

**Table S1. List of Synonymous and Nonsynonymous Mutations in r1Reovirus and r2Reovirus**

I. Synonymous mutations

<b>Gene segment</b>	<b>r1Reovirus</b>	<b>r2Reovirus</b>
L1	N/A	N/A
L2	N/A	A318G
L3	C2059T G2062C	C2059T G2062C T3550C
M1	T229C C919T	T229C C919T
M2	N/A	N/A
M3	N/A	N/A
S1	N/A	N/A
S2	See table III	N/A
S3	N/A	N/A
S4	N/A	N/A

II. Non-synonymous mutations

<b>Gene segments</b>	<b>R1Reovirus</b>	<b>R2Reovirus</b>
L1	N/A	N/A
L2	N/A	N/A
L3	G491A (A160T)	G491A (A160T)
M1	N/A	N/A
M2	N/A	N/A
M3	N/A	N/A
S1	N/A	N/A
S2	G1294A (after coding region) See table IV	N/A
S3	C508A (P161T) A775G (I250V) T1170G (after coding region)	A775G (I250V)
S4	G177A (V49I)	G177A (V49I)

III. Synonymous mutations in r1Reovirus S2 gene segment

<b>Mutation</b>	<b>Percentage</b>
G54A	45% A, 55% G
C84T	64% C, 36% T
C87T	64% C, 36% T
A90G	64% A, 36% G

C91T	65% C, 35% G
T96G	65% T, 35% G
C108T	64% C, 35% T
T114C	33% C, 66% T
A123G	67% A, 33% G
A537G	57% A, 42% G
T564C	56% T, 44% C
C573T	59% C, 41% T
T834C	69% T, 31% C
C858T	65% C, 35% T
T939C	67% T, 33% C
A945G	55% A, 45% G
A951G	55% A, 45% G
G954T	55% G, 45% T
C972T	49% C, 51% T
T981C	51% C, 48% T
T990C	50% C, 50% T
A996G	52% A, 48% G
T997C	49% C, 51% T
G1005T	48% G, 52% T
G1011A	51% A, 49% G
A1015C	47% A, 52% C
T1035C	50% C, 49% T
G1044A	45% A, 55% G
G1047A	46% A, 54% G
T1059A	49% A, 51% T
C1062T	52% C, 48% T
C1068T	51% C, 49% T
G1080A	51% A, 49% G
G1107A	51% A, 49% G
G1257A	65% A, 35% G
T1274A	65% A, 35% G

IV. Non-synonymous mutations in r1Reovirus S2 gene segment

<b>Mutation</b>	<b>Percentage</b>
G1087A (V357I)	51% A, 49% G
C1174A (H386N)	54% A, 46% C



**Table S2. Data from screening of reovirus infectivity using the NIH Clinical Collection.** Data are shown for two independent experiments (Runs). For each run, reovirus focus forming units (FFU), number of cells (DAPI), percent infectivity ( $[\text{FFU}/\text{DAPI}] \times 100$ ), and Z-score based on percent infectivity (Z percent infectivity) were calculated. Z scores for each well were calculated using the following formula:  $Z \text{ score} = (a-b)/c$ , where a is the percent infectivity (infected cells/number of cells), b is the median percent infectivity for each plate, and c is the standard deviation of percent infectivity for each plate. The average Z-score for both runs is also provided (Avg Z % Infectivity). Name for individual compounds and their PubChem ID numbers are provided.

NIH Clinical Collection Compound	PUBCHEM_SID	FFU	DAPI	Run 1		FFU	DAPI	Run 2		Average
				% Infectivity	Z % Infectivity			% Infectivity	Z % Infectivity	
(-)-Cotinine	46386857	2092	14619	14.310	0.005	3200	15961	20.049	-0.271	-0.133
(+)-cis-Diltiazem hydrochloride	104170056	3107	16205	19.173	0.309	4354	15018	28.992	0.386	0.347
(+/-)-Norepinephrine hydrochloride	104170127	1659	16363	10.139	-0.005	3611	17031	21.203	0.241	0.118
(+/-)-Vesamicol hydrochloride	46386799	3339	16652	20.052	0.310	4220	15806	26.699	0.191	0.251
1,1-Dimethyl-4-phenylpiperazinium iodide	46387026	2219	16640	13.335	-0.168	3558	17209	20.675	-0.131	-0.149
11-Deoxycortisol	46386963	1498	14406	10.398	0.015	3502	16740	20.920	-0.248	-0.116
19-Norethindrone	104170074	1177	12279	9.585	-0.299	2753	14090	19.539	-0.381	-0.340
19-Norethindrone acetate	104170073	1274	14142	9.009	-0.559	3688	17176	21.472	-0.155	-0.357
19-Nortestosterone	46386764	3024	16219	18.645	-0.313	4047	16035	25.239	-0.309	-0.311
2-Chloroadenosine	46386960	2267	13089	17.320	-0.900	3185	12461	25.560	-0.199	-0.550
2-Pyridylethylamine	46386941	2179	14932	14.593	-0.209	2770	13688	20.237	0.030	-0.089
3-Pyridinemethanol	46386968	1528	14392	10.617	0.370	3663	16448	22.270	0.262	0.316
3,5,3'-Triiodothyronine	104169993	1862	16047	11.603	0.774	3580	16147	22.171	0.604	0.689
3'-Deoxyadenosine	46386791	1256	12505	10.044	0.105	3503	16264	21.538	0.071	0.088
4-Phenylbutyric acid	104169967	1360	14260	9.537	-0.129	3506	16692	21.004	-0.069	-0.099
5-Azacytidine	104170170	1068	12621	8.462	-1.197	2646	14413	18.358	-1.152	-1.174
5-Fluoro-2-pyrimidone	46386867	2219	16295	13.618	-0.118	3498	17222	20.311	-0.212	-0.165
5-Fluorouracil	104169952	1393	15561	8.952	-0.590	3902	17874	21.831	-0.052	-0.321
5-Methoxytryptamine	46387021	2778	14304	19.421	1.353	2980	12900	23.101	1.007	1.180
5-Nonyloxytryptamine hydrochloride	46387012	1645	13694	12.013	1.026	4006	15989	25.055	1.210	1.118
6-Aminoindazole	46386887	1161	10946	10.607	0.146	3347	13783	24.284	0.938	0.542
6-Azuridine	46386950	1040	11173	9.308	-0.667	2716	14323	18.963	-0.939	-0.803
7-Nitroindazole	46387020	1763	15869	11.110	0.461	3659	16482	22.200	0.203	0.332
Acarbose	46386746	1447	14712	9.836	-0.337	3456	16945	20.395	-0.433	-0.385
Acebutolol hydrochloride	104170167	1445	16437	8.791	-0.721	3278	17207	19.050	-0.564	-0.643
Acetazolamide	104169989	1752	16398	10.684	0.285	3366	17053	19.738	-0.307	-0.011
Acetylcholine chloride	104170141	1571	16027	9.802	-0.184	3568	17766	20.083	-0.178	-0.181
Acitretin	104170221	954	10320	9.244	-0.429	3301	14286	23.107	0.316	-0.057
Actarit	46386663	2643	14689	17.993	0.891	2509	12093	20.748	0.204	0.548
Acyclovir	104170215	905	10133	8.931	-0.601	2921	14335	20.377	-0.470	-0.536
Albendazole	104170113	484	8774	5.516	-2.463	1068	7911	13.500	-2.642	-2.552
Alfuzosin	46386655	3397	16737	20.296	1.636	3240	15149	21.388	0.423	1.030
Allopurinol	104169990	1633	16071	10.161	0.007	3382	16760	20.179	-0.142	-0.067
Alosetron monohydrochloride	46386816	2464	16744	14.716	0.077	3661	17270	21.199	-0.015	0.031
Alprazolam	46386679	2743	17640	15.550	0.101	3182	15667	20.310	0.055	0.078
Altanserin hydrochloride	46386989	2605	14086	18.494	1.053	3286	13124	25.038	1.667	1.360
Altretamine	104170093	1306	13484	9.686	-0.188	3732	17032	21.912	-0.028	-0.108
AM 404	46386792	2469	16885	14.622	0.060	3562	17168	20.748	-0.115	-0.027
AM-251	46386990	1984	16774	11.828	-1.104	2334	15171	15.385	-1.624	-1.364
Amcinonide	104170128	3267	14451	22.607	1.414	4510	13593	33.179	1.388	1.401
Amiloride hydrochloride hydrate	46386846	3060	15899	19.246	-0.047	4085	15815	25.830	-0.106	-0.077
Aminoglutethimide	104170212	1002	10174	9.849	-0.098	3105	14534	21.364	-0.186	-0.142
Aminolevulinic acid	104170099	1390	14612	9.513	-0.140	3655	17987	20.320	-0.248	-0.194
Amiodarone hydrochloride	46386662	2513	16544	15.190	-1.204	4683	16432	28.499	0.374	-0.415
Amisulpride	46386656	2531	17520	14.446	-0.256	3143	15592	20.158	0.003	-0.126
Amitriptyline hydrochloride	104169995	1440	16507	8.724	-0.757	3353	17749	18.891	-0.624	-0.690
Amlexanox	46386726	3055	17095	17.871	0.852	3362	16587	20.269	0.041	0.446
Amlodipine	46386686	2279	14338	15.895	0.212	2772	13174	21.041	0.305	0.258
Amoxapine	104170044	2879	16193	17.779	-0.140	3826	14489	26.406	-0.233	-0.187
Amoxicillin	104170168	1771	16419	10.786	0.340	3624	17607	20.583	0.009	0.175
Ampicillin sodium	104170166	1056	11444	9.228	-0.718	2966	14616	20.293	-0.469	-0.593
Amproxicam	46386688	2512	17079	14.708	-0.172	3211	16208	19.811	-0.115	-0.143
Anagrelide hydrochloride	46386622	3502	17613	19.883	0.235	4408	17653	24.970	-0.401	-0.083
Anastrozole	46386543	1281	12092	10.594	0.359	3381	15069	22.437	0.306	0.333
Argatroban	46386718	3127	17578	17.789	-0.368	4230	16168	26.163	-0.327	-0.348
Aripiprazole	46386763	3374	16153	20.888	1.828	2953	13592	21.726	0.538	1.183
Artemether	46386824	3342	16282	20.526	0.513	4541	16200	28.031	0.233	0.373
Artesunate	46386645	1865	14061	13.264	-0.639	2496	12456	20.039	-0.037	-0.338
Atenolol	104170046	2987	16684	17.903	-0.100	4145	16129	25.699	-0.403	-0.251
Atomoxetine hydrochloride	46386643	1283	11505	11.152	0.487	3432	14268	24.054	0.857	0.672
Atracurium besylate	46386822	1026	10767	9.529	-0.132	3051	14760	20.671	-0.156	-0.144
Atropine	104169991	1559	13940	11.184	0.507	3696	16519	22.374	0.265	0.386
Azasetron hydrochloride	46386991	3040	17554	17.318	0.673	2926	15495	18.884	-0.431	0.121
Azathioprine	104170112	870	14394	6.044	-2.183	2895	17371	16.666	-1.539	-1.861
Azelastine hydrochloride	46386661	3778	13401	28.192	2.981	4751	11858	40.066	3.846	3.413
Azithromycin	104170210	55	11373	0.484	-6.193	518	12392	4.180	-6.153	-6.173
Balsalazide	46386828	1535	15218	10.087	0.125	3716	17221	21.578	0.081	0.103
Beclomethasone	46386972	3160	13887	22.755	1.231	4515	15021	30.058	0.842	1.036
Beclomethasone dipropionate	104170108	3182	14839	21.443	1.040	4222	13242	31.883	1.078	1.059
Benactyzine hydrochloride	46386942	3309	17489	18.920	-0.003	4448	16582	26.824	-0.129	-0.066
Benazepril hydrochloride	46386692	2940	16178	18.173	-0.244	4057	15388	26.365	-0.267	-0.255
Bendroflumazide	104170162	3170	16732	18.946	0.235	4297	15310	28.067	0.164	0.200
Benidipine hydrochloride	46386729	2208	14915	14.804	0.092	3638	15555	23.388	0.473	0.283
Benproperine phosphate	46386752	2243	16122	13.913	2.216	4376	15509	28.216	2.325	2.271
Benzbromarone	46386951	3152	16921	18.628	1.097	2618	13747	19.044	-0.376	0.360
Benztropine mesylate	104170144	1703	15721	10.833	0.287	3770	17371	21.703	0.028	0.158
Benzylimidazole	46386891	1442	14198	10.156	-0.136	3305	16286	20.294	-0.469	-0.303
Bestatin	46386830	2914	15718	18.539	-0.126	4054	15459	26.224	-0.309	-0.218
Beta-estradiol	46386902	3056	16697	18.303	-0.465	3985	16184	24.623	-0.520	-0.492
Betamethasone	104170205	1133	10531	10.759	0.400	3346	13406	24.959	0.849	0.625
Betaxolol hydrochloride	46386993	2129	16847	12.637	-0.291	3535	17047	20.737	-0.117	-0.204
Bethanechol chloride	104170158	1559	14692	10.611	0.149	3558	16932	21.013	-0.215	-0.033
Bicalutamide	46386630	970	9739	9.960	0.066	3255	15632	20.823	-0.117	-0.025
Bifemelane hydrochloride	46386922	4125	17521	23.543	1.856	5491	17516	31.348	1.784	1.820

Bifonazole	46386787	3431	17251	19.889	0.238	4032	16535	24.385	-0.601	-0.182
Bisoprolol fumarate	46386635	2729	17483	15.609	0.120	2583	14978	17.245	-0.990	-0.435
Brimonidine	104170136	3024	17114	17.670	-0.175	4313	15407	27.994	0.147	-0.014
Brucine	46386939	3349	17186	19.487	0.179	4329	15792	27.413	0.048	0.113
Budesonide	104170124	1515	13731	11.033	0.413	3659	15160	24.136	0.886	0.650
Buflomedil hydrochloride	46386737	2377	16676	14.254	-0.005	3641	16946	21.486	0.049	0.022
Bumetanide	104170048	1770	15917	11.120	0.467	3393	15858	21.396	-0.080	0.194
Bupropion hydrochloride	46386703	2495	13648	18.281	-0.209	3130	11501	27.215	-0.012	-0.110
Buspirone hydrochloride	104170171	1776	15931	11.148	0.485	4130	17529	23.561	0.683	0.584
Busulfan	104169996	1776	16484	10.774	0.333	3239	16257	19.924	-0.237	0.048
Calcipotriol	46386727	3168	15943	19.871	0.302	4427	15457	28.641	0.416	0.359
Calcitriol	46386784	2140	16933	12.638	-0.291	3475	15830	21.952	0.153	-0.069
Captopril	104170052	1649	16012	10.299	-0.047	3859	17280	22.332	0.250	0.101
Carbamazepine	104170177	1420	14442	9.832	-0.339	3450	16689	20.672	-0.335	-0.337
Carbidopa	104170225	1579	14418	10.952	0.506	4092	17858	22.914	0.260	0.383
Carinoxamine maleate	104170100	3120	17319	18.015	-0.064	3891	14868	26.170	-0.290	-0.177
Carisoprodol	104170000	2536	13797	18.381	0.054	3564	12989	27.439	0.014	0.034
Carmofur	46386675	3031	17357	17.463	-0.473	4247	16313	26.034	-0.366	-0.419
Carvedilol	46386749	1683	16972	9.916	-0.123	3381	17973	18.812	-0.654	-0.388
CCPA	46386935	1369	13492	10.147	0.153	3484	16159	21.561	0.077	0.115
Cefaclor	46386958	3056	16843	18.144	-0.253	4090	15671	26.099	-0.347	-0.300
Cefatrizine propylene glycol	46386659	2516	17111	14.704	-0.173	3314	15918	20.819	0.229	0.028
Cefazolin sodium	104170051	3147	17389	18.098	-0.038	4073	15037	27.087	-0.071	-0.054
Cefdinir	46386833	3194	17261	18.504	-0.137	4158	16112	25.807	-0.434	-0.286
Cefixime trihydrate	46386832	1350	14079	9.589	-0.105	3085	16988	18.160	-0.814	-0.459
Cefotaxime sodium	104170202	1872	15999	11.701	0.826	3701	16953	21.831	0.477	0.651
Cefoxitin sodium	104170054	3043	17342	17.547	-0.215	3736	14122	26.455	-0.222	-0.218
Cefpodoxime proxetil	46386731	2403	13373	17.969	-0.310	3332	11873	28.064	0.243	-0.033
Cefuroxime	104170159	1604	16606	9.659	-0.260	3554	17862	19.897	-0.247	-0.253
Celecoxib	104170206	1297	12844	10.098	-0.026	2932	14299	20.505	-0.020	-0.023
Cephalexin hydrate	46386774	2743	14890	18.422	1.030	2613	12636	20.679	0.181	0.605
Cerivastatin sodium	46386572	2730	14795	18.452	1.040	3607	14140	25.509	1.828	1.434
Cetirizine	104170194	1550	14739	10.516	0.268	3597	16533	21.756	-0.073	0.097
Cetiraxate hydrochloride	46386678	3337	17467	19.105	-0.110	4528	17700	25.582	-0.191	-0.150
CGS 12066B dimaleate	46386975	951	11692	8.134	-0.776	2858	14617	19.553	-0.449	-0.613
CGS 15943	46386800	2738	15750	17.384	0.549	4190	16031	26.137	1.085	0.817
Chlorambucil	104170053	1093	10543	10.367	-0.004	2915	13474	21.634	0.004	0.000
Chloramphenicol	104170151	1375	14287	9.624	-0.469	3640	16341	22.275	0.230	-0.120
Chlordiazepoxide	46386831	1464	14960	9.786	-0.014	3443	17023	20.226	-0.273	-0.143
Chlorothiazide	104169998	3207	16805	19.084	0.280	4410	15973	27.609	0.055	0.167
Chloroxine	104170003	3065	17408	17.607	-0.196	4374	15169	28.835	0.348	0.076
Chlorpheniramine maleate	46386872	2507	13409	18.696	-0.291	3321	12824	25.897	-0.083	-0.187
Chlorpromazine hydrochloride	104170050	2884	17420	16.556	-0.534	4155	15372	27.030	-0.084	-0.309
Chlorpropamide	104170001	3149	17627	17.865	-0.113	3913	14732	26.561	-0.196	-0.154
Chlorthalidone	104170188	1536	14969	10.261	0.061	3657	17498	20.900	0.128	0.094
Chlorzoxazone	104169997	1684	16393	10.273	0.067	3452	17737	19.462	-0.410	-0.172
Cilastatin sodium	46386570	2313	12905	17.923	-0.633	3365	12637	26.628	0.167	-0.233
Cimetidine	104169999	2897	16824	17.219	-0.320	4107	15440	26.600	-0.187	-0.254
Cinanserin	46386801	2134	16797	12.705	-0.279	3593	17211	20.876	-0.086	-0.183
Cisapride hydrate	46386802	3272	16478	19.857	0.986	4886	16227	30.110	1.970	1.478
Citalopram hydrobromide	46386617	2676	17052	15.693	0.147	3156	15317	20.605	0.156	0.151
Cladribine	46386544	1238	11082	11.171	0.625	3151	12712	24.788	0.922	0.774
Clarithromycin	46386761	3430	17486	19.616	1.416	2951	15049	19.609	-0.184	0.616
Clobenpropit	46387016	1784	15566	11.461	0.681	4020	17074	23.545	0.678	0.679
Clobetasol propionate	104170049	2938	12290	23.906	1.832	4085	11736	34.807	1.777	1.805
Clofazimine	46386952	1374	17415	7.890	-2.378	2633	15552	16.930	-1.097	-1.737
Clomifene citrate	104170129	1460	14973	9.751	-0.030	3482	16993	20.491	-0.204	-0.117
Clomipramine hydrochloride	104170176	1366	16638	8.210	-1.355	3257	17114	19.031	-0.914	-1.135
Clonidine hydrochloride	46386982	2458	17215	14.278	-0.311	3211	15335	20.939	0.270	-0.021
Clopidogrel	104170201	1572	14846	10.589	0.307	4158	17457	23.819	0.521	0.414
Clotrimazole	46386926	2589	15415	16.795	0.445	3692	15751	23.440	0.485	0.465
Clozapine	104170165	1340	16070	8.339	-0.962	3089	17233	17.925	-0.986	-0.974
Corticosterone	46386953	1503	14044	10.702	0.409	3879	16504	23.503	0.585	0.497
Cortisol 21-acetate	104169955	1630	13483	12.089	1.130	4333	16111	26.895	1.407	1.268
Cortisone	46386956	1629	14796	11.010	0.398	3550	16827	21.097	-0.186	0.106
Cortisone acetate	104170175	3352	17454	19.205	0.319	4230	15541	27.218	-0.039	0.140
Cromolyn sodium	104170109	1448	15286	9.473	-0.359	3533	17333	20.383	-0.065	-0.212
Crotamiton	46386684	1410	14323	9.844	0.013	3557	17398	20.445	-0.216	-0.101
Cyclophosphamide hydrate	104170160	1140	11239	10.143	-0.144	3017	14614	20.645	-0.345	-0.245
Cyproheptadine hydrochloride	46386957	1300	14714	8.835	-0.453	3125	16790	18.612	-0.696	-0.574
Cytarabine	46386862	2937	12310	23.859	1.996	3890	11800	32.966	2.338	2.167
D-Cycloserine	46386864	2524	17723	14.241	-0.323	3326	16769	19.834	-0.107	-0.215
Dactinomycin	46386883	2733	10907	25.057	3.177	3325	10282	32.338	4.156	3.666
Danazol	104170055	3254	17310	18.798	0.188	4162	15212	27.360	-0.005	0.091
Dantrolene sodium	104170142	1448	14619	9.905	-0.294	3526	16859	20.915	-0.250	-0.272
Dapsone	104169986	1193	11146	10.703	0.206	3352	14554	23.031	0.497	0.352
Daunorubicin hydrochloride	104170197	295	3477	8.484	-0.846	1709	8981	19.029	-0.858	-0.852
Deferiprone	46386865	1347	14070	9.574	-0.112	3717	17468	21.279	0.003	-0.055
Dehydrocholic acid	46386890	1035	11407	9.073	-0.814	2962	14676	20.183	-0.508	-0.661
Dehydroepiandrosterone	46387028	1510	15183	9.945	-0.268	3858	17234	22.386	0.269	0.000
Demeclocycline	104170101	1464	15273	9.586	-0.106	3596	16933	21.237	-0.008	-0.057
Desipramine hydrochloride	104170179	1614	16281	9.913	-0.124	3421	17928	19.082	-0.552	-0.338
Desloratadine	46386563	1572	16636	9.449	-1.873	1978	15801	12.518	-2.601	-2.237
Desoximetasone	46386959	1489	11217	13.274	1.596	3483	13457	25.882	1.208	1.402
Dexamethasone	104170143	1242	10381	11.964	1.061	3382	13511	25.031	0.870	0.966
Dexbrompheniramine maleate	46386574	2673	13675	19.547	0.086	3386	12781	26.492	0.121	0.103

Dexchlorpheniramine maleate	46386575	2309	17006	13.578	-0.125	3806	17303	21.996	0.163	0.019
Dextromethorphan hydrobromide, monohydrate	46386932	2575	16933	15.207	0.164	3849	17054	22.569	0.291	0.227
Dextrorphan D-tartrate	46386873	3461	17451	19.833	0.213	4283	16430	26.068	-0.025	0.094
Diazepam	46386554	2984	15856	18.819	-0.036	3956	14390	27.491	0.071	0.018
Diazoxide	46386946	1462	14515	10.072	0.118	3515	16613	21.158	-0.029	0.045
Dichloroacetic acid	46386944	2875	16028	17.937	-0.320	4056	15333	26.453	-0.240	-0.280
Diclofenac sodium	46386927	2173	13442	16.166	-0.890	3133	11768	26.623	-0.189	-0.540
Dicloxacillin sodium	104170195	1696	15265	11.110	0.512	3672	17054	21.532	0.364	0.438
Dicyclomine hydrochloride	104170002	3830	16902	22.660	1.431	4946	15477	31.957	1.095	1.263
Didanosine	46386730	2428	17477	13.893	-0.435	3005	15755	19.073	-0.366	-0.401
Diflunisal	104170004	887	10836	8.186	-1.010	2974	14925	19.926	-0.600	-0.805
Digoxin	104170057	8	9479	0.084	-4.491	91	11121	0.818	-5.355	-4.923
Dihydroxidine hydrochloride	46386992	1835	15030	12.209	-0.980	2264	12980	17.442	-0.922	-0.951
Dilantin	104170140	1673	16048	10.425	0.032	3742	17333	21.589	-0.012	0.010
Diphenhydramine hydrochloride	46386874	1146	11920	9.614	-0.284	3108	14750	21.071	0.192	-0.046
Diphenoxylate hydrochloride	46386550	3354	17418	19.256	-0.043	4320	16527	26.139	0.000	-0.022
Diphenylcyclopropenone	46386897	897	12100	7.413	-1.109	2547	14627	17.413	-1.010	-1.059
Dipyridamole	104169946	1080	11181	9.659	-0.447	3118	13799	22.596	0.343	-0.052
Disopyramide phosphate	104170181	2940	17322	16.973	-0.400	4028	14899	27.035	-0.083	-0.241
Disulfiram	46386898	3726	17283	21.559	0.977	4364	16666	26.185	0.015	0.496
DL-Penicillamine	104169974	1634	15850	10.309	0.154	3854	17415	22.130	0.035	0.094
DMSO-Mock		2	14457	0.014	-8.566	1	14359	0.007	-8.952	-8.759
DMSO-Mock		3	13247	0.023	-8.562	1	12778	0.008	-8.952	-8.757
DMSO-Mock		5	14722	0.034	-8.557	1	14374	0.007	-8.952	-8.754
DMSO-Mock		5	14419	0.035	-8.557	36	14237	0.253	-8.868	-8.712
DMSO-Mock		1	12425	0.008	-6.490	1	15209	0.007	-7.625	-7.058
DMSO-Mock		1	12211	0.008	-6.490	0	15649	0.000	-7.627	-7.059
DMSO-Mock		2	11906	0.017	-6.485	5	15134	0.033	-7.615	-7.050
DMSO-Mock		2	10999	0.018	-6.484	12	14125	0.085	-7.597	-7.041
DMSO-Mock		0	14066	0.000	-6.093	1	14360	0.007	-8.180	-7.136
DMSO-Mock		1	14197	0.007	-6.091	2	14389	0.014	-8.178	-7.134
DMSO-Mock		1	12684	0.008	-6.090	2	11909	0.017	-8.177	-7.134
DMSO-Mock		5	14111	0.035	-6.081	16	13150	0.122	-8.145	-7.113
DMSO-Mock		0	14413	0.000	-5.864	0	13412	0.000	-6.553	-6.209
DMSO-Mock		1	14919	0.007	-5.862	2	14404	0.014	-6.550	-6.206
DMSO-Mock		1	13620	0.007	-5.862	2	13294	0.015	-6.550	-6.206
DMSO-Mock		2	14500	0.014	-5.860	2	13610	0.015	-6.550	-6.205
DMSO-Mock		0	10665	0.000	-5.495	0	15530	0.000	-6.338	-5.917
DMSO-Mock		1	8725	0.011	-5.489	3	15252	0.020	-6.332	-5.911
DMSO-Mock		2	8614	0.023	-5.482	1	15372	0.007	-6.336	-5.909
DMSO-Mock		4	1857	0.215	-5.377	0	13851	0.000	-6.338	-5.858
DMSO-Mock		0	14906	0.000	-4.930	4	13249	0.030	-6.859	-5.895
DMSO-Mock		0	15148	0.000	-4.930	1	14738	0.007	-6.867	-5.899
DMSO-Mock		0	14200	0.000	-4.930	0	12652	0.000	-6.869	-5.900
DMSO-Mock		1	15221	0.007	-4.928	11	13302	0.083	-6.841	-5.885
DMSO-Mock		0	12060	0.000	-4.530	17	15361	0.111	-5.541	-5.035
DMSO-Mock		2	11643	0.017	-4.522	12	15262	0.079	-5.549	-5.036
DMSO-Mock		5	13226	0.038	-4.512	0	14479	0.000	-5.570	-5.041
DMSO-Mock		9	12277	0.073	-4.496	20	15109	0.132	-5.535	-5.016
DMSO-Mock		0	15208	0.000	-2.527	39	16632	0.234	-4.684	-3.605
DMSO-Mock		6	17101	0.035	-2.521	22	16309	0.135	-4.706	-3.613
DMSO-Mock		6	15091	0.040	-2.520	1	15474	0.006	-4.734	-3.627
DMSO-Mock		7	14972	0.047	-2.519	2	16570	0.012	-4.733	-3.626
DMSO-Mock		1036	13721	7.550	-1.381	1	15076	0.007	-7.692	-4.537
DMSO-Mock		1121	13450	8.335	-0.964	1	15610	0.006	-7.693	-4.328
DMSO-Mock		1131	12664	8.931	-0.647	0	14503	0.000	-7.695	-4.171
DMSO-Mock		1274	13302	9.578	-0.303	6	15538	0.039	-7.680	-3.992
DMSO-Reo		2551	13648	18.691	-0.293	1528	5124	29.820	1.261	0.484
DMSO-Reo		1086	11366	9.555	-0.259	2891	14485	19.959	-0.591	-0.425
DMSO-Reo		1190	11782	10.100	-0.171	3214	14386	22.341	0.253	0.041
DMSO-Reo		1164	11845	9.827	-0.110	3093	14903	20.754	-0.362	-0.236
DMSO-Reo		1064	11042	9.636	-0.083	3319	15035	22.075	0.211	0.064
DMSO-Reo		2671	13829	19.314	-0.017	1347	4411	30.537	1.506	0.745
DMSO-Reo		2128	14603	14.572	0.051	3447	15907	21.670	0.090	0.071
DMSO-Reo		2679	13721	19.525	0.076	1549	4856	31.899	1.973	1.025
DMSO-Reo		2072	14047	14.750	0.083	3352	15730	21.310	0.010	0.047
DMSO-Reo		2560	13207	19.384	0.146	3440	12393	27.758	0.151	0.148
DMSO-Reo		2335	11861	19.686	0.148	1197	3513	34.073	2.718	1.433
DMSO-Reo		2255	14693	15.347	0.189	3267	15721	20.781	-0.108	0.041
DMSO-Reo		2626	13964	18.805	0.190	3160	11272	28.034	0.156	0.173
DMSO-Reo		1203	11446	10.510	0.264	3000	14496	20.695	-0.379	-0.057
DMSO-Reo		1410	13192	10.688	0.288	3241	14916	21.728	0.438	0.363
DMSO-Reo		2522	12692	19.871	0.302	3437	12429	27.653	0.120	0.211
DMSO-Reo		2717	14094	19.278	0.342	3149	11303	27.860	0.115	0.228
DMSO-Reo		2662	13294	20.024	0.352	3486	12844	27.141	-0.034	0.159
DMSO-Reo		1234	11634	10.607	0.365	3283	15204	21.593	0.085	0.225
DMSO-Reo		1450	13288	10.912	0.407	3134	15037	20.842	0.106	0.256
DMSO-Reo		2348	13800	17.014	0.484	3373	15521	21.732	0.104	0.294
DMSO-Reo		2752	13839	19.886	0.538	3472	12784	27.159	-0.053	0.242
DMSO-Reo		1286	11623	11.064	0.576	3370	15274	22.064	0.208	0.392
DMSO-Reo		1329	11760	11.301	0.581	3067	14438	21.243	-0.134	0.223
DMSO-Reo		2525	12041	20.970	0.656	3396	11444	29.675	0.727	0.692
DMSO-Reo		1347	11741	11.473	0.688	3210	14540	22.077	0.160	0.424
DMSO-Reo		1538	13144	11.701	0.826	3100	14507	21.369	0.304	0.565
DMSO-Reo		1297	10700	12.121	1.064	3266	14369	22.729	0.383	0.723
DMSO-Reo		970	7946	12.207	1.194	2771	13438	20.621	-0.400	0.397

DMSO-Reo		2769	14439	19.177	1.274	2408	12087	19.922	-0.077	0.599
DMSO-Reo		1300	10461	12.427	1.286	3058	13811	22.142	0.183	0.734
DMSO-Reo		2946	15289	19.269	1.304	2313	11475	20.157	0.003	0.653
DMSO-Reo		1552	12136	12.788	1.404	3075	14107	21.798	0.464	0.934
DMSO-Reo		2972	14981	19.838	1.488	1967	10260	19.172	-0.333	0.578
DMSO-Reo		2818	13985	20.150	1.589	2336	10694	21.844	0.578	1.084
DMSO-Reo		2971	12775	23.256	1.623	3171	11619	27.292	-0.021	0.801
Docetaxel	46386672	465	7167	6.488	-1.536	1410	8316	16.955	-1.129	-1.333
Dofetilide	46386638	3268	17241	18.955	0.008	4437	16465	26.948	-0.092	-0.042
Dolasetron mesylate	46386881	3156	14551	21.689	1.119	3836	12928	29.672	0.548	0.834
Donepezil hydrochloride	46386644	4129	17065	24.196	2.145	4841	15139	31.977	1.999	2.072
Dopamine hydrochloride	104170043	3037	16398	18.521	0.099	3950	14911	26.491	-0.213	-0.057
Doxapram hydrochloride	46386821	1047	11320	9.249	-0.262	3156	14297	22.075	0.211	-0.025
Doxazosin	104170183	2074	16775	12.364	1.280	4603	17542	26.240	1.218	1.249
Doxepin hydrochloride	104169945	1546	14684	10.528	0.097	3963	17255	22.967	0.474	0.285
Doxorubicin hydrochloride	46386781	3010	5071	59.357	7.976	3707	7131	51.984	6.842	7.409
Doxycycline	104170107	1062	11505	9.231	-0.437	3107	14709	21.123	-0.255	-0.346
Doxylamine succinate	46386900	1244	14065	8.845	-0.448	3602	16522	21.801	0.140	-0.154
Droperidol	46386863	4336	16945	25.589	2.762	5156	16909	30.493	1.491	2.127
Duloxetine hydrochloride	46386541	2284	14329	15.940	0.293	3588	15504	23.142	0.418	0.356
DuP 697	46387010	2447	16521	14.811	0.094	3563	16797	21.212	-0.012	0.041
Duvadilan	104170012	1550	14926	10.385	0.126	3651	16325	22.364	0.676	0.401
E-4031 dihydrochloride	46387000	3461	16889	20.493	0.505	4268	16364	26.082	-0.020	0.243
E64d-Mock		0	15020	0.000	-8.572	2	14130	0.014	-8.950	-8.761
E64d-Mock		0	13528	0.000	-8.572	1	13381	0.007	-8.952	-8.762
E64d-Mock		0	14666	0.000	-8.572	1	14037	0.007	-8.952	-8.762
E64d-Mock		3	14561	0.021	-8.563	1	13998	0.007	-8.952	-8.757
E64d-Mock		0	12895	0.000	-6.496	6	15722	0.038	-7.614	-7.055
E64d-Mock		0	12257	0.000	-6.496	1	15543	0.006	-7.625	-7.060
E64d-Mock		0	11144	0.000	-6.496	0	14656	0.000	-7.627	-7.061
E64d-Mock		2	12065	0.017	-6.485	8	15582	0.051	-7.609	-7.047
E64d-Mock		0	14540	0.000	-6.093	4	14122	0.028	-8.173	-7.133
E64d-Mock		1	14636	0.007	-6.091	1	14209	0.007	-8.180	-7.135
E64d-Mock		2	13244	0.015	-6.088	0	12847	0.000	-8.182	-7.135
E64d-Mock		8	14473	0.055	-6.075	1	13770	0.007	-8.180	-7.127
E64d-Mock		0	14313	0.000	-5.864	2	12547	0.016	-6.550	-6.207
E64d-Mock		0	15025	0.000	-5.864	1	14386	0.007	-6.552	-6.208
E64d-Mock		0	14877	0.000	-5.864	0	12886	0.000	-6.553	-6.209
E64d-Mock		5	14651	0.034	-5.853	2	14406	0.014	-6.550	-6.202
E64d-Mock		0	11069	0.000	-5.495	1	15430	0.006	-6.336	-5.916
E64d-Mock		1	3239	0.031	-5.478	4	15431	0.026	-6.331	-5.904
E64d-Mock		4	9894	0.040	-5.473	0	15555	0.000	-6.338	-5.905
E64d-Mock		0	13251	0.000	-5.396	18	15849	0.114	-7.652	-6.524
E64d-Mock		0	13806	0.000	-5.396	9	16080	0.056	-7.674	-6.535
E64d-Mock		2	13007	0.015	-5.388	21	15574	0.135	-7.644	-6.516
E64d-Mock		10	12278	0.081	-5.353	3	14986	0.020	-7.687	-6.520
E64d-Mock		7	2484	0.282	-5.341	13	14292	0.091	-6.312	-5.826
E64d-Mock		0	15531	0.000	-4.930	14	14181	0.099	-6.835	-5.883
E64d-Mock		0	15245	0.000	-4.930	3	14869	0.020	-6.862	-5.896
E64d-Mock		0	14240	0.000	-4.930	0	13036	0.000	-6.869	-5.900
E64d-Mock		0	15319	0.000	-4.930	0	13576	0.000	-6.869	-5.900
E64d-Mock		0	11436	0.000	-4.530	4	15630	0.026	-5.563	-5.046
E64d-Mock		0	11613	0.000	-4.530	1	14839	0.007	-5.568	-5.049
E64d-Mock		1	12031	0.008	-4.526	2	15530	0.013	-5.566	-5.046
E64d-Mock		3	12040	0.025	-4.518	5	15360	0.033	-5.561	-5.040
E64d-Mock		2	14244	0.014	-2.525	15	16449	0.091	-4.716	-3.620
E64d-Mock		16	15244	0.105	-2.509	4	16899	0.024	-4.731	-3.620
E64d-Mock		24	14668	0.164	-2.498	26	16605	0.157	-4.701	-3.600
E64d-Mock		43	14588	0.295	-2.475	17	16933	0.100	-4.713	-3.594
E64d-Reo		19	13616	0.140	-8.510	41	5058	0.811	-8.677	-8.593
E64d-Reo		19	12552	0.151	-8.505	57	11638	0.490	-8.787	-8.646
E64d-Reo		37	12824	0.289	-8.444	29	4037	0.718	-8.708	-8.576
E64d-Reo		40	13350	0.300	-8.439	27	4413	0.612	-8.745	-8.592
E64d-Reo		0	11704	0.000	-6.496	27	14853	0.182	-7.563	-7.029
E64d-Reo		1	12067	0.008	-6.490	13	14459	0.090	-7.595	-7.043
E64d-Reo		5	12085	0.041	-6.470	20	14634	0.137	-7.579	-7.024
E64d-Reo		7	10207	0.069	-6.453	12	13824	0.087	-7.596	-7.025
E64d-Reo		14	13193	0.106	-6.059	59	13027	0.453	-8.046	-7.052
E64d-Reo		16	12506	0.128	-6.052	44	11593	0.380	-8.068	-7.060
E64d-Reo		20	12613	0.159	-6.042	31	12637	0.245	-8.108	-7.075
E64d-Reo		39	13159	0.296	-5.998	26	12956	0.201	-8.122	-7.060
E64d-Reo		10	13968	0.072	-5.841	23	12055	0.191	-6.508	-6.174
E64d-Reo		13	13819	0.094	-5.834	35	11627	0.301	-6.481	-6.158
E64d-Reo		15	13976	0.107	-5.830	23	11353	0.203	-6.505	-6.167
E64d-Reo		16	13404	0.119	-5.826	23	10884	0.211	-6.503	-6.164
E64d-Reo		0	10146	0.000	-5.495	23	14739	0.156	-6.293	-5.894
E64d-Reo		1	10139	0.010	-5.490	50	15005	0.333	-6.242	-5.866
E64d-Reo		2	9602	0.021	-5.484	16	15010	0.107	-6.307	-5.895
E64d-Reo		4	3424	0.117	-5.431	17	13892	0.122	-6.303	-5.867
E64d-Reo		0	13058	0.000	-5.396	23	15637	0.147	-7.640	-6.518
E64d-Reo		1	13256	0.008	-5.392	40	15159	0.264	-7.596	-6.494
E64d-Reo		1	12725	0.008	-5.392	9	15414	0.058	-7.673	-6.532
E64d-Reo		3	11514	0.026	-5.382	10	14164	0.071	-7.669	-6.525
E64d-Reo		11	14213	0.077	-4.905	19	10055	0.189	-6.805	-5.855
E64d-Reo		16	14977	0.107	-4.896	30	10870	0.276	-6.775	-5.835
E64d-Reo		17	14771	0.115	-4.893	20	9896	0.202	-6.800	-5.847



E64d-Reo		19	14741	0.129	-4.889	7	10461	0.067	-6.846	-5.867
E64d-Reo		1	11072	0.009	-4.526	27	15862	0.170	-5.525	-5.025
E64d-Reo		3	10351	0.029	-4.516	20	15151	0.132	-5.535	-5.026
E64d-Reo		10	11305	0.088	-4.489	39	16008	0.244	-5.506	-4.997
E64d-Reo		11	10907	0.101	-4.483	29	15819	0.183	-5.522	-5.002
E64d-Reo		7	14046	0.050	-2.519	24	16201	0.148	-4.703	-3.611
E64d-Reo		11	14437	0.076	-2.514	25	16099	0.155	-4.701	-3.608
E64d-Reo		14	14045	0.100	-2.510	21	16649	0.126	-4.708	-3.609
E64d-Reo		19	13687	0.139	-2.503	62	15391	0.403	-4.646	-3.574
Ebselen	46386980	810	11024	7.348	-1.139	3171	14917	21.258	-0.003	-0.571
Econazole nitrate	104170005	1778	16427	10.824	0.360	3805	17202	22.120	0.585	0.472
Edrophonium chloride	104170059	1409	14948	9.426	-0.180	3543	17431	20.326	-0.247	-0.213
Efavirenz	46386724	2482	16656	14.902	0.110	4212	16279	25.874	1.027	0.568
Enalapril maleate	104170123	1707	15881	10.749	0.235	3811	17452	21.837	0.075	0.155
Enalaprilat	46386741	2668	14384	18.548	0.108	3260	12213	26.693	-0.165	-0.029
Enrofloxacin	46386889	1266	11271	11.232	0.538	3104	13783	22.520	0.316	0.427
Epigallocatechin gallate	46386901	2362	13233	17.849	-0.666	3334	13124	25.404	-0.252	-0.459
Epirubicin hydrochloride	46386577	1455	4466	32.579	3.238	1978	6524	30.319	2.017	2.627
Eryped	104170095	1417	15546	9.115	-0.500	3753	17997	20.853	-0.333	-0.417
Escitalopram oxalate	46386725	2310	16807	13.744	-0.095	3766	17605	21.392	0.028	-0.033
Esmolol hydrochloride	46386551	2214	16325	13.562	-0.127	3468	16791	20.654	-0.136	-0.132
Esomeprazole magnesium	46386556	3664	17230	21.265	0.847	4711	17136	27.492	0.463	0.655
Estradiol valerate	104170058	3384	17807	19.004	0.254	4108	16173	25.400	-0.474	-0.110
Estrone 3-sulfate sodium salt	46386974	982	11179	8.784	-0.476	3070	15209	20.185	-0.284	-0.380
Eszopiclone	104170161	1230	11891	10.344	-0.019	3045	14489	21.016	-0.214	-0.116
Ethacrynic acid	104169948	1499	14710	10.190	0.173	3444	17222	19.998	-0.333	-0.080
Ethambutol	104170193	1677	16446	10.197	0.026	3566	17437	20.451	-0.040	-0.007
Ethionamide	104170006	1485	14825	10.017	-0.006	3826	16627	23.011	0.288	0.141
Ethylestrenol	46386573	1986	14191	13.995	-0.402	2309	12208	18.914	-0.421	-0.412
Ethinylestradiol	46386858	1171	14199	8.247	-0.724	3459	17165	20.151	-0.292	-0.508
Etodolac	104170216	1563	16286	9.597	-0.293	3439	17880	19.234	-0.496	-0.394
Etomidate	46386983	3082	15750	19.568	0.205	4229	15619	27.076	-0.053	0.076
Etomoxir	46386895	2941	15326	19.190	0.083	4161	14857	28.007	0.226	0.155
Etoposide	46386954	1703	9973	17.076	3.350	3478	11627	29.913	2.264	2.807
Exemestane	46386592	2393	16788	14.254	-0.318	3092	15021	20.585	0.149	-0.085
Ezetimibe	46386640	3137	16938	18.520	1.062	3069	14304	21.456	0.446	0.754
Famciclovir	46386745	2733	14827	18.433	-0.160	4242	15917	26.651	-0.181	-0.171
Famotidine	46386903	2802	14034	19.966	0.272	3316	13098	25.317	-0.282	-0.005
Felbamate	46386855	1428	14328	9.966	0.070	3544	16263	21.792	0.137	0.103
Felodipine	104170219	1343	12962	10.361	0.183	3708	17397	21.314	-0.200	-0.009
Fenofibrate	104169950	2158	15796	13.662	1.869	4542	16825	26.996	2.410	2.139
Fenoldopam mesylate	46386722	2283	16237	14.060	-0.039	3845	17450	22.034	0.172	0.066
Fenpiverinium bromide	46386658	2361	16907	13.965	-0.412	3142	15674	20.046	-0.035	-0.223
Fexofenadine hydrochloride	104170222	1463	13377	10.937	0.498	3809	15818	24.080	0.596	0.547
Finasteride	46386559	2914	16543	17.615	0.769	2869	14408	19.913	-0.080	0.344
Flecainide hydrochloride		3968	16962	23.393	1.790	4902	17170	28.550	0.825	1.308
Floxuridine	104170121	845	10139	8.334	-0.964	2319	11744	19.746	-0.304	-0.634
Flubendazole	46386742	492	6799	7.236	-3.534	1079	5714	18.883	-2.034	-2.784
Fluconazole	104170148	3150	17352	18.154	-0.020	4205	15356	27.383	0.001	-0.010
Flucytosine	46386766	1675	16534	10.131	-0.009	3390	16457	20.599	0.015	0.003
Fludarabine	104170131	1382	12438	11.111	0.594	3314	14001	23.670	0.478	0.536
Flumadine hydrochloride	104170172	2015	16454	12.246	1.116	4141	17269	23.979	1.281	1.198
Flumazenil	46386776	1304	13579	9.603	-0.098	3610	17269	20.905	-0.095	-0.097
Flunisolide	104170214	1386	15621	8.873	-0.633	3619	17420	20.775	-0.356	-0.494
Fluocinolonide acetone	104170060	2784	12011	23.179	1.598	4028	11561	34.841	1.786	1.692
Fluocinolonide acetone 21-acetate	104170119	1955	14055	13.910	2.001	3802	15636	24.316	1.407	1.704
Fluorometholone	104170223	1376	11690	11.771	0.955	3713	14544	25.529	1.013	0.984
Fluoxetine hydrochloride	104170213	1593	13765	11.573	0.847	4366	16390	26.638	1.333	1.090
Fluprelapine	46386904	2315	17112	13.529	-0.133	3680	17669	20.827	-0.097	-0.115
Fluphenazine dihydrochloride	46386937	1094	14435	7.579	-1.032	2960	17184	17.225	-1.059	-1.046
Flurbiprofen	46386788	2543	17308	14.693	-0.177	3101	15382	20.160	0.004	-0.086
Flutamide	104169949	3197	17958	17.803	-0.133	3812	14003	27.223	-0.038	-0.085
Fluticasone propionate	46386601	2273	12537	18.130	0.681	3563	14569	24.456	0.711	0.696
Fluvastatin	104170157	1507	9966	15.121	2.448	3829	12054	31.765	2.749	2.599
Fluxoxamine maleate	46386804	2405	16566	14.518	0.042	3839	16831	22.809	0.344	0.193
Folic acid	104169953	1503	12411	12.110	1.141	3962	17719	22.360	0.101	0.621
Formoterol fumarate dihydrate	46386732	2300	16625	13.835	-0.079	3431	17180	19.971	-0.288	-0.184
Furosemide	104169951	1515	14592	10.382	0.194	4020	17837	22.537	0.152	0.173
Gabexate mesilate	46386710	1302	14447	9.012	-0.371	3679	16708	22.019	0.197	-0.087
Galanthamine hydrobromide	46386805	3318	17455	19.009	-0.152	4322	16979	25.455	-0.235	-0.193
Ganciclovir	104170145	2976	16482	18.056	-0.051	3716	13930	26.676	-0.169	-0.110
Gatifloxacin	104170200	1402	14916	9.399	-0.344	3584	16724	21.430	-0.167	-0.256
Gemfibrozil	104170063	2952	17274	17.089	-0.362	3951	14987	26.363	-0.244	-0.303
Glimepiride	46386690	3503	17841	19.635	0.125	4556	17784	25.619	-0.179	-0.027
Glipizide	104170062	1569	14993	10.465	0.169	3298	17005	19.394	-0.436	-0.133
Glyburide	104170064	3199	16756	19.092	0.282	3881	14235	27.264	-0.028	0.127
Glycopyrronium bromide	46386646	3024	16125	18.753	-0.057	4127	14872	27.750	0.149	0.046
Goserelin acetate		2381	13503	17.633	-0.761	3623	13699	26.447	0.105	-0.328
GR 79236	46387015	1418	14439	9.821	-0.346	3540	16883	20.968	-0.231	-0.289
GR 89696 fumarate	46386996	3147	16489	19.085	0.050	4416	15588	28.329	0.323	0.186
Granisetron hydrochloride	46386545	2521	16332	15.436	0.204	3864	16647	23.211	0.434	0.319
Griseofulvin	104170114	1557	15416	10.100	-0.025	3432	17196	19.958	-0.224	-0.125
Halometasone monohydrate	46386633	1210	9648	12.541	1.258	3721	14437	25.774	1.180	1.219
Haloperidol hydrochloride	46386806	3242	17055	19.009	0.836	4869	16880	28.845	1.688	1.262
Hexachlorophene	104170010	668	11131	6.001	-2.207	2303	14676	15.692	-1.819	-2.013
Hexamethylenesacetamide	46386869	2131	15158	14.059	-0.040	3439	15721	21.875	0.136	0.048

Homoharringtonine	46386877	4	5267	0.076	-5.840	13	6000	0.217	-6.502	-6.171
Homoveratrylamine	46386943	3201	16609	19.273	0.110	4452	16124	27.611	0.107	0.109
Honokiol	46386673	3240	17356	18.668	-0.085	4443	16666	26.659	-0.179	-0.132
HMT dimaleate	46386998	2404	15066	15.956	0.232	2954	12892	22.913	0.943	0.588
Huperzine A	46386885	3457	18159	19.037	-0.139	4394	17531	25.064	-0.369	-0.254
Hydrochlorothiazide	104170008	1664	15816	10.521	0.270	3950	17170	23.005	0.287	0.278
Hydrocortisone	104169954	1339	10992	12.182	1.180	3490	14090	24.769	0.795	0.987
Hydrocortisone 17-valerate	104170102	3105	14507	21.403	1.027	4462	13993	31.887	1.079	1.053
Hydrocortisone hemisuccinate	104170065	2546	13105	19.428	0.391	3749	11789	31.801	1.058	0.724
Hydroflumethiazide	104169994	1838	15674	11.726	0.840	3573	15553	22.973	0.904	0.872
Hydroxyzine pamoate	104170009	1458	15656	9.313	-0.392	3730	17262	21.608	-0.116	-0.254
Hyperoside	46386811	2219	16143	13.746	-0.095	3619	17417	20.779	-0.108	-0.101
Ibuprofen	104169956	1211	12140	9.975	0.074	3315	14863	22.304	0.271	0.172
Icariin	46386578	3021	16847	17.932	0.871	3188	15364	20.750	0.205	0.538
Idarubicin hydrochloride	46386733	1299	7517	17.281	-0.531	2016	6905	29.196	0.583	0.026
Idebenone	46386682	1089	11578	9.406	-0.606	3069	14031	21.873	0.088	-0.259
Ifenprodil hemitartrate	46386807	3527	17496	20.159	1.592	3985	15278	26.083	2.023	1.808
Imatinib mesylate	46386639	1367	16866	8.105	-1.093	1943	16939	11.471	-2.181	-1.637
Imipramine hydrochloride	104170068	1318	13157	10.017	-0.069	3159	15273	20.684	0.047	-0.011
Indapamide	104170066	1266	12595	10.052	-0.051	3207	15264	21.010	0.169	0.059
Indatraline hydrochloride	46386808	2606	14520	17.948	0.649	4100	15160	27.045	1.288	0.968
Indinavir sulfate	46386606	1991	15283	13.028	-0.222	3285	15502	21.191	-0.016	-0.119
Indirubin	46386581	4016	17120	23.458	1.819	4837	16452	29.401	1.117	1.468
Indomethacin hydrate	46386809	1190	11144	10.678	0.191	3126	14965	20.889	-0.259	-0.034
Ipidacrine	46386925	3067	17058	17.980	-0.306	4206	15986	26.311	-0.283	-0.295
Ipratropium bromide	104170067	1427	14791	9.648	-0.208	3695	17250	21.420	-0.170	-0.189
Ipriflavone	46386694	1729	16681	10.365	0.116	3512	17331	20.264	-0.110	0.003
Irbesartan	46386566	2971	15576	19.074	0.046	4090	14987	27.290	0.011	0.029
Irinotecan hydrochloride	46386616	2455	12612	19.466	0.917	3802	13669	27.815	1.459	1.188
Irsogladine maleate	46386698	2734	16128	16.952	-0.637	4139	15342	26.978	-0.083	-0.360
Isoniazid	104170011	1401	15084	9.288	-0.457	3400	16541	20.555	-0.001	-0.229
Isoproterenol hydrochloride	104170013	1458	15345	9.501	-0.546	3665	16779	21.843	0.077	-0.234
Isoquercitrin	46386780	2462	17543	14.034	-0.390	3195	15681	20.375	0.077	-0.156
Isotretinoin	104170133	3003	16374	18.340	0.040	4090	14612	27.991	0.146	0.093
Isradipine	46386602	2810	16563	16.966	-0.633	4187	16092	26.019	-0.371	-0.502
Itavastatin calcium	46386827	3368	14431	23.339	1.766	4277	13469	31.754	1.923	1.844
Itopride hydrochloride	46386560	1919	14417	13.311	-0.172	3654	14620	24.993	0.831	0.329
Itraconazole	46386736	1620	16098	10.063	-2.854	3138	14302	21.941	-1.595	-2.224
Ketoconazole	46386810	3113	17103	18.201	-0.235	4578	16045	28.532	0.384	0.074
Ketoprofen	104169957	1620	15763	10.277	-0.060	3798	17480	21.728	0.037	-0.012
Ketorolac tromethamine	46386614	3361	17163	19.583	1.406	2943	15545	18.932	-0.415	0.496
Ketotifen fumarate	46386834	2491	13461	18.505	-0.375	3478	13145	26.459	0.109	-0.133
Kitasamycin	46386711	964	12174	7.919	-1.185	3038	14682	20.692	0.050	-0.568
L-694,247	46386999	3187	16932	18.822	-0.035	4699	16121	29.148	0.569	0.267
L-NMMA acetate	46386919	2105	14288	14.733	0.080	3395	16221	20.930	-0.074	0.003
L-Thyroxine	104169983	1335	14340	9.310	-0.666	3871	16941	22.850	0.433	-0.117
Labetalol hydrochloride	104170069	1732	16631	10.414	0.212	4254	18003	23.629	0.466	0.339
Lacidipine	46386664	2424	16867	14.371	-1.468	3620	15853	22.835	-1.327	-1.397
Lamivudine	46386600	2283	16380	13.938	-0.061	3448	17043	20.231	-0.230	-0.145
Lamotrigine	46386680	2936	16510	17.783	-0.369	3966	15381	25.785	-0.441	-0.405
Lansoprazole	46386562	2341	16049	14.587	0.054	3913	16039	24.397	0.698	0.376
Latanoprost	46386728	2911	17585	16.554	0.426	3097	15675	19.758	-0.133	0.146
Letrozole	46386665	1358	14055	9.662	-0.071	3647	17537	20.796	-0.124	-0.097
Levetiracetam	46386557	2587	17536	14.753	-0.157	3087	15809	19.527	-0.212	-0.185
Levocetirizine	46386593	3310	16928	19.553	0.200	4382	16426	26.677	-0.173	0.014
Levofloxacin	46386771	1318	13809	9.544	-0.125	3684	17428	21.138	-0.034	-0.080
Levonorgestrel	46386677	1580	15844	9.972	-0.251	3432	16645	20.619	-0.354	-0.303
Levosulpiride	46386685	1758	16346	10.755	0.239	3463	15864	21.829	0.073	0.156
Lidocaine	46386868	3657	17618	20.577	0.622	4461	17571	25.388	-0.257	0.182
Lincomycin hydrochloride	104170115	1624	16229	10.007	-0.075	3508	17724	19.792	-0.287	-0.181
Linezolid	46386641	3303	14991	22.033	2.198	2957	12619	23.433	1.120	1.659
Linopirdine dihydrochloride	46386985	2069	16675	12.408	-0.916	2956	15692	18.838	-0.447	-0.681
Lobeline hydrochloride	46386920	1807	14748	12.253	1.124	4381	17043	25.706	1.162	1.143
Lofepramine	46386649	3187	17699	18.007	0.896	2705	15013	18.018	-0.726	0.085
Lofexidine hydrochloride	46386875	3059	16085	19.018	0.028	4271	15272	27.966	0.214	0.121
Lomerizine dihydrochloride	46386707	1015	14579	9.962	-1.317	3289	17537	18.755	-0.658	-0.988
Lomifylline	46386754	1827	15950	11.455	0.677	3563	17066	20.878	-0.263	0.207
Loperamide hydrochloride	104170070	2	14905	0.013	-5.488	26	18123	0.143	-6.297	-5.892
Loratadine	46386837	2030	16719	12.142	-0.379	3573	17392	20.544	-0.160	-0.270
Lorazepam	46386878	2252	13012	17.307	-0.906	3480	12937	26.900	0.260	-0.323
Losartan potassium	46386652	2108	14843	14.202	-0.014	3156	15622	20.202	-0.236	-0.125
Loteprednol etabonate	46386647	1328	11144	11.917	0.970	3518	13599	25.870	1.205	1.087
Lovastatin	104170211	1645	12430	13.234	1.757	4152	13597	30.536	2.455	2.106
Loxapine succinate	46386931	1555	14211	10.942	0.356	3677	16336	22.509	0.312	0.334
Loxoprofen sodium	46386612	2312	16496	14.016	-0.047	3643	17449	20.878	-0.086	-0.067
LY 171883	46386838	2692	14115	19.072	0.276	3472	12359	28.093	0.170	0.223
Mafenide acetate	104170207	1738	15802	10.999	0.532	4153	18276	22.724	0.206	0.369
Maltol	46386945	3214	17058	18.842	-0.029	4408	16529	26.668	-0.176	-0.102
Maprotiline hydrochloride	46386839	2745	16836	16.304	0.358	4048	17362	23.315	0.457	0.407
MDL 73005EF hydrochloride	46387017	1865	15845	11.770	0.874	3990	16748	23.824	0.776	0.825
Mebendazole	104170137	547	5683	9.625	-2.765	988	4952	19.952	-1.778	-2.272
Mecillinam	46386744	1250	14049	8.897	-0.424	3844	17431	22.053	0.205	-0.109
Mecizine hydrochloride	104170138	3109	17619	17.646	-0.183	3906	15762	24.781	-0.622	-0.403
Meclofenamic acid sodium salt	104170147	3175	17752	17.885	-0.106	4181	15751	26.544	-0.200	-0.153
Medroxyprogesterone	46387018	2611	15918	16.403	0.377	3418	14982	22.814	0.909	0.643
Medroxyprogesterone 17-acetate	104170072	1753	14937	11.736	0.936	4507	17456	25.819	1.097	1.016

Medryson	104170097	1651	13688	12.062	1.114	4070	16558	24.580	0.740	0.927
Mefenamic acid	104170015	3235	17715	18.261	0.015	3981	13921	28.597	0.291	0.153
Mefloquine hydrochloride	104170120	3535	16701	21.166	0.950	5403	14731	36.678	2.225	1.588
Megestrol acetate	46386702	2901	15277	18.989	0.019	4088	15020	27.217	-0.011	0.004
Meloxicam	104170196	800	9147	8.746	-0.702	3156	14630	21.572	-0.126	-0.414
Memantine hydrochloride	104170178	3512	17820	19.708	0.481	4374	14943	29.271	0.452	0.467
Mepenzolate bromide	104170016	2801	16437	17.041	-0.378	4068	15145	26.860	-0.125	-0.251
Mepirizole	46386965	2558	12914	19.808	0.282	3465	12506	27.707	0.136	0.209
Mepivacaine hydrochloride	46386949	1650	16543	9.974	-0.092	3608	17548	20.561	0.001	-0.046
Mercaptopurine	104170111	362	13660	2.650	-3.987	1619	15940	10.157	-3.893	-3.940
Meropenem	46386666	2387	13278	17.977	-0.307	3333	12198	27.324	0.021	-0.143
Mesalazine	46386870	1314	12644	10.392	0.130	3233	15678	20.621	0.024	0.077
Mesna	104170146	1632	15438	10.571	0.124	3769	17093	22.050	0.151	0.137
Mesoridazine besylate	46386921	1046	12788	8.180	-1.046	3178	15379	20.665	0.040	-0.503
Mestanolone	46386759	2276	14641	15.545	0.099	2810	13458	20.880	0.249	0.174
Mestranol	46386940	678	13750	4.931	-2.254	2697	17223	15.659	-1.469	-1.862
Metaproterenol	104170149	3031	16220	18.687	0.152	3788	13501	28.057	0.162	0.157
Methazolamide	104170116	1007	10841	9.289	-0.405	3205	14456	22.171	0.046	-0.179
Methimazole	104170134	3276	18019	18.181	-0.011	4141	15570	26.596	-0.188	-0.099
Methocarbamol	104170007	1488	15297	9.727	-0.165	3898	17295	22.538	0.152	-0.006
Methotrexate trihydrate	46386835	1717	15835	10.843	0.294	3546	16870	21.020	-0.213	0.040
Methoxsalen	104170150	2978	16876	17.646	-0.183	3827	14673	26.082	-0.311	-0.247
Methylandrostenediol	46386580	2850	12857	22.167	1.041	3678	12005	30.637	1.016	1.029
Methylidopa	104170018	2444	14023	17.429	-0.253	3633	13050	27.839	0.110	-0.072
Methylperone hydrochloride	46387011	1506	13979	10.773	0.442	3941	16251	24.251	0.781	0.611
Methylprednisolone	104170189	1682	13252	12.692	1.460	3898	14438	26.998	1.436	1.448
Methylprednisolone acetate	104170126	1811	13815	13.109	1.713	3907	15185	25.729	1.448	1.580
Methyltestosterone	46386739	3031	13313	22.767	1.235	4375	15898	27.519	0.080	0.657
Metoclopramide hydrochloride	104170017	3179	17557	18.107	-0.035	4622	16202	28.527	0.274	0.120
Metronidazole	46386860	3376	17546	19.241	-0.049	4364	16694	26.141	0.000	-0.025
Metryapone	104169960	1537	15152	10.144	0.064	3747	16949	22.107	0.028	0.046
Mevastatin	46386660	1474	10176	14.485	2.155	3831	12663	30.253	2.353	2.254
Mexiletine hydrochloride	104170180	1788	15440	11.580	0.762	3967	17583	22.562	0.750	0.756
Miconazole nitrate	104169959	1329	12525	10.611	0.246	3228	14514	22.241	0.630	0.438
Midazolam hydrochloride	46386603	1166	11293	10.325	0.235	3331	14944	22.290	0.268	0.251
Midodrine hydrochloride	104170071	1654	15407	10.735	0.388	3881	17777	21.832	-0.051	0.168
Miglitol	46386758	1683	16187	10.397	0.015	3936	17524	22.461	0.295	0.155
Milnacipran hydrochloride	46386905	2373	16331	14.531	0.044	3652	17181	21.256	-0.002	0.021
Milrinone	46386629	2558	17465	14.646	-0.192	2913	14905	19.544	-0.206	-0.199
Minocycline hydrochloride	104169958	1316	13110	10.038	0.006	3721	17005	21.882	-0.037	-0.016
Minoxidil	104170184	1498	14862	10.079	0.028	3932	17294	22.736	0.209	0.119
Mirtazapine	46386716	2168	14351	15.107	-0.043	2499	13117	19.052	-0.374	-0.208
Mitoxantrone hydrochloride	104170122	1519	7801	19.472	0.405	1473	7316	20.134	-1.735	-0.665
MK 886	46386984	2225	16686	13.335	-0.168	3545	17518	20.236	-0.229	-0.198
Moclobemide	46386631	1451	14112	10.282	0.215	3449	16498	20.906	-0.095	0.060
Modafinil	46386605	2922	13583	21.512	0.831	3457	12518	27.616	0.109	0.470
Molindone hydrochloride	104170156	2485	13657	18.196	-0.006	3705	12713	29.143	0.422	0.208
Montelukast sodium	46386714	3278	16347	20.053	0.361	4451	15627	28.483	0.369	0.365
Mosapride citrate	46386693	2441	16681	14.633	0.062	3659	16851	21.714	0.100	0.081
Moxifloxacin hydrochloride	46386670	2387	15091	15.817	0.272	3463	16103	21.505	0.054	0.163
Moxonidine hydrochloride	46386777	2092	15165	13.795	-0.086	3549	14895	23.827	0.571	0.242
Mupirocin	104170118	1230	12303	9.998	-0.080	3098	14713	21.056	0.187	0.053
Nabumetone	104170077	1711	15624	10.951	0.506	3813	17857	21.353	-0.189	0.158
Nadolol	104169962	1093	12526	8.726	-0.714	3539	17585	20.125	-0.543	-0.628
Nafadotride	46387001	2950	16965	17.389	0.550	4479	17769	25.207	0.878	0.714
Nafcillin sodium	104170104	1637	15770	10.380	0.004	3884	17309	22.439	0.288	0.146
Naftopidil	46386715	996	10819	9.206	-0.281	3309	15065	21.965	0.182	-0.050
Nalbuphine hydrochloride	46386933	3352	16951	19.775	0.187	4136	16276	25.412	-0.250	-0.031
Nalidixic acid	104169992	3257	17801	18.297	0.027	4096	15730	26.039	-0.321	-0.147
Naloxone hydrochloride	104170085	1379	14336	9.619	-0.473	3329	16673	19.966	-0.584	-0.528
Naltrexone hydrochloride	104170191	1573	16392	9.596	-0.293	3591	18256	19.670	-0.332	-0.313
Naltrindole hydrochloride hydrate	46386854	1887	13284	14.205	-2.280	3098	13194	23.480	-0.911	-1.596
Naphazoline hydrochloride	104170021	1552	14086	11.018	0.555	3902	16854	23.152	0.493	0.524
Naproxen sodium	46386948	2504	13207	18.960	0.009	3287	12189	26.967	-0.086	-0.038
Nateglinone	46386701	1765	16319	10.816	0.355	3462	16807	20.599	0.015	0.185
Nefazodone hydrochloride	46386669	2322	15117	15.360	0.191	3663	15362	23.845	0.575	0.383
Nelfinavir mesylate	46386712	2036	16117	12.633	-0.292	3297	17605	18.728	-0.565	-0.428
Nevirapine	46386569	2403	17356	13.845	-0.451	2678	12409	21.581	0.489	0.019
Nialamide	46386894	3320	17024	19.502	0.184	4245	16216	26.178	-0.323	-0.070
Nicardipine hydrochloride	104170076	949	10972	8.649	-0.755	3040	14564	20.873	-0.327	-0.541
Nicorandil	46386683	2717	15586	17.432	-0.482	4311	16079	26.811	-0.133	-0.308
Nicotinamide	46386893	1704	16231	10.498	0.078	3655	17408	20.996	-0.221	-0.072
Nicotine	104170075	895	10335	8.660	-0.750	2901	14876	19.501	-0.722	-0.736
Nicotinic acid	104170022	3113	17453	17.836	-0.122	4345	15782	27.531	0.036	-0.043
Nifedipine	46386790	3507	17467	20.078	0.321	4537	17746	25.566	-0.197	0.062
Nifekalant hydrochloride	46386697	1956	14403	13.581	-0.124	3278	15699	20.880	-0.085	-0.105
Nimetazepam	46386768	1400	14294	9.794	-0.010	3564	16891	21.100	-0.044	-0.027
Nimodipine	46386964	2398	14611	16.412	0.380	3062	12963	23.621	1.184	0.782
Nisoldipine	46386699	1099	10292	10.678	0.191	3201	13652	23.447	0.643	0.417
Nitazoxanide	46386689	1162	16086	7.224	-1.972	2814	16695	16.855	-1.682	-1.827
Nitrazepam	46386691	2520	13585	18.550	0.108	3560	12928	27.537	0.037	0.073
Nitrendipine	46386549	1097	13063	8.398	-0.654	3421	16311	20.974	-0.077	-0.366
Nitrofurantoin	104170019	3189	18074	17.644	-0.184	3982	15196	26.204	-0.282	-0.233
Nizatidine	46386765	3087	15604	19.783	0.274	4068	16131	25.219	-0.611	-0.168
Nobiletin	46386719	3907	15309	25.521	2.121	5503	14526	37.884	3.191	2.656
Norfloxacin	104169961	1591	15487	10.273	0.067	3431	16647	20.610	0.020	0.043

Nornicotine	46386896	2192	16608	13.198	-0.192	3567	17093	20.868	-0.088	-0.140
Nortriptyline hydrochloride	104170020	1231	14551	8.460	-0.626	3002	17635	17.023	-1.112	-0.869
Ofloxacin	104169964	1633	15865	10.293	0.145	3741	17590	21.268	-0.214	-0.034
Olanzapine	46386668	3271	16989	19.254	1.299	2913	14465	20.138	-0.003	0.648
Oligomycin A		3757	15432	24.346	2.212	6101	14923	40.883	5.050	3.631
Olmesartan medoxomil	46386651	3174	17601	18.033	0.904	3379	16568	20.395	0.084	0.494
Olopatadine hydrochloride	46386826	2175	14717	14.779	-0.149	2887	12864	22.442	0.782	0.317
Omeprazole	46386973	1295	13231	9.788	-0.013	3563	16519	21.569	0.079	0.033
Ondansetron	104170204	1905	12399	15.364	2.774	3981	14475	27.503	2.599	2.687
Orlistat	46386654	2079	17662	11.771	-1.122	2629	15259	17.229	-0.995	-1.059
Ormetoprim	46386708	1491	14448	10.320	-0.034	3849	16375	23.505	0.664	0.315
Ornidazole	46386947	3046	16179	18.827	-0.034	3983	14968	26.610	-0.193	-0.113
Orphenadrine hydrochloride	104169963	1558	15614	9.978	-0.027	4009	17421	23.012	0.289	0.131
Otezepad	46386986	2222	17083	13.007	-0.722	2887	15329	18.834	-0.448	-0.585
Oxacillin sodium	104170106	1079	11166	9.663	-0.200	3015	14690	20.524	-0.428	-0.314
Oxaprozin	46386783	1453	14267	10.184	0.170	3710	16752	22.147	0.230	0.200
Oxcarbazepine	46386767	2604	16942	15.370	0.043	3366	16383	20.546	0.136	0.089
Oxiconazole nitrate	46386704	2120	16329	12.983	1.634	4114	17076	24.092	0.871	1.252
Oxybutynin hydrochloride	104170078	950	10749	8.838	-0.652	3296	14965	22.025	0.004	-0.324
Oxymetholone	46386778	2604	14169	18.378	0.053	3143	11712	26.836	-0.131	-0.039
Oxyphenonium bromide	46386961	2325	16919	13.742	-0.096	3394	17348	19.564	-0.379	-0.237
Oxytetracycline hydrochloride	104170024	1497	15288	9.792	-0.189	3528	17357	20.326	-0.087	-0.138
Ozagrel hydrochloride	46386611	2084	14966	13.925	-0.063	3442	16273	21.152	-0.025	-0.044
P1075	46386997	2710	17582	15.413	0.057	3597	13836	25.997	1.994	1.025
Palonosetron hydrochloride	46386820	3454	13106	26.354	2.389	4329	11915	36.332	2.726	2.557
Pancuronium dibromide	46386853	2145	15812	13.566	-0.127	3535	17381	20.338	-0.206	-0.166
Pantoprazole sodium	46386609	2629	17593	14.943	-0.095	3220	15939	20.202	0.018	-0.039
Parecoxib sodium	46386785	2528	13729	18.414	-0.167	3220	11854	27.164	-0.027	-0.097
Paroxetine maleate	46386841	3473	14164	24.520	2.289	4472	13503	33.119	2.391	2.340
Pazufloxacin	46386755	3116	17247	18.067	-0.278	4340	16413	26.442	-0.244	-0.261
PD 81723	46386976	2989	15383	19.431	0.161	3931	14548	27.021	-0.070	0.045
Pefloxacin mesylate	46386589	2281	16844	13.542	-0.131	3642	17396	20.936	-0.073	-0.102
Pemolide	46386687	3384	17585	19.244	-0.048	4288	17515	24.482	-0.568	-0.308
Penciclovir	46386598	2215	16122	13.739	-0.096	3430	17252	19.882	-0.308	-0.202
Penicillin G potassium	104170081	1504	15172	9.913	-0.063	3932	17908	21.957	-0.015	-0.039
Penicillin V	104170199	1552	15104	10.275	0.136	3702	16969	21.816	-0.056	0.040
Pentoxifylline	46386861	2208	16236	13.599	-0.121	3602	17495	20.589	-0.150	-0.136
Pergolide mesylate	46386979	3319	17667	18.786	-0.047	4655	16289	28.578	0.397	0.175
Perospirone hydrochloride	46386671	2604	16405	15.873	0.282	4834	17151	28.185	1.541	0.912
Perphenazine	104169970	1055	15197	6.942	-1.704	2645	16662	15.874	-1.753	-1.729
Phenelzine sulfate	46386907	3451	15941	21.649	1.017	4143	15468	26.784	0.221	0.619
Phenothiazine	46386888	1134	10975	10.333	-0.026	3034	14137	21.461	-0.057	-0.041
Phenoxybenzamine hydrochloride	104170096	1596	15233	10.477	0.246	3768	17131	21.995	-0.004	0.121
Phenprobamate	46386753	1547	14819	10.439	0.041	3616	16843	21.469	-0.054	-0.007
Phentolamine mono-hydrochloride	104170130	1865	16458	11.332	0.630	3682	17287	21.299	0.278	0.454
Phylloquinone	104170094	1429	13002	10.991	0.448	3191	14727	21.668	0.415	0.432
Physostigmine hemisulfate	46386842	2271	16531	13.738	-0.096	3688	17537	21.030	-0.052	-0.074
Piceid	46386700	1090	11519	9.463	-0.571	3212	14860	21.615	-0.003	-0.287
Picrotin - Picrotoxinin	46386843	2324	17242	13.479	-0.569	3144	16076	19.557	-0.201	-0.385
Pidotimod	46386775	2951	16971	17.388	0.696	3041	15615	19.475	-0.229	0.233
Pilocarpine hydrochloride	46386789	3026	16634	18.192	-0.238	4383	16737	26.187	-0.320	-0.279
Pinacidil monohydrate	46387019	1383	14649	9.441	-0.173	3727	16977	21.953	0.179	0.003
Pindolol	104169965	1476	16390	9.005	-0.560	3651	17465	20.905	-0.318	-0.439
Pioglitazone hydrochloride	46386618	2438	15553	15.553	0.225	3424	15468	22.136	0.194	0.210
Piperacilin sodium	104169975	1693	16334	10.365	-0.006	3702	17114	21.631	0.003	-0.001
Pireperone	46386967	1645	14160	11.617	0.831	4142	16094	25.736	1.170	1.001
Piribedil hydrochloride	46386844	2441	16388	14.895	0.108	3423	16891	20.265	-0.222	-0.057
Piroxicam	46386918	1475	14744	10.004	0.087	3713	16839	22.050	0.205	0.146
Pizotiline maleate	46386908	1999	16024	12.475	-0.320	3105	16837	18.442	-0.629	-0.474
Podofilox	104170173	320	8761	3.653	-3.454	804	7388	10.883	-3.622	-3.538
Pralidoxime chloride	104170029	1621	15961	10.156	0.005	3546	17686	20.050	-0.190	-0.093
Pramipexole	46386856	2401	13318	18.028	-0.586	3433	12527	27.405	0.433	-0.077
Pravastatin sodium	46386713	3044	15724	19.359	0.138	4143	14664	28.253	0.300	0.219
Praziquantel	104169966	3130	17786	17.598	-0.198	4048	15347	26.376	-0.240	-0.219
Prazosin hydrochloride hydrate	46386845	3629	16094	22.549	1.416	4540	15725	28.871	0.936	1.176
Prednisolone	104169971	1662	13821	12.025	1.094	3835	14856	25.814	1.096	1.095
Prednisolone acetate	104169968	3297	15429	21.369	1.016	4083	13372	30.534	0.755	0.885
Prednisolone sodium succinate	46386971	2927	13113	22.321	1.322	3615	11535	31.339	0.947	1.135
Prednisone	104169973	1758	16554	10.620	0.324	4033	17689	22.799	0.227	0.276
Prilocaine hydrochloride	104169972	1673	15884	10.533	0.277	3951	17328	22.801	0.228	0.252
Primaquine diphosphate	104170105	2640	16035	16.464	-0.564	3702	15673	23.620	-0.900	-0.732
Primidone	104170030	1703	16729	10.180	0.017	3647	17734	20.565	0.003	0.010
Priscoline hydrochloride	104170110	1021	10455	9.766	-0.144	3263	14392	22.672	0.191	0.023
Probencid	104170028	1796	16240	11.059	0.565	3519	16280	21.615	-0.114	0.226
Procanamide hydrochloride	104170033	2885	13376	21.568	1.080	3456	12776	27.051	-0.079	0.500
Procaine hydrochloride	104170025	1712	15274	11.209	0.564	3722	16703	22.283	0.646	0.605
Procabazine hydrochloride	46386582	3363	16957	19.833	0.213	4485	17121	26.196	0.019	0.116
Prochlorperazine maleate	46386924	1940	16467	11.781	-0.443	3026	17183	17.610	-0.814	-0.628
Procyclidine hydrochloride	104170083	1732	16626	10.417	0.213	4199	17681	23.749	0.501	0.357
Procyteine	46386866	1520	14734	10.316	0.231	3593	16817	21.365	0.025	0.128
Progesterone	46386909	2417	16312	14.817	0.095	3619	16449	22.001	0.164	0.129
Promethazine hydrochloride	104169969	1178	14176	8.310	-0.942	3344	16771	19.939	-0.596	-0.769
Propafenone	104170080	1517	15143	10.018	-0.006	4012	17509	22.914	0.260	0.127
Propantheline bromide	104170027	1582	15486	10.216	0.036	3682	17648	20.864	0.114	0.075
Propofol	104169947	1830	15100	12.119	1.093	3959	16763	23.617	0.703	0.898
Propranolol hydrochloride	104170185	1855	14514	12.781	1.507	4212	16599	25.375	1.323	1.415

Propylthiouracil	104170031	1692	16488	10.262	0.061	3634	18081	20.098	-0.172	-0.056
Prostaglandin E1	46386879	1063	11375	9.345	-0.644	2974	14510	20.496	-0.398	-0.521
Proxymetacaine	104170084	1106	10372	10.663	0.348	3328	14522	22.917	0.261	0.305
Pterostilbene	46386623	2289	15874	14.420	-0.265	2693	14379	18.729	-0.484	-0.374
Pyrazinamide	104170032	1369	14359	9.534	-0.271	3800	17040	22.300	0.084	-0.093
Pyridostigmine bromide	104170079	1599	15678	10.199	0.094	4027	17874	22.530	0.150	0.122
Pyrimethamine	104170026	922	14910	6.184	-2.108	2532	16506	15.340	-1.953	-2.030
Quetiapine fumarate	46386812	3284	17269	19.017	-0.149	4498	17158	26.215	0.026	-0.061
Quinapril hydrochloride	104170220	1558	14674	10.617	0.250	3412	16349	20.870	0.117	0.183
Quinidine	104169976	1382	14939	9.251	-0.703	3793	17266	21.968	0.122	-0.291
R(+)-SCH-23390 hydrochloride	46387007	3418	16212	21.083	0.767	4412	15795	27.933	0.614	0.690
Rabeprazole	46386636	1537	14361	10.703	0.409	3644	17186	21.203	-0.017	0.196
Racecadotril	46386930	1380	14510	9.511	-0.141	3292	16946	19.426	-0.482	-0.312
Racepinephrine	104170169	2693	16170	16.654	-0.502	3921	14187	27.638	0.061	-0.220
Raclopride	46386981	2553	13726	18.600	-0.333	3711	13507	27.475	0.457	0.062
Raloxifene hydrochloride	104170163	1046	15617	6.698	-2.302	1913	17668	10.827	-3.808	-3.055
Raltitrexed	46386823	2859	15993	17.877	-0.339	4071	14890	27.340	0.026	-0.157
Ramipril	46386770	2560	17448	14.672	-0.183	3105	15843	19.599	-0.187	-0.185
Ranitidine hydrochloride	104169977	2407	14211	16.938	-0.411	3450	12601	27.379	-0.001	-0.206
Ranolazine dihydrochloride	46386552	3242	16939	19.139	-0.094	4279	16614	25.755	-0.132	-0.113
Remacemide hydrochloride	46386987	3053	15769	19.361	0.004	4167	15840	26.307	0.057	0.030
Repaglinide	46386564	1142	13794	8.279	-0.709	2659	16437	16.177	-1.333	-1.021
Resveratrol	46386962	1290	13845	9.317	-0.661	3226	16752	19.257	-0.834	-0.748
Ribavirin	104170186	1278	14872	8.593	-0.826	3259	17194	18.954	-0.600	-0.713
Rifabutin	104170218	1300	14619	8.893	-0.927	3630	16928	21.444	-0.063	-0.495
Rifampicin	104169978	2989	17337	17.241	-0.313	3718	14201	26.181	-0.287	-0.300
Rifapentine	104170198	1007	10807	9.318	-0.389	2901	14319	20.260	-0.504	-0.447
Rifaximin	46386615	3054	16569	18.432	-0.161	4036	14831	27.213	-0.012	-0.086
Riluzole hydrochloride	46386847	2538	16881	15.035	0.133	3737	17568	21.272	0.002	0.067
Rimcazole dihydrochloride	46387003	2230	13542	16.467	-1.278	3292	12812	25.695	-0.153	-0.715
Risperidone	46386613	3150	14530	21.679	2.084	2838	11664	24.331	1.426	1.755
Ritonavir	46386817	2855	17818	16.023	-1.475	3533	17545	20.137	-2.056	-1.766
Rizatriptan benzoate	46386632	2562	17169	14.922	-0.102	3116	15757	19.775	-0.127	-0.115
Rofecoxib	46386634	2871	17828	16.104	0.280	3170	16115	19.671	-0.163	0.059
Rolipram	46386779	1524	14765	10.322	0.233	3619	16418	22.043	0.203	0.218
Rolitetracycline	46386966	1496	15066	9.930	0.053	3476	16277	21.355	0.023	0.038
Ropivacaine hydrochloride	46386542	2208	16518	13.367	-0.162	3732	17237	21.651	0.086	-0.038
Rosiglitazone maleate	46386628	2398	16297	14.714	0.076	3493	16880	20.693	-0.127	-0.025
Roxatidine acetate hydrochloride	46386565	3278	16946	19.344	-0.004	4162	16350	25.456	-0.234	-0.119
Ru 24969 hemisuccinate	46387004	1340	15946	8.403	-0.927	3019	16410	18.397	-0.809	-0.868
RU-486	46386955	1977	14380	13.748	1.815	4386	16709	26.249	1.304	1.560
Rufloxacin hydrochloride	46386706	1713	16054	10.670	0.186	3576	16834	21.243	-0.134	0.026
Rutin	46386546	1570	14312	10.970	0.533	3663	17247	21.238	-0.008	0.262
S(-)-Timolol maleate	104170090	1186	15171	7.818	-1.211	3368	17273	19.499	-0.723	-0.967
Salbutamol sulfate	46386798	3081	16958	18.168	-0.524	4078	16022	25.453	-0.236	-0.380
Salmeterol	46387005	3932	16830	23.363	1.426	5369	15969	33.621	1.912	1.669
Saquinavir mesylate	46386596	1028	11797	8.714	-0.508	2761	14800	18.655	-0.684	-0.596
SB 205607 dihydrobromide	46387006	1569	15977	9.820	-0.347	3654	16891	21.633	0.003	-0.172
Scopolamine hydrobromide	46386794	3427	17359	19.742	0.173	4359	17373	25.091	-0.359	-0.093
SDM25N hydrochloride	46387008	2979	17100	17.421	-0.486	4339	16406	26.448	-0.242	-0.364
Secnidazole	46386696	1746	15844	11.020	0.405	3733	17322	21.551	-0.026	0.189
Secoisolaricresinol	46386735	1458	13974	10.434	0.038	3347	16604	20.158	-0.517	-0.240
Selegiline hydrochloride	46386796	2350	13036	18.027	-0.587	3497	13079	26.738	0.205	-0.191
Sertraline hydrochloride	46386723	2237	16368	13.667	-0.109	2913	15567	18.713	-0.568	-0.339
Sibutramine	46387014	2466	12702	19.414	0.155	3423	11946	28.654	0.420	0.288
Simvastatin	104170217	1690	11344	14.898	2.526	3864	13138	29.411	3.314	2.920
SKF 83566 hydrobromide	46386977	2623	13698	19.149	0.070	3247	12551	25.870	-0.415	-0.173
Sotalol hydrochloride	46386705	994	12766	7.786	-1.256	2828	14875	19.012	-0.579	-0.917
Spectinomycin	104170086	1558	15275	10.200	0.028	3419	16948	20.173	-0.144	-0.058
Spironolactone	104169980	3559	17775	20.023	0.582	4313	15310	28.171	0.189	0.386
SR 57227A	46386849	3122	14100	22.142	1.265	3841	11538	33.290	1.414	1.339
Stanozolol	46386608	1420	14654	9.690	-0.058	3527	16573	21.282	0.003	-0.027
Stavudine	104170182	1666	16195	10.287	0.074	3627	17492	20.735	0.066	0.070
Stiripentol	46386912	2535	13383	18.942	0.003	3212	11469	28.006	0.226	0.115
Sulfacetamide	104170036	1330	14263	9.325	-0.657	3553	16505	21.527	-0.034	-0.345
Sulfamethoxazole	104170035	1202	12196	9.856	-0.155	3118	14844	21.005	0.167	0.006
Sulfasalazine	46386548	1169	12177	9.600	-0.291	3075	15203	20.226	-0.124	-0.208
Sulfipyrazone	104170037	3187	17668	18.038	-0.057	4024	15001	26.825	-0.133	-0.095
Sulfisoxazole	104170034	1664	15482	10.748	0.430	3567	17416	20.481	-0.206	0.112
Sulindac	104170038	2907	16240	17.900	-0.101	4473	15659	28.565	0.283	0.091
Sumatriptan succinate	46386597	3085	16273	18.958	-0.175	4414	15767	27.995	0.635	0.230
Symmetrel	104169987	1681	15161	11.088	0.500	3475	16645	20.877	0.120	0.310
Synephrine	46386970	2437	13784	17.680	-0.403	3363	12710	26.459	-0.238	-0.321
Tacrine hydrochloride	46386852	3732	17594	21.212	0.824	4940	17100	28.889	0.942	0.883
Tacrolimus	46386734	3146	16500	19.067	0.044	4496	15822	28.416	0.349	0.196
Tadalafil	46386604	3112	16717	18.616	1.093	2909	14696	19.795	-0.121	0.486
Tamoxifen	104170047	1006	11985	8.394	-1.240	3307	14354	23.039	0.499	-0.370
Taxifolin(+)	46386813	1326	13687	9.688	-0.429	3453	16257	21.240	-0.135	-0.282
Taxifolin(+/-)	46386773	1464	14165	10.335	0.240	3446	16667	20.676	-0.155	0.042
Tegafur	46386579	3440	17979	19.133	0.065	4433	16312	27.176	-0.023	0.021
Tegaserod maleate	46386624	2884	15161	19.022	0.839	4774	16273	29.337	1.798	1.318
Telithromycin	46386829	2638	14462	18.241	0.009	3334	11657	28.601	0.292	0.150
Telmisartan	46386620	2559	17608	14.533	-0.228	3193	16050	19.894	-0.087	-0.157
Temozolomide	46386653	2601	14488	17.953	0.878	2338	11119	21.027	0.300	0.589
Terazosin	104170187	1590	15194	10.465	0.169	3708	16889	21.955	0.523	0.346
Terbinafine hydrochloride	46386583	2625	16774	15.649	0.242	3876	17220	22.509	0.277	0.260

Terbutaline sulfate	104170117	1185	13845	8.559	-0.805	3520	16515	21.314	-0.200	-0.503
Testosterone	46501387	3083	15942	19.339	0.362	4621	15913	29.039	0.397	0.379
Tetracycline	104170039	1317	13660	9.641	-0.081	3326	17446	19.065	-0.577	-0.329
Tetrahydrozoline hydrochloride	104169982	1569	15620	10.045	-0.055	3589	17082	21.010	0.169	0.057
TFMPP hydrochloride	46386913	2776	15193	18.272	0.706	4452	16623	26.782	1.229	0.968
Thalidomide	104170098	3056	17304	17.661	-0.178	4260	15542	27.410	0.007	-0.086
Theophylline	104170040	2340	13772	16.991	-0.394	3640	12757	28.533	0.276	-0.059
Thiabendazole	104170091	1454	15011	9.686	-0.187	3524	16796	20.981	-0.296	-0.242
Thioridazine hydrochloride	104170092	980	12250	8.000	-1.142	2805	14515	19.325	-0.462	-0.802
Thiothixene	104170208	854	14015	6.093	-2.156	2142	17102	12.525	-2.731	-2.444
Tiagabine hydrochloride	46386642	2472	17164	14.402	-0.271	3047	15644	19.477	-0.229	-0.250
Tibolone	46386825	2910	15856	18.353	-0.186	4019	14643	27.447	0.058	-0.064
Ticlopidine hydrochloride	46386576	2350	16262	14.451	0.030	3542	17227	20.561	-0.157	-0.063
Tinidazole	46387025	2500	17349	14.410	-0.268	2935	14989	19.581	-0.193	-0.231
Tizanidine hydrochloride	104170152	1058	11709	9.036	-0.360	3210	14360	22.354	0.284	-0.038
Tocainide	46386772	3464	17222	20.114	0.381	4181	16494	25.349	-0.572	-0.096
Tolazamide	104170088	1463	15447	9.471	-0.305	3806	17247	22.068	0.017	-0.144
Tolbutamide	104170041	3133	17717	17.684	-0.171	3926	13413	29.270	0.452	0.141
Tolterodine tartrate	46386674	2902	17078	16.993	-1.045	4081	16476	24.769	-0.470	-0.757
Topiramate	46386619	2274	15093	15.067	-0.056	2649	11856	22.343	0.748	0.346
Topotecan hydrochloride	46386667	4461	12513	35.651	5.381	5830	12398	47.024	5.935	5.658
Torasemide	46386585	936	10973	8.530	-1.154	3039	14409	21.091	-0.188	-0.671
Toremifene citrate	46386786	1405	16753	8.387	-0.936	3390	18027	18.805	-0.656	-0.796
Tosufloxacin tosilate	46386743	2376	16863	14.090	-0.034	3564	17194	20.728	-0.119	-0.077
Tramadol hydrochloride	46386884	2592	13311	19.473	0.174	3529	12499	28.234	0.294	0.234
Tranilast	46386750	1721	15708	10.956	0.365	3745	16764	22.340	0.253	0.309
trans-Retinoic acid	104169979	3058	16772	18.233	0.006	4027	14713	27.370	-0.003	0.002
Trazodone hydrochloride	46386915	3217	16195	19.864	0.227	4338	16068	26.998	0.294	0.260
Tremulacin	46386886	2448	16520	14.818	-0.136	3115	15056	20.689	0.185	0.024
Triamcinolone acetonide	104170089	1962	13954	14.060	2.210	4054	15871	25.543	1.018	1.614
Triamterene	104170042	1865	13202	14.127	-1.316	2871	12551	22.875	-1.079	-1.197
Triclabendazole	46386738	2940	17290	17.004	0.571	3692	15958	23.136	1.019	0.795
Triclosan	104170014	3053	16187	18.861	0.208	4372	15365	28.454	0.257	0.233
Trifluoperazine hydrochloride	46386916	3016	17709	17.031	-1.028	4129	17714	23.309	-0.970	-0.999
Trihexyphenidyl hydrochloride	104169984	1711	16545	10.341	0.103	3794	17277	21.960	0.525	0.314
Trimebutine maleate	46386760	2430	16650	14.595	0.055	4057	17332	23.408	0.477	0.266
Trimethoprim	104169981	1356	12749	10.636	0.260	3305	15101	21.886	0.497	0.379
Tripeleminamine hydrochloride	46386917	2664	13799	19.306	0.121	3651	13094	27.883	0.189	0.155
Triptolide	46386571	1437	10256	14.011	-0.397	1783	8725	20.436	0.098	-0.150
Tropicamide	104170087	1678	15492	10.831	0.440	3887	17744	21.906	-0.030	0.205
Tropisetron hydrochloride	46386594	3124	16580	18.842	0.807	4988	16565	30.112	1.971	1.389
Troxipide	46386769	1665	14985	11.111	0.462	3683	17262	21.336	-0.101	0.180
Tryptoline	46386936	3212	15933	20.159	0.395	4199	14602	28.756	0.451	0.423
Urapidil hydrochloride	46386851	2421	17429	13.891	-0.069	3411	17027	20.033	-0.274	-0.172
Ursodeoxycholic acid	104169985	1083	11009	9.837	0.010	3161	14847	21.290	0.006	0.008
Valaciclovir hydrochloride	46386762	3128	16498	18.960	-0.174	4126	15790	26.130	-0.003	-0.089
Valdecoxib	46386621	3437	17135	20.058	0.363	4567	16618	27.482	0.069	0.216
Valproic acid	104170082	1077	12163	8.855	-0.643	2982	14542	20.506	-0.433	-0.538
Valsartan	46386599	2288	16956	13.494	-0.565	2901	14719	19.709	-0.150	-0.357
Vardenafil citrate	46386591	2547	16503	15.434	0.204	3889	17197	22.614	0.301	0.252
Vecuronium bromide	46386876	2419	13500	17.919	-0.326	3544	12745	27.807	0.166	-0.080
Venlafaxine hydrochloride	46386590	2391	17054	14.020	-0.046	3572	17125	20.858	-0.090	-0.068
Verapamil hydrochloride	46386795	1570	14104	11.132	0.607	4102	16332	25.116	1.008	0.807
Vidarabine	104170045	2987	15282	19.546	0.429	3879	13458	28.823	0.345	0.387
Vincristine sulfate	46386588	334	7110	4.698	-2.362	905	7266	12.455	-2.308	-2.335
Vindesine sulfate	46386586	425	4236	10.033	-2.864	969	3806	25.460	-0.539	-1.701
Vinorelbine tartrate	46386815	178	5376	3.311	-3.859	392	6039	6.491	-4.656	-4.258
Voriconazole	46386721	3172	16602	19.106	0.056	4086	14879	27.462	0.062	0.059
Warfarin sodium	104169988	3081	16818	18.320	0.034	3781	14810	25.530	-0.443	-0.205
Xanthinol nicotinate	46387024	2565	17528	14.634	-0.196	3221	16020	20.106	-0.014	-0.105
Zacopride hydrochloride hydrate	46386978	1677	12745	13.158	1.542	4020	14439	27.841	1.721	1.632
Zafirlukast	46386595	2985	17268	17.286	0.663	3311	16305	20.307	0.054	0.358
Zalcitabine	46386814	3027	15660	19.330	0.128	4043	15062	26.842	-0.123	0.002
Zaleplon	46386657	2696	14629	18.429	1.032	2428	12098	20.069	-0.027	0.503
Zardaverine	46386923	1270	13809	9.197	-0.737	3336	15681	21.274	-0.123	-0.430
Zeranol	46386627	2485	16889	14.714	-0.170	3083	15778	19.540	-0.207	-0.189
Zidovudine	104170164	1734	16193	10.708	0.298	3433	17224	19.931	-0.234	0.032
Zileuton	46386751	1178	12435	9.473	-0.358	3004	14713	20.417	-0.053	-0.206
Zolmitriptan	46386880	2532	14212	17.816	-0.128	3443	12175	28.279	0.215	0.043
Zolpidem tartrate	46386567	3170	17097	18.541	0.105	3853	14399	26.759	-0.149	-0.022
Zonisamide	104170135	1429	13998	10.209	0.181	3540	16338	21.667	0.104	0.143
Zucapsaicin	46386797	1442	14586	9.886	0.032	3401	17101	19.888	-0.362	-0.165
		<b>Std Dev</b>	2452.65			<b>Std Dev</b>	2269			
		<b>Average</b>	14826.66			<b>Average</b>	15225			
		<b>Median</b>	15279.50			<b>Median</b>	15903			