F05	X	434	440	-0.62561555	792	800	-0.02437771	2180509	-1.15436216	2774259	-1.0299168	experimental	Tocris	1229 Actinomycin D
3267 F06	X	392	400	-0.75026198	792	800	-0.02437771	3240666	0.16762375	4119853	0.59021365	experimental	Tocris	1394 (RS)-3,4-DCPG
3267 F07	X	674	680	0.08664974	511	520	-0.76997075	3426556	0.39942334	3793227	0.19694738	experimental	Tocris	1230 Methotrexate
3267 F08	X	474	480	-0.50690467	433	440	-0.97692482	1237470	0.3880935	3054413	0.3054413	experimental	Tocris	1065 (S)-3,4-DCPG
3267 F09	X	194	200	-1.33788085	594	600	-0.5497422	2489773	-0.76871867	3125188	-0.60738908	experimental	Tocris	1231 Brefeldin A
3267 F10	X	274	280	-1.10045908	393	400	-1.08306676	1323758	-2.22270652	1921659	-2.05646955	experimental	Tocris	1396 Fenretinide
3267 F11	X	436	440	-0.61968001	594	600	-0.5497422	3107255	0.00126399	3851639	0.26727696	experimental	Tocris	1232 Wortmannin
3267 F12	X	432	440	-0.6315511	590	600	-0.56035562	2684902	-0.5253983	3377765	-0.30327976	experimental	Tocris	1397 PP 1
3267 F13	X	1392	1400	2.21751009	1631	1640	2.20187899	2985046	-0.15112719	3432440	-0.23744962	experimental	Tocris	1233 Cyclochalasin D
3267 F14	X	912	920	0.79297995	1191	1200	1.03165799	2933441	-0.21547717	3554835	-0.09008283	experimental	Tocris	1398 Kenpaullone
3267 F15	X	193	200	-1.34084862	392	400	-1.08572012	1531154	-1.96408955	2189758	-1.73367133	experimental	Tocris	1234 AZ3187, free acid
3267 F16	X	380	390	-0.60091462	512	520	-0.60974338	3846332	0.4610132	4814955	0.33686955	experimental	Tocris	1395 CGP 33681 hydrochloride
3267 F17	X	354	360	-0.86303732	713	720	-0.23399283	2513693	-0.7388911	3121979	-0.6112528	experimental	Tocris	1235 Cyclopiazonic Acid
3267 F18	X	354	360	-0.86303732	552	560	-0.66118315	2034875	-1.33956365	2985080	-0.77680279	experimental	Tocris	1400 SCH 202676 hydrobromide
3267 F19	X	515	520	-0.38522662	713	720	-0.23399283	2423513	-0.85134302	3075053	-0.66775294	experimental	Tocris	1236 BHQ
3267 F20	X	513	520	-0.39116156	792	800	-0.02437771	3766085	0.82280644	4415005	0.9455844	experimental	Tocris	1401 NU 1025
3267 F21	X	351	360	-0.87194064	429	440	-0.98754594	1021974	-2.59902266	1041523	-3.11617637	experimental	Tocris	2398 SNAP 5089
3267 F22	X	790	800	0.4309113	1068	1080	0.70794855	3809686	0.87717565	4472414	1.01470634	experimental	Tocris	1402 SB 203580 hydrochloride
3267 F23	E	1280	1600	1.2382154	1396	1840	1.57824933	73652	-3.78155346	74486	-4.28051427	empty		
3267 F24	E	114168	115040	336.910973	188776	189880	498.7641	3607182	0.62465887	3628288	-0.00171574	empty		
3267 G01	N	597	600	-0.14186871	835	840	0.0897166	3549146	0.55228962	4025377	0.47646207	empty		
3267 G02	E	156	160	-1.45065619	195	200	-1.60843125	72639	-3.78281666	72864	-4.2824672	empty		
3267 G03	X	312	320	-0.98768375	552	560	-0.66118315	1291608	-2.26279666	1899908	-2.08265833	experimental	Tocris	2910 H 89 dihydrochloride
3267 G04	X	754	760	0.32407151	753	760	-0.12785859	3226134	0.14950275	4500144	1.04809398	experimental	Tocris	1074 (RS)-AMPA hydrobromide
3267 G05	X	913	920	0.79594727	751	760	-0.13316531	3525341	0.52260545	3767307	0.16573902	experimental	Tocris	946 WB 4101 hydrochloride
3267 G06	X	800	840	0.43981462	1031	1040	0.43981462	4027751	1.14809955	4613607	0.3064413	experimental	Tocris	1075 Nifedipine
3267 G07	X	712	720	-1.19942508	1072	1080	0.71856198	3915863	0.90957538	4400412	0.92801404	experimental	Tocris	947 Zanisarone
3267 G08	X	594	600	-0.15077202	633	640	-0.44626132	3302270	0.2444422	3547107	-0.09938755	experimental	Tocris	1076 Ouabain
3267 G09	X	552	560	-0.27541845	471	480	-0.87610499	3426350	0.39916646	3719647	0.10835514	experimental	Tocris	948 BRL 37344, sodium salt
3267 G10	X	756	760	0.33000705	595	600	-0.54708884	3741382	0.79200249	4285677	0.78987009	experimental	Tocris	1077 Lobeline hydrochloride
3267 G11	X	154	160	-1.45659173	233	240	-1.50760372	910882	-2.73755126	1021027	-3.14085409	experimental	Tocris	949 CP 55,940
3267 G12	X	476	480	-0.50096913	694	600	-0.5497422	3736347	0.78572399	4288308	0.79303789	experimental	Tocris	1079 (+)-SK&F 10047 hydrochloride
3267 G13	X	512	520	-0.39412933	569	680	-0.3507405	3673476	0.70732562	4058113	0.51587707	experimental	Tocris	950 Xamoterol hemifumarate
3267 G14	X	473	480	-0.50987244	551	560	-0.66383651	3003486	-0.12813303	3804510	0.21053241	experimental	Tocris	1080 (R)-(+)-8-Hydroxy-DPAT hydrobromide
3267 G15	X	635	640	-0.02909337	593	600	-0.55239556	3172599	0.08274612	4211681	0.70077697	experimental	Tocris	952 Sotalol hydrochloride
3267 G16	X	474	480	-0.50690467	793	800	-0.02172435	3839198	0.91397629	4390827	0.91647345	experimental	Tocris	1081 SKF 89976A hydrochloride
3267 G17	X	554	560	-0.2694829	631	640	-0.45156803	3671732	0.7051509	4081841	0.54444621	experimental	Tocris	955 (-)-MK 801 maleate
3267 G18	X	675	680	0.08961752	792	800	-0.02437771	3516675	0.51179919	4050355	0.50653624	experimental	Tocris	1082 CFM-2
3267 G19	X	473	480	-0.50987244	751	760	-0.13316531	3312726	0.25748054	3798888	0.20376338	experimental	Tocris	956 BD 1047 dihydrobromide
3267 G20	X	793	800	0.43981462	831	840	0.07910318	3436633	1.54673343	4109011	0.57715956	experimental	Tocris	1088 CGP 54626 hydrochloride
3267 G21	X	792	800	0.43684685	1031	920	0.29137166	3874479	0.9579707	3792027	0.19550255	experimental	Tocris	959 Spemidine trihydrochloride
3267 G22	X	948	960	0.89981929	986	1000	0.49037336	3974506	1.08270155	4258465	0.75710613	experimental	Tocris	1089 8-Bromo-cGMP, sodium salt
3267 G23	E	1190	1640	1.61802013	1323	1880	1.38455434	70853	-3.78504375	75048	-4.27983761	empty		
3267 G24	P	151163	151920	446.703701	186019	187200	491.448797	3498169	0.48872273	3698889	0.08336196	empty		
3267 H01	N	476	480	-0.50096913	635	640	-0.4409546	2938165	-0.20958648	3594841	-0.04191456	empty		
3267 H02	E	276	280	-1.09452354	155	160	-1.71456549	74506	-3.78048856	72382	-4.28304754	empty		
3267 H03	X	555	560	-0.26651513	714	720	-0.23133948	3493453	0.48284201	3818929	0.22789327	experimental	Tocris	1238 CCMQ
3267 H04	X	473	480	-0.50987244	633	640	-0.34278043	3461769	0.44332296	4463325	0.04776513	experimental	Tocris	1403 FPL 64176
3267 H05	X	394	400	-0.74326444	432	440	-0.97985897	1293790	-2.26507577	1640280	-2.39570404	experimental	Tocris	242 SB 216641 hydrochloride
3267 H06	X	353	360	-0.86600509	551	560	-0.66383651	3088966	-0.02154188	3944713	0.3793405	experimental	Tocris	1405 (-)-Terreic acid
3267 H07	X	635	640	-0.02909337	552	560	-0.66118315	3526381	0.5239023	4493628	1.04024855	experimental	Tocris	1243 (+)-PD 128907 hydrochloride
3267 H08	X	231	240	-1.22807328	391	400	-1.08837347	2583297	-0.65209687	3489171	-0.16914401	experimental	Tocris	1407 PP 2
3267 H09	X	1033	1040	1.15207992	1353	1360	1.46415502	2470214	-0.79310819	3321259	-0.37131446	experimental	Tocris	1

3267 I01	N	597	600	-0.14186871	795	800	-0.01641764	3508289	0.50134209	4019636	0.46954976	empty	
3267 I02	E	155	160	-1.45362396	274	280	-1.39881613	71992	-3.78362345	73795	-4.28134625	empty	
3267 I03	X	475	480	-0.50393699	713	720	-0.23399283	2731337	-0.46749516	3926884	0.35787392	experimental	Tocris
3267 I04	X	503	560	-0.27245688	749	760	-0.13847202	3173729	0.08415519	4293132	0.87631184	experimental	Tocris
3267 I05	X	433	440	-0.62858333	671	680	-0.34543379	7044161	-0.00261908	4018222	0.46784726	experimental	Tocris
3267 I06	X	632	640	-0.03799668	910	920	0.2887183	4587539	1.84713643	4347663	0.86450286	experimental	Tocris
3267 I07	X	551	560	-0.27838622	709	720	-0.24460626	4079014	1.21302008	4176779	0.65875405	experimental	Tocris
3267 I08	X	714	720	0.20536063	672	680	-0.34278043	4170510	1.32711302	4339839	0.85508256	experimental	Tocris
3267 I09	X	1032	1040	1.14911215	791	800	-0.02703106	3762110	0.81784972	4137136	0.61102284	experimental	Tocris
3267 I10	X	512	520	-0.39412933	552	560	-0.66118315	3773186	0.83166118	4598721	1.16678328	experimental	Tocris
3267 I11	X	474	480	-0.50690467	592	600	-0.55504891	3525061	0.5222563	3983428	0.42599437	experimental	Tocris
3267 I12	X	755	760	0.32703928	833	840	0.08440989	2290814	-0.89211775	2832215	-0.95230045	experimental	Tocris
3267 I13	X	554	560	-0.2694829	792	800	-0.02437771	2888509	-0.27150611	4016138	0.46533807	experimental	Tocris
3267 I14	X	595	600	-0.14780425	834	840	0.08706324	3170088	0.07961497	4164036	0.64341114	experimental	Tocris
3267 I15	X	634	640	-0.03206114	512	520	-0.76731739	3302637	0.24489984	3989632	0.43342415	experimental	Tocris
3267 I16	X	511	520	-0.3970971	792	800	-0.02437771	3474674	0.45942513	4127991	0.60001202	experimental	Tocris
3267 I17	X	1307	1320	1.96524947	986	1000	0.49037336	2257674	-1.05813958	2590549	-1.25110846	experimental	Tocris
3267 I18	X	3192	3200	7.59499882	2351	2360	4.11220432	8384855	6.58228249	8354469	5.68880233	experimental	Tocris
3267 I19	X	184	200	-1.36755857	303	320	-1.3218688	1066103	-2.61881335	1082414	-3.06694253	experimental	Tocris
3267 I20	X	913	920	0.79594727	1191	1200	1.03431134	2582997	-0.65247097	2880323	-0.90221296	experimental	Tocris
3267 I21	X	1151	1160	1.50227702	1147	1160	0.91756368	3853935	0.93252921	3987305	0.43062238	experimental	Tocris
3267 I22	X	627	640	-0.05283554	1225	1240	1.12452545	3976675	1.08540623	3992038	0.43632104	experimental	Tocris
3267 I23	E	1386	1920	2.19970346	1260	1840	1.21739291	73037	-3.78232036	72998	-4.28230586	empty	
3267 I24	P	179709	180640	531.421723	193619	194880	511.614303	3428721	0.40212303	3496554	-0.16025469	empty	
3267 J01	N	476	480	-0.50096913	715	720	-0.22868612	2719139	-0.48270703	3648017	-0.19461398	empty	
3267 J02	E	200	200	-1.33194341	275	280	-1.39616277	73736	-3.7814487	7480	-4.28012778	empty	
3267 J03	X	514	520	-0.38819379	511	520	-0.7699575	3275055	-0.21050586	4111179	0.75736993	experimental	Tocris
3267 J04	X	1032	1040	1.14911215	792	800	-0.02437771	3306960	0.2502905	4231776	0.72497188	experimental	Tocris
3267 J05	X	831	840	0.55258996	827	840	0.06848975	2418963	-0.85701674	3114382	-0.62039979	experimental	Tocris
3267 J06	X	1311	1320	1.97712055	1508	1520	1.8754252	3032740	-0.09165412	3677717	0.05787032	experimental	Tocris
3267 J07	X	1192	1200	1.62395568	1589	1600	2.09034704	2709602	-0.4945981	3413652	-0.26007087	experimental	Tocris
3267 J08	X	351	360	-0.87194064	789	800	-0.03233778	3069816	-0.04542139	3704324	0.08990584	experimental	Tocris
3267 J09	X	392	400	-0.75026198	632	640	-0.44891467	3852199	0.93018817	4496352	1.04352832	experimental	Tocris
3267 J10	X	665	680	-0.08961752	806	820	0.09017430	2454882	0.08961752	3632888	0.08961752	experimental	Tocris
3267 J11	X	395	400	-0.74135866	714	720	-0.23133948	3626302	0.64850097	4458300	0.99771271	experimental	Tocris
3267 J12	X	354	360	-0.86303732	512	520	-0.76731739	3284474	0.22225109	3668585	0.04687515	experimental	Tocris
3267 J13	X	196	200	-1.33194531	273	280	-1.40146948	1161278	-2.4253145	1263156	-2.84932443	experimental	Tocris
3267 J14	X	153	160	-1.45955951	271	280	-1.40677619	1801129	-1.62743833	2060882	-1.88884141	experimental	Tocris
3267 J15	X	474	480	-0.50690467	635	640	-0.4409546	3501480	0.49285146	4243005	0.73849189	experimental	Tocris
3267 J16	X	594	600	-0.15077202	791	800	-0.55770227	2849087	-0.32066423	3622476	-0.08086413	experimental	Tocris
3267 J17	X	440	450	-0.53748654	606	620	-0.60977430	3371915	0.33128755	3371915	0.08006067	experimental	Tocris
3267 J18	X	665	680	0.0599398	584	600	-0.04560456	3045742	-0.07544099	3853689	0.02893997	experimental	Tocris
3267 J19	X	754	760	0.32407151	1431	1440	1.67111679	3582033	0.59329878	4594073	1.16118696	experimental	Tocris
3267 J20	X	550	560	-0.28135399	1106	1120	0.80877608	3443212	0.4201929	3996230	0.44136832	experimental	Tocris
3267 J21	X	1072	1080	1.26782303	1347	1360	1.44823488	3389490	0.35230308	4028231	0.47989886	experimental	Tocris
3267 J22	P	588	600	-0.16857865	1303	1320	1.33148722	3240739	0.16771478	3709491	0.09612704	experimental	Tocris
3267 J23	E	1202	1720	1.6536334	1475	2172	1.78786445	73643	-3.7815647	74581	-4.28039989	empty	
3267 J24	P	173980	174920	514.383743	216630	217200	572.570678	38617306	0.94207306	4192465	0.6776404	empty	
3267 K01	N	595	600	-0.26354736	595	600	-0.54130889	3170438	0.0883514	3993365	0.43791978	experimental	Tocris
3267 K02	E	236	240	-1.21323442	275	280	-1.39616277	74536	-3.78045115	71621	-4.2839638	empty	
3267 K03	X	354	360	-0.86303732	594	600	-0.5497422	2891938	-0.26723024	3823472	0.23363616	experimental	Tocris
3267 K04	X	834	840	0.56149328	510	520	-0.77262411	2341650	-0.95342387	3083092	-0.65807377	experimental	Tocris
3267 K05	X	432	440	-0.6315511	753	760	-0.12785859	3302512	0.24474397	3812255	0.2198576	experimental	Tocris
3267 K06	X	552	560	-0.27541845	629	640	-0.45687474	2997389	-0.13573582	3152098	-0.57498874	experimental	Tocris
3267 K07	X	632	640	-0.03799668	749	760	-0.13847202	3433100	0.40759352	3578031	-0.06215424	experimental	Tocris
3267 K08	X	674	680	0.08664974	952	960	0.40015925	4364451	1.56895198	4165626	0.64532554	experimental	Tocris
3267 K09	X	634	640	-0.03206114	431	440	-0.98223923	3477525	0.46298025	3695820	0.07966668	experimental	Tocris
3267 K10	X	554	560	-0.2694829	634	640	-0.44360796	3709068	0.75170784	4675380	1.25908272	experimental	Tocris
3267 K11	X	314	320	-0.9817482	312	320	-1.2979886	1066454	-2.54355736	1285792	-2.82207009	experimental	Tocris
3267 K12	X	636	640	-0.02612559	914	920	0.29933173	3237421	0.16357732	4192789	0.67803051	experimental	Tocris
3267 K13	X	393	400	-0.74729421	669	680	-0.3507405	3117537	0.01408535	4466461	1.00753877	experimental	Tocris
3267 K14	X	1115	1120	1.39543723	1434	1440	1.67907685	3028931	-0.09640383	3833080	0.24493144	experimental	Tocris
3267 K15	X	552	560	-0.27541845	606	620	-0.98489259	3144853	0.04814764	4298074	0.80479641	experimental	Tocris
3267 K16	X	511	520	-0.3970971	678	680	-0.77793082	3505771	0.49820221	4156299	0.63409559	experimental	Tocris
3267 K17	X	752	760	0.31813597	501	520	-0.34543379	3542625	0.54415811	4106923	0.57464559	experimental	Tocris
3267 K18	X	872	880	0.67426861	711	720	-0.23929955	4164582	1.31972097	4473080	1.01550822	experimental	Tocris
3267 K19	X	752	760	0.31813597	989	1000	0.49833343	2518468	-0.73293681	2689026	-1.13253957	experimental	Tocris
3267 K20	X	593	600	-0.15373979	749	760	-0.13847202	4078236	1.21204994	3661723	0.03861312	experimental	Tocris
3267 K21	X	548	560	-0.2828954	706	720	-0.25266633	2950070	-0.19474128	3088815	-0.65154434	experimental	Tocris
3267 K22	X	750	760	0.31228042	1065	1080	0.69999898	3114833	0.01071354	2941969	-0.82798956	experimental	Tocris
3267 K23	E	1084	1520	1.30343629	1465	2000	1.76133089	72667	-3.78278174	72171	-4.28330159	empty	
3267 K24	P	145620	146600	430.253341	178068	179400	470.351964	3094923	-0.01411367	3428533	-0.24215375	empty	
3267 L01	N	515	520	-0.38522602	555	560	-0.65322308	2684547	-0.52584098	3562753	-0.08054935	empty	
3267 L02	E	275	280	-1.09749131	235	240	-1.50229701	74489	-3.78050976	70261	-4.28560128	empty	
3267 L03	X	636	640	-0.02612559	874	880	0.19319749	3169874	0.07934812	3994870	0.43973084	experimental	Tocris
3267 L04	X	392	400	-0.75026198	571	560	-0.66383651	3432546	0.4068927	3965668	0.40457087	experimental	Tocris
3267 L05	X	475	480	-0.50393699	553	560	0.6585298	2914079	-0.2396104	3606664	-0.02767936	experimental	Tocris
3267 L06	X	632	640	-0.03799668	633	640	-0.08600509	3626132	0.0974903	3626132	0.0974903	experimental	Tocris
3267 L07	X	476	480	-0.50096913	674	680	-0.33747372	3235211	0.16082157	3951517	0.38753269	experimental	Tocris
3267 L08	X	355	360	-0.86006955	592	600	-0.55504891	2754887	-0.43812898	3648218	0.02235275	experimental	Tocris
3267 L09	X	474	480	-0.50690467	714	720	-0.23133948	3434737	0.40962482	3979339	0.42103111	experimental	Tocris
3267 L10	X	435	440	-0.62264778	514	520	-0.76201068	3016490	-0.1191741	3728241	0		

3267 L19	X	513	520	-0.39116156	751	760	-0.13316531	3447065	0.42499748	4188915	0.67336611	experimental	Tocris	1302 (S)-3,4-DCPG
3267 L20	X	629	640	-0.0469	828	840	0.07114311	3286016	0.22417392	4155721	0.63339966	experimental	Tocris	1461 Linomide
3267 L21	X	1592	1600	2.51106451	1750	1760	2.51753736	3088681	-0.02189727	3623191	-0.00778042	experimental	Tocris	1304 BWB 70C
3267 L22	X	626	640	-0.05580332	1023	1040	0.585854753	1129769	-2.46460533	1797183	-2.2063419	experimental	Tocris	1467 Daunorubicin hydrochloride
3267 L23	E	1029	1026	-1.6988655	1449	2160	1.71887772	72123	3.7834601	71692	7.28387832	empty		
3267 L24	P	161314	162200	476.829556	239279	240400	632.766539	3459458	0.44045121	3735498	0.12744015	empty		
3267 M01	N	716	720	0.21129617	715	720	-0.22868612	3446551	0.42435654	4211124	0.70010633	empty		
3267 M02	E	195	200	-1.33491308	155	160	-1.71456549	72992	-3.78237648	73126	-4.28215174	empty		
3267 M03	X	434	440	-0.62561555	673	680	-0.34012707	2276539	-1.03461546	3455617	-0.20954391	experimental	Tocris	997 Mianserin hydrochloride
3267 M04	X	755	760	0.32703928	1033	1040	0.61508109	2002542	-1.37628199	2840344	-0.95034873	experimental	Tocris	1120 AM 630
3267 M05	X	431	440	-0.63451887	511	520	-0.76997075	2757734	-0.43457885	3055080	-0.69180095	experimental	Tocris	998 AH 11110 hydrochloride
3267 M06	X	956	960	0.92356147	636	640	-0.44360796	4372534	1.57903125	4187053	0.67166482	experimental	Tocris	1122 Telenzepine dihydrochloride
3267 M07	X	154	160	-1.45659173	154	160	-1.71721885	870652	-2.78771693	810972	-3.39376582	experimental	Tocris	999 Tamoxifen citrate
3267 M08	X	155	160	-1.45362396	275	280	-1.39616277	1399436	-2.12833818	1391160	-2.69520426	experimental	Tocris	1123 (S)-(+)-Niguldipine hydrochloride
3267 M09	X	676	680	0.09258529	434	440	-0.97427916	3140036	0.04214097	3454943	-0.21035542	experimental	Tocris	1000 ZD 7288
3267 M10	X	292	240	-1.33788085	234	240	-1.50495037	1227296	-2.34299191	1324877	-2.77501072	experimental	Tocris	1124 (R)-(-)-Niguldipine hydrochloride
3267 M11	X	593	600	-0.15373979	551	560	-0.66383651	2810980	-0.66818259	3423328	-0.24842071	experimental	Tocris	1001 Chlorisondamine diiodide
3267 M12	X	995	1000	1.03930458	1794	1800	2.63428502	3187478	0.10129981	4200570	0.68739903	experimental	Tocris	1125 Quercetin
3267 M13	X	392	400	-0.75026198	586	600	-0.57096905	2647085	-0.57255503	3107253	-0.62898329	experimental	Tocris	1002 L-745,870 thiydrochloride
3267 M14	X	754	760	0.32407151	1153	1160	0.93348381	3641050	0.66689131	4467852	1.00921357	experimental	Tocris	1126 Dexamethasone
3267 M15	X	513	520	-0.39116156	388	400	-1.09633354	2030793	-1.34105379	2445761	-1.425437	experimental	Tocris	1003 L-741,626
3267 M16	X	512	520	-0.39412933	828	840	0.07114311	3506219	0.49876086	4157578	0.63563554	experimental	Tocris	1127 Yohimbine hydrochloride
3267 M17	X	673	680	0.08368197	670	680	-0.34808714	2599552	-0.63182735	3047021	-0.7015042	experimental	Tocris	1004 L-741,742 hydrochloride
3267 M18	X	553	560	-0.27245068	1072	1080	0.71856198	3833132	0.90641216	4441998	0.97808076	experimental	Tocris	1129 BRL 54443
3267 M19	X	512	520	-0.39412933	631	640	-0.45156803	3602023	0.61822574	3909392	0.36681309	experimental	Tocris	1006 BWB 7378 dihydrochloride
3267 M20	X	910	920	0.79594727	712	720	-0.404664619	11760315	1.17603115	4187051	0.5774442	experimental	Tocris	1130 LY 294002 hydrochloride
3267 M21	X	908	920	0.81110841	708	720	-0.24775961	2318681	0.98205557	2268224	-3.81919621	experimental	Tocris	1007 N-Desmethyloclozapine
3267 M22	X	909	920	0.78407618	986	1000	0.49037336	4571556	1.82720608	4308382	0.81720751	experimental	Tocris	1131 KU14R
3267 M23	E	1331	1800	2.036476	1470	2080	1.77459767	73053	-3.78230041	72226	-4.28323537	empty		
3267 M24	P	156840	157800	463.551743	204321	205680	540.010519	3048200	-0.07237593	3392576	-0.28544692	empty		
3267 N01	N	516	520	-0.38225824	915	920	0.30198508	2355016	-0.93675685	2904557	-0.87303459	empty		
3267 N02	E	156	160	-1.45065619	195	200	-1.60843125	69425	-3.78682443	70875	-4.28486201	empty		
3267 N03	X	555	560	-0.26651513	471	480	-0.87610499	3454731	0.43455677	4097748	0.56359865	experimental	Tocris	1305 Monastrol
3267 N04	X	385	400	-0.87194064	593	600	-0.45422158	3183433	1.58431218	3197497	0.6289114	experimental	Tocris	1470 Flecainide acetate
3267 N05	X	1035	1040	1.15801546	992	1000	0.50894685	2476485	-0.78528843	2793247	-1.00705475	experimental	Tocris	1307 Ciglitazone
3267 N06	X	430	440	-0.63748664	592	600	-0.55504891	2748684	-0.44586394	3156968	-0.56912513	experimental	Tocris	1471 Etomidate
3267 N07	X	395	400	-0.74135866	515	520	-0.75935733	2826110	-0.3493159	3492512	-0.16512136	experimental	Tocris	1309 PNDOS
3267 N08	X	394	400	-0.74432644	553	560	-0.6585298	2454630	-0.812541	3216295	-0.49769387	experimental	Tocris	1472 Suramin hexasodium salt
3267 N09	X	473	480	-0.50987244	994	1000	0.51160021	3486520	0.47419676	4241535	0.73672197	experimental	Tocris	1310 UCL 1684
3267 N10	X	393	400	-0.74729421	633	640	-0.44626132	2640875	-0.58029873	3410481	-0.26388883	experimental	Tocris	1475 (-)-[R,4S]-Chromanol 293B
3267 N11	X	664	670	0.32061114	610	620	-0.32061114	3402268	0.36136881	4173107	0.89190321	experimental	Tocris	1312 WY 14643
3267 N12	X	312	320	-0.98765975	310	320	-1.30329531	766830	-2.9178004	967650	-3.2051214	experimental	Tocris	1477 GR 127935 hydrochloride
3267 N13	X	595	600	-0.14780425	554	560	-0.65587644	3657611	0.68754241	4214765	0.70449019	experimental	Tocris	1317 CP 94253 hydrochloride
3267 N14	X	392	400	-0.75026198	590	600	-0.56035562	2222349	-1.10218886	3036519	-0.71414889	experimental	Tocris	1479 Mefipristone
3267 N15	X	753	760	0.32110374	1151	1160	0.9281771	3017255	-0.11096347	3971716	0.41185282	experimental	Tocris	1321 XM 336372
3267 N16	X	312	320	-0.98768375	510	520	-0.77262411	1103506	-2.49735456	1356649	-2.7367564	experimental	Tocris	1480 FIT
3267 N17	X	513	520	-0.39116156	712	720	-0.23399283	3382551	0.34455034	3905771	0.33245331	experimental	Tocris	1322 GR 113808
3267 N18	X	548	560	-0.28748954	546	560	-0.67710329	2578979	-0.6574813	3622208	-0.66653821	experimental	Tocris	1483 GR 89656 fumarate
3267 N19	X	593	600	-0.15373979	550	560	-0.66468986	3148803	0.3835207	4274775	0.71767438	experimental	Tocris	1323 Butabindole oxalate
3267 N20	X	391	400	-0.75322975	711	720	-0.23929955	2006850	-1.37091004	2884346	-0.89736917	experimental	Tocris	1484 Olethethanolamide
3267 N21	X	592	600	-0.15670757	710	720	-0.2419529	3430022	0.40374534	4270571	0.77168207	experimental	Tocris	1324 RX 821002 hydrochloride
3267 N22	X	549	560	-0.28432176	947	960	0.38689247	2706813	-0.4980759	3184421	-0.536071	experimental	Tocris	1493 CGP 78608
3267 N23	E	1424	1920	2.3124788	1328	2000	1.39782112	68138	-3.78842928	70798	-4.28495472	empty		
3267 N24	P	166638	167520	492.629974	225763	227000	596.903779	3522595	0.51918127	3882661	0.30462826	empty		
3267 O01	N	636	640	-0.02612559	755	760	-0.12255188	3311167	0.25553651	3450898	-0.21522571	empty		
3267 O02	E	235	240	-1.2162022	193	200	-1.61373796	71318	-3.78446391	69316	-4.28673908	empty		
3267 O03	X	754	760	0.32407151	1434	1440	1.67907685	2945109	-0.2009275	3728119	0.11855565	experimental	Tocris	1014 QX 314 bromide
3267 O04	X	913	920	0.79594727	991	1000	0.50364014	2931468	-0.21793745	4032731	0.48531648	experimental	Tocris	1132 RS 16566 hydrochloride
3267 O05	X	589	600	-0.16561088	630	640	-0.45422138	2991027	-0.14366905	3016512	-0.73823784	experimental	Tocris	1015 RS 16566 hydrochloride
3267 O06	X	1067	1080	1.25298417	587	600	-0.56831569	3870973	0.95359882	3918345	0.34759274	experimental	Tocris	1133 BRL 44408 maleate
3267 O07	X	791	800	0.43387908	553	560	-0.6585298	2883785	-0.2773968	2908412	-0.86839307	experimental	Tocris	1018 LY 225910
3267 O08	X	1153	1160	1.50821257	754	760	-0.12520524	3769354	0.82688279	3925092	0.3557163	experimental	Tocris	1134 CGP 12177 hydrochloride
3267 O09	X	871	880	0.67130084	514	520	-0.76997075	3651810	0.68030873	3737470	0.12981449	experimental	Tocris	1024 CGP 20712 dihydrochloride
3267 O10	X	1072	1080	1.26782303	590	600	-0.56035562	3330497	0.27964047	3640760	0.01337312	experimental	Tocris	1139 L-NIL hydrochloride
3267 O11	X	670	680	0.07477866	591	600	-0.55770227	2858593	-0.30881052	3606372	-0.02803093	experimental	Tocris	1025 Nisoxetine hydrochloride
3267 O12	X	554	560	-0.2694829	514	520	-0.76201068	3024023	-0.10229951	3762179	0.15956478	experimental	Tocris	1140 8-Bromo-cAMP, sodium salt
3267 O13	X	673	680	0.08368197	593	600	-0.55239556	2968547	-0.17170098	3927406	0.35850242	experimental	Tocris	1026 HomoAMPA
3267 O14	X	720	730	0.19052177	540	560	-0.67444993	3004320	-0.17093006	3822232	0.23187016	experimental	Tocris	1141 Dibutyryl-cAMP, sodium salt
3267 O15	X	850	1160	1.50227702	1670	1680	2.30526888	3066541	-0.04950522	3732419	0.12373296	experimental	Tocris	1027 PHCC
3267 O16	X	782	800	0.67428954	748	760	-0.14112327	3289869	0.2289785	3983045	0.42543223	experimental	Tocris	1142 N-kymenazoline hydrochloride
3267 O17	X	788	800	0.15497576	747	760	-0.65437973	3524808	0.3835207	4053273	0.51004959	experimental	Tocris	1028 CCZOC
3267 O18	X	2312	2320	4.9478604	2510	2520	4.53408793	2278043	-1.03274001	2354041	-1.53587029	experimental	Tocris	2926 FPA 124
3267 O19	X	906	920	0.77517287	1386	1400	1.55171577	3724950	0.77151225	3682656	0.063817	experimental	Tocris	1029 Methyllycaonitine citrate
3267 O20	X	1072	1080	1.26782303	988	1000	0.49568007	3254707	0.18513248	3056353	-0.69026823	experimental	Tocris	1144 U0126
3267 O21	X	791	800	0.43387908	908	920	0.28341159	3630710	0.65399763					

3267 P13	X	392	400	-0.75026198	752	760	-0.13051195	2655437	-0.56214033	3275107	-0.42688268	experimental	Tocris	1345	AF-DX 384
3267 P14	X	1634	1640	2.93571093	1593	1600	2.10096046	2523282	-0.72693389	3173864	-0.5487819	experimental	Tocris	1505	Mycophenolic acid
3267 P15	X	790	800	-0.4309113	1067	1080	0.7052952	2759323	-0.43259741	3384600	-0.29505024	experimental	Tocris	1347	Nafadotride
3267 P16	X	554	560	-0.2698929	1233	1240	1.1457523	2854928	-0.31338067	3464860	-0.19641509	experimental	Tocris	1506	Tarazosin hydrochloride
3267 P17	X	515	520	-0.38522602	1092	600	-0.55504891	2920057	-0.22166664	3741015	-0.13408277	experimental	Tocris	1348	IL-65 fumarate
3267 P18	X	390	400	-0.75619752	749	760	-0.13847202	3469663	0.45317655	4114636	0.58393225	experimental	Tocris	1507	FR 122047 hydrochloride
3267 P19	X	674	680	0.08664974	751	760	-0.13316531	3101750	-0.00560059	3554199	-0.09084859	experimental	Tocris	1349	(R)-(-)-Rolipram
3267 P20	X	592	600	-0.15670757	950	960	0.39485254	2892480	-0.26655438	3413113	-0.26071984	experimental	Tocris	1508	GW 9662
3267 P21	X	872	880	0.67426861	1547	1560	1.97890608	2743717	-0.45205765	3585104	-0.05363816	experimental	Tocris	1350	(S)-(+)-Rolipram
3267 P22	X	1392	1400	2.21751009	2427	2440	4.31385938	2772743	-0.41586305	3387466	-0.29159957	experimental	Tocris	1509	TMS
3267 P23	E	1035	1520	1.15801546	1694	2360	2.36894942	67740	-3.78892557	67059	-4.28945665	empty			
3267 P24	E	164176	164600	485.323319	224797	225440	594.340637	2737772	-0.4594709	3175174	-0.55310436	empty			
3268 A01	N	678	680	-0.0563533	718	720	0.01534378	1325582	-1.0411509	2554338	0.35770075	empty			
3268 A02	E	157	160	-0.11557422	116	120	-0.38702915	113361	-3.5603463	141645	-3.23487198	empty			
3268 A03	X	318	320	-0.0972737	678	680	-0.01139197	1441769	-0.79969513	2490496	0.26263809	experimental	Tocris	1510	Ozagrel hydrochloride
3268 A04	X	237	240	-0.10648079	276	280	-0.28008618	877174	-1.97301676	956694	-2.02123941	experimental	Tocris	1701	A 77636 hydrochloride
3268 A05	X	156	160	-0.11568788	236	240	-0.30682193	833212	-2.06437706	875146	-2.14266684	experimental	Tocris	1511	SR 59230A hydrochloride
3268 A06	X	676	680	-0.05658063	475	480	-0.14707586	1592433	-0.48659046	1876423	-0.65173515	experimental	Tocris	1702	N6 -Cyclopropyladenosine
3268 A07	X	673	680	-0.05692164	955	960	0.17375305	1553396	-0.56771579	1975125	-0.50476489	experimental	Tocris	1512	SB 205384
3268 A08	X	755	760	-0.04760088	715	720	0.0133386	1520129	-0.63685011	1927174	-0.57616538	experimental	Tocris	1703	2-Chloro-N6-cyclopropyladenosine
3268 A09	X	555	560	-0.07033444	475	480	-0.14707586	1268055	-1.1607015	1512894	-1.19304081	experimental	Tocris	1515	CGP 7930
3268 A10	X	555	560	-0.07033444	436	640	-0.0394645	1556896	-0.56044221	1793870	-0.77465906	experimental	Tocris	1704	Acetaminophen
3268 A11	X	675	680	-0.0566943	635	440	-0.1738116	1588375	-0.49502365	2182025	-0.19668455	experimental	Tocris	1516	CGP 13501
3268 A12	X	636	640	-0.06112734	516	520	-0.11967173	1659297	-0.34763603	2405427	0.13596778	experimental	Tocris	1707	Sulindac
3268 A13	X	475	480	-0.07942786	715	720	0.0133386	1417955	-0.84918455	2033023	-0.41855302	experimental	Tocris	1516	SDZ 21009
3268 A14	X	495	600	-0.06556039	396	600	-0.09878925	1369734	-0.95363025	1823777	-0.40231999	experimental	Tocris	2108	Midonetacin
3268 A15	X	437	440	-0.08397457	435	440	-0.1738116	1494852	-0.68057985	2484022	-0.24763781	experimental	Tocris	1518	5-iodo-A-85380 dihydrochloride
3268 A16	X	717	720	-0.05192025	675	680	-0.01339715	1478849	-0.72263677	2252834	-0.09124781	experimental	Tocris	1709	CL 218872
3268 A17	X	355	360	-0.09306799	474	480	-0.14774426	1659935	-0.34631016	1747461	-0.84376347	experimental	Tocris	1524	LY 288513
3268 A18	X	437	440	-0.08374723	755	760	0.04007434	1621096	-0.42702401	1833987	-0.71492364	experimental	Tocris	1710	CV 1808
3268 A19	X	316	320	-0.09750104	555	560	-0.09360438	1727086	-0.20675929	2029181	-0.42427388	experimental	Tocris	1526	Mevastatin
3268 A20	X	475	480	-0.07942786	435	440	-0.1738116	1192930	-1.31682366	1231648	-1.61182446	experimental	Tocris	1742	RG-9544 hydrochloride
3268 A21	X	636	640	-0.06112734	677	680	-0.01206036	1773418	-0.11047374	2070891	-0.36216643	experimental	Tocris	1529	SMC-162
3268 A22	E	480	480	-0.08021762	352	480	-0.08021762	10224371	1.66711293	16671929	1.90077399	experimental	Tocris	1743	Bay 11-7085
3268 A23	E	1583	2840	0.04651605	636	1440	-0.0394645	119605	-3.54737023	114370	-3.27548528	empty			
3268 A24	P	430063	431280	48.7508914	275440	276040	183.637763	1535203	-0.60552385	1711180	-0.89778697	empty			
3268 B01	N	476	480	-0.07931419	635	640	-0.04013289	1688863	-0.286193	1818824	-0.7375018	empty			
3268 B02	E	117	120	-0.12012093	116	120	-0.38702915	126322	-3.5334112	119113	-3.26842281	empty			
3268 B03	X	402	440	-0.08772561	315	320	-0.25401883	1413158	-0.85915351	1605286	-1.05546633	experimental	Tocris	1965	Simvastatin
3268 B04	X	517	520	-0.07465381	496	440	-0.17314321	1403562	-0.87099568	1675496	-0.95092152	experimental	Tocris	2194	R 59-022
3268 B05	X	394	400	-0.08863495	514	400	-0.19548217	1769660	-0.11628349	217818	-1.25253828	experimental	Tocris	1514	Etilprodil hydrochloride
3268 B06	X	433	440	-0.08420191	534	600	-0.06753703	2187009	0.74903664	2622433	0.45909775	experimental	Tocris	2195	Eliprodil
3268 B07	X	835	840	-0.03850745	474	480	-0.14774426	1825672	-0.0018813	2133676	-0.26867767	experimental	Tocris	1969	SL 327
3268 B08	X	432	440	-0.08431557	394	400	-0.20121574	1777083	-0.10285727	2363884	0.074109	experimental	Tocris	2196	3-MATIDA
3268 B09	X	556	560	-0.07022077	476	480	-0.14640747	1860793	0.07110593	2177643	-0.20320948	experimental	Tocris	1970	Norketamine hydrochloride
3268 B10	X	394	400	-0.08863495	314	320	-0.25468723	1618155	-0.4331359	1726098	-0.87557362	experimental	Tocris	2197	L 755507
3268 B11	X	475	480	-0.07942786	436	440	-0.17314321	1902765	0.15833068	2159929	-0.22958616	experimental	Tocris	1971	(+)-Anabasine hydrochloride
3268 B12	X	154	160	-0.11591522	354	160	-0.3616302	935493	-1.85102025	1751544	-1.99897841	experimental	Tocris	2198	Mibepradil dihydrochloride
3268 B13	X	474	480	-0.07931419	676	680	-0.07931419	1896562	-0.0546719	2040262	-0.40777393	experimental	Tocris	1972	Tianeptine
3268 B14	X	154	160	-0.11591522	74	80	-0.41510168	986008	-1.74684174	1026255	-1.91766098	experimental	Tocris	2199	CGP 71683 hydrochloride
3268 B15	X	516	520	-0.07476748	635	640	-0.04013289	1904308	0.16153729	2710835	0.59072951	experimental	Tocris	1974	SANT-1
3268 B16	X	393	400	-0.08874862	753	760	0.03873755	1827015	0.00090967	2333256	0.02850298	experimental	Tocris	2200	PD 160170
3268 B17	X	435	440	-0.08397457	714	720	0.0126702	1758298	-0.1418956	2148175	-0.24708822	experimental	Tocris	1975	6-Iodo-nordihydrocapsaicin
3268 B18	X	62	520	-0.12637266	513	520	-0.12167691	1875346	0.10134947	2299292	-0.02207044	experimental	Tocris	2201	PHU 22394 hydrochloride
3268 B19	X	475	480	-0.07942786	595	600	-0.06686863	1784992	-0.08642106	2157443	-0.23238789	experimental	Tocris	1979	L-803,087 trifluoroacetate
3268 B20	X	715	720	-0.05214759	553	560	-0.09494116	1668283	-0.32986163	2040262	-0.40777393	experimental	Tocris	2202	Zatebradine hydrochloride
3268 B21	X	393	400	-0.08874862	393	400	-0.20188413	1738945	-0.18211433	1890497	-0.63077854	experimental	Tocris	1982	Rboxetine mesylate
3268 B22	X	546	560	-0.07135745	752	760	0.03806916	1821096	-0.01139099	2095299	-0.32582218	experimental	Tocris	2203	PALDA
3268 B23	E	1337	2560	0.01855378	555	1160	-0.09360438	126513	-3.53301427	125182	-3.25938588	empty			
3268 B24	P	415517	417480	47.0974797	204653	205880	136.324187	1716271	-0.22923465	1958241	-0.52990568	empty			
3268 C01	N	517	520	-0.07465381	756	760	0.04074273	1722745	-0.21578061	3022730	1.05515058	empty			
3268 C02	E	83	120	-0.12398563	156	160	-0.36029341	124792	-3.53659079	124575	-3.26028973	empty			
3268 C03	X	12115	12120	1.24366523	398	400	-0.19548217	1897209	0.14678439	3032779	1.07011386	experimental	Tocris	1530	Lovastatin
3268 C04	X	79	120	-0.1244403	112	120	-0.38970273	927185	-1.86908565	1085273	-1.82978139	experimental	Tocris	1744	Bay 11-7821
3268 C05	X	795	800	-0.04305417	755	760	0.04007434	2035258	0.43367301	2529910	0.32132672	experimental	Tocris	1531	Icilin
3268 C06	X	593	600	-0.06601506	474	480	-0.14774426	1581914	-0.50845068	2166835	-0.21930292	experimental	Tocris	1746	Nemonapride
3268 C07	X	313	320	-0.09784204	275	280	-0.28075458	1466997	-0.74726718	1929329	-0.57295652	experimental	Tocris	1540	DCPIB
3268 C08	X	636	640	-0.06112734	356	360	-0.2266147	1645940	-0.37539408	1819908	-0.18494652	experimental	Tocris	1747	Isoproterenol hydrochloride
3268 C09	X	115	120	-0.12034826	116	120	-0.38702915	1069567	-1.57319234	1190736	-1.6727438	experimental	Tocris	1541	HA14-1
3268 C10	X	437	440	-0.08374723	397	440	-0.1921056	1070961	-1.57029508	1170866	-1.6308276	experimental	Tocris	1748	IG 132
3268 C11	X	474	480	-0.07954153	474	480	-0.14774426	1802936	-0.04913047	2492296	0.26531834	experimental	Tocris	1742	Spilimicin
3268 C12	X	511	520	-0.07533582	513	520	-0.12167691	1577944	-0.51670099	2425392	0.16569627	experimental	Tocris	2737	TC 2559 difumarate
3268 C13	X	555	560	-0.07033444	274	280	-0.28142297	1898479	0.14942366	3098391	1.1678121	experimental	Tocris	1544	(*)-Bay K 8644

3268 D07	X	312	320	-0.09795571	435	440	-0.1738116	1965279	0.28824509	2800701	0.7245427	experimental	Tocris	1995	Ro 19-4605
3268 D08	X	635	640	-0.06124101	676	680	-0.01272875	2082007	0.53082515	3314160	1.48909866	experimental	Tocris	2214	ABT 724 trihydrochloride
3268 D09	X	234	240	-0.1068218	233	240	-0.30882711	1352333	-0.985579	1211761	-1.64143694	experimental	Tocris	1996	ZK 93426 hydrochloride
3268 D10	X	120	120	-0.12048286	115	120	-0.38769755	929452	-1.86437445	862411	-2.01272662	experimental	Tocris	2227	CI 976
3268 D11	X	480	480	-0.07976886	552	560	-0.05609592	2017508	2.396368	263368	0.53494002	experimental	Tocris	1997	Ro 15-4513
3268 D12	X	1754	1760	0.06595325	1434	1440	0.49391357	2175650	0.72543077	2962548	0.96553777	experimental	Tocris	2228	Leflunomide
3268 D13	X	511	520	-0.07533582	432	440	-0.17581679	2515764	1.43224382	2986952	1.00187606	experimental	Tocris	1999	Linopiridine dihydrochloride
3268 D14	X	375	480	-0.07942786	675	680	-0.01339715	1609071	-0.45201395	2119138	-0.29032519	experimental	Tocris	2229	GW 0742
3268 D15	X	395	400	-0.08852128	554	560	-0.09427277	2203701	0.78372538	2937423	0.92812589	experimental	Tocris	2000	XE 991 dihydrochloride
3268 D16	X	514	520	-0.07499481	632	640	-0.04213807	2149060	0.67017236	3912579	2.38016262	experimental	Tocris	2237	BRL 50481
3268 D17	X	352	360	-0.093409	592	600	-0.06887381	1888067	0.12778581	2708807	0.58770976	experimental	Tocris	2001	GS59783
3268 D18	X	765	1240	-0.04646442	1393	1400	0.46509944	1638309	-0.39125256	2497855	-0.32509851	experimental	Tocris	2238	GW 441756
3268 D19	X	6152	6160	0.56586419	231	240	-0.31016389	857239	-2.01444498	880074	-2.1353289	experimental	Tocris	2002	Ro 31-8220 mesylate
3268 D20	X	538	560	-0.07226679	486	560	-0.13927353	2574513	1.55433394	2801401	0.72558502	experimental	Tocris	2239	GW 583340 dihydrochloride
3268 D21	X	353	360	-0.09329533	473	480	-0.14841265	1787261	-0.08170571	2045898	-0.39938176	experimental	Tocris	2004	Isradipine
3268 D22	X	509	520	-0.07556315	632	640	-0.04213807	1669278	-0.32689386	1866712	-0.66619513	experimental	Tocris	2241	DMAB-anabaseine dihydrochloride
3268 D23	E	648	1200	-0.05976333	579	1000	-0.07756293	130732	-3.52424649	125002	-3.25965391	empty			
3268 D24	P	186241	187480	21.0361831	142150	143000	94.5475836	1852881	0.05466349	2180494	-0.19896425	empty			
3268 E01	N	556	560	-0.07022077	637	640	-0.03087961	1737280	-0.18557448	3171036	1.2759827	empty			
3268 E02	E	117	120	-0.12012093	157	160	-0.35962502	131244	-3.52318247	134557	-3.24542623	empty			
3268 E03	X	114	120	-0.12046193	196	200	-0.33355767	1037202	-1.64045216	1334053	-1.45934046	experimental	Tocris	1549	CD 437
3268 E04	X	475	480	-0.07942786	513	520	-0.12167691	1841051	0.0300788	2635218	0.47813352	experimental	Tocris	1762	Acifran
3268 E05	X	552	560	-0.07067544	676	680	-0.01272875	1958391	0.27393069	2953755	0.95244473	experimental	Tocris	1550	SC 560
3268 E06	X	152	160	-0.11614256	154	160	-0.3616302	882288	-1.96238903	959028	-2.01776401	experimental	Tocris	2747	NNC 05-2090 hydrochloride
3268 E07	X	676	680	-0.05658063	474	480	-0.14774426	2627368	1.66417536	2917356	0.89824552	experimental	Tocris	1551	STO-609 acetate
3268 E08	X	471	480	-0.07988253	594	600	-0.07988253	1720255	-2.22095324	3917462	-1.14458738	experimental	Tocris	1567	Mefenidine dihydrochloride
3268 E09	X	1315	1320	0.01605349	1476	1480	0.5219861	806453	0.8521587	2352092	0.80555035	experimental	Tocris	1554	Picostatin
3268 E10	X	589	600	-0.06646973	390	400	-0.20388932	2321057	1.02761052	276764	0.07988643	experimental	Tocris	1769	Flurbiprofen
3268 E11	X	394	400	-0.08863495	675	680	-0.01339715	1797957	-0.05947765	2804270	0.72985705	experimental	Tocris	1555	AG 825
3268 E12	X	472	480	-0.07976886	392	400	-0.20255253	1226281	-1.24751477	1410295	-1.34581382	experimental	Tocris	1770	Deguelin
3268 E13	X	354	360	-0.09318166	454	360	-0.22795148	1649971	-0.36701699	2492571	0.26572782	experimental	Tocris	1558	Tracazolate hydrochloride
3268 E14	X	514	520	-0.07499481	374	480	-0.14774426	1685788	-0.29258335	159154	-0.23074016	experimental	Tocris	1771	S 14506 hydrochloride
3268 E15	X	475	480	-0.07942786	352	360	-0.22928827	1960684	0.27906999	2667674	0.52646148	experimental	Tocris	1561	(S)-SNAP 5114
3268 E16	X	440	440	-0.04762085	515	520	-0.07522115	2180642	0.80056425	2445336	1.18298621	experimental	Tocris	1772	Radipridil hydrochloride
3268 E17	X	674	680	-0.05680797	510	520	-0.12368209	1947427	0.25114569	2795064	0.71614904	experimental	Tocris	1579	HEMADO
3268 E18	X	671	680	-0.05714897	1151	1160	0.30475819	1714624	-0.23265738	2143873	-0.25349403	experimental	Tocris	1777	Artcigenin
3268 E19	X	818	840	-0.04043981	765	840	0.04675827	1083564	-1.54410426	1437780	-1.30488783	experimental	Tocris	1580	Purvalanol A
3268 E20	X	391	400	-0.08897595	23911	23920	15.5173959	1405239	-0.8756105	1730486	-0.86903975	experimental	Tocris	1778	Ro 106-9920
3268 E21	X	674	680	-0.05680797	645	720	-0.03344895	2295936	0.97540494	2896728	0.8675298	experimental	Tocris	1581	Purvalanol B
3268 E22	X	871	880	-0.03441541	592	600	-0.06887381	2223501	0.82487305	2326666	0.01869027	experimental	Tocris	1997	NNC 711
3268 E23	E	1200	-0.05820433	24687	569	569	126614	-3.53280437	126614	-3.26546877	empty				
3268 E24	P	181144	182560	20.4568184	145222	146080	96.6008886	2351125	1.09009679	2626160	0.46464588	empty			
3268 F01	N	637	640	-0.06101368	396	400	-0.19987895	2474133	1.34572773	2587699	0.40737629	empty			
3268 F02	E	156	160	-0.11568788	117	120	-0.38636076	134415	-3.51659261	120404	-3.26650047	empty			
3268 F03	X	477	480	-0.07920052	456	360	-0.2266147	1688060	-0.28786176	2022851	-0.43369944	experimental	Tocris	2005	Ro 04-5595
3268 F04	X	310	320	-0.09818304	335	440	-0.1738116	2350529	1.0888582	3023308	1.05601124	experimental	Tocris	2242	Octopamine hydrochloride
3268 F05	X	1835	1840	-0.07516034	354	360	-0.22795148	1673546	-1.31802425	1995361	-0.47433507	experimental	Tocris	2006	Paxilline
3268 F06	X	440	-0.08442924	594	594	600	-0.06753703	2480088	1.3581032	3265877	1.42286212	experimental	Tocris	2251	Isiplatin
3268 F07	X	555	560	-0.07033444	1155	1160	0.30743111	2187598	0.75026066	2856248	0.46464588	experimental	Tocris	2007	Fluticasone propionate
3268 F08	X	474	480	-0.07954153	553	560	-0.09494116	1448087	-0.78656528	1840969	-0.70452723	experimental	Tocris	2252	Doxorubicin hydrochloride
3268 F09	X	548	560	-0.07113011	430	440	-0.17715357	2121216	0.61230793	3175736	1.28298114	experimental	Tocris	2008	SKF 86002 dihydrochloride
3268 F10	X	1793	1800	0.07038629	1196	1200	0.3348359	2011445	0.38418566	2298186	-0.02371731	experimental	Tocris	2254	ACDPD hydrochloride
3268 F11	X	592	600	-0.06612873	313	320	-0.25535562	3793963	4.08855239	4542776	3.31854498	experimental	Tocris	2009	PSB 1115
3268 F12	X	315	320	-0.09761471	274	280	-0.28142297	1446061	-0.79077564	1605685	-1.05487221	experimental	Tocris	2255	CGS 9343B
3268 F13	X	395	400	-0.08852128	755	760	0.04007434	2142466	0.65946894	3220320	1.34936806	experimental	Tocris	2752	MRS 1754
3268 F14	X	755	760	-0.04762088	514	520	-0.12100851	2241248	0.86175424	3245330	1.38809774	experimental	Tocris	2261	L-692,585
3268 F15	X	313	320	-0.09784204	473	480	-0.14841265	1889579	0.13092799	2490078	0.26201567	experimental	Tocris	2011	Tomoxetine hydrochloride
3268 F16	X	954	960	-0.02498099	952	960	0.17174787	1914822	-1.8338712	2541434	0.33848631	experimental	Tocris	2266	DY131
3268 F17	X	674	680	-0.05680797	594	600	-0.06753703	2134747	0.64042758	2811615	0.74079397	experimental	Tocris	2012	PSB 11
3268 F18	X	192	200	-0.11159584	192	200	-0.33623124	866481	-1.99523858	934049	-2.0549585	experimental	Tocris	2268	NNC 55-0396 dihydrochloride
3268 F19	X	432	440	-0.08431557	459	480	-0.15777016	2113429	0.59612526	2271712	-0.0631379	experimental	Tocris	2013	Guggulsterone
3268 F20	X	915	920	-0.02941403	766	840	0.04742273	2021103	0.40425658	2567474	0.37726065	experimental	Tocris	2270	SCH 58261
3268 F21	X	431	440	-0.08442924	594	760	0.03740077	2106678	0.58209556	2444607	0.19430798	experimental	Tocris	2018	Mirtazepine
3268 F22	X	630	640	-0.06180935	550	560	-0.09694634	2044951	0.45381666	2446299	0.19682742	experimental	Tocris	2018	GW 4471
3268 F23	E	681	1560	-0.05601229	591	1040	-0.06954221	131624	-3.52239277	121771	-3.26446497	empty			
3268 F24	P	299080	300280	33.862343	151400	152280	100.730224	1964761	0.2871686	2477963	0.24397607	empty			
3268 G01	N	477	480	-0.07920052	677	680	-0.01206036	1789891	-0.07624013	3288213	1.45046279	empty			
3268 G02	E	116	120	-0.1202346	75	80	-0.41443229	131083	-3.52351705	191770	-3.16023434	empty			
3268 G03	X	596	600	-0.06567406	756	760	0.04074273	1862998	0.07568829	3572897	1.87436586	experimental	Tocris	2681	17-PA
3268 G04	X	515	520	-0.07488115	585	585	-0.09360438	1903654	0.1617817	250586	0.96303024	experimental	Tocris	1780	NBQX-0532
3268 G05	X	440	440	-0.07078111	476	480	-0.14640747	1541534	-0.59236699	3582783	1.88922503	experimental	Tocris	1586	SKF 83566 hydrobromide
3268 G06	X	555	560	-0.07033444	354	360	-0.22795148	2044847	0.45360054	2939489	0.93120222	experimental	Tocris	1794	Ro 26-4590 trifluoroacetate
3268 G07	X	155	160	-0.11580155	74	80	-0.41510168	923924	-1.87586254	1048842	-1.88402825	experimental	Tocris	1588	Ind

3268 H01	N	276	280	-0.10204775	596	600	-0.06620024	1871357	0.09305967	2922670	0.90615822	empty								
3268 H02	E	117	120	-0.12012093	116	120	-0.38702915	130587	-3.52454782	118129	-3.26988801	empty								
3268 H03	X	395	400	-0.08852128	432	440	-0.17581679	1884515	0.12040417	2674296	0.53632184	experimental	Tocris	2019					PSB 36	
3268 H04	X	196	200	-0.11114117	155	160	-0.3609618	2215574	0.80839943	2129791	-0.18065365	experimental	Tocris	2272					Ro 08-2750	
3268 H05	X	115	120	-0.12034826	115	120	-0.38769755	924610	-1.87443692	966072	-2.0073238	experimental	Tocris	2020					CI 5	
3268 H06	X	596	600	-0.06567406	797	800	0.06814687	1762714	-0.13271842	2535586	0.32977846	experimental	Tocris	2275					TBB	
3268 H07	X	153	160	-0.11602889	114	120	-0.38836594	932468	-1.8581067	1008604	-1.94394385	experimental	Tocris	2021					LE 135	
3268 H08	X	596	600	-0.06567406	475	480	-0.14707586	2155143	0.68281383	3413217	1.63659752	experimental	Tocris	2276					FPL 55712	
3268 H09	X	435	440	-0.08397457	876	880	0.12094996	2001800	0.36414176	2692760	0.56381529	experimental	Tocris	2022					SR 202	
3268 H10	X	154	160	-0.11591522	192	200	-0.33623124	1005417	-1.70650663	1183461	-1.6837565	experimental	Tocris	2280					Raloxifene hydrochloride	
3268 H11	X	396	400	-0.08840761	676	680	-0.01272875	1975135	0.30872749	2769562	0.67817579	experimental	Tocris	2283					Medetomidine hydrochloride	
3268 H12	X	354	360	-0.05318166	392	400	-0.20255253	2563242	1.53091094	3314304	1.48933975	experimental	Tocris	2281					2'-MeCCPA	
3268 H13	X	1155	1160	-0.00213376	1075	1080	0.25396028	1896523	0.14535877	3127371	1.21096419	experimental	Tocris	2025					Cinalukast	
3268 H14	X	433	440	-0.08420191	552	560	-0.09560956	2234542	0.64781807	3861502	2.30410742	experimental	Tocris	2282					Moxonidine hydrochloride	
3268 H15	X	554	560	-0.07044481	631	640	-0.04280646	2363003	1.11478124	3527311	1.80648693	experimental	Tocris	2037					SDZ 205-557 hydrochloride	
3268 H16	X	514	520	-0.07499481	514	520	-0.12100851	2502409	1.40448992	3679460	2.03304139	experimental	Tocris	2284					SEW 2871	
3268 H17	X	876	880	-0.03384707	555	560	-0.09360438	1525291	-0.62612262	1749143	-0.84125892	experimental	Tocris	2029					CI 898 trihydrochloride	
3268 H18	X	391	400	-0.08897595	352	360	-0.22928827	2164412	0.70207635	2931612	0.91947313	experimental	Tocris	2288					O-1918	
3268 H19	X	1034	1040	-0.01588756	1053	1080	0.23925562	1296175	-1.1022635	1256037	-1.42660562	experimental	Tocris	2072					Aminopurvalanol A	
3268 H20	X	512	520	-0.07522215	3072	3080	1.58874225	2166453	0.70631788	2597015	0.42124809	experimental	Tocris	2289					Lamotrigine isethionate	
3268 H21	X	712	720	-0.05248859	704	720	0.00598627	1998938	0.35819405	2354384	0.05996321	experimental	Tocris	2073					(R)-(-)-Apomorphine hydrochloride	
3268 H22	X	829	840	-0.03918946	1109	1120	0.27668566	2421002	1.23531274	3322426	1.50140698	experimental	Tocris	2291					1,2,3,4,5,6-Hexabromocyclohexane	
3268 H23	E	887	1600	-0.03259673	471	880	-0.14974944	130950	-3.52379345	124428	-3.26050861	empty								
3268 H24	P	240641	242200	27.219711	136810	137720	90.9783619	1927232	0.1998254	2485981	0.25591512	empty								
3268 I01	N	637	640	-0.06101368	437	440	-0.17247482	1857173	0.06358297	3408865	1.63011726	empty								
3268 I02	E	113	120	-0.12034826	113	120	-0.38702915	124991	-3.5361728	117293	-3.26988801	empty								
3268 I03	X	716	720	-0.05203392	1555	1560	0.5747892	1802664	0.04969573	3092401	1.15889281	experimental	Tocris	1615						SB 366791
3268 I04	X	475	480	-0.07942786	553	560	-0.09494116	1992299	0.34439711	2793208	0.7133854	experimental	Tocris	1808						E-4031 dihydrochloride
3268 I05	X	234	240	-0.1068218	355	360	-0.22728309	1853119	0.05515809	2826137	0.76241767	experimental	Tocris	1616						SB 216763
3268 I06	X	593	600	-0.06601506	553	560	-0.09494116	2103145	0.57475341	2742434	0.63778138	experimental	Tocris	1809						Altanserin hydrochloride
3268 I07	X	954	960	-0.02498099	635	640	-0.04013289	2514206	1.42900604	2950508	0.94760985	experimental	Tocris	1617						SB 415286
3268 I08	X	472	480	-0.07976886	474	480	-0.14774426	2116203	0.60189009	2864529	0.81958452	experimental	Tocris	1810						Raclopridol
3268 I09	X	514	520	-0.07499481	391	400	-0.20322092	2211716	0.80038187	2647906	0.49702633	experimental	Tocris	1620						Alprostadil
3268 I10	X	716	720	-0.04760888	996	1000	0.29241577	1818742	0.24963694	2921071	1.19519356	experimental	Tocris	1813						Imidubin-3'-oxime
3268 I11	X	555	560	-0.07033444	513	520	-0.12167691	2051502	0.46743072	2921714	0.90473471	experimental	Tocris	1621						Streptozocin
3268 I12	X	194	200	-0.11136851	155	160	-0.3609618	1350857	-0.98862528	1329376	-1.46630466	experimental	Tocris	1814						N-ArachidonylGABA
3268 I13	X	432	440	-0.08431557	393	400	-0.20188413	2348095	1.08379995	3756153	0.65820938	experimental	Tocris	1622						Remacemide hydrochloride
3268 I14	X	434	440	-0.08408824	431	440	-0.17648518	1974862	0.30816015	2567058	0.37664122	experimental	Tocris	1816						ICI 63197
3268 I15	X	833	840	-0.03873479	875	1640	0.62425032	1944850	0.24579026	2718724	0.60247647	experimental	Tocris	1625						DFB
3268 I16	X	274	280	-0.02127508	311	320	-0.25669241	1219900	-1.26077554	1397391	-1.36502827	experimental	Tocris	1819						Demethylasterriquinone B1
3268 I17	X	234	240	-0.1068218	235	240	-0.37490324	1876589	-1.97166099	2400258	-2.00654236	experimental	Tocris	1634						GTP 14564
3268 I18	X	395	400	-0.08852128	395	400	-0.20054735	1983229	3.25548816	2585528	4.4041458	experimental	Tocris	1821						YM 975
3268 I19	X	592	600	-0.06612873	471	480	-0.14974944	2211572	0.80008261	2818115	0.75047267	experimental	Tocris	1636						IEM 1460
3268 I20	X	713	720	-0.05237492	586	600	-0.07288418	1894116	0.14035663	1901336	-0.30521847	experimental	Tocris	1838						IRL-2500
3268 I21	X	697	720	-0.05419361	471	480	-0.14974944	2158807	0.69042823	2984749	0.99859573	experimental	Tocris	1638						U 186664
3268 I22	X	867	880	-0.03487008	800	840	0.07015205	2088877	0.54510215	2368849	0.08150203	experimental	Tocris	1842						RHC 80267
3268 I23	E	940	1840	-0.02657234	659	1120	-0.02409414	129070	-3.5277004	120570	-3.26625329	empty								
3268 I24	P	304968	306460	34.531619	155713	156600	103.613006	1946701	0.24963694	2789590	0.08739959	empty								
3268 J01	N	637	640	-0.06112734	356	360	-0.0266147	1895100	0.14677971	2788977	0.70708831	empty								
3268 J02	E	156	160	-0.11568788	156	160	-0.36029341	130676	-3.52436287	116366	-3.27251317	empty								
3268 J03	X	395	400	-0.08852128	633	640	-0.04146968	2000117	0.36064421	2388762	0.11115309	experimental	Tocris	2074						SKF 83959 hydrobromide
3268 J04	X	594	600	-0.06590139	354	360	-0.22795148	2204912	0.78624203	2852485	0.80218669	experimental	Tocris	2292						AQ-RA 741
3268 J05	X	835	840	-0.03850745	475	480	-0.14707586	2283985	0.95056879	2706011	0.58354643	experimental	Tocris	2076						Y-26763
3268 J06	X	592	600	-0.06612873	595	600	-0.06686863	2396003	1.18336069	3073907	1.13135468	experimental	Tocris	2293						Zebularine
3268 J07	X	744	760	-0.04885122	388	400	-0.2052261	2303429	0.99097663	2853449	0.80308606	experimental	Tocris	2077						Y-27152
3268 J08	X	553	560	-0.07056177	554	560	-0.09427277	2036071	0.43352556	3251075	1.39516319	experimental	Tocris	2294						Cordycepin
3268 J09	X	514	520	-0.07499481	595	600	-0.06686863	2218425	0.81432428	2802523	0.72725571	experimental	Tocris	2078						UBP 296
3268 J10	X	634	640	-0.06135468	392	400	-0.20255253	2139332	0.64995597	3100018	1.17023475	experimental	Tocris	2295						(±)-Cloprosteno sodium salt
3268 J11	X	474	480	-0.07954153	514	520	-0.12034012	2150723	0.67362835	2885866	0.85135596	experimental	Tocris	2079						UBP 302
3268 J12	X	554	560	-0.07044481	514	560	-0.09427277	2158066	0.68888831	2748997	0.64755388	experimental	Tocris	2296						Prostaglandin E2
3268 J13	X	995	1000	-0.02032061	875	880	0.12028157	1840924	0.02981487	2548973	0.34971211	experimental	Tocris	3037						SU 5416
3268 J14	X	351	360	-0.09352266	668	680	-0.0180759	1967226	0.29229128	2857034	0.80842424	experimental	Tocris	2299						SCH 39166 hydrobromide
3268 J15	X	1153	1160	-0.0023611	2390	2400	-0.13289783	1894734	0.14164093	2400456	1.12856581	experimental	Tocris	2086						TD 14564
3268 J16	X	473	480	-0.07955519	710	720	0.00999663	1912872	0.17933469	2402634	0.15881146	experimental	Tocris	2301						T 0070907
3268 J17	X	394	400	-0.08863495	394	400	-0.20121574	2052785	0.47009701	2584423	0.40249823	experimental	Tocris	2088						DMNB
3268 J18	X	514	520	-0.07499481	593	600	-0.06820542	2328247	1.04255253	2858898										

3268 K19	X	673	680	-0.05692164	393	400	-0.20188413	1849555	0.04775151	1895567	-0.62322916	experimental	Tocris	1660	Salmeterol
3268 K20	X	671	680	-0.05714897	349	360	-0.23129345	2313230	1.01134472	2270430	-0.06504683	experimental	Tocris	1866	MRS 1845
3268 K21	X	1426	1480	0.02867021	2073	2080	0.92101707	3503792	3.48552914	3179161	1.28808017	experimental	Tocris	1661	SB 206553 hydrochloride
3268 K22	X	466	480	-0.08045087	518	560	-0.11833494	941226	-1.83990613	957969	-2.01934089	experimental	Tocris	1867	NSC 663284
3268 K23	E	1024	1840	-0.01702424	419	880	-0.1845059	128314	152927149	122021	-0.26409271	empty			
3268 K24	P	276884	278200	31.3393727	155527	156560	103.488684	1991271	0.34226076	2492995	0.26635917	empty			
3268 L01	N	356	360	-0.09295433	475	480	-0.14707586	1811660	-0.03100055	2268980	-0.06720593	experimental	Tocris	2096	DAU 5884 hydrochloride
3268 L02	E	277	280	-0.10193408	157	160	-0.35962502	126748	-3.3252529	118485	-3.26935792	experimental	Tocris	2309	SR 142948
3268 L03	X	476	480	-0.07931419	356	360	-0.2266147	2161068	0.69512696	2287017	-0.04034829	experimental	Tocris	2310	SK1 II
3268 L04	X	473	480	-0.07965519	154	560	-0.09427277	2203136	0.78255121	2851722	0.80051451	experimental	Tocris	2311	SR 49059
3268 L05	X	1155	1160	-0.00213376	1055	1040	0.22722454	1852171	0.05318799	2264906	-0.07327224	experimental	Tocris	2098	Apoptosis Activator 2
3268 L06	X	552	560	-0.07067544	433	440	-0.17514839	2098172	0.56441869	237844	0.69351578	experimental	Tocris	2312	L-168,049
3268 L07	X	466	480	-0.08045087	389	400	-0.20455771	2382639	1.15558809	2275417	-0.05762104	experimental	Tocris	2098	Apoptosis Activator 2
3268 L08	X	553	560	-0.07056177	434	440	-0.17448	2465919	1.32865768	2930658	0.9180526	experimental	Tocris	2311	L-168,049
3268 L09	X	394	400	-0.08863495	515	520	-0.12034012	2213057	0.80316869	2825152	0.76095098	experimental	Tocris	2132	Amisulpride
3268 L10	X	472	480	-0.07976886	351	360	-0.22995666	2162076	0.69722175	2797710	0.72008901	experimental	Tocris	2312	DNQX disodium salt
3268 L11	X	1355	1360	0.0205998	1396	1400	0.46851462	1797573	-0.06027567	2838614	0.7809963	experimental	Tocris	2137	2,3-DCE hydrochloride
3268 L12	X	473	480	-0.07965519	354	360	-0.22795148	2292310	0.96786951	2892512	0.86125205	experimental	Tocris	2313	QX 314 chloride
3268 L13	X	195	200	-0.11125484	115	120	-0.38769755	850799	-2.02782837	937334	-2.04932252	experimental	Tocris	2139	Lylamine hydrochloride
3268 L14	X	316	320	-0.09750104	756	760	0.04074273	1323903	-1.04464014	2011332	-0.45085158	experimental	Tocris	2314	LOE 908 hydrochloride
3268 L15	X	314	320	-0.09772837	354	360	-0.22795148	1093411	-1.52364057	1418883	-1.33302603	experimental	Tocris	2141	Paroxetine maleate
3268 L16	X	512	520	-0.07522215	710	720	0.00999663	2910214	2.25197605	3145601	1.23810921	experimental	Tocris	2143	Immethidine dihydrobromide
3268 L17	X	1312	1320	0.01571208	1553	1560	0.57345241	2098877	0.5658838	2537112	0.33205072	experimental	Tocris	2135	SCS
3268 L18	X	1110	1120	-0.00724881	912	920	0.14501213	1630052	-0.40841197	2035403	-0.41500913	experimental	Tocris	2116	AMG 9810
3268 L19	X	632	640	-0.06158202	394	400	-0.20121574	2235717	0.85025991	2487452	0.25810548	experimental	Tocris	2147	Nicorandil
3268 L20	X	561	600	-0.06965243	394	440	-0.22121574	2446070	0.28740083	2446070	0.2956568	experimental	Tocris	2318	Pravastatin sodium salt
3268 L21	X	11810	11840	-0.20899656	510	520	-0.1236899	2190384	0.75605048	2240517	-0.10958819	experimental	Tocris	2148	(4S)-Mefl 5652
3268 L22	X	398	440	-0.08818028	511	520	-0.12301369	1712776	-0.23649783	1925365	-0.57885904	experimental	Tocris	2322	BTS 54-505
3268 L23	E	763	1280	-0.04669153	608	1160	-0.05817952	129770	-3.52624568	123652	-3.2616644	empty			
3268 L24	P	173159	174640	19.549181	187246	188120	124.68946	2019609	0.4011518	2425576	0.16597205	empty			
3268 M01	N	477	480	-0.07920052	677	680	-0.01206036	1773652	-0.10998745	2987730	1.00303453	empty			
3268 M02	E	116	120	-0.1202346	156	160	-0.36029341	123780	-3.53869389	1281159	-3.25495304	experimental	Tocris	1662	SKF 77434 hydrobromide
3268 M03	X	436	440	-0.0838609	517	520	-0.11900333	1775492	-0.10616363	3174472	1.28109901	experimental	Tocris	1868	U0124
3268 M04	X	391	400	-0.08897595	432	440	-0.17581679	1813532	-0.02711023	2522446	0.31021266	experimental	Tocris	1663	BW 373U86
3268 M05	X	554	560	-0.0704481	554	560	-0.09427277	1773231	-0.11086236	2683442	0.54994051	experimental	Tocris	1869	Isapirone
3268 M07	X	433	440	-0.08420191	473	480	-0.14841265	1935904	0.22719899	2205411	-0.16186209	experimental	Tocris	1664	GW 1929
3268 M08	X	714	720	-0.05226126	554	560	-0.09427277	2171214	0.71621203	2847454	0.79415933	experimental	Tocris	1870	BTS
3268 M09	X	473	480	-0.07965519	553	560	-0.09494116	1246957	-1.20454663	1688203	-0.93200042	experimental	Tocris	1671	PD 102807
3268 M10	X	795	800	-0.04305417	795	800	0.06681008	1773427	-0.11045504	2408059	0.1398869	experimental	Tocris	1937	NSC 693868
3268 M11	X	400	480	-0.08885229	448	432	-0.08885229	1959962	0.27719549	2181822	0.2181822	experimental	Tocris	1672	ZD 2079 hydrochloride
3268 M12	X	351	360	-0.09352266	353	360	-0.22861988	1352343	-1.21241872	1587887	-1.08137987	experimental	Tocris	1941	m-3M3FBS
3268 M13	X	475	480	-0.07942786	396	400	-0.19987895	1747891	-0.16352307	2429829	0.17230309	experimental	Tocris	2719	RWJ 21757
3268 M14	X	435	440	-0.08397457	394	400	-0.20121574	2010837	0.38292214	2575151	0.38869194	experimental	Tocris	1942	o-3M3FBS
3268 M15	X	476	480	-0.07931419	435	440	-0.1738116	1914824	0.18339127	2357834	0.06510036	experimental	Tocris	1674	LE 300
3268 M16	X	514	520	-0.07499481	914	920	0.14634892	1593913	-0.48351477	1701868	-0.91165282	experimental	Tocris	1944	Lorazidine
3268 M17	X	432	440	-0.08431557	350	360	-0.23062506	4676778	5.92318773	4621619	3.43594459	experimental	Tocris	1675	YM 97099
3268 M18	X	632	640	-0.06158202	394	400	-0.20121574	2010837	0.38292214	2575151	0.38869194	experimental	Tocris	1942	o-3M3FBS
3268 M19	X	514	520	-0.07499481	914	920	0.14634892	1593913	-0.48351477	1701868	-0.91165282	experimental	Tocris	1944	Lorazidine
3268 M20	X	453	480	-0.08192855	675	680	-0.01339715	2032641	0.42823445	2641641	0.48769756	experimental	Tocris	1952	DCB
3268 M21	X	7680	7720	7.3954858	313	320	-0.25535562	935231	-1.85236473	989601	-1.97223989	experimental	Tocris	1677	GW 7647
3268 M22	X	930	960	-0.02770901	832	840	0.09154064	2152428	0.67717162	2269725	-0.0660966	experimental	Tocris	1953	DMeOB
3268 M23	E	798	1480	-0.04271316	654	1080	-0.02743341	127985	-3.52995521	119702	-3.26754577	empty			
3268 M24	P	230901	232040	26.1125867	143228	144200	95.2681118	2050959	0.46630228	2292206	-0.03262171	empty			
3268 N01	N	475	480	-0.07942786	515	520	-0.12034012	1850595	0.0499128	2541687	0.33886303	empty			
3268 N02	E	237	240	-0.10648079	157	160	-0.35962502	125159	-3.5358281	111577	-3.27964414	experimental	Tocris	2150	nTZDpa
3268 N03	X	195	200	-0.11125484	154	160	-0.3616302	1202033	-1.29790612	958884	-2.01797843	experimental	Tocris	2150	nTZDpa
3268 N04	X	634	640	-0.06135468	795	800	0.06681008	1976452	0.31146443	2641882	0.48805641	experimental	Tocris	2324	Necrostatin-1
3268 N05	X	874	880	-0.03407441	753	760	0.03873755	2152520	0.67736281	2826811	0.76342128	experimental	Tocris	2151	API-2
3268 N06	X	513	520	-0.07510848	593	600	-0.06820542	1862677	0.0750212	2319859	0.00855444	experimental	Tocris	2327	WIN 55,212-3 mesylate
3268 N07	X	514	520	-0.07499481	754	760	0.03940595	1544538	-0.58612418	1998517	-0.4699335	experimental	Tocris	2152	NSC 625987
3268 N08	X	554	560	-0.0704481	632	640	-0.04213807	2285062	0.95280697	2843324	0.78800963	experimental	Tocris	2329	Ro 10-5824
3268 N09	X	514	520	-0.07499481	754	760	0.03940595	1544538	-0.58612418	1998517	-0.4699335	experimental	Tocris	2152	NSC 625987
3268 N10	X	514	520	-0.07499481	754	760	0.03940595	1544538	-0.58612418	1998517	-0.4699335	experimental	Tocris	2152	NSC 625987
3268 N11	X	151	160	-0.11625622	113	120	-0.38903434	981342	-1.75653846	1144995	-1.74085353	experimental	Tocris	2155	NTNCB hydrochloride
3268 N12	X	1755	1760	0.06606691	1236	1240	0.36157165	2280617	0.94356952	2651090	0.5017674	experimental	Tocris	2333	JM1 26259685
3268 N13	X	751	760	-0.04805555	512	520	-0.1223453	1747815	-0.16368101	2587827	0.40756689	experimental	Tocris	2156	Embelin
3268 N14	X	474	480	-0.07949481	475	480	-0.14707586	1808658	-0.03723291	2487366	0.25797742	experimental	Tocris	2337	Trequinsin hydrochloride
3268 N15	X	234	240	-0.1068218	194	200	-0.33489446	856935	-2.01507675	914978	-2.08335579	experimental	Tocris	2160	Bax channel blocker
3268 N16	X	555	560	-0.07033444	714	720	0.01267078	2336640	1.05999457	3245025	0.57275543	experimental	Tocris	2154	ZD 2079 hydrochloride
3268 N17	X	314	320	-0.09772837	354	360	-0.06753703	1925026	0.20459271	2612210	0.44387398	experimental	Tocris	2330	DMP 543
3268 N18	X	554	560	-0.0704481	474	480	-0.14774426	2195060	0.76576795	2805335	0.73144287	experimental	Tocris	2342	4-Methylhistamine dihydrochloride
3268 N19	X	393	400	-0.08874862	472	480	-0.14908104	2002818	0.36625733	2435601	0.18089777	experimental	Tocris	2162	INCA-6
3268 N20	X	594	600	-0.06590139	633	640	-0.04146968	2372700	1.1349332	26					

3268 O13	X	474	480	-0.07954153	594	600	-0.06753703	1664984	-0.3358175	2230003	-0.12524386	experimental	Tocris	1695	Cisapride
3268 O14	X	594	600	-0.06590139	714	720	0.0126702	1855166	0.0594121	2393579	0.11832575	experimental	Tocris	1960	SB 334867
3268 O15	X	508	520	-0.07567682	348	360	-0.23196185	1450666	-0.78120569	1929428	-0.57280911	experimental	Tocris	1697	Noscapine hydrochloride
3268 O16	X	554	560	-0.07044481	434	440	-0.174448	1701456	-0.26003266	1923495	-0.58164352	experimental	Tocris	1961	EMD 386088 hydrochloride
3268 O17	X	513	520	-0.07510848	434	440	-0.174448	1644770	-0.37782553	17050803	-0.90686112	experimental	Tocris	1698	L 655240
3268 O18	X	872	880	-0.03430175	591	600	-0.06954221	2114504	0.59835928	2532665	0.325429	experimental	Tocris	1962	SB 239063
3268 O19	X	793	800	-0.0432815	952	960	0.17174787	1661276	-0.34352334	2140260	-0.25887389	experimental	Tocris	1699	CGS 15943
3268 O20	X	591	600	-0.06624239	872	880	0.11827639	2120478	0.61077424	2514518	0.29840757	experimental	Tocris	1963	SB 408124
3268 O21	X	873	880	-0.03418808	713	720	0.01200181	2133366	0.63755763	2524459	0.31321002	experimental	Tocris	1700	BIIE 0246 formate
3268 O22	X	269	280	-0.10284342	430	440	-0.17715357	884491	-1.95781083	819732	-2.22517996	experimental	Tocris	1964	Gossypol
3268 O23	E	579	1240	-0.06760641	495	1040	-0.13370799	122367	-3.54163034	115023	-3.27451294	empty			
3268 O24	P	224360	25.172554		184174	185360	122.636155	1930523	0.21601639	215174	-0.21284201	empty			
3268 P01	N	637	640	-0.06101368	837	840	0.09488261	1638789	-0.39025504	1943546	-0.55178698	empty			
3268 P02	E	196	200	-0.11114117	115	120	-0.38769755	114783	-3.55739115	110696	-3.28095598	empty			
3268 P03	X	517	520	-0.07465381	637	640	-0.0387961	1489117	-0.70129817	1762904	-0.82076837	experimental	Tocris	2173	WAY 629 hydrochloride
3268 P04	X	356	360	-0.09295433	396	400	-0.19987895	1650847	-0.36519652	2081309	-0.34665371	experimental	Tocris	2347	Salubralin
3268 P05	X	516	520	-0.07476748	615	520	-0.12034012	1780064	-0.09666226	2291002	-0.0344145	experimental	Tocris	2175	Tetrabenzazine
3268 P06	X	396	400	-0.08840761	677	680	-0.01206036	1623175	-0.42270351	2196202	-0.17557457	experimental	Tocris	2348	Galvestin
3268 P07	X	116	120	-0.1202346	115	120	-0.38769755	772637	-2.19028191	829805	-2.21018096	experimental	Tocris	2176	BVT 948
3268 P08	X	397	400	-0.08829395	477	480	-0.14573907	2007301	0.37555735	2399315	0.12686682	experimental	Tocris	2372	ABT 702 dihydrochloride
3268 P09	X	317	320	-0.09738737	276	280	-0.28008618	922934	-1.87791993	1043484	-1.89200648	experimental	Tocris	2183	ZK 164015
3268 P10	X	276	280	-0.10204775	354	360	-0.22795148	1115692	-1.47733698	1422633	-1.32744217	experimental	Tocris	2373	T 0901317
3268 P11	X	596	600	-0.06567406	1116	1120	0.28136442	1845471	0.03926429	2406042	0.13688353	experimental	Tocris	2184	SN-6
3268 P12	X	516	520	-0.06567406	475	480	-0.14774426	1170149	-1.36416634	1390648	-1.37058068	experimental	Tocris	2374	GW 405833
3268 P13	X	395	320	-0.09761471	434	440	-0.1738116	1470073	-0.74087474	1932273	-0.56857282	experimental	Tocris	2186	CMPD-1
3268 P14	X	489	490	-0.08010987	380	480	-0.13573381	1466580	-0.7467767	2144428	-0.2373549	experimental	Tocris	2382	EMD 386088 hydrochloride
3268 P15	X	2756	2760	0.17984837	2916	2920	1.48447285	6330319	-0.40224605	2345130	0.04618372	experimental	Tocris	2190	SR 27897
3268 P16	X	469	480	-0.08010987	389	400	-0.20455771	1493330	-0.69254286	1389537	-1.37672311	experimental	Tocris	2385	AMN 082 dihydrochloride
3268 P17	X	555	560	-0.07033444	474	480	-0.14774426	1790511	-0.07495167	1979413	-0.49837993	experimental	Tocris	2191	S-Trityl-L-cysteine
3268 P18	X	834	840	-0.03862112	1115	1120	0.28069602	1894507	0.14116919	2278064	-0.05367958	experimental	Tocris	2386	Fenobam
3268 P19	X	593	600	-0.06601506	632	640	-0.04213807	1885492	0.12243453	2278572	-0.05292315	experimental	Tocris	2192	4-HQN
3268 P20	X	794	800	-0.04316783	514	520	-0.12100851	1940934	0.23765216	2194521	-0.17807763	experimental	Tocris	2387	LY 320135
3268 P21	X	792	800	-0.04339517	594	600	-0.06753703	1841049	0.03007464	2034451	-0.41642669	experimental	Tocris	2193	Carmoxirole hydrochloride
3268 P22	X	967	960	-0.17287949	833	960	-0.02531999	1853879	0.05661495	1975765	-0.1071929	experimental	Tocris	2190	MPMQ
3268 P23	E	1097	2200	-0.00872649	597	1360	-0.06553185	115994	-3.55487449	111264	-3.28011021	empty			
3268 P24	P	377984	378640	42.8311864	261219	261760	174.132538	1611095	-0.44780774	1785927	-0.78648643	empty			
3269 A01	N	1078	1080	-0.16672673	478	480	-0.12688049	1708070	-0.71193879	1558701	-0.80099304	empty			
3269 A02	E	155	160	-0.20215828	237	240	-0.15290061	78199	-2.35401324	120197	-2.26564312	empty			
3269 A03	X	553	560	-0.1868801	595	600	-0.11424831	1143491	-1.280745	1059406	-1.30936316	experimental	Tocris	2392	JTE 013
3269 A04	E	515	520	-0.18833883	355	360	-0.14016047	1917564	-0.50087623	1704961	-0.65207463	empty			
3269 A05	X	497	480	-0.19286107	557	600	-0.13573381	1605731	-0.81504404	1815968	-0.79499802	experimental	Tocris	2394	SDZ NKT 343
3269 A06	E	277	280	-0.19747502	357	560	-0.11835107	1833884	-0.58518278	1899663	-0.45383375	empty			
3269 A07	X	197	200	-0.20054601	196	200	-0.15732727	969894	-1.45564179	939992	-1.43094762	experimental	Tocris	2395	Sertraline hydrochloride
3269 A08	E	556	560	-0.18676494	556	560	-0.11845904	1876795	-0.54195048	1955727	-0.39675074	empty			
3269 A09	X	593	600	-0.18534461	435	440	-0.13152308	2241561	-0.17445335	1851161	-0.50321732	experimental	Tocris	2396	Glimepiride
3269 A10	X	764	1200	-0.17878037	476	480	-0.12709642	2035050	-0.38251057	1905434	-0.44795786	empty			
3269 A11	X	148808	149480	5.50424154	494	520	-0.12515301	2011077	-0.40666307	2066553	-0.28391038	experimental	Tocris	2397	Eplerenone
3269 A12	E	229149	230160	8.58832238	386	400	-0.13573381	1906426	-0.51209763	1835868	-0.5189715	empty			
3269 A13	X	197988	199280	7.392131	357	360	-0.13994453	135215	-0.07029835	1972729	-0.598940761	experimental	Tocris	2400	FK 888
3269 A14	E	215194	216040	8.05262643	357	360	-0.13994453	1954542	-0.46362136	1749772	-0.60644915	empty			
3269 A15	X	91224	92240	3.29374241	396	400	-0.13573381	2128615	-0.28824501	1961734	-0.39063456	experimental	Tocris	2403	MRS 3777 hemioxalate
3269 A16	E	133506	134360	4.91683779	437	440	-0.13130715	2089183	-0.32797226	1860213	-0.49400079	empty			
3269 A17	X	201195	202480	7.51524144	316	320	-0.14437119	1949166	-0.46903762	2033618	-0.317444	experimental	Tocris	2404	Ambroxol hydrochloride
3269 A18	E	308444	309040	11.63225	155	480	-0.16175393	1953222	-0.46495125	1974214	-0.37792772	empty			
3269 A19	X	2021	2920	-0.13052742	111555	111560	11.865805	2102330	-0.31472682	2246093	-0.10110708	experimental	Tocris	2408	Ro 90-7501
3269 A20	E	787	800	-0.17789746	353	680	-0.1403764	2180531	-0.2359403	2141921	-0.2071725	empty			
3269 A21	X	793	800	-0.17767613	874	880	-0.08412543	2065260	-0.35207438	2414861	0.07072843	experimental	Tocris	2759	B-HT 920
3269 A22	E	868	880	-0.17478808	748	760	-0.09772931	2071172	-0.34611811	2120616	-0.22886474	empty			
3269 A23	E	749	1680	-0.17935618	1439	2440	-0.0231239	79132	-2.35307326	110332	-2.27568742	empty			
3269 A24	P	318137	319000	12.0043389	342509	343280	36.8012883	1684473	-0.73571247	1863215	-0.49094423	empty			
3269 B01	N	475	480	-0.18987432	557	560	-0.11835107	2024155	-0.39348715	2157770	-0.19103543	empty			
3269 B02	E	73	80	-0.20530605	114	120	-0.16618059	85280	-2.34687922	83291	-2.30321992	empty			
3269 B03	X	1546	1600	-0.14876143	426	1280	-0.04191021	1765184	-0.6533967	1765255	-0.58966556	experimental	Tocris	2550	SUN-B 8155
3269 B04	E	642	680	-0.18346363	514	520	-0.1229367	193907	0.78502322	2629514	0.28928296	empty			
3269 B05	X	146	160	-0.20250377	114	120	-0.16618059	988368	-1.43702947	941404	-1.42950995	experimental	Tocris	2554	CD 1530
3269 B06	E	477	480	-0.18979755	356	360	-0.1400525	2601665	0.18834689	2273903	-0.07279161	empty			
3269 B07	X	236	240	-0.19904891	235	240	-0.15311655	1019958	-1.40520294	1022938	-1.346494	experimental	Tocris	2558	10-DEBC hydrochloride
3269 B08	E	389	440	-0.19317564	595	600	-0.11424831	2619415	0.20622979	2311790	-0.03421598	empty			
3269 B09	X	615	680	-0.18450009	514	620	-0.1229367	1826716	-0.59240444	1787776	-0.5677544	experimental	Tocris	2559	TPCA-1
3269 B10	E	54	54	0.734075	493	520	-0.12526098	2754691	0.34251865	2137130	-0.00761715	empty			
3269 B11	X	0	680	-0.20092899	7944	7960	0.67920349	1914536	-0.5039269	1987431	-0.36447049	experimental	Tocris	2560	SB 218078
3269 B12	E	187	440	-0.20810833	494	520	-0.12515301	2497194	0.08309367	2322268	-0.02354753	empty			
3269 B13	X	0	160	-0.20810833	115	120	-0.16607263	923185	-1.50270052	923169	-1.44807639	experimental	Tocris	2561	Calmidazolium chloride
3269 B14	E	0	520	-0.20810833	396	400	-0.13573381	2771326	0.3592782	2480629	0.13769182	empty			
3269 B15	X	333	640	-0.19532533	436	440									

3269 C07	X	149	200	-0.20238861	393	400	-0.13605771	1382408	-1.04003914	1476901	-0.88427982	experimental	Tocris	2417	BIBU 1361 dihydrochloride
3269 C08	E	16017	16080	0.4067424	430	480	-0.13206292	2332742	-0.08258964	2395121	0.05062964	empty			
3269 C09	X	20539	20640	0.58033016	634	640	-0.11003759	2055688	-0.36171805	1911178	-0.444210946	experimental	Tocris	2418	LY 303511
3269 C10	E	17760	17880	0.47361552	424	440	-0.12711072	2412100	-0.00263746	2165073	-0.18335969	empty			Scriptaid
3269 C11	X	97889	99880	0.55153962	3893	3920	-0.24272789	1733990	-0.56822472	1503033	-0.85767285	experimental	Tocris	2421	
3269 C12	E	11921	12000	0.24950768	425	440	-0.13260276	2545537	0.13179864	2384139	0.03944803	empty			
3269 C13	X	6442	6480	0.0391832	396	400	-0.13573381	2998136	0.58778641	2666358	0.32679661	experimental	Tocris	2429	Fexofenadine hydrochloride
3269 C14	E	461	520	-0.19041174	356	360	-0.1400525	2491192	0.07704673	2283379	-0.06314337	empty			
3269 C15	X	12746	12800	0.28117727	190	200	-0.15797508	1672311	-0.74796553	1372353	-0.99072808	experimental	Tocris	2435	CCT 018159
3269 C16	E	15792	15920	0.39810524	596	600	-0.11414035	2582615	0.16915425	2454777	0.11136994	empty			
3269 C17	X	20261	20360	0.56965846	442	200	-0.16315751	2862007	0.45063816	2343935	-0.00148671	experimental	Tocris	2436	AC 55649
3269 C18	X	14854	14920	0.36209788	17914	18120	1.75542168	2881024	0.46979755	255507	0.20882668	empty			
3269 C19	X	459	520	-0.19048852	503	560	-0.12418131	3198578	0.7897292	2728505	0.39007318	experimental	Tocris	2438	TMPh hydrochloride
3269 C20	E	912	920	-0.17309903	498	560	-0.12472114	2819876	0.40819171	2825842	0.48917937	empty			
3269 C21	X	584	600	-0.1856901	5312	5320	0.39503351	946209	-1.47950413	982542	-1.38762423	experimental	Tocris	2440	NNC 26-9100
3269 C22	E	700	720	-0.18123716	736	760	-0.09902492	2590040	0.17663485	2756444	0.41852	empty			
3269 C23	E	751	1640	-0.1792794	699	1280	-0.10301971	86900	-2.34524709	111671	-2.27432408	empty			
3269 C24	P	301533	303160	11.3669548	195297	196680	20.9072039	2469769	0.05546333	2840870	0.50448052	empty			
3269 D01	N	502	600	-0.18883786	797	800	-0.09243892	2544689	0.13094429	2617007	0.27654861	empty			
3269 D02	E	157	160	-0.20208151	156	160	-0.16164597	86638	-2.34551106	85330	-2.30114386	empty			
3269 D03	X	106	160	-0.20403927	146	160	-0.16272564	1581208	-0.83975065	1420603	-0.94160109	experimental	Tocris	2574	PSB 06126
3269 D04	E	405	440	-0.19256144	615	520	-0.1228857	3316654	0.90868928	2914062	0.57900285	empty			
3269 D05	X	787	800	-0.17789746	535	640	-0.10992962	2525002	0.11110988	2398819	0.05439485	experimental	Tocris	2577	Cetirizine dihydrochloride
3269 D06	E	472	480	-0.18998948	350	360	-0.14059234	2893209	0.48207379	2974434	0.64047216	empty			
3269 D07	X	874	880	-0.17455775	1031	1080	-0.06728253	2503044	0.08898747	2526383	0.18427744	experimental	Tocris	2578	Benazepril hydrochloride
3269 D08	E	440	450	-0.1947495	15713	15720	1.51800156	3001061	0.59073331	3245448	0.89668608	empty			
3269 D09	X	295	360	-0.19678405	428	480	-0.13227886	819782	-0.59890336	1830786	-0.52396265	experimental	Tocris	2579	Zamifenacin fumarate
3269 D10	E	424	480	-0.19183208	513	520	-0.12310163	2884625	0.47342551	3035324	0.70246889	empty			
3269 D11	X	657	720	-0.18288782	504	520	-0.12407334	2114820	-0.3021433	1931676	-0.42123889	experimental	Tocris	2580	Tenidap
3269 D12	E	480	520	-0.18968238	235	240	-0.15311655	3128228	0.71885246	2642957	0.30297027	empty			
3269 D13	X	536	560	-0.18753269	396	400	-0.13573381	2032740	-0.38483787	1622984	-0.73554164	experimental	Tocris	2581	PAC 1
3269 D14	E	591	600	-0.18542138	430	440	-0.13206292	3319354	0.91140949	3071761	0.73956817	empty			
3269 D15	X	1409	1480	-0.1540205	2195	2200	0.05849939	2631640	0.21854632	2337871	-0.00776093	experimental	Tocris	2582	Lansoprazole
3269 D16	X	10480	10480	0.19188822	973	10480	0.19188822	2915085	0.5071396	3727404	0.0399112	experimental	Tocris	2583	Omeprazole
3269 D17	X	2504	2600	-0.11198632	431	640	-0.13195495	2434833	0.02026575	2629021	0.28878097	empty			
3269 D18	E	1415	1480	-0.15379018	70422	70480	7.42478541	3122316	0.17289619	3257355	0.9285355	empty			
3269 D19	X	4510	4520	-0.03498123	389	640	-0.13648958	2068264	-0.34904788	1887578	-0.46613841	experimental	Tocris	2586	CFM 1571 hydrochloride
3269 D20	E	733	760	-0.17997038	14992	15000	1.44015712	2959668	0.54903039	3612692	1.29033106	empty			
3269 D21	X	3105	3120	-0.0889155	857	920	-0.08596088	2942634	0.53186885	2944625	0.61012136	experimental	Tocris	2591	TCS 359
3269 D22	E	3022	3040	-0.09210165	727	760	-0.09999663	3067408	0.65757708	4031280	1.71652727	empty			
3269 D23	X	1550	1560	-0.17820456	973	1350	-0.17820456	87501	-7.34641359	1863629	-7.34641359	empty			
3269 D24	P	262371	263920	9.86362806	211392	212600	22.6449378	2454022	0.03959843	2476434	0.133942057	empty			
3269 E01	N	33219	33240	1.06708219	515	520	-0.1228857	2119503	-0.29742524	2349610	0.00429143	empty			
3269 E02	E	61	160	-0.2057667	197	200	-0.15721931	87111	-2.34503451	133941	-2.25164931	empty			
3269 E03	X	717	720	-0.18058457	556	600	-0.1400525	3241760	0.83323452	2383627	0.03892672	experimental	Tocris	2441	JNJ 10191584 maleate
3269 E04	E	395	400	-0.19294531	396	600	-0.11414035	2779420	0.3674328	2216431	-0.13130821	empty			
3269 E05	X	274	280	-0.19759019	272	280	-0.14912176	1375533	-1.04696562	1387850	-0.9749494	experimental	Tocris	2442	CGP 53353
3269 E06	X	434	440	-0.19144882	874	880	-0.08412543	2848504	0.43703406	3543398	0.81861629	empty			
3269 E07	X	873	880	-0.17459614	911	920	-0.08013064	2632586	2.93064792	52077	2.93064792	experimental	Tocris	2443	RITA
3269 E08	E	592	600	-0.185383	427	480	-0.13238682	2728927	0.31656174	2793868	0.45662421	empty			
3269 E09	X	1036	1040	-0.168339	1074	1080	-0.06253197	3028896	0.61877672	2452724	0.10927962	experimental	Tocris	2447	YM 298198, Desmethyl-
3269 E10	E	352	360	-0.19459597	832	840	-0.08866006	2627817	0.2146947	2689656	0.35051807	empty			
3269 E11	X	955	960	-0.17144838	674	680	-0.1057189	2501564	0.08749639	2825648	-0.06083313	experimental	Tocris	2448	YM 298198 hydrochloride
3269 E12	E	553	560	-0.1868801	395	400	-0.13584178	2693797	0.28116871	2453214	0.10977853	empty			
3269 E13	X	555	560	-0.18680333	396	400	-0.13573381	2422776	0.00811848	2204752	-0.14319949	experimental	Tocris	2451	LY 344864 hydrochloride
3269 E14	E	393	400	-0.19302209	395	400	-0.13584178	2530917	0.11708917	2772404	0.43477009	empty			
3269 E15	X	671	680	-0.18235039	590	600	-0.11478815	2647382	0.23440619	2085049	-0.2650782	experimental	Tocris	2452	LY 2183240
3269 E16	E	684	720	-0.18185136	632	640	-0.11025352	2961895	0.55127406	2519807	0.17758191	empty			
3269 E17	X	787	800	-0.17789746	753	760	-0.09718948	3376427	0.96809982	2724247	0.38573779	experimental	Tocris	2456	Co 101244 hydrochloride
3269 E18	E	480	480	-0.19006626	391	600	-0.13627365	3368369	0.96079148	2916377	0.58135992	empty			
3269 E19	X	659	680	-0.18281104	509	520	-0.1235335	2605076	0.19178343	2458699	0.11536322	experimental	Tocris	2457	Arcyriaflavin A
3269 E20	E	672	680	-0.18231201	671	720	-0.1060428	3101264	0.69168657	3140832	0.80989459	empty			
3269 E21	X	688	720	-0.18169781	409	840	-0.09144331	1684452	-0.73573363	1990295	-0.36155443	experimental	Tocris	2458	ZM 447439
3269 E22	E	855	880	-0.17528711	8228	8240	0.7098662	3055580	0.64566052	2882544	0.54691198	empty			
3269 E23	E	563	1240	-0.18649623	1173	1840	-0.05184321	84406	-2.34775977	111026	-2.27498081	empty			
3269 E24	P	229043	230320	8.58425332	217883	219120	23.3457537	2643984	0.23098274	2772762	0.43513459	empty			
3269 F01	N	6542	6640	0.04302194	712	760	-0.10161614	2522824	0.10891557	2750275	0.41223887	empty			
3269 F02	E	139	160	-0.20277248	156	160	-0.16164597	84004	-2.34816478	82571	-2.303953	empty			
3269 F03	X	315	320	-0.1960163	396	400	-0.13573381	2392860	-0.02202151	2286196	-0.06027517	experimental	Tocris	2592	TCB2
3269 F04	E	355	360	-0.19448081	354	360	-0.14026584	28980074	0.56959818	3542271	0.58681578	empty			
3269 F05	X	306	400	-0.19290692	595	600	-0.11424831	2633834	0.23068575	2596481	0.25564953	experimental	Tocris	2596	Mexiletine hydrochloride
3269 F06	E	395	400	-0.19294531	313	520	-0.12310163	2936524	0.5257131	3440652	1.11516408	empty			
3269 F07	X	632	640	-0.1838475	512	520	-0.1232096	2166180	-0.25039875	2427460	0.08355643	experimental	Tocris	2600	Clofarabine
3269 F08	E	595	600	-0.18526783	555	560	-0.11856701	3231168	0.82256321	3102524	0.77089031	empty			
3269 F09	X	192	200	-0.20073795	191	200	-0.15786711	1101050	-1.32350378	1150119	-1.21700138	experimental	Tocris	2605	PD 198306
3269 F10	E	436	440	-0.19137143	635										

3269 J19	X	474	480	-0.18991271	1818	1840	0.01779571	2852356	0.4409149	2049060	-0.30172133	experimental	Tocris	2655	Naproxen sodium
3269 J20	E	632	640	-0.1838475	5091	5120	0.37117274	3080895	0.67116506	3348547	1.021385	empty			
3269 J21	X	952	960	-0.17156354	1711	1840	0.00624321	2461719	0.04735306	2349875	0.00456125	experimental	Tocris	2657	JX 401
3269 J22	E	908	920	-0.17325258	866	880	-0.06498917	3332624	0.92477885	3037717	0.70429468	empty			
3269 J23	E	464	1280	-0.19029658	811	1400	-0.09092737	83579	-2.34859296	104579	-2.28154499	empty			
3269 J24	P	275666	277480	10.37782721	197708	199160	21.1675131	2602092	0.18877708	2653929	0.31414147	empty			
3269 K01	N	128073	128080	4.70827913	357	360	-0.13994453	2553101	0.13941927	2445408	0.10183065	empty			
3269 K02	E	0	200	-0.20810833	117	120	-0.16585669	84426	-2.34773962	131560	-2.25407358	empty			
3269 K03	X	24035	24040	0.71453245	315	320	-0.14447916	2955369	0.5446992	2241186	-0.10610327	experimental	Tocris	2491	Xaliproden hydrochloride
3269 K04	E	365	440	-0.19409693	994	1000	-0.07116936	3044348	0.63434442	2583168	0.24209456	empty			
3269 K05	X	632	640	-0.1838475	672	680	-0.10593483	3587254	1.18131536	2506145	0.1636716	experimental	Tocris	2492	MNITMT
3269 K06	E	713	720	-0.18093842	753	760	-0.09718948	2553053	0.14541583	3076830	0.74334967	empty			
3269 K07	X	714	720	-0.18069974	553	560	-0.11878294	2850880	0.43942785	2956764	0.62248099	experimental	Tocris	2493	VUF 5681 dihydrobromide
3269 K08	E	834	840	-0.17609325	633	640	-0.11014556	3014089	0.60385886	2907655	0.57247939	empty			
3269 K09	X	514	520	-0.18837721	794	800	-0.09276282	3230414	0.82180356	2963931	0.62977826	experimental	Tocris	2494	VUF 8430 dihydrobromide
3269 K10	E	514	520	-0.18837721	713	720	-0.10150817	2972086	0.56154137	2803163	0.46608816	empty			
3269 K11	X	471	480	-0.19002787	431	440	-0.13195495	2894431	0.48330493	2655429	0.31566896	experimental	Tocris	2495	Melperone hydrochloride
3269 K12	E	474	480	-0.18991271	594	600	-0.11435628	2943973	0.53321787	2898516	0.56317428	empty			
3269 K13	X	635	640	-0.18373234	475	480	-0.12720439	2826673	0.41503961	2766830	0.42809478	experimental	Tocris	2496	DR 2313
3269 K14	E	353	360	-0.19455758	353	360	-0.1403764	3349400	0.94168046	2618822	0.2783966	empty			
3269 K15	X	593	600	-0.18534461	634	640	-0.11003759	3309744	0.90172754	2813090	0.47619559	experimental	Tocris	2498	PNU 120596
3269 K16	E	473	480	-0.1899511	593	600	-0.11446425	3129692	0.72032742	2687990	0.34882179	empty			
3269 K17	X	394	400	-0.1929837	513	520	-0.12310163	3334908	0.92707995	4480822	2.17424009	experimental	Tocris	2499	ZM 306416 hydrochloride
3269 K18	E	475	480	-0.18987432	792	800	-0.09297875	3159646	0.74050557	3640533	1.3186781	empty			
3269 K19	X	552	560	-0.18691849	613	640	-0.1123049	2653478	0.24504783	2999884	0.66638474	experimental	Tocris	2500	BAY 59-3074
3269 K20	E	713	720	-0.18074912	5618	5680	-0.14497722	3798915	0.38107377	4778626	0.64398455	empty			
3269 K21	X	681	680	-0.18235039	734	760	-0.09924086	2974310	0.56378202	3906342	1.58931841	experimental	Tocris	2501	BAY 36-7620
3269 K22	E	1029	1040	-0.16860771	787	800	-0.09351859	2964176	0.55357214	3301682	0.97366819	empty			
3269 K23	E	814	1640	-0.176861	909	1760	-0.08034658	81611	-2.35057569	114603	-2.27133879	empty			
3269 K24	P	280065	281600	10.5428544	288648	290040	30.9860607	2862270	0.45090313	2828666	0.4920547	empty			
3269 L01	N	267	640	-0.1978589	556	560	-0.11845904	2490993	0.07684624	2751912	0.41390563	empty			
3269 L02	E	156	160	-0.2021199	157	160	-0.161538	80152	-2.35204562	80940	-2.30561365	empty			
3269 L03	X	447	520	-0.19094917	316	320	-0.14437119	1563070	-0.85802446	1705664	-0.65135885	experimental	Tocris	2661	UCL 2077
3269 L04	E	552	560	-0.18691849	475	480	-0.14878294	3159646	0.74050557	3640533	1.3186781	empty			
3269 L05	X	1033	1040	-0.16845416	632	440	-0.13184699	2815309	0.40359052	2305332	-0.04079136	experimental	Tocris	2662	PHTPP
3269 L06	E	472	480	-0.18998948	794	800	-0.09276282	2857711	0.44631	3127373	0.79619096	empty			
3269 L07	X	312	320	-0.19613146	512	520	-0.1232096	2122651	-0.29425367	2076420	-0.27386404	experimental	Tocris	2664	Cabergoline
3269 L08	E	434	440	-0.1914482	355	360	-0.14016047	3306176	0.89813282	3347399	1.02021613	empty			
3269 L09	X	115	120	-0.20369378	153	160	-0.16196987	1312834	-1.11013407	1010515	-1.3591428	experimental	Tocris	2665	BMS 191011
3269 L10	E	475	480	-0.18987432	554	560	-0.11867497	3415037	1.00780891	2663592	0.32398033	empty			
3269 L11	X	554	560	-0.18687432	792	800	-0.11457722	1649063	-0.7713876	1578626	0.64795853	experimental	Tocris	2764	GP 1a
3269 L12	E	474	480	-0.18991271	795	800	-0.13163105	3659763	1.25436726	2883324	0.54770616	empty			
3269 L13	X	393	400	-0.19302209	395	400	-0.13584178	3353952	0.94626654	2523153	0.18098873	experimental	Tocris	2668	Artemisinin
3269 L14	E	794	800	-0.17762875	434	440	-0.13163105	3559155	1.15300597	3228703	0.89936272	empty			
3269 L15	X	752	760	-0.17924102	674	680	-0.1057189	3147401	0.73816902	2457999	0.1146505	experimental	Tocris	2669	TC 1
3269 L16	E	832	840	-0.17617002	593	600	-0.11446425	3287717	0.87953561	2638843	0.2987815	empty			
3269 L17	X	794	800	-0.17762875	594	600	-0.11435628	2734763	0.32244144	2850469	0.51425399	experimental	Tocris	2671	Budesonide
3269 L18	E	472	480	-0.18998948	592	600	-0.11457722	3224573	0.81591883	4727623	0.94769553	empty			
3269 L19	X	914	920	-0.17302226	673	680	-0.10582686	672367	0.31096011	2820950	0.57546774	experimental	Tocris	2673	Acarbose
3269 L20	E	632	640	-0.1838475	658	680	-0.10744637	3146407	0.73716757	3591447	1.26869992	empty			
3269 L21	X	432	440	-0.19152498	352	360	-0.14048437	1061410	-1.36344058	1071934	-1.29660746	experimental	Tocris	2676	Y 134
3269 L22	E	670	680	-0.18238878	909	920	-0.08034658	3076907	0.6671472	3250232	0.92128303	empty			
3269 L23	E	703	1440	-0.181122	938	1760	-0.07721552	85019	-2.34714218	101448	-2.2847329	empty			
3269 L24	P	249449	251000	9.36758628	278251	279760	29.8635246	2277047	-0.13870165	2692833	0.35375281	empty			
3269 M01	N	436	440	-0.19137143	716	720	-0.10118427	2468170	0.05385236	2334265	-0.01133248	empty			
3269 M02	E	116	120	-0.20365339	156	160	-0.16164597	84014	-2.3481547	129033	-2.25664651	empty			
3269 M03	X	513	520	-0.1884156	354	360	-0.14026844	4109348	1.70731847	2458786	0.1154518	experimental	Tocris	2503	(-)-Bicuculline methiodide
3269 M04	E	633	640	-0.18380911	594	600	-0.11435628	3099520	0.68992951	2699374	0.3604127	empty			
3269 M05	X	832	840	-0.17617002	594	600	-0.11435628	3308017	0.89998761	3461090	1.13597356	experimental	Tocris	2504	Irsogladine maleate
3269 M06	E	551	560	-0.18695688	392	400	-0.13616568	2816379	0.40466853	2957181	0.62290557	empty			
3269 M07	X	1194	1200	-0.16227379	875	880	-0.08401747	2667093	0.25426477	2981461	0.64762688	experimental	Tocris	2506	SSR 69071
3269 M08	E	713	720	-0.18073812	512	520	-0.1232096	2778515	0.36652103	3382632	1.05608952	empty			
3269 M09	X	352	360	-0.19459597	752	760	-0.09728745	3060883	0.65100322	3813243	1.49452726	experimental	Tocris	2507	J 104129 fumarate
3269 M10	E	435	440	-0.19140982	474	480	-0.12731236	3200418	0.79158297	3095878	0.76412351	empty			
3269 M11	X	475	480	-0.18987432	314	320	-0.14458713	2853052	0.44161611	2920163	0.58521474	experimental	Tocris	2508	Trap 101
3269 M12	E	514	520	-0.18837721	355	360	-0.14016047	2767878	0.35580439	2933413	0.59870557	empty			
3269 M13	X	515	520	-0.18833883	355	360	-0.14016047	2948556	0.53783519	3209405	0.87971397	experimental	Tocris	2510	Taliniflumate
3269 M14	E	473	480	-0.1899511	475	480	-0.12720439	2712268	0.29977801	2959103	0.62486251	empty			
3269 M15	X	512	520	-0.18845399	553	560	-0.11878294	2787012	0.37508165	3209661	0.67997462	experimental	Tocris	2513	Acyclovir
3269 M16	E	493	500	-0.18534461	434	440	-0.11652195	2781917	0.36594885	4708132	0.36931971	empty			
3269 M17	X	352	360	-0.19459597	394	400	-0.13594974	2924726	-0.39291187	2014071	-0.33734628	experimental	Tocris	2514	L 161982
3269 M18	E	515	520	-0.18833883	674	680	-0.1057189	3129661	0.72029619	3580609	1.25766493	empty			
3269 M19	X	513	520	-0.1884156	513	520	-0.12310163	1985422	-0.43251015	2438850	0.09515345	experimental	Tocris	2517	RS 504393
3269 M20	E	753	760	-0.17920263	834	840	-0.08844413	2948787	0.53806792	3372684	1.04596071	empty			
3269 M21	X	711	720	-0.1808149	551	560	-0.11899888	1640911	-0.77960064	1905896	-0.44748746	experimental	Tocris	2519	T 98475
3269 M22	E	669	680	-0.18242717	1029	1040	-0.0673905	3114592	0.70511436	3276698	0.94823008	empty			

3269 N13	X	475	480	-0.18987432	554	560	-0.11867497	2789726	0.37781597	2931992	0.59725874	experimental	Tocris	2687	Pentylentetrazole
3269 N14	X	473	480	-0.1899511	473	480	-0.12742033	2699502	0.28691643	3011139	0.67784431	empty			
3269 N15	X	755	760	-0.17912585	755	760	-0.09697354	10637548	8.28439753	10747332	8.55464945	experimental	Tocris	2688	CPT 11
3269 N16	E	633	640	-0.18380911	593	640	-0.18380911	3604059	1.19824618	3192760	0.06683913	empty			
3269 N17	X	673	680	-0.18227362	473	480	-0.12742033	3166897	0.75781099	2765029	0.42726104	experimental	Tocris	2691	Moexipril hydrochloride
3269 N18	E	433	440	-0.19148659	674	680	-0.1057189	3273971	0.86586669	3117692	0.786334	empty			
3269 N19	X	314	320	-0.19605469	273	280	-0.14901379	994708	-1.430642	942672	-1.42821891	experimental	Tocris	2693	PHA 665752
3269 N20	E	552	560	-0.18691849	432	440	-0.13184699	3361630	0.95400203	2958759	0.62451225	empty			
3269 N21	X	1072	1080	-0.16695705	712	720	-0.10161614	1755380	-0.66427456	1500021	-0.8607396	experimental	Tocris	2694	PD 407824
3269 N22	E	827	840	-0.17636196	587	600	-0.11511205	2752560	0.34037169	3121730	0.7904454	empty			
3269 N23	E	786	1680	-0.17793594	974	1720	-0.0733287	83150	-2.34902517	96327	-2.28994698	empty			
3269 N24	P	303714	305120	11.4507545	252353	253760	-0.03683575	2715609	0.30314403	2752240	0.41423959	empty			
3269 O01	N	476	480	-0.18983593	835	840	-0.08833616	2161263	-0.25535257	2288727	-0.05769817	empty			
3269 O02	E	194	200	-0.20066118	114	120	-0.16618059	82539	-2.34964075	123395	-2.26238699	empty			
3269 O03	X	1114	1120	-0.16534478	875	880	-0.08401747	2932083	0.52123885	2592102	0.25119094	experimental	Tocris	2520	PD 166793
3269 O04	E	513	520	-0.1884156	513	520	-0.12310163	2439387	0.02485385	2321093	-0.02474389	empty			
3269 O05	X	274	280	-0.19759019	194	200	-0.15754321	1593320	-0.82754797	1486041	-0.8749737	experimental	Tocris	2521	NSC 3852
3269 O06	E	352	360	-0.19459597	512	520	-0.1232096	2506413	0.0923817	2506046	0.1635708	empty			
3269 O07	X	1594	1600	-0.14691894	1312	1320	-0.03683575	2715609	0.30314403	2752240	0.41423959	experimental	Tocris	2524	A 205804
3269 O08	E	711	720	-0.1808149	1272	1280	-0.04115444	2604274	0.19097542	2674853	0.33544601	empty			
3269 O09	X	549	560	-0.18703365	468	480	-0.12796016	2774888	0.36286687	2647414	0.30750828	experimental	Tocris	2531	Ganaxalone
3269 O10	E	714	720	-0.18069974	434	440	-0.13163105	2489054	0.07489273	2477590	0.13459758	empty			
3269 O11	X	392	400	-0.19306047	393	400	-0.13605771	2682756	0.27004505	2491642	0.14890499	experimental	Tocris	2533	DPO-1
3269 O12	E	515	520	-0.18833883	354	360	-0.14026844	2618323	0.20512961	2289844	-0.05656087	empty			
3269 O13	X	274	280	-0.19759019	434	440	-0.13163105	2084519	-0.33267118	1857515	-0.49674783	experimental	Tocris	2536	Domperidone
3269 O14	E	676	680	-0.18215846	135	640	-0.10992962	2674193	0.26141793	2323800	-0.02198769	empty			
3269 O15	X	154	160	-0.20219667	113	120	-0.16628856	940698	-1.48505639	959532	-1.41105246	experimental	Tocris	2539	IKK 16
3269 O16	E	393	400	-0.19302209	634	640	-0.11003759	2902275	0.49120767	2478407	0.13542943	empty			
3269 O17	X	833	840	-0.17613164	632	640	-0.11025352	2292487	-0.12314604	2493874	0.15117756	experimental	Tocris	2542	KI 8751
3269 O18	E	753	760	-0.17920263	592	600	-0.11457222	2879891	0.46865607	2622976	0.2826261	empty			
3269 O19	X	628	640	-0.18400105	707	720	-0.10215597	2603253	0.18994678	2508649	0.16622111	experimental	Tocris	2545	Lofepramine
3269 O20	E	553	560	-0.1868801	831	840	-0.08876803	2630547	0.21744514	2628728	0.28848265	empty			
3269 O21	X	470	480	-0.19006626	1030	1040	-0.06728253	2368363	-0.04670193	2643399	0.30342031	experimental	Tocris	2547	6-Hydroxydopamine hydrochloride
3269 O22	E	950	960	-0.17164031	1027	1040	-0.06760643	2432734	0.01815104	2614969	0.27447357	empty			
3269 O23	E	598	1280	-0.18515267	847	1600	-0.08704055	83961	-2.3482081	108998	-2.27704567	empty			
3269 O24	P	228536	230680	8.56479091	253287	255080	27.1682285	2251285	-0.16465654	2152890	-0.19600413	empty			
3269 P01	N	598	600	-0.18515267	877	880	-0.08380153	2013969	-0.40374941	2055139	-0.29553184	empty			
3269 P02	E	157	160	-0.20208151	194	200	-0.15721931	74555	-2.35768453	76125	-2.31051616	empty			
3269 P03	X	194	200	-0.20066118	194	200	-0.15754321	1035010	-1.39003824	927852	-1.44330827	experimental	Tocris	2700	Calcipitriol
3269 P04	E	675	680	-0.18219684	836	840	-0.08822819	2431880	0.01729064	2628882	0.28863945	empty			
3269 P05	X	836	840	-0.17601648	595	600	-0.11424831	2251876	-0.16406111	2466162	0.12296187	experimental	Tocris	2706	Temozolomide
3269 P06	E	516	520	-0.18830044	676	680	-0.10550296	2560943	0.14731999	2702508	0.36360367	empty			
3269 P07	X	273	280	-0.19762857	353	360	-0.1403764	2369305	-0.04575288	2435413	0.09165398	experimental	Tocris	2709	Cilastatin sodium
3269 P08	E	435	440	-0.19140982	272	280	-0.14912176	2488971	0.0748091	2579857	0.23872338	empty			
3269 P09	X	716	720	-0.18062296	1076	1080	-0.06231604	2735016	0.32269634	2321513	-0.02431625	experimental	Tocris	2718	LY 364947
3269 P10	E	473	480	-0.1899511	593	600	-0.11446425	2496222	0.0821144	2362273	0.01718459	empty			
3269 P11	X	1076	1080	-0.1668035	956	960	-0.07527211	1172986	-1.25102916	1490279	-0.87065867	experimental	Tocris	2721	SB 225002
3269 P12	E	594	600	-0.18530622	355	360	-0.14016047	2507939	0.09391913	2488687	0.14589628	empty			
3269 P13	X	516	520	-0.18830044	436	440	-0.13141512	2213090	-0.20313752	2290405	-0.05598967	experimental	Tocris	2725	CGP 57380
3269 P14	E	475	480	-0.18987432	635	640	-0.10992962	2624265	0.2111161	2433194	0.08939465	empty			
3269 P15	X	396	400	-0.19290692	476	480	-0.12709642	1984948	-0.4329877	2085616	-0.26450089	experimental	Tocris	2742	Reserpine
3269 P16	E	636	640	-0.18369395	593	600	-0.11446425	2525962	0.11207707	2545646	0.20389056	empty			
3269 P17	X	674	680	-0.18223523	1195	1200	-0.04946792	1998311	-0.41952465	2403807	0.05947351	experimental	Tocris	2743	Caffeic acid phenethyl ester
3269 P18	E	508	520	-0.18860754	627	640	-0.11079336	2675696	0.26293218	2884599	0.54900433	empty			
3269 P19	X	254	2560	-0.11006695	2754	2760	0.11885312	2284486	-0.13120695	2407244	0.06297298	experimental	Tocris	2748	KF 38789
3269 P20	E	748	760	-0.17939457	787	800	-0.09351859	2701792	0.28922357	2607045	0.26640354	empty			
3269 P21	X	914	920	-0.17302226	711	720	-0.10172411	2254254	-0.16166531	2364474	0.01942556	experimental	Tocris	2755	DCA
3269 P22	E	828	840	-0.17632357	1349	1360	-0.03284096	2475540	0.06127754	2308984	-0.03707298	empty			
3269 P23	E	1097	2360	-0.16599737	1058	2120	-0.06425945	78222	-2.35399007	95107	-2.29118915	empty			
3269 P24	P	433565	434240	16.4353179	363095	363840	39.0239035	2029245	-0.38835903	1994594	-0.3571773	empty			