

Antimalarial drugs with whole protein 6vw1 grid, Table S1

Entry Name	docking score	glide gscore
6vw1.1		
Conformer3D_CID_6178	-5.129	-5.129
Conformer3D_CID_5467	-4.869	-4.869
Conformer3D_CID_6882	-4.786	-4.786
Conformer3D_CID_4069	-4.599	-4.599
Conformer3D_CID_2165	-4.2	-4.2
Conformer3D_CID_1226	-4.05	-4.05
Conformer3D_CID_4465	-3.866	-3.866
Conformer3D_CID_2719	-3.828	-3.828
Conformer3D_CID_6395	-3.828	-3.828
Conformer3D_CID_4993	-3.682	-3.682
Conformer3D_CID_3739	-3.636	-3.636
Conformer3D_CID_4908	-3.63	-3.63
Conformer3D_CID_3085	-3.62	-3.62
Conformer3D_CID_3034	-3.038	-3.038
Conformer3D_CID_7498	-3.024	-3.024

Antimalarial drugs with whole protein 6y84 grid, Table S2

Entry Name	docking score	glide gscore
6y84.1		
Conformer3D_CID_5467	-6.831	-6.831
Conformer3D_CID_1226	-6.296	-6.296
Conformer3D_CID_2165	-5.545	-5.545
Conformer3D_CID_4908	-5.498	-5.498
Conformer3D_CID_4993	-5.403	-5.403
Conformer3D_CID_4465	-5.005	-5.005
Conformer3D_CID_2719	-4.831	-4.831
Conformer3D_CID_6395	-4.831	-4.831
Conformer3D_CID_3739	-4.765	-4.765
Conformer3D_CID_4069	-4.521	-4.521
Conformer3D_CID_3034	-4.491	-4.491
Conformer3D_CID_6882	-4.162	-4.162
Conformer3D_CID_3085	-3.871	-3.871
Conformer3D_CID_7498	-3.727	-3.727
Conformer3D_CID_6178	-1.737	-1.737

Antimalarial drugs with residue protein 6vw1 grid, Table S3

Entry Name	docking score	glide gscore
6vw1.1		
Conformer3D_CID_4993	-5.063	-5.063
Conformer3D_CID_5467	-3.749	-3.749
Conformer3D_CID_3739	-3.656	-3.656
Conformer3D_CID_4465	-3.466	-3.466
Conformer3D_CID_2165	-3.211	-3.211
Conformer3D_CID_4908	-3.111	-3.111
Conformer3D_CID_1226	-3.018	-3.018
Conformer3D_CID_4069	-3.014	-3.014
Conformer3D_CID_2719	-2.908	-2.908
Conformer3D_CID_6395	-2.908	-2.908
Conformer3D_CID_3034	-2.793	-2.793
Conformer3D_CID_6882	-2.769	-2.769
Conformer3D_CID_7498	-2.394	-2.394
Conformer3D_CID_6178	-2.328	-2.328
Conformer3D_CID_3085	0.356	0.356

Antimalarial drugs with residue protein 6y84 grid, Table S4

Entry Name	docking score	glide gscore
6y84.1.1		
Conformer3D_CID_5467	-5.782	-5.782
Conformer3D_CID_4465	-5.558	-5.558
Conformer3D_CID_1226	-4.968	-4.968
Conformer3D_CID_2165	-4.814	-4.814
Conformer3D_CID_3034	-4.238	-4.238
Conformer3D_CID_4908	-4.165	-4.165
Conformer3D_CID_6178	-4.127	-4.127
Conformer3D_CID_2719	-4.111	-4.111
Conformer3D_CID_6395	-4.111	-4.111
Conformer3D_CID_3739	-3.992	-3.992
Conformer3D_CID_6882	-3.947	-3.947
Conformer3D_CID_4069	-3.94	-3.94
Conformer3D_CID_4993	-3.634	-3.634
Conformer3D_CID_7498	-3.386	-3.386
Conformer3D_CID_3085	-2.545	-2.545

FDA approved drugs with 6vw1, Table S5

FORMULA	DRUGBANK_ID	GENERIC_NAME	docking score	glide gscore
C25H48N6O10	DB12615	Plazomicin	-9.035	-9.935
C25H48N6O10	DB12615	Plazomicin	-9.168	-9.66
C29H40N4O7	DB12455	Omadacycline	-7.241	-9.178
C25H48N6O10	DB12615	Plazomicin	-5.948	-8.514
C25H48N6O10	DB12615	Plazomicin	-7.112	-8.194
C22H42N4O8S2	DB11190	Pantethine	-8.188	-8.188
C32H35N5O5	DB09272	Eluxadoline	-7.408	-8.166
C17H22I3N3O8	DB11705	Iomeprol	-8.076	-8.076
C6H8CaO8	DB13962	Calcium saccharate	-7.951	-7.951
C37H48I6N6O18	DB09487	Iotrolan	-6.759	-7.653
C50H71N13O12	DB11842	Angiotensin II	-6.841	-7.491
C11H16N8O8	DB14075	Imidurea	-6.843	-7.482
C18H24I3N3O9	DB09134	Ioversol	-7.378	-7.378
C11H8Na4O8P2	DB09332	Kappadione	-4.711	-7.335
C25H48N6O10	DB12615	Plazomicin	-4.584	-7.141
C32H35N5O5	DB09272	Eluxadoline	-6.364	-7.092
C38H73N21O10S2	DB12865	Etelcalcetide	-4.827	-7.036
C11H16N8O8	DB14075	Imidurea	-5.148	-7.015
C17H22I3N3O8	DB08947	Iopamidol	-6.973	-6.973
C6H12O6	DB13178	Inositol	-6.93	-6.93
C36H70O19	DB11602	Hydroxyethyl cellulose	-6.912	-6.912
C18H24I3N3O8	DB09156	Iopromide	-6.801	-6.801
C20H25N7O6	DB11256	Levemefolic acid	-4.551	-6.783
C20H23N7O7	DB11596	Levoleucovorin	-6.684	-6.684
C49H62N10O16S3	DB09142	Sincalide	-4.521	-6.642
C25H48N6O10	DB12615	Plazomicin	-5.248	-6.621
CH6O7P2Tc	DB09139	Technetium Tc-99m oxidronate	-5.571	-6.615
C6H12O7	DB13180	Gluconic Acid	-6.601	-6.601
C32H50O13	DB12434	Steviolbioside	-6.577	-6.581
C12H22FeO14	DB14488	Ferrous gluconate	-6.569	-6.569
C12H22O14Zn	DB11248	Zinc gluconate	-6.569	-6.569
C12H22CuO14	DB11246	Copper gluconate	-6.552	-6.552
C12H22MnO14	DB11141	Manganese gluconate	-6.551	-6.551
C12H22CaO14	DB11126	Calcium gluconate	-6.551	-6.551
C6H11KO7	DB13620	Potassium gluconate	-6.532	-6.532

C43H67N11O12S2	DB09059	Atosiban	-6.475	-6.475
CH6O7P2	DB14159	Oxidronic acid	-5.424	-6.468
C15H30N2O5	DB12839	Pegvaliase	-6.418	-6.418
C18H33CrO21	DB14528	Chromium gluconate	-6.416	-6.416
C12H26MgO16	DB13749	Magnesium gluconate	-6.374	-6.374
C12H29Fe5Na2O23	DB09146	Iron saccharate	-6.369	-6.369
C18H37N5O8	DB13270	Dibekacin	-4.82	-6.362
C30H44N2O10	DB13265	Hexobendine	-4.047	-6.339
C23H36N2O4	DB09039	Eliglustat	-6.221	-6.227
C11H20O10	DB12767	Gaxilose	-6.195	-6.195
C14H23N3O10	DB14007	Pentetic acid	-5.378	-6.194
C18H24I3N3O8	DB09135	Ioxilan	-6.181	-6.181
C23H30N12O8S2	DB09050	Ceftolozane	-6.154	-6.155
Al2H2Mg2O12Si3	DB14116	Silodrate	-6.114	-6.114
C50H71N13O12	DB11842	Angiotensin II	-5.428	-6.111
CH6O7P2Tc	DB09139	Technetium Tc-99m oxidronate	-5.972	-6.083
C14H23N3O10	DB14007	Pentetic acid	-3.866	-6.042
C29H40N4O7	DB12455	Omadacycline	-3.656	-6.036
C19H20Br2N6O4S	DB08932	Macitentan	-5.831	-6.03
C50H68N14O10	DB11653	Bremelanotide	-5.218	-6.029
C25H30N4O9S2	DB12127	Sultamicillin	-5.287	-6.008
C12H16O7	DB11217	Arbutin	-6.006	-6.006
C11H16N8O8	DB14075	Imidurea	-5.707	-5.993
C32H43N5O5	DB11274	Dihydro-alpha-ergocryptine	-3.56	-5.989
C26H25F3N6O5	DB09335	Alatrofloxacin	-5.791	-5.927
C49H62N10O16S3	DB09142	Sincalide	-5.909	-5.926
C22H25ClO7	DB11827	Ertugliflozin	-5.913	-5.913
C16H22N6O4	DB09421	Protirelin	-5.194	-5.87
C14H20InN3O10	DB09425	Indium In-111 pentetate	-5.04	-5.856
C19H23N4O6PS	DB11748	Benfotiamine	-4.611	-5.853
O7P2Tc	DB09165	Technetium Tc-99m pyrophosphate	-3.516	-5.853
C11H12O8P2	DB14650	Menadiol diphosphate	-4.496	-5.839
C11H8Na4O8P2	DB09332	Kappadione	-4.496	-5.839
C24H33Cl2NO5	DB09082	Vilanterol	-5.833	-5.838
C4H4Na2O6	DB13707	Sodium tartrate	-5.836	-5.836
C11H18N2O9	DB12362	Diaminopropanol tetraacetic acid	-3.582	-5.829
C32H35N5O5	DB09272	Eluxadoline	-4.491	-5.795
C12H16O7	DB14109	alpha-Arbutin	-5.785	-5.785
C14H26N4O11P2	DB12153	Citicoline	-5.78	-5.78
C11H12O8P2	DB14650	Menadiol diphosphate	-3.136	-5.76
C28H32O15	DB08995	Diosmin	-5.75	-5.75
C50H68N14O10	DB11653	Bremelanotide	-5.19	-5.74
C46H65N13O12S2	DB14642	Lypressin	-5.545	-5.738
C31H41N5O5	DB11273	Dihydroergocornine	-3.296	-5.729
C26H25F3N6O5	DB09335	Alatrofloxacin	-3.735	-5.717
C22H32N2O2	DB12313	Dopexamine	-5.711	-5.711
C18H37N5O8	DB13270	Dibekacin	-4.206	-5.687
C25H48N6O10	DB12615	Plazomicin	-3.532	-5.679
C26H27N3O5S	DB09183	Dasabuvir	-5.637	-5.647
C6H11FO5	DB09502	Fludeoxyglucose F-18	-5.643	-5.645
C23H28N8O4	DB12483	Copanlisib	-2.884	-5.607
CH6O7P2	DB14159	Oxidronic acid	-5.494	-5.605
C6H11FeNO7	DB09501	Ferric ammonium citrate	-5.588	-5.588
C8H14N4O7	DB14173	Diazolidinylurea	-5.576	-5.576
C8H14CaO10	DB11168	Calcium threonate	-5.554	-5.554
C14H19BCl2N2O4	DB09570	Ixazomib	-5.549	-5.549
C27H26ClF3N6O3	DB12095	Telotristat ethyl	-5.104	-5.539
C46H65N13O12S2	DB14642	Lypressin	-4.777	-5.534
C10H15N3O5	DB12783	Benserazide	-4.38	-5.531
C16H22N6O4	DB09421	Protirelin	-4.897	-5.53
C20H28I3N3O9	DB12407	Iobitridol	-5.491	-5.491
C27H26ClF3N6O3	DB12095	Telotristat ethyl	-3.213	-5.483
C8H10N6	DB12945	Dihydralazine	-4.994	-5.451

C18H26N2O5Tc	DB09164	Technetium Tc-99m disofenin	-3.902	-5.444
C42H62O16	DB13751	Glycyrrhizic acid	-5.435	-5.438
C10H14O3	DB13583	Mephenesin	-5.432	-5.432
C18H23NO3	DB08941	Isoxsuprine	-5.38	-5.415
C15H17N3O6S	DB14082	Betiatide	-5.41	-5.41
C49H55N9O7	DB11574	Elbasvir	-4.063	-5.353
Al2H2MgO9Si2	DB13595	Almasilate	-5.339	-5.339
C12H16BNO5S	DB12107	Vaborbactam	-5.32	-5.321
C6H6N2O3	DB09055	Acipimox	-5.279	-5.282
C23H28N8O4	DB12483	Copanlisib	-4.845	-5.276
C3H7Na2O6P	DB09561	Sodium glycerophosphate	-5.168	-5.275
C12H10O14Zn3	DB11154	Zinc citrate	-5.264	-5.264
C6H5Na3O7	DB09154	Sodium citrate	-5.264	-5.264
C3H7CaO6P	DB11264	Calcium glycerophosphate	-4.184	-5.262
C22H28O5	DB12952	Methylprednisone	-5.251	-5.251
C18H24N2O5	DB09477	Enalaprilat	-4.247	-5.223
C15H16O9	DB13155	Esculin	-5.202	-5.213
C3H7CaO6P	DB11264	Calcium glycerophosphate	-5.095	-5.2
O7P2Tc	DB09165	Technetium Tc-99m pyrophosphate	-4.962	-5.195
C14H20InN3O10	DB09425	Indium In-111 pentetate	-3.01	-5.186
C15H14O6	DB14086	Cianidanol	-5.178	-5.178
C28H27N3O3	DB13931	Netarsudil	-5.141	-5.152
C27H31FN4O8	DB12329	Eravacycline	-3.886	-5.123
C11H12O8P2	DB14650	Menadiol diphosphate	-3.684	-5.102
C11H8Na4O8P2	DB09332	Kappadione	-3.684	-5.102
CH6O8P2Tc	DB09138	Technetium Tc-99m medronate	-4.572	-5.099
CH6O6P2	DB14078	Medronic acid	-4.572	-5.098
C14H23N3O10	DB14007	Pentetic acid	-4.853	-5.091
C14H20InN3O10	DB09425	Indium In-111 pentetate	-4.853	-5.091
C16H14O3	DB08981	Fenbufen	-5.089	-5.089
C32H35N5O5	DB09272	Eluxadoline	-3.656	-5.087
C20H41N5O7	DB13274	Micronomicin	-3.463	-5.074
C18H24Fe4O42P6	DB13995	Ferric pyrophosphate citrate	-5.065	-5.065
C12H10Ca3O14	DB11093	Calcium Citrate	-5.065	-5.065
C12H8BiK5O14	DB09275	Bismuth subcitrate potassium	-5.065	-5.065
C11H18N2O9	DB12362	Diaminopropanol tetraacetic acid	-4.962	-5.051
C10H14N2O4	DB13253	Proxibarbal	-4.897	-5.042
C21H27FO5	DB09378	Fluprednisolone	-5.038	-5.038
C17H26N4O3S2	DB08966	Fursultiamine	-4.937	-5.029
C49H55N9O7	DB11574	Elbasvir	-3.864	-5.008
C14H11FN2OS	DB09151	Flutemetamol (18F)	-2.782	-5.004
C24H29N3O8	DB12035	Sarecycline	-3.886	-4.972
C17H14BrN3O2S	DB11560	Lesinurad	-4.971	-4.971
C27H31FN4O8	DB12329	Eravacycline	-4.827	-4.96
C15H18N2O9	DB09144	Uridine triacetate	-4.935	-4.938
C6H12O6	DB11735	Galactose	-4.932	-4.932
C18H12ClF3N4O4	DB11943	Delafloxacin	-4.886	-4.93
C12H14MgO12	DB14484	Magnesium ascorbate	-4.921	-4.921
C20H41N5O7	DB13274	Micronomicin	-3.181	-4.915
C7H11N3O6S	DB09060	Avibactam	-4.906	-4.906
CH6O8P2Tc	DB09138	Technetium Tc-99m medronate	-4.584	-4.898
CH6O6P2	DB14078	Medronic acid	-4.583	-4.897
C11H18N2O9	DB12362	Diaminopropanol tetraacetic acid	-3.464	-4.894
C20H22O8	DB11263	Polydatin	-4.888	-4.888
C10H14N2Na2O8	DB14600	Edetate disodium anhydrous	-2.663	-4.877
C20H41N5O7	DB13274	Micronomicin	-3.055	-4.872
C9H11ClN4O2	DB09343	Tipiracil	-4.063	-4.871
C30H26N2O13	DB11184	Oftasceine	-3.582	-4.854
C15H16O9	DB13155	Esculin	-2.505	-4.854
C11H18N2O9	DB12362	Diaminopropanol tetraacetic acid	-2.645	-4.835
C17H16FN6O6P	DB09042	Tedizolid phosphate	-4.747	-4.832
C20H17F3N2O4	DB08976	Floctafenine	-2.623	-4.832
C18H37N5O8	DB13270	Dibekacin	-3.253	-4.819

C5H10O5	DB09419	Xylose	-4.81	-4.81
C29H40N4O7	DB12455	Omadacycline	-3.548	-4.805
C30H29CIN6O3	DB11828	Neratinib	-3.899	-4.801
C26H27N3O5S	DB09183	Dasabuvir	-2.379	-4.798
C18H32Fe4O31	DB14520	Tetraferic tricitrate decahydrate	-4.787	-4.787
C36H72NO8P	DB11283	DL-dimyristoylphosphatidylcholine	-4.786	-4.786
C9H10O4	DB11323	Glycol salicylate	-4.781	-4.782
C8H8O3	DB13218	Mandelic acid	-4.779	-4.779
C23H26FN6O9P	DB12010	Fostamatinib	-3.422	-4.776
C6H5Li3O7	DB14507	Lithium citrate	-4.762	-4.762
C6H5K3O7	DB09125	Potassium Citrate	-4.762	-4.762
C14H12O4	DB11221	Dioxybenzone	-2.86	-4.758
C21H29O8P	DB14631	Prednisolone phosphate	-4.684	-4.75
C26H25F3N6O5	DB09335	Alatrofloxacin	-3.677	-4.75
C23H27ClO7	DB09038	Empagliflozin	-4.74	-4.74
C14H12O4	DB11221	Dioxybenzone	-4.676	-4.738
C33H54O5	DB14001	alpha-Tocopherol succinate	-4.727	-4.727
C2H7N5	DB13100	Biguanide	-4.713	-4.716
C14H27N3O2	DB13247	Pramiracetam	-4.71	-4.714
C4H9Al2CIN4O7	DB11205	Alcloxa	-4.434	-4.707
C13H21NO3	DB13139	Levosalbutamol	-4.686	-4.686
C21H30O4S	DB09091	Tixocortol	-2.191	-4.686
C3H7Na2O6P	DB09561	Sodium glycerophosphate	-3.614	-4.681
C52H78N10O17	DB13156	Inosine pranobex	-4.677	-4.677
C22H29FN3O9P	DB08934	Sofosbuvir	-4.665	-4.668
C10H15N3O5	DB12783	Benserazide	-4.576	-4.668
C23H23ClFNO5	DB09101	Elvitegravir	-3.705	-4.661
C5H8FNO2	DB13146	Fluciclovine (18F)	-4.658	-4.658
C4H6N4O3	DB11100	Allantoin	-2.995	-4.651
C23H26FN6O9P	DB12010	Fostamatinib	-4.577	-4.641
C24H38N2O4	DB11915	Valbenazine	-4.377	-4.625
C24H38N2O4	DB11915	Valbenazine	-2.178	-4.615
C22H18FN7O	DB09054	Idelalisib	-4.587	-4.608
C23H28N8O4	DB12483	Copanlisib	-4.188	-4.603
C26H30N6O3	DB13074	Macimorelin	-3.599	-4.596
C13H21N5O4	DB09092	Xanthinol	-3.348	-4.59
C32H30F5N3O5	DB11979	Elagolix	-3.849	-4.581
C10H10N2O	DB12243	Edaravone	-4.227	-4.578
C16H22I2N6O4S	DB09546	Iobenguane sulfate I-123	-4.574	-4.574
C21H26N2O5	DB09080	Olodaterol	-1.947	-4.571
C10H12ClNO4	DB14656	Chlorphenesin carbamate	-4.563	-4.563
C8H17FeN3O6S2	DB11197	Ferrous cysteine glycinate	-2.344	-4.563
C24H29NO5	DB09292	Sacubitril	-2.339	-4.553
C19H12O8	DB11994	Diacerein	-4.526	-4.526
C27H31FN4O8	DB12329	Eravacycline	-2.4	-4.521
C21H31O8P	DB14542	Hydrocortisone phosphate	-3.183	-4.516
C26H34O8	DB14644	Methylprednisolone hemisuccinate	-4.509	-4.51
C10H8N2O2S2	DB11327	Dipyrrithione	-4.49	-4.49
C50H68N14O10	DB11653	Bremelanotide	-3.867	-4.488
C7H6O3	DB11268	Protocatechualdehyde	-4.376	-4.483
C6H8N2	DB14141	p-Phenylenediamine	-3.494	-4.479
C22H28O5	DB09383	Meprednisone	-4.449	-4.449
C17H20N2O5S	DB13337	Pheneticillin	-4.448	-4.448
C21H20O6	DB11672	Curcumin	-3.211	-4.444
C10H9N5O	DB11336	Kinetin	-4.417	-4.438
C21H27N	DB09016	Butriptyline	-4.434	-4.435
C37H48I6N6O18	DB09487	Iotrolan	-4.285	-4.433
C14H14N4O4	DB12954	Terizidone	-4.431	-4.431
C19H23N4O6PS	DB11748	Benfotiamine	-3.165	-4.431
C4H9Al2CIN4O7	DB11205	Alcloxa	-2.779	-4.43
C15H10Cl2N4O6	DB11632	Opicapone	-3.469	-4.429
C20H25N7O6	DB11256	Levomefolic acid	-4.412	-4.428
C32H43N5O5	DB11275	Epicriptine	-2.007	-4.428

C10H12CaN2Na2O8	DB14598	Edetate calcium disodium anhydrous	-2.212	-4.426
C29H40N4O7	DB12455	Omadacycline	-4.298	-4.424
C18H37N5O8	DB13270	Dibekacin	-4.188	-4.414
C13H21N5O4	DB09092	Xanthinol	-4.327	-4.405
C14H10O3	DB11157	Anthralin	-4.396	-4.396
C12H14N2O7	DB14486	Niacinamide ascorbate	-4.39	-4.39
C12H14O12Zn	DB14485	Zinc ascorbate	-4.39	-4.39
C30H53N3O6	DB09026	Aliskiren	-4.375	-4.38
C16H16N4O	DB14753	Hydroxystilbamidine	-4.375	-4.375
C35H38N4O6	DB09238	Manidipine	-3.088	-4.368
C11H12O8P2	DB14650	Menadiol diphosphate	-4.225	-4.363
C11H8Na4O8P2	DB09332	Kappadione	-4.225	-4.363
C15H10Cl2N4O6	DB11632	Opicapone	-4.194	-4.349
C4H6N4O3	DB11100	Allantoin	-4.077	-4.347
C6H10O4	DB09401	Isosorbide	-4.346	-4.346
AlO4P	DB14517	Aluminium phosphate	-2.734	-4.342
HNa2O4P	DB14502	Sodium phosphate, dibasic	-2.734	-4.342
CaH5O6P	DB14481	Calcium phosphate dihydrate	-2.734	-4.342
Ca3O8P2	DB11348	Calcium Phosphate	-2.734	-4.342
H2NaO4P	DB09449	Sodium phosphate, monobasic	-2.734	-4.342
HK2O4P	DB09414	Dipotassium phosphate	-2.734	-4.342
H2KO4P	DB09413	Monopotassium phosphate	-2.734	-4.342
H3O4P	DB09394	Phosphoric acid	-2.734	-4.342
C10H14N2O4	DB13253	Proxibarbal	-3.025	-4.341
C26H30N6O3	DB13074	Macimorelin	-4.216	-4.338
C20H17F3N2O4	DB08976	Floctafenine	-4.32	-4.335
C19H17F6N7O	DB13874	Enasidenib	-4.329	-4.329
C49H55N9O7	DB11574	Elbasvir	-2.897	-4.308
C24H21I6N5O8	DB09313	Ioxaglic acid	-4.306	-4.306
C12H10Mg3O14	DB11110	Magnesium citrate	-4.303	-4.303
C24H29N7O2	DB09073	Palbociclib	-2.381	-4.292
C21H31O8P	DB14542	Hydrocortisone phosphate	-4.224	-4.29
C4H6O4S2	DB14089	Dimercaptosuccinic acid	-4.28	-4.28
C27H41NO8	DB11660	Latanoprostene Bunod	-4.276	-4.276
C32H30F5N3O5	DB11979	Elagolix	-4.054	-4.262
C9H12ClN5O	DB09242	Moxonidine	-2.935	-4.258
C22H23ClN2O8	DB09093	Chlortetracycline	-4.118	-4.254
C8H18O10S2	DB12097	Mannitol busulfan	-4.244	-4.244
C7H7BrN4O2	DB14018	Bromotheophylline	-4.204	-4.235
C25H36O6	DB14540	Hydrocortisone butyrate	-4.234	-4.234
C18H21ClN2	DB08936	Chlorcyclizine	-3.759	-4.227
C11H14ClN5	DB14763	Cycloguanil	-3.774	-4.224
C31H35F6N4O5P	DB14019	Fosnetupitant	-4.197	-4.218
C32H34N4O6	DB11691	Naldemedine	-3.692	-4.216
C15H14N2O2	DB14575	Eslicarbazepine	-4.211	-4.211
C21H21N3O3	DB12924	Ozenoxacin	-3.598	-4.195
C16H22N6O4	DB09421	Protirelin	-3.548	-4.192
C21H26F3N5	DB09195	Lorpirazole	-4.075	-4.189
Mg2O8Si3	DB09281	Magnesium trisilicate	-4.188	-4.188
C12H17NO3	DB13278	Bucetin	-4.184	-4.184
C32H34N4O6	DB11691	Naldemedine	-2.295	-4.182
C21H22N6O	DB11978	Glasdegib	-3.143	-4.175
C22H30FO8P	DB14669	Betamethasone phosphate	-2.827	-4.167
C26H27F3N2O6	DB11712	Tezacaftor	-4.158	-4.158
C20H4Cl4I4O5	DB11182	Rose bengal free acid	-4.15	-4.156
C21H19ClN4O4	DB09078	Lenvatinib	-4.15	-4.15
C20H33N3O3S	DB09097	Quinagolide	-4.107	-4.145
C7H7BrN4O2	DB14018	Bromotheophylline	-2.363	-4.14
C22H28F2O4	DB09095	Difluocortolone	-4.139	-4.139
C11H16N2O5	DB13421	Edoxudine	-4.136	-4.137
C14H12O6S	DB11185	Sulisobenzone	-4.082	-4.122
C22H30FO8P	DB14669	Betamethasone phosphate	-4.057	-4.122
C10H10N2O	DB12243	Edaravone	-3.323	-4.116

C14H23N3O10	DB14007	Pentetic acid	-2.267	-4.106
C14H20InN3O10	DB09425	Indium In-111 pentetate	-2.267	-4.106
C15H10Cl2N4O6	DB11632	Opicapone	-1.856	-4.098
C25H34O8	DB14545	Hydrocortisone succinate	-4.094	-4.095
C22H24FN3O2	DB12867	Benperidol	-4.071	-4.088
C18H12ClF3N4O4	DB11943	Delafloxacin	-2.523	-4.088
C25H26F6N2O2	DB09291	Rolapitant	-3.992	-4.074
C6H10CaO6	DB13231	Calcium lactate	-4.072	-4.073
C3H5KO3	DB09483	Potassium lactate	-4.072	-4.073
C7H6O3	DB11268	Protocatechualdehyde	-2.995	-4.061
C27H36O7	DB14643	Methylprednisolone aceponate	-4.052	-4.052
C23H30N2O4	DB09209	Pholcodine	-3.95	-4.052
C34H53NO11	DB09049	Naloxegol	-1.502	-4.049
C18H37N5O8	DB13270	Dibekacin	-2.294	-4.046
C12H14FeO12	DB14490	Ferrous ascorbate	-4.038	-4.038
C6H7NaO6	DB14482	Sodium ascorbate	-4.038	-4.038
C30H26N2O13	DB11184	Oftasceine	-3.948	-4.037
C12H18O3	DB11299	Vanillyl butyl ether	-4.033	-4.033
C10H16N2O	DB11738	Rilmenidine	-4.02	-4.021
C12H18IN	DB09480	Iofetamine I-123	-4.019	-4.019
C23H23ClFNO5	DB09101	Elvitegravir	-3.875	-4.012
C17H16FN6O6P	DB09042	Tedizolid phosphate	-2.816	-4.009
C18H23NO3	DB08941	Isoxsuprine	-2.316	-4.009
C13H10O3	DB11071	Phenyl salicylate	-3.977	-4.001
C16H17N7O2S	DB11817	Baricitinib	-4	-4
C20H26O3	DB13952	Estradiol acetate	-3.997	-3.997
C10H10N2O	DB12243	Edaravone	-2.46	-3.993
C34H53NO11	DB09049	Naloxegol	-2.744	-3.99
C10H15NO2	DB11610	Oxilofrine	-3.969	-3.98
C2H8N2	DB14189	Ethylenediamine	-3.273	-3.973
C13H10N2O3S	DB11115	Ensulizole	-2.676	-3.952
C23H30N8O	DB11730	Ribociclib	-2.547	-3.948
C21H30O4S	DB09091	Tixocortol	-3.933	-3.942
C22H23ClN2O8	DB09093	Chlortetracycline	-1.65	-3.942
C22H24FN3O2	DB12867	Benperidol	-1.795	-3.931
C17H26N4O3S2	DB08966	Fursultiamine	-2.782	-3.928
C43H49N2O6S2	DB09374	Indocyanine green acid form	-3.924	-3.924
C12H6N2O8SSr2	DB09267	Strontium ranelate	-3.918	-3.918
C20H15NO4	DB09219	Bisoxatin	-3.909	-3.914
C18H29NO3	DB09351	Levobetaxolol	-3.909	-3.911
C17H11ClF3N5O3	DB12301	Doravirine	-3.908	-3.908
C17H16N2O3	DB09119	Eslicarbazepine acetate	-3.908	-3.908
C23H30N2O4	DB09209	Pholcodine	-2.307	-3.908
C24H31FO6	DB14657	Paramethasone acetate	-3.906	-3.906
C11H13NO4	DB11102	N-acetyltirosine	-3.904	-3.904
C32H35N5O5	DB09272	Eluxadoline	-2.624	-3.897
C11H10FNO2S	DB13228	Flosequinan	-3.891	-3.891
H2O3S2	DB09499	Thiosulfuric acid	-3.889	-3.889
C8H10O2	DB11304	Phenoxyethanol	-3.887	-3.887
C21H27ClO5	DB00873	Loteprednol	-3.886	-3.886
C20H19F2N3O5	DB08930	Dolutegravir	-1.905	-3.874
C13H19NO3	DB09185	Viloxazine	-3.85	-3.873
C20H19FN4O4	DB09047	Finafloxacin	-2.207	-3.869
C21H29O8P	DB14631	Prednisolone phosphate	-2.495	-3.83
C40H52F4N6O9S	DB12026	Voxilaprevir	-3.825	-3.828
C19H23N4O6PS	DB11748	Benfotiamine	-1.504	-3.828
C21H29N6O5P	DB09299	Tenofovir alafenamide	-3.824	-3.824
C40H43N7O7S	DB09297	Paritaprevir	-1.106	-3.822
C21H20O6	DB11672	Curcumin	-3.47	-3.814
C27H34N4O	DB12492	Piritramide	-2.102	-3.814
C32H43N5O5	DB11274	Dihydro-alpha-ergocryptine	-3.77	-3.813
C15H19BrN2O5Tc	DB09137	Technetium Tc-99m mebrofenin	-2.264	-3.806
C12H11I3N2O5	DB13444	Ioxitalamic acid	-3.803	-3.803

C18H24N2O5	DB09477	Enalaprilat	-3.672	-3.799
C23H32O6	DB14539	Hydrocortisone acetate	-3.798	-3.798
C10H14Cl2NO2PS	DB11768	Zytron	-3.796	-3.796
C3H8O3	DB09462	Glycerin	-3.796	-3.796
C14H12O2	DB14020	Benzoin	-3.792	-3.792
C10H14N2Na2O8	DB14600	Edetate disodium anhydrous	-3.776	-3.79
C8H10N6	DB12945	Dihydralazine	-3.415	-3.788
C24H29N3O8	DB12035	Sarecycline	-3.675	-3.786
C21H21N3O3	DB12924	Ozenoxacin	-3.427	-3.786
C32H34N4O6	DB11691	Naldemedine	-1.376	-3.785
C7H8O2	DB11359	Guaiacol	-3.782	-3.783
C24H29N7O2	DB09073	Palbociclib	-3.375	-3.782
C17H15FN6O3	DB14569	Tedizolid	-3.779	-3.779
CCaN2	DB09116	Calcium carbimide	-3.779	-3.779
C49H55N9O7	DB11574	Elbasvir	-2.529	-3.772
C27H26ClF3N6O3	DB12095	Telotristat ethyl	-1.5	-3.771
C22H23NO4S2	DB13166	Zofenopril	-3.768	-3.768
C30H44N2O10	DB13265	Hexobendine	-1.236	-3.767
C17H15BrF2N4O3	DB11967	Binimetinib	-3.754	-3.763
C12H14CaO12	DB14483	Calcium ascorbate	-3.76	-3.76
C18H18ClN3S	DB13256	Clothiapine	-3.719	-3.753
C10H7Cl2NO	DB13306	Chlorquinaldol	-2.958	-3.747
C22H29FO4	DB08971	Fluocortolone	-3.745	-3.745
C16H12Cl2N2O2	DB13872	Lormetazepam	-3.745	-3.745
C17H15BrF2N4O3	DB11967	Binimetinib	-1.236	-3.744
C28H40O7	DB14543	Hydrocortisone probutate	-3.743	-3.743
C29H39ClN7O2P	DB12267	Brigatinib	-3.725	-3.739
C21H18F3N3O5	DB11799	Bictegravir	-1.768	-3.736
C21H28O3	DB11636	Nomegestrol	-3.729	-3.729
C21H34O5	DB09081	Idebenone	-3.725	-3.725
O7P2Tc	DB09165	Technetium Tc-99m pyrophosphate	-3.021	-3.722
C14H11FN2OS	DB09151	Flutemetamol (18F)	-3.705	-3.719
C14H14O2	DB14120	Phenylethyl resorcinol	-3.71	-3.712
HNaO3S	DB14015	Sodium bisulfite	-3.711	-3.711
C10H15NO2	DB11610	Oxilofrine	-1.361	-3.706
C24H25ClFN5O2	DB11963	Dacomitinib	-3.597	-3.705
C21H28O2	DB09070	Tibolone	-3.695	-3.695
C22H27F3O4S	DB13867	Fluticasone	-3.691	-3.691
C25H30N4O9S2	DB12127	Sultamicillin	-3.481	-3.689
C21H21N3O3	DB12924	Ozenoxacin	-1.982	-3.689
C26H38O6	DB14544	Hydrocortisone valerate	-3.686	-3.686
C19H31N	DB12728	Fenpropidin	-3.681	-3.681
C18H24NO4	DB11315	Methscopolamine	-3.675	-3.675
C21H19ClFN4O4S	DB11629	Laropiprant	-3.673	-3.675
C21H22F2N6O2	DB14723	Larotrectinib	-3.668	-3.668
C9H11ClN4O2	DB09343	Tipiracil	-3.489	-3.664
C16H19NO2	DB13219	Medifoxamine	-3.305	-3.664
C8H8O3	DB09543	Methyl salicylate	-2.49	-3.663
C9H8N2	DB12537	Benzodiazepine	-3.66	-3.66
C20H41N5O7	DB13274	Micronomicin	-3.474	-3.657
C7H6BFO2	DB09041	Tavaborole	-3.656	-3.656
C10H15N	DB09571	Levmetamfetamine	-3.643	-3.644
C16H22N4O	DB11235	Thonzylamine	-3.633	-3.637
BH3O3	DB11326	Boric acid	-3.63	-3.63
C22H18FN7O	DB09054	Idelalisib	-1.629	-3.626
C19H20Br2N6O4S	DB08932	Macitentan	-2.883	-3.625
C20H22O3	DB09495	Avobenzzone	-2.353	-3.617
C21H45N3	DB08958	Hexetidine	-3.215	-3.608
C34H53NO11	DB09049	Naloxegol	-3.511	-3.597
C21H18ClNO6	DB13783	Acemetacin	-3.593	-3.593
C8H8O2	DB09269	Phenylacetic acid	-3.589	-3.59
C19H23N4O6PS	DB11748	Benfotiamine	-3.408	-3.587
C9H19NO4	DB09357	Dexpanthenol	-3.583	-3.583

C3H6BrNO4	DB13960	Bronopol	-3.581	-3.581
C19H18N6O6S2	DB14725	Cefamandole nafate	-3.566	-3.566
C22H17F2N5OS	DB11633	Isavuconazole	-3.559	-3.559
C29H32Cl2N2O5S	DB13125	Lusutrombopag	-3.555	-3.555
C8H9FN2O3	DB09256	Tegafur	-1.753	-3.55
C19H22F3N5O2S	DB12015	Alpelisib	-3.549	-3.549
C10H14N2O2	DB14754	Solriamfetol	-3.531	-3.549
C12H13I3N2O2	DB09333	Iopodic acid	-3.467	-3.549
C20H23NO	DB13114	Amitriptylinoxide	-3.547	-3.547
C16H14O3	DB09214	Dexketoprofen	-3.542	-3.543
C32H35N5O5	DB09272	Eluxadoline	-2.248	-3.541
C14H18O3	DB09118	Stiripentol	-3.534	-3.534
B4Na2O7	DB14505	Sodium borate	-3.526	-3.526
C13H9Cl3N2O	DB11155	Triclocarban	-3.523	-3.523
C12H24N2O4S2	DB11164	Bicisate	-2.765	-3.518
C22H22N6O5S2	DB13682	Cefpirome	-3.515	-3.515
C20H26O2	DB09371	Norethynodrel	-3.507	-3.507
C25H31NO6	DB11921	Deflazacort	-3.502	-3.503
C10H13NO4S2	DB13284	Meticrane	-3.5	-3.501
C15H19BrN2O5Tc	DB09137	Technetium Tc-99m mebrofenin	-3.453	-3.499
C29H33FO9S	DB14703	Dexamethasone metasulfobenzoate	-3.494	-3.494
C16H10N2O8S2	DB11577	Indigotindisulfonic Acid	-3.49	-3.49
C28H41N3O3	DB12532	Oxetacaine	-3.42	-3.488
C20H19FN4O4	DB09047	Finaxofloxacin	-1.117	-3.487
C16H28N2O2	DB13288	Tromantadine	-1.241	-3.485
C38H50N6O9S	DB11575	Grazoprevir	-3.473	-3.48
C22H27ClFN7O4S	DB11718	Encorafenib	-3.042	-3.476
C29H50O2	DB14476	DL-alpha-Tocopherol	-3.474	-3.474
C24H23FN4O3	DB09074	Olaparib	-3.472	-3.472
C26H32N4O4S	DB11362	Selexipag	-3.464	-3.469
C19H21NS	DB09167	Dosulepin	-3.462	-3.466
C32H43N5O5	DB11275	Epicriptine	-1.712	-3.451
ClKO4	DB09418	Potassium perchlorate	-3.442	-3.442
C6H6O2	DB11085	Resorcinol	-3.425	-3.428
C35H46ClN5O9S	DB11586	Asunaprevir	-0.701	-3.419
C30H29ClN6O3	DB11828	Neratinib	-3.233	-3.415
C38H50N6O9S	DB11575	Grazoprevir	-0.695	-3.413
C21H18F3N3O5	DB11799	Bictegravir	-3.059	-3.412
C6H6O2	DB09526	Hydroquinone	-3.408	-3.408
C20H19FN4O4	DB09047	Finaxofloxacin	-3.206	-3.408
C6H10N2O2	DB09210	Piracetam	-3.397	-3.397
C20H25NO2	DB09123	Dienogest	-3.393	-3.393
C10H22O3	DB13163	Terpin hydrate	-3.379	-3.379
C7H11N3O3	DB12834	Secnidazole	-3.369	-3.369
C32H43N5O5	DB11274	Dihydro-alpha-ergocryptine	-1.631	-3.369
C49H55N9O7	DB11574	Elbasvir	-1.963	-3.354
C21H26N2O5	DB09080	Olodaterol	-3.341	-3.348
C6H5ClO	DB13154	Parachlorophenol	-3.336	-3.338
C14H12O3	DB14176	Benzylparaben	-3.304	-3.328
C10H8BrNO	DB13222	Tilbroquinol	-3.121	-3.328
C27H18InN3O3	DB09473	Indium In-111 oxyquinoline	-3.299	-3.317
C21H30O2	DB09061	Cannabidiol	-3.309	-3.309
C21H26FNO3	DB09148	Florbetaben (18F)	-3.305	-3.309
C27H33N2O7S2	DB13967	Patent Blue	-3.093	-3.309
C24H34O5	DB11622	Dehydrocholic acid	-3.304	-3.308
C20H41N5O7	DB13274	Micronomicin	-1.788	-3.306
C17H27NO3	DB09345	Pramocaine	-2.883	-3.304
C17H12I2O3	DB13277	Benziodarone	-0.762	-3.304
C30H29ClN6O3	DB11828	Neratinib	-1.486	-3.3
C27H34N4O	DB12492	Piritramide	-1.09	-3.3
C21H24O4	DB14083	Bisphenol A diglycidyl ether	-3.29	-3.29
C31H41N5O5	DB11273	Dihydroergocormine	-3.243	-3.287
C27H26ClF3N6O3	DB12095	Telotristat ethyl	-2.847	-3.285

C13H16ClNO	DB11823	Esketamine	-2.204	-3.285
C21H27NO2	DB08954	Ifenprodil	-3.283	-3.283
C29H35F3N2O3	DB12371	Siponimod	-0.681	-3.283
C14H19N3O	DB13216	Oxolamine	-1.172	-3.269
C22H26ClFO4	DB13158	Clobetasone	-3.268	-3.268
C14H12O6S	DB11185	Sulisobenzone	-1.642	-3.267
C12H13FN4O5	DB09327	Tegafur-uracil	-1.47	-3.267
C12H13I3N2O2	DB09333	Iopodic acid	-2.047	-3.26
C20H19FN4O4	DB09047	Finafloxacin	-2.333	-3.255
C8H8O3	DB14212	Methylparaben	-3.228	-3.252
C23H32O2	DB09124	Medrogestone	-3.25	-3.25
C12H13I3N2O3	DB09403	Iocetamic acid	-3.248	-3.249
C20H19F2N3O5	DB08930	Dolutegravir	-2.96	-3.247
C19H15F3N2O3	DB12020	Tecovirimat	-3.245	-3.245
C27H32F2N8	DB12001	Abemaciclib	-3.04	-3.242
C24H29NO5	DB09292	Sacubitril	-3.226	-3.24
C19H27NO3	DB12161	Deutetrabenazine	-3.185	-3.235
C4H7NaO3	DB09072	Sodium oxybate	-3.229	-3.231
C10H7Cl2NO	DB13306	Chlorquinaldol	-3.047	-3.228
C24H38N2O4	DB11915	Valbenazine	-2.55	-3.225
C14H10O4	DB09096	Benzoyl peroxide	-3.219	-3.219
C22H30O4	DB09015	Canrenoic acid	-3.213	-3.218
C11H14ClN5	DB14763	Cycloguanil	-1.188	-3.214
C13H13N3	DB14191	Diphenylguanidine	-3.211	-3.211
C5H7N3	DB11640	Amifampridine	-3.206	-3.208
C12H19NO	DB11587	Etafedrine	-1.715	-3.2
H32Mo7N6O28	DB11128	Ammonium molybdate	-3.191	-3.193
H3N	DB09326	Ammonia N-13	-3.191	-3.193
C24H25ClFN5O2	DB11963	Dacomitinib	-1.437	-3.187
AlO4P	DB14517	Aluminium phosphate	-3.145	-3.186
HNa2O4P	DB14502	Sodium phosphate, dibasic	-3.145	-3.186
CaH5O6P	DB14481	Calcium phosphate dihydrate	-3.145	-3.186
Ca3O8P2	DB11348	Calcium Phosphate	-3.145	-3.186
H2NaO4P	DB09449	Sodium phosphate, monobasic	-3.145	-3.186
HK2O4P	DB09414	Dipotassium phosphate	-3.145	-3.186
H2KO4P	DB09413	Monopotassium phosphate	-3.145	-3.186
H3O4P	DB09394	Phosphoric acid	-3.145	-3.186
C11H14O3	DB14084	Butylparaben	-3.164	-3.181
C28H37N3O3	DB11591	Bilastine	-1.425	-3.174
C14H7Cl2NO3	DB11644	Tafamidis	-3.172	-3.172
C18H22F2N4O	DB09040	Efinaconazole	-1.393	-3.17
C2H8N2	DB14189	Ethylenediamine	-2.951	-3.168
C29H44N8O3	DB12141	Gilteritinib	-0.487	-3.167
C26H38O4	DB14677	Gestonorone caproate	-3.159	-3.159
C16H25NO3	DB09205	Moxisylyte	-3.137	-3.157
C12H8N2O4Zn	DB11175	Zinc picolinate	-3.14	-3.15
C17H15NO5	DB13657	Benorilate	-3.148	-3.148
C28H27N3O3	DB13931	Netarsudil	-0.785	-3.147
C4H4FeO4	DB14489	Ferrous succinate	-3.145	-3.145
C21H30NO4	DB09300	Butylscopolamine	-3.145	-3.145
C12H19NO	DB11587	Etafedrine	-3.087	-3.138
C29H39ClN7O2P	DB12267	Brigatinib	-0.889	-3.137
C12H24N2O4S2	DB11164	Bicisate	-2.896	-3.136
C23H36N2O4	DB09039	Eliglustat	-0.452	-3.136
C7H7NO2	DB13882	Methyl nicotinate	-3.133	-3.133
C9H13NO	DB09352	Hydroxyamphetamine	-3.131	-3.131
C35H43N5O4	DB11855	Revefenacin	-1.28	-3.119
C22H28ClFO4	DB11750	Clobetasol	-3.116	-3.116
C5H4ClNO2	DB09257	Gimeracil	-3.114	-3.114
C32H34N4O6	DB11691	Naldemedine	-0.489	-3.114
C10H14CaO6	DB13800	Calcium levulinate	-3.111	-3.113
C15H18N2	DB14195	4-(Isopropylamino)diphenylamine	-2.84	-3.112
C8H9N3O4	DB09220	Nicorandil	-3.111	-3.111

C3H4O2	DB09348	Propiolactone	-3.104	-3.104
C21H21N3O3	DB12924	Ozenoxacin	-1.057	-3.104
C45H50ClN7O7S	DB11581	Venetoclax	-3.09	-3.101
C18H12CrN3O6	DB14529	Chromium nicotinate	-0.65	-3.098
CK2O3	DB13977	Potassium carbonate	-2.981	-3.092
CNa2O3	DB09460	Sodium carbonate	-2.981	-3.092
CLi2O3	DB14509	Lithium carbonate	-2.98	-3.092
CH24Al2Mg6O24	DB13322	Hydrotalcite	-2.98	-3.092
CHKO3	DB11098	Potassium bicarbonate	-2.98	-3.092
CMgO3	DB09481	Magnesium carbonate	-2.98	-3.092
C7H16N4O4S2	DB12473	Taurolidine	-2.518	-3.092
C12H13FN4O5	DB09327	Tegafur-uracil	-3.06	-3.089
C8H8O3	DB09543	Methyl salicylate	-3.001	-3.089
C17H19NO	DB12293	Nefopam	-1.621	-3.087
C49H54N8O8	DB11613	Velpatasvir	-0.824	-3.084
C44H32N4O4	DB11630	Temoporfin	-3.079	-3.079
C6H12O3	DB09117	Paraldehyde	-3.078	-3.078
C10H8BrNO	DB13222	Tilbroquinol	-2.352	-3.077
C7H6Cl2O	DB13269	Dichlorobenzyl alcohol	-3.076	-3.076
C11H17NO	DB11278	DL-Methylephedrine	-1.926	-3.074
C9H7NO	DB11145	Oxyquinoline	-0.993	-3.072
C27H18InN3O3	DB09473	Indium In-111 oxyquinoline	-0.993	-3.072
C18H12Cl2N2O	DB12792	Boscalid	-3.068	-3.068
C40H50N8O6	DB09102	Daclatasvir	-1.786	-3.068
C22H17ClN6O	DB11952	Duvelisib	-1.069	-3.066
C17H28N2O	DB08987	Etidocaine	-0.891	-3.064
C19H18FN3O	DB12332	Rucaparib	-0.876	-3.062
C24H29Cl2FO5	DB08973	Fluclorolone acetone	-3.06	-3.06
C22H29NO5	DB09089	Trimebutine	-2.812	-3.05
C10H12O4	DB12328	Cantharidin	-3.049	-3.049
C26H33NO6	DB09236	Lacidipine	-3.036	-3.036
C19H30O5	DB09350	Piperonyl butoxide	-3.032	-3.032
C20H34O5	DB12789	Dinoprost	-3.026	-3.029
C24H18F2N2O5	DB09280	Lumacaftor	-3.028	-3.028
C17H15ClO4	DB13873	Fenofibric acid	-3.027	-3.027
C23H17FN6O	DB11791	Capmatinib	-3.022	-3.027
FNa2O3P	DB09484	Sodium fluorophosphate	-0.928	-3.026
C18H21N3O	DB13225	Dibenzepin	-0.811	-3.022
C18H27NO3	DB09120	Zucapsaicin	-3.02	-3.02
C9H5I2NO	DB09115	Diiodohydroxyquinoline	-2.441	-3.02
C12H11I3N2O4	DB09346	Metrizoic acid	-3.016	-3.016
CK2O3	DB13977	Potassium carbonate	-1.962	-3.006
CNa2O3	DB09460	Sodium carbonate	-1.962	-3.006
CLi2O3	DB14509	Lithium carbonate	-1.962	-3.006
CH24Al2Mg6O24	DB13322	Hydrotalcite	-1.962	-3.006
CHKO3	DB11098	Potassium bicarbonate	-1.962	-3.006
CMgO3	DB09481	Magnesium carbonate	-1.962	-3.006
C25H26F6N2O2	DB09291	Rolapitant	-1.79	-3.005
C8H9FN2O3	DB09256	Tegafur	-2.969	-2.998
C23H28O6	DB14646	Prednisone acetate	-2.994	-2.994
C14H27NaO5S	DB13157	Sodium lauryl sulfoacetate	-2.99	-2.99
C40H52N2O4	DB13947	Testosterone enantate benzilic acid hydrazone	-2.982	-2.982
C30H32F6N4O	DB09048	Netupitant	-1.088	-2.98
C14H22N2O3	DB09069	Trimetazidine	-2.52	-2.976
C35H41N5O5	DB13345	Dihydroergocristine	-0.743	-2.975
C15H19NO2	DB09071	Tasimelteon	-2.967	-2.969
C41H50N6O2	DB11262	Bisotrizole	-2.948	-2.967
C26H26ClN3	DB11614	Rupatadine	-1.805	-2.967
C7H16N4O2	DB11815	Tilarginine	-2.966	-2.966
C16H14N2O3	DB13501	Bendazac	-2.964	-2.964
C13H18O2	DB09213	Dexibuprofen	-2.961	-2.962
C14H8N2S4	DB14201	2,2'-Dibenzothiazyl disulfide	-2.958	-2.958
C49H55N9O7	DB11574	Elbasvir	-1.568	-2.956

C18H15NO8S2	DB09268	Picosulfuric acid	-2.935	-2.947
C24H29N7O2	DB09073	Palbociclib	-2.475	-2.945
C21H22N6O	DB11978	Glasdegib	-2.318	-2.945
C41H50N6O2	DB11262	Bisoctrizole	-0.888	-2.938
C10H9N5O	DB11336	Kinetin	-0.939	-2.937
C27H34N4O	DB12492	Piritramide	-1.337	-2.933
C10H14N2O2	DB14754	Solriamfetol	-0.846	-2.932
C47H72NO10P	DB14096	1,2-icosapentoyl-sn-glycero-3-phosphoserine	-0.642	-2.926
C25H27N3O2S	DB09128	Brexiprazole	-1.984	-2.925
C9H7NO	DB11145	Oxyquinoline	-2.906	-2.924
C10H12CaN2Na2O8	DB14598	Edetate calcium disodium anhydrous	-2.9	-2.914
C11H12N2OS2	DB14202	Morpholinylmercaptobenzothiazole	-2.912	-2.912
C35H43N5O4	DB11855	Revefenacin	-2.84	-2.912
C20H27NO5	DB13279	Carbocromen	-2.899	-2.902
C40H50N8O6	DB09102	Daclatasvir	-1.65	-2.902
C16H25GdN4O8	DB09132	Gadoteric acid	-1.5	-2.902
C9H10O	DB14186	Cinnamyl alcohol	-2.899	-2.899
C12H18O	DB13908	Amylmetacresol	-2.89	-2.89
C20H22O3	DB09495	Avobenzone	-1.668	-2.885
C14H12O4	DB11221	Dioxybenzone	-1.178	-2.885
C29H44N8O3	DB12141	Gilteritinib	-0.624	-2.885
C38H8N2OS	DB13838	Noxytiolin	-2.882	-2.882
C13H12N2O3S	DB09355	Sulfabenzamide	-2.882	-2.882
CH6N2O3	DB11129	Carbamide peroxide	-2.877	-2.877
CH4N2O	DB09513	Urea C-14	-2.877	-2.877
CH4N2O	DB09510	Urea C-13	-2.877	-2.877
C36H51Cl2N3O4	DB14185	Aripiprazole lauroxil	-2.117	-2.876
C22H17ClN6O	DB11952	Duvelisib	-2.85	-2.871
C27H38O6	DB14632	Prednisolone tebutate	-2.863	-2.863
C9H16N2O2	DB13221	Apronalide	-2.862	-2.862
C20H33N3O3S	DB09097	Quinagolide	-0.841	-2.862
C5H11NO2S	DB13972	Racemethionine	-2.861	-2.861
FNa2O3P	DB09484	Sodium fluorophosphate	-2.836	-2.854
C14H12ClNO2	DB09216	Tolfenamic Acid	-2.848	-2.849
C16H21NO3	DB11181	Homatropine	-2.847	-2.847
C24H31NO4	DB11269	Diethylamino hydroxybenzoyl hexyl benzoate	-2.835	-2.847
C16H24N2	DB08944	Isoaminile	-0.993	-2.847
C12H18O2	DB11254	Hexylresorcinol	-2.841	-2.842
C3H3F5	DB13117	Pentafluoropropane	-2.827	-2.827
C17H26N2O4S	DB13273	Sultopride	-2.826	-2.827
C28H41N3O3	DB12532	Oxetacaine	-1.51	-2.824
C15H24N2O2	DB09085	Tetracaine	-2.81	-2.82
C14H9Cl2N3S2	DB08933	Luliconazole	-2.816	-2.816
C11H12I3NO2	DB08946	Iopanoic acid	-2.814	-2.814
C14H17N5O3S	DB14203	Disperse Blue 106	-2.807	-2.807
C11H17NO	DB11278	DL-Methylephedrine	-2.714	-2.806
C12H17NO	DB11282	Diethyltoluamide	-2.801	-2.801
C2H6O3S2	DB09110	Coenzyme M	-2.798	-2.8
C15H18I3NO3	DB09340	Tyropanoic acid	-2.796	-2.797
C9H12N2S	DB12667	Protionamide	-2.791	-2.792
C4H7Cl3O	DB11386	Chlorobutanol	-2.786	-2.786
C26H36O3	DB13954	Estradiol cypionate	-2.786	-2.786
C18H18ClN3S	DB13256	Clothiapine	-1.047	-2.778
C35H41N5O5	DB13345	Dihydroergocristine	-1.036	-2.778
C21H19FN6O2	DB12130	Lorlatinib	-2.276	-2.772
C28H36ClN5O3S	DB09063	Ceritinib	-2.771	-2.771
C11H11ClO3	DB13167	Alclofenac	-2.768	-2.769
C23H22ClN5O3	DB12364	Betrixaban	-2.759	-2.759
C10H10N2O	DB12243	Edaravone	-1.448	-2.756
C12H8N2O4Zn	DB11175	Zinc picolinate	-0.306	-2.754
C21H45N3	DB08958	Hexetidine	-2.318	-2.751
C9H10O3	DB13628	Ethyl hydroxybenzoate	-2.73	-2.748
C4H2FeO4	DB14491	Ferrous fumarate	-2.745	-2.745

C16H23NO2	DB08988	Ethoheptazine	-2.74	-2.745
C7H8O2	DB09516	Mequinol	-2.74	-2.74
C14H22N2O3	DB09069	Trimetazidine	-2.335	-2.737
C13H10N2O3S	DB11115	Ensulizole	-2.324	-2.735
C20H22O3	DB09495	Avobenzone	-2.452	-2.733
C21H19FN6O2	DB12130	Lorlatinib	-2.397	-2.733
C6H6Br2N2	DB14199	Bromothalonil	-2.726	-2.726
AuH4Na3O8S4	DB13743	Sodium aurotiosulfate	-2.619	-2.725
C21H34O2	DB11859	Brexanolone	-2.724	-2.724
C29H44N8O3	DB12141	Gilteritinib	-0.031	-2.723
C29H28F4N4O4	DB12070	Letermovir	-2.715	-2.716
C8H11NO5S	DB09324	Sulbactam	-2.715	-2.715
C7H5NS2	DB11496	2-mercaptobenzothiazole	-2.7	-2.7
C10H12O3	DB14177	Propylparaben	-2.681	-2.699
C40H80NO8P	DB09114	Colfosceril palmitate	-2.697	-2.697
C18H15NO8S2	DB09268	Picosulfuric acid	-0.357	-2.697
C17H12I2O3	DB13277	Benziodarone	-2.685	-2.693
C18H21ClN2	DB08936	Chlorcyclizine	-2.298	-2.693
C20H28O	DB12474	Lynestrenol	-2.69	-2.69
K2O4S	DB14499	Potassium sulfate	-2.681	-2.681
NiO4S	DB14180	Nickel sulfate	-2.681	-2.681
FeO4S	DB13257	Ferrous sulfate anhydrous	-2.681	-2.681
CrO4S	DB14530	Chromous sulfate	-2.681	-2.681
Fe2H10O17S3	DB11171	Ferric sulfate	-2.681	-2.681
BaO4S	DB11150	Barium sulfate	-2.681	-2.681
Al2O12S3	DB11239	Aluminum sulfate	-2.681	-2.681
Na2O4S	DB09472	Sodium sulfate	-2.681	-2.681
O4SZn	DB09322	Zinc sulfate	-2.681	-2.681
Al5H33Mg10O40S2	DB08938	Magaldrate	-2.681	-2.681
AlKO8S2	DB09087	Potassium alum	-2.681	-2.681
C20H25N3S	DB12710	Perazine	-0.336	-2.68
C22H23ClN2O8	DB09093	Chlortetracycline	-0.976	-2.679
C14H30O4S	DB11328	Tetradecyl hydrogen sulfate (ester)	-2.677	-2.677
C17H28N2O	DB08987	Etidocaine	-2.66	-2.675
C16H26N2O3	DB09342	Propoxycaïne	-0.677	-2.664
C18H12CrN3O6	DB14529	Chromium nicotinate	-2.649	-2.658
C20H31NO3	DB11186	Pentoxifyverine	-0.013	-2.657
C45H50ClN7O7S	DB11581	Venetoclax	-0.297	-2.655
C14H9Cl3N2O5	DB12245	Triclabendazole	-1.855	-2.652
C9H12ClN5O	DB09242	Moxonidine	-2.583	-2.65
C8H8O3	DB14212	Methylparaben	-0.726	-2.649
C7H16N4O4S2	DB12473	Taurolidine	-1.793	-2.644
C11H17NO	DB13624	Methoxyphenamine	-2.642	-2.642
C18H26N2O5Tc	DB09164	Technetium Tc-99m disofenin	-2.59	-2.636
C21H23BrFNO2	DB12401	Bromperidol	-0.382	-2.634
C19H18FN3O	DB12332	Rucaparib	-2.617	-2.632
C14H22N2O3	DB09069	Trimetazidine	-0.42	-2.632
C13H20N2O3S	DB09009	Articaine	-1.136	-2.631
C30H32F6N4O	DB09048	Netupitant	-2.602	-2.628
C4H10O2	DB14110	Butylene glycol	-2.623	-2.623
C22H27ClFN7O4S	DB11718	Encorafenib	-2.224	-2.613
C18H14Cl4N2O	DB08943	Isoconazole	-2.395	-2.603
C49H54F2N8O6	DB09027	Ledipasvir	-1.422	-2.603
C28H37N3O3	DB11591	Bilastine	-2.557	-2.599
C17H19NO	DB12293	Nefopam	-2.547	-2.599
C20H38O7S	DB11089	Docusate	-2.594	-2.594
C24H31FO6	DB14649	Dexamethasone acetate	-2.591	-2.591
C14H9Cl3N2O5	DB12245	Triclabendazole	-2.406	-2.587
C21H23BrFNO2	DB12401	Bromperidol	-2.571	-2.584
C23H30N2O4	DB09209	Pholcodine	-1.106	-2.579
C35H43N5O4	DB11855	Revefenacin	-0.969	-2.577
C24H29N3O8	DB12035	Sarecycline	0.055	-2.575
C32H34N4O6	DB11691	Naldemedine	-2.18	-2.571

C20H25NO	DB11609	Normethadone	-2.566	-2.57
C16H18N2O7S2	DB12343	Temocillin	-2.569	-2.569
C20H23CIN2O4	DB09555	Dexchlorpheniramine maleate	-2.568	-2.568
C18H18CINOS	DB09225	Zotepine	-2.563	-2.563
C26H23N7O2	DB11703	Acalabrutinib	-2.545	-2.559
C23H29NO3	DB12278	Propiverine	-2.549	-2.556
C19H22N2O3	DB13286	Bumadizone	-2.551	-2.551
C47H72NO10P	DB14096	1,2-icosapentoyl-sn-glycero-3-phosphoserine	-2.538	-2.55
C50H71N13O12	DB11842	Angiotensin II	-1.868	-2.546
C8H9ClO	DB11121	Chloroxylenol	-2.543	-2.545
C16H24N2	DB08944	Isoaminile	-2.518	-2.544
C17H25NO2	DB11096	Meradimate	-2.541	-2.541
C29H34Cl2N6O3S2	DB11995	Avatrombopag	-2.537	-2.541
C13H14Cl2O3	DB09064	Ciprofibrate	-2.537	-2.537
C12H12N4O3	DB11989	Benznidazole	-2.528	-2.528
C49H54F2N8O6	DB09027	Ledipasvir	-1.171	-2.528
C27H33N2O6S2	DB09136	Isosulfan blue	-2.309	-2.523
C38H46F4N6O9S	DB13879	Glecaprevir	-2.519	-2.522
C27H31FN4O8	DB12329	Eravacycline	0.011	-2.522
C13H10N2O3S	DB11115	Ensulizole	-1.954	-2.521
C7H10O6S3	DB13267	Ritiometan	-2.519	-2.519
C20H25N3S	DB12710	Perazine	-2.238	-2.518
C10H12O2	DB09086	Eugenol	-2.516	-2.516
C10H20O2	DB14187	Hydroxycitronellal	-2.514	-2.514
C12H14O4	DB11285	Ethyl ferulate	-2.512	-2.513
C6H8N2	DB14141	p-Phenylenediamine	-2.386	-2.511
C18H21N3O	DB13225	Dibenzepin	-2.492	-2.507
C19H20N4O	DB11793	Niraparib	-2.503	-2.503
C31H41N5O5	DB11273	Dihydroergocornine	-0.762	-2.5
C45H54F2N4O8	DB11641	Vinflunine	-0.283	-2.499
C19H19NS	DB13292	Pimethixene	-0.023	-2.498
C13H16ClNO	DB11823	Esketamine	-2.379	-2.483
C34H67O10P	DB11284	DL-dimyristoylphosphatidylglycerol	-2.47	-2.47
C16H19NO2	DB13219	Medifoxamine	-1.998	-2.464
C20H25N3S	DB12710	Perazine	-1.853	-2.463
C28H37N3O3	DB11591	Bilastine	0.01	-2.454
C17H24O3	DB11201	Menthyl salicylate	-2.449	-2.451
C27H30Cl2O6	DB14512	Mometasone furoate	-2.449	-2.449
C24H31N3OS	DB13213	Butaperazine	-1.839	-2.448
C40H53N7O5S2	DB09065	Cobicistat	-2.135	-2.446
C21H24O2	DB11619	Gestrinone	-2.437	-2.437
C49H55N9O7	DB11574	Elbasvir	-1.157	-2.437
C40H43N7O7S	DB09297	Paritaprevir	-2.429	-2.435
C32H55N4O	DB09552	Thonzonium	-2.43	-2.43
C40H50N8O6	DB09102	Daclatasvir	-1.559	-2.424
C16H28N2O2	DB13288	Tromantadine	-2.408	-2.422
C26H26N2O6S	DB09319	Carindacillin	-2.173	-2.422
C23H32O3	DB13956	Estradiol valerate	-2.416	-2.416
C20H24N	DB13720	Diphemanil	-2.405	-2.405
C30H44N2O10	DB13265	Hexobendine	-2.383	-2.404
C7H16N4O4S2	DB12473	Taurolidine	-1.835	-2.404
C4H4CINOS	DB14197	Methylchloroisothiazolinone	-2.403	-2.403
C18H40O4P2	DB11180	Tetofosmin	-1.543	-2.402
C36H84O10P4Tc	DB09160	Technetium Tc-99m tetrafosmin	-1.543	-2.402
C19H14F2N6O	DB11760	Talazoparib	-2.393	-2.393
C20H19FN8O2	DB08931	Riociguat	-2.389	-2.391
C9H10O3	DB13628	Ethyl hydroxybenzoate	-0.323	-2.388
C10H12O2	DB14188	Isoeugenol	-2.385	-2.386
C29H33FN2O4	DB09030	Vorapaxar	-2.352	-2.363
C12H17NO3	DB13346	Bufexamac	-2.356	-2.361
C9H17Cl2N4	DB14198	Quaternium-15	-2.355	-2.355
C6H18O4Si3	DB09512	Simethicone	-2.354	-2.354
C9H15NO2	DB13262	Aceclidine	-2.352	-2.354

C27H32F2N8	DB12001	Abemaciclib	0.3	-2.351
C10H13N3O2	DB13211	Guanoxan	-2.347	-2.347
C22H24N2O2	DB09488	Acrivastine	-2.338	-2.344
C17H21NO	DB11160	Phenyltoloxamine	-0.33	-2.343
C29H34NO2	DB09076	Umeclidinium	-2.332	-2.332
C21H15F4N5O2S	DB11901	Apalutamide	-2.329	-2.329
C13H16N2S2	DB14200	Thiohexam	-2.327	-2.327
C16H26N2O3	DB09342	Propoxycaine	-2.3	-2.321
C27H23F2N3O7S	DB13997	Baloxavir marboxil	-2.318	-2.318
C15H20O3	DB11207	Amiloxate	-2.312	-2.312
C4F10	DB12821	Perflubutane	-2.312	-2.312
C24H30CIN7O4S	DB09075	Edoxaban	-1.638	-2.308
C13H18CIN3O4S2	DB13532	Cyclopenanthiazide	-2.296	-2.306
C14H19N3O	DB13216	Oxolamine	-2.288	-2.306
C14H18O	DB14175	alpha-Amyl cinnamaldehyde	-2.304	-2.304
C21H35NO	DB09056	Amorolfine	-1.496	-2.303
C28H34O8S2	DB09534	Ecamsule	-2.299	-2.299
C10H12O3	DB14177	Propylparaben	-0.212	-2.294
C35H41N5O5	DB13345	Dihydroergocristine	-2.245	-2.292
C10H8OS3	DB13853	Anethole trithione	-2.281	-2.281
C29H42O6	DB14541	Hydrocortisone cypionate	-2.27	-2.27
C18H33NO3	DB11272	Methyl undecenoyl leucinate	-2.27	-2.27
Al2ClH7O6	DB11573	Aluminum chlorohydrate	-2.267	-2.267
H2O	DB09145	Water	-2.267	-2.267
H8O4Tc	DB09314	Technetium Tc-99m pertechnetate	-2.267	-2.267
C8H17FeN3O6S2	DB11197	Ferrous cysteine glycinate	-2.244	-2.258
C19H19NS	DB13292	Pimethixene	-2.245	-2.255
O2Si	DB11132	Silicon dioxide	-2.252	-2.252
C27H31FN4O8	DB12329	Eravacycline	-0.106	-2.248
C25H24N6O2	DB09053	Ibrutinib	-2.247	-2.247
C45H54F2N4O8	DB11641	Vinflunine	-2.043	-2.247
C11H14O3	DB14084	Butylparaben	-0.161	-2.244
F6S	DB11104	Sulfur hexafluoride	-2.242	-2.242
C15H26O	DB13153	Levomenol	-2.235	-2.235
C27H36N2O5	DB09083	Ivabradine	-2.234	-2.235
C15H12F3NO4S	DB12938	Isoxaflutole	-2.229	-2.229
C12H24N2O4S2	DB11164	Bicisate	-0.485	-2.229
C24H45BiO6	DB13910	Valproate bismuth	-2.223	-2.225
C32H39NO2	DB11742	Ebastine	0.281	-2.224
C20H25FN2O3	DB09149	Florbetapir (18F)	-2.216	-2.219
C21H38N	DB13282	Benzododecinium	-2.215	-2.215
C15H9FO2	DB13136	Fluindione	-2.213	-2.214
C23H29NO3	DB12278	Propiverine	0.379	-2.206
C17H28O5	DB13851	Artemotil	-2.204	-2.204
C26H26CIN3	DB11614	Rupatadine	-0.399	-2.204
C9H5I2NO	DB09115	Diiodohydroxyquinoline	-1.924	-2.203
C27H34N4O	DB12492	Piritramide	-2.105	-2.2
C36H51Cl2N3O4	DB14185	Aripiprazole lauroxil	-2.004	-2.197
C20H2Br4Cl4Na2O5	DB13911	Phloxine B	-2.195	-2.196
C36H84O10P4Tc	DB09160	Technetium Tc-99m tetrofosmin	-1.603	-2.196
C19H27NO3	DB12161	Deutetrabenazine	-0.698	-2.193
C6H9AlO6	DB14518	Aluminum acetate	-2.186	-2.189
C2H3KO2	DB14498	Potassium acetate	-2.186	-2.189
C4H6O4Zn	DB14487	Zinc acetate	-2.186	-2.189
C4H6MgO4	DB13996	Magnesium acetate	-2.186	-2.189
C4H14MgO8	DB09409	Magnesium acetate tetrahydrate	-2.186	-2.189
C2H3NaO2	DB09395	Sodium acetate	-2.186	-2.189
C13H19NO3	DB09185	Viloxazine	-0.254	-2.187
C15H23N3OS	DB13858	Dimazole	-0.173	-2.186
C36H84O10P4Tc	DB09160	Technetium Tc-99m tetrofosmin	-1.636	-2.182
C14H12O3	DB14176	Benzyiparaben	-0.26	-2.177
HLiO	DB14506	Lithium hydroxide	-2.175	-2.175
FeHO2	DB14695	Ferric oxyhydroxide	-2.175	-2.175

HKO	DB11153	Potassium hydroxide	-2.175	-2.175
HNaO	DB11151	Sodium hydroxide	-2.175	-2.175
H2MgO2	DB09104	Magnesium hydroxide	-2.175	-2.175
C18H40O4P2	DB11180	Tetrofosmin	-1.578	-2.171
C2HCl3	DB13323	Trichloroethylene	-2.17	-2.17
C20H33N3O3S	DB09097	Quinagolide	-0.088	-2.165
C29H44N8O3	DB12141	Gilteritinib	-2.136	-2.162
C27H33N2	DB11279	Brilliant green cation	-1.947	-2.161
C27H32F2N8	DB12001	Abemaciclib	-0.008	-2.161
C23H38O5	DB08964	Gemprost	-2.153	-2.153
ClO	DB11123	Hypochlorite	-2.153	-2.153
C14H21NO2	DB09088	Amylocaine	0.184	-2.152
C11H15NO2	DB11148	Butamben	-2.15	-2.15
C24H30ClN7O4S	DB09075	Edoxaban	-1.912	-2.142
C18H22N2S	DB09068	Vortioxetine	0.543	-2.136
C49H54N8O8	DB11613	Velpatasvir	-1.523	-2.126
C18H40O4P2	DB11180	Tetrofosmin	-1.571	-2.117
C21H22N6O	DB11978	Glasdegib	-1.665	-2.103
C24H19NO5	DB14627	Oxyphenisatin acetate	-2.092	-2.092
C26H23N7O2	DB11703	Acalabrutinib	0.139	-2.083
C14H21NO2	DB09088	Amylocaine	-2.067	-2.079
C15H24N2O2	DB09085	Tetracaine	0.341	-2.077
C15H20O3	DB13063	Parthenolide	-2.07	-2.07
C24H39N3O3Si3	DB11585	Drometrizole trisiloxane	-2.063	-2.063
C18H21ClN2	DB08936	Chlorcyclizine	-0.027	-2.059
C38H49N3O5	DB11206	Bemotrizinol	-2.043	-2.043
C18H21NO	DB11584	Pipradrol	-2.037	-2.041
C25H30N6O2	DB12147	Erdafitinib	-2.036	-2.036
C12H19NO4	DB14006	Choline salicylate	-2.024	-2.024
C5H14NO	DB09563	Choline C-11	-2.024	-2.024
C5H14ClNO	DB09277	Choline C 11	-2.024	-2.024
C24H44BCuF4N4O4	DB14106	Tetrakis(2-methoxyisobutylisocyanide)copper(I)	-2.02	-2.02
C36H66N6O6Tc	DB09161	Technetium Tc-99m sestamibi	-2.02	-2.02
C26H32N2O8	DB13711	Tritoqualine	-1.847	-2.014
H4OSi	DB11343	Silanol	-2.01	-2.01
C18H22O	DB11219	Enzacamene	-2.009	-2.009
C15H18N2	DB14195	4-(Isopropylamino)diphenylamine	-1.405	-1.997
C11H9B3N2O4	DB09133	Iothalamic acid	-1.994	-1.994
CHCl3	DB11387	Chloroform	-1.993	-1.993
C25H46N	DB11583	Cetalkonium	-1.992	-1.992
C32H39NO2	DB11742	Ebastine	-1.982	-1.991
C25H28O3	DB13953	Estradiol benzoate	-1.983	-1.983
C38H74NaO10P	DB14105	Sodium 1,2-Dipalmitoyl-sn-glycero-3-phospho-	-1.955	-1.956
C20H19F2N3O5	DB08930	Dolutegravir	-1.29	-1.915
C21H18F3N3O5	DB11799	Bictegravir	-1.375	-1.899
C17H21NO	DB11160	Phenyltoloxamine	-1.873	-1.893
C16H18ClN3S	DB09241	Methylene blue	-1.863	-1.882
C26H26F3N3O3	DB09143	Sonidegib	-1.875	-1.875
C41H67NO15	DB13179	Troleandomycin	-0.995	-1.871
C30H34N4O2	DB11363	Alectinib	-0.983	-1.863
C17H13N3O5S2	DB13248	Phthalylsulfathiazole	-1.565	-1.861
C35H38N4O6	DB09238	Manidipine	-1.719	-1.859
C31H52O3	DB14002	D-alpha-Tocopherol acetate	-1.849	-1.849
C13H15N3O4S	DB14033	Acetyl sulfisoxazole	-1.842	-1.842
C12H20N2S4	DB14174	Dipentamethylenethiuram disulfide	-1.842	-1.842
C6H12N2S3	DB14178	Tetramethylthiuram monosulfide	-1.836	-1.836
C26H41BrNO4	DB09090	Pinaverium	-1.83	-1.83
C18H14Cl4N2O	DB08943	Isoconazole	-1.1	-1.823
C40H50N8O6	DB09102	Daclatasvir	-0.696	-1.817
C27H33N2O6S2	DB09136	Isosulfan blue	-1.109	-1.815
C27H42NO2	DB11125	Benzethonium	-1.799	-1.799
C29H35F3N2O3	DB12371	Siponimod	-1.79	-1.797
C30H34N4O2	DB11363	Alectinib	-1.645	-1.797

C25H27N3O2S	DB09128	Brexpiprazole	-1.659	-1.794
C49H54N8O8	DB11613	Velpatasvir	-0.396	-1.781
C17H27NO3	DB09345	Pramocaine	-1.37	-1.771
C19H20Cl2N2O5	DB13258	Etofamide	-1.762	-1.762
AuH4Na3O8S4	DB13743	Sodium aurotiosulfate	-0.686	-1.76
C6H15NO3	DB13747	Trolamine	-0.452	-1.746
C24H31N3OS	DB13213	Butaperazine	0.6	-1.744
C16H18ClN3S	DB09241	Methylene blue	0.323	-1.743
C18H22F2N4O	DB09040	Efinaconazole	-1.703	-1.733
C14H20Br2N2	DB09019	Bromhexine	0.232	-1.716
C19H23N3O	DB09084	Benzylamine	-1.695	-1.695
C27H33N2	DB11279	Brilliant green cation	-0.981	-1.688
C17H20N2O2	DB11699	Tropisetron	-1.678	-1.683
C25H25F3N4O6	DB11637	Delamanid	0.688	-1.681
C12H17NO3	DB12911	Nicoboxil	-1.68	-1.68
C20H31NO3	DB11186	Pentoxifyverine	-1.671	-1.678
C17H27NO2	DB11570	Padimate O	-1.669	-1.669
C19H25N3O2S2	DB08967	Dimetotiazine	-1.664	-1.665
CO2	DB09157	Carbon dioxide	-1.66	-1.66
C9H8O	DB14184	Cinnamaldehyde	-1.66	-1.66
C19H28O8	DB09274	Artesunate	-1.658	-1.659
C29H38N4O6S	DB09320	Procaine benzylpenicillin	-1.657	-1.657
C24H31N3OS	DB13213	Butaperazine	-1.373	-1.653
C18H22N2S	DB09068	Vortioxetine	-1.641	-1.647
C45H54F2N4O8	DB11641	Vinflunine	-0.583	-1.642
C12H9NO2	DB12300	P-nitrobiphenyl	-1.639	-1.639
S8Tc	DB09397	Technetium Tc-99m sulfur colloid	-1.631	-1.631
S8	DB09353	Octasulfur	-1.631	-1.631
C23H30N8O	DB11730	Ribociclib	-1.556	-1.625
C21H24N2	DB13246	Quinupramine	-1.61	-1.61
C30H48O3	DB13946	Testosterone undecanoate	-1.596	-1.596
C49H54N8O8	DB11613	Velpatasvir	-0.382	-1.59
C23H23ClN6O2	DB09034	Suvorexant	-1.561	-1.561
C23H32Cl2N6O6P	DB14674	Estramustine phosphate	-1.391	-1.54
C21H35NO	DB09056	Amorolfine	-1.356	-1.531
C49H55N9O7	DB11574	Elbasvir	-0.158	-1.526
C27H42Cl2N2O6	DB14658	Chloramphenicol palmitate	-1.524	-1.524
C28H33N7O2	DB09330	Osimertinib	-1.507	-1.514
C57H65F5N10O8	DB13878	Pibrentasvir	-0.357	-1.501
CHI3	DB13813	Iodoform	-1.488	-1.488
C10H18O	DB14183	Geraniol	-1.484	-1.484
C10H16O	DB14156	Synthetic camphor	-1.475	-1.475
C27H40O3	DB13943	Testosterone cypionate	-1.467	-1.467
C32H43N5O5	DB11275	Epicriptine	-1.423	-1.466
C2H2F4	DB13116	Norflurane	-1.463	-1.463
C2H5Cl	DB13259	Ethyl chloride	-1.451	-1.451
C29H24Cl2N2O7S	DB11611	Lifitegrast	-1.45	-1.45
CO	DB11588	Carbon monoxide	-1.426	-1.426
C18H22N2	DB14196	N-Cyclohexyl-N'-phenyl-1,4-phenylenediamine	-1.217	-1.415
C31H38O7	DB11260	Diacetyl benzoyl lathyrol	-1.386	-1.386
C11H14N2S	DB11156	Pyrantel	-1.375	-1.376
C31H33N5O4	DB09079	Nintedanib	-0.543	-1.367
C18H26O3	DB09496	Octinoxate	-1.361	-1.361
C30H50O2	DB14555	Ursadiol	-1.333	-1.333
C4H10FeN2O8S	DB14501	Ferrous glycine sulfate	-1.31	-1.31
C4H8FeN2O4	DB11210	Ferrous bisglycinate	-1.31	-1.31
C2H8AlClNO4Zr	DB11200	Aluminum zirconium octachlorohydrax gly	-1.31	-1.31
C4H8MgN2O4	DB11189	Magnesium glycinate	-1.31	-1.31
C6H12N2S4	DB13245	Thiram	-1.307	-1.307
C40H53N7O5S2	DB09065	Cobicistat	-0.753	-1.282
C13H20N2O3S	DB09009	Articaine	-1.217	-1.267
C15H23N3OS	DB13858	Dimazole	-1.238	-1.258
C26H32N2O8	DB13711	Tritoqualine	-0.425	-1.257

O2	DB09140	Oxygen	-1.238	-1.238
C18H22N2	DB14196	N-Cyclohexyl-N'-phenyl-1,4-phenylenediamine	-0.489	-1.235
C26H26ClN3	DB11614	Rupatadine	-1.092	-1.215
C27H32F2N8	DB12001	Abemaciclib	-0.389	-1.207
C18H30O2	DB13854	Gamolenic acid	-1.198	-1.202
C24H25ClFN5O2	DB11963	Dacomitinib	0.099	-1.184
C21H26F3N5	DB09195	Lorpiprazole	-0.131	-1.172
C31H33N5O4	DB09079	Nintedanib	1.372	-1.138
C13H21NO6	DB11079	Trolamine salicylate	0.176	-1.117
C14H20Br2N2	DB09019	Bromhexine	-1.089	-1.112
C21H35N2O3	DB09376	Lapyrium	-1.103	-1.103
C49H55N9O7	DB11574	Elbasvir	0.168	-1.086
C13H10O3	DB11071	Phenyl salicylate	0.842	-1.052
C25H35NO5	DB12554	Mebeverine	-1.017	-1.02
C21H46NO4P	DB09031	Miltefosine	-0.998	-0.998
H2O2	DB11091	Hydrogen peroxide	-0.996	-0.996
C35H46ClN5O9S	DB11586	Asunaprevir	-0.961	-0.967
C26H26N2O6S	DB09319	Carindacillin	-0.329	-0.964
C24H31NO4	DB11269	Diethylamino hydroxybenzoyl hexyl benzoate	1.333	-0.956
C13H18ClN3O4S2	DB13532	Cyclopenthiiazide	1.49	-0.952
C37H34N2Na2O9S3	DB11183	Light green SF yellowish	-0.939	-0.941
Si	DB12982	Silicon	-0.915	-0.915
C26H40O3	DB13944	Testosterone enanthate	-0.912	-0.912
NO2	DB12529	Nitrite	-0.901	-0.901
C	DB09278	Activated charcoal	-0.889	-0.889
C21H28O2	DB09389	Norgestrel	-0.87	-0.87
C17H26ClNO	DB11642	Pitolisant	-0.837	-0.838
P	DB14151	Phosphorus	-0.812	-0.812
C25H25F3N4O6	DB11637	Delamanid	-0.758	-0.769
C23H36O3	DB14655	Drostanolone propionate	-0.755	-0.755
Bi5H9N4O22	DB13209	Bismuth subnitrate	-0.661	-0.661
CrN3O9	DB14527	Chromic nitrate	-0.661	-0.661
KNO3	DB11090	Potassium nitrate	-0.661	-0.661
C40H50N8O6	DB09102	Daclatasvir	0.517	-0.651
C35H38N4O6	DB09238	Manidipine	0.843	-0.55
C27H33N2O7S2	DB13967	Patent Blue	0.167	-0.542
C28H22ClF3N6O3	DB14568	Ivosidenib	-0.52	-0.52
C40H50N8O6	DB09102	Daclatasvir	0.376	-0.464
N2	DB09152	Nitrogen	-0.417	-0.417
C29H33FN2O4	DB09030	Vorapaxar	1.944	-0.413
C9H14N4O4	DB09282	Molsidomine	-0.405	-0.405
C21H38N	DB11073	Cetylpyridinium	-0.341	-0.341
HNO2	DB09112	Nitrous acid	-0.34	-0.34
C23H32Cl2NO6P	DB14674	Estramustine phosphate	0.674	-0.22
C31H35F6N4O5P	DB14019	Fosnetupitant	1.806	-0.175
C22H40NO	DB11594	Domiphen	-0.149	-0.149
C25H29NO3	DB11226	Ethylhexyl methoxycrylene	-0.079	-0.079
C11H20O2	DB11117	Undecylenic acid	0.067	0.063
C16H34O	DB09494	Cetyl alcohol	0.078	0.078
C16H25GdN4O8	DB09132	Gadoteric acid	0.183	0.118
C17H13N3O5S2	DB13248	Phthalylsulfathiazole	1.146	0.592
C14H11Cl2NO4	DB14638	Diloxanide furoate	0.644	0.644
C17H34O2	DB13966	Isopropyl myristate	0.772	0.772
C18H32O2	DB14104	Linoleic acid	0.981	0.977
C16H25NO3	DB09205	Moxisylyte	3.169	1.156
C22H19NO4	DB09020	Bisacodyl	1.187	1.176
C40H77O10P	DB11331	1-Palmitoyl-2-oleoyl-sn-glycero-3-(phospho-rac	1.195	1.195
C6H15NO3	DB13747	Trolamine	1.445	1.374
C10H11I2NO3	DB09366	Propylidone	1.414	1.414
C13H21NO6	DB11079	Trolamine salicylate	1.518	1.447
C18H40N	DB13970	Diocetyltrimonium	1.496	1.496
C22H29NO5	DB09089	Trimebutine	2.436	1.781
C32H48O4	DB13955	Estradiol dieneanthate	2.5	2.5

C31H33N5O4	DB09079	Nintedanib	4.503	3.649
C22H19NO4	DB09020	Bisacodyl	7.208	4.867
C41H67NO15	DB13179	Troleandomycin	5.432	5.279

FDA approved drugs with 6vw1, Table S6

FORMULA	DRUGBANK_ID	GENERIC_NAME	docking score	glide gscore
C23H45N5O14	DB01421	Paromomycin	-9.02	-10.01
C22H30MnN4O14P2	DB06796	Mangafodipir	-7.181	-9.089
C22H30MnN4O14P2	DB06796	Mangafodipir	-7.846	-9.032
C27H33N9O15P2	DB03147	Flavin adenine dinucleotide	-8.986	-8.986
C17H34N4O10	DB03615	Ribostamycin	-6.763	-8.781
C23H45N5O14	DB01421	Paromomycin	-6.056	-8.661
C27H30O16	DB01698	Rutin	-6.587	-8.507
C23H45N5O14	DB01421	Paromomycin	-7.422	-8.505
C22H30MnN4O14P2	DB06796	Mangafodipir	-5.945	-8.455
C23H45N5O14	DB01421	Paromomycin	-6.022	-8.213
C5H13O14P3	DB01632	5-O-phosphono-alpha-D-ribofuranosyl diphosp	-5.843	-8.179
C28H44N2O23	DB08818	Hyaluronic acid	-8.121	-8.121
C5H13O14P3	DB01632	5-O-phosphono-alpha-D-ribofuranosyl diphosp	-6.761	-8.042
C5H13O14P3	DB01632	5-O-phosphono-alpha-D-ribofuranosyl diphosp	-6.805	-8.038
C17H21N4O9P	DB03247	Flavin mononucleotide	-6.931	-8.006
C22H30MnN4O14P2	DB06796	Mangafodipir	-6.961	-7.985
C18H36N4O11	DB01172	Kanamycin	-6.414	-7.983
C18H36N4O11	DB01172	Kanamycin	-6.417	-7.931
C23H45N5O14	DB01421	Paromomycin	-6.113	-7.858
C23H23N7O5	DB06813	Pralatrexate	-7.787	-7.829
C12H22O11	DB02772	Sucrose	-7.817	-7.817
C27H30O16	DB01698	Rutin	-7.774	-7.803
C12H17N3O4S	DB01598	Imipenem	-7.746	-7.747
C18H36N4O11	DB01172	Kanamycin	-6.118	-7.669
C52H76O24	DB06810	Plicamycin	-5.89	-7.603
C17H25Cl2F3N5O12P3S	DB06441	Cangrelor	-5.256	-7.482
C23H45N5O14	DB01421	Paromomycin	-5.222	-7.467
C22H30MnN4O14P2	DB06796	Mangafodipir	-6.279	-7.465
C18H36N4O11	DB01172	Kanamycin	-7.231	-7.38
C21H39N7O12	DB01082	Streptomycin	-7.2	-7.364
C19H24N2O4	DB00983	Formoterol	-5.016	-7.324
C23H45N5O14	DB01421	Paromomycin	-5.179	-7.295
C5H13O14P3	DB01632	5-O-phosphono-alpha-D-ribofuranosyl diphosp	-7.113	-7.292
C52H76O24	DB06810	Plicamycin	-7.156	-7.208
C20H32N6O12S2	DB03310	Glutathione disulfide	-7.145	-7.149
C23H45N5O14	DB01421	Paromomycin	-4.736	-7.137
C26H27NO9	DB01177	Idarubicin	-7.104	-7.132
C33H38GdN3Na3O14P	DB06705	Gadofosveset trisodium	-5.733	-7.125
C17H34N4O10	DB03615	Ribostamycin	-5.521	-7.123
C17H34N4O10	DB03615	Ribostamycin	-5.475	-7.039
C28H54N8	DB06809	Plerixafor	-5.499	-6.973
C52H76O24	DB06810	Plicamycin	-4.839	-6.943
C11H15N5O5	DB01280	Nelarabine	-6.83	-6.83
C17H34N4O10	DB03615	Ribostamycin	-4.864	-6.762
C28H54N8	DB06809	Plerixafor	-4.09	-6.761
C6H17N2O12P4Sm	DB05273	Samarium (153Sm) lexicidronam	-6.687	-6.705
C33H38GdN3Na3O14P	DB06705	Gadofosveset trisodium	-4.537	-6.678
C9H13N5O4	DB01004	Ganciclovir	-6.654	-6.654
C5H15N2O3PS	DB01143	Amifostine	-5.018	-6.643
C21H24N4O2S	DB08893	Mirabegron	-5.769	-6.62
C7H9ClO6P2S	DB01133	Tiludronic acid	-5.18	-6.57
C14H22N6O5	DB01610	Valganciclovir	-5.821	-6.53
C6H12O6	DB04173	Fructose	-6.516	-6.516

C2H8O7P2	DB01077	Etidronic acid	-5.867	-6.506
C23H45N5O14	DB01421	Paromomycin	-5.052	-6.49
C22H28N4O6	DB01204	Mitoxantrone	-6.464	-6.464
Al2H4O9Si2	DB01575	Kaolin	-6.449	-6.449
C17H34N4O10	DB03615	Ribostamycin	-6.028	-6.449
C6H17N2O12P4Sm	DB05273	Samarium (153Sm) lexidronam	-3.824	-6.412
C19H26I3N3O9	DB01362	Iohexol	-6.407	-6.407
C28H34O15	DB04703	Hesperidin	-6.378	-6.378
C10H12FN5O4	DB01073	Fludarabine	-6.363	-6.363
C5H9NO4S	DB04339	Carbocysteine	-6.34	-6.347
C21H39N7O12	DB01082	Streptomycin	-5.437	-6.276
C18H34N2O6S	DB01627	Lincomycin	-6.247	-6.257
C17H25Cl2F3N5O12P3S	DB06441	Cangrelor	-6.175	-6.189
C14H22N6O5	DB01610	Valganciclovir	-5.955	-6.169
C23H45N5O14	DB01421	Paromomycin	-4.315	-6.165
C27H29NO11	DB00997	Doxorubicin	-6.126	-6.153
C23H45N5O14	DB01421	Paromomycin	-5.471	-6.102
C17H34N4O10	DB03615	Ribostamycin	-5.34	-6.06
C28H54N8	DB06809	Plerixafor	-3.343	-6.036
C15H24N4O6S2	DB06211	Doripenem	-5.608	-6.008
C17H21N4O9P	DB03247	Flavin mononucleotide	-5.9	-6.006
C47H74O19	DB01078	Deslanoside	-5.984	-5.984
C21H27N3O7S	DB01602	Bacampicillin	-5.227	-5.952
C23H28F2N6O4S	DB08816	Ticagrelor	-5.715	-5.937
C12H22O11	DB04465	Lactose	-5.913	-5.913
C22H30MnN4O14P2	DB06796	Mangafodipir	-3.425	-5.869
C18H23NO4	DB01102	Arbutamine	-5.848	-5.855
C25H24FNO4	DB08860	Pitavastatin	-5.844	-5.854
H4O7P2	DB04160	Pyrophosphoric acid	-3.516	-5.853
C6H10O6	DB04564	Gluconolactone	-5.827	-5.827
C52H74Cl2O18	DB08874	Fidaxomicin	-3.114	-5.796
C25H32F3N3O4	DB06207	Silodosin	-5.752	-5.755
C10H14N2O5	DB01265	Telbivudine	-5.731	-5.732
C17H21NO4	DB01288	Fenoterol	-5.707	-5.728
C21H22Cl2FN5O	DB08865	Crizotinib	-5.349	-5.685
C28H54N8	DB06809	Plerixafor	-4.42	-5.685
C9H11NO5	DB06262	Droxidopa	-5.673	-5.673
C38H50N6O5	DB01232	Saquinavir	-5.637	-5.65
C54H69N11O10S2	DB06791	Lanreotide	-4.94	-5.65
C22H30MnN4O14P2	DB06796	Mangafodipir	-4.151	-5.612
C7H9ClO6P2S	DB01133	Tiludronic acid	-5.534	-5.593
C22H21N8O8PS4	DB06590	Ceftaroline fosamil	-5.268	-5.569
C19H23N5O3	DB01157	Trimetrexate	-3.298	-5.565
C2H8O7P2	DB01077	Etidronic acid	-5.315	-5.561
C9H9Cl2N3O	DB01018	Guanfacine	-5.519	-5.519
C28H54N8	DB06809	Plerixafor	-3.376	-5.509
C22H21N8O8PS4	DB06590	Ceftaroline fosamil	-4.958	-5.503
C19H24N2O4	DB00983	Formoterol	-5.484	-5.496
C21H24N4O2S	DB08893	Mirabegron	-5.324	-5.492
C45H69N11O12S	DB01282	Carbetocin	-5.48	-5.48
C14H10N2O6	DB01250	Olsalazine	-5.479	-5.479
C9H17NO5	DB01783	Pantothenic acid	-5.471	-5.472
C12H14N4O4S	DB01299	Sulfadoxine	-4.381	-5.47
C17H21NO4	DB01288	Fenoterol	-2.831	-5.47
C18H34N2O6S	DB01627	Lincomycin	-3.051	-5.463
C22H30MnN4O14P2	DB06796	Mangafodipir	-3.386	-5.456
C25H22N4O4	DB06210	Eltrombopag	-5.444	-5.449
C9H8N2O2	DB01230	Pemoline	-5.446	-5.448
C5H15N2O3PS	DB01143	Amifostine	-5.405	-5.445
C22H31N3O5	DB01340	Cilazapril	-4.766	-5.421
C6H14O6	DB01638	Sorbitol	-5.405	-5.405
C28H54N8	DB06809	Plerixafor	-4.659	-5.397
C23H23N7O5	DB06813	Pralatrexate	-3.788	-5.383

C20H20N6O9S	DB04570	Latamoxef	-5.372	-5.373
C20H14I6N2O6	DB04711	Iodipamide	-5.363	-5.363
C8H8N4	DB01275	Hydralazine	-4.814	-5.338
C22H30MnN4O14P2	DB06796	Mangafodipir	-4.29	-5.315
C17H21NO4	DB01288	Fenoterol	-3.097	-5.314
C8H12N4O4	DB01262	Decitabine	-2.807	-5.309
C25H34FN3O2	DB05316	Pimavanserin	-5.304	-5.307
C33H38GdN3Na3O14P	DB06705	Gadofosveset trisodium	-5.214	-5.306
H4O7P2	DB04160	Pyrophosphoric acid	-5.052	-5.286
C19H20N2O3S	DB01132	Pioglitazone	-3.404	-5.279
C22H24CIN5O2	DB01184	Domperidone	-5.259	-5.277
C29H44O12	DB01092	Ouabain	-5.26	-5.26
C23H22F7N4O6P	DB06717	Fosaprepitant	-2.763	-5.25
C24H26FNO4	DB01095	Fluvastatin	-5.246	-5.247
C24H26N2O4	DB01136	Carvedilol	-5.18	-5.223
C52H74N16O15S2	DB02638	Terlipressin	-4.184	-5.219
C17H17N7O8S4	DB01330	Cefotetan	-5.207	-5.207
C11H13BrN2O5	DB03312	Brivudine	-5.172	-5.19
C32H40BrN5O5	DB01200	Bromocriptine	-4.309	-5.146
C18H18N8O7S3	DB01212	Ceftriaxone	-5.142	-5.142
C19H21CIFN3O3	DB06771	Besifloxacin	-3.807	-5.14
C8H11NO2	DB00988	Dopamine	-5.132	-5.132
C12H20N2O3	DB01291	Pirbuterol	-4.761	-5.124
C27H33N3O8	DB01301	Rolitetraacycline	-4.184	-5.122
C9H11NO4	DB01235	Levodopa	-5.099	-5.099
C6H8O7	DB04272	Citric acid	-5.082	-5.082
C27H33N3O8	DB01301	Rolitetraacycline	-4.831	-5.051
C4H3N3O4	DB03209	Oteracil	-2.868	-5.049
C16H15F6N5O	DB01261	Sitagliptin	-5.037	-5.04
C6H18N4	DB06824	Triethylenetetramine	-3.32	-5.038
C15H28N4O4	DB06614	Peramivir	-5.021	-5.021
C24H21F2NO3	DB00973	Ezetimibe	-5.018	-5.019
C18H21NO5	DB06814	Protokylol	-2.704	-5.012
C4H3N3O4	DB03209	Oteracil	-2.526	-5.005
C38H52N6O7	DB01072	Atazanavir	-4.964	-4.972
C19H24N2O4	DB01274	Arformoterol	-2.657	-4.965
C18H23NO4	DB01102	Arbutamine	-2.231	-4.944
C16H18FN3O2	DB04953	Ezogabine	-2.346	-4.928
C10H13N3	DB04840	Debrisoquine	-4.919	-4.919
C3H7NO3	DB03929	D-Serine	-4.917	-4.917
C35H44I6N6O15	DB01249	Iodixanol	-4.915	-4.915
C18H33CIN2O5S	DB01190	Clindamycin	-4.903	-4.914
C40H59NO11	DB08871	Eribulin	-2.341	-4.912
C8H10IN3	DB06704	Iobenguane	-4.907	-4.907
C13H18Cl2N2O2	DB01042	Melphalan	-4.9	-4.9
C18H21NO5	DB06814	Protokylol	-4.882	-4.894
C6H18N4	DB06824	Triethylenetetramine	-4.807	-4.894
C18H28N2O4	DB01193	Acebutolol	-4.873	-4.874
C16H19N3O4S	DB01333	Cefradine	-4.592	-4.869
C25H34O6	DB05013	Ingenol mebutate	-4.858	-4.858
C15H18N8O5	DB06213	Regadenoson	-4.856	-4.856
C9H7N7O2S	DB00993	Azathioprine	-3.108	-4.85
C30H34N2O3	DB06401	Bazedoxifene	-2.379	-4.835
C53H67N9O10S	DB01369	Quinupristin	-2.877	-4.83
C31H36N2O11	DB01051	Novobiocin	-2.403	-4.828
C12H18N2O2S	DB01154	Thiamylal	-4.783	-4.823
C12H18N4O7P2S	DB01987	Coccarboxylase	-4.716	-4.806
C14H8O4	DB04816	Dantron	-4.8	-4.8
C9H13N3O5	DB00987	Cytarabine	-4.784	-4.784
C16H15N2O6P	DB01320	Fosphenytoin	-4.727	-4.776
C15H25N3O	DB01255	Lisdexamfetamine	-4.678	-4.773
C18H18N6O8S3	DB01328	Cefonicid	-4.757	-4.757
C17H19N5O2	DB06193	Pixantrone	-4.74	-4.74

C24H25ClFN5O3	DB08916	Afatinib	-2.92	-4.735
C21H25ClO6	DB06292	Dapagliflozin	-4.731	-4.731
C16H22N2O3	DB01366	Procaterol	-2.87	-4.73
C12H21N3O5S3	DB01194	Brinzolamide	-2.399	-4.715
C9H13NO3	DB06707	Levonordefrin	-2.619	-4.714
C22H30MnN4O14P2	DB06796	Mangafodipir	-2.356	-4.705
C23H27N3O7	DB01017	Minocycline	-4.587	-4.698
C19H33NO2	DB08868	Fingolimod	-4.652	-4.695
C7H10N2O2S	DB06795	Mafenide	-4.662	-4.692
C20H33NO3	DB04822	Oxeladin	-4.683	-4.69
C26H27N5O2	DB06684	Vilazodone	-4.583	-4.685
C23H18ClF2N3O3S	DB08881	Vemurafenib	-4.236	-4.68
C35H35F2N8O5S	DB06636	Isavuconazonium	-2.773	-4.677
C13H21O5P	DB06716	Fospropofol	-3.266	-4.675
C24H25FO5S	DB08907	Canagliflozin	-4.666	-4.666
C8H12N4O4	DB01262	Decitabine	-4.237	-4.656
C20H32F2O5	DB01046	Lubiprostone	-4.649	-4.652
C29H39NO9	DB04865	Omacetaxine mepesuccinate	-3.602	-4.639
C5H4N4S	DB01033	Mercaptopurine	-4.516	-4.631
C19H25NOS	DB05271	Rotigotine	-1.909	-4.627
C17H15N3O6	DB01014	Balsalazide	-4.624	-4.625
C6H13NO5	DB01296	Glucosamine	-4.453	-4.62
C18H26ClN3O	DB01611	Hydroxychloroquine	-2.376	-4.617
C15H22FN3O6	DB01101	Capecitabine	-4.604	-4.604
C22H25F2NO4	DB04861	Nebivolol	-4.553	-4.573
C10H22N4	DB01170	Guanethidine	-4.547	-4.569
C12H21N3O5S3	DB01194	Brinzolamide	-2.83	-4.564
C22H29N3O6S	DB01604	Pivampicillin	-3.841	-4.562
C5H9N3	DB05381	Histamine	-4.054	-4.561
C25H27N9O8S2	DB01329	Cefoperazone	-4.549	-4.549
C24H34N2O	DB01244	Bepidil	-4.548	-4.548
C22H22F3N	DB01012	Cinacalcet	-4.531	-4.542
C6H13NO4	DB05018	Migalstat	-4.538	-4.54
C16H15N2O6P	DB01320	Fosphenytoin	-3.007	-4.54
C23H20F3N5O2S2	DB08912	Dabrafenib	-4.132	-4.537
C5H9NO4S	DB04339	Carbocisteine	-1.838	-4.532
C19H20N2O3S	DB01132	Pioglitazone	-4.086	-4.526
C21H23N3O2	DB06603	Panobinostat	-4.524	-4.524
C15H25N3O	DB01255	Lisdexamfetamine	-3.384	-4.517
C6H5GaO7	DB06784	Gallium citrate Ga 67	-4.516	-4.516
C25H36N6O4S	DB06267	Udenafil	-4.51	-4.515
C22H29FO5	DB01234	Dexamethasone	-4.514	-4.514
C12H20N2O3	DB01291	Pirbuterol	-3.988	-4.513
C16H21Cl2N3O2	DB06769	Bendamustine	-4.029	-4.473
C23H28F2N6O4S	DB08816	Ticagrelor	-3.752	-4.467
C23H26ClN7O3	DB06237	Avanafil	-2.182	-4.466
C12H18N2O2S	DB01154	Thiamylal	-2.439	-4.464
C4H4FN3O	DB01099	Flucytosine	-4.46	-4.46
C11H13BrN2O5	DB03312	Brivudine	-2.378	-4.447
C24H28F3N3O3	DB06608	Tafenoquine	-4.437	-4.444
C19H20ClNO4	DB01393	Bezafibrate	-4.438	-4.438
C35H35F2N8O5S	DB06636	Isavuconazonium	-2.661	-4.434
C23H16O11	DB01003	Cromoglicic acid	-4.433	-4.433
C41H64O13	DB01396	Digitoxin	-4.428	-4.428
C19H26N2S	DB01186	Pergolide	-2.088	-4.428
C6H10N2O5	DB06775	Carglumic acid	-4.424	-4.424
C16H24N10O4	DB01223	Aminophylline	-4.391	-4.423
C5H4N4S	DB01033	Mercaptopurine	-3.379	-4.418
C19H23N5O3	DB01157	Trimetrexate	-2.386	-4.415
C19H19ClN2	DB00967	Desloratadine	-4.411	-4.413
C2H4Cl3O4P	DB06753	Triclofos	-4.346	-4.41
C54H69N11O10S2	DB06791	Lanreotide	-4.196	-4.409
C7H7NO2	DB08797	Salicylamide	-2.76	-4.407

C15H22N2O	DB08918	Levomilnacipran	-4.403	-4.404
C28H54N8	DB06809	Plerixafor	-2.259	-4.404
C35H35F2N8O5S	DB06636	Isavuconazonium	-3.9	-4.403
C19H24N2O4	DB01274	Arformoterol	-4.388	-4.401
C5H9NO3S	DB06823	Tiopronin	-2.071	-4.393
C9H15NO3S	DB01197	Captopril	-4.386	-4.386
C23H30GdN3O11	DB08884	Gadoxetic acid	-3.497	-4.383
C22H29N3O6S	DB01604	Pivampicillin	-4.172	-4.38
C6H12O6	DB01914	D-glucose	-4.376	-4.376
C12H14N4O4S	DB06150	Sulfadimethoxine	-3.301	-4.375
C18H18N6O5S2	DB01326	Cefamandole	-4.371	-4.371
C14H10N4O5	DB01219	Dantrolene	-3.086	-4.367
C10H13NO4	DB00968	Methyl dopa	-4.362	-4.362
C14H10O5	DB01399	Salsalate	-2.467	-4.361
C24H28N2O3	DB05039	Indacaterol	-4.312	-4.355
C17H20N2S	DB01069	Promethazine	-4.353	-4.354
C12H20N2O3	DB01291	Pirbuterol	-2.528	-4.353
C10H16N2O8	DB00974	Edetic Acid	-2.136	-4.351
C5H9N3	DB05381	Histamine	-3.018	-4.349
C15H15NO2S	DB06413	Armodafinil	-4.337	-4.337
C52H74Cl2O18	DB08874	Fidaxomicin	-4.315	-4.333
C18H33ClN2O5S	DB01190	Clindamycin	-1.976	-4.332
C17H19FN2O2	DB06654	Safinamide	-4.142	-4.327
C17H18N4O	DB00969	Alosetron	-3.292	-4.326
C23H30GdN3O11	DB08884	Gadoxetic acid	-2.602	-4.325
C19H18N6O5S3	DB01066	Cefditoren	-4.323	-4.323
C56H87NO16	DB06287	Temsirolimus	-4.306	-4.307
C45H57NO14	DB06772	Cabazitaxel	-4.297	-4.299
C14H20N2O2	DB00960	Pindolol	-4.294	-4.295
C16H17N3O5S	DB01140	Cefadroxil	-4.073	-4.282
C16H23N5O	DB01079	Tegaserod	-4.272	-4.272
C24H32O6	DB01260	Desonide	-4.265	-4.265
C24H28N2O3	DB05039	Indacaterol	-2.481	-4.262
C20H14O4	DB04824	Phenolphthalein	-3.436	-4.26
C11H6ClN3O6	DB06794	Lodoxamide	-4.258	-4.258
C18H18ClNS	DB01239	Chlorprothixene	-4.244	-4.248
C9H7N7O2S	DB00993	Azathioprine	-3.878	-4.248
C8H12N2	DB06698	Betahistine	-4.245	-4.245
C17H18N4O	DB00969	Alosetron	-3.943	-4.238
C15H14N4O6S2	DB01415	Ceftibuten	-4.23	-4.23
C28H54N8	DB06809	Plerixafor	-1.799	-4.228
C10H22N4	DB01170	Guanethidine	-2.26	-4.223
C18H27NO3	DB06774	Capsaicin	-4.218	-4.219
C43H51N3O11	DB01220	Rifaximin	-3.417	-4.212
C38H50N6O5	DB01232	Saquinavir	-1.952	-4.212
C21H15N3O4	DB01609	Deferasirox	-4.203	-4.209
C6H13NO5	DB01296	Glucosamine	-3.366	-4.2
C26H27NO9	DB01177	Idarubicin	-2.357	-4.197
C20H24N2	DB08801	Dimetindene	-3.677	-4.191
C15H14N2O2	DB06802	Nepafenac	-4.186	-4.186
C18H20FN5O4	DB01155	Gemifloxacin	-2.583	-4.186
C23H30GdN3O11	DB08884	Gadoxetic acid	-3.13	-4.183
C29H26ClFN4O4S	DB01259	Lapatinib	-3.01	-4.178
C9H7N7O2S	DB00993	Azathioprine	-3.649	-4.175
C23H23N3O5	DB01030	Topotecan	-3.344	-4.175
C16H14N2O4	DB01025	Amlexanox	-2.054	-4.167
C5H6N2	DB06637	Dalfampridine	-4.154	-4.158
C23H30GdN3O11	DB08884	Gadoxetic acid	-1.699	-4.155
C24H28N2O3	DB05039	Indacaterol	-1.816	-4.154
C37H42F2N8O4	DB01263	Posaconazole	-4.132	-4.15
C16H24N10O4	DB01223	Aminophylline	-2.31	-4.143
C20H29FO3	DB01185	Fluoxymesterone	-4.142	-4.142
C19H25N5O4	DB01162	Terazosin	-1.897	-4.126

C11H17NO3	DB01064	Isoprenaline	-4.124	-4.124
C17H20O6	DB01024	Mycophenolic acid	-4.091	-4.122
C16H24N2O2	DB01618	Molindone	-2.657	-4.122
C18H20FN5O4	DB01155	Gemifloxacin	-4.075	-4.116
C4H3N3O4	DB03209	Oteracil	-4.03	-4.109
C16H20N6O	DB08895	Tofacitinib	-4.088	-4.099
C27H29F3O6S	DB08906	Fluticasone furoate	-4.092	-4.092
C11H11N5	DB01438	Phenazopyridine	-4.082	-4.088
C24H26N2O4	DB01136	Carvedilol	-2.512	-4.086
C10H15NO	DB01364	Ephedrine	-4.079	-4.085
C30H32N2O2	DB01081	Diphenoxylate	-3.7	-4.084
C53H83NO14	DB01590	Everolimus	-4.082	-4.083
C20H23N5O6S	DB01061	Azlocillin	-4.081	-4.081
C12H18N4O7P2S	DB01987	Cocarboxylase	-1.956	-4.078
C22H25CIN2OS	DB01624	Zuclopenthixol	-3.847	-4.075
C20H31NO4	DB06217	Vernakalant	-1.348	-4.074
C3H6O3	DB04398	Lactic acid	-4.072	-4.073
C13H21O5P	DB06716	Fospropofol	-3.995	-4.052
C21H32N2O	DB06718	Stanozolol	-3.661	-4.051
C16H20N6O	DB08895	Tofacitinib	-1.709	-4.05
C9H13NO3	DB06707	Levonordefrin	-4.024	-4.041
C17H20O6	DB01024	Mycophenolic acid	-2.264	-4.023
C15H18N2O	DB04864	Huperzine A	-2.902	-4.021
C15H24N4O6S2	DB06211	Doripenem	-3.587	-4.009
C11H16CIN5	DB01131	Proguanil	-2.017	-4.003
C20H32O5	DB01240	Epoprostenol	-3.998	-4
C8H14N2O2	DB01202	Levetiracetam	-3.999	-3.999
C14H16N2O6S3	DB01145	Sulfoxone	-3.998	-3.998
C14H17N3O	DB00998	Frovatriptan	-3.995	-3.995
C43H74N2O14	DB06145	Spiramycin	-1.456	-3.991
C5H9NO3S	DB06151	Acetylcysteine	-3.978	-3.978
C12H6Cl4O2S	DB04813	Bithionol	-2.417	-3.966
C6H11NO3	DB00992	Methyl aminolevulinate	-3.61	-3.962
C20H33N3O4	DB04846	Celiprolol	-3.96	-3.961
C13H11N3O4	DB08910	Pomalidomide	-3.958	-3.958
C14H10O5	DB01399	Salsalate	-3.932	-3.956
C22H30N2O5S2	DB01348	Spirapril	-3.799	-3.941
C21H25N3O2S	DB01224	Quetiapine	-3.841	-3.93
C18H19N3O5S	DB01150	Cefprozil	-3.648	-3.93
C14H12O3	DB01428	Oxybenzone	-3.892	-3.928
C16H14F3N3O2S	DB05351	Dexlansoprazole	-3.888	-3.908
C18H21N3O3S	DB01129	Rabeprazole	-2.204	-3.905
C34H50N4O9S	DB01764	Dalfopristin	-3.234	-3.892
C8H7CIN2O2S	DB01119	Diazoxide	-3.881	-3.889
C13H11N3	DB01123	Proflavine	-3.855	-3.886
C23H30GdN3O11	DB08884	Gadoxetic acid	-3.491	-3.879
C18H20FN3O4	DB01165	Ofloxacin	-3.735	-3.878
C33H35FN2O5	DB01076	Atorvastatin	-3.868	-3.87
C19H21NO4	DB01183	Naloxone	-2.781	-3.868
C18H15NO3	DB00991	Oxaprozin	-3.864	-3.865
C15H16Cl2N2O8	DB07565	Chloramphenicol succinate	-3.862	-3.863
C16H18FN3O3	DB01059	Norfloxacin	-3.76	-3.859
C17H19FN2O2	DB06654	Safinamide	-3.069	-3.847
C22H28FN3O6S	DB01098	Rosuvastatin	-3.843	-3.845
C12H12N2O3	DB01174	Phenobarbital	-3.664	-3.835
C11H14CIN	DB04871	Lorcaserin	-3.833	-3.834
C15H14N4O2S	DB06729	Sulfaphenazole	-3.779	-3.832
C27H29NO11	DB00997	Doxorubicin	-1.982	-3.822
C23H22F7N4O6P	DB06717	Fosaprepitant	-1.299	-3.818
C17H25NO3	DB01210	Levobunolol	-3.814	-3.815
C15H22O3	DB01241	Gemfibrozil	-3.8	-3.803
C22H25F2NO4	DB04861	Nebivolol	-1.776	-3.8
C3H7NO2	DB04827	Urethane	-3.799	-3.799

C18H20FN3O4	DB01137	Levofloxacin	-3.653	-3.797
C23H18CIF2N3O3S	DB08881	Vemurafenib	-3.417	-3.796
C9H5Cl2NO	DB01243	Chloroxine	-2.844	-3.792
C27H36O8	DB01130	Prednicarbate	-3.79	-3.79
C16H17BrN2	DB04832	Zimelidine	-3.755	-3.788
C30H21I7N2Na2O8	DB01583	Liotrix	-2.796	-3.784
C31H48O6	DB02703	Fusidic acid	-1.755	-3.784
C17H26N4O	DB01084	Emedastine	-3.488	-3.782
C16H19N3O5S	DB01060	Amoxicillin	-3.587	-3.779
C19H25N5O4	DB01162	Terazosin	-2.702	-3.776
C7H9NO2	DB08826	Deferiprone	-3.775	-3.775
C28H54N8	DB06809	Plerixafor	-1.585	-3.774
C23H22F7N4O6P	DB06717	Fosaprepitant	-3.321	-3.766
C15H16N2O6S2	DB01607	Ticarcillin	-3.761	-3.761
C20H24O2	DB00977	Ethinylestradiol	-3.759	-3.759
C2H4O3	DB03085	Glycolic acid	-3.757	-3.757
C16H14O3	DB01009	Ketoprofen	-3.753	-3.753
C25H34O6	DB01222	Budesonide	-3.752	-3.752
C18H14F4N2O4S	DB01128	Bicalutamide	-3.739	-3.739
C9H13N	DB01576	Dextroamphetamine	-3.737	-3.737
C10H8F2N4O	DB06201	Rufinamide	-3.733	-3.733
C17H25NO3	DB00979	Cyclopentolate	-1.708	-3.732
C16H32O2	DB03796	Palmitic Acid	-3.723	-3.727
H4O7P2	DB04160	Pyrophosphoric acid	-3.021	-3.722
C19H20N2O3S	DB01132	Pioglitazone	-3.237	-3.72
C17H27NO4	DB01203	Nadolol	-3.714	-3.715
C22H26ClN7O2S	DB01254	Dasatinib	-3.292	-3.714
C17H17ClN6O3	DB01198	Zopiclone	-3.359	-3.709
C13H21NO3	DB01001	Salbutamol	-3.706	-3.706
C13H15N3O4S	DB01382	Glymidine	-3.257	-3.702
C7H7NO2	DB08797	Salicylamide	-3.662	-3.7
C12H18N4O7P2S	DB01987	Coccarboxylase	-2.413	-3.698
C4H3N3O4	DB03209	Oteracil	-2.166	-3.697
C13H18ClNO	DB01156	Bupropion	-3.458	-3.696
C53H67N9O10S	DB01369	Quinupristin	-3.223	-3.696
C27H33N3O8	DB01301	Rolitetraacycline	-2.104	-3.688
C14H10BNO3	DB05219	Crisaborole	-3.682	-3.682
C10H16N2O3	DB01353	Butobarbital	-3.646	-3.681
C6H9NO6	DB01020	Isosorbide Mononitrate	-3.669	-3.669
C10H7F3O4	DB08814	Triflusal	-3.668	-3.668
C13H10N2O4	DB01041	Thalidomide	-3.667	-3.667
C6H11NO3	DB00992	Methyl aminolevulinate	-3.177	-3.652
C21H26NO4	DB06800	Methylnaltrexone	-1.071	-3.637
C20H26N2O2	DB01426	Ajmaline	-3.135	-3.633
C13H18N2O3	DB06218	Lacosamide	-3.631	-3.631
C14H12O3	DB02709	Resveratrol	-3.63	-3.63
C32H31BrN2O2	DB08903	Bedaquiline	-3.626	-3.63
C20H26N2O2	DB01426	Ajmaline	-3.198	-3.625
C8H11NO4S2	DB05057	Erdosteine	-3.621	-3.621
C17H27NO4	DB01214	Metipranolol	-3.619	-3.621
C21H25NO3	DB06230	Nalmefene	-1.671	-3.618
C26H26F2N2	DB04841	Flunarizine	-3.528	-3.616
C11H16N2O	DB01056	Tocainide	-3.459	-3.616
C16H23NO	DB01209	Dezocine	-3.606	-3.606
C16H18FN3O3	DB01059	Norfloxacin	-2.496	-3.601
C18H20FN3O4	DB01165	Ofloxacin	-2.38	-3.601
C31H48O6	DB02703	Fusidic acid	-3.579	-3.599
C20H27N	DB01616	Alverine	-3.593	-3.594
C5H9NO3S	DB06823	Tiopronin	-3.578	-3.589
C10H16NO	DB01010	Edrophonium	-2.291	-3.582
C4H11NO3	DB03754	Tromethamine	-2.927	-3.579
C2H4Cl3O4P	DB06753	Triclofos	-2.232	-3.578
C13H15N3O4S	DB01382	Glymidine	-3.194	-3.575

C12H6Cl4O2S	DB04813	Bithionol	-3.042	-3.573
C16H26N2O5S	DB01597	Cilastatin	-0.863	-3.573
C16H22N2O3	DB01366	Procaterol	-3.545	-3.571
C23H23N3O5	DB01030	Topotecan	-3.296	-3.564
C25H24FNO4	DB08860	Pitavastatin	-1.105	-3.561
C21H22Cl2FN5O	DB08865	Crizotinib	-3.06	-3.556
C21H25NO3	DB06230	Nalmefene	-3.522	-3.553
C16H19N3O5S	DB01060	Amoxicillin	-2.784	-3.55
C23H27N	DB01091	Butenafine	-3.413	-3.547
C23H23N3O5	DB01030	Topotecan	-2.27	-3.547
C21H26NO4	DB06800	Methylalantrexone	-3.529	-3.537
C11H16N2O	DB01056	Tocainide	-2.676	-3.537
C20H21FN6O5	DB06817	Raltegravir	-2.943	-3.536
C11H18N2O3	DB01351	Amobarbital	-1.812	-3.526
C19H28NO3	DB00986	Glycopyrronium	-3.519	-3.519
C39H37F6N3O2	DB08827	Lomitapide	-3.509	-3.512
C17H14Cl2F2N2O3	DB01656	Roflumilast	-3.511	-3.511
C19H22NO4S2	DB01409	Tiotropium	-3.489	-3.489
C28H24FN3O5	DB08875	Cabozantinib	-3.436	-3.481
C23H27FN4O3	DB01267	Paliperidone	-1.059	-3.481
C22H22N2O4	DB06403	Ambrisentan	-3.48	-3.48
C9H5ClINO	DB04815	Clioquinol	-2.683	-3.473
C22H30MnN4O14P2	DB06796	Mangafodipir	-2.125	-3.472
C3H8OS2	DB06782	Dimercaprol	-0.807	-3.463
C19H23N3O2	DB01253	Ergometrine	-3.208	-3.462
C18H20FN3O4	DB01165	Ofloxacin	-1.92	-3.462
C20H21NO4	DB01113	Papaverine	-3.369	-3.46
C16H14N2O4	DB01025	Amlexanox	-3.432	-3.449
C19H24N6O5S2	DB01413	Cefepime	-3.444	-3.444
C20H24N2	DB08801	Dimetindene	-3.058	-3.444
C17H19NO4	DB01192	Oxymorphone	-3.32	-3.44
C22H22O8	DB01179	Podofilox	-3.438	-3.438
C17H11N5	DB01006	Letrozole	-3.437	-3.437
C10H17NO2	DB01107	Methyprylon	-3.436	-3.436
C22H18N6	DB08864	Rilpivirine	-3.432	-3.432
C15H13ClFNO2	DB01283	Lumiracoxib	-3.429	-3.431
C20H30O2	DB06710	Methyltestosterone	-3.427	-3.427
C7H7NO2	DB02362	Aminobenzoic acid	-3.424	-3.426
C17H17N3O6S2	DB01139	Cefapirin	-3.41	-3.419
C12H13N3O2	DB01247	Isocarboxazid	-3.417	-3.417
C23H22F7N4O6P	DB06717	Fosaprepitant	-3.003	-3.415
C20H14O4	DB04824	Phenolphthalein	-3.233	-3.403
C21H23N7O2S	DB06589	Pazopanib	-0.759	-3.401
C23H29N3O2S	DB01063	Acetophenazine	-1.427	-3.397
C19H25NO2	DB06152	Nylidrin	-3.387	-3.395
C12H7Cl3O2	DB08604	Triclosan	-2.835	-3.394
C16H17BrN2	DB04832	Zimelidine	-1.673	-3.393
C21H27NO3	DB01182	Propafenone	-3.389	-3.392
C27H42N2O5S	DB04845	Ixabepilone	-3.387	-3.392
C28H29NO4S	DB06249	Arzoxifene	-0.929	-3.392
C15H18N2O	DB04864	Huperzine A	-3.288	-3.385
C7H10N2O2S	DB06795	Mafenide	-1.591	-3.381
C24H28N2O3	DB08820	Ivacaftor	-3.379	-3.379
C23H26ClN7O3	DB06237	Avanafil	-1.482	-3.379
C16H13Cl2NO4	DB06736	Aceclofenac	-3.378	-3.378
C22H24N2O7S	DB05676	Apremilast	-3.37	-3.37
C27H44O2	DB01436	Alfacalcidol	-3.368	-3.368
C24H45NO8	DB01160	Dinoprost tromethamine	-3.365	-3.368
C21H25ClN2O3	DB04890	Bepotastine	-3.362	-3.367
C22H30O5	DB00959	Methylprednisolone	-3.362	-3.362
C16H17N3O7S2	DB01331	Cefoxitin	-3.349	-3.349
C14H10F3NO2	DB02266	Flufenamic Acid	-3.346	-3.347
C18H20FN3O4	DB01137	Levofloxacin	-2.114	-3.335

C21H26NO3	DB04843	Mepenzolate	-3.332	-3.332
C28H54N8	DB06809	Plerixafor	-1.269	-3.324
C30H21I7N2Na2O8	DB01583	Liotrix	-3.199	-3.322
C22H18N4OS	DB06626	Axitinib	-3.318	-3.321
C14H16O3	DB01322	Kava	-3.317	-3.317
C32H38N2O8	DB01089	Deserpidine	-1.59	-3.315
C19H21NO4	DB01183	Naloxone	-3.19	-3.314
C28H29F2N3O	DB01100	Pimozide	-3.301	-3.308
C11H16ClN5	DB01131	Proguanil	-1.259	-3.308
C16H17N3O5S	DB01140	Cefadroxil	-2.582	-3.306
C7H15Cl2N2O2P	DB01181	Ifosfamide	-3.305	-3.305
C11H16ClN5	DB01131	Proguanil	-1.04	-3.305
C21H27NO	DB01231	Diphenidol	-3.303	-3.304
C19H21ClFN3O3	DB06771	Besifloxacin	-3.237	-3.303
C17H19N5	DB01217	Anastrozole	-3.299	-3.299
C25H43N13O10	DB06827	Viomycin	-2.888	-3.299
C19H21NS	DB06153	Pizotifen	-3.288	-3.296
C7H8O	DB06770	Benzyl alcohol	-3.293	-3.293
CH4N2O2	DB01005	Hydroxyurea	-3.284	-3.292
C26H23FIN5O4	DB08911	Trametinib	-3.286	-3.286
C16H16N4O8S	DB01112	Cefuroxime	-3.283	-3.283
C13H18Br2N2O	DB06742	Ambroxol	-3.273	-3.283
C16H15ClN2OS	DB01559	Clotiazepam	-3.279	-3.28
C17H25NO3	DB00979	Cyclopentolate	-3.26	-3.28
C5H7NO3	DB03088	Pidolic Acid	-3.276	-3.276
C34H50N4O9S	DB01764	Dalfopristin	-3.031	-3.268
C23H26ClN7O3	DB06237	Avanafil	-3.223	-3.261
C23H28F2N6O4S	DB08816	Ticagrelor	-0.722	-3.259
C31H36N2O11	DB01051	Novobiocin	-0.56	-3.259
C16H16N2O3S	DB04854	Febuxostat	-3.252	-3.253
C10H14O	DB02513	Thymol	-3.252	-3.252
C22H24BrFN4O2	DB05294	Vandetanib	-3.248	-3.248
C52H74Cl2O18	DB08874	Fidaxomicin	-0.762	-3.247
C15H17N5O6S2	DB01416	Cefpodoxime	-3.246	-3.246
C12H18Cl2N2O	DB01407	Clenbuterol	-3.239	-3.24
C6H6N2O	DB02701	Nicotinamide	-3.235	-3.235
C4H8O3	DB01440	gamma-Hydroxybutyric acid	-3.229	-3.231
C25H32N2O4	DB06274	Alvimopan	-3.224	-3.228
C17H19F2N3O3	DB00978	Lomefloxacin	-3.148	-3.218
C21H32O3	DB06412	Oxymetholone	-2.447	-3.217
C26H28Cl2N4O4	DB01026	Ketoconazole	-2.664	-3.213
C13H17N	DB01037	Selegiline	-2.097	-3.195
C11H12N4O2S	DB01581	Sulfamerazine	-0.771	-3.195
ClH4N	DB06767	Ammonium chloride	-3.191	-3.193
C22H32O4	DB01088	Iloprost	-3.19	-3.193
C10H16N2O3	DB01353	Butobarbital	-1.505	-3.193
C21H25ClN2O3	DB06282	Levocetirizine	-1.323	-3.182
C40H57N5O7	DB08889	Carfilzomib	-3.177	-3.18
C22H23NO7	DB06174	Noscapine	-3.013	-3.18
C32H40BrN5O5	DB01200	Bromocriptine	-0.584	-3.174
C9H23NO3PS	DB01057	Echothiophate	-3.172	-3.172
C25H25N5O4	DB06605	Apixaban	-3.171	-3.171
C17H18N6	DB08877	Ruxolitinib	-3.169	-3.169
C15H14FN3O3	DB01205	Flumazenil	-3.168	-3.169
C15H9FN2O3	DB05016	Ataluren	-3.167	-3.167
C22H31N3O5	DB01340	Cilazapril	-2.925	-3.164
C18H26ClN3O3	DB06480	Prucalopride	-0.453	-3.164
C19H20N2O3S	DB01132	Pioglitazone	-1.245	-3.163
C43H53NO14	DB01248	Docetaxel	-3.16	-3.162
C19H22FN3O4	DB01044	Gatifloxacin	-3.069	-3.162
C15H10O2	DB07776	Flavone	-3.16	-3.16
C26H27N5O2	DB06684	Vilazodone	-2.058	-3.153
C19H15NO6	DB01418	Acenocoumarol	-3.129	-3.15

C19H33NO2	DB08868	Fingolimod	-1.574	-3.15
C19H25NOS	DB05271	Rotigotine	-3.141	-3.147
C31H36N2O11	DB01051	Novobiocin	-3.131	-3.147
C11H12N2O3	DB02959	Oxitriptan	-3.145	-3.145
C19H22FN3O4	DB01044	Gatifloxacin	-1.996	-3.142
C8H8C13N3O4S2	DB01021	Trichlormethiazide	-2.892	-3.141
C17H17N3O6S2	DB01139	Cefapirin	-0.641	-3.141
C13H15NO2	DB01437	Glutethimide	-3.139	-3.139
C23H20N2O3S	DB01138	Sulfinpyrazone	-3.137	-3.139
C31H46O2	DB01022	Phylloquinone	-3.136	-3.136
C20H21FN6O5	DB06817	Raltegravir	-2.863	-3.135
C18H19N3O5S	DB01150	Cefprozil	-2.56	-3.135
C22H30MnN4O14P2	DB06796	Mangafodipir	-0.994	-3.129
C10H16NO	DB01010	Edrophonium	-3.057	-3.128
C18H34O2	DB04224	Oleic Acid	-3.12	-3.123
C13H18Br2N2O	DB06742	Ambroxol	-0.716	-3.122
C30H26F6N4O2	DB01419	Antrafenine	-1.383	-3.116
C13H11N3	DB01123	Proflavine	-1.346	-3.113
C12H12N2O3	DB01174	Phenobarbital	-2.283	-3.105
C6H6O	DB03255	Phenol	-3.101	-3.102
C29H26ClFN4O4S	DB01259	Lapatinib	-3.008	-3.097
C15H10ClN3O3	DB01068	Clonazepam	-3.096	-3.096
C12H7Cl3O2	DB08604	Triclosan	-2.804	-3.096
C15H12BrNO3	DB00963	Bromfenac	-3.095	-3.095
C23H30O6	DB01380	Cortisone acetate	-3.094	-3.094
C19H22F2N4O3	DB01208	Sparfloxacin	-3.012	-3.094
C3La2O9	DB06792	Lanthanum carbonate	-2.981	-3.092
CCaO3	DB06724	Calcium Carbonate	-2.981	-3.092
CHNaO3	DB01390	Sodium bicarbonate	-2.981	-3.092
C22H31NO	DB01036	Tolterodine	-3.089	-3.089
C21H15ClF4N4O3	DB08896	Regorafenib	-3.087	-3.087
C25H32ClN5O2	DB01149	Nefazodone	-2.683	-3.087
C24H40O4	DB01586	Ursodeoxycholic acid	-3.079	-3.083
C30H32Cl3NO	DB06708	Lumefantrine	-3.05	-3.074
C13H16N2O2	DB01065	Melatonin	-3.073	-3.073
C28H54N8	DB06809	Plerixafor	-0.599	-3.064
C13H18ClNO	DB01156	Bupropion	-2.394	-3.052
C22H26ClN7O2S	DB01254	Dasatinib	-0.954	-3.051
C10H15NO	DB01364	Ephedrine	-0.389	-3.051
C17H20ClNO	DB04837	Clofedanol	-3.046	-3.05
C17H17Cl2N	DB01104	Sertraline	-0.75	-3.048
C12H19N3O	DB01168	Procarbazine	-2.536	-3.046
C20H21F3N4O	DB04908	Flibanserin	-0.672	-3.045
C21H32N2O	DB06718	Stanozolol	-2.607	-3.042
C15H14N2O4S	DB05015	Belinostat	-0.779	-3.033
C16H18N2O4S	DB01053	Benzympenicillin	-3.032	-3.032
C24H40N8O4	DB00975	Dipyridamole	-3.028	-3.028
C16H12ClNO3	DB04812	Benoxaprofen	-3.027	-3.027
C21H26N2O3	DB01392	Yohimbine	-1.114	-3.019
C32H36N4O5	DB01346	Quinidine barbiturate	-0.742	-3.017
C7H8ClN3O4S2	DB00999	Hydrochlorothiazide	-0.764	-3.015
C14H12O3	DB04571	Trioxsalen	-3.01	-3.01
C11H13N	DB01626	Pargyline	-2.105	-3.007
C3La2O9	DB06792	Lanthanum carbonate	-1.962	-3.006
CCaO3	DB06724	Calcium Carbonate	-1.962	-3.006
CHNaO3	DB01390	Sodium bicarbonate	-1.962	-3.006
CH4N2O2	DB01005	Hydroxyurea	-0.507	-3.005
C19H18ClN3O5S	DB01147	Cloxacillin	-3.002	-3.002
C4H6N2	DB01213	Fomepizole	-2.999	-2.999
C32H38N2O8	DB01089	Deserpidine	-2.965	-2.998
C32H44O7	DB01410	Ciclesonide	-2.997	-2.997
C3H9NO3	DB06768	Ammonium lactate	-2.997	-2.997
C18H22O5S	DB04574	Estrone sulfate	-2.996	-2.996

C10H12O2	DB06819	Phenylbutyric acid	-2.994	-2.996
C26H29Cl2N5O3	DB06616	Bosutinib	-0.948	-2.996
C33H30N4O2	DB00966	Telmisartan	-2.279	-2.989
C10H11N3O3S	DB01015	Sulfamethoxazole	-0.453	-2.988
C12H19N3O	DB01168	Procarbazine	-2.194	-2.987
C18H20FN3O4	DB01165	Ofloxacin	-0.434	-2.986
C11H12N4O3S	DB06821	Sulfameter	-2.534	-2.982
C22H30N2O5S2	DB01348	Spirapril	-2.066	-2.982
C29H41F2N5O	DB04835	Maraviroc	-2.981	-2.981
C24H35N5O5	DB04898	Ximelagatran	-2.763	-2.981
C11H12N4O3S	DB06821	Sulfameter	-2.604	-2.979
C27H46O	DB04540	Cholesterol	-2.978	-2.978
C5H9N3	DB05381	Histamine	-2.523	-2.978
C9H13NO2	DB01031	Ethinamate	-2.977	-2.977
C27H37N3O7S	DB01264	Darunavir	-2.975	-2.975
C17H27N3O4S	DB06288	Amisulpride	-2.971	-2.972
C2H7NO3S	DB01956	Taurine	-2.971	-2.972
C14H14N2O	DB01011	Metirapone	-2.965	-2.97
C22H25N2O5	DB01116	Trimethaphan	-2.963	-2.963
C18H24O3	DB04573	Estriol	-2.962	-2.962
C16H18N2	DB04821	Nomifensine	-1.03	-2.961
C22H30MnN4O14P2	DB06796	Mangafodipir	-0.533	-2.958
C28H35NO3	DB08867	Ulipristal	-0.763	-2.957
C20H22N8O6S2	DB04918	Ceftobiprole	-2.954	-2.954
C24H32ClFO5	DB06786	Halcinonide	-2.953	-2.953
C3H8O2	DB01839	Propylene glycol	-2.953	-2.953
C28H28N2O2	DB01501	Difenoxin	-0.785	-2.953
C21H26N2O3	DB01392	Yohimbine	-2.927	-2.952
C3H8O	DB03175	Propyl alcohol	-2.95	-2.95
C18H20FN3O4	DB01137	Levofloxacin	-0.394	-2.946
C16H21Cl2N3O2	DB06769	Bendamustine	-2.562	-2.945
C11H12Cl2N2O	DB04948	Lofexidine	-2.938	-2.94
C18H15Cl3N2S	DB06820	Sulconazole	-2.608	-2.939
C28H29NO4S	DB06249	Arzoxifene	-0.251	-2.938
C22H32O3	DB01420	Testosterone propionate	-2.937	-2.937
C38H69NO13	DB01211	Clarithromycin	-0.301	-2.936
C19H18N2O4S	DB08439	Parecoxib	-2.918	-2.935
C2H3Cl3O2	DB01563	Chloral hydrate	-2.934	-2.934
C17H21NO	DB01075	Diphenhydramine	-0.695	-2.932
C12H13NO2	DB05246	Methsuximide	-2.928	-2.928
C15H11N3O3	DB01595	Nitrazepam	-2.928	-2.928
C26H44O4	DB05990	Obeticholic acid	-2.921	-2.925
C6H12F2N2O2	DB06243	Eflornithine	-2.639	-2.919
C28H44O3	DB08804	Nandrolone decanoate	-2.914	-2.914
C10H16N2O8	DB00974	Edetic Acid	-2.9	-2.914
C11H20N2O2	DB05541	Brivaracetam	-2.912	-2.912
C25H36N3O9PS	DB01319	Fosamprenavir	-2.838	-2.912
C16H18N4O2	DB04820	Nialamide	-2.906	-2.906
C13H19ClN2O2	DB01161	Chloroprocaine	-2.883	-2.904
C19H19N	DB01619	Phenindamine	-1.107	-2.901
C21H23Cl2NO6	DB04920	Clevidipine	-2.9	-2.9
C13H18O2	DB01050	Ibuprofen	-2.897	-2.897
C23H32O4	DB06780	Desoxycorticosterone acetate	-2.892	-2.892
C58H66N10O9	DB06663	Pasireotide	-2.892	-2.892
C18H26ClN3O	DB01611	Hydroxychloroquine	-1.187	-2.89
C4H9NO2	DB02530	gamma-Aminobutyric acid	-2.886	-2.886
C19H29IO2	DB01187	Iophendylate	-2.879	-2.879
C19H25NO2	DB06152	Nylidrin	-0.311	-2.879
CH4N2O	DB03904	Urea	-2.877	-2.877
C30H32Cl3NO	DB06708	Lumefantrine	-0.967	-2.868
C16H20N2	DB01620	Pheniramine	-2.866	-2.866
C9H17NO4	DB08842	Acetylcarnitine	-2.861	-2.861
C19H23N3O2	DB01253	Ergometrine	-2.233	-2.859

C3H4C12F2O	DB01028	Methoxyflurane	-2.858	-2.858
C5H11NO2S	DB02893	D-Methionine	-2.856	-2.856
C12H12N2O2S	DB04880	Enoximone	-2.853	-2.853
C15H14N2O4S	DB05015	Belinostat	-0.314	-2.846
C20H26N2O2	DB01426	Ajmaline	-1.306	-2.843
C16H14F3N3O2S	DB05351	Dexlansoprazole	-0.805	-2.838
C28H35NO3	DB08867	Ulipristal	-2.822	-2.837
C18H23NO3	DB01551	Dihydrocodeine	-2.822	-2.836
C21H25N3O2S	DB01224	Quetiapine	-1.655	-2.836
C10H12CIN3O3S	DB01325	Quinethazone	-2.83	-2.832
C34H41N7O5	DB06695	Dabigatran etexilate	-1.359	-2.83
C22H27NO2	DB01406	Danazol	-2.829	-2.829
C29H31F2N3O	DB04842	Fluspirilene	-2.822	-2.827
C19H22F2N4O3	DB01208	Sparfloxacin	-1.617	-2.827
C23H33N2O	DB01625	Isopropamide	-2.826	-2.826
C22H25NO6	DB01394	Colchicine	-2.824	-2.824
C10H9N3O	DB01427	Amrinone	-2.819	-2.819
C14H12O3S	DB01600	Tiaprofenic acid	-2.819	-2.819
C26H30NO4S2	DB08897	Aclidinium	-2.815	-2.815
C30H26F6N4O2	DB01419	Antrafenine	-0.841	-2.812
C17H20BrNO	DB01237	Bromodiphenhydramine	-0.585	-2.81
C20H21FN2O	DB01175	Escitalopram	-2.807	-2.809
C22H25CIN2OS	DB01624	Zuclopthixol	-1.309	-2.809
C30H26F6N4O2	DB01419	Antrafenine	-2.211	-2.808
C18H26CIN3O	DB01611	Hydroxychloroquine	-2.753	-2.803
C18H20FN3O4	DB01137	Levofloxacin	-1.26	-2.802
C24H31NO4	DB06751	Drotaverine	-2.8	-2.8
C25H28N8O2	DB08882	Linagliptin	-2.798	-2.799
C16H26N2O5S	DB01597	Cilastatin	-2.792	-2.799
C34H41N7O5	DB06695	Dabigatran etexilate	-0.439	-2.799
C18H25N3O2	DB06335	Saxagliptin	-2.685	-2.797
C14H21N3O3	DB01096	Oxamniquine	-2.793	-2.793
C16H21NO2	DB00980	Ramelteon	-2.787	-2.787
C20H21NO4	DB01113	Papaverine	-1.631	-2.785
C24H31NO	DB05812	Abiraterone	-2.763	-2.784
C21H23N3OS	DB01608	Periciazine	-2.779	-2.78
C26H28Cl2N4O4	DB01026	Ketoconazole	-0.081	-2.779
C16H18N2	DB04821	Nomifensine	-2.752	-2.775
C14H12F3N3O5	DB05154	Pretomanid	-2.774	-2.774
C6H12F2N2O2	DB06243	Eflornithine	-2.192	-2.771
C10H9AgN4O2S	DB05245	Silver sulfadiazine	-2.612	-2.767
C24H25ClFN5O3	DB08916	Afatinib	-1.857	-2.76
C2H2Cl2O2	DB08809	Dichloroacetic acid	-2.757	-2.757
C18H29NO2	DB01359	Penbutolol	-2.754	-2.755
C19H14Cl2N2O3S	DB08828	Vismodegib	-2.754	-2.754
C24H26ClFN4O	DB06144	Sertindole	-2.739	-2.744
C20H20FNO3S	DB06209	Prasugrel	-2.518	-2.744
C16H12O3	DB01125	Anisindione	-0.401	-2.743
C28H24FN3O5	DB08875	Cabozantinib	-1.192	-2.742
C15H21N3O	DB01087	Primaquine	-2.741	-2.741
C14H20N2O3	DB02546	Vorinostat	-2.74	-2.74
C21H25CIN2O3	DB06282	Levocetirizine	-2.27	-2.734
C27H40O4	DB06789	Hydroxyprogesterone caproate	-2.728	-2.728
C10H21N	DB06714	Propylhexedrine	-2.728	-2.728
C19H19N	DB01619	Phenindamine	-2.24	-2.724
C37H48N4O5	DB01601	Lopinavir	-2.723	-2.723
C18H15CIN2O6S2	DB06268	Sitaxentan	-2.716	-2.716
C20H21F3N4O	DB04908	Flibanserin	-2.703	-2.714
C32H40BrN5O5	DB01200	Bromocriptine	-2.534	-2.713
C16H12FN3O3	DB01544	Flunitrazepam	-2.71	-2.71
C13H12N2O5S	DB04743	Nimesulide	-2.51	-2.71
C14H12O3	DB01428	Oxybenzone	-1.027	-2.708
C6H12N4	DB06799	Methenamine	-0.444	-2.707

C11H16N2O2	DB01085	Pilocarpine	-1.947	-2.703
C4H3F7O	DB01236	Sevoflurane	-2.701	-2.701
C11H12ClNO3S	DB01178	Chlormezanone	-2.7	-2.7
C11H16N2O2	DB01085	Pilocarpine	-2.503	-2.697
C17H17ClN6O3	DB01198	Zopiclone	-2.218	-2.696
C19H18ClN3O5S	DB06228	Rivaroxaban	-2.694	-2.694
C30H24N4O8	DB08822	Azilsartan medoxomil	-2.69	-2.69
C23H27FN4O3	DB01267	Paliperidone	-2.68	-2.69
C16H27NO6	DB08872	Gabapentin enacarbil	-2.684	-2.687
C22H27FN4O2	DB01268	Sunitinib	-2.682	-2.686
C19H20N2O3	DB03585	Oxyphenbutazone	-0.13	-2.684
C14H23NO	DB06204	Tapentadol	-2.683	-2.683
C33H30N4O2	DB00966	Telmisartan	-0.526	-2.683
CuO4S	DB06778	Cupric sulfate	-2.681	-2.681
C9H10N2O2	DB01121	Phenacemide	-2.675	-2.675
C26H29Cl2N5O3	DB06616	Bosutinib	-2.561	-2.674
C27H33N3O8	DB01301	Rolitetraacycline	-0.25	-2.672
C13H13N5O5S2	DB01332	Ceftizoxime	-2.671	-2.671
C8H8N4	DB01275	Hydralazine	-2.34	-2.665
C13H21N3O	DB01035	Procainamide	-2.659	-2.663
C18H26ClN3O3	DB06480	Prucalopride	-2.652	-2.658
C23H29N3O2S	DB01063	Acetophenazine	-2.321	-2.657
C17H19F2N3O3	DB00978	Lomefloxacin	-1.293	-2.648
C43H65N5O10	DB00976	Telithromycin	-2.367	-2.645
C12H14N4O4S	DB06150	Sulfadimethoxine	-0.759	-2.644
C19H28O2	DB01708	Prasterone	-2.642	-2.642
C9H11NO2	DB01086	Benzocaine	-2.641	-2.641
C19H27NO3	DB04844	Tetrabenazine	-2.591	-2.641
C28H22F3N7O	DB04868	Nilotinib	-1.717	-2.641
C40H59NO11	DB08871	Eribulin	-2.631	-2.639
C16H19N3O4S	DB01333	Cefradine	-2.054	-2.639
C24H23ClO2	DB04938	Ospemifene	-2.638	-2.638
C9H17NO2	DB00996	Gabapentin	-2.637	-2.637
C9H10Cl2N4	DB00964	Apraclonidine	-2.632	-2.636
C25H32ClFO5	DB01013	Clobetasol propionate	-2.633	-2.633
C32H36N4O5	DB01346	Quinidine barbiturate	-2.618	-2.632
C16H13Cl3N2OS	DB01007	Tioconazole	-2.017	-2.632
C18H20N2O6	DB01054	Nitrendipine	-2.63	-2.63
C35H35F2N8O5S	DB06636	Isavuconazonium	-2.197	-2.629
C27H40O3	DB02300	Calcipotriol	-2.628	-2.628
C20H18NO4	DB04115	Berberine	-2.625	-2.625
C9H5Cl2NO	DB01243	Chloroxine	-2.489	-2.623
C19H21N3O	DB06766	Alcaftadine	-2.613	-2.621
C36H53N7O6	DB05521	Telaprevir	-2.62	-2.62
C13H19N5	DB06762	Pinacidil	-2.615	-2.62
C17H18N4O	DB00969	Alosetron	-1.717	-2.62
C10H12N4O5S	DB01606	Tazobactam	-2.618	-2.618
C13H12N2O5S	DB04743	Nimesulide	-1.872	-2.615
C19H21N3O	DB06766	Alcaftadine	-0.095	-2.614
C33H30N4O2	DB00966	Telmisartan	-0.741	-2.613
C11H13ClF3N3O4S3	DB01324	Polythiazide	-2.607	-2.61
C22H23NO7	DB06174	Noscapine	-1.777	-2.61
C16H25NO2	DB06700	Desvenlafaxine	-2.608	-2.608
C17H24O3	DB04838	Cyclandelate	-2.606	-2.606
C27H34F2O7	DB06781	Difluprednate	-2.605	-2.605
C21H16F4N4O2S	DB08899	Enzalutamide	-2.6	-2.6
C13H17N3O	DB01424	Aminophenazone	-2.535	-2.597
C21H27N5O4S	DB01067	Glipizide	-0.627	-2.596
C23H36N2O2	DB01216	Finasteride	-2.593	-2.593
C13H17N3O	DB01424	Aminophenazone	-1.221	-2.588
C17H19NO4	DB01192	Oxymorphone	-1.503	-2.586
C13H16ClNO	DB01221	Ketamine	-1.504	-2.585
C13H8Cl2N2O4	DB06803	Niclosamide	-1.256	-2.584

C3H8OS2	DB06782	Dimercaprol	-2.572	-2.578
C28H29F2N3O	DB01100	Pimozide	0.067	-2.578
C14H18N6O	DB01048	Abacavir	-2.571	-2.576
C13H17N3O4S	DB04817	Metamizole	-2.571	-2.573
C13H17CIN2O2	DB01171	Moclobemide	-2.383	-2.572
C20H33NO3	DB04822	Oxeladin	0.072	-2.572
C14H10N4O5	DB01219	Dantrolene	-2.498	-2.57
C30H26F6N4O2	DB01419	Antrafenine	-2.206	-2.565
C21H23NO5	DB01452	Diamorphine	-1.214	-2.565
C20H24O2	DB00990	Exemestane	-2.564	-2.564
C28H22F3N7O	DB04868	Nilotinib	-2.42	-2.56
C38H52N6O7	DB01072	Atazanavir	0.02	-2.557
C18H21N3O3S	DB01129	Rabeprazole	-2.52	-2.555
C28H44O2	DB06410	Doxercalciferol	-2.551	-2.551
C15H21N3O3S	DB01120	Gliclazide	-0.622	-2.545
C18H23NO	DB01173	Orphenadrine	-0.304	-2.541
C20H20FNO3S	DB06209	Prasugrel	-1.859	-2.539
C22H25CIN2OS	DB01624	Zuclopenthixol	-1.691	-2.538
C26H26F2N2	DB04841	Flunarizine	-1.316	-2.537
C19H26O3	DB08905	Formestane	-2.534	-2.534
C12H14N4O3S	DB01298	Sulfacytine	-0.878	-2.533
C19H27NO3	DB04844	Tetrabenazine	-1.034	-2.529
C21H25NO3	DB06230	Nalmefene	0.033	-2.523
C16H11CIN4	DB01215	Estazolam	-2.521	-2.522
C12H6Cl4O2S	DB04813	Bithionol	-2.133	-2.522
C24H40O5	DB02659	Cholic Acid	-2.516	-2.52
C16H18FN3O2	DB04953	Ezogabine	-2.511	-2.52
C24H40O4	DB06777	Chenodeoxycholic acid	-2.515	-2.519
C5H11NO2	DB06756	Glycine betaine	-2.516	-2.516
C4H11NO3	DB03754	Tromethamine	-2.276	-2.516
C23H15N3O	DB08883	Perampanel	-2.508	-2.508
C22H38O5	DB06826	Unoprostone	-2.501	-2.504
C15H22N2O	DB00961	Mepivacaine	-1.37	-2.501
C30H34N2O3	DB06401	Bazedoxifene	-2.489	-2.499
C16H24N2O2	DB01618	Molindone	-2.442	-2.495
C19H19N	DB01619	Phenindamine	-2.039	-2.495
C23H27N	DB01091	Butenafine	-1.545	-2.494
C20H24N2	DB08801	Dimetindene	-0.59	-2.494
C22H24CIN5O2	DB01184	Domperidone	-0.389	-2.494
C19H20N2O3	DB03585	Oxyphenbutazone	-2.482	-2.49
C15H18Cl6N2O5	DB01495	Dichloralphenazone	-2.489	-2.489
C19H24N2OS	DB01403	Methotrimeprazine	-2.488	-2.489
C16H12O3	DB01125	Anisidione	-2.476	-2.487
C23H29N3O2S2	DB01623	Thiothixene	-1.223	-2.481
C12H14N4O2S	DB01582	Sulfamethazine	-2.168	-2.48
C13H19CIN2O2	DB01161	Chloroprocaine	-0.492	-2.479
C24H31NO	DB05812	Abiraterone	-0.48	-2.479
C26H26F2N2	DB04841	Flunarizine	0.182	-2.478
C17H26N4O	DB01084	Emedastine	-1.898	-2.469
C12H14N4O2S	DB01582	Sulfamethazine	-0.62	-2.458
C25H28N6O	DB01029	Irbesartan	-2.451	-2.457
C12H13NO2S	DB04657	Carboxin	-2.455	-2.455
C26H29Cl2N5O3	DB06616	Bosutinib	-1.301	-2.455
C17H22N2S	DB04826	Thenalidine	-2.447	-2.447
C18H23NO	DB01173	Orphenadrine	-2.432	-2.446
C12H11NO	DB04951	Pirfenidone	-2.439	-2.439
C9H5ClINO	DB04815	Clioquinol	-2.257	-2.438
C11H12N2O	DB01435	Antipyrine	-2.433	-2.433
C13H13N3	DB01273	Varenicline	-2.433	-2.433
C12H9F3N2O2	DB01097	Leflunomide	-2.428	-2.428
C16H26O5	DB06697	Artemether	-2.424	-2.424
C17H25N3O2	DB04876	Vildagliptin	-0.879	-2.424
C34H41N7O5	DB06695	Dabigatran etexilate	-0.884	-2.421

C15H14N4O2S	DB06729	Sulfaphenazole	-0.958	-2.417
C18H23FINO2	DB08824	Ioflupane I-123	-2.396	-2.409
C16H19CIN2	DB01114	Chlorphenamine	-2.404	-2.404
C33H60O10	DB06804	Nonoxynol-9	-2.403	-2.403
C24H25NO4	DB01148	Flavoxate	-2.391	-2.401
C19H26N2S	DB01186	Pergolide	-2.39	-2.401
C6H14O6S2	DB01008	Busulfan	-2.4	-2.4
C18H15CIN2O2S	DB01628	Etoricoxib	-2.4	-2.4
C35H42N2O9	DB01180	Rescinnamine	-0.645	-2.398
C11H16CIN5	DB01131	Proguanil	-2.167	-2.389
C22H22F3N	DB01012	Cinacalcet	-0.016	-2.384
C18H21N5O2	DB06203	Alogliptin	-2.381	-2.381
C13H17CIN2O2	DB01171	Moclobemide	-1.608	-2.378
C28H44O	DB04038	Ergosterol	-2.375	-2.375
C25H36N3O9PS	DB01319	Fosamprenavir	-1.104	-2.372
C21H29NO2	DB06713	Norelgestromin	-2.371	-2.371
C11H12N4O2S	DB01581	Sulfamerazine	0.006	-2.37
C28H31NO2	DB06202	Lasofoxifene	-2.357	-2.362
C20H31NO4	DB06217	Vernakalant	-2.349	-2.355
C12H14N4O4S	DB06150	Sulfadimethoxine	-2.218	-2.354
C11H16CIN5	DB01131	Proguanil	-1.27	-2.349
C3H2F6O	DB01189	Desflurane	-2.348	-2.348
C2H6OS	DB01093	Dimethyl sulfoxide	-2.344	-2.344
C19H35N	DB01074	Perhexiline	-2.341	-2.341
C22H24CIN3O	DB00972	Azelastine	-2.339	-2.34
C14H14N2	DB06711	Naphazoline	-2.338	-2.338
C20H15BrN6O	DB06414	Etravirine	-2.333	-2.333
C11H13N	DB01626	Pargyline	-2.182	-2.328
C16H24N2	DB06694	Xylometazoline	-2.321	-2.321
C21H32Cl2N4O	DB06016	Cariprazine	-2.27	-2.321
C22H19ClO3	DB01117	Atovaquone	-2.318	-2.318
C21H32O3	DB06412	Oxymetholone	-0.059	-2.312
C26H30Cl2F3NO	DB01218	Halofantrine	-2.31	-2.311
C13H8Cl2N2O4	DB06803	Niclosamide	-2.242	-2.308
C26H28Cl2N4O4	DB01026	Ketoconazole	-1.978	-2.303
C34H41N7O5	DB06695	Dabigatran etexilate	-0.743	-2.302
C19H23NO	DB01146	Diphenylpyraline	-2.296	-2.3
C24H28CIN5O3	DB00985	Dimenhydrinate	-2.286	-2.299
C17H21NO	DB01075	Diphenhydramine	-2.284	-2.298
C28H42Cl2N4O2	DB01122	Ambenonium	-2.295	-2.295
C17H19NO4	DB01192	Oxymorphone	-0.019	-2.293
C27H30F6N2O2	DB01126	Dutasteride	-2.289	-2.289
C21H23NO5	DB01452	Diamorphine	-2.222	-2.286
C23H31Cl2NO3	DB01196	Estramustine	-2.28	-2.28
C28H46O	DB01070	Dihydrotachysterol	-2.28	-2.28
C14H19NO2	DB06701	Dexmethylphenidate	-2.276	-2.277
C10H11N3O3S	DB01015	Sulfamethoxazole	-2.267	-2.275
C29H39NO9	DB04865	Omacetaxine mepesuccinate	-2.16	-2.273
C26H29F2N7	DB01430	Almitrine	-0.608	-2.267
C26H28Cl2N4O4	DB01026	Ketoconazole	0.208	-2.266
C15H14N2O4S	DB05015	Belinostat	-2.241	-2.263
C29H27F3N6O	DB08901	Ponatinib	-1.509	-2.263
C23H26N2O2	DB01591	Solifenacin	-2.259	-2.262
C20H28O2	DB00982	Isotretinoin	-2.258	-2.261
C12H17NO2	DB01188	Ciclopirox	-2.259	-2.259
C18H20N2	DB06148	Mianserin	-1.371	-2.257
C7H6O2	DB03793	Benzoic Acid	-2.255	-2.256
C11H21NO3	DB06261	Hexaminolevulinate	-1.875	-2.252
C5H5NOS	DB06815	Pyrithione	-2.247	-2.247
C18H15Cl3N2S	DB06820	Sulconazole	-1.744	-2.247
C9H16CIN3O2	DB01206	Lomustine	-2.246	-2.246
C23H27Cl2N3O2	DB01238	Aripiprazole	-1.488	-2.246
C17H17Cl2N	DB01104	Sertraline	-2.233	-2.245

C18H25N3O2	DB06335	Saxagliptin	-1.202	-2.243
C6H18N4	DB06824	Triethylenetetramine	-0.748	-2.238
C20H33N2O	DB06787	Hexocyclium	-0.734	-2.238
C22H18N2	DB04794	Bifonazole	-1.733	-2.23
C6H6Cl2N2O4S2	DB01144	Diclofenamide	0.379	-2.23
C15H17NO2	DB06594	Agomelatine	-2.227	-2.227
C27H45N5O5	DB08873	Boceprevir	-2.227	-2.227
C19H15NO6	DB01418	Acenocoumarol	-0.219	-2.218
C10H9AgN4O2S	DB05245	Silver sulfadiazine	-1.348	-2.217
C19H18N2O4S	DB08439	Parecoxib	-0.103	-2.216
C23H20F3N5O2S2	DB08912	Dabrafenib	-1.795	-2.211
C13H17N	DB01037	Selegiline	-2.105	-2.206
C19H21NO	DB01142	Doxepin	-2.194	-2.197
C17H18N2O6	DB01115	Nifedipine	-2.195	-2.195
C17H15N5O	DB00962	Zaleplon	-2.195	-2.195
C24H40O4	DB03619	Deoxycholic Acid	-2.189	-2.193
C11H21NO3	DB06261	Hexaminolevulinate	-1.747	-2.193
C15H23N3O4S	DB01000	Cyclacillin	-0.964	-2.191
C2H4O2	DB03166	Acetic acid	-2.186	-2.189
C24H25ClFN5O3	DB08916	Afatinib	-2.006	-2.188
C17H20F6N2O3	DB01195	Flecainide	-2.186	-2.186
C38H47N5O7S2	DB06290	Simeprevir	0.485	-2.186
C20H24N2	DB08801	Dimetindene	0.355	-2.183
C34H41N7O5	DB06695	Dabigatran etexilate	-1.531	-2.178
C24H33N3O3S2	DB01621	Pipotiazine	-2.176	-2.176
AlH3O3	DB06723	Aluminum hydroxide	-2.175	-2.175
C24H28ClN5O3	DB00985	Dimenhydrinate	0.063	-2.175
C19H25N5O4	DB01162	Terazosin	-2.051	-2.173
C7H8ClN3O4S2	DB00999	Hydrochlorothiazide	-2.156	-2.17
C14H10BrN3O	DB01558	Bromazepam	-2.169	-2.169
C13H10ClN3O4S2	DB06725	Lornoxicam	-2.168	-2.169
C19H21NS	DB06153	Pizotifen	0.406	-2.169
C25H34F2O5	DB08819	Tafluprost	-2.167	-2.167
C22H21Cl3N4O	DB06155	Rimonabant	-2.162	-2.162
C20H15Cl3N2OS	DB01153	Sertaconazole	-1.9	-2.16
C25H29I2NO3	DB01118	Amiodarone	-0.147	-2.16
C18H22N2	DB01151	Desipramine	-2.159	-2.159
C25H32O2	DB04575	Quinestrol	-2.156	-2.156
C10H20N2O4	DB06797	Mebutamate	-2.156	-2.156
C23H29N3O2S2	DB01623	Thiothixene	-2.047	-2.146
C23H28ClN3O5S	DB01016	Glyburide	-2.123	-2.144
C18H22N2	DB01176	Cyclizine	-1.749	-2.144
C20H15Cl3N2OS	DB01153	Sertaconazole	-1.529	-2.143
C26H29F2N7	DB01430	Almitrine	-2.098	-2.141
C15H23N3O4S	DB01000	Cyclacillin	-2.06	-2.14
C15H22N2O	DB00961	Mepivacaine	-2.043	-2.138
C53H67N9O10S	DB01369	Quinupristin	-1.735	-2.131
C18H15Cl3N2O	DB01127	Econazole	-1.408	-2.131
C12H21N5O3	DB01303	Oxtriphylline	-2.128	-2.128
C11H17BrN	DB01158	Bretylium	-2.125	-2.125
C25H29I2NO3	DB01118	Amiodarone	-2.103	-2.123
C30H47NO4S	DB01256	Retapamulin	-2.117	-2.118
C18H28N2O	DB01002	Levobupivacaine	-0.67	-2.111
C31H48O2S2	DB01599	Probucol	-2.107	-2.107
C24H25NO4	DB01148	Flavoxate	0.327	-2.102
C21H26O2	DB01357	Mestranol	-2.083	-2.083
C33H30N4O2	DB00966	Telmisartan	-1.806	-2.08
C25H32ClN5O2	DB01149	Nefazodone	-1.659	-2.077
C18H22N2	DB01176	Cyclizine	-0.046	-2.077
C28H54N8	DB06809	Plerixafor	0.114	-2.077
C43H74N2O14	DB06145	Spiramycin	-0.445	-2.07
C13H16N2	DB06764	Tetryzoline	-2.069	-2.069
C17H11ClF4N2S	DB01589	Quazepam	-2.065	-2.065

C21H32O3	DB06412	Oxymetholone	-1.858	-2.065
C18H14Cl4N2O	DB01110	Miconazole	-1.339	-2.062
C21H32O2	DB02789	Pregnenolone	-2.061	-2.061
C26H32F2O7	DB01047	Fluocinonide	-2.061	-2.061
C8H7ClN2O2S	DB01119	Diazoxide	0.51	-2.059
C19H23ClN2	DB01242	Clomipramine	-2.058	-2.058
C12H9F3N2O2	DB08880	Teriflunomide	-2.052	-2.058
C9H19N	DB06706	Isometheptene	-2.055	-2.055
C6H11NO2	DB01080	Vigabatrin	-2.051	-2.051
C28H28N2O2	DB01501	Difenoxin	-2.032	-2.048
C58H80N2O14	DB01226	Mivacurium	-2.041	-2.041
C12H21N3O5S3	DB01194	Brinzolamide	-1.993	-2.039
C21H20ClNO5	DB06216	Asenapine	-2.034	-2.038
C14H22ClN3O2	DB01233	Metoclopramide	-2.028	-2.032
C20H21ClO4	DB01039	Fenofibrate	-2.03	-2.03
C11H12N4O2S	DB01581	Sulfamerazine	-1.803	-2.025
C26H29MgNO10	DB01401	Choline magnesium trisalicylate	-2.024	-2.024
C20H33N2O	DB06787	Hexocyclium	-1.971	-2.02
C12H13N	DB01367	Rasagiline	-1.601	-2.018
C34H41N7O5	DB06695	Dabigatran etexilate	0.128	-2.016
C15H22N2O	DB04896	Milnacipran	-2.013	-2.014
C19H17ClN2O	DB01588	Prazepam	-2.01	-2.01
C17H20N2O6S	DB01603	Meticillin	-2.009	-2.009
C12H19N3O	DB01168	Procabazine	-1.325	-2.009
C19H19N	DB01619	Phenindamine	-0.176	-1.997
C2HBrClF3	DB01159	Halothane	-1.994	-1.994
C18H20N2	DB06148	Mianserin	-1.84	-1.991
C24H30O3	DB01395	Drospirenone	-1.99	-1.99
C14H14N8O4S3	DB01327	Cefazolin	-1.982	-1.982
C3H6O2	DB03766	Propanoic acid	-1.975	-1.978
C18H28N2O	DB01002	Levobupivacaine	-1.902	-1.956
C23H27N3O7	DB01017	Minocycline	0.682	-1.948
C18H15Cl3N2O	DB01127	Econazole	-1.737	-1.945
C30H62O10	DB06811	Polidocanol	-1.941	-1.941
C38H47N5O7S2	DB06290	Simeprevir	-1.929	-1.936
C11H17N	DB01365	Mephentermine	-1.929	-1.929
C30H32N2O2	DB01081	Diphenoxylate	-1.491	-1.929
C11H18N2O3	DB01351	Amobarbital	-1.891	-1.925
CH2O	DB03843	Formaldehyde	-1.919	-1.919
C23H27Cl2N3O2	DB01238	Aripiprazole	-1.725	-1.918
C17H26ClN	DB01105	Sibutramine	-1.913	-1.915
C24H29ClO4	DB04839	Cyproterone acetate	-1.897	-1.897
C6H6Cl2N2O4S2	DB01144	Diclofenamide	-1.89	-1.897
C27H33N3O6S	DB01251	Gliquidone	0.215	-1.89
C12H14N4O4S	DB01299	Sulfadoxine	-1.735	-1.887
C35H38Cl2N8O4	DB01167	Itraconazole	0.099	-1.873
C18H22N2	DB01176	Cyclizine	-1.401	-1.87
C25H28N6O	DB01029	Irbesartan	0.844	-1.864
C18H22N2S	DB01246	Alimemazine	-1.862	-1.863
C22H18N2	DB04794	Bifonazole	-1.528	-1.863
C6H8O4	DB08908	Dimethyl fumarate	-1.858	-1.858
C12H16F3N	DB01191	Dexfenfluramine	-1.853	-1.854
C30H40N4	DB04209	Dequalinium	-1.851	-1.851
C21H27N5O4S	DB01067	Glipizide	-1.812	-1.834
C13H16ClNO	DB01221	Ketamine	-1.718	-1.822
C29H27F3N6O	DB08901	Ponatinib	0.682	-1.822
C5H8N4O12	DB06154	Pentaerythritol tetranitrate	-1.815	-1.815
C10H15N	DB01577	Metamfetamine	-1.812	-1.812
C15H32N2	DB01090	Pentolinium	-1.796	-1.796
C14H22N2O3	DB01297	Practolol	-1.789	-1.791
C23H31NO3	DB00957	Norgestimate	-1.79	-1.79
C16H13Cl3N2OS	DB01007	Tioconazole	-1.527	-1.786
C4H6N4O12	DB01613	Erythryl tetranitrate	-1.775	-1.775

C19H24N2O2	DB01058	Praziquantel	-1.775	-1.775
C7H17N2O2	DB01019	Bethanechol	-1.772	-1.772
C33H38O6	DB08909	Glycerol phenylbutyrate	-1.767	-1.767
C17H19N3	DB08799	Antazoline	-1.764	-1.764
C15H23NO3	DB01580	Oxprenolol	-1.761	-1.762
C21H27N3O7S	DB01602	Bacampicillin	-1.556	-1.762
C6H12N4	DB06799	Methenamine	-1.748	-1.761
C12H17NO	DB01579	Phendimetrazine	-1.545	-1.76
C35H30N4O4	DB06595	Midostaurin	-1.748	-1.748
C9H9N3O2S2	DB06147	Sulfathiazole	-1.519	-1.745
C17H23N3O	DB06691	Mepyramine	-1.738	-1.743
C21H25CIN2O3	DB06282	Levocetirizine	-1.33	-1.741
C26H25CIN2O3	DB06212	Tolvaptan	-1.728	-1.728
C8H18NO2	DB06709	Methacholine	-1.719	-1.719
C20H27NO3	DB01108	Trilostane	-1.719	-1.719
C47H64N4O12	DB01201	Rifapentine	0.873	-1.716
C12H14N4O3S	DB01298	Sulfacytine	-1.67	-1.708
C23H29N3O2S	DB01063	Acetophenazine	-1.16	-1.708
C22H28N2O2	DB01228	Encainide	-1.7	-1.701
C18H19Cl2NO4	DB01023	Felodipine	-1.691	-1.691
C21H33N3O5S	DB01605	Pivmecillinam	-1.69	-1.69
C62H86N12O16	DB00970	Dactinomycin	-1.684	-1.684
C19H23N5O3	DB01157	Trimetrexate	-1.649	-1.682
C14H22N2O2	DB00989	Rivastigmine	-0.178	-1.678
C27H33N3O6S	DB01251	Gliquidone	-1.63	-1.647
C12H17NO	DB01579	Phendimetrazine	-0.94	-1.646
C7H16NO2	DB03128	Acetylcholine	-1.624	-1.624
C27H34O3	DB00984	Nandrolone phenpropionate	-1.616	-1.616
C20H27N5O2	DB01166	Cilostazol	-1.603	-1.603
C22H31NO3	DB01062	Oxybutynin	-0.363	-1.596
C17H18N2O5S	DB02925	Piretanide	-1.594	-1.594
C18H23NO3	DB01551	Dihydrocodeine	0.651	-1.571
C35H42N2O9	DB01180	Rescinnamine	-1.538	-1.569
C21H32Cl2N4O	DB06016	Cariprazine	-0.05	-1.528
C3H8O	DB02325	Isopropyl alcohol	-1.523	-1.523
C23H31NO2	DB01227	Levacetylmethadol	-1.483	-1.486
C43H74N2O14	DB06145	Spiramycin	-1.432	-1.481
C35H62N4O4	DB01338	Pipecuronium	-1.269	-1.477
C10H16O	DB01744	Camphor	-1.475	-1.475
C22H32O2	DB03756	Doconexent	-1.468	-1.47
C24H27FN2O4	DB04946	Iloperidone	0.804	-1.47
C28H54N8	DB06809	Plerixafor	-0.743	-1.449
C13H19NO4S	DB01032	Probenecid	-1.446	-1.446
C12H14N4O2S	DB01582	Sulfamethazine	-0.739	-1.415
C19H21NO4	DB01183	Naloxone	0.693	-1.411
C8H8Cl3N3O4S2	DB01021	Trichlormethiazide	-0.759	-1.392
C29H27F3N6O	DB08901	Ponatinib	-1.18	-1.387
C24H27FN2O4	DB04946	Iloperidone	-1.36	-1.372
C11H12N4O2S	DB01581	Sulfamerazine	-0.598	-1.358
C12H19N2O2	DB01400	Neostigmine	-1.343	-1.343
C18H36O2	DB03193	Stearic acid	-1.336	-1.339
C12H14N4O4S	DB01299	Sulfadoxine	0.277	-1.328
C56H78N2O16	DB01135	Doxacurium	-1.315	-1.315
C12H18N2O3S	DB01124	Tolbutamide	0.764	-1.315
C26H28N3	DB06816	Pyrvinium	-1.299	-1.299
C26H29FN2O2	DB01106	Levocabastine	-1.273	-1.273
N2O	DB06690	Nitrous oxide	-1.219	-1.219
C17H25N3O2	DB04876	Vildagliptin	-1.155	-1.2
C12H18N2O3S	DB01124	Tolbutamide	-1.149	-1.167
C24H27N	DB04825	Prenylamine	-1.163	-1.163
C9H9N3O2S2	DB06147	Sulfathiazole	-0.474	-1.155
C31H44N2O5S	DB04855	Dronedarone	0.132	-1.151
C28H54N8	DB06809	Plerixafor	1.603	-1.119

C22H26CIN7O2S	DB01254	Dasatinib	-0.644	-1.079
C12H24O2	DB03017	Lauric acid	-1.062	-1.066
C29H53NO5	DB01083	Orlistat	-1.056	-1.056
C35H62N4O4	DB01338	Pipecuronium	1.044	-1.041
C38H69NO13	DB01211	Clarithromycin	-1.008	-1.015
C64H82N18O13	DB06825	Triptorelin	-0.463	-0.998
C18H14Cl4N2O	DB01110	Miconazole	-0.787	-0.994
C12H13N	DB01367	Rasagiline	-0.579	-0.983
C21H20Cl2O3	DB04930	Permethrin	-0.973	-0.973
C6H12N3PS	DB04572	Thiotepa	-0.944	-0.944
C35H62N4O4	DB01338	Pipecuronium	1.761	-0.943
C23H28CIN3O5S	DB01016	Glyburide	1.063	-0.92
C28H36N4O2S	DB08815	Lurasidone	-0.913	-0.913
C28H29NO4S	DB06249	Arzoxifene	-0.874	-0.89
C14H22N2O2	DB00989	Rivastigmine	-0.785	-0.834
C35H62N4O4	DB01338	Pipecuronium	0.072	-0.737
C12H21N	DB01043	Memantine	-0.706	-0.706
C15H21N3O2	DB00981	Physostigmine	1.794	-0.704
GaN3O9	DB05260	Gallium nitrate	-0.661	-0.661
C23H29N3O2S2	DB01623	Thiothixene	1.408	-0.604
C34H57N2O4	DB01339	Vecuronium	-0.572	-0.576
C43H65N5O10	DB00976	Telithromycin	0.057	-0.525
C20H41NO3	DB06689	Ethanolamine oleate	-0.484	-0.487
C5H11NO2	DB01612	Amyl Nitrite	-0.423	-0.423
C22H31NO3	DB01062	Oxybutynin	-0.343	-0.422
C13H11NO3	DB06807	Phenyl aminosaliclylate	1.544	-0.407
C47H51NO14	DB01229	Paclitaxel	-0.286	-0.287
C24H35N5O5	DB04898	Ximelagatran	0.443	-0.256
C26H37NO3	DB06702	Fesoterodine	-0.205	-0.207
C21H23N7O2S	DB06589	Pazopanib	-0.192	-0.199
C21H21F3IN3O2	DB05239	Cobimetinib	-0.055	-0.058
C35H38Cl2N8O4	DB01167	Itraconazole	0.086	0.065
C17H20BrNO	DB01237	Bromodiphenhydramine	0.08	0.066
C24H28F3N3O3	DB06608	Tafenoquine	2.796	0.119
C18H23FINO2	DB08824	Ioflupane I-123	2.444	0.207
C31H44N2O5S	DB04855	Dronedarone	0.551	0.479
C22H34O2	DB08887	Icosapent ethyl	0.509	0.509
C22H48N	DB04221	Didecyldimethylammonium	0.659	0.659
C13H11NO3	DB06807	Phenyl aminosaliclylate	0.699	0.676
C15H21N3O3S	DB01120	Gliclazide	0.769	0.745
C35H60N2O4	DB01337	Pancuronium	0.758	0.758
C19H19N3O6	DB06712	Nilvadipine	1.284	1.284
C16H38N2	DB01245	Decamethonium	1.635	1.635
C47H64N4O12	DB01201	Rifapentine	2.59	1.73
C43H58N4O12	DB01045	Rifampicin	4.618	2.394
C19H42N	DB01718	Cetrimonium	2.422	2.422
C47H64N4O12	DB01201	Rifapentine	3.611	2.534
C34H41N7O5	DB06695	Dabigatran etexilate	3.553	2.818
C47H64N4O12	DB01201	Rifapentine	3.772	3.425
C47H64N4O12	DB01201	Rifapentine	6.282	4.289
C15H21N3O2	DB00981	Physostigmine	5.624	5.615
C37H61N2O4	DB04834	Rapacuronium	8.081	8.077

FDA approved drugs with 6vw1, Table S7

FORMULA	DRUGBANK_ID	GENERIC_NAME	docking score	glide gscore
C23H46N6O13	DB00452	Framycetin	-8.719	-11.233
C23H46N6O13	DB00452	Framycetin	-8.588	-10.865
C25H43NO18	DB00284	Acarbose	-10.017	-10.649
C23H46N6O13	DB00452	Framycetin	-8.226	-10.442

C23H46N6O13	DB00452	Framycetin	-7.873	-9.698
C25H43NO18	DB00284	Acarbose	-9.3	-9.551
C23H46N6O13	DB00452	Framycetin	-6.151	-8.782
C10H17N3O6S	DB00143	Glutathione	-5.387	-8.09
C21H29N7O14P2	DB00157	NADH	-8.042	-8.042
C22H43N5O13	DB00479	Amikacin	-5.523	-7.762
C31H53N3O49S8	DB00569	Fondaparinux	-7.094	-7.76
C29H39N5O8	DB00560	Tigecycline	-6.485	-7.592
C18H37N5O9	DB00684	Tobramycin	-6.062	-7.59
C20H22N8O5	DB00563	Methotrexate	-7.482	-7.547
C23H46N6O13	DB00452	Framycetin	-6.115	-7.455
C10H15N5O3	DB00299	Penciclovir	-7.412	-7.412
C36H47N5O4	DB00224	Indinavir	-7.013	-7.403
C29H39N5O8	DB00560	Tigecycline	-7.261	-7.395
C23H46N6O13	DB00452	Framycetin	-5.215	-7.375
C23H46N6O13	DB00452	Framycetin	-5.501	-7.362
C15H22N6O5S	DB00118	Ademetionine	-4.893	-7.296
C66H75Cl2N9O24	DB00512	Vancomycin	-4.65	-7.271
C8H10NO6P	DB00114	Pyridoxal phosphate	-4.764	-7.263
C7H11NO7P2	DB00884	Risedronic acid	-7.042	-7.23
C17H20N4O6	DB00140	Riboflavin	-7.159	-7.159
C21H43N5O7	DB00798	Gentamicin	-6.921	-7.096
C22H43N5O13	DB00479	Amikacin	-6.984	-7.048
C27H29NO10	DB00694	Daunorubicin	-6.984	-7.012
C14H26CaO16	DB00326	Calcium glucoheptonate	-7.007	-7.007
C4H13NO7P2	DB00630	Alendronic acid	-6.167	-6.91
C7H11NO7P2	DB00884	Risedronic acid	-6.078	-6.871
C3H11NO7P2	DB00282	Pamidronic acid	-6.755	-6.866
C12H22O11	DB00581	Lactulose	-6.855	-6.855
C49H66N10O10S2	DB00104	Octreotide	-6.087	-6.797
C22H43N5O13	DB00479	Amikacin	-5.23	-6.732
C27H29NO11	DB00445	Epirubicin	-6.692	-6.719
C23H46N6O13	DB00452	Framycetin	-4.513	-6.693
C5H10N2O7P2	DB00399	Zoledronic acid	-5.267	-6.631
C5H10N2O7P2	DB00399	Zoledronic acid	-5.068	-6.599
C23H46N6O13	DB00452	Framycetin	-5.86	-6.545
C23H46N6O13	DB00452	Framycetin	-5.546	-6.532
C10H13N5O4	DB00194	Vidarabine	-6.486	-6.486
C21H22N4O6S	DB00293	Raltitrexed	-6.414	-6.478
C4H7NO4	DB00128	Aspartic acid	-6.37	-6.37
C8H14N3O6P	DB00369	Cidofovir	-6.072	-6.368
C8H11N5O3	DB00787	Acyclovir	-6.355	-6.355
C3H11NO7P2	DB00282	Pamidronic acid	-5.297	-6.351
C50H88N28O15	DB00314	Capreomycin	-5.834	-6.347
C18H37N5O9	DB00684	Tobramycin	-3.72	-6.318
C9H23NO7P2	DB00710	Ibandronate	-6.213	-6.304
C8H5F3N2OS	DB00740	Riluzole	-6.263	-6.263
C14H24N2O7	DB00919	Spectinomycin	-5.974	-6.225
C13H20N6O4	DB00577	Valaciclovir	-5.445	-6.17
C4H13NO7P2	DB00630	Alendronic acid	-5.967	-6.166
C21H43N5O7	DB00798	Gentamicin	-4.527	-6.14
C14H24N2O7	DB00919	Spectinomycin	-4.713	-6.082
C28H31FN4O	DB00637	Astemizole	-5.74	-6.066
C8H14N3O6P	DB00369	Cidofovir	-5.513	-6.066
C8H10NO6P	DB00114	Pyridoxal phosphate	-5.961	-6.053
C12H15N5O3	DB00442	Entecavir	-6.051	-6.051
C9H15N5O3	DB00360	Sapropterin	-6.039	-6.051
C19H25BN4O4	DB00188	Bortezomib	-6.043	-6.043
C8H17NO5	DB00491	Miglitol	-4.474	-6.033
C5H11NO2S	DB00859	Penicillamine	-3.787	-6.006
C5H10N2O7P2	DB00399	Zoledronic acid	-5.459	-6.003
C52H88N10O15	DB00520	Caspofungin	-5.942	-5.95
C5H10N2O7P2	DB00399	Zoledronic acid	-5.434	-5.94

C21H41N5O7	DB00955	Netilmicin	-3.403	-5.934
C8H12N4O5	DB00928	Azacitidine	-5.508	-5.925
C49H66N10O10S2	DB00104	Octreotide	-5.691	-5.904
C9H11F2N3O4	DB00441	Gemcitabine	-3.183	-5.904
C47H73NO17	DB00681	Amphotericin B	-4.258	-5.898
C18H23N9O4S3	DB00229	Cefotiam	-5.796	-5.896
C21H41N5O7	DB00955	Netilmicin	-5.181	-5.891
C46H64N14O12S2	DB00035	Desmopressin	-5.888	-5.888
C10H11ClFN5O3	DB00631	Clofarabine	-5.887	-5.887
C8H12N4O5	DB00811	Ribavirin	-5.866	-5.866
C10H14N5O7P	DB00131	Adenosine phosphate	-5.773	-5.865
C23H46N6O13	DB00452	Framycetin	-4.822	-5.863
C4H8N2O3	DB00174	Asparagine	-5.858	-5.858
C9H13NO3	DB00668	Epinephrine	-5.833	-5.845
C50H88N28O15	DB00314	Capreomycin	-4.32	-5.841
C29H38N4O10	DB00256	Lymecycline	-4.631	-5.76
C47H75NO17	DB00646	Nystatin	-3.995	-5.753
C66H75Cl2N9O24	DB00512	Vancomycin	-5.34	-5.732
C6H9N3O2	DB00117	Histidine	-5.274	-5.731
C10H14N5O7P	DB00131	Adenosine phosphate	-4.577	-5.726
C21H43N5O7	DB00798	Gentamicin	-4.206	-5.715
C21H21ClN2O8	DB00618	Demeclocycline	-4.18	-5.713
C29H32O13	DB00773	Etoposide	-5.708	-5.709
C19H24N4O2	DB00738	Pentamidine	-5.692	-5.692
C33H47NO13	DB00826	Natamycin	-4.048	-5.689
C8H15N7O2S3	DB00927	Famotidine	-4.7	-5.68
C19H29NO5	DB00449	Dipivefrin	-5.672	-5.678
C29H39N5O8	DB00560	Tigecycline	-3.71	-5.676
C20H21N5O6	DB00642	Pemetrexed	-5.648	-5.648
C14H19N5O4	DB00426	Famciclovir	-5.647	-5.647
C22H25N3O7S	DB00303	Ertapenem	-4.141	-5.642
C19H24N2O3	DB00598	Labetalol	-5.611	-5.639
C3H7NO3	DB00133	Serine	-5.633	-5.633
C11H16N4O4	DB00380	Dexrazoxane	-4.68	-5.608
C19H19N7O6	DB00158	Folic acid	-5.425	-5.603
C21H41N5O7	DB00955	Netilmicin	-4.925	-5.563
C12H20N4O7	DB00558	Zanamivir	-5.551	-5.551
C22H28GdN3O11	DB00743	Gadobenic acid	-5.354	-5.534
C26H44O9	DB00410	Mupirocin	-5.528	-5.532
CH3O5P	DB00529	Foscarnet	-5.481	-5.488
C19H19N7O6	DB00158	Folic acid	-4.126	-5.471
C34H36F3NO13	DB00385	Valrubicin	-5.468	-5.469
C12H12N2O3	DB00779	Nalidixic acid	-5.406	-5.451
C19H19N7O6	DB00158	Folic acid	-4.298	-5.439
C21H29FO5	DB00687	Fludrocortisone	-5.426	-5.426
CH4Cl2O6P2	DB00720	Clodronic acid	-5.422	-5.426
C10H12ClN5O3	DB00242	Cladribine	-5.422	-5.422
C20H34GdN5O10	DB00538	Gadoversetamide	-2.721	-5.418
C8H15NO6	DB00141	N-Acetylglucosamine	-5.396	-5.397
C4H9NO3	DB00156	L-Threonine	-5.395	-5.395
C18H23NO3	DB00841	Dobutamine	-5.38	-5.38
C23H36O7	DB00175	Pravastatin	-5.372	-5.374
C14H24N2O7	DB00919	Spectinomycin	-4.536	-5.367
C12H13ClN4	DB00205	Pyrimethamine	-4.577	-5.363
C14H20GdN3O10	DB00789	Gadopentetic acid	-3.185	-5.361
C20H22N8O5	DB00563	Methotrexate	-3.921	-5.357
C22H28GdN3O11	DB00743	Gadobenic acid	-3.752	-5.356
C13H20N6O4	DB00577	Valaciclovir	-5.148	-5.354
C18H22O4	DB00179	Masoprocol	-5.346	-5.346
C20H34GdN5O10	DB00538	Gadoversetamide	-3.092	-5.318
C14H11ClN2O4S	DB00310	Chlorthalidone	-5.273	-5.275
C35H36ClNO3S	DB00471	Montelukast	-5.273	-5.273
C29H38N4O10	DB00256	Lymecycline	-3.136	-5.266

C17H19N3O3S	DB00736	Esomeprazole	-5.161	-5.254
C9H15N5O	DB00350	Minoxidil	-5.245	-5.245
C9H23NO7P2	DB00710	Ibandronate	-4.061	-5.231
C9H11FN2O5	DB00322	Floxuridine	-5.192	-5.222
C9H15N5O3	DB00360	Sapropterin	-2.899	-5.217
C20H32O5	DB00917	Dinoprostone	-5.21	-5.213
C47H73NO17	DB00681	Amphotericin B	-5.167	-5.205
C10H14O4	DB00874	Guaifenesin	-5.15	-5.15
C18H37N5O9	DB00684	Tobramycin	-4.879	-5.15
C21H43N5O7	DB00798	Gentamicin	-3.449	-5.146
C13H8F2O3	DB00861	Diflunisal	-5.133	-5.133
C10H17N3O6S	DB00143	Glutathione	-5.083	-5.089
C9H13N3O3	DB00943	Zalcitabine	-5.085	-5.085
C15H11I4NO4	DB00509	Dextrothyroxine	-4.094	-5.082
C21H22N4O6S	DB00293	Raltitrexed	-3.734	-5.082
C18H37N5O9	DB00684	Tobramycin	-3.496	-5.08
C32H41NO2	DB00342	Terfenadine	-5.074	-5.077
C14H20GdN3O10	DB00789	Gadopentetic acid	-4.25	-5.066
C66H75Cl2N9O24	DB00512	Vancomycin	-3.288	-5.053
C11H12Cl2N2O5	DB00446	Chloramphenicol	-5.044	-5.044
C8H10FN3O3S	DB00879	Emtricitabine	-5.03	-5.03
C20H24N2OS	DB00777	Propiomazine	-5.019	-5.021
C18H37N5O9	DB00684	Tobramycin	-3.406	-5.017
C11H16N4O4	DB00552	Pentostatin	-3.282	-5.016
C20H34GdN5O10	DB00538	Gadoversetamide	-3.138	-5.012
C11H12N2O2S	DB00744	Zileuton	-4.986	-5.005
C7H7NO3	DB00244	Mesalazine	-4.988	-4.991
C12H9N3O	DB00235	Milrinone	-4.969	-4.988
C22H28GdN3O11	DB00743	Gadobenic acid	-3.529	-4.983
C5H9NO4	DB00142	Glutamic Acid	-4.977	-4.977
C22H30Cl2N10	DB00878	Chlorhexidine	-4.943	-4.953
C10H21NO4	DB00419	Miglustat	-2.896	-4.942
C16H17N3O4S	DB00567	Cephalexin	-4.325	-4.941
C12H11N7	DB00384	Triamterene	-4.939	-4.939
C8H15N3O7	DB00428	Streptozocin	-4.934	-4.934
C22H24N2O9	DB00595	Oxytetracycline	-4.647	-4.918
C11H12N2O2	DB00150	L-Tryptophan	-4.916	-4.916
C21H41N5O7	DB00955	Netilmicin	-2.984	-4.906
C5H10N2O3	DB00130	L-Glutamine	-4.895	-4.895
C3H6N2O2	DB00260	Cycloserine	-4.231	-4.869
C13H24NO10P	DB00144	Phosphatidyl serine	-4.851	-4.864
C22H29ClO5	DB00240	Alclometasone	-4.836	-4.836
C21H28O5	DB00860	Prednisolone	-4.832	-4.832
C15H17FN4O3	DB00467	Enoxacin	-2.18	-4.815
C17H14N2O3	DB00817	Rosoxacin	-3.525	-4.8
C11H16N4O4	DB00380	Dexrazoxane	-4.189	-4.797
C19H24N2O3	DB00598	Labetalol	-2.86	-4.797
C19H20FNO3	DB00715	Paroxetine	-4.795	-4.796
C52H98N16O13	DB00803	Colistin	-3.283	-4.794
C10H19N3O2	DB00226	Guanadrel	-4.786	-4.786
C21H27ClN2O2	DB00557	Hydroxyzine	-4.463	-4.781
C22H28F2O5	DB00223	Diflorasone	-4.777	-4.777
C16H15F2N3O4S	DB00213	Pantoprazole	-4.474	-4.776
C15H22N6O5S	DB00118	Ademetionine	-4.752	-4.762
C10H21NO4	DB00419	Miglustat	-4.741	-4.76
C11H15NO5	DB00423	Methocarbamol	-4.74	-4.74
C8H11N3O3S	DB00709	Lamivudine	-4.736	-4.736
C7H6O3	DB00936	Salicylic acid	-4.735	-4.735
C22H36N2O5S	DB00775	Tirofiban	-4.73	-4.73
C29H38N4O10	DB00256	Lymecycline	-2.869	-4.728
C23H32N2O5	DB00178	Ramipril	-4.519	-4.725
C7H4ClNO2	DB00356	Chlorzoxazone	-4.687	-4.72
C8H11NO3	DB00165	Pyridoxine	-4.005	-4.72

C19H27N3O5S2	DB00204	Dofetilide	-4.651	-4.717
C8H15N7O2S3	DB00927	Famotidine	-3.906	-4.713
C16H16ClNO3	DB00800	Fenoldopam	-2.701	-4.689
C20H34GdN5O10	DB00538	Gadoversetamide	-3.171	-4.685
C20H25ClN2O5	DB00381	Amlodipine	-4.679	-4.684
C28H46N6O8S	DB00895	Benzyloxyethyl Polylysine	-4.673	-4.673
C21H21ClN2O8	DB00618	Demeclocycline	-3.637	-4.669
C26H34FNO5	DB00439	Cerivastatin	-4.636	-4.659
C9H7Cl2N5	DB00555	Lamotrigine	-2.837	-4.657
C15H18N4O5	DB00305	Mitomycin	-4.631	-4.648
C22H28F2O5	DB00663	Flumethasone	-4.647	-4.647
C24H26N6O3	DB00275	Olmesartan	-3.526	-4.64
C21H21ClN2O8	DB00618	Demeclocycline	-4.442	-4.638
C7H7NO3	DB00233	Aminosalicylic Acid	-4.635	-4.636
C8H10N4O2	DB00824	Enprofylline	-4.577	-4.636
C8H11NO3	DB00368	Norepinephrine	-2.541	-4.636
C22H22N6O7S2	DB00438	Ceftazidime	-4.635	-4.635
C24H26N6O3	DB00275	Olmesartan	-4.532	-4.63
C12H20N2O3S	DB00489	Sotalol	-4.607	-4.628
C12H18N2O3	DB00418	Secobarbital	-4.523	-4.625
C21H30O5	DB00741	Hydrocortisone	-4.623	-4.623
C5H9N3	DB00272	Betazole	-4.213	-4.623
C22H24N2O9	DB00595	Oxytetracycline	-2.239	-4.617
C21H43N5O7	DB00798	Gentamicin	-2.621	-4.61
C24H33N3O4	DB00243	Ranolazine	-2.755	-4.609
C8H17NO5	DB00491	Miglitol	-4.557	-4.601
C16H14ClN3O	DB00475	Chlordiazepoxide	-3.015	-4.591
C9H13NO3	DB00668	Epinephrine	-2.245	-4.59
C13H21NO3	DB00221	Isoetarine	-4.586	-4.586
C16H14ClN3O	DB00475	Chlordiazepoxide	-4.529	-4.577
C18H19N3O6S	DB00689	Cephaloglycin	-4.325	-4.575
C10H13N5O4	DB00640	Adenosine	-4.572	-4.572
C8H9NO5	DB00766	Clavulanic acid	-4.568	-4.568
C20H34GdN5O10	DB00538	Gadoversetamide	-4.468	-4.568
C11H10BrN5	DB00484	Brimonidine	-4.507	-4.556
C10H24N2O2	DB00330	Ethambutol	-4.377	-4.555
C13H24NO10P	DB00144	Phosphatidyl serine	-2.267	-4.551
C25H24N8O7S2	DB00430	Cefpiramide	-4.546	-4.546
C22H24ClFN4O3	DB00317	Gefitinib	-4.138	-4.544
C8H11NO3	DB00165	Pyridoxine	-1.889	-4.543
C18H37N5O9	DB00684	Tobramycin	-3.189	-4.541
C12H13ClN4	DB00205	Pyrimethamine	-3.804	-4.54
C18H19N3O	DB00904	Ondansetron	-4.41	-4.535
C8H12N4O5	DB00928	Azacitidine	-1.851	-4.535
C15H17N7O5S3	DB00274	Cefmetazole	-4.534	-4.534
C41H64O14	DB00390	Digoxin	-4.534	-4.534
C25H31F3O5S	DB00588	Fluticasone propionate	-4.532	-4.532
C12H12N2O3	DB00779	Nalidixic acid	-2.97	-4.531
C15H18N4O5	DB00305	Mitomycin	-2.393	-4.531
C5H5N5	DB00173	Adenine	-2.532	-4.529
C22H28GdN3O11	DB00743	Gadobenidic acid	-3.105	-4.527
C26H34FNO5	DB00439	Cerivastatin	-2.587	-4.523
C26H29N3O6	DB00622	Nicardipine	-3.828	-4.521
C22H26F3N3OS	DB00623	Fluphenazine	-4.181	-4.517
C20H15F3N4O3	DB00685	Trovafloxacin	-2.475	-4.514
C33H47NO13	DB00826	Natamycin	-4.472	-4.51
C26H37N5O2	DB00248	Cabergoline	-4.272	-4.506
C17H19NO3	DB00295	Morphine	-4.444	-4.503
C5H4N4O	DB00437	Allopurinol	-4.396	-4.499
C20H21N7O6S2	DB00923	Ceforanide	-4.468	-4.492
C20H23N	DB00321	Amitriptyline	-4.476	-4.48
C12H15N3O2S	DB00518	Albendazole	-2.589	-4.475
C10H13N5O4	DB00495	Zidovudine	-4.466	-4.467

C5H9NO2	DB00172	Proline	-4.462	-4.462
C8H10NO6P	DB00114	Pyridoxal phosphate	-3.016	-4.431
C7H8N4O2	DB00277	Theophylline	-4.391	-4.423
C37H49N7O9S	DB00183	Pentagastrin	-4.421	-4.422
C3H7NO2S	DB00151	L-Cysteine	-2.202	-4.421
C14H18N2O3	DB00474	Methohexital	-4.358	-4.415
C36H41N3O6	DB00528	Lercanidipine	-4.384	-4.414
C21H27NO4	DB00844	Nalbuphine	-4.384	-4.414
C14H11NO5	DB00323	Tolcapone	-1.859	-4.414
C5H4N4O	DB00437	Allopurinol	-3.231	-4.409
C10H11F3N2O5	DB00432	Trifluridine	-3.208	-4.402
C21H41N5O7	DB00955	Netilmicin	-1.993	-4.402
C6H14O6	DB00742	Mannitol	-4.401	-4.401
C10H14N2O4	DB00190	Carbidopa	-4.394	-4.394
C17H21NO3	DB00867	Ritodrine	-4.369	-4.382
C22H29FO5	DB00443	Betamethasone	-4.381	-4.381
C26H37N5O2	DB00248	Cabergoline	-3.711	-4.379
C8H10N4O2	DB00824	Enprofylline	-2.906	-4.379
C4H11N5	DB00331	Metformin	-4.367	-4.37
C4H6N2S	DB00763	Methimazole	-4.363	-4.363
C22H25N3O7S	DB00303	Ertapenem	-4.314	-4.363
C21H41N5O7	DB00955	Netilmicin	-3.26	-4.354
C5H9NO3	DB00855	Aminolevulinic acid	-4.106	-4.324
C9H9Cl2N3	DB00575	Clonidine	-4.291	-4.314
C32H39NO4	DB00950	Fexofenadine	-4.313	-4.313
C15H15NO2S	DB00745	Modafinil	-4.312	-4.312
C27H41NO6	DB00769	Hydrocortamate	-4.213	-4.311
C11H16N4O4	DB00552	Pentostatin	-4.265	-4.297
C20H23NS	DB00340	Metixene	-4.291	-4.292
C23H31NO7	DB00688	Mycophenolate mofetil	-4.219	-4.289
C4H9N3O2	DB00148	Creatine	-4.286	-4.286
C14H11NO5	DB00323	Tolcapone	-2.744	-4.281
C4H6O4S2	DB00566	Succimer	-4.28	-4.28
C20H36N2O3S	DB00308	Ibutilide	-4.258	-4.269
C13H17N5O8S2	DB00355	Aztreonam	-4.268	-4.268
C8H10NO6P	DB00114	Pyridoxal phosphate	-2.309	-4.267
C5H9NO3	DB00855	Aminolevulinic acid	-3.558	-4.257
C8H6N4O5	DB00698	Nitrofurantoin	-4.184	-4.256
C24H31FO6	DB00180	Flunisolide	-4.247	-4.247
C17H25N3O2S	DB00952	Naratriptan	-4.241	-4.242
C13H13N3O3	DB00480	Lenalidomide	-4.239	-4.239
C10H15N3	DB00217	Bethanidine	-4.23	-4.23
C16H20N4O3S	DB00214	Torasemide	-1.605	-4.229
C10H12N4O3	DB00900	Didanosine	-3.02	-4.228
C16H16ClNO3	DB00800	Fenoldopam	-4.198	-4.224
C24H34N2O5	DB00519	Trandolapril	-4.01	-4.215
C19H23NO3	DB00234	Reboxetine	-2.5	-4.209
C17H14N2O3	DB00817	Rosoxacin	-4.135	-4.208
C21H41N5O7	DB00955	Netilmicin	-2.437	-4.205
C25H48N6O8	DB00746	Deferoxamine	-4.203	-4.203
C17H23NO	DB00854	Levorphanol	-4.192	-4.197
C26H29NO	DB00675	Tamoxifen	-4.177	-4.197
C11H16N2O3	DB00241	Butalbital	-4.128	-4.183
C21H26O5	DB00635	Prednisone	-4.182	-4.182
C20H28N2O5	DB00584	Enalapril	-3.431	-4.182
C25H37NO4	DB00938	Salmeterol	-4.174	-4.179
C9H11F2N3O4	DB00441	Gemcitabine	-4.173	-4.179
C23H34O5	DB00374	Treprostinil	-4.161	-4.161
CH5N3	DB00536	Guanidine	-4.16	-4.16
C17H20N2O2	DB00809	Tropicamide	-1.598	-4.157
C11H17NO3	DB00816	Orciprenaline	-1.944	-4.155
C10H14N4O4	DB00651	Dyphylline	-4.147	-4.147
C13H6Cl6O2	DB00756	Hexachlorophene	-1.622	-4.144

C7H8N4O2	DB00277	Theophylline	-2.31	-4.143
C24H30F2O6	DB00591	Fluocinolone acetonide	-4.131	-4.131
C21H27FO6	DB00620	Triamcinolone	-4.122	-4.122
C16H17N9O5S3	DB00267	Cefmenoxime	-4.12	-4.12
C14H13N5O5S2	DB00535	Cefdinir	-4.119	-4.119
C6H12N2O4S2	DB00138	Cystine	-2.319	-4.114
C21H27CIN2O2	DB00557	Hydroxyzine	-3.504	-4.108
C6H13N3O3	DB00155	L-Citrulline	-4.103	-4.103
C22H22FN3O2	DB00450	Droperidol	-2.989	-4.101
C22H24N2O8	DB00759	Tetracycline	-3.957	-4.096
C5H11NO2S	DB00134	Methionine	-4.088	-4.088
C14H13N3O4S2	DB00814	Meloxicam	-1.918	-4.087
C6H8CIN7O	DB00594	Amiloride	-4.083	-4.084
C17H18F3NO	DB00472	Fluoxetine	-4.081	-4.082
C20H22CIN3O	DB00613	Amodiaquine	-3.488	-4.082
C6H13NO2	DB00167	Isoleucine	-4.078	-4.078
C18H23N9O4S3	DB00229	Cefotiam	-2.973	-4.075
C21H41N5O7	DB00955	Netilmicin	-1.605	-4.055
C8H11NO3	DB00368	Norepinephrine	-4.036	-4.053
C14H16N4	DB00724	Imiquimod	-3.555	-4.041
C6H8O6	DB00126	Ascorbic acid	-4.038	-4.038
C27H29NO11	DB00445	Epirubicin	-2.192	-4.032
C15H17FN4O3	DB00467	Enoxacin	-3.983	-4.03
C12H18N2O4	DB00211	Midodrine	-3.922	-4.03
C24H33N3O4	DB00243	Ranolazine	-3.995	-4.026
C14H20GdN3O10	DB00789	Gadopentetic acid	-3.787	-4.025
C18H31NO4	DB00612	Bisoprolol	-4.022	-4.023
C17H21NO4	DB00747	Scopolamine	-3.803	-4.016
C12H18N2O4	DB00211	Midodrine	-2.952	-4.013
C22H22N2O8	DB00931	Metacycline	-3.709	-4.004
C17H19N3O3S	DB00338	Omeprazole	-3.964	-3.998
C23H32N2O5	DB00178	Ramipril	-3.269	-3.995
C36H47N5O4	DB00224	Indinavir	-2.845	-3.991
C9H9Cl2N3	DB00575	Clonidine	-2.057	-3.99
C9H8CIN5S	DB00697	Tizanidine	-3.152	-3.989
C17H25N3O5S	DB00760	Meropenem	-2.188	-3.989
C8H11NO3	DB00165	Pyridoxine	-3.756	-3.98
C20H17FO3S	DB00605	Sulindac	-3.976	-3.976
C27H41NO6	DB00769	Hydrocortamate	-2.86	-3.975
C52H98N16O13	DB00803	Colistin	-2.642	-3.974
C22H22N2O8	DB00931	Metacycline	-1.703	-3.968
C14H20GdN3O10	DB00789	Gadopentetic acid	-2.125	-3.965
C3H7O4P	DB00828	Fosfomycin	-3.336	-3.962
C8H11Cl2N3O2	DB00791	Uracil mustard	-2.029	-3.961
C5H5N5S	DB00352	Tioguanine	-1.782	-3.957
C16H15N3	DB00751	Epinastine	-3.915	-3.954
C9H10N2O3	DB00345	Aminohippuric acid	-3.949	-3.949
C27H29NO10	DB00694	Daunorubicin	-2.108	-3.948
C15H12ClNO2	DB00821	Carprofen	-3.943	-3.944
C6H12N2O4S2	DB00138	Cystine	-3.914	-3.944
C13H22N4O3S	DB00863	Ranitidine	-3.488	-3.94
C20H22CIN3O	DB00613	Amodiaquine	-1.374	-3.939
C17H21NO3	DB00674	Galantamine	-3.921	-3.938
C13H16N2	DB00633	Dexmedetomidine	-3.149	-3.936
C20H15F3N4O3	DB00685	Trovafloxacin	-2.039	-3.935
C21H21CIN2O8	DB00618	Demeclocycline	-1.526	-3.93
C32H45N3O4S	DB00220	Nelfinavir	-1.696	-3.928
C19H21N	DB00540	Nortriptyline	-3.92	-3.92
C18H19N3O3S	DB00412	Rosiglitazone	-2.543	-3.92
C23H31NO7	DB00688	Mycophenolate mofetil	-2.202	-3.91
C16H14F3N3O2S	DB00448	Lansoprazole	-3.888	-3.908
C18H29NO3	DB00195	Betaxolol	-3.904	-3.906
C6H10N6O	DB00851	Dacarbazine	-3.87	-3.903

C26H35F3O6	DB00287	Travoprost	-3.899	-3.899
C17H20FN3O3	DB00487	Pefloxacin	-2.336	-3.894
C12H12N2O2S	DB00250	Dapsone	-3.886	-3.886
C5H5N5S	DB00352	Tioguanine	-3.868	-3.886
C10H14N2	DB00184	Nicotine	-1.977	-3.885
C22H24N2O8	DB00759	Tetracycline	-2.806	-3.853
C17H17ClO6	DB00400	Griseofulvin	-3.846	-3.846
C6H9N3O2	DB00117	Histidine	-2.119	-3.84
C19H21N5O4	DB00457	Prazosin	-1.539	-3.839
C10H16N2O3	DB00237	Butabarbital	-3.795	-3.83
C21H23ClFNO2	DB00502	Haloperidol	-3.815	-3.828
C21H27N3O2	DB00247	Methysergide	-3.576	-3.828
C15H12N2O2	DB00776	Oxcarbazepine	-3.824	-3.824
C18H19ClN4	DB00363	Clozapine	-3.795	-3.821
C21H31N3O5	DB00722	Lisinopril	-2.823	-3.82
C17H19N3O3S	DB00736	Esomeprazole	-2.048	-3.817
C17H23NO3	DB00572	Atropine	-3.811	-3.814
C9H11N2O5	DB00249	Idoxuridine	-1.605	-3.814
C7H15NO3	DB00583	Levocarnitine	-3.809	-3.809
C9H11ClO3	DB00856	Chlorphenesin	-3.801	-3.801
C11H12N2S	DB00848	Levamisole	-3.716	-3.798
C16H15N5O7S2	DB00671	Cefixime	-3.795	-3.795
C32H32O13S	DB00444	Teniposide	-3.794	-3.795
C41H76N2O15	DB00778	Roxithromycin	-1.155	-3.794
C20H30O2	DB00159	Icosapent	-3.789	-3.792
C18H21NO3	DB00318	Codeine	-3.742	-3.787
C16H15F2N3O4S	DB00213	Pantoprazole	-2.095	-3.787
C12H9N3O5S	DB00507	Nitazoxanide	-1.598	-3.782
C6H10N6O	DB00851	Dacarbazine	-2.034	-3.78
C11H12N2O2S	DB00744	Zileuton	-1.715	-3.776
C17H20N2O2	DB00809	Tropicamide	-3.766	-3.774
C11H17NO3	DB00723	Methoxamine	-1.364	-3.773
C10H16N6S	DB00501	Cimetidine	-3.216	-3.769
C12H10N2O5	DB00827	Cinoxacin	-1.922	-3.766
C17H21NO3	DB00674	Galantamine	-1.65	-3.766
C22H32O3	DB00253	Medrysone	-3.765	-3.765
C8H8Cl2N4	DB00629	Guanabenz	-3.76	-3.76
C22H24N2O8	DB00254	Doxycycline	-3.526	-3.758
C11H16N4O4	DB00380	Dexrazoxane	-2.565	-3.758
C17H22N4O	DB00805	Minaprine	-3.661	-3.756
C12H10N2O5	DB00827	Cinoxacin	-3.726	-3.753
C17H19NO3	DB00295	Morphine	-1.18	-3.752
C10H11F3N2O5	DB00432	Trifluridine	-3.667	-3.751
C16H17N3O4S	DB00567	Cephalexin	-3.487	-3.746
C17H19N3O3S	DB00736	Esomeprazole	-2.349	-3.744
C9H18N6	DB00488	Altretamine	-3.694	-3.743
C20H30NO3	DB00332	Ipratropium	-3.741	-3.741
C18H19N3O3S	DB00412	Rosiglitazone	-3.217	-3.741
C9H13N	DB00182	Amphetamine	-3.737	-3.738
C13H22N4O3S	DB00863	Ranitidine	-1.699	-3.731
C24H33FO6	DB00846	Flurandrenolide	-3.729	-3.729
C17H17ClN6O3	DB00402	Eszopiclone	-3.376	-3.726
C15H12N2O	DB00564	Carbamazepine	-3.707	-3.707
C20H23N7O7	DB00650	Leucovorin	-3.707	-3.707
C13H24N4O3S	DB00373	Timolol	-3.703	-3.704
C12H11ClN2O5S	DB00695	Furosemide	-3.703	-3.703
C10H18O21S4	DB00686	Pentosan Polysulfate	-3.698	-3.698
C16H24N2O3	DB00521	Carteolol	-3.697	-3.698
C2H5NO2	DB00551	Acetohydroxamic acid	-3.681	-3.684
C20H25N3O2	DB00353	Methylergometrine	-3.43	-3.683
C15H10Cl2N2O2	DB00186	Lorazepam	-3.677	-3.677
C23H27N5O7S	DB00319	Piperacillin	-3.674	-3.675
C16H20FN3O4	DB00601	Linezolid	-3.673	-3.673

C6H14N2O2	DB00123	L-Lysine	-3.673	-3.673
C20H24N2O	DB00192	Indecainide	-3.67	-3.671
C22H22N2O8	DB00931	Metacycline	-1.334	-3.668
C10H12N2O4	DB00649	Stavudine	-3.664	-3.665
C37H48N6O5S2	DB00503	Ritonavir	-3.663	-3.663
C20H23NO4	DB00704	Naltrexone	-1.933	-3.663
C18H14N4O5S	DB00795	Sulfasalazine	-2.355	-3.662
C18H20O2	DB00255	Diethylstilbestrol	-3.66	-3.661
C11H16N4O4	DB00380	Dexrazoxane	-2.78	-3.653
C21H27N3O2	DB00247	Methysergide	-3.024	-3.651
C15H19N5	DB00953	Rizatriptan	-3.644	-3.648
C12H20N2O3S	DB00489	Sotalol	-1.661	-3.644
C19H22FN3O3	DB00365	Grepafloxacin	-2.63	-3.638
C17H21NO3	DB00867	Ritodrine	-1.33	-3.637
C20H26N2	DB00726	Trimipramine	-3.635	-3.635
C5H11Cl2N	DB00888	Mechlorethamine	-2.282	-3.627
C11H17NO3	DB00723	Methoxamine	-3.615	-3.626
C24H31ClO7	DB14596	Loteprednol etabonate	-3.625	-3.625
C21H21N	DB00735	Naftifine	-3.544	-3.624
C15H14ClN3O4S3	DB00562	Benzthiazide	-3.072	-3.62
C24H36O3	DB00486	Nabilone	-3.616	-3.616
C17H14F3N3O2S	DB00482	Celecoxib	-3.615	-3.616
C19H19NOS	DB00920	Ketotifen	-1.033	-3.608
C17H23NO3	DB00424	Hyoscyamine	-3.604	-3.607
C45H54N4O8	DB00361	Vinorelbine	-2.163	-3.598
C16H18N2O5S	DB00417	Phenoxymethylpenicillin	-3.597	-3.597
C10H16N6S	DB00501	Cimetidine	-1.091	-3.596
C8H8N2O3S	DB00909	Zonisamide	-3.59	-3.591
C22H24N2O9	DB00595	Oxytetracycline	-2.932	-3.591
C5H4N4O	DB00437	Allopurinol	-1.145	-3.587
C33H37N5O5	DB00320	Dihydroergotamine	-1.397	-3.583
C15H16O2	DB00461	Nabumetone	-3.582	-3.582
C17H17NO2	DB00714	Apomorphine	-2.017	-3.581
C22H29FO4	DB00547	Desoximetasone	-3.579	-3.579
C17H20FN3O3	DB00487	Pefloxacin	-3.411	-3.572
C21H30O2	DB00470	Dronabinol	-3.571	-3.571
C23H25N5O5	DB00590	Doxazosin	-2.531	-3.569
C11H16N2O3	DB00241	Butalbital	-2.128	-3.569
C9H11FN2O5	DB00322	Floxuridine	-1.779	-3.565
C21H41N5O7	DB00955	Netilmicin	-1.432	-3.562
C21H27ClN2O2	DB00557	Hydroxyzine	-1.836	-3.561
C9H8O4	DB00945	Acetylsalicylic acid	-3.56	-3.56
C5H5N5	DB00173	Adenine	-3.535	-3.555
C20H12O5	DB00693	Fluorescein	-3.338	-3.554
C14H14O3	DB00788	Naproxen	-3.548	-3.548
C8H17NO2	DB00230	Pregabalin	-3.544	-3.544
C12H17N4OS	DB00152	Thiamine	-3.521	-3.54
C19H27N5O4	DB00346	Alfuzosin	-3.539	-3.539
C17H17NO2	DB00714	Apomorphine	-3.493	-3.537
C23H24N2O4S	DB00876	Eprosartan	-1.792	-3.527
C10H13ClN2O3S	DB00672	Chlorpropamide	-0.889	-3.525
C23H25F3N2OS	DB00875	Flupentixol	-3.284	-3.523
C8H14O2S2	DB00166	Lipoic Acid	-3.516	-3.519
C19H32N2O5	DB00790	Perindopril	-3.263	-3.518
C25H30NO3	DB00209	Trospium	-3.516	-3.516
C15H17FN4O3	DB00467	Enoxacin	-1.893	-3.516
C17H28N2O3	DB00892	Oxybuprocaine	-1.527	-3.514
C14H10F3NO5	DB00348	Nitisinone	-3.51	-3.51
C17H24BrNO3	DB00725	Homatropine methylbromide	-3.504	-3.505
C10H21N3O	DB00711	Diethylcarbamazine	-3.151	-3.503
C4H6O4	DB00139	Succinic acid	-0.831	-3.5
C6H13NO2	DB00149	L-Leucine	-3.499	-3.499
C3H6N2O2	DB00260	Cycloserine	-3.246	-3.493

C15H14ClN3O4S	DB00833	Cefaclor	-3.26	-3.492
C26H29N3O6	DB00622	Nicardipine	-3.267	-3.488
C22H38O5	DB00929	Misoprostol	-3.487	-3.487
C18H24BrNO4	DB00462	Methscopolamine bromide	-3.486	-3.486
C9H13NO2	DB00610	Metaraminol	-1.077	-3.486
C17H20FN3O3	DB00487	Pefloxacin	-2.351	-3.478
C21H26O3	DB00459	Acitretin	-3.474	-3.477
C29H50O2	DB00163	Vitamin E	-3.474	-3.474
C16H21NO2	DB00571	Propranolol	-3.471	-3.473
C23H31NO7	DB00688	Mycophenolate mofetil	-1.717	-3.472
C20H12O5	DB00693	Fluorescein	-2.754	-3.464
C9H13NO2	DB00388	Phenylephrine	-0.795	-3.456
C15H12I3NO4	DB00279	Liothyronine	-3.347	-3.45
C27H44O3	DB00910	Paricalcitol	-3.448	-3.448
C10H12N4O3	DB00900	Didanosine	-3.364	-3.447
C19H22FN3O3	DB00365	Grepafloxacin	-3.325	-3.444
C21H28N2O5	DB00662	Trimethobenzamide	-1.43	-3.443
C25H47NO8	DB00429	Carboprost tromethamine	-3.437	-3.44
C12H18N2O3	DB00418	Secobarbital	-1.933	-3.437
C20H32N5O8P	DB00718	Adefovir dipivoxil	-3.434	-3.434
C6H6N6O2	DB00853	Temozolomide	-3.433	-3.434
C17H17ClN6O3	DB00402	Eszopiclone	-2.954	-3.432
C5H5N3O	DB00339	Pyrazinamide	-3.428	-3.428
C11H10BrN5	DB00484	Brimonidine	-1.924	-3.425
C23H25N5O5	DB00590	Doxazosin	-1.208	-3.425
C2H7NS	DB00847	Cysteamine	-0.807	-3.425
C26H28ClNO	DB00539	Toremifene	-3.403	-3.424
C13H12F2N6O	DB00196	Fluconazole	-3.42	-3.42
C21H31N3O5	DB00722	Lisinopril	-3.296	-3.418
C19H25NO	DB00504	Levallorphan	-1.582	-3.418
C9H13NO2	DB00610	Metaraminol	-3.403	-3.414
C25H30N3	DB00406	Gentian violet cation	-1.132	-3.412
C19H19N3O5S	DB00713	Oxacillin	-3.41	-3.41
C9H18N2O4	DB00371	Meprobamate	-3.409	-3.409
C17H21NO3	DB00749	Etodolac	-3.407	-3.408
C29H33ClN2O2	DB00836	Loperamide	-3.376	-3.405
C21H25N5O8S2	DB00948	Mezlocillin	-3.402	-3.402
C9H11N2O5	DB00249	Idoxuridine	-3.387	-3.401
C3H7O4P	DB00828	Fosfomycin	-3.144	-3.398
C5H11NO2	DB00161	L-Valine	-3.395	-3.395
C13H16N2O2	DB00357	Aminoglutethimide	-3.394	-3.395
C13H14N2O3	DB00849	Methylphenobarbital	-3.306	-3.394
C8H15NO2	DB00302	Tranexamic acid	-3.393	-3.393
C19H19NOS	DB00920	Ketotifen	-3.383	-3.391
C8H6N4O5	DB00698	Nitrofurantoin	-2.109	-3.39
C18H18O2	DB00890	Dienestrol	-3.386	-3.386
C20H15F3N4O3	DB00685	Trovafloxacin	-3.34	-3.386
C21H27NO4	DB00844	Nalbuphine	-1.428	-3.386
C10H12ClNO2	DB00181	Baclofen	-3.378	-3.378
C32H47F5O3S	DB00947	Fulvestrant	-3.378	-3.378
C18H25NO	DB00514	Dextromethorphan	-3.368	-3.372
C24H28N2O5	DB00542	Benazepril	-3.007	-3.364
C14H18N2O3	DB00474	Methohexital	-1.951	-3.363
C21H21NO2S	DB00799	Tazarotene	-3.362	-3.362
C16H25NO4	DB00187	Esmolol	-3.36	-3.362
C22H28O2	DB00294	Etonogestrel	-3.359	-3.359
C12H18O	DB00818	Propofol	-3.356	-3.356
C9H13NO	DB00397	Phenylpropranolamine	-0.947	-3.356
C21H23NO3	DB00768	Olopatadine	-3.354	-3.354
C9H11N	DB00752	Tranlycypromine	-3.324	-3.353
C11H16N4O4	DB00380	Dexrazoxane	-1.775	-3.353
C12H10F3N3O4	DB00665	Nilutamide	-3.351	-3.352
C11H18N2O3	DB00312	Pentobarbital	-1.659	-3.347

C12H21NO8S	DB00273	Topiramate	-0.922	-3.344
C12H14N2O2	DB00794	Primidone	-3.342	-3.342
C22H22N2O8	DB00931	Metacycline	-2.705	-3.34
C19H21N5O4	DB00457	Prazosin	-2.097	-3.339
C10H15NO	DB00852	Pseudoephedrine	-3.315	-3.322
C20H28N2O5	DB00584	Enalapril	-3.122	-3.318
C11H11F3N2O3	DB00499	Flutamide	-3.317	-3.317
C17H20N4S	DB00334	Olanzapine	-1.655	-3.314
C7H10N2OS	DB00550	Propylthiouracil	-1.645	-3.314
C17H19N3O3S	DB00338	Omeprazole	-1.602	-3.313
C21H34NO3	DB00219	Oxyphenonium	-3.31	-3.31
C23H24N2O4S	DB00876	Eprosartan	-3.272	-3.304
C20H28N2O5S	DB00706	Tamsulosin	-3.3	-3.3
C9H11NO3	DB00135	Tyrosine	-3.299	-3.299
C20H21N7O6S2	DB00923	Ceforanide	-1.384	-3.293
C19H30N5O10P	DB00300	Tenofovir disoproxil	-3.291	-3.291
C10H16N2O3S	DB00121	Biotin	-3.285	-3.288
C17H16CIN3O	DB00543	Amoxapine	-3.274	-3.288
C18H18CIN3O	DB00408	Loxapine	-3.256	-3.288
C22H24N2O8	DB00759	Tetracycline	-0.956	-3.285
C14H22N2O3	DB00335	Atenolol	-3.278	-3.279
C13H12Cl2O4	DB00903	Etacrynic acid	-3.275	-3.275
C23H29ClFN3O4	DB00604	Cisapride	-2.108	-3.273
C9H13NO2	DB00388	Phenylephrine	-3.263	-3.269
C21H24FN3O4	DB00218	Moxifloxacin	-3.168	-3.269
C12H17N4OS	DB00152	Thiamine	-1.217	-3.267
C8H15N7O2S3	DB00927	Famotidine	-2.776	-3.261
C21H26CIN3OS	DB00850	Perphenazine	-1.289	-3.259
C6H6N4O4	DB00336	Nitrofuraf	-3.258	-3.258
C16H13CIN2O	DB00579	Mazindol	-0.642	-3.257
C6H14N4O2	DB00125	L-Arginine	-3.256	-3.256
C22H29FO4	DB00324	Fluorometholone	-3.256	-3.256
C22H26N2O2S	DB00216	Eletriptan	-3.25	-3.252
C9H13NO	DB00397	Phenylpropanolamine	-3.237	-3.247
C15H11I4NO4	DB00451	Levothyroxine	-2.259	-3.247
C4H3FN2O2	DB00544	Fluorouracil	-2.499	-3.242
C11H12N2O2	DB00754	Ethotoin	-3.24	-3.24
C36H47N5O4	DB00224	Indinavir	-2.598	-3.24
C19H23N3O4S	DB00739	Hetacillin	-3.233	-3.237
C14H18N4O3	DB00440	Trimethoprim	-2.6	-3.232
C19H12O6	DB00266	Dicoumarol	-2.173	-3.232
C10H20O	DB00825	Levomethol	-3.231	-3.231
C11H12N4O3S	DB00664	Sulfametopyrazine	-3.115	-3.228
C21H19N3O3S	DB00276	Amsacrine	-1.179	-3.225
C12H9N3O	DB00235	Milrinone	-1.159	-3.224
C8H10N2O3S	DB00634	Sulfacetamide	-1.132	-3.224
C13H6Cl6O2	DB00756	Hexachlorophene	-3.211	-3.22
C17H26N2O	DB00296	Ropivacaine	-1.775	-3.216
C18H24O2	DB00783	Estradiol	-3.215	-3.215
C19H28O2	DB00624	Testosterone	-3.212	-3.212
C28H30N2O2	DB00496	Darifenacin	-3.209	-3.211
C29H39N5O8	DB00560	Tigecycline	-0.559	-3.211
C18H14N4O5S	DB00795	Sulfasalazine	-2.439	-3.201
C24H34O3	DB00896	Rimexolone	-3.2	-3.2
C13H12O2	DB00600	Monobenzene	-3.197	-3.197
C10H19O6PS2	DB00772	Malathion	-3.194	-3.194
C17H25N3O5S	DB00760	Meropenem	-3.159	-3.188
C17H21NO4	DB00907	Cocaine	-1.765	-3.184
C13H14N2O3	DB00849	Methylphenobarbital	-2.006	-3.182
C19H27NO	DB00652	Pentazocine	-3.169	-3.18
C22H26NO3	DB00771	Clidinium	-3.177	-3.177
C17H19CIN2S	DB00477	Chlorpromazine	-3.176	-3.177
C11H18N2O3	DB00312	Pentobarbital	-3.141	-3.176

C14H9CIF3NO2	DB00625	Efavirenz	-3.174	-3.174
C21H31N5O2	DB00490	Buspirone	-2.839	-3.169
C12H19NO3	DB00871	Terbutaline	-3.151	-3.165
C15H13N3O4S	DB00554	Piroxicam	-3.159	-3.164
C26H28ClNO	DB00882	Clomifene	-3.141	-3.162
C14H11Cl2NO2	DB00939	Meclofenamic acid	-3.16	-3.161
C21H25N	DB00857	Terbinafine	-3.038	-3.159
C17H29GdN4O7	DB00597	Gadoteridol	-0.672	-3.157
C17H21NO4	DB00747	Scopolamine	-2.446	-3.156
C11H8O2	DB00170	Menadione	-3.15	-3.15
C7H15Cl2N2O2P	DB00531	Cyclophosphamide	-3.146	-3.146
C17H16ClN3O	DB00543	Amoxapine	-0.896	-3.146
C4H6O4	DB00139	Succinic acid	-3.138	-3.145
C12H21NO8S	DB00273	Topiramate	-3.133	-3.143
C17H29GdN4O7	DB00597	Gadoteridol	-1.035	-3.143
C16H13ClN2O2	DB00349	Clobazam	-2.757	-3.142
C16H14F3N5O	DB00582	Voriconazole	-3.14	-3.14
C32H45N3O4S	DB00220	Nelfinavir	-3.126	-3.14
C5H11NO4S	DB00659	Acamprosate	-3.137	-3.137
C4H6N4O3S2	DB00819	Acetazolamide	-1.716	-3.134
C15H12N2O2	DB00252	Phenytoin	-1.612	-3.133
C52H98N16O13	DB00803	Colistin	-0.709	-3.132
C20H24ClN3S	DB00433	Prochlorperazine	-0.787	-3.131
C16H13ClN2O2	DB00231	Temazepam	-3.129	-3.129
C4H3FN2O2	DB00544	Fluorouracil	-2.927	-3.127
C15H23N3O4S	DB00391	Sulpiride	-3.126	-3.126
CH3O5P	DB00529	Foscarnet	-0.436	-3.124
C19H24N2O	DB00377	Palonosetron	-3.122	-3.123
C15H15NO2	DB00784	Mefenamic acid	-3.121	-3.121
C14H22N2O	DB00281	Lidocaine	-3.1	-3.121
C17H16F6N2O	DB00358	Mefloquine	-3.116	-3.119
C8H8F3N3O4S2	DB00774	Hydroflumethiazide	-3.068	-3.114
C20H26N4O	DB00589	Lisuride	-2.674	-3.112
C12H15N3O2S	DB00518	Albendazole	-1.695	-3.109
C28H27NO4S	DB00481	Raloxifene	-0.646	-3.108
C16H16N2O6S2	DB00456	Cefalotin	-3.107	-3.107
C18H19N3O6S	DB00689	Cephaloglycin	-2.471	-3.103
C3H4O3	DB00119	Pyruvic acid	-3.1	-3.1
C16H15F2N3O4S	DB00213	Pantoprazole	-1.013	-3.099
C6H5NO2	DB00627	Niacin	-0.65	-3.098
C29H38N4O10	DB00256	Lymecycline	-2.935	-3.097
C22H23ClN6O	DB00678	Losartan	-3.095	-3.095
C6H7N3O	DB00951	Isoniazid	-3.092	-3.092
C7H11NO3	DB00617	Paramethadione	-3.091	-3.091
C23H21F7N4O3	DB00673	Aprepitant	-3.087	-3.087
C19H29NO5	DB00449	Dipivefrin	-0.422	-3.084
C19H22ClN5O	DB00656	Trazodone	-2.665	-3.083
C43H66O14	DB00511	Acetyldigitoxin	-3.081	-3.081
C21H24FN3O4	DB00218	Moxifloxacin	-1.982	-3.08
C13H18N4O3	DB00806	Pentoxifylline	-3.079	-3.079
C10H15NO	DB00852	Pseudoephedrine	-0.412	-3.074
C46H56N4O10	DB00541	Vincristine	-1.974	-3.068
C19H21N3O5	DB00270	Isradipine	-3.067	-3.067
C11H13N3O3S	DB00263	Sulfisoxazole	-3.066	-3.066
C22H28N2O2	DB00913	Anileridine	-1.054	-3.065
C28H35FO7	DB00288	Amcinonide	-3.063	-3.063
C6H9NO3	DB00347	Trimethadione	-3.057	-3.057
C2H7NS	DB00847	Cysteamine	-3.035	-3.057
C17H18FN3O3	DB00537	Ciprofloxacin	-1.952	-3.057
C8H10N2O3S	DB00634	Sulfacetamide	-3.035	-3.053
C22H24ClFN4O3	DB00317	Gefitinib	-2.631	-3.046
C7H11NO2	DB00593	Ethosuximide	-3.045	-3.045
C19H16O4	DB00682	Warfarin	-3.025	-3.045

C46H56N4O10	DB00541	Vincristine	-1.339	-3.041
C19H17NO7	DB00716	Nedocromil	-3.038	-3.038
C6H13NO2	DB00513	Aminocaproic Acid	-3.034	-3.034
C14H21N3O2S	DB00669	Sumatriptan	-3.026	-3.03
C10H16N2O3	DB00237	Butabarbital	-1.35	-3.03
C20H23NO4	DB00704	Naltrexone	-2.974	-3.022
C20H22N8O5	DB00563	Methotrexate	-0.557	-3.018
C11H9I3N2O4	DB00271	Diatrizoate	-3.014	-3.014
C28H37ClO7	DB00394	Beclomethasone dipropionate	-3.014	-3.014
C8H15N7O2S3	DB00927	Famotidine	-1.713	-3.012
C8H12N2	DB00780	Phenelzine	-2.002	-3.009
C22H28ClFO4	DB00838	Clocortolone	-3.006	-3.006
C33H34N6O6	DB00796	Candesartan cilexetil	-2.846	-3.002
C16H16ClN3O4	DB00447	Loracarbef	-2.449	-3.001
C19H21N3O	DB00425	Zolpidem	-2.656	-3
C11H16N2O3	DB00306	Talbutal	-1.557	-2.998
C17H20FN3O3	DB00487	Pefloxacin	-0.534	-2.992
C27H44O2	DB00146	Calcifediol	-2.989	-2.989
C22H22FN3O2	DB00450	Droperidol	-2.89	-2.988
C20H25N3O2	DB00353	Methylethylmetrine	-2.357	-2.985
C10H15N5	DB00914	Phenformin	-0.449	-2.985
C15H14O3	DB00573	Fenoprofen	-2.981	-2.981
C28H44O	DB00153	Ergocalciferol	-2.98	-2.98
C14H12N6O	DB00922	Levosimendan	-2.897	-2.978
C20H26N4O	DB00589	Lisuride	-2.587	-2.971
C16H13N3O3	DB00643	Mebendazole	-2.306	-2.965
C17H20N2O5S	DB00887	Bumetanide	-2.962	-2.962
C23H25F3N2OS	DB00875	Flupentixol	-2.152	-2.961
C16H19N3O4S	DB00415	Ampicillin	-2.733	-2.96
C15H12I3NO4	DB00279	Liothyronine	-1.868	-2.959
C17H29GdN4O7	DB00597	Gadoteridol	-2.926	-2.957
C14H18N4O3	DB00440	Trimethoprim	-2.486	-2.956
C30H53NO11	DB00868	Benzonatate	-2.954	-2.954
C15H11I4NO4	DB00509	Dextrothyroxine	-2.827	-2.951
C27H34N2O7	DB00691	Moexipril	-2.795	-2.949
C5H9N3	DB00272	Betazole	-2.538	-2.948
C19H27NO3	DB00731	Nateglinide	-2.946	-2.946
C21H19N3O3S	DB00276	Amsacrine	-2.926	-2.945
C20H22ClN3O	DB00613	Amodiaquine	-2.65	-2.941
C7H6ClN3O4S2	DB00880	Chlorothiazide	-2.621	-2.935
C22H25N3O4S	DB00680	Moricizine	-1.391	-2.93
C18H18ClN3O	DB00408	Loxapine	-1.182	-2.929
C24H34N2O5	DB00519	Trandolapril	-2.195	-2.923
C15H14N4O	DB00238	Nevirapine	-2.921	-2.921
C8H10N4O2	DB00824	Enprofylline	-0.27	-2.92
C7H6ClN3O4S2	DB00880	Chlorothiazide	-2.381	-2.915
C33H35N5O5	DB00696	Ergotamine	-2.05	-2.915
C13H20N2O2	DB00721	Procaine	-2.892	-2.913
C7H4ClNO2	DB00356	Chlorzoxazone	-1.188	-2.91
C20H22N2	DB00719	Azatadine	-2.905	-2.909
C37H67NO13	DB00199	Erythromycin	-2.902	-2.908
C9H7Cl2N5	DB00555	Lamotrigine	-2.876	-2.905
C15H11I4NO4	DB00451	Levothyroxine	-2.777	-2.901
C14H11Cl2NO2	DB00586	Diclofenac	-2.898	-2.899
C21H26ClN3OS	DB00850	Perphenazine	-2.555	-2.891
C10H7Cl2N3O	DB00261	Anagrelide	-2.888	-2.888
C10H15N5	DB00914	Phenformin	-2.87	-2.887
C22H26F3N3OS	DB00623	Fluphenazine	-0.915	-2.885
C10H13NO3	DB00765	Metyrosine	-2.881	-2.881
C20H24N2O2	DB00908	Quinidine	-2.866	-2.881
C13H20N2O	DB00750	Prilocaine	-1.51	-2.881
C18H13Cl4N3O	DB00239	Oxiconazole	-1.84	-2.878
C22H28Cl2O4	DB00764	Mometasone	-2.876	-2.876

C8H12N2	DB00780	Phenelzine	-2.094	-2.874
C10H16Br2N2O2	DB00236	Pipobroman	-2.872	-2.872
C19H27N3O5S2	DB00204	Dofetilide	-1.324	-2.872
C9H11Cl2N3O4S2	DB00232	Methyclothiazide	-2.87	-2.87
C16H26N2O3	DB00807	Proparacaine	-2.849	-2.868
C21H25CIN2O3	DB00341	Cetirizine	-1.009	-2.868
C28H28O3	DB00210	Adapalene	-2.867	-2.867
C21H29NO2	DB00611	Butorphanol	-2.856	-2.867
C22H28N6O3S	DB00705	Delavirdine	-2.702	-2.863
C21H21CIN2O8	DB00618	Demeclocycline	-0.348	-2.861
C17H19N3	DB00370	Mirtazapine	-1.594	-2.857
C18H13CIFN3	DB00683	Midazolam	-2.64	-2.851
C25H30N2O5	DB00881	Quinapril	-1.974	-2.848
C29H33CIN2O2	DB00836	Loperamide	-1.057	-2.847
C19H27NO	DB00652	Pentazocine	-0.507	-2.847
C32H26N4O2	DB00872	Conivaptan	-1.927	-2.841
C16H14N2O3S	DB00580	Valdecoxib	-2.839	-2.839
C14H12N6O	DB00922	Levosimendan	-1.617	-2.838
C18H28N2O	DB00297	Bupivacaine	-1.396	-2.837
C29H35NO2	DB00834	Mifepristone	-0.683	-2.837
C53H72N2O12	DB00565	Cisatracurium	-2.836	-2.836
C19H17CIFN3O5S	DB00301	Flucloxacillin	-2.836	-2.836
C26H40O5	DB00654	Latanoprost	-2.836	-2.836
C19H21N5O2	DB00670	Pirenzepine	-2.55	-2.835
C18H22CINO	DB00925	Phenoxybenzamine	-2.46	-2.834
C21H27NO	DB00333	Methadone	-2.823	-2.826
C4H10N2	DB00592	Piperazine	-2.81	-2.823
C10H8N6O	DB00885	Pemirolast	-2.821	-2.822
C21H23CIFNO2	DB00502	Haloperidol	-0.57	-2.822
C22H23N3O4	DB00530	Erlotinib	-2.82	-2.82
C19H12O6	DB00266	Dicoumarol	-2.697	-2.811
C6H9N3O2	DB00117	Histidine	-2.376	-2.811
C24H32O4S	DB00421	Spirolactone	-2.81	-2.81
C8H10N2S	DB00609	Ethionamide	-2.81	-2.81
C23H25F3N2OS	DB00875	Flupentixol	-1.289	-2.81
C17H19NO3	DB00295	Morphine	-1.32	-2.807
C14H10Cl4	DB00648	Mitotane	-2.804	-2.804
C55H75N17O13	DB00644	Gonadorelin	-1.976	-2.803
C16H19CIN2O	DB00748	Carbinoxamine	-2.796	-2.802
C27H36N2O4	DB00912	Repaglinide	-2.786	-2.795
C16H13CIN2O2	DB00349	Clobazam	-2.357	-2.794
C21H25CIN2O3	DB00341	Cetirizine	-2.382	-2.793
C20H24N2O2	DB00468	Quinine	-0.516	-2.793
C18H22O2	DB00655	Estrone	-2.792	-2.792
C6H9N3O3	DB00916	Metronidazole	-2.79	-2.79
C16H13CIN2O	DB00579	Mazindol	-2.78	-2.788
C19H24O3	DB00894	Testolactone	-2.778	-2.778
C22H26N2O4S	DB00343	Diltiazem	-2.76	-2.778
C12H8O4	DB00553	Methoxsalen	-2.775	-2.775
C33H37N5O5	DB00320	Dihydroergotamine	-1.045	-2.772
C16H19BrN2	DB00835	Brompheniramine	-2.769	-2.769
C23H32N6O4S	DB00862	Vardenafil	-1.996	-2.767
C11H16N2O3	DB00306	Talbutal	-2.712	-2.766
C16H19BrN2	DB00405	Dexbrompheniramine	-2.765	-2.765
C27H34N2O7	DB00691	Moexipril	-1.885	-2.759
C19H32N2O5	DB00790	Perindopril	-2.135	-2.758
C10H17N3S	DB00413	Pramipexole	-2.753	-2.753
C6H8N2O2S	DB00259	Sulfanilamide	-2.752	-2.752
C24H30N2O2	DB00561	Doxapram	-2.4	-2.749
C14H12O3S	DB00870	Suprofen	-2.748	-2.748
C20H30O	DB00162	Vitamin A	-2.748	-2.748
C30H46NO7P	DB00492	Fosinopril	-2.747	-2.747
C19H16CINO4	DB00328	Indometacin	-2.746	-2.746

C11H18N2O2S	DB00599	Thiopental	-2.719	-2.746
C17H28N2O3	DB00892	Oxybuprocaine	-2.722	-2.743
C10H16N2O4S3	DB00869	Dorzolamide	-2.675	-2.739
C15H13FO2	DB00712	Flurbiprofen	-2.736	-2.736
C11H18N2O2S	DB00599	Thiopental	-0.474	-2.736
C8H11Cl2N3O2	DB00791	Uracil mustard	-2.711	-2.734
C16H26N2O3	DB00807	Proparacaine	-0.695	-2.734
C18H16O3	DB00946	Phenprocoumon	-1.231	-2.732
C19H25NO	DB00504	Levallorphan	-2.701	-2.728
C20H28O2	DB00523	Alitretinoin	-2.717	-2.722
C8H9NO2	DB00316	Acetaminophen	-2.72	-2.72
C14H11NO5	DB00323	Tolcapone	-2.66	-2.715
C17H19NO3	DB00327	Hydromorphone	-2.658	-2.709
C11H17NO	DB00379	Mexiletine	-2.703	-2.708
C18H26ClN3	DB00608	Chloroquine	-2.664	-2.7
C20H21FN2O	DB00215	Citalopram	-2.696	-2.698
C25H30N2O5	DB00881	Quinapril	-2.543	-2.697
C20H26O2	DB00717	Norethisterone	-2.685	-2.685
C25H35N3O6S	DB00701	Amprenavir	-2.685	-2.685
C17H18FN3O3	DB00537	Ciprofloxacin	-2.586	-2.685
C19H20N2O2	DB00812	Phenylbutazone	-0.086	-2.685
C12H21N5O2S2	DB00585	Nizatidine	-2.683	-2.683
C16H16ClNO2S	DB00758	Clopidogrel	-0.734	-2.683
MgO4S	DB00653	Magnesium sulfate	-2.681	-2.681
C21H29N3O	DB00280	Disopyramide	-2.676	-2.681
C9H16O4	DB00548	Azelaic acid	-0.083	-2.681
C18H19N3O3S	DB00412	Rosiglitazone	-1.341	-2.676
C5H8N4O3S2	DB00703	Methazolamide	-1.465	-2.675
C16H15N3	DB00751	Epinastine	-1.029	-2.673
C9H4Cl3IO	DB00793	Haloprogin	-2.672	-2.672
C7H10N2O2S	DB00389	Carbimazole	-2.671	-2.671
C7H10N2OS	DB00550	Propylthiouracil	-2.632	-2.67
C26H28N2	DB00568	Cinnarizine	-1.446	-2.667
C38H72N2O12	DB00207	Azithromycin	-0.017	-2.662
C9H10N4O2S2	DB00576	Sulfamethizole	-2.644	-2.661
C23H29ClFN3O4	DB00604	Cisapride	-2.571	-2.661
C6H5NO2	DB00627	Niacin	-2.649	-2.659
C11H15NO	DB00830	Phenmetrazine	0.073	-2.654
C17H14O4S	DB00533	Rofecoxib	-2.652	-2.652
C26H28ClNO	DB00539	Toremifene	-0.634	-2.647
C27H22Cl2N4	DB00845	Clofazimine	-2.644	-2.646
C24H30N2O2	DB00561	Doxapram	-2.163	-2.643
C16H24N2O	DB00935	Oxymetazoline	-2.641	-2.641
C17H22N2O	DB00366	Doxylamine	-2.637	-2.64
C12H16F3N	DB00574	Fenfluramine	-2.63	-2.63
C8H10N4O2	DB00201	Caffeine	-2.629	-2.629
C18H16O3	DB00946	Phenprocoumon	-2.58	-2.629
C16H15F2N3O4S	DB00213	Pantoprazole	-1.921	-2.628
C18H19NOS	DB00476	Duloxetine	-2.625	-2.626
C13H11N3O4S2	DB00469	Tenoxicam	-2.619	-2.621
C14H16N4	DB00724	Imiquimod	-2.277	-2.62
C16H28N2O4	DB00198	Oseltamivir	-2.536	-2.618
C16H16ClN3O4	DB00447	Loracarbef	-2.32	-2.617
C11H11NO2	DB00832	Phensuximide	-2.612	-2.612
C17H18N2O6S	DB00578	Carbenicillin	-2.609	-2.609
C14H14ClNS	DB00208	Ticlopidine	-2.434	-2.608
C20H24N2O2	DB00468	Quinine	-2.587	-2.602
C13H16N2	DB00633	Dexmedetomidine	-1.878	-2.597
C29H31N7O	DB00619	Imatinib	-1.84	-2.594
C15H11ClN2O2	DB00842	Oxazepam	-2.591	-2.591
C9H8ClN5S	DB00697	Tizanidine	-2.426	-2.591
C16H13N3O3	DB00643	Mebendazole	-1.902	-2.585
C27H36N2O4	DB00912	Repaglinide	-0.043	-2.582

C19H20N2O3	DB00757	Dolasetron	-1.662	-2.581
C19H23NO3	DB00234	Reboxetine	-2.545	-2.579
C12H13CIN4	DB00205	Pyrimethamine	-2.099	-2.577
C21H26NO3	DB00940	Methantheleine	-2.572	-2.572
C24H28O2	DB00307	Bexarotene	-2.568	-2.569
C16H28N2O4	DB00198	Oseltamivir	-1.353	-2.565
C20H28N2O3	DB00383	Oxyphencyclimine	-2.563	-2.563
C20H28O2	DB00755	Tretinoin	-2.558	-2.563
C19H21N	DB00344	Protriptyline	-2.561	-2.561
C15H21F3N2O2	DB00176	Fluvoxamine	-2.557	-2.56
C21H21N	DB00434	Cyproheptadine	-0.085	-2.56
C5H11NO2S	DB00859	Penicillamine	-2.544	-2.558
C6H14FO3P	DB00677	Isoflurophate	-2.554	-2.554
C23H25N5O5	DB00590	Doxazosin	-2.424	-2.554
C5H12N2O2	DB00129	Ornithine	-2.553	-2.553
C15H14CIN3O4S	DB00833	Cefaclor	-1.881	-2.549
C16H14F3N3O2S	DB00448	Lansoprazole	-0.513	-2.546
C22H28N6O3S	DB00705	Delavirdine	-1.669	-2.54
C19H30O3	DB00621	Oxandrolone	-2.537	-2.537
C16H25NO2	DB00193	Tramadol	-2.533	-2.535
C19H21N5O2	DB00670	Pirenzepine	-1.893	-2.534
C19H16O4	DB00682	Warfarin	-0.534	-2.532
C15H12N2O2	DB00252	Phenytoin	-2.16	-2.525
C17H21NO	DB00289	Atomoxetine	-2.52	-2.52
C14H16N2O2	DB00292	Etomidate	-0.139	-2.52
C7H9ClO	DB00189	Ethchlorvynol	-2.518	-2.518
C16H13CIN2O	DB00829	Diazepam	-2.513	-2.513
C22H25N3O4S	DB00680	Moricizine	-1.349	-2.507
C29H31N7O	DB00619	Imatinib	-0.003	-2.507
C12H14N2O2	DB00532	Mephenytoin	-2.501	-2.501
C15H14CIN3O4S3	DB00562	Benzthiazide	-2.197	-2.5
C20H29N3O2	DB00527	Cinchocaine	-2.495	-2.499
C8H12N2	DB00780	Phenelzine	-2.143	-2.498
C41H42N4O8	DB00460	Verteporfin	-2.496	-2.497
C22H30N6O4S	DB00203	Sildenafil	-2.314	-2.496
C15H10O2	DB00498	Phenindione	-2.493	-2.494
C19H27N5	DB00298	Dapiprazole	-1.621	-2.491
C24H28N2O5	DB00542	Benazepril	-2.019	-2.489
C10H21N3O	DB00711	Diethylcarbamazine	-2.013	-2.489
C24H32O4	DB00823	Ethynodiol diacetate	-2.488	-2.488
C4H10N2	DB00592	Piperazine	-0.136	-2.482
C46H58N4O9	DB00570	Vinblastine	-0.456	-2.481
C6H6Cl6	DB00431	Lindane	-2.479	-2.479
C14H22N2O	DB00281	Lidocaine	-0.477	-2.478
C10H17NOS	DB00185	Cevimeline	-2.476	-2.477
C27H44O3	DB00136	Calcitriol	-2.475	-2.475
C10H14N2	DB00184	Nicotine	-2.448	-2.473
C18H19CIN4	DB00363	Clozapine	-0.602	-2.471
C21H29NO2	DB00611	Butorphanol	-0.085	-2.464
C16H11CIN2O3	DB00628	Clorazepic acid	-2.462	-2.462
C8H8F3N3O4S2	DB00774	Hydroflumethiazide	-0.85	-2.46
C24H30O6	DB00700	Eplerenone	-2.455	-2.455
C4H6N4O3S2	DB00819	Acetazolamide	-1.11	-2.455
C21H21N	DB00434	Cyproheptadine	-2.441	-2.451
C8H16O2	DB00313	Valproic Acid	-2.448	-2.45
C16H19N3O4S	DB00415	Ampicillin	-1.77	-2.447
C26H29NO	DB00675	Tamoxifen	-0.433	-2.446
C21H16ClF3N4O3	DB00398	Sorafenib	-0.127	-2.44
C21H22N2O5S	DB00607	Nafcillin	-2.438	-2.438
C24H26BrN3O3	DB00699	Nicergoline	-0.855	-2.436
C8H13N3O4S	DB00911	Tinidazole	-2.435	-2.435
C14H19NO2	DB00422	Methylphenidate	-2.431	-2.432
C18H21NO4	DB00497	Oxycodone	-2.334	-2.431

C4H6N4O3S2	DB00819	Acetazolamide	-0.29	-2.429
C28H33CIN2	DB00354	Buclizine	-2.233	-2.427
C33H40N2O9	DB00206	Reserpine	-2.384	-2.421
C19H20N2O2	DB00812	Phenylbutazone	-2.408	-2.415
C16H13N3O3	DB00643	Mebendazole	-1.801	-2.415
C14H12O2	DB00676	Benzyl benzoate	-2.41	-2.41
C24H34N4O5S	DB00222	Glimepiride	-2.386	-2.41
C4H6N4O3S2	DB00819	Acetazolamide	-2.156	-2.41
C13H19NO	DB00937	Diethylpropion	-1.503	-2.409
C3H2CIF5O	DB00753	Isoflurane	-2.404	-2.404
C20H34O5	DB00770	Alprostadil	-2.396	-2.4
C22H23CIN2O2	DB00455	Loratadine	-2.374	-2.4
C15H15NO3	DB00500	Tolmetin	-2.396	-2.397
C17H19N3	DB00370	Mirtazapine	-2.307	-2.395
C9H16O4	DB00548	Azelaic acid	-2.386	-2.394
C22H24N2O8	DB00759	Tetracycline	0.006	-2.394
C13H20N2O	DB00750	Prilocaine	-2.332	-2.393
C21H16CIF3N4O3	DB00398	Sorafenib	-2.38	-2.392
C22H30O	DB00304	Desogestrel	-2.386	-2.386
C31H33N3O6S	DB00549	Zafirlukast	-2.372	-2.379
C19H29NO	DB00387	Procyclidine	-2.375	-2.376
C29H31N7O	DB00619	Imatinib	-2.169	-2.376
C19H27N5	DB00298	Dapiprazole	-2.074	-2.374
C17H12Cl2N4	DB00897	Triazolam	-2.369	-2.371
C37H67NO13	DB00199	Erythromycin	0.277	-2.367
C16H17N5O7S2	DB00493	Cefotaxime	-2.364	-2.364
C3H2CIF5O	DB00228	Enflurane	-2.35	-2.35
C26H31Cl2N5O3	DB00251	Terconazole	-2.103	-2.35
C33H37N5O5	DB00320	Dihydroergotamine	-2.295	-2.345
C19H17Cl3N2S	DB00639	Butoconazole	-1.964	-2.343
C21H25N	DB00857	Terbinafine	-1.342	-2.342
C33H34N6O6	DB00796	Candesartan cilexetil	-1.474	-2.34
C24H36O5	DB00227	Lovastatin	-2.339	-2.339
C19H27N5	DB00298	Dapiprazole	-1.278	-2.338
C15H21NO2	DB00454	Meperidine	-2.314	-2.329
C14H14CINS	DB00208	Ticlopidine	-1.519	-2.329
C14H18N4O3	DB00440	Trimethoprim	-1.378	-2.322
C22H28N2O	DB00813	Fentanyl	-0.21	-2.318
C14H29NaO4S	DB00464	Sodium Tetradecyl Sulfate	-2.316	-2.316
C28H33CIN2	DB00354	Buclizine	-1.499	-2.314
C22H30N6O4S	DB00203	Sildenafil	-1.495	-2.314
C17H27NO2	DB00285	Venlafaxine	-2.312	-2.313
C14H19Cl2NO2	DB00291	Chlorambucil	-2.303	-2.305
C19H17Cl2N3O5S	DB00485	Dicloxacillin	-2.303	-2.303
C19H22CIN5O	DB00656	Trazodone	-1.896	-2.299
C21H23CIFN3O	DB00690	Flurazepam	0	-2.297
C16H20N4O3S	DB00214	Torsemide	-1.875	-2.285
C18H21NO3	DB00956	Hydrocodone	-2.252	-2.282
C14H16N2O2	DB00292	Etomidate	-2.27	-2.281
C36H41N3O6	DB00528	Lercanidipine	-0.491	-2.278
C23H32N6O4S	DB00862	Vardenafil	-1.409	-2.274
C22H28N2O2	DB00913	Anileridine	-2.251	-2.272
C24H32O4	DB00351	Megestrol acetate	-2.264	-2.264
C15H25NO3	DB00264	Metoprolol	-2.262	-2.264
C45H54N4O8	DB00361	Vinorelbine	-2.12	-2.262
C21H28O2	DB00378	Dydrogesterone	-2.26	-2.26
C4H6N4O3S2	DB00819	Acetazolamide	-1.038	-2.26
C21H21CIN4OS	DB00246	Ziprasidone	-1.583	-2.253
C14H13N3O4S2	DB00814	Meloxicam	-2.232	-2.248
C18H13CIFN3	DB00683	Midazolam	-1.535	-2.248
C36H42N2	DB00941	Hexafluoronium	-2.241	-2.241
C22H29N3S2	DB00372	Thiethylperazine	-1.954	-2.235
C24H26BrN3O3	DB00699	Nicergoline	-2.188	-2.231

C16H16ClNO2S	DB00758	Clopidogrel	-2.197	-2.22
C10H10N4O2S	DB00359	Sulfadiazine	-1.348	-2.217
C14H16ClN3O4S2	DB00606	Cyclothiazide	0.087	-2.217
C22H26F3N3OS	DB00623	Fluphenazine	-1.665	-2.213
C13H17NO	DB00265	Crotamiton	-2.211	-2.211
C9H11N	DB00752	Tranlycypromine	-0.402	-2.211
C19H27N3O5S2	DB00204	Dofetilide	-0.168	-2.211
C15H21NO2	DB00454	Meperidine	-0.018	-2.211
C20H24N2O2	DB00908	Quinidine	0.069	-2.208
C12H9N3O5S	DB00507	Nitazoxanide	-2.189	-2.204
C18H19N3O3S	DB00412	Rosiglitazone	-1.625	-2.191
C4H6CaO4	DB00258	Calcium acetate	-2.186	-2.189
C13H16N2	DB00633	Dexmedetomidine	-1.699	-2.188
C23H27FN4O2	DB00734	Risperidone	0.234	-2.188
C18H28N2O	DB00297	Bupivacaine	-2.131	-2.186
C18H19N3O	DB00904	Ondansetron	-1.198	-2.182
C23H27FN4O2	DB00734	Risperidone	-2.169	-2.179
C10H7N3S	DB00730	Thiabendazole	-2.177	-2.178
C23H32N6O4S	DB00862	Vardenafil	-0.512	-2.178
C22H17ClN2	DB00257	Clotrimazole	-1.774	-2.172
C23H32N6O4S	DB00862	Vardenafil	0.549	-2.168
C17H22N4O	DB00805	Minaprine	-0.98	-2.164
C19H21N5O2	DB00670	Pirenzepine	-0.291	-2.162
C23H30NO3	DB00782	Propantheline	-2.161	-2.161
C19H21N5O4	DB00457	Prazosin	-2.068	-2.16
C22H23ClN2O2	DB00455	Loratadine	-0.29	-2.16
C27H38N2O4	DB00661	Verapamil	-2.145	-2.15
C33H40N2O9	DB00206	Reserpine	-0.467	-2.141
C17H13ClN4	DB00404	Alprazolam	-2.138	-2.14
C20H25NO2S2	DB00906	Tiagabine	-2.138	-2.138
C13H20N2O2	DB00721	Procaine	-0.148	-2.135
C12H15NO3	DB00660	Metaxalone	-2.12	-2.12
C13H14N2	DB00382	Tacrine	-2.119	-2.12
C25H30N3	DB00406	Gentian violet cation	-2.101	-2.114
C22H24N2O8	DB00254	Doxycycline	0.409	-2.113
C17H12ClF3N2O	DB00801	Halazepam	-2.112	-2.112
C5H14NO	DB00122	Choline	-2.11	-2.11
C26H28ClNO	DB00882	Clomifene	-0.097	-2.11
C27H44O	DB00169	Cholecalciferol	-2.109	-2.109
C12H15N3O2S	DB00518	Albendazole	-2.018	-2.102
C21H23ClFN3O	DB00690	Flurazepam	-2.085	-2.098
C21H21N	DB00735	Naftifine	-0.861	-2.091
C16H20N4O3S	DB00214	Torsemide	-1.661	-2.087
C20H23NO4	DB00704	Naltrexone	0.131	-2.085
C16H21N3O2	DB00315	Zolmitriptan	-2.079	-2.083
C3F8	DB00556	Perflutren	-2.078	-2.078
C9H10N4O2S2	DB00576	Sulfamethizole	0.045	-2.076
C5H8N4O3S2	DB00703	Methazolamide	-1.837	-2.073
C18H19F3N2S	DB00508	Triflupromazine	-2.066	-2.067
C20H31NO	DB00376	Trihexyphenidyl	-2.059	-2.06
C23H32N6O4S	DB00862	Vardenafil	-0.207	-2.057
C18H24N4O	DB00889	Granisetron	-2.051	-2.052
C19H21N3O	DB00425	Zolpidem	-1.565	-2.052
C9H11NO2	DB00120	L-Phenylalanine	-2.041	-2.041
C5H8N4O3S2	DB00703	Methazolamide	-0.72	-2.034
C6H12ClNO	DB00658	Sevelamer	-2.023	-2.025
C17H20N4S	DB00334	Olanzapine	-1.982	-2.025
C22H27ClF2O4	DB00596	Ulobetasol	-2.019	-2.019
C12H15ClO3	DB00636	Clofibrate	-2.018	-2.018
C23H32N6O4S	DB00862	Vardenafil	-0.251	-2.009
C19H17Cl3N2S	DB00639	Butoconazole	-1.553	-1.997
C15H13NO3	DB00465	Ketorolac	-1.988	-1.989
C3H7NO2S	DB00151	L-Cysteine	-1.972	-1.986

C16H23NO2	DB00473	Hexylcaine	-1.982	-1.983
C11H12N4O3S	DB00664	Sulfametopyrazine	-0.946	-1.981
C22H24N2O9	DB00595	Oxytetracycline	0.335	-1.981
C23H32N6O4S	DB00862	Vardenafil	-1.298	-1.977
C33H35N5O5	DB00696	Ergotamine	0.366	-1.973
C21H25CIN2O3	DB00341	Cetirizine	-1.503	-1.968
C66H83N17O13	DB00666	Nafarelin	-1.341	-1.968
C10H15N	DB00191	Phentermine	-1.966	-1.966
C26H31Cl2N5O3	DB00251	Terconazole	-0.806	-1.964
C43H55N5O7	DB00309	Vindesine	0.596	-1.963
C10H20N2S4	DB00822	Disulfiram	-1.962	-1.962
C11H12N2S	DB00848	Levamisole	-0.75	-1.962
C6H8N2O8	DB00883	Isosorbide dinitrate	-1.961	-1.961
C21H29NO	DB00810	Biperiden	-1.952	-1.954
C19H24N2S	DB00392	Profenamine	-1.951	-1.952
C18H27NO2	DB00645	Dyclonine	-1.945	-1.951
C3H5N3O9	DB00727	Nitroglycerin	-1.949	-1.949
C22H26N2O4S	DB00343	Diltiazem	0.149	-1.947
C20H23N	DB00934	Maprotiline	-1.945	-1.945
C13H19NO	DB00937	Diethylpropion	-1.798	-1.942
C22H17CIN2	DB00257	Clotrimazole	-1.512	-1.935
C9H18N6	DB00488	Altretamine	-0.429	-1.934
C20H24CIN3S	DB00433	Prochlorperazine	-1.636	-1.916
C18H14N4O5S	DB00795	Sulfasalazine	-1.625	-1.914
C26H28N2	DB00568	Cinnarizine	-1.819	-1.907
C20H36N2O3S	DB00308	Ibutilide	0.458	-1.904
C5H9Cl2N3O2	DB00262	Carmustine	-1.903	-1.903
C21H26CINO	DB00283	Clemastine	-1.899	-1.9
C21H26N2OS2	DB00933	Mesoridazine	-1.896	-1.897
C24H29N5O3	DB00177	Valsartan	-1.896	-1.896
C24H29NO3	DB00843	Donepezil	-1.888	-1.891
C33H35N5O5	DB00696	Ergotamine	-1.7	-1.877
C45H54N4O8	DB00361	Vinorelbine	-0.577	-1.876
C5H8N4O3S2	DB00703	Methazolamide	-0.422	-1.872
C5H11Cl2N	DB00888	Mechlorethamine	-1.806	-1.87
C21H28N2O5	DB00662	Trimethobenzamide	-1.849	-1.869
C16H16CIN3O3S	DB00808	Indapamide	-1.865	-1.868
C12H25NaO4S	DB00815	Sodium lauryl sulfate	-1.861	-1.861
C17H19NO3	DB00327	Hydromorphone	-0.122	-1.86
C15H14F3N3O4S2	DB00436	Bendroflumethiazide	-1.79	-1.858
C11H21N	DB00657	Mecamylamine	-1.857	-1.857
C21H27NO4	DB00844	Nalbuphine	0.705	-1.855
C45H54N4O8	DB00361	Vinorelbine	0.766	-1.826
C21H30O2	DB00396	Progesterone	-1.824	-1.824
C16H23BrN2O3	DB00409	Remoxipride	-1.821	-1.822
C15H14F3N3O4S2	DB00436	Bendroflumethiazide	-0.447	-1.821
C10H16N6S	DB00501	Cimetidine	-1.031	-1.816
C16H24N2O	DB00268	Ropinirole	-1.808	-1.81
C21H24F3N3S	DB00831	Trifluoperazine	0.534	-1.809
C11H15NO	DB00830	Phenmetrazine	-1.797	-1.803
C17H20N2S	DB00420	Promazine	-1.8	-1.801
C19H24N2	DB00458	Imipramine	-1.799	-1.799
C17H26N2O	DB00296	Ropivacaine	-1.741	-1.795
C16H16CIN3O3S	DB00524	Metolazone	-1.785	-1.787
C22H29N3S2	DB00372	Thiethylperazine	0.558	-1.786
C7H9N2O	DB00733	Pralidoxime	-1.554	-1.779
C26H31Cl2N5O3	DB00251	Terconazole	-0.805	-1.768
C25H27CIN2	DB00737	Meclizine	-1.572	-1.765
C10H12N2	DB00797	Tolazoline	-1.762	-1.762
C20H24N2O6	DB00401	Nisoldipine	-1.757	-1.757
C21H24F3N3S	DB00831	Trifluoperazine	-1.473	-1.753
C17H25N3O2S	DB00918	Almotriptan	-1.74	-1.744
C26H28N2	DB00568	Cinnarizine	0.918	-1.742

C6H15N2O2	DB00411	Carbamoylcholine	-1.738	-1.738
C32H26N4O2	DB00872	Conivaptan	-1.34	-1.731
C19H22N2	DB00427	Tripolidine	-1.727	-1.729
C17H21N	DB00865	Benzphetamine	-0.098	-1.711
C20H24CIN3S	DB00433	Prochlorperazine	-1.097	-1.707
C21H28O2	DB00367	Levonorgestrel	-1.692	-1.692
C29H41NO4	DB00921	Buprenorphine	-1.685	-1.685
C21H24F3N3S	DB00831	Trifluoperazine	-1.059	-1.669
C25H37NO4	DB00905	Bimatoprost	-1.666	-1.666
C22H29NO2	DB00647	Dextropropoxyphene	-1.66	-1.665
C11H14N2O4	DB00949	Felbamate	-1.663	-1.663
C17H19N3O	DB00692	Phentolamine	-1.661	-1.661
C17H19N3	DB00370	Mirtazapine	0.816	-1.659
C11H11N3O2S	DB00891	Sulfapyridine	-0.612	-1.65
C2H7NS	DB00847	Cysteamine	0.537	-1.646
C18H20N2S	DB00902	Methdilazine	-1.641	-1.642
C14H15N3O5	DB00494	Entacapone	-1.635	-1.635
C31H33F3N2O5S	DB00932	Tipranavir	-0.7	-1.632
C10H16N6S	DB00501	Cimetidine	-0.936	-1.618
C17H21N	DB00865	Benzphetamine	-1.569	-1.61
C14H21N3O3S	DB00839	Tolazamide	0.32	-1.6
C25H27CIN2	DB00737	Meclizine	0.563	-1.599
C22H25N3O4S	DB00680	Moricizine	0.095	-1.596
C22H29N3S2	DB00372	Thiethylperazine	-0.983	-1.593
C25H27CIN2	DB00737	Meclizine	-0.775	-1.59
C10H13CIN2O3S	DB00672	Chlorpropamide	-1.579	-1.586
C51H79NO13	DB00877	Sirolimus	-1.582	-1.583
C11H11N3O2S	DB00891	Sulfapyridine	-1.424	-1.581
C12H21N	DB00478	Rimantadine	-1.576	-1.576
C10H16N2O4S3	DB00869	Dorzolamide	-0.151	-1.563
C7H9N2O	DB00733	Pralidoxime	-0.875	-1.557
C16H21N3	DB00792	Tripeleminamine	-1.55	-1.555
C14H30N2O4	DB00202	Succinylcholine	-1.543	-1.543
C19H29NO	DB00942	Cycrimine	-1.524	-1.525
C18H13Cl4N3O	DB00239	Oxiconazole	-1.402	-1.515
C21H25NO	DB00245	Benzatropine	-1.49	-1.491
C19H35NO2	DB00804	Dicyclomine	-1.469	-1.486
C22H19N3O4	DB00820	Tadalafil	-1.485	-1.485
C21H21CIN4OS	DB00246	Ziprasidone	-1.235	-1.466
C18H27NO2	DB00645	Dyclonine	1.244	-1.462
C22H25N3O4S	DB00680	Moricizine	-1.27	-1.46
C3H7NO2	DB00160	L-Alanine	-1.445	-1.445
C21H31N5O2	DB00490	Buspirone	-0.918	-1.423
C17H32BrNO2	DB00517	Anisotropine methylbromide	-1.418	-1.418
C29H35NO2	DB00834	Mifepristone	-1.39	-1.406
C28H33CIN2	DB00354	Buclizine	0.784	-1.378
C30H60I3N3O3	DB00483	Gallamine Triethiodide	-1.373	-1.373
C46H58N4O9	DB00570	Vinblastine	-0.479	-1.347
C19H35NO2	DB00804	Dicyclomine	0.773	-1.345
C18H26CIN3	DB00608	Chloroquine	0.352	-1.324
C25H38O5	DB00641	Simvastatin	-1.32	-1.32
C10H10N4O2S	DB00359	Sulfadiazine	-1.16	-1.316
C2H5NO2	DB00145	Glycine	-1.31	-1.31
C24H34N4O5S	DB00222	Glimepiride	0.638	-1.285
C21H26CIN3OS	DB00850	Perphenazine	-0.687	-1.234
C14H16CIN3O4S2	DB00606	Cyclothiazide	-1.204	-1.217
C31H33F3N2O5S	DB00932	Tipranavir	-1.055	-1.193
C21H26N2S2	DB00679	Thioridazine	-1.178	-1.179
C32H26N4O2	DB00872	Conivaptan	-0.269	-1.046
C9H13N2O2	DB00545	Pyridostigmine	-0.957	-0.957
C21H32N6O3	DB00802	Alfentanil	0.402	-0.918
C22H28N2O	DB00813	Fentanyl	-0.896	-0.913
C46H58N4O9	DB00570	Vinblastine	-0.652	-0.913

C19H17NOS	DB00525	Tolnaftate	-0.902	-0.902
C28H31FN4O	DB00637	Astemizole	-0.387	-0.901
C20H28N2O5	DB00899	Remifentanil	-0.557	-0.843
C18H21NO4	DB00497	Oxycodone	0.338	-0.783
C18H21NO3	DB00318	Codeine	0.769	-0.775
C12H24N2O4	DB00395	Carisoprodol	-0.763	-0.763
C14H21N3O3S	DB00839	Tolazamide	-0.658	-0.682
C28H27NO4S	DB00481	Raloxifene	-0.658	-0.673
C31H33N3O6S	DB00549	Zafirlukast	2.012	-0.649
C2H6O	DB00898	Ethanol	-0.632	-0.632
C10H17N	DB00915	Amantadine	-0.531	-0.531
C22H30N2O2S	DB00708	Sufentanil	-0.482	-0.521
C10H24N2O2	DB00330	Ethambutol	0.348	-0.451
C22H30N2O2S	DB00708	Sufentanil	1.218	-0.416
C27H29N5O6S	DB00559	Bosentan	-0.284	-0.284
C22H46O	DB00632	Docosanol	-0.283	-0.283
C17H19NO3	DB00327	Hydromorphone	1.986	-0.118
C12H19NO3	DB00871	Terbutaline	2.149	-0.066
C11H17NO3	DB00816	Orciprenaline	-0.039	-0.053
C32H53N2O4	DB00728	Rocuronium	0.206	0.059
C33H38N4O6	DB00762	Irinotecan	0.307	0.304
C11H11N3O2S	DB00891	Sulfapyridine	2.005	0.337
C17H21NO4	DB00907	Cocaine	0.442	0.385
C23H36N6O5S	DB00278	Argatroban	0.45	0.45
C20H28N2O5	DB00899	Remifentanil	1.088	0.52
C21H32N6O3	DB00802	Alfentanil	0.703	0.636
C18H30O2	DB00132	Alpha-Linolenic Acid	0.683	0.68
C20H21N	DB00924	Cyclobenzaprine	0.746	0.742
C24H34O4	DB00603	Medroxyprogesterone acetate	0.771	0.771
C15H20N2O4S	DB00414	Acetohexamide	0.783	0.778
C21H26N2O7	DB00393	Nimodipine	0.858	0.858
C65H82N2O18S2	DB00732	Atracurium besylate	0.953	0.953
C52H88N10O15	DB00520	Caspofungin	3.772	1.179
C43H55N5O7	DB00309	Vindesine	1.713	1.523
C18H22ClNO	DB00925	Phenoxybenzamine	2.203	1.754
C32H52N4O4	DB00944	Demecarium	1.99	1.99
C19H20N2O3	DB00757	Dolasetron	2.171	2.03
C32H53N2O4	DB00728	Rocuronium	5.871	4.973

FDA approved drugs with 6y84, Table S8

FORMULA	DRUGBANK_ID	GENERIC_NAME	docking score	glide gscore
C23H45N5O14	DB01421	Paromomycin	-9.463	-11.579
C23H45N5O14	DB01421	Paromomycin	-9.859	-10.848
C23H45N5O14	DB01421	Paromomycin	-8.866	-10.611
C23H45N5O14	DB01421	Paromomycin	-8.223	-10.413
C27H30O16	DB01698	Rutin	-9.824	-9.853
C28H44N2O23	DB08818	Hyaluronic acid	-9.786	-9.786
C52H76O24	DB06810	Plicamycin	-7.673	-9.777
C5H15N2O3PS	DB01143	Amifostine	-9.588	-9.628
C21H39N7O12	DB01082	Streptomycin	-8.624	-9.463
C52H74N16O15S2	DB02638	Terlipressin	-9.292	-9.406
C23H45N5O14	DB01421	Paromomycin	-6.785	-9.389
C17H34N4O10	DB03615	Ribostamycin	-8.836	-9.257
C52H76O24	DB06810	Plicamycin	-7.44	-9.153
C17H34N4O10	DB03615	Ribostamycin	-7.077	-9.095
C52H74N16O15S2	DB02638	Terlipressin	-8.028	-9.063
C22H28N4O6	DB01204	Mitoxantrone	-8.991	-8.991
C17H34N4O10	DB03615	Ribostamycin	-7.409	-8.973
C27H30O16	DB01698	Rutin	-6.914	-8.834
C23H45N5O14	DB01421	Paromomycin	-7.35	-8.788
C35H44I6N6O15	DB01249	Iodixanol	-8.717	-8.717

C17H34N4O10	DB03615	Ribostamycin	-6.982	-8.584
C27H33N9O15P2	DB03147	Flavin adenine dinucleotide	-8.524	-8.524
C12H22O11	DB04465	Lactose	-8.514	-8.514
C23H45N5O14	DB01421	Paromomycin	-5.946	-8.347
C23H45N5O14	DB01421	Paromomycin	-6.209	-8.059
C18H36N4O11	DB01172	Kanamycin	-6.497	-8.048
C17H34N4O10	DB03615	Ribostamycin	-7.261	-7.981
C27H29NO11	DB00997	Doxorubicin	-7.951	-7.978
C21H39N7O12	DB01082	Streptomycin	-7.683	-7.848
C18H36N4O11	DB01172	Kanamycin	-6.276	-7.845
C5H13O14P3	DB01632	5-O-phosphono-alpha-D-ribofuranosyl diphosp	-5.452	-7.787
C23H28F2N6O4S	DB08816	Ticagrelor	-7.054	-7.77
C17H34N4O10	DB03615	Ribostamycin	-5.696	-7.595
C23H45N5O14	DB01421	Paromomycin	-6.865	-7.495
C6H17N2O12P4Sm	DB05273	Samarium (153Sm) lexicronam	-7.466	-7.484
C59H89N19O13S	DB06196	Icatibant	-7.351	-7.476
C18H23NO4	DB01102	Arbutamine	-4.743	-7.456
C52H76O24	DB06810	Plicamycin	-7.279	-7.332
C6H17N2O12P4Sm	DB05273	Samarium (153Sm) lexicronam	-4.734	-7.323
C12H22O11	DB02772	Sucrose	-7.282	-7.282
C17H25Cl2F3N5O12P3S	DB06441	Cangrelor	-5.01	-7.237
C26H27NO9	DB01177	Idarubicin	-7.19	-7.217
C18H21NO5	DB06814	Protokylol	-4.825	-7.133
C28H34O15	DB04703	Hesperidin	-7.067	-7.067
C35H35F2N8O5S	DB06636	Isavuconazonium	-6.538	-7.042
C5H13O14P3	DB01632	5-O-phosphono-alpha-D-ribofuranosyl diphosp	-5.706	-6.939
C27H29NO11	DB00997	Doxorubicin	-5.075	-6.915
C23H45N5O14	DB01421	Paromomycin	-5.772	-6.854
C18H34N2O6S	DB01627	Lincomycin	-4.437	-6.85
C23H23N7O5	DB06813	Pralatrexate	-6.756	-6.798
C26H27NO9	DB01177	Idarubicin	-4.934	-6.775
C64H82N18O13	DB06825	Triptorelin	-6.135	-6.762
C5H13O14P3	DB01632	5-O-phosphono-alpha-D-ribofuranosyl diphosp	-5.453	-6.734
C17H25Cl2F3N5O12P3S	DB06441	Cangrelor	-6.706	-6.72
C70H94N18O16	DB06788	Histrelin	-5.293	-6.693
C18H21NO5	DB06814	Protokylol	-6.678	-6.69
C64H82N18O13	DB06825	Triptorelin	-5.848	-6.674
C23H27N3O7	DB01017	Minocycline	-6.561	-6.672
C43H74N2O14	DB06145	Spiramycin	-4.13	-6.665
C23H27N3O7	DB01017	Minocycline	-5.568	-6.654
C20H32N6O12S2	DB03310	Glutathione disulfide	-6.645	-6.649
C15H18N8O5	DB06213	Regadenoson	-6.63	-6.63
C18H36N4O11	DB01172	Kanamycin	-6.465	-6.614
C17H21NO4	DB01288	Fenoterol	-3.953	-6.592
C19H24N2O4	DB01274	Arformoterol	-4.223	-6.531
C15H24N4O6S2	DB06211	Doripenem	-6.123	-6.523
C41H64O13	DB01396	Digitoxin	-6.484	-6.484
C52H74Cl2O18	DB08874	Fidaxomicin	-6.399	-6.417
C20H14I6N2O6	DB04711	Iodipamide	-6.389	-6.389
C20H22N8O6S2	DB04918	Ceftobiprole	-6.32	-6.32
C70H94N18O16	DB06788	Histrelin	-5.015	-6.316
C19H26I3N3O9	DB01362	Iohexol	-6.254	-6.254
C14H22N6O5	DB01610	Valganciclovir	-5.534	-6.243
C18H18N6O8S3	DB01328	Cefonicid	-6.201	-6.201
C22H21N8O8PS4	DB06590	Ceftaroline fosamil	-5.863	-6.164
C23H22F7N4O6P	DB06717	Fosaprepitant	-5.707	-6.152
C38H50N6O5	DB01232	Saquinavir	-3.822	-6.082
C18H23NO4	DB01102	Arbutamine	-6.049	-6.055
C19H21NO4	DB01183	Naloxone	-5.904	-6.028
C12H17N3O4S	DB01598	Imipenem	-6.004	-6.004
C25H34F2O5	DB08819	Tafluprost	-5.984	-5.984
C23H23N7O5	DB06813	Pralatrexate	-4.382	-5.977
C32H40BrN5O5	DB01200	Bromocriptine	-5.134	-5.971

C6H14O6	DB01638	Sorbitol	-5.92	-5.92
C25H34O6	DB05013	Ingenol mebutate	-5.912	-5.912
C29H44O12	DB01092	Ouabain	-5.907	-5.907
C52H74Cl2O18	DB08874	Fidaxomicin	-3.411	-5.896
C12H18N4O7P2S	DB01987	Cocarboxylase	-4.597	-5.882
C17H21NO4	DB01288	Fenoterol	-3.633	-5.849
C19H33NO2	DB08868	Fingolimod	-5.796	-5.839
C23H28F2N6O4S	DB08816	Ticagrelor	-5.604	-5.826
C24H28F3N3O3	DB06608	Tafenoquine	-3.123	-5.8
C11H15N5O5	DB01280	Nelarabine	-5.799	-5.799
C17H21N4O9P	DB03247	Flavin mononucleotide	-4.724	-5.799
C23H23N3O5	DB01030	Topotecan	-4.489	-5.766
C17H21N4O9P	DB03247	Flavin mononucleotide	-5.654	-5.759
C27H37N3O7S	DB01264	Darunavir	-5.744	-5.744
C23H45N5O14	DB01421	Paromomycin	-3.488	-5.734
C16H17N3O5S	DB01140	Cefadroxil	-5.516	-5.725
C38H69NO13	DB01211	Clarithromycin	-5.677	-5.684
C23H30GdN3O11	DB08884	Gadoxetic acid	-5.292	-5.679
C17H27NO4	DB01203	Nadolol	-5.673	-5.674
C18H33ClN2O5S	DB01190	Clindamycin	-3.305	-5.661
C25H28N8O2	DB08882	Linagliptin	-5.658	-5.658
C10H12FN5O4	DB01073	Fludarabine	-5.656	-5.656
C24H25FO5S	DB08907	Canagliflozin	-5.649	-5.649
C21H27NO3	DB01182	Propafenone	-5.637	-5.641
C21H24N4O2S	DB08893	Mirabegron	-5.454	-5.622
C58H66N10O9	DB06663	Pasireotide	-5.615	-5.615
C15H23N3O4S	DB01000	Cyclacillin	-4.382	-5.609
C19H24N2O4	DB00983	Formoterol	-3.277	-5.585
C5H13O14P3	DB01632	5-O-phosphono-alpha-D-ribofuranosyl diphosph	-5.405	-5.583
C16H17N3O5S	DB01140	Cefadroxil	-4.854	-5.578
C24H40O5	DB02659	Cholic Acid	-5.561	-5.566
C15H16Cl2N2O8	DB07565	Chloramphenicol succinate	-5.561	-5.561
C25H27N9O8S2	DB01329	Cefoperazone	-5.56	-5.56
C24H28F3N3O3	DB06608	Tafenoquine	-5.553	-5.559
C8H12N4O4	DB01262	Decitabine	-3.052	-5.554
C32H40BrN5O5	DB01200	Bromocriptine	-5.36	-5.539
C30H34N2O3	DB06401	Bazedoxifene	-5.524	-5.534
C7H9ClO6P2S	DB01133	Tiludronic acid	-4.135	-5.525
C24H28N2O3	DB05039	Indacaterol	-3.742	-5.523
C6H13NO5	DB01296	Glucosamine	-4.664	-5.498
C18H19N3O5S	DB01150	Cefprozil	-5.215	-5.497
C23H29N3O2S	DB01063	Acetophenazine	-4.931	-5.479
C19H23N5O3	DB01157	Trimetrexate	-3.212	-5.479
C6H13NO5	DB01296	Glucosamine	-5.299	-5.466
C21H25ClO6	DB06292	Dapagliflozin	-5.451	-5.451
C19H24N2O4	DB01274	Arformoterol	-5.435	-5.447
C19H22FN3O4	DB01044	Gatifloxacin	-4.292	-5.438
C19H18N6O5S3	DB01066	Cefditoren	-5.429	-5.429
C18H36N4O11	DB01172	Kanamycin	-3.915	-5.429
C18H24O3	DB04573	Estriol	-5.428	-5.428
C27H40O3	DB02300	Calcipotriol	-5.425	-5.425
C33H30N4O2	DB00966	Telmisartan	-5.14	-5.414
C14H8O4	DB04816	Dantron	-5.409	-5.409
C16H18FN3O3	DB01059	Norfloxacin	-4.296	-5.4
C25H29I2NO3	DB01118	Amiodarone	-3.386	-5.399
C47H74O19	DB01078	Deslanoside	-5.383	-5.383
C21H25N3O2S	DB01224	Quetiapine	-4.194	-5.375
C24H23ClO2	DB04938	Ospemifene	-5.371	-5.371
C14H18N6O	DB01048	Abacavir	-5.36	-5.365
C22H31N3O5	DB01340	Cilazapril	-5.117	-5.355
C22H31NO3	DB01062	Oxybutynin	-4.12	-5.353
C18H18N8O7S3	DB01212	Ceftriaxone	-5.349	-5.349
C32H40BrN5O5	DB01200	Bromocriptine	-2.757	-5.347

C18H26ClN3O	DB01611	Hydroxychloroquine	-3.637	-5.34
C21H25NO3	DB06230	Nalmefene	-5.277	-5.308
C18H18N6O5S2	DB01326	Cefamandole	-5.291	-5.291
C38H50N6O5	DB01232	Saquinavir	-5.278	-5.291
C15H17N5O6S2	DB01416	Cefpodoxime	-5.29	-5.29
C21H25NO3	DB06230	Nalmefene	-3.336	-5.283
C17H21NO4	DB01288	Fenoterol	-5.261	-5.282
C33H30N4O2	DB00966	Telmisartan	-3.384	-5.256
C12H7Cl3O2	DB08604	Triclosan	-4.695	-5.254
C16H19N3O5S	DB01060	Amoxicillin	-4.48	-5.245
C25H32F3N3O4	DB06207	Silodosin	-5.24	-5.244
C22H24BrFN4O2	DB05294	Vandetanib	-5.242	-5.242
C9H13N3O5	DB00987	Cytarabine	-5.232	-5.232
C28H29NO4S	DB06249	Arzoxifene	-2.543	-5.23
C14H10BN03	DB05219	Crisaborole	-5.229	-5.229
C10H13NO4	DB00968	Methyldopa	-5.226	-5.226
C17H20O6	DB01024	Mycophenolic acid	-5.192	-5.224
C20H20FN03S	DB06209	Prasugrel	-4.995	-5.221
C6H12O6	DB04173	Fructose	-5.213	-5.213
C22H24ClN5O2	DB01184	Domperidone	-3.108	-5.213
C22H29FO5	DB01234	Dexamethasone	-5.209	-5.209
C64H82N18O13	DB06825	Triptorelin	-4.669	-5.204
C22H30N2O5S2	DB01348	Spirapril	-4.285	-5.202
C15H21N3O	DB01087	Primaquine	-5.19	-5.19
C27H30F6N2O2	DB01126	Dutasteride	-5.187	-5.187
C14H16N2O6S3	DB01145	Sulfoxone	-5.186	-5.186
C24H25ClFN5O3	DB08916	Afatinib	-3.366	-5.181
C20H24O2	DB00977	Ethinylestradiol	-5.171	-5.171
C17H19F2N3O3	DB00978	Lomefloxacin	-3.817	-5.171
C22H26ClN7O2S	DB01254	Dasatinib	-4.734	-5.168
C33H38GdN3Na3O14P	DB06705	Gadofosveset trisodium	-3.025	-5.166
C43H53NO14	DB01248	Docetaxel	-5.156	-5.158
C2H8O7P2	DB01077	Etidronic acid	-4.91	-5.156
C21H20Cl2O3	DB04930	Permethrin	-5.155	-5.155
C22H21N8O8PS4	DB06590	Ceftaroline fosamil	-4.609	-5.154
C21H23Cl2NO6	DB04920	Clevidipine	-5.151	-5.151
C19H25N5O4	DB01162	Terazosin	-4.074	-5.147
C16H19N3O4S	DB01333	Cefradine	-4.855	-5.132
C16H23N5O	DB01079	Tegaserod	-5.128	-5.128
C18H23NO3	DB01551	Dihydrocodeine	-2.906	-5.128
C24H31NO	DB05812	Abiraterone	-3.127	-5.127
C33H60O10	DB06804	Nonoxynol-9	-5.12	-5.12
C34H50N4O9S	DB01764	Dalfopristin	-4.878	-5.115
C24H45NO8	DB01160	Dinoprost tromethamine	-5.11	-5.113
C22H30MnN4O14P2	DB06796	Mangafodipir	-3.761	-5.108
C13H10N2O4	DB01041	Thalidomide	-5.105	-5.105
C13H11N3O4	DB08910	Pomalidomide	-5.097	-5.097
C22H31N3O5	DB01340	Cilazapril	-4.436	-5.091
C19H20N2O3	DB03585	Oxyphenbutazone	-2.536	-5.091
C19H23N5O3	DB01157	Trimetrexate	-3.058	-5.087
C14H14N8O4S3	DB01327	Cefazolin	-5.086	-5.086
C22H26ClN7O2S	DB01254	Dasatinib	-2.988	-5.085
C27H33N3O8	DB01301	Rolitetraacycline	-4.142	-5.08
C19H33NO2	DB08868	Fingolimod	-3.499	-5.075
C19H23N3O2	DB01253	Ergometrine	-4.444	-5.07
C25H29I2NO3	DB01118	Amiodarone	-5.048	-5.068
C23H20F3N5O2S2	DB08912	Dabrafenib	-4.658	-5.064
C27H46O	DB04540	Cholesterol	-5.061	-5.061
C9H13NO3	DB06707	Levonordefrin	-5.043	-5.06
C22H25F2NO4	DB04861	Nebivolol	-5.04	-5.06
C52H74Cl2O18	DB08874	Fidaxomicin	-2.363	-5.044
C19H21NO4	DB01183	Naloxone	-3.955	-5.042
C22H32O4	DB01088	Iloprost	-5.029	-5.032

C2H8O7P2	DB01077	Etidronic acid	-4.389	-5.029
C19H22F2N4O3	DB01208	Sparfloxacin	-4.934	-5.016
C21H15N3O4	DB01609	Deferasirox	-5.009	-5.015
C17H19FN2O2	DB06654	Safinamide	-4.828	-5.014
C13H21O5P	DB06716	Fospropofol	-3.588	-4.997
C18H34N2O6S	DB01627	Lincomycin	-4.981	-4.991
C70H94N18O16	DB06788	Histrelin	-3.605	-4.988
C25H25N5O4	DB06605	Apixaban	-4.987	-4.987
C17H17N3O6S2	DB01139	Cefapirin	-4.978	-4.987
C20H26N2O2	DB01426	Ajmaline	-4.488	-4.987
C26H29Cl2N5O3	DB06616	Bosutinib	-4.872	-4.985
C18H20FN3O4	DB01137	Levofloxacin	-2.428	-4.98
C18H20FN3O4	DB01165	Ofloxacin	-2.428	-4.98
C22H25F2NO4	DB04861	Nebivolol	-2.956	-4.979
C31H48O6	DB02703	Fusidic acid	-4.958	-4.977
C18H27NO3	DB06774	Capsaicin	-4.973	-4.973
C23H26ClN7O3	DB06237	Avanafil	-4.933	-4.97
C13H11N3	DB01123	Proflavine	-3.197	-4.964
C19H20N2O3	DB03585	Oxyphenbutazone	-4.954	-4.962
C19H22NO4S2	DB01409	Tiotropium	-4.958	-4.958
C22H31NO	DB01036	Tolterodine	-4.956	-4.956
C22H26ClN7O2S	DB01254	Dasatinib	-4.527	-4.949
C18H19N3O5S	DB01150	Cefprozil	-4.37	-4.944
C19H25NOS	DB05271	Rotigotine	-2.224	-4.942
C17H19FN2O2	DB06654	Safinamide	-4.159	-4.938
C11H13BrN2O5	DB03312	Brivudine	-2.863	-4.933
C59H89N19O13S	DB06196	Icatibant	-3.944	-4.926
C6H12O6	DB01914	D-glucose	-4.925	-4.925
C22H22N2O4	DB06403	Ambrisentan	-4.923	-4.923
C17H18N6	DB08877	Ruxolitinib	-4.922	-4.922
C22H30O5	DB00959	Methylprednisolone	-4.921	-4.921
C18H20FN5O4	DB01155	Gemifloxacin	-3.312	-4.915
C22H30N2O5S2	DB01348	Spirapril	-4.767	-4.909
C21H25ClN2O3	DB04890	Bepotastine	-4.902	-4.907
C53H83NO14	DB01590	Everolimus	-4.904	-4.906
C28H31NO2	DB06202	Lasofoxifene	-4.898	-4.903
C15H14N4O6S2	DB01415	Ceftibuten	-4.9	-4.9
C22H25NO6	DB01394	Colchicine	-4.89	-4.89
C54H69N11O10S2	DB06791	Lanreotide	-4.178	-4.887
C20H21FN6O5	DB06817	Raltegravir	-4.29	-4.883
C16H19N3O4S	DB01333	Cefradine	-4.297	-4.881
C33H30N4O2	DB00966	Telmisartan	-2.714	-4.871
C13H13N5O5S2	DB01332	Ceftizoxime	-4.866	-4.866
C20H32O5	DB01240	Epoprostenol	-4.861	-4.864
C18H33ClN2O5S	DB01190	Clindamycin	-4.846	-4.857
C16H16N4O8S	DB01112	Cefuroxime	-4.855	-4.855
C19H24N6O5S2	DB01413	Cefepime	-4.845	-4.845
C16H14N2O4	DB01025	Amlexanox	-4.827	-4.844
C29H39NO9	DB04865	Omacetaxine mepesuccinate	-4.718	-4.831
C19H20N2O3S	DB01132	Pioglitazone	-4.39	-4.83
C17H17N3O6S2	DB01139	Cefapirin	-2.33	-4.829
C17H17ClN6O3	DB01198	Zopiclone	-4.35	-4.828
C15H14N2O4S	DB05015	Belinostat	-2.571	-4.824
C7H9ClO6P2S	DB01133	Tiludronic acid	-4.751	-4.811
C35H35F2N8O5S	DB06636	Isavuconazonium	-3.038	-4.811
C18H21N3O3S	DB01129	Rabeprazole	-3.108	-4.808
C21H32O3	DB06412	Oxymetholone	-4.03	-4.8
C15H15NO2S	DB06413	Armodafinil	-4.796	-4.796
C17H19N5O2	DB06193	Pixantrone	-4.795	-4.795
C23H30O6	DB01380	Cortisone acetate	-4.795	-4.795
C16H20N6O	DB08895	Tofacitinib	-4.783	-4.794
C16H27NO6	DB08872	Gabapentin enacarbil	-4.788	-4.791
C12H18N4O7P2S	DB01987	Cocarboxylase	-4.696	-4.787

C47H64N4O12	DB01201	Rifapentine	-3.709	-4.786
C21H32O3	DB06412	Oxymetholone	-4.577	-4.785
C20H31NO4	DB06217	Vernakalant	-4.777	-4.783
C27H45N5O5	DB08873	Boceprevir	-4.78	-4.78
C17H19NO4	DB01192	Oxymorphone	-4.656	-4.775
C30H34N2O3	DB06401	Bazedoxifene	-2.314	-4.771
C23H20N2O3S	DB01138	Sulfapyrazone	-4.768	-4.77
C16H19N3O5S	DB01060	Amoxicillin	-4.573	-4.765
C19H20N2O3S	DB01132	Pioglitazone	-4.281	-4.764
C24H40O4	DB03619	Deoxycholic Acid	-4.758	-4.762
C25H32CIN5O2	DB01149	Nefazodone	-4.359	-4.762
C29H53NO5	DB01083	Orlistat	-4.761	-4.761
C11H17NO3	DB01064	Isoprenaline	-4.757	-4.757
C24H21F2NO3	DB00973	Ezetimibe	-4.756	-4.757
C27H44O2	DB01436	Alfacalcidol	-4.755	-4.755
C11H13BrN2O5	DB03312	Brivudine	-4.735	-4.753
C22H28FN3O6S	DB01098	Rosuvastatin	-4.746	-4.748
C38H52N6O7	DB01072	Atazanavir	-2.157	-4.734
C18H28N2O4	DB01193	Acebutolol	-4.727	-4.729
C15H17NO2	DB06594	Agomelatine	-4.726	-4.726
C28H29NO4S	DB06249	Arzoxifene	-4.71	-4.726
C21H32O3	DB06412	Oxymetholone	-2.465	-4.718
C5H9NO4S	DB04339	Carbocisteine	-2.024	-4.718
C12H18N4O7P2S	DB01987	Cocarboxylase	-2.583	-4.705
C24H28N2O3	DB05039	Indacaterol	-4.658	-4.7
C21H23N3O2	DB06603	Panobinostat	-4.698	-4.698
C32H36N4O5	DB01346	Quinidine barbiturate	-2.42	-4.695
C27H33N3O8	DB01301	Rolitetraacycline	-4.474	-4.694
C18H20FN3O4	DB01137	Levofloxacin	-3.473	-4.694
C18H20FN3O4	DB01165	Ofloxacin	-3.473	-4.694
C25H24FNO4	DB08860	Pitavastatin	-4.672	-4.682
C30H32N2O2	DB01081	Diphenoxylate	-4.233	-4.672
C30H21I7N2Na2O8	DB01583	Liotrix	-3.679	-4.667
C26H23FIN5O4	DB08911	Trametinib	-4.665	-4.665
C24H40O4	DB01586	Ursodeoxycholic acid	-4.661	-4.665
C16H18FN3O3	DB01059	Norfloracin	-4.565	-4.665
C30H26F6N4O2	DB01419	Antrafenine	-2.693	-4.665
C19H15NO6	DB01418	Acenocoumarol	-4.643	-4.663
C26H30NO4S2	DB08897	Aclidinium	-4.649	-4.649
C22H31NO3	DB01062	Oxybutynin	-4.57	-4.649
C31H46O2	DB01022	Phylloquinone	-4.648	-4.648
C16H14F3N3O2S	DB05351	Dexlansoprazole	-2.615	-4.648
C9H11NO5	DB06262	Droxidopa	-4.643	-4.643
C20H15Cl3N2OS	DB01153	Sertaconazole	-4.023	-4.638
C21H32O2	DB02789	Pregnenolone	-4.636	-4.636
C23H29N3O2S	DB01063	Acetophenazine	-2.666	-4.636
C15H25N3O	DB01255	Lisdexamfetamine	-4.54	-4.635
C20H21NO4	DB01113	Papaverine	-4.534	-4.626
C21H24N4O2S	DB08893	Mirabegron	-3.773	-4.624
C19H15NO6	DB01418	Acenocoumarol	-2.621	-4.619
C23H33N2O	DB01625	Isopropamide	-4.617	-4.617
C30H21I7N2Na2O8	DB01583	Liotrix	-4.492	-4.616
C20H26N2O2	DB01426	Ajmaline	-3.079	-4.615
C26H32F2O7	DB01047	Fluocinonide	-4.614	-4.614
C15H24N4O6S2	DB06211	Doripenem	-4.19	-4.612
C24H25ClFN5O3	DB08916	Afatinib	-4.428	-4.611
C19H23N5O3	DB01157	Trimetrexate	-4.577	-4.61
C31H44N2O5S	DB04855	Dronedarone	-4.535	-4.608
C33H30N4O2	DB00966	Telmisartan	-3.893	-4.603
C25H32O2	DB04575	Quinestrol	-4.602	-4.602
C9H11NO4	DB01235	Levodopa	-4.598	-4.598
C19H22F2N4O3	DB01208	Sparfloxacin	-3.386	-4.596
C13H17N3O4S	DB04817	Metamizole	-4.593	-4.595

C19H24N2OS	DB01403	Methotrimeprazine	-4.593	-4.594
C19H20N2O3S	DB01132	Pioglitazone	-2.715	-4.59
C27H34F2O7	DB06781	Difluprednate	-4.58	-4.58
C19H24N2O4	DB00983	Formoterol	-4.563	-4.575
C19H20CINO4	DB01393	Bezafibrate	-4.574	-4.574
C25H34O6	DB01222	Budesonide	-4.568	-4.568
C22H24CIN5O2	DB01184	Domperidone	-4.547	-4.564
C39H43N3O11S	DB05109	Trabectedin	-4.419	-4.564
C28H54N8	DB06809	Plerixafor	-2.097	-4.562
C17H20O6	DB01024	Mycophenolic acid	-2.8	-4.56
C19H28NO3	DB00986	Glycopyrronium	-4.552	-4.552
C13H12N2O5S	DB04743	Nimesulide	-3.805	-4.547
C29H39NO9	DB04865	Omacetaxine mepesuccinate	-3.501	-4.539
C15H23N3O4S	DB01000	Cyclacillin	-4.448	-4.528
C24H31NO4	DB06751	Drotaverine	-4.524	-4.524
C20H30O2	DB06710	Methyltestosterone	-4.517	-4.517
C24H40N8O4	DB00975	Dipyridamole	-4.513	-4.513
C22H18N4OS	DB06626	Axitinib	-4.507	-4.51
C16H24N2O2	DB01618	Molindone	-4.454	-4.506
C20H33N3O4	DB04846	Celiprolol	-4.504	-4.505
C22H30MnN4O14P2	DB06796	Mangafodipir	-2.155	-4.504
C17H25NO3	DB01210	Levobunolol	-4.5	-4.501
C31H36N2O11	DB01051	Novobiocin	-4.484	-4.501
C15H28N4O4	DB06614	Peramivir	-4.5	-4.5
C16H12O3	DB01125	Anisindione	-4.488	-4.5
C17H20N2O6S	DB01603	Meticillin	-4.499	-4.499
C24H26N2O4	DB01136	Carvedilol	-2.921	-4.496
C17H25NO3	DB00979	Cyclopentolate	-4.476	-4.495
C20H14O4	DB04824	Phenolphthalein	-3.67	-4.494
C7H7NO2	DB08797	Salicylamide	-2.846	-4.493
C9H13NO3	DB06707	Levonordefrin	-2.398	-4.492
C26H29Cl2N5O3	DB06616	Bosutinib	-3.335	-4.49
C45H69N11O12S	DB01282	Carbetocin	-4.489	-4.489
C16H20N6O	DB08895	Tofacitinib	-2.146	-4.487
C19H18CIN3O5S	DB01147	Cloxacillin	-4.481	-4.481
C37H41N2O6	DB01199	Tubocurarine	-1.867	-4.479
C16H18FN3O2	DB04953	Ezogabine	-1.895	-4.476
C18H15Cl3N2S	DB06820	Sulconazole	-3.971	-4.473
C12H12N2O2S	DB04880	Enoximone	-4.463	-4.463
C28H29F2N3O	DB01100	Pimozide	-1.807	-4.452
C23H22F7N4O6P	DB06717	Fosaprepitant	-1.931	-4.451
C24H40O4	DB06777	Chenodeoxycholic acid	-4.445	-4.449
C20H31NO4	DB06217	Vernakalant	-1.721	-4.447
C14H10BrN3O	DB01558	Bromazepam	-4.446	-4.446
C38H69NO13	DB01211	Clarithromycin	-1.81	-4.445
C20H20N6O9S	DB04570	Latamoxef	-4.443	-4.444
C15H14FN3O3	DB01205	Flumazenil	-4.441	-4.442
C28H24FN3O5	DB08875	Cabozantinib	-2.885	-4.435
C19H21ClFN3O3	DB06771	Besifloxacin	-4.368	-4.434
C26H37NO3	DB06702	Fesoterodine	-4.425	-4.427
C21H23N3OS	DB01608	Periciazine	-4.422	-4.424
C11H20N2O2	DB05541	Brivaracetam	-4.419	-4.419
C15H22N2O	DB04896	Milnacipran	-4.418	-4.419
C17H20BrNO	DB01237	Bromodiphenhydramine	-4.401	-4.415
C27H33N3O8	DB01301	Rolitetracline	-1.992	-4.414
C14H10O5	DB01399	Salsalate	-4.384	-4.409
C19H25NO2	DB06152	Nylidrin	-1.84	-4.409
C32H44O7	DB01410	Ciclesonide	-4.404	-4.404
C22H18N2	DB04794	Bifonazole	-3.901	-4.398
C10H14N2O5	DB01265	Telbivudine	-4.393	-4.394
C20H21F3N4O	DB04908	Flibanserin	-4.38	-4.391
C21H22Cl2FN5O	DB08865	Crizotinib	-4.051	-4.387
C24H31NO	DB05812	Abiraterone	-4.359	-4.38

C22H25CIN2OS	DB01624	Zuclopenthixol	-4.151	-4.378
C28H35NO3	DB08867	Ulipristal	-2.183	-4.377
C23H26CIN7O3	DB06237	Avanafil	-2.093	-4.377
C14H22N6O5	DB01610	Valganciclovir	-4.162	-4.376
C17H18N4O	DB00969	Alosetron	-3.472	-4.375
H4O7P2	DB04160	Pyrophosphoric acid	-2.038	-4.375
C28H29NO4S	DB06249	Arzoxifene	-1.909	-4.372
C19H25NO2	DB06152	Nylidrin	-4.36	-4.368
C28H22F3N7O	DB04868	Nilotinib	-3.441	-4.366
C20H24N2	DB08801	Dimetindene	-1.828	-4.366
C20H29FO3	DB01185	Fluoxymesterone	-4.364	-4.364
C19H27NO3	DB04844	Tetrabenazine	-2.868	-4.363
C16H26N2O5S	DB01597	Cilastatin	-1.651	-4.361
C19H28O2	DB01708	Prasterone	-4.36	-4.36
C18H15NO3	DB00991	Oxaprozin	-4.357	-4.359
C17H26N4O	DB01084	Emedastine	-3.787	-4.358
C22H30MnN4O14P2	DB06796	Mangafodipir	-2.896	-4.357
C21H25NO3	DB06230	Nalmefene	-1.8	-4.356
C14H12O3	DB02709	Resveratrol	-4.352	-4.352
C14H10F3NO2	DB02266	Flufenamic Acid	-4.351	-4.352
C22H27NO2	DB01406	Danazol	-4.351	-4.351
C18H28N2O	DB01002	Levobupivacaine	-4.296	-4.351
C43H74N2O14	DB06145	Spiramycin	-2.726	-4.351
C24H28N2O3	DB05039	Indacaterol	-2.008	-4.346
C32H36N4O5	DB01346	Quinidine barbiturate	-4.328	-4.343
C8H12N4O4	DB01262	Decitabine	-3.922	-4.341
C21H15ClF4N4O3	DB08896	Regorafenib	-4.34	-4.34
C21H32N2O	DB06718	Stanozolol	-3.903	-4.338
C19H21NO4	DB01183	Naloxone	-2.234	-4.337
C12H19N3O	DB01168	Procarbazine	-3.824	-4.334
C35H38Cl2N8O4	DB01167	Itraconazole	-2.357	-4.329
C17H14Cl2F2N2O3	DB01656	Roflumilast	-4.327	-4.327
C37H41N2O6	DB01199	Tubocurarine	-4.132	-4.322
C17H18N4O	DB00969	Alosetron	-3.286	-4.32
C22H25CIN2OS	DB01624	Zuclopenthixol	-2.819	-4.32
C16H13Cl2NO4	DB06736	Aceclofenac	-4.318	-4.318
C33H38O6	DB08909	Glycerol phenylbutyrate	-4.317	-4.317
C22H38O5	DB06826	Unoprostone	-4.314	-4.317
C11H16N2O	DB01056	Tocainide	-4.159	-4.317
C12H6Cl4O2S	DB04813	Bithionol	-2.764	-4.314
C15H16N2O6S2	DB01607	Ticarcillin	-4.313	-4.313
C9H13N5O4	DB01004	Ganciclovir	-4.312	-4.312
C16H24N2O2	DB01618	Molindone	-2.847	-4.312
C17H19NO4	DB01192	Oxymorphone	-3.227	-4.31
C23H27FN4O3	DB01267	Paliperidone	-1.888	-4.31
C15H22FN3O6	DB01101	Capecitabine	-4.308	-4.308
C22H32O2	DB03756	Doconexent	-4.301	-4.304
C17H27N3O4S	DB06288	Amisulpride	-4.302	-4.303
C28H44O3	DB08804	Nandrolone decanoate	-4.302	-4.302
C19H25N5O4	DB01162	Terazosin	-2.069	-4.298
C20H33NO3	DB04822	Oxeladin	-1.651	-4.295
C21H26O2	DB01357	Mestranol	-4.294	-4.294
C17H24O3	DB04838	Cyclandelate	-4.292	-4.293
C37H41N2O6	DB01199	Tubocurarine	-3.277	-4.289
C18H21N3O3S	DB01129	Rabeprazole	-4.248	-4.283
C16H17BrN2	DB04832	Zimelidine	-4.249	-4.282
C19H20N2O3S	DB01132	Pioglitazone	-2.36	-4.278
C28H42Cl2N4O2	DB01122	Ambenonium	-4.275	-4.275
C28H44O	DB04038	Ergosterol	-4.271	-4.271
C14H20N2O2	DB00960	Pindolol	-4.269	-4.27
C10H16N2O3	DB01353	Butobarbital	-2.58	-4.268
C18H20FN5O4	DB01155	Gemifloxacin	-4.221	-4.262
C22H24N2O7S	DB05676	Apremilast	-4.261	-4.261

C25H36N3O9PS	DB01319	Fosamprenavir	-2.993	-4.261
C17H20CINO	DB04837	Clofedanol	-4.256	-4.26
C14H12O3	DB04571	Trioxsalen	-4.254	-4.254
C18H25N3O2	DB06335	Saxagliptin	-3.212	-4.253
C16H17N3O7S2	DB01331	Cefoxitin	-4.251	-4.251
C16H22N2O3	DB01366	Procaterol	-2.388	-4.249
C15H25N3O	DB01255	Lisdexamfetamine	-3.115	-4.248
C21H26NO4	DB06800	Methylnaltrexone	-4.237	-4.244
C25H24FNO4	DB08860	Pitavastatin	-1.788	-4.244
C22H28N2O2	DB01228	Encainide	-4.239	-4.24
C17H27NO4	DB01214	Metipranolol	-4.238	-4.24
C20H32F2O5	DB01046	Lubiprostone	-4.236	-4.239
C16H17BrN2	DB04832	Zimelidine	-2.512	-4.232
C17H20F6N2O3	DB01195	Flecainide	-4.23	-4.23
C14H10N2O6	DB01250	Olsalazine	-4.229	-4.229
C20H15Cl3N2OS	DB01153	Sertaconazole	-3.96	-4.219
C16H12ClNO3	DB04812	Benoxaprofen	-4.213	-4.214
C16H14N2O4	DB01025	Amlexanox	-2.095	-4.209
C24H25NO4	DB01148	Flavoxate	-1.776	-4.206
C31H36N2O11	DB01051	Novobiocin	-1.776	-4.201
C14H12O3	DB01428	Oxybenzone	-4.163	-4.198
C34H50N4O9S	DB01764	Dalfopristin	-3.539	-4.197
C16H21Cl2N3O2	DB06769	Bendamustine	-3.748	-4.192
C20H21F3N4O	DB04908	Flibanserin	-1.815	-4.189
C16H15N2O6P	DB01320	Fosphenytoin	-2.652	-4.186
C19H23N3O2	DB01253	Ergometrine	-3.932	-4.185
C17H25N3O2	DB04876	Vildagliptin	-2.635	-4.18
C27H42N2O5S	DB04845	Ixabepilone	-4.169	-4.175
C13H21O5P	DB06716	Fospropofol	-4.117	-4.175
C39H43N3O11S	DB05109	Trabectedin	-2.16	-4.175
C17H17Cl2N	DB01104	Sertraline	-1.87	-4.168
C28H44O2	DB06410	Doxercalciferol	-4.164	-4.164
C17H18N4O	DB00969	Alosetron	-3.867	-4.162
C70H94N18O16	DB06788	Histrelin	-2.779	-4.162
C16H14F3N3O2S	DB05351	Dexlansoprazole	-4.141	-4.161
C34H41N7O5	DB06695	Dabigatran etexilate	-2.69	-4.161
C18H15Cl3N2O	DB01127	Econazole	-3.951	-4.158
C5H15N2O3PS	DB01143	Amifostine	-2.533	-4.158
C23H29N3O2S	DB01063	Acetophenazine	-3.819	-4.155
C19H21ClFN3O3	DB06771	Besifloxacin	-2.819	-4.152
C11H6ClN3O6	DB06794	Lodoxamide	-4.149	-4.149
C15H9FN2O3	DB05016	Ataluren	-4.147	-4.147
C17H19F2N3O3	DB00978	Lomefloxacin	-4.076	-4.146
C14H22ClN3O2	DB01233	Metoclopramide	-4.139	-4.143
C28H28N2O2	DB01501	Difenoxin	-1.974	-4.142
C15H14N2O2	DB06802	Nepafenac	-4.139	-4.139
C27H29F3O6S	DB08906	Fluticasone furoate	-4.138	-4.138
C27H36O8	DB01130	Prednicarbate	-4.131	-4.131
C13H16N2O2	DB01065	Melatonin	-4.125	-4.125
C23H26ClN7O3	DB06237	Avanafil	-2.227	-4.124
C10H8F2N4O	DB06201	Rufinamide	-4.12	-4.12
C9H7N7O2S	DB00993	Azathioprine	-3.594	-4.12
C37H42F2N8O4	DB01263	Posaconazole	-4.101	-4.119
C70H94N18O16	DB06788	Histrelin	-2.136	-4.117
C31H48O2S2	DB01599	Probucol	-4.115	-4.115
C13H18ClNO	DB01156	Bupropion	-3.458	-4.115
C13H16ClNO	DB01221	Ketamine	-3.033	-4.114
C26H28Cl2N4O4	DB01026	Ketoconazole	-1.414	-4.113
C18H19Cl2NO4	DB01023	Felodipine	-4.109	-4.109
C13H15NO2	DB01437	Glutethimide	-4.109	-4.109
C18H15Cl3N2O	DB01127	Econazole	-3.386	-4.109
C23H23N3O5	DB01030	Topotecan	-3.276	-4.108
C12H18Cl2N2O	DB01407	Clenbuterol	-4.104	-4.105

C16H22N2O3	DB01366	Procaterol	-4.077	-4.103
C43H65N5O10	DB00976	Telithromycin	-3.52	-4.102
C12H12N2O3	DB01174	Phenobarbital	-3.276	-4.097
C23H22F7N4O6P	DB06717	Fosaprepitant	-3.681	-4.093
C25H28N6O	DB01029	Irbesartan	-4.083	-4.089
C15H10ClN3O3	DB01068	Clonazepam	-4.087	-4.087
C16H12O3	DB01125	Anisindione	-1.745	-4.087
C17H26ClN	DB01105	Sibutramine	-4.084	-4.085
C9H5Cl2NO	DB01243	Chloroxine	-3.137	-4.085
C13H17ClN2O2	DB01171	Moclobemide	-3.894	-4.083
C10H12N4O5S	DB01606	Tazobactam	-4.081	-4.081
C18H23NO	DB01173	Orphenadrine	-4.066	-4.079
C17H18N2O6	DB01115	Nifedipine	-4.073	-4.073
C21H25ClN2O3	DB06282	Levocetirizine	-3.6	-4.065
C20H21ClO4	DB01039	Fenofibrate	-4.063	-4.063
C23H16O11	DB01003	Cromoglicic acid	-4.063	-4.063
C18H23NO3	DB01551	Dihydrocodeine	-4.048	-4.063
H4O7P2	DB04160	Pyrophosphoric acid	-3.828	-4.061
C29H27F3N6O	DB08901	Ponatinib	-3.852	-4.059
C7H15Cl2N2O2P	DB01181	Ifosfamide	-4.058	-4.058
C13H17N3O	DB01424	Aminophenazone	-3.995	-4.057
C18H14Cl4N2O	DB01110	Miconazole	-3.334	-4.057
C21H27N3O7S	DB01602	Bacampicillin	-3.332	-4.057
C21H23NO5	DB01452	Diamorphine	-3.983	-4.047
C15H10O2	DB07776	Flavone	-4.046	-4.046
C13H12N2O5S	DB04743	Nimesulide	-3.845	-4.044
C22H23NO7	DB06174	Noscapine	-3.206	-4.038
C14H14N2O	DB01011	Metirapone	-4.032	-4.037
C19H21NO	DB01142	Doxepin	-4.033	-4.036
C17H25NO3	DB00979	Cyclopentolate	-2.011	-4.035
C21H25N3O2S	DB01224	Quetiapine	-3.944	-4.033
C22H30MnN4O14P2	DB06796	Mangafodipir	-3.008	-4.032
C16H14O3	DB01009	Ketoprofen	-4.03	-4.031
C12H19N3O	DB01168	Procarbazine	-3.346	-4.031
C15H18N2O	DB04864	Huperzine A	-2.912	-4.031
C13H8Cl2N2O4	DB06803	Niclosamide	-2.703	-4.031
C24H32O6	DB01260	Desonide	-4.028	-4.028
C16H21NO2	DB00980	Ramelteon	-4.028	-4.028
C23H15N3O	DB08883	Perampanel	-4.028	-4.028
C53H67N9O10S	DB01369	Quinupristin	-3.555	-4.028
C10H20N2O4	DB06797	Mebutamate	-4.027	-4.027
C28H54N8	DB06809	Plerixafor	-3.32	-4.027
C19H26N2S	DB01186	Pergolide	-1.677	-4.017
C19H23ClN2	DB01242	Clomipramine	-4.014	-4.014
C13H18N2O3	DB06218	Lacosamide	-4.013	-4.013
C15H11N3O3	DB01595	Nitrazepam	-4.013	-4.013
C15H23NO3	DB01580	Oxprenolol	-4.011	-4.013
C21H32N2O	DB06718	Stanozolol	-3.616	-4.006
C24H26FNO4	DB01095	Fluvastatin	-4.002	-4.004
C17H15N5O	DB00962	Zaleplon	-3.999	-3.999
C37H41N2O6	DB01199	Tubocurarine	-2.204	-3.995
C25H36N6O4S	DB06267	Udenafil	-3.986	-3.991
C18H25N3O2	DB06335	Saxagliptin	-3.877	-3.99
C6H10N2O5	DB06775	Carglumic acid	-3.989	-3.989
C25H32ClFO5	DB01013	Clobetasol propionate	-3.983	-3.983
C13H21NO3	DB01001	Salbutamol	-3.979	-3.979
C38H52N6O7	DB01072	Atazanavir	-3.97	-3.978
C26H44O4	DB05990	Obeticholic acid	-3.971	-3.976
C18H22O5S	DB04574	Estrone sulfate	-3.975	-3.975
C20H33NO3	DB04822	Oxeladin	-3.968	-3.974
C11H18N2O3	DB01351	Amobarbital	-2.255	-3.969
C22H32O3	DB01420	Testosterone propionate	-3.962	-3.962
C62H86N12O16	DB00970	Dactinomycin	-3.96	-3.96

C36H53N7O6	DB05521	Telaprevir	-3.959	-3.959
C20H21FN2O	DB01175	Escitalopram	-3.956	-3.958
C26H27N5O2	DB06684	Vilazodone	-2.862	-3.957
C25H22N4O4	DB06210	Eltrombopag	-3.951	-3.956
C21H27NO	DB01231	Diphenidol	-3.954	-3.955
C11H12N2O3	DB02959	Oxtripitan	-3.954	-3.954
C19H18N2O4S	DB08439	Parecoxib	-1.838	-3.951
C8H14N2O2	DB01202	Levetiracetam	-3.95	-3.95
C24H29ClO4	DB04839	Cyproterone acetate	-3.948	-3.948
C12H9F3N2O2	DB08880	Teriflunomide	-3.943	-3.948
C24H28ClN5O3	DB00985	Dimenhydrinate	-1.71	-3.947
C21H27N3O7S	DB01602	Bacampicillin	-3.739	-3.946
C70H94N18O16	DB06788	Histrelin	-2.644	-3.945
C17H17N7O8S4	DB01330	Cefotetan	-3.941	-3.941
C6H13NO4	DB05018	Migalastat	-3.938	-3.941
C9H9Cl2N3O	DB01018	Guanfacine	-3.939	-3.939
C15H12BrNO3	DB00963	Bromfenac	-3.936	-3.937
C22H18N2	DB04794	Bifonazole	-3.599	-3.934
C18H15ClN2O2S	DB01628	Etoricoxib	-3.933	-3.933
C18H20FN3O4	DB01137	Levofloxacin	-3.789	-3.932
C18H20FN3O4	DB01165	Ofloxacin	-3.789	-3.932
C14H12F3N3O5	DB05154	Pretomanid	-3.929	-3.929
C20H33N2O	DB06787	Hexocyclium	-3.878	-3.926
C12H14N4O4S	DB01299	Sulfadoxine	-2.829	-3.918
C16H25NO2	DB06700	Desvenlafaxine	-3.917	-3.917
C19H19N	DB01619	Phenindamine	-3.434	-3.917
C22H18N6	DB08864	Rilpivirine	-3.913	-3.913
C9H5ClINO	DB04815	Clioquinol	-3.122	-3.912
C9H17NO5	DB01783	Pantothenic acid	-3.91	-3.911
C12H19N3O	DB01168	Procarbazine	-3.118	-3.911
C26H28Cl2N4O4	DB01026	Ketoconazole	-3.359	-3.908
C24H25ClFN5O3	DB08916	Afatinib	-3.003	-3.905
C16H12FN3O3	DB01544	Flunitrazepam	-3.903	-3.903
C30H62O10	DB06811	Polidocanol	-3.899	-3.899
C8H10IN3	DB06704	Iobenguane	-3.896	-3.896
C23H28ClN3O5S	DB01016	Glyburide	-1.913	-3.896
C18H23FINO2	DB08824	Ioflupane I-123	-3.881	-3.895
C15H22N2O	DB00961	Mepivacaine	-3.798	-3.893
C14H21N3O3	DB01096	Oxamniquine	-3.891	-3.891
C12H12N2O3	DB01174	Phenobarbital	-3.721	-3.891
C14H10O5	DB01399	Salsalate	-1.993	-3.887
C43H65N5O10	DB00976	Telithromycin	-3.609	-3.886
C31H36N2O11	DB01051	Novobiocin	-1.188	-3.886
C16H15N2O6P	DB01320	Fosphenytoin	-3.835	-3.884
C30H24N4O8	DB08822	Azilsartan medoxomil	-3.881	-3.881
C26H28Cl2N4O4	DB01026	Ketoconazole	-1.405	-3.88
C37H48N4O5	DB01601	Lopinavir	-3.877	-3.877
C9H23NO3PS	DB01057	Echothiophate	-3.876	-3.876
C18H23FINO2	DB08824	Ioflupane I-123	-1.638	-3.875
C23H31NO3	DB00957	Norgestimate	-3.873	-3.873
C11H16N2O	DB01056	Tocainide	-3.012	-3.873
C16H18N2	DB04821	Nomifensine	-1.942	-3.873
C17H20BrNO	DB01237	Bromodiphenhydramine	-1.647	-3.872
C24H30O3	DB01395	Drospirenone	-3.87	-3.87
C22H34O2	DB08887	Icosapent ethyl	-3.869	-3.869
C33H38GdN3Na3O14P	DB06705	Gadofosveset trisodium	-3.77	-3.862
CHNaO3	DB01390	Sodium bicarbonate	-2.815	-3.858
CCaO3	DB06724	Calcium Carbonate	-2.815	-3.858
C3La2O9	DB06792	Lanthanum carbonate	-2.815	-3.858
C16H26O5	DB06697	Artemether	-3.852	-3.852
C19H19N	DB01619	Phenindamine	-2.058	-3.852
C32H31BrN2O2	DB08903	Bedaquiline	-3.846	-3.85
C25H28N6O	DB01029	Irbesartan	-1.14	-3.848

C22H25CIN2OS	DB01624	Zuclopenthixol	-2.999	-3.846
C29H27F3N6O	DB08901	Ponatinib	-3.085	-3.84
C18H28N2O	DB01002	Levobupivacaine	-2.399	-3.84
C19H26O3	DB08905	Formestane	-3.838	-3.838
C23H36N2O2	DB01216	Finasteride	-3.835	-3.835
C19H27NO3	DB04844	Tetrabenazine	-3.784	-3.834
C8H11NO2	DB00988	Dopamine	-3.828	-3.828
C17H21NO	DB01075	Diphenhydramine	-3.81	-3.823
C10H12CIN3O3S	DB01325	Quinethazone	-3.82	-3.822
C12H20N2O3	DB01291	Pirbuterol	-1.997	-3.822
C21H26NO3	DB04843	Mepenzolate	-3.82	-3.82
C27H40O4	DB06789	Hydroxyprogesterone caproate	-3.819	-3.819
C12H20N2O3	DB01291	Pirbuterol	-3.451	-3.814
C13H17CIN2O2	DB01171	Moclobemide	-3.039	-3.809
C23H32O4	DB06780	Desoxycorticosterone acetate	-3.806	-3.806
C15H22O3	DB01241	Gemfibrozil	-3.803	-3.806
C18H15Cl3N2S	DB06820	Sulconazole	-3.473	-3.804
C20H14O4	DB04824	Phenolphthalein	-3.627	-3.796
C33H38GdN3Na3O14P	DB06705	Gadofosveset trisodium	-2.402	-3.794
C18H21N5O2	DB06203	Alogliptin	-3.789	-3.789
C23H27N	DB01091	Butenafine	-2.841	-3.789
C33H35FN2O5	DB01076	Atorvastatin	-3.783	-3.785
C19H29IO2	DB01187	Iophendylate	-3.781	-3.781
C20H27NO3	DB01108	Trilostane	-3.778	-3.778
C15H13ClFNO2	DB01283	Lumiracoxib	-3.776	-3.777
C5H9NO3S	DB06151	Acetylcysteine	-3.776	-3.776
C19H22FN3O4	DB01044	Gatifloxacin	-3.684	-3.776
C15H22N2O	DB00961	Mepivacaine	-2.642	-3.774
C22H29N3O6S	DB01604	Pivampicillin	-3.048	-3.769
C10H13N3	DB04840	Debrisoquine	-3.768	-3.768
C39H37F6N3O2	DB08827	Lomitapide	-3.763	-3.766
C20H24N2	DB08801	Dimetindene	-1.862	-3.766
C16H18FN3O2	DB04953	Ezogabine	-3.756	-3.765
C10H7F3O4	DB08814	Triflusal	-3.764	-3.764
C15H18N2O	DB04864	Huperzine A	-3.659	-3.756
C18H26CIN3O3	DB06480	Prucalopride	-1.043	-3.755
C16H18N2	DB04821	Nomifensine	-3.728	-3.751
C18H15CIN2O6S2	DB06268	Sitaxentan	-3.749	-3.749
C13H11N3	DB01123	Proflavine	-3.718	-3.749
C22H29N3O6S	DB01604	Pivampicillin	-3.541	-3.749
C12H14N4O4S	DB06150	Sulfadimethoxine	-2.666	-3.739
C17H11N5	DB01006	Letrozole	-3.737	-3.737
C17H19N3	DB08799	Antazoline	-3.733	-3.734
C31H44N2O5S	DB04855	Dronedarone	-2.45	-3.733
C21H16F4N4O2S	DB08899	Enzalutamide	-3.732	-3.732
C11H16N2O2	DB01085	Pilocarpine	-2.977	-3.732
C27H34O3	DB00984	Nandrolone phenpropionate	-3.73	-3.73
C16H13Cl3N2OS	DB01007	Tioconazole	-3.463	-3.722
C37H41N2O6	DB01199	Tubocurarine	-1.547	-3.721
C30H26F6N4O2	DB01419	Antrafenine	-3.122	-3.719
C24H28N2O3	DB08820	Ivacaftor	-3.718	-3.718
C19H19CIN2	DB00967	Desloratadine	-3.714	-3.715
C13H10CIN3O4S2	DB06725	Lornoxicam	-3.713	-3.715
C28H54N8	DB06809	Plerixafor	-1.565	-3.71
C17H21NO	DB01075	Diphenhydramine	-1.469	-3.707
C22H23NO7	DB06174	Noscapine	-3.538	-3.705
C13H18Cl2N2O2	DB01042	Melphalan	-3.703	-3.703
C21H26N2O3	DB01392	Yohimbine	-3.678	-3.702
C18H14Cl4N2O	DB01110	Miconazole	-3.492	-3.699
C25H34FN3O2	DB05316	Pimavanserin	-3.694	-3.697
C14H17N3O	DB00998	Frovatriptan	-3.696	-3.696
C6H9NO6	DB01020	Isosorbide Mononitrate	-3.695	-3.695
C18H20FN3O4	DB01137	Levofloxacin	-2.15	-3.691

C18H20FN3O4	DB01165	Ofloxacin	-2.15	-3.691
C12H6Cl4O2S	DB04813	Bithionol	-3.159	-3.69
C18H22N2	DB01151	Desipramine	-3.687	-3.687
C6H6N2O	DB02701	Nicotinamide	-3.685	-3.685
C21H26NO4	DB06800	Methylnaltrexone	-1.119	-3.684
C18H22N2S	DB01246	Alimemazine	-3.682	-3.683
C6H12F2N2O2	DB06243	Eflornithine	-3.402	-3.682
C22H22F3N	DB01012	Cinacalcet	-3.667	-3.678
C12H13N3O2	DB01247	Isocarboxazid	-3.677	-3.677
C16H15F6N5O	DB01261	Sitagliptin	-3.672	-3.675
C12H14N4O3S	DB01298	Sulfacytine	-3.636	-3.674
C20H24N2	DB08801	Dimetindene	-3.288	-3.674
C35H38Cl2N8O4	DB01167	Itraconazole	-3.651	-3.672
C19H21N3O	DB06766	Alcaftadine	-3.66	-3.669
C28H35NO3	DB08867	Ulipristal	-3.653	-3.668
C15H14N2O4S	DB05015	Belinostat	-3.645	-3.667
C18H23NO	DB01173	Orphenadrine	-1.428	-3.665
C24H28ClN5O3	DB00985	Dimenhydrinate	-3.65	-3.664
C6H12F2N2O2	DB06243	Eflornithine	-3.084	-3.663
C15H14N2O4S	DB05015	Belinostat	-1.127	-3.659
C10H16N2O8	DB00974	Edetic Acid	-3.643	-3.657
C23H31NO2	DB01227	Levacetylmethadol	-3.652	-3.656
C24H26ClFN4O	DB06144	Sertindole	-3.648	-3.653
C11H12Cl2N2O	DB04948	Lofexidine	-3.649	-3.651
C29H27F3N6O	DB08901	Ponatinib	-1.148	-3.651
C28H54N8	DB06809	Plerixafor	-2.175	-3.65
C20H24O2	DB00990	Exemestane	-3.647	-3.647
C12H11NO	DB04951	Pirfenidone	-3.646	-3.646
C20H26N2O2	DB01426	Ajmaline	-3.215	-3.642
C16H16N2O3S	DB04854	Febuxostat	-3.636	-3.637
C12H14N4O2S	DB01582	Sulfamethazine	-3.325	-3.637
C12H14N4O4S	DB06150	Sulfadimethoxine	-1.751	-3.635
C10H15NO	DB01364	Ephedrine	-3.626	-3.632
C24H25NO4	DB01148	Flavoxate	-3.621	-3.631
C7H10N2O2S	DB06795	Mafenide	-1.842	-3.631
C59H79N15O21S6	DB08890	Linaclotide	-3.319	-3.629
C10H14O	DB02513	Thymol	-3.626	-3.626
C10H9N3O	DB01427	Amrinone	-3.625	-3.625
C13H18Br2N2O	DB06742	Ambroxol	-3.613	-3.623
C14H10N4O5	DB01219	Dantrolene	-3.55	-3.622
C18H26ClN3O	DB01611	Hydroxychloroquine	-1.381	-3.622
C29H41F2N5O	DB04835	Maraviroc	-3.616	-3.616
C20H23N5O6S	DB01061	Azlocillin	-3.612	-3.612
C40H59NO11	DB08871	Eribulin	-1.036	-3.607
C38H47N5O7S2	DB06290	Simeprevir	-0.935	-3.606
C2H4Cl3O4P	DB06753	Triclofos	-2.259	-3.604
C13H15N3O4S	DB01382	Glymidine	-3.155	-3.6
C43H74N2O14	DB06145	Spiramycin	-3.55	-3.599
C15H14N4O2S	DB06729	Sulfaphenazole	-2.139	-3.598
C29H26ClFN4O4S	DB01259	Lapatinib	-3.506	-3.595
C30H26F6N4O2	DB01419	Antrafenine	-3.235	-3.594
C19H18ClN3O5S	DB06228	Rivaroxaban	-3.589	-3.589
C15H18Cl6N2O5	DB01495	Dichloralphenazone	-3.587	-3.587
C11H12N2O	DB01435	Antipyrine	-3.582	-3.582
C12H14N4O2S	DB01582	Sulfamethazine	-2.904	-3.58
C16H20N2	DB01620	Pheniramine	-3.578	-3.578
C13H18O2	DB01050	Ibuprofen	-3.575	-3.576
C14H12O3S	DB01600	Tiaprofenic acid	-3.574	-3.574
C32H38N2O8	DB01089	Deserpidine	-3.538	-3.571
C17H19NO4	DB01192	Oxymorphone	-1.291	-3.565
C9H10N2O2	DB01121	Phenacemide	-3.562	-3.562
C20H20FNO3S	DB06209	Prasugrel	-2.88	-3.56
C23H23N3O5	DB01030	Topotecan	-3.282	-3.55

C21H25CIN2O3	DB06282	Levocetirizine	-1.688	-3.547
C30H47NO4S	DB01256	Retapamulin	-3.543	-3.545
C7H9NO2	DB08826	Deferiprone	-3.541	-3.541
C20H33N2O	DB06787	Hexocyclium	-2.035	-3.539
C26H29Cl2N5O3	DB06616	Bosutinib	-1.484	-3.533
C37H42F2N8O4	DB01263	Posaconazole	-1.442	-3.531
C11H18N2O3	DB01351	Amobarbital	-3.495	-3.529
C17H19N5	DB01217	Anastrozole	-3.524	-3.524
C22H22F3N	DB01012	Cinacalcet	-1.155	-3.523
C6H18N4	DB06824	Triethylenetetramine	-1.802	-3.521
C13H19CIN2O2	DB01161	Chloroprocaine	-1.535	-3.521
C23H26N2O2	DB01591	Solifenacin	-3.513	-3.516
C17H18N2O5S	DB02925	Piretanide	-3.513	-3.513
C24H26N2O4	DB01136	Carvedilol	-3.467	-3.51
C54H69N11O10S2	DB06791	Lanreotide	-3.297	-3.51
C6H6Cl2N2O4S2	DB01144	Diclofenamide	-0.899	-3.509
C18H20N2O6	DB01054	Nitrendipine	-3.507	-3.507
C16H15CIN2OS	DB01559	Clotiazepam	-3.506	-3.507
C23H30GdN3O11	DB08884	Gadoxetic acid	-1.05	-3.506
C7H7NO2	DB02362	Aminobenzoic acid	-3.5	-3.502
C16H18N4O2	DB04820	Nialamide	-3.501	-3.501
C9H8N2O2	DB01230	Pemoline	-3.496	-3.499
C16H24N10O4	DB01223	Aminophylline	-3.466	-3.498
C23H22F7N4O6P	DB06717	Fosaprepitant	-1.011	-3.497
C19H19N	DB01619	Phenindamine	-1.674	-3.495
C16H13Cl3N2OS	DB01007	Tioconazole	-2.879	-3.494
C24H32ClFO5	DB06786	Halcinonide	-3.492	-3.492
C23H29N3O2S2	DB01623	Thiothixene	-2.233	-3.491
C13H16CINO	DB01221	Ketamine	-3.383	-3.487
C40H57N5O7	DB08889	Carfilzomib	-3.481	-3.484
C12H21N3O5S3	DB01194	Brinzolamide	-1.162	-3.478
C19H19N3O6	DB06712	Nilvadipine	-3.475	-3.476
C22H30MnN4O14P2	DB06796	Mangafodipir	-1.342	-3.476
C5H9NO4S	DB04339	Carbocisteine	-3.468	-3.475
C16H11CIN4	DB01215	Estazolam	-3.473	-3.473
C21H21F3IN3O2	DB05239	Cobimetinib	-3.47	-3.472
C9H5Cl2NO	DB01243	Chloroxine	-3.336	-3.469
C12H7Cl3O2	DB08604	Triclosan	-3.175	-3.467
C21H29NO2	DB06713	Norelgestromin	-3.464	-3.464
C12H20N2O3	DB01291	Pirbuterol	-2.937	-3.462
C18H20N2	DB06148	Mianserin	-2.573	-3.459
C14H19NO2	DB06701	Dexmethylphenidate	-3.457	-3.457
C23H31Cl2NO3	DB01196	Estramustine	-3.455	-3.455
C10H15NO	DB01364	Ephedrine	-0.793	-3.455
C28H54N8	DB06809	Plerixafor	-1.319	-3.452
C34H41N7O5	DB06695	Dabigatran etexilate	-2.714	-3.449
C34H41N7O5	DB06695	Dabigatran etexilate	-2.795	-3.442
C9H5ClINO	DB04815	Clioquinol	-3.255	-3.437
C9H15NO3S	DB01197	Captopril	-3.435	-3.435
C38H47N5O7S2	DB06290	Simeprevir	-3.427	-3.434
C20H27N5O2	DB01166	Cilostazol	-3.432	-3.432
C16H26N2O5S	DB01597	Cilastatin	-3.426	-3.432
C22H30MnN4O14P2	DB06796	Mangafodipir	-1.008	-3.432
H4O7P2	DB04160	Pyrophosphoric acid	-2.727	-3.428
C21H20CINO5	DB06216	Asenapine	-3.423	-3.427
C10H22N4	DB01170	Guanethidine	-1.463	-3.426
C23H18ClF2N3O3S	DB08881	Vemurafenib	-3.043	-3.423
C13H18Br2N2O	DB06742	Ambroxol	-1.015	-3.421
C22H30MnN4O14P2	DB06796	Mangafodipir	-0.977	-3.421
C10H17NO2	DB01107	Methyprylon	-3.419	-3.419
C22H27FN4O2	DB01268	Sunitinib	-3.415	-3.419
C23H28F2N6O4S	DB08816	Ticagrelor	-0.879	-3.416
C10H16N2O8	DB00974	Edetic Acid	-1.2	-3.414

C19H21N3O	DB06766	Alcaftadine	-0.892	-3.41
C29H26ClFN4O4S	DB01259	Lapatinib	-2.239	-3.408
C11H16ClN5	DB01131	Proguanil	-2.327	-3.405
C22H30MnN4O14P2	DB06796	Mangafodipir	-1.494	-3.402
C11H13ClF3N3O4S3	DB01324	Polythiazide	-3.398	-3.401
C3H7NO3	DB03929	D-Serine	-3.4	-3.4
C12H17NO	DB01579	Phendimetrazine	-2.694	-3.4
C26H28Cl2N4O4	DB01026	Ketoconazole	-3.074	-3.398
C12H14N4O3S	DB01298	Sulfacytine	-1.735	-3.389
C17H17Cl2N	DB01104	Sertraline	-3.373	-3.386
C14H16O3	DB01322	Kava	-3.385	-3.385
C11H12N4O2S	DB01581	Sulfamerazine	-3.16	-3.382
C12H18N2O2S	DB01154	Thiamylal	-3.332	-3.372
C27H33N3O6S	DB01251	Gliquidone	-1.263	-3.369
C16H18N2O4S	DB01053	Benzylpenicillin	-3.365	-3.365
C22H30MnN4O14P2	DB06796	Mangafodipir	-2.34	-3.364
C9H16ClN3O2	DB01206	Lomustine	-3.36	-3.36
C8H11NO4S2	DB05057	Erdosteine	-3.356	-3.356
C20H28O2	DB00982	Isotretinoin	-3.345	-3.349
C13H17N3O	DB01424	Aminophenazone	-1.981	-3.348
C12H14N4O4S	DB06150	Sulfadimethoxine	-3.21	-3.346
C7H7NO2	DB08797	Salicylamide	-3.307	-3.345
C7H8O	DB06770	Benzyl alcohol	-3.338	-3.338
C23H27FN4O3	DB01267	Paliperidone	-3.322	-3.332
C22H24ClN3O	DB00972	Azelastine	-3.33	-3.331
C12H18N2O2S	DB01154	Thiamylal	-1.302	-3.327
C10H12O2	DB06819	Phenylbutyric acid	-3.322	-3.325
C17H26N4O	DB01084	Emedastine	-3.026	-3.32
C9H13N	DB01576	Dextroamphetamine	-3.318	-3.319
C34H41N7O5	DB06695	Dabigatran etexilate	-1.775	-3.312
C20H21NO4	DB01113	Papaverine	-2.154	-3.308
C11H12ClNO3S	DB01178	Chlormezanone	-3.3	-3.3
C19H14Cl2N2O3S	DB08828	Vismodegib	-3.283	-3.283
C6H8O7	DB04272	Citric acid	-3.28	-3.28
C6H5GaO7	DB06784	Gallium citrate Ga 67	-3.28	-3.28
C8H8N4	DB01275	Hydralazine	-2.757	-3.28
C9H13NO2	DB01031	Ethinamate	-3.279	-3.279
C9H7N7O2S	DB00993	Azathioprine	-1.533	-3.275
C12H13NO2	DB05246	Methsuximide	-3.27	-3.27
C9H7N7O2S	DB00993	Azathioprine	-2.896	-3.266
C5H9N3	DB05381	Histamine	-1.932	-3.264
C35H42N2O9	DB01180	Rescinnamine	-1.51	-3.263
C22H30MnN4O14P2	DB06796	Mangafodipir	-0.753	-3.263
C14H23NO	DB06204	Tapentadol	-3.262	-3.262
C15H22N2O	DB08918	Levomilnacipran	-3.256	-3.257
C17H23N3O	DB06691	Mepyramine	-3.25	-3.256
C20H17ClN2O3	DB01587	Ketazolam	-3.255	-3.255
C4H11NO3	DB03754	Tromethamine	-3.015	-3.255
C12H14N4O4S	DB01299	Sulfadoxine	-1.648	-3.253
C18H20N2	DB06148	Mianserin	-3.096	-3.247
C10H16NO	DB01010	Edrophonium	-3.175	-3.246
CH4N2O2	DB01005	Hydroxyurea	-3.234	-3.242
C14H14N2	DB06711	Naphazoline	-3.241	-3.241
C21H22Cl2FN5O	DB08865	Crizotinib	-2.745	-3.24
C22H19ClO3	DB01117	Atovaquone	-3.239	-3.239
C6H18N4	DB06824	Triethylenetetramine	-1.747	-3.237
C6H10O6	DB04564	Gluconolactone	-3.236	-3.236
C8H8N4	DB01275	Hydralazine	-2.911	-3.236
C17H20N2S	DB01069	Promethazine	-3.234	-3.235
C18H22N2	DB01176	Cyclizine	-1.199	-3.23
C22H30MnN4O14P2	DB06796	Mangafodipir	-2.041	-3.227
C10H16N2O3	DB01353	Butobarbital	-3.187	-3.222
C3H6O3	DB04398	Lactic acid	-3.208	-3.208

C20H27N	DB01616	Alverine	-3.203	-3.204
C5H9N3	DB05381	Histamine	-2.689	-3.197
C21H32Cl2N4O	DB06016	Cariprazine	-1.718	-3.196
C16H24N10O4	DB01223	Aminophylline	-1.363	-3.196
C11H12N4O2S	DB01581	Sulfamerazine	-0.82	-3.196
C4H3N3O4	DB03209	Oteracil	-1.015	-3.195
C26H30Cl2F3NO	DB01218	Halofantrine	-3.191	-3.192
C5H9N3	DB05381	Histamine	-2.734	-3.189
C26H27N5O2	DB06684	Vilazodone	-3.076	-3.178
C16H19CIN2	DB01114	Chlorphenamine	-3.173	-3.173
C6H11NO3	DB00992	Methyl aminolevulinate	-2.694	-3.169
C18H29NO2	DB01359	Penbutolol	-3.167	-3.168
C40H59NO11	DB08871	Eribulin	-3.159	-3.167
C18H22N2	DB01176	Cyclizine	-2.772	-3.167
C7H8CIN3O4S2	DB00999	Hydrochlorothiazide	-0.915	-3.165
C20H24N2	DB08801	Dimetindene	-2.648	-3.162
C10H9AgN4O2S	DB05245	Silver sulfadiazine	-2.293	-3.162
C8H7CIN2O2S	DB01119	Diazoxide	-0.589	-3.159
C12H14N4O4S	DB01299	Sulfadoxine	-3.006	-3.158
C10H15N	DB01577	Metamfetamine	-3.155	-3.155
C11H14CIN	DB04871	Lorcaserin	-3.154	-3.155
C8H8Cl3N3O4S2	DB01021	Trichlormethiazide	-2.906	-3.155
C12H21N3O5S3	DB01194	Brinzolamide	-3.107	-3.152
C20H21FN6O5	DB06817	Raltegravir	-2.88	-3.151
C24H35N5O5	DB04898	Ximelagatran	-2.453	-3.151
C19H26N2S	DB01186	Pergolide	-3.134	-3.145
C14H22N2O2	DB00989	Rivastigmine	-1.613	-3.113
C12H16F3N	DB01191	Dexfenfluramine	-3.107	-3.107
C18H14F4N2O4S	DB01128	Bicalutamide	-3.106	-3.106
C18H26CIN3O3	DB06480	Prucalopride	-3.098	-3.105
C3H9NO3	DB06768	Ammonium lactate	-3.101	-3.101
C12H14N4O2S	DB01582	Sulfamethazine	-1.257	-3.095
C17H11ClF4N2S	DB01589	Quazepam	-3.094	-3.094
C6H6O	DB03255	Phenol	-3.092	-3.093
C12H9F3N2O2	DB01097	Leflunomide	-3.092	-3.092
C16H24N2	DB06694	Xylometazoline	-3.091	-3.091
C12H13N	DB01367	Rasagiline	-2.673	-3.09
C19H21NS	DB06153	Pizotifen	-3.081	-3.089
C16H21Cl2N3O2	DB06769	Bendamustine	-2.701	-3.084
C13H13N3	DB01273	Varenicline	-3.077	-3.077
C8H7CIN2O2S	DB01119	Diazoxide	-3.065	-3.073
C3H8O2	DB01839	Propylene glycol	-3.07	-3.07
C40H48N2O6	DB01336	Metocurine	-3.069	-3.069
C15H21N3O3S	DB01120	Gliclazide	-3.046	-3.069
C21H25CIN2O3	DB06282	Levocetirizine	-2.654	-3.065
C12H17NO2	DB01188	Ciclopirox	-3.062	-3.062
C19H24N2O2	DB01058	Praziquantel	-3.057	-3.057
C11H16CIN5	DB01131	Proguanil	-1.068	-3.055
C11H12N4O2S	DB01581	Sulfamerazine	-0.629	-3.053
C9H11NO2	DB01086	Benzocaine	-3.048	-3.048
C3H7NO2	DB04827	Urethane	-3.045	-3.045
C3H8O	DB03175	Propyl alcohol	-3.041	-3.041
C23H27N	DB01091	Butenafine	-2.896	-3.029
C20H15BrN6O	DB06414	Etravirine	-3.024	-3.024
C43H51N3O11	DB01220	Rifaximin	-2.227	-3.023
C11H16CIN5	DB01131	Proguanil	-0.757	-3.021
C2H4Cl3O4P	DB06753	Triclofos	-2.948	-3.013
C11H16CIN5	DB01131	Proguanil	-0.962	-3.012
C26H25CIN2O3	DB06212	Tolvaptan	-3.008	-3.008
C5H9NO3S	DB06823	Tiopronin	-2.996	-3.008
C4H3N3O4	DB03209	Oteracil	-2.928	-3.007
C26H26F2N2	DB04841	Flunarizine	-0.34	-3
C21H23N7O2S	DB06589	Pazopanib	-2.991	-2.998

C19H18N2O4S	DB08439	Parecoxib	-2.981	-2.998
C28H46O	DB01070	Dihydrotachysterol	-2.997	-2.997
C5H7NO3	DB03088	Pidolic Acid	-2.993	-2.993
C30H40N4	DB04209	Dequalinium	-2.981	-2.981
C4H4FN3O	DB01099	Flucytosine	-2.98	-2.981
C20H18NO4	DB04115	Berberine	-2.979	-2.979
C19H35N	DB01074	Perhexiline	-2.977	-2.977
C12H13NO2S	DB04657	Carboxin	-2.975	-2.975
C17H25N3O2	DB04876	Vildagliptin	-2.926	-2.972
C43H51N3O11	DB01220	Rifaximin	-1.931	-2.971
C9H17NO4	DB08842	Acetylcarnitine	-2.968	-2.968
C27H33N3O6S	DB01251	Gliquidone	-2.949	-2.966
C21H33N3O5S	DB01605	Pivmecillinam	-2.965	-2.965
C24H27FN2O4	DB04946	Iloperidone	-0.684	-2.958
C5H4N4S	DB01033	Mercaptopurine	-2.842	-2.957
C26H28N3	DB06816	Pyrvinium	-2.956	-2.956
C7H10N2O2S	DB06795	Mafenide	-2.926	-2.956
C24H27N	DB04825	Prenylamine	-2.942	-2.942
C11H16N2O2	DB01085	Pilocarpine	-2.742	-2.936
C19H21NS	DB06153	Pizotifen	-0.357	-2.933
C14H22N2O3	DB01297	Practolol	-2.925	-2.927
C24H27FN2O4	DB04946	Iloperidone	-2.91	-2.923
C14H10N4O5	DB01219	Dantrolene	-1.632	-2.913
C18H22N2	DB01176	Cyclizine	-2.439	-2.907
C13H19CIN2O2	DB01161	Chloroprocaine	-2.884	-2.905
C6H18N4	DB06824	Triethylenetetramine	-2.807	-2.894
C35H35F2N8O5S	DB06636	Isavuconazonium	-0.989	-2.894
C19H19N	DB01619	Phenindamine	-2.435	-2.891
C22H22O8	DB01179	Podofilox	-2.883	-2.883
C9H17NO2	DB00996	Gabapentin	-2.881	-2.881
C23H18CIF2N3O3S	DB08881	Vemurafenib	-2.431	-2.875
C22H30MnN4O14P2	DB06796	Mangafodipir	-0.806	-2.875
C9H10Cl2N4	DB00964	Apraclonidine	-2.863	-2.866
C9H9N3O2S2	DB06147	Sulfathiazole	-2.178	-2.859
C4H6N2	DB01213	Fomepizole	-2.849	-2.849
C2H7NO3S	DB01956	Taurine	-2.847	-2.848
C11H16CIN5	DB01131	Proguanil	-2.625	-2.848
C5H9NO3S	DB06823	Tiopronin	-0.526	-2.848
C10H22N4	DB01170	Guanethidine	-2.822	-2.844
C11H11N5	DB01438	Phenazopyridine	-2.831	-2.836
C2H4O3	DB03085	Glycolic acid	-2.835	-2.835
C5H5NOS	DB06815	Pyrrithione	-2.832	-2.832
C45H57NO14	DB06772	Cabazitaxel	-2.825	-2.828
C7H6O2	DB03793	Benzoic Acid	-2.822	-2.822
C13H21N3O	DB01035	Procainamide	-2.814	-2.817
C4H8O3	DB01440	gamma-Hydroxybutyric acid	-2.811	-2.813
C12H17NO	DB01579	Phendimetrazine	-2.597	-2.812
C8H12N2	DB06698	Betahistine	-2.809	-2.809
C4H3N3O4	DB03209	Oteracil	-1.259	-2.79
C25H32CIN5O2	DB01149	Nefazodone	-2.371	-2.789
C53H67N9O10S	DB01369	Quinupristin	-0.832	-2.784
C13H18CINO	DB01156	Bupropion	-2.544	-2.781
C11H12N4O3S	DB06821	Sulfameter	-2.327	-2.776
C30H32Cl3NO	DB06708	Lumefantrine	-0.869	-2.77
C28H54N8	DB06809	Plerixafor	-0.7	-2.754
C6H14O6S2	DB01008	Busulfan	-2.744	-2.744
C4H3N3O4	DB03209	Oteracil	-0.264	-2.744
C5H4N4S	DB01033	Mercaptopurine	-1.698	-2.737
C3H8OS2	DB06782	Dimercaprol	-2.728	-2.735
C23H28CIN3O5S	DB01016	Glyburide	-2.71	-2.731
C11H12N4O2S	DB01581	Sulfamerazine	-1.951	-2.711
C4H11NO3	DB03754	Tromethamine	-2.056	-2.708
C35H35F2N8O5S	DB06636	Isavuconazonium	-2.273	-2.705

C28H54N8	DB06809	Plerixafor	0.03	-2.693
C4H9NO2	DB02530	gamma-Aminobutyric acid	-2.682	-2.682
C12H21N5O3	DB01303	Oxtriphylline	-2.681	-2.681
C26H29MgNO10	DB01401	Choline magnesium trisalicylate	-2.681	-2.681
C23H27Cl2N3O2	DB01238	Aripiprazole	-2.479	-2.672
C22H48N	DB04221	Didecyldimethylammonium	-2.664	-2.664
C23H20F3N5O2S2	DB08912	Dabrafenib	-2.248	-2.664
C13H17N	DB01037	Selegiline	-2.555	-2.656
C19H25N5O4	DB01162	Terazosin	-2.525	-2.647
C19H17ClN2O	DB01588	Prazepam	-2.644	-2.644
C10H16O	DB01744	Camphor	-2.642	-2.642
C28H22F3N7O	DB04868	Nilotinib	-2.489	-2.629
C35H60N2O4	DB01337	Pancuronium	-2.628	-2.628
C22H21Cl3N4O	DB06155	Rimonabant	-2.623	-2.623
C5H6N2	DB06637	Dalfampridine	-2.62	-2.623
C3H8OS2	DB06782	Dimercaprol	0.037	-2.619
C13H16N2	DB06764	Tetryzoline	-2.608	-2.608
C26H26F2N2	DB04841	Flunarizine	-1.388	-2.608
C70H94N18O16	DB06788	Histrelin	-0.654	-2.602
C23H29N3O2S2	DB01623	Thiothixene	-0.588	-2.6
C34H41N7O5	DB06695	Dabigatran etexilate	-0.456	-2.599
C35H62N4O4	DB01338	Pipecuronium	-2.36	-2.567
C13H11NO3	DB06807	Phenyl aminosalicylate	-0.615	-2.566
C10H11N3O3S	DB01015	Sulfamethoxazole	-0.028	-2.564
C5H11NO2	DB06756	Glycine betaine	-2.561	-2.561
C58H80N2O14	DB01226	Mivacurium	-2.555	-2.555
C8H8Cl3N3O4S2	DB01021	Trichlormethiazide	-1.912	-2.545
C35H62N4O4	DB01338	Pipecuronium	-1.73	-2.539
C25H32N2O4	DB06274	Alvimopan	-2.532	-2.537
C22H30MnN4O14P2	DB06796	Mangafodipir	-1.339	-2.524
C28H28N2O2	DB01501	Difenoxin	-2.504	-2.52
C23H29N3O2S2	DB01623	Thiothixene	-2.416	-2.514
C10H11N3O3S	DB01015	Sulfamethoxazole	-2.504	-2.513
C19H23NO	DB01146	Diphenylpyraline	-2.499	-2.502
C18H26ClN3O	DB01611	Hydroxychloroquine	-2.443	-2.493
C6H11NO3	DB00992	Methyl aminolevulinate	-2.139	-2.492
C3H4Cl2F2O	DB01028	Methoxyflurane	-2.482	-2.482
C10H9AgN4O2S	DB05245	Silver sulfadiazine	-2.326	-2.482
C25H36N3O9PS	DB01319	Fosamprenavir	-2.395	-2.469
C11H12N4O3S	DB06821	Sulfamer	-2.089	-2.465
C23H27N3O7	DB01017	Minocycline	0.174	-2.456
C35H42N2O9	DB01180	Rescinnamine	-2.421	-2.453
C11H21NO3	DB06261	Hexaminolevulinate	-1.996	-2.442
C14H20N2O3	DB02546	Vorinostat	-2.439	-2.439
C13H19N5	DB06762	Pinacidil	-2.431	-2.437
C10H21N	DB06714	Propylhexedrine	-2.413	-2.413
C12H21N	DB01043	Memantine	-2.401	-2.401
C18H18ClNS	DB01239	Chlorprothixene	-2.383	-2.387
C21H27N5O4S	DB01067	Glipizide	-0.413	-2.382
C11H17BrN	DB01158	Bretylium	-2.379	-2.379
C19H25NOS	DB05271	Rotigotine	-2.368	-2.374
C11H13N	DB01626	Pargyline	-2.228	-2.373
C13H19NO4S	DB01032	Probenecid	-2.371	-2.371
C7H17N2O2	DB01019	Bethanechol	-2.366	-2.366
C2H3Cl3O2	DB01563	Chloral hydrate	-2.329	-2.329
C6H12N3PS	DB04572	Thiotepa	-2.324	-2.324
C35H62N4O4	DB01338	Pipecuronium	-0.217	-2.302
C4H6N4O12	DB01613	Erythryl tetranitrate	-2.298	-2.298
C9H9N3O2S2	DB06147	Sulfathiazole	-2.059	-2.285
C12H13N	DB01367	Rasagiline	-1.879	-2.283
C21H32Cl2N4O	DB06016	Cariprazine	-2.221	-2.272
C28H24FN3O5	DB08875	Cabozantinib	-2.225	-2.27
C26H29F2N7	DB01430	Almitrine	-2.22	-2.263

CuO4S	DB06778	Cupric sulfate	-2.256	-2.256
C7H8ClN3O4S2	DB00999	Hydrochlorothiazide	-2.24	-2.254
C13H17N	DB01037	Selegiline	-1.156	-2.254
C34H41N7O5	DB06695	Dabigatran etexilate	-0.695	-2.254
C5H11NO2S	DB02893	D-Methionine	-2.236	-2.236
CH4N2O	DB03904	Urea	-2.23	-2.23
ClH4N	DB06767	Ammonium chloride	-2.222	-2.224
C28H54N8	DB06809	Plerixafor	-0.027	-2.216
C12H21N3O5S3	DB01194	Brinzolamide	-0.479	-2.213
C15H21N3O3S	DB01120	Gliclazide	-0.29	-2.213
C24H34N2O	DB01244	Bepidil	-2.21	-2.21
C22H25N2OS	DB01116	Trimethaphan	-2.208	-2.208
C2H2Cl2O2	DB08809	Dichloroacetic acid	-2.183	-2.183
C9H19N	DB06706	Isometheptene	-2.18	-2.18
C11H17N	DB01365	Mephentermine	-2.173	-2.173
C20H41NO3	DB06689	Ethanolamine oleate	-2.153	-2.156
C11H21NO3	DB06261	Hexaminolevulinate	-1.746	-2.123
C2H4O2	DB03166	Acetic acid	-2.113	-2.116
C14H12O3	DB01428	Oxybenzone	-0.431	-2.111
C6H6Cl2N2O4S2	DB01144	Diclofenamide	-2.103	-2.11
C23H30GdN3O11	DB08884	Gadoxetic acid	-1.218	-2.103
C28H54N8	DB06809	Plerixafor	-1.356	-2.094
C16H32O2	DB03796	Palmitic Acid	-2.088	-2.091
C2H6OS	DB01093	Dimethyl sulfoxide	-2.089	-2.089
C4H3F7O	DB01236	Sevoflurane	-2.087	-2.087
C26H26F2N2	DB04841	Flunarizine	-1.993	-2.081
C21H27N5O4S	DB01067	Glipizide	-2.057	-2.079
C30H32Cl3NO	DB06708	Lumefantrine	-2.034	-2.059
C18H34O2	DB04224	Oleic Acid	-2.022	-2.025
C12H18N2O3S	DB01124	Tolbutamide	-2.004	-2.022
C17H22N2S	DB04826	Thenalidine	-2.019	-2.019
C53H67N9O10S	DB01369	Quinupristin	-1.588	-1.984
C24H36N4O6S2	DB06176	Romidepsin	-1.981	-1.981
C29H31F2N3O	DB04842	Fluspirilene	-1.955	-1.96
C8H18NO2	DB06709	Methacholine	-1.959	-1.959
C12H19N2O2	DB01400	Neostigmine	-1.957	-1.957
C12H24O2	DB03017	Lauric acid	-1.939	-1.943
C23H27Cl2N3O2	DB01238	Aripiprazole	-1.164	-1.923
C26H29F2N7	DB01430	Almitrine	-0.258	-1.917
C11H13N	DB01626	Pargyline	-0.984	-1.887
C23H30GdN3O11	DB08884	Gadoxetic acid	-0.155	-1.878
C6H11NO2	DB01080	Vigabatrin	-1.865	-1.865
C23H30GdN3O11	DB08884	Gadoxetic acid	-0.806	-1.859
C15H14N4O2S	DB06729	Sulfaphenazole	-1.804	-1.857
C40H56	DB06755	Beta carotene	-1.829	-1.829
C18H36O2	DB03193	Stearic acid	-1.82	-1.823
C56H78N2O16	DB01135	Doxacurium	-1.811	-1.811
C15H21N3O2	DB00981	Physostigmine	0.692	-1.805
C27H33N3O8	DB01301	Rolitetraacycline	-0.22	-1.804
C15H32N2	DB01090	Pentolinium	-1.8	-1.8
C14H22N2O2	DB00989	Rivastigmine	-1.706	-1.755
CH2O	DB03843	Formaldehyde	-1.754	-1.754
C31H48O6	DB02703	Fusidic acid	0.287	-1.743
CH4N2O2	DB01005	Hydroxyurea	0.755	-1.743
C43H58N4O12	DB01045	Rifampicin	-0.84	-1.726
C39H43N3O11S	DB05109	Trabectedin	-0.718	-1.722
C13H15N3O4S	DB01382	Glymidine	-1.312	-1.693
C21H26N2O3	DB01392	Yohimbine	0.226	-1.679
C5H8N4O12	DB06154	Pentaerythritol tetranitrate	-1.672	-1.672
C13H11NO3	DB06807	Phenyl aminosaliclylate	-1.61	-1.632
C3H2F6O	DB01189	Desflurane	-1.627	-1.627
C3H6O2	DB03766	Propanoic acid	-1.608	-1.611
GaN3O9	DB05260	Gallium nitrate	-1.603	-1.603

C6H12N4	DB06799	Methenamine	0.683	-1.58
C28H29F2N3O	DB01100	Pimozide	-1.522	-1.529
C6H12N4	DB06799	Methenamine	-1.475	-1.488
C43H58N4O12	DB01045	Rifampicin	-1.103	-1.47
C30H32N2O2	DB01081	Diphenoxylate	-1.08	-1.464
CHNaO3	DB01390	Sodium bicarbonate	-1.33	-1.442
CCaO3	DB06724	Calcium Carbonate	-1.33	-1.442
C3La2O9	DB06792	Lanthanum carbonate	-1.33	-1.442
C3H8O	DB02325	Isopropyl alcohol	-1.417	-1.417
C7H16NO2	DB03128	Acetylcholine	-1.337	-1.337
C28H54N8	DB06809	Plerixafor	1.363	-1.308
C32H38N2O8	DB01089	Deserpidine	0.468	-1.257
N2O	DB06690	Nitrous oxide	-1.233	-1.233
C2HBrClF3	DB01159	Halothane	-1.216	-1.216
C15H21N3O2	DB00981	Physostigmine	-1.119	-1.128
I2	DB05382	Iodine	-1.121	-1.121
C47H64N4O12	DB01201	Rifapentine	-0.765	-1.113
C30H26F6N4O2	DB01419	Antrafenine	0.621	-1.112
C59H79N15O21S6	DB08890	Linaclotide	-0.525	-1.056
C21H23N7O2S	DB06589	Pazopanib	1.741	-0.901
C16H38N2	DB01245	Decamethonium	-0.888	-0.888
C28H54N8	DB06809	Plerixafor	1.394	-0.797
C28H54N8	DB06809	Plerixafor	0.474	-0.791
C13H8Cl2N2O4	DB06803	Niclosamide	-0.696	-0.763
C19H42N	DB01718	Cetrimonium	-0.758	-0.758
C5H11NO2	DB01612	Amyl Nitrite	-0.702	-0.702
C12H18N2O3S	DB01124	Tolbutamide	1.379	-0.701
C34H41N7O5	DB06695	Dabigatran etexilate	1.68	-0.68
C17H15N3O6	DB01014	Balsalazide	-0.655	-0.656
C24H33N3O3S2	DB01621	Pipotiazine	-0.575	-0.575
Al2H4O9Si2	DB01575	Kaolin	-0.561	-0.561
C12H6Cl4O2S	DB04813	Bithionol	-0.11	-0.499
C26H29FN2O2	DB01106	Levocabastine	-0.444	-0.444
C10H16NO	DB01010	Edrophonium	1.032	-0.259
C28H54N8	DB06809	Plerixafor	2.219	-0.211
C24H35N5O5	DB04898	Ximelagatran	0.03	-0.188
C28H36N4O2S	DB08815	Lurasidone	-0.155	-0.155
C17H17ClN6O3	DB01198	Zopiclone	0.262	-0.088
C28H54N8	DB06809	Plerixafor	2.729	0.036
C56H87NO16	DB06287	Temsirolimus	0.212	0.21
C43H58N4O12	DB01045	Rifampicin	1.602	0.511
C47H64N4O12	DB01201	Rifapentine	1.548	0.688
C70H94N18O16	DB06788	Histrelin	2.727	0.746
C47H51NO14	DB01229	Paclitaxel	1.027	1.026
C37H61N2O4	DB04834	Rapacuronium	1.237	1.233
C35H62N4O4	DB01338	Pipecuronium	4.064	1.359
C21H23NO5	DB01452	Diamorphine	3.039	1.688
C47H64N4O12	DB01201	Rifapentine	3.909	1.916
C25H43N13O10	DB06827	Viomycin	2.351	1.941
C6H8O4	DB08908	Dimethyl fumarate	2.072	2.072
C34H57N2O4	DB01339	Vecuronium	4.081	4.077

FDA approved drugs with 6y84, Table S9

FORMULA	DRUGBANK_ID	GENERIC_NAME	docking score	glide gscore
C37H48I6N6O18	DB09487	Iotrolan	-10.853	-11.001
C36H70O19	DB11602	Hydroxyethyl cellulose	-10.119	-10.119
C11H20O10	DB12767	Gaxilose	-9.728	-9.728
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-9.464	-10.795

C18H24I3N3O8	DB09156	Iopromide	-9.338	-9.338
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-8.948	-10.607
C17H22I3N3O8	DB08947	Iopamidol	-8.567	-8.567
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-8.32	-10.178
C28H32O15	DB08995	Diosmin	-8.28	-8.28
C49H62N10O16S3	DB09142	Sinacalide	-8.216	-8.233
C22H42N4O8S2	DB11190	Pantethine	-7.813	-7.813
C65H90N14O19S2	DB14554	Dotatate	-7.75	-9.43
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-7.701	-9.451
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-7.659	-9.487
C32H50O13	DB12434	Steviolbioside	-7.617	-7.621
C20H25N7O6	DB11256	Levomefolic acid	-7.599	-7.615
C42H62O16	DB13751	Glycyrrhizic acid	-7.592	-7.596
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-7.448	-9.16
C25H48N6O10	DB12615	Plazomicin	-7.418	-9.565
C65H90N14O19S2	DB14554	Dotatate	-7.416	-9.18
C37H48I6N6O18	DB09487	Iotrolan	-7.311	-8.205
C29H40N4O7	DB12455	Omadacycline	-7.305	-7.431
C18H24I3N3O8	DB09135	Ioxilan	-7.278	-7.278
C65H90N14O19S2	DB14554	Dotatate	-7.201	-8.913
C12H29Fe5Na2O23	DB09146	Iron saccharate	-7.1	-7.1
C24H21I6N5O8	DB09313	Ioxaglic acid	-7.031	-7.031
C17H22I3N3O8	DB11705	Iomeprol	-6.993	-6.993
C20H28I3N3O9	DB12407	Iobitridol	-6.975	-6.975
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-6.956	-8.765
C12H22MnO14	DB11141	Manganese gluconate	-6.921	-6.921
C12H22CaO14	DB11126	Calcium gluconate	-6.921	-6.921
C17H15BrF2N4O3	DB11967	Binimetinib	-6.917	-6.926
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-6.886	-8.531
C65H90N14O19S2	DB14554	Dotatate	-6.737	-8.553
C50H71N13O12	DB11842	Angiotensin II	-6.731	-7.381
C26H27F3N2O6	DB11712	Tezacaftor	-6.622	-6.622
C43H67N11O12S2	DB09059	Atosiban	-6.574	-6.574
C13H21NO3	DB13139	Levosalbutamol	-6.417	-6.417
C15H14O6	DB14086	Cianidanol	-6.402	-6.402
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-6.347	-7.944
C11H16N8O8	DB14075	Imidurea	-6.328	-6.614
C20H23N7O7	DB11596	Levoleucovorin	-6.327	-6.327
C50H68N14O10	DB11653	Bremelanotide	-6.325	-6.946
C14H26N4O11P2	DB12153	Citicoline	-6.259	-6.259
C46H65N13O12S2	DB14642	Lypressin	-6.25	-6.443
C32H30F5N3O5	DB11979	Elagolix	-6.24	-6.448
C65H90N14O19S2	DB14554	Dotatate	-6.221	-7.618
C6H12O6	DB13178	Inositol	-6.186	-6.186
C18H24I3N3O9	DB09134	Ioversol	-6.185	-6.185
C12H16O7	DB14109	alpha-Arbutin	-6.165	-6.165
C25H48N6O10	DB12615	Plazomicin	-6.157	-6.648
C29H40N4O7	DB12455	Omadacycline	-6.125	-7.382
C26H30N6O3	DB13074	Macimorelin	-6.109	-6.231
C10H15N3O5	DB12783	Benserazide	-6.104	-6.196
C21H29N6O5P	DB09299	Tenofovir alafenamide	-6.037	-6.037
C11H16N8O8	DB14075	Imidurea	-6.021	-6.66
C20H22O8	DB11263	Polydatin	-6.013	-6.013
C12H26MgO16	DB13749	Magnesium gluconate	-6.004	-6.004
C24H33Cl2NO5	DB09082	Vilanterol	-5.933	-5.939
C28H27N3O3	DB13931	Netarsudil	-5.817	-5.828
C15H18N2O9	DB09144	Uridine triacetate	-5.806	-5.808
C12H22O14Zn	DB11248	Zinc gluconate	-5.75	-5.75
C25H48N6O10	DB12615	Plazomicin	-5.732	-6.631
C8H18O10S2	DB12097	Mannitol busulfan	-5.719	-5.719
C6H11KO7	DB13620	Potassium gluconate	-5.69	-5.69
C21H30NO4	DB09300	Butylscopolamine	-5.689	-5.689
C19H23N4O6PS	DB11748	Benfotiamine	-5.662	-6.928

C30H53N3O6	DB09026	Aliskiren	-5.645	-5.65
C23H32O3	DB13956	Estradiol valerate	-5.62	-5.62
C22H28O5	DB09383	Meprednisone	-5.611	-5.611
C15H16O9	DB13155	Esculin	-5.609	-5.62
C29H42O6	DB14541	Hydrocortisone cypionate	-5.588	-5.588
C23H27ClO7	DB09038	Empagliflozin	-5.582	-5.582
C23H26FN6O9P	DB12010	Fostamatinib	-5.574	-6.928
C27H41NO8	DB11660	Latanoprostene Bunod	-5.557	-5.557
C23H23ClFNO5	DB09101	Elvitegravir	-5.495	-6.451
C34H53NO11	DB09049	Naloxegol	-5.494	-5.581
C23H30N12O8S2	DB09050	Ceftolozane	-5.473	-5.475
C11H8Na4O8P2	DB09332	Kappadione	-5.47	-6.813
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-5.46	-7.224
C28H33N7O2	DB09330	Osimertinib	-5.445	-5.453
C22H25ClO7	DB11827	Ertugliflozin	-5.414	-5.414
C10H8N2O2S2	DB11327	Dipyrrithione	-5.404	-5.404
C12H22FeO14	DB14488	Ferrous gluconate	-5.39	-5.39
C6H12O6	DB11735	Galactose	-5.387	-5.387
C19H23N4O6PS	DB11748	Benfotiamine	-5.382	-6.623
C29H44N8O3	DB12141	Gilteritinib	-5.381	-5.407
C23H23ClFNO5	DB09101	Elvitegravir	-5.374	-5.51
C28H41N3O3	DB12532	Oxetacaine	-5.372	-5.44
C30H44N2O10	DB13265	Hexobendine	-5.36	-5.381
C34H67O10P	DB11284	DL-dimyristoylphosphatidylglycerol	-5.35	-5.35
C52H78N10O17	DB13156	Inosine pranobex	-5.347	-5.347
C65H90N14O19S2	DB14554	Dotatate	-5.324	-6.954
C8H14N4O7	DB14173	Diazolidinylurea	-5.314	-5.314
C11H12O8P2	DB14650	Menadiol diphosphate	-5.305	-6.724
C11H8Na4O8P2	DB09332	Kappadione	-5.305	-6.724
C20H17F3N2O4	DB08976	Floctafenine	-5.3	-5.314
C18H33CrO21	DB14528	Chromium gluconate	-5.294	-5.294
C56H98N16O13	DB00781	Polymyxin B	-5.282	-5.291
C18H37N5O8	DB13270	Dibekacin	-5.277	-6.758
C22H29FN3O9P	DB08934	Sofosbuvir	-5.254	-5.257
C21H28O3	DB11636	Nomegestrol	-5.246	-5.246
C29H34Cl2N6O3S2	DB11995	Avatrombopag	-5.233	-5.237
C6H12O7	DB13180	Gluconic Acid	-5.224	-5.224
C11H18N2O9	DB12362	Diaminopropanol tetraacetic acid	-5.21	-5.299
C32H43N5O5	DB11275	Epicriptine	-5.188	-5.231
C65H90N14O19S2	DB14554	Dotatate	-5.18	-6.944
C6H8CaO8	DB13962	Calcium saccharate	-5.17	-5.171
C16H22N6O4	DB09421	Protirelin	-5.158	-5.833
C7H6O3	DB11268	Protocatechualdehyde	-5.156	-5.263
C20H34O5	DB12789	Dinoprost	-5.138	-5.141
C29H32Cl2N2O5S	DB13125	Lusutrombopag	-5.132	-5.132
C12H22CuO14	DB11246	Copper gluconate	-5.129	-5.129
C14H19BCl2N2O4	DB09570	Ixazomib	-5.128	-5.128
C26H25F3N6O5	DB09335	Alatrofloxacin	-5.117	-5.254
C25H30N4O9S2	DB12127	Sultamicillin	-5.117	-5.325
C17H15FN6O3	DB14569	Tedizolid	-5.109	-5.109
C23H38O5	DB08964	Gemprost	-5.104	-5.104
C35H46ClN5O9S	DB11586	Asunaprevir	-5.101	-5.107
C26H30N6O3	DB13074	Macimorelin	-5.052	-6.049
C27H33N2O7S2	DB13967	Patent Blue	-5.051	-5.267
C12H16O7	DB11217	Arbutin	-5.046	-5.046
C22H28O5	DB12952	Methylprednisone	-5.041	-5.041
C12H11I3N2O5	DB13444	Ioxitalamic acid	-5.031	-5.031
C23H30N2O4	DB09209	Pholcodine	-5.021	-5.122
C32H30F5N3O5	DB11979	Elagolix	-5.014	-5.746
C19H22N2O3	DB13286	Bumadizone	-4.993	-4.993
C32H43N5O5	DB11274	Dihydro-alpha-ergocryptine	-4.991	-5.035
C26H34O8	DB14644	Methylprednisolone hemisuccinate	-4.983	-4.984
C21H19ClN4O4	DB09078	Lenvatinib	-4.954	-4.954

C14H7Cl2NO3	DB11644	Tafamidis	-4.953	-4.953
C26H25F3N6O5	DB09335	Alatrofloxacin	-4.902	-6.884
C19H20Cl2N2O5	DB13258	Etofamide	-4.897	-4.897
C23H32O6	DB14539	Hydrocortisone acetate	-4.895	-4.895
C21H30O2	DB09061	Cannabidiol	-4.884	-4.884
C22H18FN7O	DB09054	Idelalisib	-4.883	-4.904
C23H28N8O4	DB12483	Copanlisib	-4.88	-5.311
C14H12O6S	DB11185	Sulisobenzone	-4.873	-4.912
C30H26N2O13	DB11184	Oftasceine	-4.871	-4.961
C50H71N13O12	DB11842	Angiotensin II	-4.865	-5.548
C29H24Cl2N2O7S	DB11611	Lifitegrast	-4.854	-4.854
C14H10O3	DB11157	Anthralin	-4.837	-4.837
C29H39ClN7O2P	DB12267	Brigatinib	-4.825	-4.838
C22H29NO5	DB09089	Trimebutine	-4.824	-5.479
C29H33FO9S	DB14703	Dexamethasone metasulfobenzoate	-4.823	-4.823
C28H40O7	DB14543	Hydrocortisone probutate	-4.818	-4.818
C65H90N14O19S2	DB14554	Dotatate	-4.817	-6.567
C20H41N5O7	DB13274	Micronomicin	-4.81	-6.627
C26H32N2O8	DB13711	Tritoqualine	-4.808	-5.64
C26H25F3N6O5	DB09335	Alatrofloxacin	-4.805	-5.879
C26H36O3	DB13954	Estradiol cypionate	-4.805	-4.805
C11H8Na4O8P2	DB09332	Kappadione	-4.802	-4.939
C24H31FO6	DB14657	Paramethasone acetate	-4.788	-4.788
C18H32Fe4O31	DB14520	Tetraferic tricitrate decahydrate	-4.788	-4.788
C21H26FNO3	DB09148	Florbetaben (18F)	-4.781	-4.785
C42H30N6O12	DB08949	Inositol nicotinate	-4.776	-4.777
C12H6N2O8SSr2	DB09267	Strontium ranelate	-4.776	-4.776
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-4.768	-6.62
C19H28O8	DB09274	Artesunate	-4.766	-4.767
C20H25FN2O3	DB09149	Florbetapir (18F)	-4.75	-4.754
C17H12I2O3	DB13277	Benziodarone	-4.75	-4.758
C20H23NO	DB13114	Amitriptylinoxide	-4.737	-4.737
C27H31FN4O8	DB12329	Eravacycline	-4.729	-5.967
C16H17N7O2S	DB11817	Baricitinib	-4.725	-4.725
C6H5Li3O7	DB14507	Lithium citrate	-4.724	-4.724
C6H5K3O7	DB09125	Potassium Citrate	-4.724	-4.724
C14H11FN2OS	DB09151	Flutemetamol (18F)	-4.72	-4.734
C36H51Cl2N3O4	DB14185	Aripiprazole lauroxil	-4.718	-4.911
C21H31O8P	DB14542	Hydrocortisone phosphate	-4.706	-4.772
C14H20InN3O10	DB09425	Indium In-111 pentetate	-4.706	-4.944
C19H20Br2N6O4S	DB08932	Macitentan	-4.7	-4.9
C15H10Cl2N4O6	DB11632	Opicapone	-4.69	-4.844
C24H31N3OS	DB13213	Butaperazine	-4.689	-4.969
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-4.686	-6.318
C11H12O8P2	DB14650	Menadiol diphosphate	-4.674	-6.017
C24H31FO6	DB14649	Dexamethasone acetate	-4.672	-4.672
C17H20N2O5S	DB13337	Pheneticillin	-4.668	-4.668
C18H18ClNOS	DB09225	Zotepine	-4.667	-4.667
C17H11ClF3N5O3	DB12301	Doravirine	-4.646	-4.646
C11H12O8P2	DB14650	Menadiol diphosphate	-4.645	-4.782
C12H16BNO5S	DB12107	Vaborbactam	-4.632	-4.633
C22H17ClN6O	DB11952	Duvelisib	-4.63	-4.651
C21H21N3O3	DB12924	Ozenoxacin	-4.624	-5.221
C21H31O8P	DB14542	Hydrocortisone phosphate	-4.619	-5.952
C16H12Cl2N2O2	DB13872	Lormetazepam	-4.616	-4.616
C20H25NO2	DB09123	Dienogest	-4.611	-4.611
C5H10O5	DB09419	Xylose	-4.601	-4.601
C21H27FO5	DB09378	Fluprednisolone	-4.601	-4.601
C22H30O4	DB09015	Canrenoic acid	-4.596	-4.6
C15H30N2O5	DB12839	Pegvaliase	-4.592	-4.592
C30H48O3	DB13946	Testosterone undecanoate	-4.586	-4.586
C24H25ClFN5O2	DB11963	Dacomitinib	-4.582	-4.691
C21H34O5	DB09081	Idebenone	-4.58	-4.58

C38H73N21O10S2	DB12865	Etelcalcetide	-4.569	-6.778
C15H14N2O2	DB14575	Eslicarbazepine	-4.567	-4.567
C28H36ClN5O3S	DB09063	Ceritinib	-4.566	-4.566
C7H11N3O6S	DB09060	Avibactam	-4.561	-4.561
C24H29NO5	DB09292	Sacubitril	-4.559	-4.574
C21H29O8P	DB14631	Prednisolone phosphate	-4.553	-4.619
C6H6N2O3	DB09055	Acipimox	-4.543	-4.546
C14H17N5O3S	DB14203	Disperse Blue 106	-4.54	-4.54
C25H48N6O10	DB12615	Plazomicin	-4.539	-7.096
C50H68N14O10	DB11653	Bremelanotide	-4.53	-5.08
C21H27NO2	DB08954	Ifenprodil	-4.525	-4.525
C16H22N6O4	DB09421	Protirelin	-4.524	-5.168
C23H28O6	DB14646	Prednisone acetate	-4.522	-4.522
C6H11FO5	DB09502	Fludeoxyglucose F-18	-4.522	-4.524
C22H28F2O4	DB09095	Difluocortolone	-4.517	-4.517
C26H40O3	DB13944	Testosterone enanthate	-4.515	-4.515
C14H12O2	DB14020	Benzoin	-4.51	-4.51
C16H21NO3	DB11181	Homatropine	-4.506	-4.506
C32H35N5O5	DB09272	Eluxadoline	-4.499	-5.803
C25H34O8	DB14545	Hydrocortisone succinate	-4.498	-4.499
C12H13I3N2O3	DB09403	Iocetamic acid	-4.496	-4.497
C22H22N6O5S2	DB13682	Cefpirome	-4.493	-4.493
C22H29NO5	DB09089	Trimebutine	-4.48	-4.718
C23H36N2O4	DB09039	Eliglustat	-4.48	-4.486
C32H35N5O5	DB09272	Eluxadoline	-4.476	-5.235
C38H49N3O5	DB11206	Bemotrizinol	-4.467	-4.467
C19H23N3O	DB09084	Benzydamine	-4.453	-4.453
C21H27ClO5	DB00873	Loteprednol	-4.45	-4.45
C13H21N5O4	DB09092	Xanthinol	-4.446	-4.524
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-4.441	-6.214
C18H22F2N4O	DB09040	Efinaconazole	-4.44	-4.471
C18H23NO3	DB08941	Isoxsuprine	-4.439	-4.474
C25H48N6O10	DB12615	Plazomicin	-4.437	-5.519
C21H22F2N6O2	DB14723	Larotrectinib	-4.436	-4.436
C21H30O4S	DB09091	Tixocortol	-4.425	-4.434
C17H13N3O5S2	DB13248	Phthalylsulfathiazole	-4.424	-4.72
C26H38O6	DB14544	Hydrocortisone valerate	-4.423	-4.423
C20H25N7O6	DB11256	Levomefolic acid	-4.421	-6.653
C24H31NO4	DB11269	Diethylamino hydroxybenzoyl hexyl benzoate	-4.419	-4.431
C25H30N4O9S2	DB12127	Sultamicillin	-4.418	-5.139
C19H23N4O6PS	DB11748	Benfotiamine	-4.416	-4.596
C14H23N3O10	DB14007	Pentetic acid	-4.409	-4.647
C34H53NO11	DB09049	Naloxegol	-4.406	-5.652
C37H47NO12	DB11753	Rifamycin	-4.404	-4.513
C12H18O	DB13908	Amylmetacresol	-4.403	-4.403
C16H25NO3	DB09205	Moxisylyte	-4.403	-4.423
C20H25NO	DB11609	Normethadone	-4.399	-4.402
C15H19NO2	DB09071	Tasimelteon	-4.378	-4.379
C15H17N3O6S	DB14082	Betiotide	-4.372	-4.372
C10H15N3O5	DB12783	Benserazide	-4.368	-5.519
C11H8Na4O8P2	DB09332	Kappadione	-4.363	-6.987
C18H29NO3	DB09351	Levobetaxolol	-4.353	-4.355
C11H12O8P2	DB14650	Menadiol diphosphate	-4.353	-6.977
C16H14O3	DB08981	Fenbufen	-4.346	-4.347
C22H29FO4	DB08971	Fluocortolone	-4.346	-4.346
C22H30FO8P	DB14669	Betamethasone phosphate	-4.344	-5.684
C16H14N2O3	DB13501	Bendazac	-4.344	-4.344
C24H29N3O8	DB12035	Sarecycline	-4.343	-5.429
C20H25N3S	DB12710	Perazine	-4.343	-4.623
C21H28O2	DB09389	Norgestrel	-4.333	-4.333
C11H13NO4	DB11102	N-acetyltyrosine	-4.329	-4.329
C16H28N2O2	DB13288	Tromantadine	-4.329	-4.342
C10H12ClNO4	DB14656	Chlorphenesin carbamate	-4.327	-4.327

C17H16N2O3	DB09119	Eslicarbazepine acetate	-4.324	-4.324
C14H14N4O4	DB12954	Terizidone	-4.323	-4.323
C15H10Cl2N4O6	DB11632	Opicapone	-4.319	-5.279
C29H38N4O6S	DB09320	Procaine benzylpenicillin	-4.316	-4.316
C21H24O4	DB14083	Bisphenol A diglycidyl ether	-4.316	-4.316
C20H19FN4O4	DB09047	Finaxofloxacin	-4.314	-5.237
C12H14CaO12	DB14483	Calcium ascorbate	-4.313	-4.313
C19H12O8	DB11994	Diacerein	-4.309	-4.309
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-4.308	-5.644
C24H23FN4O3	DB09074	Olaparib	-4.306	-4.306
C10H14O3	DB13583	Mephenesin	-4.303	-4.303
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-4.302	-5.538
C12H14O4	DB11285	Ethyl ferulate	-4.294	-4.295
C16H18N2O7S2	DB12343	Temocillin	-4.288	-4.288
C50H67N7O8	DB09296	Ombitasvir	-4.271	-4.271
C22H27F3O4S	DB13867	Fluticasone	-4.264	-4.264
C20H33N3O3S	DB09097	Quinagolide	-4.256	-4.295
C24H38N2O4	DB11915	Valbenazine	-4.25	-4.498
C13H21N5O4	DB09092	Xanthinol	-4.246	-5.488
C23H29NO3	DB12278	Propiverine	-4.242	-4.25
C14H14O2	DB14120	Phenylethyl resorcinol	-4.235	-4.238
C32H34N4O6	DB11691	Naldemedine	-4.227	-4.618
C18H12ClF3N4O4	DB11943	Delafloxacin	-4.227	-4.271
C40H53N7O5S2	DB09065	Cobicistat	-4.224	-4.754
C25H48N6O10	DB12615	Plazomicin	-4.223	-5.595
C20H28O	DB12474	Lynestrenol	-4.22	-4.22
C3H7Na2O6P	DB09561	Sodium glycerophosphate	-4.218	-4.325
C24H18F2N2O5	DB09280	Lumacaftor	-4.216	-4.216
C21H29O8P	DB14631	Prednisolone phosphate	-4.214	-5.55
C24H29Cl2FO5	DB08973	Fluclorolone acetoneide	-4.208	-4.208
C21H20O6	DB11672	Curcumin	-4.201	-4.544
C35H41N5O5	DB13345	Dihydroergocristine	-4.199	-4.247
C14H18O3	DB09118	Stiripentol	-4.198	-4.198
C18H21N3O	DB13225	Dibenzepin	-4.179	-4.193
C3H6BrNO4	DB13960	Bronopol	-4.179	-4.179
C20H15NO4	DB09219	Bisoxatin	-4.179	-4.183
C25H29NO3	DB11226	Ethylhexyl methoxycrylene	-4.174	-4.174
C10H9N5O	DB11336	Kinetin	-4.174	-4.194
C18H37N5O8	DB13270	Dibekacin	-4.17	-5.712
C11H10FNO2S	DB13228	Flosequinan	-4.165	-4.165
C9H11ClN4O2	DB09343	Tipiracil	-4.165	-4.34
C21H19ClFNO4S	DB11629	Laropiprant	-4.161	-4.163
C13H10N2O3S	DB11115	Ensulizole	-4.157	-4.568
C30H32F6N4O	DB09048	Netupitant	-4.157	-4.183
BH3O3	DB11326	Boric acid	-4.155	-4.155
C23H26FN6O9P	DB12010	Fostamatinib	-4.152	-4.215
C27H36O7	DB14643	Methylprednisolone aceponate	-4.15	-4.15
C16H22N6O4	DB09421	Protirelin	-4.147	-4.781
C19H17F6N7O	DB13874	Enasidenib	-4.145	-4.145
C21H27N	DB09016	Butriptyline	-4.142	-4.143
C15H23N3OS	DB13858	Dimazole	-4.138	-4.158
C49H62N10O16S3	DB09142	Sincalide	-4.136	-6.257
C21H21N3O3	DB12924	Ozenoxacin	-4.135	-4.494
C20H19FN4O4	DB09047	Finaxofloxacin	-4.132	-4.335
C14H22N2O3	DB09069	Trimetazidine	-4.126	-4.528
C25H36O6	DB14540	Hydrocortisone butyrate	-4.113	-4.113
C20H27NO5	DB13279	Carbocromen	-4.111	-4.114
C22H30FO8P	DB14669	Betamethasone phosphate	-4.11	-4.175
C24H29N7O2	DB09073	Palbociclib	-4.109	-4.579
C37H47NO12	DB11753	Rifamycin	-4.109	-6.779
C19H20N4O	DB11793	Niraparib	-4.104	-4.104
C26H26F3N3O3	DB09143	Sonidegib	-4.097	-4.097
C10H14Cl2NO2PS	DB11768	Zytron	-4.095	-4.095

C11H16N8O8	DB14075	Imidurea	-4.095	-5.962
C46H65N13O12S2	DB14642	Lypressin	-4.092	-4.849
C38H50N6O9S	DB11575	Grazoprevir	-4.091	-4.097
C27H33N2O7S2	DB13967	Patent Blue	-4.09	-4.799
HNao3S	DB14015	Sodium bisulfite	-4.09	-4.09
C9H12N2S	DB12667	Protonamide	-4.09	-4.09
C18H37N5O8	DB13270	Dibekacin	-4.087	-4.313
C17H28N2O	DB08987	Etidocaine	-4.087	-4.102
CH6O7P2	DB14159	Oxidronic acid	-4.085	-4.196
CH6O7P2Tc	DB09139	Technetium Tc-99m oxidronate	-4.085	-4.196
C33H57N3O9	DB08965	Fusafungine	-4.08	-4.08
C23H17FN6O	DB11791	Capmatinib	-4.074	-4.08
C27H40O3	DB13943	Testosterone cypionate	-4.072	-4.072
C12H10Ca3O14	DB11093	Calcium Citrate	-4.067	-4.067
C15H12F3NO4S	DB12938	Isoxoflutole	-4.065	-4.065
C21H21N3O3	DB12924	Ozenoxacin	-4.061	-5.769
C12H8BiK5O14	DB09275	Bismuth subcitrate potassium	-4.058	-4.058
C12H14MgO12	DB14484	Magnesium ascorbate	-4.057	-4.057
C12H14N2O7	DB14486	Niacinamide ascorbate	-4.051	-4.051
C8H8O3	DB09543	Methyl salicylate	-4.05	-4.138
C11H9I3N2O4	DB09133	Iothalamic acid	-4.047	-4.047
C59H92O4	DB11340	Ubiquinol	-4.045	-4.045
C7H8O2	DB11359	Guaiaacol	-4.045	-4.045
C49H55N9O7	DB11574	Elbasvir	-4.037	-5.425
C10H12CaN2Na2O8	DB14598	Edetate calcium disodium anhydrous	-4.03	-4.045
C16H14O3	DB09214	Dexketoprofen	-4.03	-4.031
C11H12I3NO2	DB08946	Iopanoic acid	-4.022	-4.022
C15H18I3NO3	DB09340	Tyropanoic acid	-4.02	-4.021
C23H32Cl2NO6P	DB14674	Estramustine phosphate	-4.012	-4.906
C11H16N2O5	DB13421	Edoxudine	-4.011	-4.012
C12H11I3N2O4	DB09346	Metrizoic acid	-3.998	-3.998
C16H22I2N6O4S	DB09546	Iobenguane sulfate I-123	-3.986	-3.986
CH6O6P2	DB14078	Medronic acid	-3.983	-4.296
CH6O8P2Tc	DB09138	Technetium Tc-99m medronate	-3.983	-4.296
C65H90N14O19S2	DB14554	Dotatate	-3.978	-5.719
C18H27NO3	DB09120	Zucapsaicin	-3.976	-3.976
C32H35N5O5	DB09272	Eluxadoline	-3.975	-5.268
C18H24Fe4O42P6	DB13995	Ferric pyrophosphate citrate	-3.973	-3.973
C21H35N2O3	DB09376	Lapyrium	-3.969	-3.969
C26H33NO6	DB09236	Lacidipine	-3.962	-3.962
C21H45N3	DB08958	Hexetidine	-3.962	-4.355
C25H31NO6	DB11921	Deflazacort	-3.96	-3.961
C21H19FN6O2	DB12130	Lorlatinib	-3.959	-4.454
C28H22ClF3N6O3	DB14568	Ivosidenib	-3.957	-3.957
C15H9FO2	DB13136	Fluindione	-3.957	-3.958
C19H20Br2N6O4S	DB08932	Macitentan	-3.952	-4.694
C14H27N3O2	DB13247	Pramiracetam	-3.949	-3.953
C8H14CaO10	DB11168	Calcium threonate	-3.943	-3.943
C29H44N8O3	DB12141	Gilteritinib	-3.935	-6.195
C22H24N2O2	DB09488	Acrivastine	-3.932	-3.938
C12H10O14Zn3	DB11154	Zinc citrate	-3.929	-3.929
C6H5Na3O7	DB09154	Sodium citrate	-3.929	-3.929
C14H27NaO5S	DB13157	Sodium lauryl sulfoacetate	-3.926	-3.926
C25H26F6N2O2	DB09291	Rolapitant	-3.926	-5.142
C14H12O4	DB11221	Dioxybenzone	-3.912	-3.974
C12H24N2O4S2	DB11164	Bicisate	-3.91	-4.151
C24H34O5	DB11622	Dehydrocholic acid	-3.909	-3.913
C6H10O4	DB09401	Isosorbide	-3.908	-3.908
C24H30ClN7O4S	DB09075	Edoxaban	-3.903	-4.573
C27H30Cl2O6	DB14512	Mometasone furoate	-3.903	-3.903
C21H28O2	DB09070	Tibolone	-3.9	-3.9
C32H35N5O5	DB09272	Eluxadoline	-3.895	-4.622
C22H26ClFO4	DB13158	Clobetasone	-3.888	-3.888

C28H37N3O3	DB11591	Bilastine	-3.883	-3.925
C18H22N2	DB14196	N-Cyclohexyl-N'-phenyl-1,4-phenylenediamine	-3.882	-4.08
C49H55N9O7	DB11574	Elbasvir	-3.875	-5.286
C6H11FeNO7	DB09501	Ferric ammonium citrate	-3.874	-3.874
C20H26O2	DB09371	Norethynodrel	-3.868	-3.868
C15H20O3	DB13063	Parthenolide	-3.865	-3.865
C29H50O2	DB14476	DL-alpha-Tocopherol	-3.865	-3.865
C31H41N5O5	DB11273	Dihydroergocornine	-3.861	-3.904
C14H12ClNO2	DB09216	Tolfenamic Acid	-3.858	-3.859
CH6O6P2	DB14078	Medronic acid	-3.856	-4.382
C18H22N2S	DB09068	Vortioxetine	-3.855	-3.862
C21H15F4N5O2S	DB11901	Apalutamide	-3.849	-3.849
C10H13N3O2	DB13211	Guanoxan	-3.843	-3.843
C26H32N4O4S	DB11362	Selexipag	-3.842	-3.847
C20H23ClN2O4	DB09555	Dexchlorpheniramine maleate	-3.839	-3.839
C26H26ClN3	DB11614	Rupatadine	-3.83	-3.953
O7P2Tc	DB09165	Technetium Tc-99m pyrophosphate	-3.828	-4.061
C23H32O2	DB09124	Medrogestone	-3.827	-3.827
C7H6Cl2O	DB13269	Dichlorobenzyl alcohol	-3.824	-3.824
C27H32F2N8	DB12001	Abemaciclib	-3.818	-4.02
C8H8O3	DB13218	Mandelic acid	-3.815	-3.815
C20H19FN4O4	DB09047	Finafloxacin	-3.815	-6.185
C13H14Cl2O3	DB09064	Ciprofibrate	-3.814	-3.814
C25H27N3O2S	DB09128	Brexiprazole	-3.812	-3.948
C27H23F2N3O7S	DB13997	Baloxavir marboxil	-3.811	-3.811
C9H10O4	DB11323	Glycol salicylate	-3.811	-3.812
C3H7CaO6P	DB11264	Calcium glycerophosphate	-3.809	-3.914
C26H23N7O2	DB11703	Acalabrutinib	-3.803	-3.817
C17H26N4O3S2	DB08966	Fursultiamine	-3.803	-3.895
C23H36O3	DB14655	Drostanolone propionate	-3.793	-3.793
C27H42Cl2N2O6	DB14658	Chloramphenicol palmitate	-3.778	-3.778
C27H38O6	DB14632	Prednisolone tebutate	-3.776	-3.776
C27H18InN3O3	DB09473	Indium In-111 oxyquinoline	-3.775	-3.793
C22H32N2O2	DB12313	Dopexamine	-3.774	-3.774
C18H14Cl4N2O	DB08943	Isoconazole	-3.773	-4.496
C22H17F2N5OS	DB11633	Isavuconazole	-3.771	-3.771
C12H14O12Zn	DB14485	Zinc ascorbate	-3.753	-3.753
C6H7NaO6	DB14482	Sodium ascorbate	-3.753	-3.753
C12H14FeO12	DB14490	Ferrous ascorbate	-3.748	-3.748
C28H41N3O3	DB12532	Oxetacaine	-3.741	-5.055
C21H34O2	DB11859	Brexanolone	-3.74	-3.74
C17H14BrN3O2S	DB11560	Lesinurad	-3.736	-3.736
C14H22N2O3	DB09069	Trimetazidine	-3.734	-4.189
C19H21NS	DB09167	Dosulepin	-3.732	-3.736
C32H55N4O	DB09552	Thonzonium	-3.726	-3.726
C17H15BrF2N4O3	DB11967	Binimetinib	-3.725	-6.233
C20H41N5O7	DB13274	Micronomicin	-3.717	-5.328
C15H26O	DB13153	Levomenol	-3.717	-3.717
C10H22O3	DB13163	Terpin hydrate	-3.714	-3.714
C26H38O4	DB14677	Gestonorone caproate	-3.712	-3.712
C22H28ClFO4	DB11750	Clobetasol	-3.709	-3.709
C10H11I2NO3	DB09366	Propylidone	-3.708	-3.708
C11H12N2OS2	DB14202	Morpholinylmercaptobenzothiazole	-3.708	-3.708
C10H15NO2	DB11610	Oxilofrine	-3.707	-3.719
C9H7NO	DB11145	Oxyquinoline	-3.707	-3.725
C30H50O2	DB14555	Ursadiol	-3.705	-3.705
C36H84O10P4Tc	DB09160	Technetium Tc-99m tetrofosmin	-3.705	-4.298
C10H13NO4S2	DB13284	Meticrane	-3.704	-3.705
C21H20O6	DB11672	Curcumin	-3.701	-4.934
C27H42NO2	DB11125	Benzethonium	-3.696	-3.696
C12H12N4O3	DB11989	Benznidazole	-3.691	-3.691
C16H16N4O	DB14753	Hydroxystilbamidine	-3.688	-3.688
C13H16ClNO	DB11823	Esketamine	-3.682	-3.786

C12H18O2	DB11254	Hexylresorcinol	-3.681	-3.682
C10H8BrNO	DB13222	Tilbroquinol	-3.68	-3.886
C29H34NO2	DB09076	Umeclidinium	-3.674	-3.674
C14H18O	DB14175	alpha-Amyl cinnamaldehyde	-3.674	-3.674
C25H35NO5	DB12554	Mebeverine	-3.674	-3.677
C4H4Na2O6	DB13707	Sodium tartrate	-3.67	-3.67
C18H37N5O8	DB13270	Dibekacin	-3.669	-5.235
C12H18O3	DB11299	Vanillyl butyl ether	-3.668	-3.669
C17H26N2O4S	DB13273	Sultopride	-3.666	-3.667
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-3.663	-5.293
C7H8O2	DB09516	Mequinol	-3.663	-3.663
C44H32N4O4	DB11630	Temoporfin	-3.662	-3.662
C10H12O2	DB14188	Isoeugenol	-3.661	-3.662
C26H41BrNO4	DB09090	Pinaverium	-3.651	-3.651
C30H29ClN6O3	DB11828	Neratinib	-3.649	-3.831
C6H10N2O2	DB09210	Piracetam	-3.646	-3.646
C10H14N2Na2O8	DB14600	Edetate disodium anhydrous	-3.643	-3.657
C38H73N21O10S2	DB12865	Etelcalcetide	-3.642	-3.657
C29H33FN2O4	DB09030	Vorapaxar	-3.639	-3.65
C27H26ClF3N6O3	DB12095	Telotristat ethyl	-3.634	-4.072
C5H7N3	DB11640	Amifampridine	-3.632	-3.635
C27H32F2N8	DB12001	Abemaciclib	-3.617	-4.436
C45H54F2N4O8	DB11641	Vinflunine	-3.614	-4.975
C25H26F6N2O2	DB09291	Rolapitant	-3.603	-3.684
C26H27N3O5S	DB09183	Dasabuvir	-3.603	-3.613
C17H20N2O2	DB11699	Tropisetron	-3.593	-3.598
C18H22O	DB11219	Enzacamene	-3.584	-3.584
C18H12ClF3N4O4	DB11943	Delafloxacin	-3.581	-5.147
C23H23ClN6O2	DB09034	Suvorexant	-3.57	-3.57
C15H18N2	DB14195	4-(Isopropylamino)diphenylamine	-3.566	-3.838
C20H19FN8O2	DB08931	Riociguat	-3.565	-3.567
C17H24O3	DB11201	Menthyl salicylate	-3.564	-3.565
C21H18ClNO6	DB13783	Acemetacin	-3.559	-3.559
C17H16FN6O6P	DB09042	Tedizolid phosphate	-3.549	-4.742
C40H53N7O5S2	DB09065	Cobicistat	-3.541	-3.853
C57H65F5N10O8	DB13878	Pibrentasvir	-3.538	-4.053
C6H6O2	DB11085	Resorcinol	-3.537	-3.541
C18H21NO	DB11584	Pipradrol	-3.535	-3.539
C13H18O2	DB09213	Dexibuprofen	-3.526	-3.527
C9H13NO	DB09352	Hydroxyamphetamine	-3.522	-3.522
C15H24N2O2	DB09085	Tetracaine	-3.52	-3.53
C19H27NO3	DB12161	Deutetabenazine	-3.517	-3.567
C36H84O10P4Tc	DB09160	Technetium Tc-99m tetrofosmin	-3.514	-4.06
C35H43N5O4	DB11855	Revefenacin	-3.513	-3.585
C14H30O4S	DB11328	Tetradecyl hydrogen sulfate (ester)	-3.511	-3.511
C26H26N2O6S	DB09319	Carindacillin	-3.505	-3.753
C18H24N2O5	DB09477	Enalaprilat	-3.499	-4.475
C13H10N2O3S	DB11115	Ensulizole	-3.494	-4.061
C17H16FN6O6P	DB09042	Tedizolid phosphate	-3.492	-3.577
C18H24NO4	DB11315	Methscopolamine	-3.492	-3.492
C25H25F3N4O6	DB11637	Delamanid	-3.49	-3.501
C20H41N5O7	DB13274	Micronomicin	-3.49	-5.007
C23H28N8O4	DB12483	Copanlisib	-3.49	-3.905
C22H27ClFN7O4S	DB11718	Encorafenib	-3.486	-3.875
AlO4P	DB14517	Aluminium phosphate	-3.48	-5.089
HNa2O4P	DB14502	Sodium phosphate, dibasic	-3.48	-5.089
CaH5O6P	DB14481	Calcium phosphate dihydrate	-3.48	-5.089
Ca3O8P2	DB11348	Calcium Phosphate	-3.48	-5.089
H2NaO4P	DB09449	Sodium phosphate, monobasic	-3.48	-5.089
HK2O4P	DB09414	Dipotassium phosphate	-3.48	-5.089
H2KO4P	DB09413	Monopotassium phosphate	-3.48	-5.089
H3O4P	DB09394	Phosphoric acid	-3.48	-5.089
C24H31N3OS	DB13213	Butaperazine	-3.477	-4.087

C30H44N2O10	DB13265	Hexobendine	-3.47	-6.002
C15H19BrN2O5Tc	DB09137	Technetium Tc-99m mebprofenin	-3.469	-3.514
C15H20O3	DB11207	Amiloxate	-3.461	-3.461
C19H15F3N2O3	DB12020	Tecovirimat	-3.46	-3.46
C12H17NO3	DB13346	Bufexamac	-3.456	-3.461
C19H14F2N6O	DB11760	Talazoparib	-3.454	-3.454
C18H40O4P2	DB11180	Tetrofosmin	-3.452	-4.045
C18H26O3	DB09496	Octinoxate	-3.452	-3.452
C17H27NO3	DB09345	Pramocaine	-3.438	-3.838
C11H11ClO3	DB13167	Alclofenac	-3.438	-3.438
C17H28O5	DB13851	Artemotil	-3.437	-3.437
C19H31N	DB12728	Fenpropidin	-3.434	-3.435
C18H21ClN2	DB08936	Chlorcyclizine	-3.43	-3.824
C24H39N3O3Si3	DB11585	Drometrizole trisiloxane	-3.428	-3.428
C49H55N9O7	DB11574	Elbasvir	-3.425	-4.793
C18H18ClN3S	DB13256	Clothiapine	-3.425	-3.458
C21H46NO4P	DB09031	Miltefosine	-3.423	-3.423
C12H17NO3	DB13278	Bucetin	-3.423	-3.423
C13H19NO3	DB09185	Viloxazine	-3.422	-3.445
CH6O7P2	DB14159	Oxidronic acid	-3.416	-4.461
CH6O7P2Tc	DB09139	Technetium Tc-99m oxidronate	-3.416	-4.461
C6H5ClO	DB13154	Parachlorophenol	-3.414	-3.417
C20H19FN4O4	DB09047	Finafloxacin	-3.411	-5.073
C21H21N3O3	DB12924	Ozenoxacin	-3.409	-5.457
C32H34N4O6	DB11691	Naldemedine	-3.401	-3.925
C18H15NO8S2	DB09268	Picosulfuric acid	-3.399	-3.411
C19H22F3N5O2S	DB12015	Alpelisib	-3.398	-3.398
C31H35F6N4O5P	DB14019	Fosnetupitant	-3.395	-3.416
C20H41N5O7	DB13274	Micronomicin	-3.393	-3.577
C12H17NO	DB11282	Diethyltoluamide	-3.392	-3.392
H2O3S2	DB09499	Thiosulfuric acid	-3.387	-3.387
C8H9ClO	DB11121	Chloroxylenol	-3.386	-3.387
C17H21NO	DB11160	Phenyltoloxamine	-3.384	-3.404
C29H40N4O7	DB12455	Omadacycline	-3.383	-5.321
C10H7Cl2NO	DB13306	Chlorquinaldol	-3.382	-4.172
C4H9Al2ClN4O7	DB11205	Alcloxa	-3.38	-3.654
C8H11NO5S	DB09324	Sulbactam	-3.379	-3.379
CH6O8P2Tc	DB09138	Technetium Tc-99m medronate	-3.379	-3.906
C28H27N3O3	DB13931	Netarsudil	-3.375	-5.737
C7H7BrN4O2	DB14018	Bromotheophylline	-3.374	-3.405
C27H33N2	DB11279	Brilliant green cation	-3.371	-3.586
C31H33N5O4	DB09079	Nintedanib	-3.368	-4.223
C21H19FN6O2	DB12130	Lorlatinib	-3.362	-3.699
C20H38O7S	DB11089	Docusate	-3.361	-3.361
C12H13I3N2O2	DB09333	Iopodic acid	-3.356	-3.438
C19H30O5	DB09350	Piperonyl butoxide	-3.356	-3.356
C18H14Cl4N2O	DB08943	Isoconazole	-3.341	-3.548
C38H74NaO10P	DB14105	Sodium 1,2-Dipalmitoyl-sn-glycero-3-phospho-	-3.337	-3.337
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-3.334	-5.15
C27H36N2O5	DB09083	Ivabradine	-3.329	-3.33
C45H54F2N4O8	DB11641	Vinflunine	-3.323	-5.54
C13H12N2O3S	DB09355	Sulfabenzamide	-3.321	-3.321
C13H16N2S2	DB14200	Thiohexam	-3.319	-3.319
C19H18FN3O	DB12332	Rucaparib	-3.314	-3.329
C10H12O2	DB09086	Eugenol	-3.311	-3.311
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-3.31	-5.086
C40H77O10P	DB11331	1-Palmitoyl-2-oleoyl-sn-glycero-3-(phospho-rac	-3.309	-3.309
C32H35N5O5	DB09272	Eluxadoline	-3.307	-4.739
C23H30N8O	DB11730	Ribociclib	-3.305	-3.374
C3H7Na2O6P	DB09561	Sodium glycerophosphate	-3.296	-4.363
C14H8N2S4	DB14201	2,2'-Dibenzothiazyl disulfide	-3.292	-3.292
C14H10O4	DB09096	Benzoyl peroxide	-3.289	-3.289
C4H6O4S2	DB14089	Dimercaptosuccinic acid	-3.288	-3.288

C21H23BrFNO2	DB12401	Bromperidol	-3.288	-3.301
C12H10Mg3O14	DB11110	Magnesium citrate	-3.28	-3.28
C23H36N2O4	DB09039	Eliglustat	-3.277	-5.961
C8H9FN2O3	DB09256	Tegafur	-3.277	-3.306
C11H18N2O9	DB12362	Diaminopropanol tetraacetic acid	-3.264	-4.694
C29H28F4N4O4	DB12070	Letermovir	-3.264	-3.264
C24H38N2O4	DB11915	Valbenazine	-3.262	-3.937
C10H14N2O4	DB13253	Proxibarbal	-3.261	-4.577
C12H13FN4O5	DB09327	Tegafur-uracil	-3.252	-3.281
C49H54N8O8	DB11613	Velpatasvir	-3.252	-4.637
C21H22N6O	DB11978	Glasdegib	-3.251	-4.283
C57H65F5N10O8	DB13878	Pibrentasvir	-3.239	-4.382
C13H18ClN3O4S2	DB13532	Cyclopenothiazide	-3.234	-3.244
C49H54N8O8	DB11613	Velpatasvir	-3.233	-3.837
C10H20O2	DB14187	Hydroxycitronellal	-3.231	-3.231
C8H10N6	DB12945	Dihydralazine	-3.231	-3.604
C16H23NO2	DB08988	Ethoheptazine	-3.23	-3.236
C12H19NO	DB11587	Etafedrine	-3.224	-3.275
C10H8OS3	DB13853	Anethole trithione	-3.221	-3.221
C25H46N	DB11583	Cetalkonium	-3.22	-3.22
C21H22N6O	DB11978	Glasdegib	-3.22	-3.846
C50H68N14O10	DB11653	Bremelanotide	-3.22	-4.031
C7H10O6S3	DB13267	Ritiometan	-3.218	-3.219
C14H9Cl3N2OS	DB12245	Triclabendazole	-3.218	-3.399
C16H22N4O	DB11235	Thonzylamine	-3.215	-3.22
C10H14N2O2	DB14754	Solriamfetol	-3.213	-3.231
C20H31NO3	DB11186	Pentoxifyverine	-3.211	-3.218
C11H15NO2	DB11148	Butamben	-3.21	-3.21
C6H10CaO6	DB13231	Calcium lactate	-3.208	-3.208
C3H5KO3	DB09483	Potassium lactate	-3.208	-3.208
C10H14N2O4	DB13253	Proxibarbal	-3.206	-3.351
C14H19N3O	DB13216	Oxolamine	-3.206	-3.223
C10H12O4	DB12328	Cantharidin	-3.203	-3.203
C20H22O3	DB09495	Avobenzone	-3.201	-3.482
C4H6N4O3	DB11100	Allantoin	-3.199	-3.469
C21H18F3N3O5	DB11799	Bictegravir	-3.198	-5.166
C23H32Cl2NO6P	DB14674	Estramustine phosphate	-3.192	-3.341
C8H10O2	DB11304	Phenoxyethanol	-3.186	-3.186
C16H10N2O8S2	DB11577	Indigotindisulfonic Acid	-3.183	-3.183
C20H2Br4Cl4Na2O5	DB13911	Phloxine B	-3.179	-3.18
C9H10O	DB14186	Cinnamyl alcohol	-3.169	-3.169
C31H41N5O5	DB11273	Dihydroergocornine	-3.166	-4.904
C14H11Cl2NO4	DB14638	Diloxanide furoate	-3.162	-3.162
C22H23NO4S2	DB13166	Zofenopril	-3.156	-3.156
C9H5I2NO	DB09115	Diiodohydroxyquinoline	-3.153	-3.732
C8H8O2	DB09269	Phenylacetic acid	-3.149	-3.15
C20H4Cl4I4O5	DB11182	Rose bengal free acid	-3.144	-3.149
C18H12Cl2N2O	DB12792	Boscalid	-3.139	-3.139
C24H45BiO6	DB13910	Valproate bismuth	-3.138	-3.14
C7H6BFO2	DB09041	Tavaborole	-3.132	-3.132
C27H34N4O	DB12492	Piritramide	-3.132	-4.728
C6H6O2	DB09526	Hydroquinone	-3.124	-3.124
C3H8O3	DB09462	Glycerin	-3.121	-3.121
C30H29ClN6O3	DB11828	Neratinib	-3.119	-4.022
C24H29NO5	DB09292	Sacubitril	-3.114	-5.328
C14H12O3	DB14176	Benzylparaben	-3.106	-3.13
C17H25NO2	DB11096	Meradimate	-3.104	-3.104
C18H40O4P2	DB11180	Tetrofosmin	-3.103	-3.649
C43H49N2O6S2	DB09374	Indocyanine green acid form	-3.1	-3.1
C12H20N2S4	DB14174	Dipentamethylenethiuram disulfide	-3.096	-3.096
C17H27NO2	DB11570	Padimate O	-3.092	-3.092
C22H23ClN2O8	DB09093	Chlortetracycline	-3.091	-3.227
C19H23N4O6PS	DB11748	Benfotiamine	-3.09	-5.415

C65H90N14O19S2	DB14554	Dotatate	-3.09	-4.863
C16H24N2	DB08944	Isoaminile	-3.081	-3.107
C22H27CIFN7O4S	DB11718	Encorafenib	-3.076	-3.51
C25H48N6O10	DB12615	Plazomicin	-3.075	-5.641
C3H7CaO6P	DB11264	Calcium glycerophosphate	-3.072	-4.15
C9H10O3	DB13628	Ethyl hydroxybenzoate	-3.071	-3.089
C32H39NO2	DB11742	Ebastine	-3.07	-3.078
C9H16N2O2	DB13221	Apronalide	-3.068	-3.068
C24H29N3O8	DB12035	Sarecycline	-3.058	-3.17
C18H33NO3	DB11272	Methyl undecenoyl leucinate	-3.057	-3.057
C9H11CIN4O2	DB09343	Tipiracil	-3.056	-3.864
C9H5I2NO	DB09115	Diiodoxyhydroxyquinoline	-3.055	-3.334
C8H9N3O4	DB09220	Nicorandil	-3.054	-3.054
C40H52F4N6O9S	DB12026	Voxilaprevir	-3.053	-3.056
C4H4FeO4	DB14489	Ferrous succinate	-3.042	-3.042
C21H24O2	DB11619	Gestrinone	-3.039	-3.039
C7H11N3O3	DB12834	Secnidazole	-3.038	-3.038
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-3.027	-4.768
C21H35NO	DB09056	Amorolfine	-3.026	-3.833
C27H26CIF3N6O3	DB12095	Telotristat ethyl	-3.024	-3.46
C6H18O4Si3	DB09512	Simethicone	-3.02	-3.02
C14H23N3O10	DB14007	Pentetic acid	-3.015	-5.192
C14H20InN3O10	DB09425	Indium In-111 pentetate	-3.015	-5.192
C40H50N8O6	DB09102	Daclatasvir	-3.014	-4.296
C14H20Br2N2	DB09019	Bromhexine	-3.012	-3.035
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-3.012	-4.854
C21H18F3N3O5	DB11799	Bictegravir	-3.004	-3.528
C21H35NO	DB09056	Amorolfine	-3.002	-3.178
C57H65F5N10O8	DB13878	Pibrentasvir	-3.002	-4.626
C10H12O3	DB14177	Propylparaben	-2.995	-3.012
C17H26N4O3S2	DB08966	Fursultiamine	-2.994	-4.141
C24H30CIN7O4S	DB09075	Edoxaban	-2.994	-3.224
C32H34N4O6	DB11691	Naldemedine	-2.993	-4.88
C6H6Br2N2	DB14199	Bromothalonil	-2.989	-2.989
C17H15ClO4	DB13873	Fenofibric acid	-2.988	-2.988
C14H9Cl2N3S2	DB08933	Luliconazole	-2.987	-2.987
C22H19NO4	DB09020	Bisacodyl	-2.984	-2.996
C23H30N2O4	DB09209	Pholcodine	-2.977	-4.577
C13H9Cl3N2O	DB11155	Triclocarban	-2.97	-2.97
C12H24N2O4S2	DB11164	Bicisate	-2.963	-3.717
C5H4ClNO2	DB09257	Gimeracil	-2.962	-2.962
C32H43N5O5	DB11275	Epicriptine	-2.96	-4.698
C16H18CIN3S	DB09241	Methylene blue	-2.955	-2.973
C11H14CIN5	DB14763	Cycloguanil	-2.947	-3.398
C17H19NO	DB12293	Nefopam	-2.946	-2.998
C21H18F3N3O5	DB11799	Bictegravir	-2.939	-3.293
C10H30O5Si5	DB11244	Cyclomethicone 5	-2.935	-2.935
C9H8N2	DB12537	Benzodiazepine	-2.934	-2.934
C12H17NO3	DB12911	Nicoboxil	-2.931	-2.931
C18H26N2O5Tc	DB09164	Technetium Tc-99m disofenin	-2.924	-4.466
C18H12CrN3O6	DB14529	Chromium nicotinate	-2.924	-2.934
C41H50N6O2	DB11262	Bisotrizole	-2.919	-2.938
C6H8N2	DB14141	p-Phenylenediamine	-2.916	-3.041
C16H26N2O3	DB09342	Propoxycaine	-2.906	-2.927
C12H18IN	DB09480	Iofetamine I-123	-2.905	-2.905
C49H55N9O7	DB11574	Elbasvir	-2.901	-4.293
C13H15N3O4S	DB14033	Acetyl sulfisoxazole	-2.901	-2.901
C17H26CINO	DB11642	Pitolisant	-2.9	-2.901
C20H33N3O3S	DB09097	Quinagolide	-2.881	-4.902
C29H39CIN7O2P	DB12267	Brigatinib	-2.876	-5.124
C49H54N8O8	DB11613	Velpatasvir	-2.874	-4.371
C11H17NO	DB13624	Methoxyphenamine	-2.862	-2.862
C13H20N2O3S	DB09009	Articaine	-2.849	-2.899

C10H14CaO6	DB13800	Calcium levulinate	-2.849	-2.851
C27H33N2O6S2	DB09136	Isosulfan blue	-2.84	-3.054
C11H18N2O9	DB12362	Diaminopropanol tetraacetic acid	-2.84	-5.087
C24H25ClFN5O2	DB11963	Dacomitinib	-2.826	-4.108
C62H80InN12O19S2	DB11835	Indium In-111 pentetreotide	-2.816	-4.603
CK2O3	DB13977	Potassium carbonate	-2.815	-3.858
CNa2O3	DB09460	Sodium carbonate	-2.815	-3.858
CLi2O3	DB14509	Lithium carbonate	-2.814	-3.858
CH24Al2Mg6O24	DB13322	Hydrotalcite	-2.814	-3.858
CHKO3	DB11098	Potassium bicarbonate	-2.814	-3.858
CMgO3	DB09481	Magnesium carbonate	-2.814	-3.858
C4H7NaO3	DB09072	Sodium oxybate	-2.811	-2.813
C31H35F6N4O5P	DB14019	Fosnetupitant	-2.806	-4.787
C26H32N2O8	DB13711	Tritoqualine	-2.796	-2.962
C27H31FN4O8	DB12329	Eravacycline	-2.795	-2.929
C15H23N3OS	DB13858	Dimazole	-2.794	-4.807
C25H24N6O2	DB09053	Ibrutinib	-2.787	-2.787
C24H29N7O2	DB09073	Palbociclib	-2.783	-3.189
C18H37N5O8	DB13270	Dibekacin	-2.779	-4.531
C10H18O	DB14183	Geraniol	-2.777	-2.777
C17H15NO5	DB13657	Benorilate	-2.776	-2.776
C10H7Cl2NO	DB13306	Chlorquinaldol	-2.775	-2.957
C28H34O8S2	DB09534	Ecamsule	-2.767	-2.767
C11H17NO	DB11278	DL-Methylephedrine	-2.757	-2.849
C13H16ClNO	DB11823	Esketamine	-2.752	-3.834
C22H18FN7O	DB09054	Idelalisib	-2.747	-4.744
C35H38N4O6	DB09238	Manidipine	-2.742	-2.883
C33H54O5	DB14001	alpha-Tocopherol succinate	-2.739	-2.739
C20H22O3	DB09495	Avobenzon	-2.729	-3.993
C12H8N2O4Zn	DB11175	Zinc picolinate	-2.727	-2.737
O7P2Tc	DB09165	Technetium Tc-99m pyrophosphate	-2.727	-3.428
C8H17FeN3O6S2	DB11197	Ferrous cysteine glycinate	-2.719	-2.733
C4H7Cl3O	DB11386	Chlorobutanol	-2.717	-2.717
C2H6O3S2	DB09110	Coenzyme M	-2.715	-2.717
C18H26N2O5Tc	DB09164	Technetium Tc-99m disofenin	-2.714	-2.76
C21H24N2	DB13246	Quinupramine	-2.712	-2.712
C2H7N5	DB13100	Biguanide	-2.709	-2.713
C20H25N3S	DB12710	Perazine	-2.707	-3.316
C8H8O3	DB14212	Methylparaben	-2.702	-2.726
C12H9NO2	DB12300	P-nitrobiphenyl	-2.69	-2.69
C12H19NO4	DB14006	Choline salicylate	-2.681	-2.681
C5H14NO	DB09563	Choline C-11	-2.681	-2.681
C5H14ClNO	DB09277	Choline C 11	-2.681	-2.681
C31H38O7	DB11260	Diacetyl benzoyl lathyrol	-2.677	-2.677
C4H4ClNOS	DB14197	Methylchloroisothiazolinone	-2.675	-2.675
C21H45N3	DB08958	Hexetidine	-2.659	-3.092
C11H14N2S	DB11156	Pyrantel	-2.656	-2.656
C15H19BrN2O5Tc	DB09137	Technetium Tc-99m mebprofenin	-2.654	-4.196
C22H40NO	DB11594	Domiphen	-2.654	-2.654
C10H15N	DB09571	Levmetamfetamine	-2.652	-2.652
C10H16O	DB14156	Synthetic camphor	-2.642	-2.642
C10H10N2O	DB12243	Edaravone	-2.635	-2.987
C18H30O2	DB13854	Gamolenic acid	-2.627	-2.631
C15H18N2	DB14195	4-(Isopropylamino)diphenylamine	-2.617	-3.208
C19H27NO3	DB12161	Deutetrabenazine	-2.614	-4.109
C14H12O4	DB11221	Dioxybenzone	-2.613	-4.511
C9H14N4O4	DB09282	Molsidomine	-2.613	-2.613
C32H43N5O5	DB11274	Dihydro-alpha-ergocryptine	-2.608	-5.036
C17H27NO3	DB09345	Pramocaine	-2.605	-3.026
C14H21NO2	DB09088	Amylocaine	-2.601	-2.613
C9H12ClN5O	DB09242	Moxonidine	-2.6	-2.667
C18H21N3O	DB13225	Dibenzepin	-2.596	-4.807
C38H46F4N6O9S	DB13879	Glecaprevir	-2.595	-2.598

C24H38N2O4	DB11915	Valbenazine	-2.59	-5.027
C32H35N5O5	DB09272	Eluxadolone	-2.588	-3.861
S8Tc	DB09397	Technetium Tc-99m sulfur colloid	-2.582	-2.582
S8	DB09353	Octasulfur	-2.582	-2.582
C14H12O6S	DB11185	Sulisobenzone	-2.579	-4.204
C4H2FeO4	DB14491	Ferrous fumarate	-2.577	-2.577
AlO4P	DB14517	Aluminium phosphate	-2.564	-2.604
HNa2O4P	DB14502	Sodium phosphate, dibasic	-2.564	-2.604
CaH5O6P	DB14481	Calcium phosphate dihydrate	-2.564	-2.604
Ca3O8P2	DB11348	Calcium Phosphate	-2.564	-2.604
H2NaO4P	DB09449	Sodium phosphate, monobasic	-2.564	-2.604
HK2O4P	DB09414	Dipotassium phosphate	-2.564	-2.604
H2KO4P	DB09413	Monopotassium phosphate	-2.564	-2.604
H3O4P	DB09394	Phosphoric acid	-2.564	-2.604
C27H26ClF3N6O3	DB12095	Telotristat ethyl	-2.563	-4.835
C16H19NO2	DB13219	Medifoxamine	-2.561	-3.028
C9H15NO2	DB13262	Aceclidine	-2.553	-2.555
C11H17NO	DB11278	DL-Methylephedrine	-2.551	-3.699
C34H53NO11	DB09049	Naloxegol	-2.546	-5.093
C10H8BrNO	DB13222	Tilbroquinol	-2.54	-3.265
C7H6O3	DB11268	Protocatechualdehyde	-2.535	-3.601
C22H24FN3O2	DB12867	Benperidol	-2.516	-2.533
C9H8O	DB14184	Cinnamaldehyde	-2.513	-2.513
C14H12O4	DB11221	Dioxybenzone	-2.509	-4.215
C30H26N2O13	DB11184	Oftasceine	-2.508	-3.781
C20H17F3N2O4	DB08976	Floctafenine	-2.504	-4.714
C30H34N4O2	DB11363	Alectinib	-2.503	-2.656
C21H22N6O	DB11978	Glasdegib	-2.5	-2.939
C23H22CIN5O3	DB12364	Betrixaban	-2.487	-2.488
C49H54F2N8O6	DB09027	Ledipasvir	-2.482	-3.632
C5H11NO2S	DB13972	Racemethionine	-2.465	-2.465
C13H10N2O3S	DB11115	Ensulizole	-2.459	-3.736
C3H4O2	DB09348	Propiolactone	-2.452	-2.452
C6H12N2S4	DB13245	Thiram	-2.449	-2.449
C5H8FN02	DB13146	Fluciclovine (18F)	-2.448	-2.448
C29H44N8O3	DB12141	Gilteritinib	-2.444	-5.136
C45H50CIN7O7S	DB11581	Venetoclax	-2.429	-2.44
C14H9Cl3N2OS	DB12245	Triclabendazole	-2.426	-3.223
C40H80NO8P	DB09114	Colfosceril palmitate	-2.417	-2.417
C20H24N	DB13720	Diphemanil	-2.417	-2.417
B4Na2O7	DB14505	Sodium borate	-2.407	-2.407
C3H3F5	DB13117	Pentafluoropropane	-2.405	-2.405
C13H20N2O3S	DB09009	Articaine	-2.397	-3.892
C18H21CIN2	DB08936	Chlorcyclizine	-2.396	-2.864
O2Si	DB11132	Silicon dioxide	-2.391	-2.391
C32H48O4	DB13955	Estradiol dianthate	-2.384	-2.384
C9H19NO4	DB09357	Dexpanthenol	-2.381	-2.381
C49H54F2N8O6	DB09027	Ledipasvir	-2.375	-4.619
C40H50N8O6	DB09102	Daclatasvir	-2.372	-3.494
C22H24FN3O2	DB12867	Benperidol	-2.37	-4.506
C30H34N4O2	DB11363	Alectinib	-2.369	-3.249
C23H30N2O4	DB09209	Pholcodine	-2.368	-3.841
FNa2O3P	DB09484	Sodium fluorophosphate	-2.368	-2.386
C20H22O3	DB09495	Avobenzon	-2.363	-3.58
C18H22N2	DB14196	N-Cyclohexyl-N'-phenyl-1,4-phenylenediamine	-2.358	-3.104
C40H50N8O6	DB09102	Daclatasvir	-2.356	-3.196
Al2ClH7O6	DB11573	Aluminum chlorohydrate	-2.342	-2.342
H8O4Tc	DB09314	Technetium Tc-99m pertechnetate	-2.342	-2.342
H2O	DB09145	Water	-2.342	-2.342
C49H54F2N8O6	DB09027	Ledipasvir	-2.325	-3.581
C32H43N5O5	DB11275	Epicriptine	-2.316	-4.737
C12H13I3N2O2	DB09333	Iopodic acid	-2.311	-3.524
C24H25ClFN5O2	DB11963	Dacomitinib	-2.311	-4.06

C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-2.31	-4.074
C7H7NO2	DB13882	Methyl nicotinate	-2.303	-2.303
C4H6N4O3	DB11100	Allantoin	-2.301	-3.957
C20H19F2N3O5	DB08930	Dolutegravir	-2.279	-4.247
C4H10O2	DB14110	Butylene glycol	-2.279	-2.279
C7H16N4O4S2	DB12473	Taurolidine	-2.278	-2.853
C22H23ClN2O8	DB09093	Chlortetracycline	-2.27	-3.518
C19H18FN3O	DB12332	Rucaparib	-2.264	-4.449
C49H54N8O8	DB11613	Velpatasvir	-2.26	-3.411
C18H23NO3	DB08941	Isoxsuprine	-2.26	-3.953
C35H43N5O4	DB11855	Revefenacin	-2.259	-4.097
K2O4S	DB14499	Potassium sulfate	-2.256	-2.256
NiO4S	DB14180	Nickel sulfate	-2.256	-2.256
FeO4S	DB13257	Ferrous sulfate anhydrous	-2.256	-2.256
CrO4S	DB14530	Chromous sulfate	-2.256	-2.256
Fe2H10O17S3	DB11171	Ferric sulfate	-2.256	-2.256
BaO4S	DB11150	Barium sulfate	-2.256	-2.256
Al2O12S3	DB11239	Aluminum sulfate	-2.256	-2.256
Na2O4S	DB09472	Sodium sulfate	-2.256	-2.256
O4SZn	DB09322	Zinc sulfate	-2.256	-2.256
Al5H33Mg10O40S2	DB08938	Magaldrate	-2.256	-2.256
AlKO8S2	DB09087	Potassium alum	-2.256	-2.256
C24H44BCuF4N4O4	DB14106	Tetrakis(2-methoxyisobutylisocyanide)copper(I)	-2.252	-2.252
C36H66N6O6Tc	DB09161	Technetium Tc-99m sestamibi	-2.252	-2.252
C25H27N3O2S	DB09128	Brexpiprazole	-2.252	-3.193
Al2H2MgO9Si2	DB13595	Almasilate	-2.247	-2.247
C44H88NO8P	DB14099	1,2-Distearoyllecithin	-2.245	-2.245
C35H38N4O6	DB09238	Manidipine	-2.242	-3.522
CH6N2O3	DB11129	Carbamide peroxide	-2.23	-2.23
CH4N2O	DB09513	Urea C-14	-2.23	-2.23
CH4N2O	DB09510	Urea C-13	-2.23	-2.23
C30H44N2O10	DB13265	Hexobendine	-2.229	-4.521
C7H7BrN4O2	DB14018	Bromotheophylline	-2.228	-4.005
C11H14ClN5	DB14763	Cycloguanil	-2.223	-4.249
C18H22F2N4O	DB09040	Efinaconazole	-2.222	-3.999
C21H38N	DB11073	Cetylpyridinium	-2.222	-2.222
H32Mo7N6O28	DB11128	Ammonium molybdate	-2.222	-2.224
H3N	DB09326	Ammonia N-13	-2.222	-2.224
C29H35F3N2O3	DB12371	Siponimod	-2.214	-2.222
C21H26F3N5	DB09195	Lorpiprazole	-2.201	-2.315
C65H87LuN14O19S2	DB13985	Lutetium Lu 177 dotatate	-2.193	-3.591
C49H55N9O7	DB11574	Elbasvir	-2.187	-3.477
C27H34N4O	DB12492	Piritramide	-2.187	-2.281
C16H25NO3	DB09205	Moxisylyte	-2.182	-4.195
C11H18N2O9	DB12362	Diaminopropanol tetraacetic acid	-2.169	-4.359
C6H12O3	DB09117	Paraldehyde	-2.162	-2.162
C9H12ClN5O	DB09242	Moxonidine	-2.162	-3.484
C40H50N8O6	DB09102	Daclatasvir	-2.16	-3.025
C18H32O2	DB14104	Linoleic acid	-2.16	-2.163
C13H13N3	DB14191	Diphenylguanidine	-2.157	-2.157
C16H19NO2	DB13219	Medifoxamine	-2.153	-2.512
C7H5NS2	DB11496	2-mercaptobenzothiazole	-2.151	-2.151
C21H26N2O5	DB09080	Olodaterol	-2.146	-4.77
C15H10Cl2N4O6	DB11632	Opicapone	-2.145	-4.387
C8H8O3	DB09543	Methyl salicylate	-2.136	-3.309
C2HCl3	DB13323	Trichloroethylene	-2.136	-2.136
C28H37N3O3	DB11591	Bilastine	-2.131	-3.88
C12H13FN4O5	DB09327	Tegafur-uracil	-2.128	-3.926
C8H9FN2O3	DB09256	Tegafur	-2.128	-3.926
C10H10N2O	DB12243	Edaravone	-2.123	-3.431
C6H9AlO6	DB14518	Aluminum acetate	-2.113	-2.116
C2H3KO2	DB14498	Potassium acetate	-2.113	-2.116
C4H6O4Zn	DB14487	Zinc acetate	-2.113	-2.116

C4H6MgO4	DB13996	Magnesium acetate	-2.113	-2.116
C4H14MgO8	DB09409	Magnesium acetate tetrahydrate	-2.113	-2.116
C2H3NaO2	DB09395	Sodium acetate	-2.113	-2.116
C49H54N8O8	DB11613	Velpatasvir	-2.108	-4.197
C7H16N4O2	DB11815	Tilarginine	-2.108	-2.108
C35H46CIN5O9S	DB11586	Asunaprevir	-2.105	-4.823
C20H26O3	DB13952	Estradiol acetate	-2.096	-2.096
C22H17CIN6O	DB11952	Duvelisib	-2.095	-4.092
C26H26CIN3	DB11614	Rupatadine	-2.09	-3.253
C35H43N5O4	DB11855	Revefenacin	-2.089	-3.697
C6H12N2S3	DB14178	Tetramethylthiuram monosulfide	-2.065	-2.065
C29H33FN2O4	DB09030	Vorapaxar	-2.064	-4.421
C23H28N8O4	DB12483	Copanlisib	-2.046	-4.769
C7H16N4O4S2	DB12473	Taurolidine	-2.044	-2.613
C6H8N2	DB14141	p-Phenylenediamine	-2.042	-3.027
C9H17Cl2N4	DB14198	Quaternium-15	-2.039	-2.039
O7P2Te	DB09165	Technetium Tc-99m pyrophosphate	-2.038	-4.375
C20H31NO3	DB11186	Pentoxifyverine	-2.035	-4.678
C35H41N5O5	DB13345	Dihydroergocristine	-2.011	-3.753
C41H50N6O2	DB11262	Bisotrizole	-2.006	-4.057
C10H16N2O	DB11738	Rilmenidine	-1.954	-1.955
C32H43N5O5	DB11274	Dihydro-alpha-ergocryptine	-1.943	-3.681
AuH4Na3O8S4	DB13743	Sodium aurotiosulfate	-1.912	-2.018
C37H34N2Na2O9S3	DB11183	Light green SF yellowish	-1.909	-1.911
C8H10N6	DB12945	Dihydralazine	-1.894	-2.351
CCaN2	DB09116	Calcium carbimide	-1.888	-1.888
C18H24N2O5	DB09477	Enalaprilat	-1.886	-2.012
C4H9Al2CIN4O7	DB11205	Alcloxa	-1.884	-3.535
C10H12CaN2Na2O8	DB14598	Edetate calcium disodium anhydrous	-1.873	-4.088
C3H8N2OS	DB13838	Noxytiolin	-1.87	-1.87
C19H19NS	DB13292	Pimethixene	-1.867	-1.877
ClKO4	DB09418	Potassium perchlorate	-1.866	-1.866
C25H28O3	DB13953	Estradiol benzoate	-1.862	-1.862
C45H50CIN7O7S	DB11581	Venetoclax	-1.853	-4.211
C21H26N2O5	DB09080	Olodaterol	-1.848	-1.855
C24H31N3OS	DB13213	Butaperazine	-1.843	-4.187
C21H30O4S	DB09091	Tixocortol	-1.809	-4.305
C2H8N2	DB14189	Ethylenediamine	-1.803	-2.503
C2H8N2	DB14189	Ethylenediamine	-1.803	-2.02
CHI3	DB13813	Iodoform	-1.797	-1.797
C24H29N7O2	DB09073	Palbociclib	-1.796	-3.708
C16H24N2	DB08944	Isoaminile	-1.796	-3.65
C17H28N2O	DB08987	Etidocaine	-1.789	-3.962
C18H22N2S	DB09068	Vortioxetine	-1.773	-4.453
C6H15NO3	DB13747	Trolamine	-1.762	-1.832
C13H21NO6	DB11079	Trolamine salicylate	-1.754	-1.825
Mg2O8Si3	DB09281	Magnesium trisilicate	-1.753	-1.753
C21H38N	DB13282	Benzododecinium	-1.735	-1.735
C20H19F2N3O5	DB08930	Dolutegravir	-1.714	-2.001
C34H28N6O14S4	DB09158	Trypan blue free acid	-1.704	-3.555
C10H9N5O	DB11336	Kinetin	-1.695	-3.692
C16H28N2O2	DB13288	Tromantadine	-1.684	-3.927
CHCl3	DB11387	Chloroform	-1.676	-1.676
C7H16N4O4S2	DB12473	Taurolidine	-1.674	-2.524
C49H55N9O7	DB11574	Elbasvir	-1.652	-2.905
C17H21NO	DB11160	Phenyltoloxamine	-1.64	-3.653
C10H10N2O	DB12243	Edaravone	-1.639	-2.432
C45H54F2N4O8	DB11641	Vinflunine	-1.638	-1.843
C57H65F5N10O8	DB13878	Pibrentasvir	-1.634	-3.068
C17H19NO	DB12293	Nefopam	-1.633	-3.099
C10H15NO2	DB11610	Oxilofrine	-1.629	-3.974
C12H19NO	DB11587	Etafedrine	-1.609	-3.094
C27H31FN4O8	DB12329	Eravacycline	-1.606	-4.139

C14H11FN2OS	DB09151	Flutemetamol (18F)	-1.603	-3.824
Bi5H9N4O22	DB13209	Bismuth subnitrate	-1.603	-1.603
CrN3O9	DB14527	Chromic nitrate	-1.603	-1.603
KNO3	DB11090	Potassium nitrate	-1.603	-1.603
C14H20InN3O10	DB09425	Indium In-111 pentetate	-1.595	-2.411
C49H54N8O8	DB11613	Velpatasvir	-1.58	-3.839
C49H54N8O8	DB11613	Velpatasvir	-1.574	-2.782
CO2	DB09157	Carbon dioxide	-1.568	-1.568
C17H34O2	DB13966	Isopropyl myristate	-1.562	-1.562
C27H34N4O	DB12492	Piritramide	-1.557	-3.766
C10H10N2O	DB12243	Edaravone	-1.555	-3.088
C16H34O	DB09494	Cetyl alcohol	-1.533	-1.533
C63H87N13O19S2	DB12602	Pentetreotide	-1.518	-1.584
C36H51Cl2N3O4	DB14185	Aripiprazole lauroxil	-1.493	-2.251
C27H33N2O6S2	DB09136	Isosulfan blue	-1.486	-2.192
C13H10O3	DB11071	Phenyl salicylate	-1.485	-1.51
C38H80N	DB14143	Distearyltrimonium	-1.441	-1.441
C11H20O2	DB11117	Undecylenic acid	-1.413	-1.416
C49H54F2N8O6	DB09027	Ledipasvir	-1.397	-2.577
ClO	DB11123	Hypochlorite	-1.377	-1.377
C11H14O3	DB14084	Butylparaben	-1.375	-3.458
C26H27N3O5S	DB09183	Dasabuvir	-1.366	-3.785
C31H33N5O4	DB09079	Nintedanib	-1.365	-2.189
C2H5Cl	DB13259	Ethyl chloride	-1.365	-1.365
C13H19NO3	DB09185	Viloxazine	-1.365	-3.298
C4H10FeN2O8S	DB14501	Ferrous glycine sulfate	-1.363	-1.363
C4H8FeN2O4	DB11210	Ferrous bisglycinate	-1.363	-1.363
C2H8AlClNO4Zr	DB11200	Aluminum zirconium octachlorohydrate gly	-1.363	-1.363
C4H8MgN2O4	DB11189	Magnesium glycinate	-1.363	-1.363
C14H21NO2	DB09088	Amylocaine	-1.346	-3.683
C15H24N2O2	DB09085	Tetracaine	-1.342	-3.76
C9H10O3	DB13628	Ethyl hydroxybenzoate	-1.336	-3.401
CK2O3	DB13977	Potassium carbonate	-1.33	-1.442
CNa2O3	DB09460	Sodium carbonate	-1.33	-1.442
CLi2O3	DB14509	Lithium carbonate	-1.33	-1.442
CH24Al2Mg6O24	DB13322	Hydrotalcite	-1.33	-1.442
CHKO3	DB11098	Potassium bicarbonate	-1.33	-1.442
CMgO3	DB09481	Magnesium carbonate	-1.33	-1.442
O2	DB09140	Oxygen	-1.31	-1.31
C27H31FN4O8	DB12329	Eravacycline	-1.308	-3.45
C20H19F2N3O5	DB08930	Dolutegravir	-1.306	-1.932
C10H14N2Na2O8	DB14600	Edetate disodium anhydrous	-1.29	-3.505
C27H26ClF3N6O3	DB12095	Telotristat ethyl	-1.29	-3.559
C21H26F3N5	DB09195	Loripiprazole	-1.279	-2.32
C35H38N4O6	DB09238	Manidipine	-1.273	-2.666
C16H26N2O3	DB09342	Propoxycaine	-1.268	-3.254
C10H14N2O2	DB14754	Solriamfetol	-1.261	-3.347
C8H8O3	DB14212	Methylparaben	-1.261	-3.184
C20H33N3O3S	DB09097	Quinagolide	-1.245	-3.322
C49H54N8O8	DB11613	Velpatasvir	-1.212	-2.388
C17H12I2O3	DB13277	Benziodarone	-1.198	-3.74
H4OSi	DB11343	Silanol	-1.192	-1.192
C57H65F5N10O8	DB13878	Pibrentasvir	-1.125	-1.888
C27H34N4O	DB12492	Piritramide	-1.114	-2.826
C20H25N3S	DB12710	Perazine	-1.112	-3.456
C49H55N9O7	DB11574	Elbasvir	-1.11	-2.39
C9H7NO	DB11145	Oxyquinoline	-1.093	-3.172
C27H18InN3O3	DB09473	Indium In-111 oxyquinoline	-1.093	-3.172
C14H23N3O10	DB14007	Pentetic acid	-1.068	-1.884
C36H72N8O8P	DB11283	DL-dimyrystoylphosphatidylcholine	-1.065	-1.065
C19H25N3O2S2	DB08967	Dimetotiazine	-1.047	-1.048
C27H32F2N8	DB12001	Abemaciclib	-1.041	-3.693
C18H18ClN3S	DB13256	Clothiapine	-1.035	-2.766

C14H19N3O	DB13216	Oxolamine	-1.034	-3.131
C40H50N8O6	DB09102	Daclatasvir	-1.023	-2.276
C28H37N3O3	DB11591	Bilastine	-1.022	-3.487
C30H32F6N4O	DB09048	Netupitant	-1.003	-2.895
C16H25GdN4O8	DB09132	Gadoteric acid	-1.002	-1.067
C14H20Br2N2	DB09019	Bromhexine	-0.985	-2.932
C41H67NO15	DB13179	Troleandomycin	-0.983	-1.137
C40H43N7O7S	DB09297	Paritaprevir	-0.978	-0.985
C26H23N7O2	DB11703	Acalabrutinib	-0.968	-3.191
C17H13N3O5S2	DB13248	Phthalylsulfathiazole	-0.965	-1.518
C18H15NO8S2	DB09268	Picosulfuric acid	-0.957	-3.298
C20H41N5O7	DB13274	Micronomicin	-0.956	-2.69
C12H24N2O4S2	DB11164	Bicisate	-0.955	-2.698
CO	DB11588	Carbon monoxide	-0.949	-0.949
NO2	DB12529	Nitrite	-0.948	-0.948
C8H17FeN3O6S2	DB11197	Ferrous cysteine glycinate	-0.888	-3.107
C49H55N9O7	DB11574	Elbasvir	-0.888	-2.131
C25H25F3N4O6	DB11637	Delamanid	-0.884	-3.252
F6S	DB11104	Sulfur hexafluoride	-0.849	-0.849
C25H30N6O2	DB12147	Erdafitinib	-0.844	-0.844
C32H39NO2	DB11742	Ebastine	-0.806	-3.311
C4F10	DB12821	Perflubutane	-0.801	-0.801
C41H67NO15	DB13179	Troleandomycin	-0.727	-1.604
C31H33N5O4	DB09079	Nintedanib	-0.712	-3.222
N2	DB09152	Nitrogen	-0.709	-0.709
C32H34N4O6	DB11691	Naldemedine	-0.675	-3.084
C24H31NO4	DB11269	Diethylamino hydroxybenzoyl hexyl benzoate	-0.662	-2.951
C49H55N9O7	DB11574	Elbasvir	-0.658	-1.802
C21H23BrFNO2	DB12401	Bromperidol	-0.653	-2.905
C50H71N13O12	DB11842	Angiotensin II	-0.647	-1.325
C19H18N6O6S2	DB14725	Cefamandole nafate	-0.631	-0.631
C29H40N4O7	DB12455	Omadacycline	-0.629	-3.009
C40H43N7O7S	DB09297	Paritaprevir	-0.626	-3.341
FH	DB11072	Hydrogen fluoride	-0.616	-0.616
C27H32F2N8	DB12001	Abemaciclib	-0.583	-2.736
C15H16O9	DB13155	Esculin	-0.557	-2.906
C40H52N2O4	DB13947	Testosterone enantate benzilic acid hydrazone	-0.538	-0.538
C32H34N4O6	DB11691	Naldemedine	-0.535	-3.16
C18H21ClN2	DB08936	Chlorcyclizine	-0.535	-2.566
HNO2	DB09112	Nitrous acid	-0.469	-0.469
C65H87GaN14O19S2	DB13925	Dotatate gallium Ga-68	-0.422	-1.633
C22H23ClN2O8	DB09093	Chlortetracycline	-0.401	-2.105
C14H23N3O10	DB14007	Pentetic acid	-0.385	-2.224
C2H2F4	DB13116	Norflurane	-0.378	-0.378
C29H35F3N2O3	DB12371	Siponimod	-0.367	-2.969
C36H84O10P4Tc	DB09160	Technetium Tc-99m tetrofosmin	-0.351	-1.211
C18H40N	DB13970	Diocetyltrimonium	-0.332	-0.332
C19H19NS	DB13292	Pimethixene	-0.33	-2.805
FN2O3P	DB09484	Sodium fluorophosphate	-0.319	-2.418
H2O2	DB11091	Hydrogen peroxide	-0.313	-0.313
AuH4Na3O8S4	DB13743	Sodium aurotiolate	-0.308	-1.382
C18H12CrN3O6	DB14529	Chromium nicotinate	-0.216	-2.664
C30H29ClN6O3	DB11828	Neratinib	-0.203	-2.017
C31H41N5O5	DB11273	Dihydroergocornine	-0.2	-2.633
C23H29NO3	DB12278	Propiverine	-0.196	-2.78
C34H28N6O14S4	DB09158	Trypan blue free acid	-0.191	-0.246
C18H40O4P2	DB11180	Tetrofosmin	-0.17	-1.029
C27H33N2	DB11279	Brilliant green cation	-0.133	-0.84
C26H26N2O6S	DB09319	Carindacillin	-0.128	-0.763
C45H54F2N4O8	DB11641	Vinflunine	-0.113	-1.172
C12H8N2O4Zn	DB11175	Zinc picolinate	-0.108	-2.556
C16H25GdN4O8	DB09132	Gadoteric acid	-0.062	-1.464
C49H54F2N8O6	DB09027	Ledipasvir	-0.05	-1.407

C14H20InN3O10	DB09425	Indium In-111 pentetate	-0.028	-1.867
C29H44N8O3	DB12141	Gilteritinib	0.021	-2.659
C65H87GaN14O19S2	DB13925	Dotatate gallium Ga-68	0.041	-2.623
C35H41N5O5	DB13345	Dihydroergocristine	0.117	-2.115
C14H22N2O3	DB09069	Trimetazidine	0.212	-2
C13H21NO6	DB11079	Trolamine salicylate	0.266	-1.027
C40H50N8O6	DB09102	Daclatasvir	0.271	-0.897
C37H47NO12	DB11753	Rifamycin	0.288	-0.862
C23H30N8O	DB11730	Ribociclib	0.429	-0.972
C49H54F2N8O6	DB09027	Ledipasvir	0.435	-1.105
C49H54F2N8O6	DB09027	Ledipasvir	0.451	-1.617
C13H18CIN3O4S2	DB13532	Cyclophentiazide	0.468	-1.973
C24H29N3O8	DB12035	Sarecycline	0.493	-2.137
Al2H2Mg2O12Si3	DB14116	Silodrate	0.497	0.497
C16H18CIN3S	DB09241	Methylene blue	0.504	-1.562
C13H10O3	DB11071	Phenyl salicylate	0.524	-1.37
C6H15NO3	DB13747	Trolamine	0.529	-0.765
C47H72NO10P	DB14096	1,2-icosapentoyl-sn-glycero-3-phosphoserine	0.717	0.704
C26H26CIN3	DB11614	Rupatadine	0.858	-0.947
C65H87GaN14O19S2	DB13925	Dotatate gallium Ga-68	0.891	-0.692
C38H50N6O9S	DB11575	Grazoprevir	0.949	-1.77
C22H23CIN2O8	DB09093	Chlortetracycline	0.988	-1.304
C31H52O3	DB14002	D-alpha-Tocopherol acetate	1.065	1.065
C65H87GaN14O19S2	DB13925	Dotatate gallium Ga-68	1.118	0.112
C59H90O4	DB09270	Ubidecarenone	1.618	1.618
C27H31FN4O8	DB12329	Eravacycline	1.682	-0.44
C49H54F2N8O6	DB09027	Ledipasvir	1.716	1.129
C10H12O3	DB14177	Propylparaben	1.73	-0.352
C11H14O3	DB14084	Butylparaben	1.842	1.824
C14H12O3	DB14176	Benzylparaben	2.086	0.169
C47H72NO10P	DB14096	1,2-icosapentoyl-sn-glycero-3-phosphoserine	3.332	1.048
C63H87N13O19S2	DB12602	Pentetreotide	3.976	2.518
C24H19NO5	DB14627	Oxyphenisatin acetate	4.049	4.049
C22H19NO4	DB09020	Bisacodyl	4.239	1.899

FDA approved drugs with 6y84, Table S10

FORMULA	DRUGBANK_ID	GENERIC_NAME	docking score	glide gscore
C25H43NO18	DB00284	Acarbose	-12.507	-13.139
C25H43NO18	DB00284	Acarbose	-10.525	-10.775
C52H98N16O13	DB00803	Colistin	-10.271	-12.63
C55H84N17O21S3	DB00290	Bleomycin	-9.182	-10.542
C21H29N7O14P2	DB00157	NADH	-9.031	-9.031
C55H75N17O13	DB00644	Gonadorelin	-8.688	-9.315
C66H75Cl2N9O24	DB00512	Vancomycin	-8.66	-9.053
C31H53N3O49S8	DB00569	Fondaparinux	-8.617	-9.283
C23H46N6O13	DB00452	Framycetin	-8.609	-9.949
C23H46N6O13	DB00452	Framycetin	-8.533	-10.713
C23H46N6O13	DB00452	Framycetin	-8.478	-9.518
C22H43N5O13	DB00479	Amikacin	-8.44	-8.504
C12H22O11	DB00581	Lactulose	-8.109	-8.109
C27H29NO10	DB00694	Daunorubicin	-8.065	-8.093
C22H43N5O13	DB00479	Amikacin	-7.947	-10.186
C27H29NO11	DB00445	Epirubicin	-7.915	-7.942
C50H88N28O15	DB00314	Capreomycin	-7.898	-8.41
C55H75N17O13	DB00644	Gonadorelin	-7.869	-8.696
C59H84N18O14	DB00014	Goserelin	-7.577	-8.403
C23H46N6O13	DB00452	Framycetin	-7.439	-9.655
C37H49N7O9S	DB00183	Pentagastrin	-7.436	-7.437

C52H88N10O15	DB00520	Casposfungin	-7.431	-7.439
C29H39N5O8	DB00560	Tigecycline	-7.182	-7.316
C18H22O4	DB00179	Masoprocol	-7.141	-7.141
C14H26CaO16	DB00326	Calcium glucoheptonate	-7.034	-7.034
C23H46N6O13	DB00452	Framycetin	-7.015	-9.175
C20H23N7O7	DB00650	Leucovorin	-6.876	-6.876
C29H39N5O8	DB00560	Tigecycline	-6.62	-7.728
C8H12N4O5	DB00811	Ribavirin	-6.58	-6.58
C46H64N14O12S2	DB00035	Desmopressin	-6.555	-6.556
C23H34O5	DB00374	Treprostinil	-6.359	-6.359
C18H23NO3	DB00841	Dobutamine	-6.355	-6.355
C52H98N16O13	DB00803	Colistin	-6.346	-7.552
C14H13N5O5S2	DB00535	Cefdinir	-6.333	-6.333
C25H24N8O7S2	DB00430	Cefpiramide	-6.316	-6.316
C15H22N6O5S	DB00118	Ademetionine	-6.309	-6.319
C23H36O7	DB00175	Pravastatin	-6.267	-6.269
C23H46N6O13	DB00452	Framycetin	-6.238	-8.752
C23H24N2O4S	DB00876	Eprosartan	-6.219	-6.251
C25H37NO4	DB00905	Bimatoprost	-6.206	-6.206
C21H27NO4	DB00844	Nalbuphine	-6.194	-6.224
C47H73NO17	DB00681	Amphotericin B	-6.158	-6.196
C50H88N28O15	DB00314	Capreomycin	-6.144	-7.665
C34H36F3NO13	DB00385	Valrubicin	-6.091	-6.091
C66H83N17O13	DB00666	Nafarelin	-6.046	-6.673
C66H83N17O13	DB00666	Nafarelin	-5.984	-6.52
C14H11NO5	DB00323	Tolcapone	-5.984	-6.039
C10H13N5O4	DB00640	Adenosine	-5.955	-5.955
C10H14N5O7P	DB00131	Adenosine phosphate	-5.928	-6.02
C8H17NO5	DB00491	Miglitol	-5.903	-5.948
C23H46N6O13	DB00452	Framycetin	-5.88	-8.51
C17H20N4O6	DB00140	Riboflavin	-5.877	-5.877
C19H25BN4O4	DB00188	Bortezomib	-5.864	-5.864
C20H21N7O6S2	DB00923	Ceforanide	-5.82	-5.844
C26H35F3O6	DB00287	Travoprost	-5.816	-5.816
C52H98N16O13	DB00803	Colistin	-5.759	-7.092
C8H14N3O6P	DB00369	Cidofovir	-5.748	-6.044
C16H21N3O2	DB00315	Zolmitriptan	-5.744	-5.748
C7H11NO7P2	DB00884	Risedronic acid	-5.728	-6.521
C20H21N5O6	DB00642	Pemetrexed	-5.692	-5.692
C12H18N2O4	DB00211	Midodrine	-5.69	-5.798
C27H44O3	DB00910	Paricalcitol	-5.685	-5.685
C66H75Cl2N9O24	DB00512	Vancomycin	-5.682	-7.784
C21H25N5O8S2	DB00948	Mezlocillin	-5.655	-5.655
C21H22N4O6S	DB00293	Raltitrexed	-5.655	-5.719
C23H46N6O13	DB00452	Framycetin	-5.654	-7.93
C24H36O5	DB00227	Lovastatin	-5.615	-5.615
C4H13NO7P2	DB00630	Alendronic acid	-5.613	-6.356
C27H44O2	DB00146	Calcifediol	-5.611	-5.611
C66H75Cl2N9O24	DB00512	Vancomycin	-5.596	-7.361
C26H44O9	DB00410	Mupirocin	-5.589	-5.592
C10H11ClFN5O3	DB00631	Clofarabine	-5.568	-5.568
C17H19NO3	DB00295	Morphine	-5.567	-5.626
C14H24N2O7	DB00919	Spectinomycin	-5.565	-5.815
C33H47NO13	DB00826	Natamycin	-5.559	-5.597
C21H41N5O7	DB00955	Netilmicin	-5.553	-6.263
C8H15NO6	DB00141	N-Acetylglucosamine	-5.544	-5.544
C52H98N16O13	DB00803	Colistin	-5.539	-6.788
C7H11NO7P2	DB00884	Risedronic acid	-5.522	-5.71
C52H98N16O13	DB00803	Colistin	-5.51	-7.398
C9H11F2N3O4	DB00441	Gemcitabine	-5.504	-5.51
C10H12ClN5O3	DB00242	Cladribine	-5.485	-5.485
C31H53N3O49S8	DB00569	Fondaparinux	-5.438	-6.06
C19H29NO5	DB00449	Dipivefrin	-5.431	-5.437

C18H29NO3	DB00195	Betaxolol	-5.406	-5.408
C4H13NO7P2	DB00630	Alendronic acid	-5.388	-5.587
C20H25CIN2O5	DB00381	Amlodipine	-5.387	-5.391
C6H14O6	DB00742	Mannitol	-5.383	-5.383
C22H24N2O8	DB00759	Tetracycline	-5.382	-6.428
C25H47NO8	DB00429	Carboprost tromethamine	-5.362	-5.365
C20H30O	DB00162	Vitamin A	-5.355	-5.355
C32H45N3O4S	DB00220	Nelfinavir	-5.345	-5.358
C22H25N3O7S	DB00303	Ertapenem	-5.341	-5.39
C43H66O14	DB00511	Acetyldigitoxin	-5.333	-5.333
C23H32N2O5	DB00178	Ramipril	-5.327	-5.532
C22H26N2O2S	DB00216	Eletriptan	-5.322	-5.324
C10H11F3N2O5	DB00432	Trifluridine	-5.308	-5.393
C19H17NO7	DB00716	Nedocromil	-5.305	-5.305
C22H36N2O5S	DB00775	Tirofiban	-5.303	-5.303
C22H22N2O8	DB00931	Metacycline	-5.278	-5.913
C8H15N3O7	DB00428	Streptozocin	-5.255	-5.255
C17H21NO3	DB00867	Ritodrine	-5.254	-5.266
C20H34O5	DB00770	Alprostadil	-5.252	-5.256
C18H31NO4	DB00612	Bisoprolol	-5.216	-5.218
C32H47F5O3S	DB00947	Fulvestrant	-5.193	-5.193
C36H47N5O4	DB00224	Indinavir	-5.185	-5.827
C18H24O2	DB00783	Estradiol	-5.173	-5.173
C41H64O14	DB00390	Digoxin	-5.169	-5.169
C10H17N3O6S	DB00143	Glutathione	-5.165	-5.171
C32H39NO4	DB00950	Fexofenadine	-5.16	-5.16
C17H23NO3	DB00424	Hyoscyamine	-5.146	-5.148
C17H25N3O2S	DB00918	Almotriptan	-5.135	-5.139
C9H11N2O5	DB00249	Idoxuridine	-5.134	-5.148
C15H12I3NO4	DB00279	Liothyronine	-5.13	-5.232
C32H32O13S	DB00444	Teniposide	-5.127	-5.127
C12H20N4O7	DB00558	Zanamivir	-5.121	-5.122
C15H15NO2S	DB00745	Modafinil	-5.111	-5.111
C21H26N2O7	DB00393	Nimodipine	-5.106	-5.106
C37H48N6O5S2	DB00503	Ritonavir	-5.104	-5.104
C19H19N7O6	DB00158	Folic acid	-5.1	-5.278
C18H23N9O4S3	DB00229	Cefotiam	-5.086	-5.186
C21H21CIN2O8	DB00618	Demeclocycline	-5.084	-5.281
C52H98N16O13	DB00803	Colistin	-5.084	-6.479
C22H24N2O9	DB00595	Oxytetracycline	-5.081	-5.74
C29H32O13	DB00773	Etoposide	-5.073	-5.073
C30H53NO11	DB00868	Benzonatate	-5.07	-5.07
C10H14N5O7P	DB00131	Adenosine phosphate	-5.068	-6.217
C17H20N2O2	DB00809	Tropicamide	-5.063	-5.071
C20H29N3O2	DB00527	Cinchocaine	-5.062	-5.066
C19H24N4O2	DB00738	Pentamidine	-5.059	-5.059
C25H37NO4	DB00938	Salmeterol	-5.05	-5.055
C16H17N9O5S3	DB00267	Cefmenoxime	-5.047	-5.047
C18H20O2	DB00255	Diethylstilbestrol	-5.046	-5.047
C21H21CIN2O8	DB00618	Demeclocycline	-5.044	-6.077
C52H98N16O13	DB00803	Colistin	-5.043	-6.33
C10H18O21S4	DB00686	Pentosan Polysulfate	-5.039	-5.039
C10H13N5O4	DB00495	Zidovudine	-5.038	-5.038
C33H37N5O5	DB00320	Dihydroergotamine	-5.037	-5.087
C17H25N3O2S	DB00952	Naratriptan	-5.032	-5.034
C10H14N4O4	DB00651	Dyphylline	-5.026	-5.026
C27H44O3	DB00136	Calcitriol	-5.003	-5.003
C18H37N5O9	DB00684	Tobramycin	-5.002	-6.529
C21H41N5O7	DB00955	Netilmicin	-4.991	-6.759
C11H12CI2N2O5	DB00446	Chloramphenicol	-4.988	-4.988
C23H46N6O13	DB00452	Framycetin	-4.971	-5.957
C16H18N2O5S	DB00417	Phenoxymethylpenicillin	-4.969	-4.969
C3H11NO7P2	DB00282	Pamidronic acid	-4.967	-6.021

C9H15N5O3	DB00360	Sapropterin	-4.966	-4.978
C17H18N2O6S	DB00578	Carbenicillin	-4.963	-4.963
C21H29NO	DB00810	Biperiden	-4.959	-4.96
C26H40O5	DB00654	Latanoprost	-4.948	-4.948
C20H22CIN3O	DB00613	Amodiaquine	-4.937	-5.228
C27H41NO6	DB00769	Hydrocortamate	-4.933	-5.031
C17H23NO3	DB00572	Atropine	-4.928	-4.93
C52H98N16O13	DB00803	Colistin	-4.923	-6.317
C20H23NO4	DB00704	Naltrexone	-4.908	-4.956
C12H20N2O3S	DB00489	Sotalol	-4.905	-4.926
C27H36N2O4	DB00912	Repaglinide	-4.9	-4.908
C16H14CIN3O	DB00475	Chlordiazepoxide	-4.899	-4.946
C21H29FO5	DB00687	Fludrocortisone	-4.897	-4.897
C27H29NO10	DB00694	Daunorubicin	-4.897	-6.737
C23H21F7N4O3	DB00673	Aprepitant	-4.894	-4.894
C19H20N2O2	DB00812	Phenylbutazone	-4.892	-4.9
C17H21NO4	DB00747	Scopolamine	-4.888	-5.101
C17H25N3O5S	DB00760	Meropenem	-4.865	-4.894
C3H11NO7P2	DB00282	Pamidronic acid	-4.856	-4.966
C10H15N5O3	DB00299	Penciclovir	-4.846	-4.846
C27H29NO11	DB00445	Epirubicin	-4.832	-6.672
C8H14N3O6P	DB00369	Cidofovir	-4.831	-5.384
C16H15N5O7S2	DB00671	Cefixime	-4.819	-4.819
C19H25NO	DB00504	Levallorphan	-4.812	-4.839
C20H24N2O	DB00192	Indecainide	-4.811	-4.811
C9H13NO3	DB00668	Epinephrine	-4.811	-4.822
C22H29ClO5	DB00240	Alclometasone	-4.807	-4.807
C13H8F2O3	DB00861	Diflunisal	-4.807	-4.807
C29H38N4O10	DB00256	Lymecycline	-4.8	-4.962
C9H11FN2O5	DB00322	Floxuridine	-4.799	-4.828
C17H17NO2	DB00714	Apomorphine	-4.797	-6.361
CH4Cl2O6P2	DB00720	Clodronic acid	-4.796	-4.801
C16H17N5O7S2	DB00493	Cefotaxime	-4.795	-4.795
C26H28ClNO	DB00539	Toremifene	-4.79	-4.81
C52H98N16O13	DB00803	Colistin	-4.755	-6.195
C21H27CIN2O2	DB00557	Hydroxyzine	-4.747	-5.065
C18H23N9O4S3	DB00229	Cefotiam	-4.743	-5.845
C20H28N2O5	DB00584	Enalapril	-4.737	-4.932
C9H23NO7P2	DB00710	Ibandronate	-4.736	-4.827
C14H21N3O2S	DB00669	Sumatriptan	-4.725	-4.729
C20H12O5	DB00693	Fluorescein	-4.703	-4.919
C33H35N5O5	DB00696	Ergotamine	-4.698	-4.875
C21H26O5	DB00635	Prednisone	-4.694	-4.694
C21H43N5O7	DB00798	Gentamicin	-4.687	-4.863
C22H28GdN3O11	DB00743	Gadobenic acid	-4.682	-4.862
C11H16N4O4	DB00552	Pentostatin	-4.68	-4.712
C22H26N2O4S	DB00343	Diltiazem	-4.678	-4.696
C16H21NO2	DB00571	Propranolol	-4.678	-4.679
C22H22N6O7S2	DB00438	Ceftazidime	-4.676	-4.676
C49H66N10O10S2	DB00104	Octreotide	-4.673	-4.886
C21H30O5	DB00741	Hydrocortisone	-4.673	-4.673
C52H98N16O13	DB00803	Colistin	-4.672	-6.183
C19H32N2O5	DB00790	Perindopril	-4.668	-4.922
C22H43N5O13	DB00479	Amikacin	-4.666	-6.168
C22H29FO5	DB00443	Betamethasone	-4.664	-4.664
C18H19N3O6S	DB00689	Cephaloglycin	-4.66	-4.91
C22H24N2O8	DB00254	Doxycycline	-4.66	-4.892
C15H17FN4O3	DB00467	Enoxacin	-4.653	-4.701
C14H24N2O7	DB00919	Spectinomycin	-4.647	-5.479
C13H24NO10P	DB00144	Phosphatidyl serine	-4.646	-4.659
C19H22FN3O3	DB00365	Grepafloxacin	-4.643	-5.651
C22H28F2O5	DB00223	Diflorasone	-4.631	-4.631
C18H19NOS	DB00476	Duloxetine	-4.63	-4.631

C23H27N5O7S	DB00319	Piperacillin	-4.629	-4.63
C10H13N5O4	DB00194	Vidarabine	-4.628	-4.628
C5H10N2O7P2	DB00399	Zoledronic acid	-4.625	-5.132
C9H23NO7P2	DB00710	Ibandronate	-4.623	-5.792
C23H32N2O5	DB00178	Ramipril	-4.618	-5.344
C15H12N2O2	DB00776	Oxcarbazepine	-4.617	-4.617
C14H11Cl2NO2	DB00939	Meclofenamic acid	-4.614	-4.615
C18H22O2	DB00655	Estrone	-4.614	-4.614
C17H18FN3O3	DB00537	Ciprofloxacin	-4.608	-5.712
C20H32O5	DB00917	Dinoprostone	-4.605	-4.608
C31H53N3O49S8	DB00569	Fondaparinux	-4.597	-5.265
C12H15N5O3	DB00442	Entecavir	-4.596	-4.596
C26H37N5O2	DB00248	Cabergoline	-4.593	-5.261
C20H30NO3	DB00332	Ipratropium	-4.591	-4.591
C21H24F3N3S	DB00831	Trifluoperazine	-4.59	-4.87
C9H13N3O3	DB00943	Zalcitabine	-4.588	-4.588
C18H21NO3	DB00318	Codeine	-4.587	-4.633
C19H27NO	DB00652	Pentazocine	-4.577	-4.588
C21H19N3O3S	DB00276	Amsacrine	-4.576	-4.595
C19H19N7O6	DB00158	Folic acid	-4.571	-5.916
C16H24N2O3	DB00521	Carteolol	-4.57	-4.571
C21H28N2O5	DB00662	Trimethobenzamide	-4.569	-4.589
C16H19ClN2O	DB00748	Carbinoxamine	-4.561	-4.566
C22H28ClFO4	DB00838	Clocortolone	-4.56	-4.56
C13H21NO3	DB00221	Isoetarine	-4.558	-4.558
C18H18O2	DB00890	Dienestrol	-4.558	-4.558
C20H24ClN3S	DB00433	Prochlorperazine	-4.556	-4.836
C8H11NO3	DB00368	Norepinephrine	-4.553	-4.57
C28H44O	DB00153	Ergocalciferol	-4.547	-4.547
C23H36N6O5S	DB00278	Argatroban	-4.546	-4.546
C24H33FO6	DB00846	Flurandrenolide	-4.545	-4.545
C19H17Cl2N3O5S	DB00485	Dicloxacillin	-4.544	-4.544
C10H21NO4	DB00419	Miglustat	-4.534	-4.553
C22H30Cl2N10	DB00878	Chlorhexidine	-4.533	-4.543
C17H21NO3	DB00749	Etodolac	-4.521	-4.522
C15H11I4NO4	DB00509	Dextrothyroxine	-4.521	-4.645
C11H13N3O3S	DB00263	Sulfisoxazole	-4.52	-4.52
C26H28ClNO	DB00882	Clomifene	-4.52	-4.54
C20H25N3O2	DB00353	Methylephedrine	-4.518	-4.771
C19H28O2	DB00624	Testosterone	-4.518	-4.518
C11H15NO5	DB00423	Methocarbamol	-4.514	-4.514
C15H11I4NO4	DB00451	Levothyroxine	-4.505	-4.629
C10H14O4	DB00874	Guafenesin	-4.504	-4.504
C22H30O	DB00304	Desogestrel	-4.502	-4.502
C49H66N10O10S2	DB00104	Octreotide	-4.496	-5.206
C21H27N3O2	DB00247	Methysergide	-4.495	-4.748
C10H12N2O4	DB00649	Stavudine	-4.494	-4.496
C18H19N3O3S	DB00412	Rosiglitazone	-4.492	-5.016
C21H26ClN3OS	DB00850	Perphenazine	-4.491	-5.038
C22H26F3N3OS	DB00623	Fluphenazine	-4.49	-5.037
C19H22FN3O3	DB00365	Grepafloxacin	-4.486	-4.606
C21H27FO6	DB00620	Triamcinolone	-4.485	-4.485
C18H24BrNO4	DB00462	Methscopolamine bromide	-4.483	-4.483
C19H24N2O3	DB00598	Labetalol	-4.483	-4.511
C19H23N3O4S	DB00739	Hetacillin	-4.482	-4.485
C27H44O	DB00169	Cholecalciferol	-4.479	-4.479
C8H9NO5	DB00766	Clavulanic acid	-4.46	-4.46
C26H34FNO5	DB00439	Cerivastatin	-4.459	-4.482
C20H22N8O5	DB00563	Methotrexate	-4.458	-4.523
C46H58N4O9	DB00570	Vinblastine	-4.456	-5.873
C30H46NO7P	DB00492	Fosinopril	-4.444	-4.445
C22H28F2O5	DB00663	Flumethasone	-4.444	-4.444
C28H37ClO7	DB00394	Beclomethasone dipropionate	-4.44	-4.44

C20H21FN2O	DB00215	Citalopram	-4.439	-4.441
C20H26O2	DB00717	Norethisterone	-4.438	-4.438
C21H28O2	DB00367	Levonorgestrel	-4.41	-4.41
C25H48N6O8	DB00746	Deferoxamine	-4.409	-4.409
C19H29NO	DB00942	Cycrimine	-4.407	-4.408
C11H17NO3	DB00816	Orciprenaline	-4.403	-4.417
C20H28N2O3	DB00383	Oxyphencyclimine	-4.395	-4.395
C19H16O4	DB00682	Warfarin	-4.391	-4.412
C43H55N5O7	DB00309	Vindesine	-4.391	-5.188
C7H15Cl2N2O2P	DB00531	Cyclophosphamide	-4.391	-4.391
C16H13N3O3	DB00643	Mebendazole	-4.39	-5.073
C16H25NO2	DB00193	Tramadol	-4.389	-4.392
C55H75N17O13	DB00644	Gonadorelin	-4.387	-4.922
C16H16ClN3O4	DB00447	Loracarbef	-4.381	-4.932
C22H29N3S2	DB00372	Thiethylperazine	-4.38	-4.66
C25H30N2O5	DB00881	Quinapril	-4.378	-4.531
C15H15NO2	DB00784	Mefenamic acid	-4.375	-4.376
C28H46N6O8S	DB00895	Benzylpenicilloyl Polylysine	-4.374	-4.374
C14H10F3NO5	DB00348	Nitisinone	-4.368	-4.368
C15H17N7O5S3	DB00274	Cefmetazole	-4.363	-4.363
C27H41NO6	DB00769	Hydrocortamate	-4.363	-5.478
C29H39N5O8	DB00560	Tigecycline	-4.361	-6.327
C11H16N4O4	DB00380	Dexrazoxane	-4.361	-4.969
C12H8O4	DB00553	Methoxsalen	-4.361	-4.361
C27H29N5O6S	DB00559	Bosentan	-4.359	-4.359
C16H11ClN2O3	DB00628	Clorazepic acid	-4.358	-4.358
C52H98N16O13	DB00803	Colistin	-4.356	-6.643
C22H24ClFN4O3	DB00317	Gefitinib	-4.353	-4.759
C18H19N3O3S	DB00412	Rosiglitazone	-4.347	-4.914
C8H12N4O5	DB00928	Azacitidine	-4.341	-4.758
C16H23BrN2O3	DB00409	Remoxipride	-4.338	-4.339
C20H24N2O6	DB00401	Nisoldipine	-4.336	-4.336
C22H24N2O8	DB00254	Doxycycline	-4.336	-5.03
C21H26NO3	DB00940	Methantheleine	-4.335	-4.335
C13H13N3O3	DB00480	Lenalidomide	-4.335	-4.335
C12H17N4OS	DB00152	Thiamine	-4.331	-4.35
C21H27NO4	DB00844	Nalbuphine	-4.33	-6.289
C5H10N2O7P2	DB00399	Zoledronic acid	-4.328	-4.873
C20H24N2O2	DB00468	Quinine	-4.328	-4.343
C9H18N2O4	DB00371	Meprobamate	-4.328	-4.328
C22H38O5	DB00929	Misoprostol	-4.327	-4.327
C16H16ClN3O4	DB00447	Loracarbef	-4.324	-4.621
C10H16Br2N2O2	DB00236	Pipobroman	-4.321	-4.321
C29H38N4O10	DB00256	Lymecycline	-4.317	-6.446
C8H11N3O3S	DB00709	Lamivudine	-4.308	-4.308
C17H18F3NO	DB00472	Fluoxetine	-4.306	-4.306
C16H16N2O6S2	DB00456	Cefalotin	-4.305	-4.305
C15H21F3N2O2	DB00176	Fluvoxamine	-4.294	-4.297
C16H13ClN2O	DB00579	Mazindol	-4.292	-4.3
C22H29FO4	DB00547	Desoximetasone	-4.292	-4.292
C22H24ClFN4O3	DB00317	Gefitinib	-4.291	-4.706
C17H19NO3	DB00295	Morphine	-4.288	-5.775
C21H27ClN2O2	DB00557	Hydroxyzine	-4.288	-4.891
C23H46N6O13	DB00452	Framycetin	-4.286	-6.147
C15H14ClN3O4S	DB00833	Cefaclor	-4.281	-4.514
C17H20FN3O3	DB00487	Pefloxacin	-4.281	-5.408
C22H23ClN6O	DB00678	Losartan	-4.279	-4.279
C19H12O6	DB00266	Dicoumarol	-4.279	-4.393
C13H18N4O3	DB00806	Pentoxifylline	-4.278	-4.278
C14H19Cl2N2O2	DB00291	Chlorambucil	-4.269	-4.272
C8H15N7O2S3	DB00927	Famotidine	-4.262	-4.747
C17H19N3O3S	DB00338	Omeprazole	-4.256	-4.29
C21H28O5	DB00860	Prednisolone	-4.254	-4.254

C31H33F3N2O5S	DB00932	Tipranavir	-4.254	-4.392
C15H12N2O	DB00564	Carbamazepine	-4.252	-4.252
C11H12N2O2S	DB00744	Zileuton	-4.252	-4.271
C21H30O2	DB00470	Dronabinol	-4.248	-4.248
C19H21N3O5	DB00270	Isradipine	-4.239	-4.239
C23H31NO7	DB00688	Mycophenolate mofetil	-4.236	-4.305
C13H14N2O3	DB00849	Methyphenobarbital	-4.236	-4.323
C15H14N4O	DB00238	Nevirapine	-4.233	-4.233
C18H19N3O3S	DB00412	Rosiglitazone	-4.231	-5.565
C22H22FN3O2	DB00450	Droperidol	-4.23	-4.329
C26H29NO	DB00675	Tamoxifen	-4.229	-4.249
C11H17NO3	DB00723	Methoxamine	-4.227	-4.237
C25H38O5	DB00641	Simvastatin	-4.226	-4.226
C21H21N	DB00735	Naftifine	-4.224	-4.304
C26H31Cl2N5O3	DB00251	Terconazole	-4.224	-4.47
C52H98N16O13	DB00803	Colistin	-4.217	-6.601
C8H5F3N2OS	DB00740	Riluzole	-4.214	-4.214
C20H21N7O6S2	DB00923	Ceforanide	-4.214	-6.123
C7H10N2OS	DB00550	Propylthiouracil	-4.213	-4.251
C16H17N3O4S	DB00567	Cephalexin	-4.204	-4.82
C21H26N2OS2	DB00933	Mesoridazine	-4.196	-4.197
C18H19N3O	DB00904	Ondansetron	-4.195	-4.32
C20H17FO3S	DB00605	Sulindac	-4.189	-4.189
C17H20FN3O3	DB00487	Pefloxacin	-4.187	-4.348
C22H29FO4	DB00324	Fluorometholone	-4.184	-4.184
C24H31FO6	DB00180	Flunisolide	-4.184	-4.184
C21H41N5O7	DB00955	Netilmicin	-4.184	-5.278
C10H16N2O3S	DB00121	Biotin	-4.181	-4.184
C13H16N2	DB00633	Dexmedetomidine	-4.18	-4.899
C13H12Cl2O4	DB00903	Etacrynic acid	-4.166	-4.166
C21H21ClN4OS	DB00246	Ziprasidone	-4.166	-4.397
C14H22N2O3	DB00335	Atenolol	-4.161	-4.162
C11H9B3N2O4	DB00271	Diatrizoate	-4.148	-4.148
C21H24FN3O4	DB00218	Moxifloxacin	-4.144	-5.242
C16H14F3N3O2S	DB00448	Lansoprazole	-4.141	-4.161
C17H14O4S	DB00533	Rofecoxib	-4.141	-4.141
C5H10N2O7P2	DB00399	Zoledronic acid	-4.139	-5.503
C25H30NO3	DB00209	Trospium	-4.136	-4.136
C22H28Cl2O4	DB00764	Mometasone	-4.133	-4.133
C8H11NO3	DB00165	Pyridoxine	-4.126	-4.841
C28H35FO7	DB00288	Amcinonide	-4.124	-4.124
C22H23N3O4	DB00530	Erlotinib	-4.124	-4.124
C18H19ClN4	DB00363	Clozapine	-4.123	-4.149
C15H16O2	DB00461	Nabumetone	-4.122	-4.122
C20H28N2O5	DB00584	Enalapril	-4.117	-4.868
C24H30O6	DB00700	Eplerenone	-4.116	-4.116
C22H26F3N3OS	DB00623	Fluphenazine	-4.114	-4.45
C13H20N6O4	DB00577	Valaciclovir	-4.111	-4.317
C18H24N4O	DB00889	Granisetron	-4.108	-4.109
C47H75NO17	DB00646	Nystatin	-4.107	-4.139
C15H14ClN3O4S	DB00833	Cefaclor	-4.107	-4.775
C20H30O2	DB00159	Icosapent	-4.107	-4.11
C20H32N5O8P	DB00718	Adefovir dipivoxil	-4.105	-4.105
C9H11ClO3	DB00856	Chlorphenesin	-4.102	-4.102
C9H7Cl2N5	DB00555	Lamotrigine	-4.099	-4.127
C5H10N2O7P2	DB00399	Zoledronic acid	-4.099	-5.631
C7H7NO3	DB00233	Aminosalicylic Acid	-4.094	-4.095
C20H24N2O2	DB00908	Quinidine	-4.086	-4.101
C19H12O6	DB00266	Dicoumarol	-4.084	-5.143
C21H22N2O5S	DB00607	Nafcillin	-4.082	-4.082
C14H18N4O3	DB00440	Trimethoprim	-4.08	-4.55
C8H11Cl2N3O2	DB00791	Uracil mustard	-4.072	-4.096
C33H47NO13	DB00826	Natamycin	-4.061	-5.702

C9H13NO2	DB00610	Metaraminol	-4.058	-4.068
C19H21N	DB00540	Nortriptyline	-4.057	-4.057
C14H14O3	DB00788	Naproxen	-4.055	-4.056
C12H14N2O2	DB00794	Primidone	-4.052	-4.052
C11H14N2O4	DB00949	Felbamate	-4.052	-4.052
C22H29NO2	DB00647	Dextropropoxyphene	-4.05	-4.054
C24H34O4	DB00603	Medroxyprogesterone acetate	-4.049	-4.049
C24H34N2O5	DB00519	Trandolapril	-4.049	-4.254
C14H18N4O3	DB00440	Trimethoprim	-4.045	-4.677
C21H41N5O7	DB00955	Netilmicin	-4.045	-6.575
C17H19CIN2S	DB00477	Chlorpromazine	-4.042	-4.043
C19H30O3	DB00621	Oxandrolone	-4.038	-4.038
C21H30O2	DB00396	Progesterone	-4.038	-4.038
C17H21NO3	DB00674	Galantamine	-4.035	-4.052
C13H17NO	DB00265	Crotamiton	-4.035	-4.035
C15H14O3	DB00573	Fenoprofen	-4.034	-4.035
C17H14N2O3	DB00817	Rosoxacin	-4.034	-5.308
C24H32O4	DB00823	Ethynodiol diacetate	-4.034	-4.034
C23H25N5O5	DB00590	Doxazosin	-4.031	-5.07
C24H28N2O5	DB00542	Benazepril	-4.03	-4.387
C19H17CIFN3O5S	DB00301	Flucloxacillin	-4.026	-4.026
C8H15N7O2S3	DB00927	Famotidine	-4.024	-5.004
C21H34NO3	DB00219	Oxyphenonium	-4.018	-4.018
C36H47N5O4	DB00224	Indinavir	-4.014	-5.16
C19H21N3O	DB00425	Zolpidem	-4.013	-4.356
C19H27NO3	DB00731	Nateglinide	-4.012	-4.012
C8H17NO5	DB00491	Miglitol	-4.009	-5.568
C24H26N6O3	DB00275	Olmesartan	-4.009	-5.122
C17H14F3N3O2S	DB00482	Celecoxib	-4.006	-4.007
C21H27NO	DB00333	Methadone	-4.005	-4.008
C18H16O3	DB00946	Phenprocoumon	-4	-4.049
C13H16N2O2	DB00357	Aminoglutethimide	-3.998	-3.999
C17H25N3O5S	DB00760	Meropenem	-3.998	-5.799
C19H16CINO4	DB00328	Indometacin	-3.995	-3.996
C21H31N3O5	DB00722	Lisinopril	-3.995	-4.991
C18H37N5O9	DB00684	Tobramycin	-3.991	-4.262
C12H12N2O2S	DB00250	Dapsone	-3.99	-3.99
C21H26CIN3OS	DB00850	Perphenazine	-3.987	-4.324
C11H11NO2	DB00832	Phensuximide	-3.983	-3.983
C17H17ClO6	DB00400	Griseofulvin	-3.982	-3.982
C20H21N	DB00924	Cyclobenzaprine	-3.973	-3.977
C14H22N2O	DB00281	Lidocaine	-3.972	-3.993
C9H15N5O	DB00350	Minoxidil	-3.97	-3.97
C21H23NO3	DB00768	Olopatadine	-3.965	-3.965
C22H26NO3	DB00771	Clidinium	-3.964	-3.964
C19H17Cl3N2S	DB00639	Butoconazole	-3.964	-4.408
C12H11N7	DB00384	Triamterene	-3.962	-3.963
C15H12I3NO4	DB00279	Liothyronine	-3.96	-5.051
C17H21NO	DB00289	Atomoxetine	-3.954	-3.955
C35H36CINO3S	DB00471	Montelukast	-3.954	-3.954
C10H19N3O2	DB00226	Guanadrel	-3.952	-3.952
C21H28O2	DB00378	Dydrogesterone	-3.951	-3.951
C11H12N4O3S	DB00664	Sulfametopyrazine	-3.948	-4.062
C18H37N5O9	DB00684	Tobramycin	-3.946	-5.557
C47H73NO17	DB00681	Amphotericin B	-3.939	-5.579
C14H11Cl2NO2	DB00586	Diclofenac	-3.938	-3.94
C8H10FN3O3S	DB00879	Emtricitabine	-3.935	-3.935
C10H19O6PS2	DB00772	Malathion	-3.934	-3.934
C17H28N2O3	DB00892	Oxybuprocaine	-3.933	-3.954
C17H21NO4	DB00747	Scopolamine	-3.931	-4.641
C14H18N2O3	DB00474	Methohexital	-3.927	-3.984
C19H21N5O2	DB00670	Pirenzepine	-3.925	-4.21
C16H16CINO2S	DB00758	Clopidogrel	-3.924	-3.947

C19H19N7O6	DB00158	Folic acid	-3.92	-5.061
C9H4Cl3IO	DB00793	Haloproglin	-3.916	-3.916
C14H16N4	DB00724	Imiquimod	-3.914	-4.4
C18H19N3O6S	DB00689	Cephaloglycin	-3.913	-4.546
C22H28N6O3S	DB00705	Delavirdine	-3.91	-4.072
C21H22N4O6S	DB00293	Raltitrexed	-3.91	-5.258
C17H14N2O3	DB00817	Rosoxacin	-3.902	-3.976
C10H13NO3	DB00765	Metyrosine	-3.899	-3.899
C15H19N5	DB00953	Rizatriptan	-3.899	-3.903
C15H15NO3	DB00500	Tolmetin	-3.898	-3.899
C21H21ClN4OS	DB00246	Ziprasidone	-3.893	-4.563
C16H16ClNO3	DB00800	Fenoldopam	-3.891	-3.917
C17H20N4S	DB00334	Olanzapine	-3.889	-3.932
C14H24N2O7	DB00919	Spectinomycin	-3.886	-5.255
C17H26N2O	DB00296	Ropivacaine	-3.882	-3.937
C10H15NO	DB00852	Pseudoephedrine	-3.879	-3.885
C17H19NO3	DB00327	Hydromorphone	-3.877	-3.928
C17H16F6N2O	DB00358	Mefloquine	-3.875	-3.878
C8H15N7O2S3	DB00927	Famotidine	-3.874	-4.68
C8H10NO6P	DB00114	Pyridoxal phosphate	-3.867	-5.283
C12H10F3N3O4	DB00665	Nilutamide	-3.863	-3.863
C16H19N3O4S	DB00415	Ampicillin	-3.862	-4.538
C17H16ClN3O	DB00543	Amoxapine	-3.853	-3.866
C20H28O2	DB00523	Alitretinoin	-3.853	-3.857
C15H13FO2	DB00712	Flurbiprofen	-3.852	-3.852
C19H24O3	DB00894	Testolactone	-3.852	-3.852
C19H35NO2	DB00804	Dicyclomine	-3.849	-3.865
C25H35N3O6S	DB00701	Amprenavir	-3.847	-3.847
C16H20FN3O4	DB00601	Linezolid	-3.846	-3.846
C17H19N3O	DB00692	Phentolamine	-3.844	-3.844
C13H20N2O	DB00750	Prilocaine	-3.84	-3.902
C59H84N18O14	DB00014	Goserelin	-3.837	-4.372
C8H11N5O3	DB00787	Acyclovir	-3.835	-3.835
C20H26N4O	DB00589	Lisuride	-3.831	-4.269
C14H12O3S	DB00870	Suprofen	-3.829	-3.829
C21H27ClN2O2	DB00557	Hydroxyzine	-3.828	-5.553
C15H12ClNO2	DB00821	Carprofen	-3.827	-3.828
C11H16N4O4	DB00380	Dexrazoxane	-3.826	-4.699
C12H15N3O2S	DB00518	Albendazole	-3.826	-3.911
C12H18O	DB00818	Propofol	-3.82	-3.82
C12H15NO3	DB00660	Metaxalone	-3.819	-3.819
C16H13ClN2O2	DB00231	Temazepam	-3.817	-3.817
C24H31ClO7	DB14596	Loteprednol etabonate	-3.816	-3.816
C8H6N4O5	DB00698	Nitrofurantoin	-3.81	-3.883
C15H11I4NO4	DB00451	Levothyroxine	-3.81	-4.798
C16H19BrN2	DB00405	Dexbrompheniramine	-3.805	-3.805
C8H12N4O5	DB00928	Azacitidine	-3.8	-6.484
C13H20N6O4	DB00577	Valaciclovir	-3.796	-4.522
C6H6N6O2	DB00853	Temozolomide	-3.796	-3.797
C22H27ClF2O4	DB00596	Ulobetasol	-3.793	-3.793
C11H11F3N2O3	DB00499	Flutamide	-3.79	-3.79
C17H27NO2	DB00285	Venlafaxine	-3.789	-3.789
C16H13ClN2O2	DB00349	Clobazam	-3.786	-4.224
C20H24N2OS	DB00777	Propiomazine	-3.784	-3.785
C25H31F3O5S	DB00588	Fluticasone propionate	-3.783	-3.783
C13H24N4O3S	DB00373	Timolol	-3.781	-3.782
C17H18FN3O3	DB00537	Ciprofloxacin	-3.781	-3.88
C12H13ClN4	DB00205	Pyrimethamine	-3.776	-4.255
C15H10O2	DB00498	Phenindione	-3.772	-3.773
C15H17FN4O3	DB00467	Enoxacin	-3.762	-5.385
C9H13NO2	DB00388	Phenylephrine	-3.759	-3.766
C16H17N3O4S	DB00567	Cephalexin	-3.759	-4.017
C19H24N2O	DB00377	Palonosetron	-3.758	-3.759

C20H34GdN5O10	DB00538	Gadoversetamide	-3.757	-5.271
C52H98N16O13	DB00803	Colistin	-3.754	-6.177
C6H8O6	DB00126	Ascorbic acid	-3.753	-3.753
C18H18ClN3O	DB00408	Loxapine	-3.752	-3.785
C8H10NO6P	DB00114	Pyridoxal phosphate	-3.75	-3.842
C8H10NO6P	DB00114	Pyridoxal phosphate	-3.747	-5.705
C12H12N2O3	DB00779	Nalidixic acid	-3.747	-3.792
C21H26ClNO	DB00283	Clemastine	-3.746	-3.747
C12H11ClN2O5S	DB00695	Furosemide	-3.742	-3.742
C18H21NO4	DB00497	Oxycodone	-3.737	-3.833
C6H8ClN7O	DB00594	Amiloride	-3.737	-3.738
C15H14ClN3O4S3	DB00562	Benzthiazide	-3.736	-4.039
C19H30N5O10P	DB00300	Tenofovir disoproxil	-3.735	-3.735
C18H19N3O	DB00904	Ondansetron	-3.735	-4.718
C22H32O3	DB00253	Medrysone	-3.729	-3.729
C28H27NO4S	DB00481	Raloxifene	-3.724	-3.739
C17H12ClF3N2O	DB00801	Halazepam	-3.723	-3.723
C32H26N4O2	DB00872	Conivaptan	-3.722	-4.635
C14H11ClN2O4S	DB00310	Chlorthalidone	-3.721	-3.723
C23H30NO3	DB00782	Propantheline	-3.72	-3.72
C19H29NO	DB00387	Procyclidine	-3.719	-3.719
C13H6Cl6O2	DB00756	Hexachlorophene	-3.714	-3.723
C14H13N3O4S2	DB00814	Meloxicam	-3.714	-3.729
C19H24N2	DB00458	Imipramine	-3.712	-3.712
C19H21N	DB00344	Protriptyline	-3.709	-3.709
C16H20N4O3S	DB00214	Torsemide	-3.704	-4.13
C24H34N2O5	DB00519	Trandolapril	-3.701	-4.429
C16H19N3O4S	DB00415	Ampicillin	-3.699	-3.927
C11H8O2	DB00170	Menadiolone	-3.691	-3.691
C15H21NO2	DB00454	Meperidine	-3.691	-3.705
C36H42N2	DB00941	Hexafluoronium	-3.686	-3.686
C18H37N5O9	DB00684	Tobramycin	-3.684	-6.282
C20H31NO	DB00376	Trihexyphenidyl	-3.684	-3.685
C17H32BrNO2	DB00517	Anisotropine methylbromide	-3.684	-3.684
C19H32N2O5	DB00790	Perindopril	-3.682	-4.305
C23H25F3N2O5	DB00875	Flupentixol	-3.666	-3.905
C12H12N2O3	DB00779	Nalidixic acid	-3.662	-5.223
C20H25NO2S2	DB00906	Tiagabine	-3.662	-3.662
C11H12N2O2	DB00754	Ethotoin	-3.659	-3.659
C22H28N2O2	DB00913	Anileridine	-3.657	-3.679
C29H38N4O10	DB00256	Lymecycline	-3.655	-5.515
C17H20N2S	DB00420	Promazine	-3.652	-3.653
C9H13NO	DB00397	Phenylpropanolamine	-3.649	-3.659
C12H9N3O	DB00235	Milrinone	-3.648	-3.666
C20H28O2	DB00755	Tretinoin	-3.647	-3.651
C10H14N2O4	DB00190	Carbidopa	-3.645	-3.645
C5H5N5S	DB00352	Tioguanine	-3.642	-3.66
C14H16N4	DB00724	Imiquimod	-3.64	-3.984
C24H36O3	DB00486	Nabilone	-3.639	-3.639
C16H21N3	DB00792	Tripelennamine	-3.636	-3.641
C15H11I4NO4	DB00509	Dextrothyroxine	-3.636	-4.624
C18H28N2O	DB00297	Bupivacaine	-3.635	-3.689
C17H22N4O	DB00805	Minaprine	-3.632	-3.726
C20H26N2	DB00726	Trimipramine	-3.631	-3.631
C24H26BrN3O3	DB00699	Nicergoline	-3.63	-5.211
C8H8Cl2N4	DB00629	Guanabenz	-3.627	-3.627
C24H32O4S	DB00421	Spirolactone	-3.624	-3.624
C20H36N2O3S	DB00308	Ibutilide	-3.622	-3.633
C12H9N3O5S	DB00507	Nitazoxanide	-3.621	-3.636
C12H10N2O5	DB00827	Cinoxacin	-3.618	-5.462
C16H15F2N3O4S	DB00213	Pantoprazole	-3.618	-3.92
C18H37N5O9	DB00684	Tobramycin	-3.616	-4.969
C16H14F3N5O	DB00582	Voriconazole	-3.615	-3.615

C18H14N4O5S	DB00795	Sulfasalazine	-3.613	-4.92
C10H7Cl2N3O	DB00261	Anagrelide	-3.613	-3.613
C9H8O4	DB00945	Acetylsalicylic acid	-3.606	-3.606
C14H10Cl4	DB00648	Mitotane	-3.603	-3.603
C9H11NO3	DB00135	Tyrosine	-3.602	-3.602
C6H12N2O4S2	DB00138	Cystine	-3.598	-3.627
C14H11NO5	DB00323	Tolcapone	-3.594	-5.131
C27H38N2O4	DB00661	Verapamil	-3.593	-3.598
C17H19N3O3S	DB00736	Esomeprazole	-3.592	-3.685
C22H28N2O	DB00813	Fentanyl	-3.588	-3.605
C17H24BrNO3	DB00725	Homatropine methylbromide	-3.587	-3.588
C22H30N6O4S	DB00203	Sildenafil	-3.586	-3.768
C12H14N2O2	DB00532	Mephenytoin	-3.574	-3.574
C16H16ClN3O3S	DB00524	Metolazone	-3.569	-3.571
C18H19N3O3S	DB00412	Rosiglitazone	-3.568	-4.945
C15H25NO3	DB00264	Metoprolol	-3.566	-3.567
C12H10N2O5	DB00827	Cinoxacin	-3.565	-3.592
C29H50O2	DB00163	Vitamin E	-3.562	-3.562
C24H34O3	DB00896	Rimexolone	-3.562	-3.562
C19H20FNO3	DB00715	Paroxetine	-3.562	-3.563
C20H23N	DB00934	Maprotiline	-3.56	-3.56
C65H82N2O18S2	DB00732	Atracurium besylate	-3.557	-3.557
C24H30F2O6	DB00591	Fluocinolone acetonide	-3.556	-3.556
C11H12N2O2	DB00150	L-Tryptophan	-3.554	-3.554
C19H27N3O5S2	DB00204	Dofetilide	-3.554	-3.62
C12H18N2O4	DB00211	Midodrine	-3.554	-4.615
C7H11NO2	DB00593	Ethosuximide	-3.553	-3.554
C20H15F3N4O3	DB00685	Trovafloxacin	-3.549	-3.595
C11H18N2O2S	DB00599	Thiopental	-3.547	-3.574
C22H17ClN2	DB00257	Clotrimazole	-3.546	-3.97
C14H16ClN3O4S2	DB00606	Cyclothiazide	-3.543	-3.555
C12H18N2O3	DB00418	Secobarbital	-3.542	-3.644
C15H22N6O5S	DB00118	Ademetionine	-3.53	-5.932
C29H31N7O	DB00619	Imatinib	-3.528	-4.283
C9H10N2O3	DB00345	Aminohippuric acid	-3.526	-3.526
C10H20O	DB00825	Levomenthol	-3.524	-3.524
C7H7NO3	DB00244	Mesalazine	-3.524	-3.527
C15H12N2O2	DB00252	Phenytoin	-3.519	-3.884
C10H12N4O3	DB00900	Didanosine	-3.518	-3.601
C6H14FO3P	DB00677	Isoflurophate	-3.511	-3.511
C10H17N3S	DB00413	Pramipexole	-3.508	-3.508
C20H26N4O	DB00589	Lisuride	-3.503	-3.887
C20H23N	DB00321	Amitriptyline	-3.502	-3.505
C17H22N2O	DB00366	Doxylamine	-3.5	-3.504
C8H15NO2	DB00302	Tranexamic acid	-3.497	-3.497
C17H20N2O5S	DB00887	Bumetanide	-3.491	-3.491
C18H19F3N2S	DB00508	Triflupromazine	-3.487	-3.488
C10H16N2O3	DB00237	Butabarbital	-3.487	-3.522
C21H27N3O2	DB00247	Methysergide	-3.486	-4.114
C16H13ClN2O	DB00829	Diazepam	-3.486	-3.486
C16H13N3O3	DB00643	Mebendazole	-3.482	-4.096
C21H26N2S2	DB00679	Thioridazine	-3.48	-3.481
C15H20N2O4S	DB00414	Acetohehexamide	-3.474	-3.479
C6H6N4O4	DB00336	Nitrofurural	-3.473	-3.473
C16H13ClN2O2	DB00349	Clobazam	-3.47	-3.855
C11H16N2O3	DB00306	Talbutal	-3.47	-3.525
C6H7N3O	DB00951	Isoniazid	-3.47	-3.471
C19H21N3O	DB00425	Zolpidem	-3.468	-3.954
C7H8N4O2	DB00277	Theophylline	-3.466	-3.498
C17H17ClN6O3	DB00402	Eszopiclone	-3.459	-3.937
C9H13N	DB00182	Amphetamine	-3.458	-3.459
C21H29NO2	DB00611	Butorphanol	-3.458	-3.469
C15H14ClN3O4S3	DB00562	Benzthiazide	-3.452	-4

C12H19NO3	DB00871	Terbutaline	-3.449	-3.463
C8H10N2S	DB00609	Ethionamide	-3.446	-3.447
C66H75Cl2N9O24	DB00512	Vancomycin	-3.446	-5.928
C24H26BrN3O3	DB00699	Nicergoline	-3.445	-3.487
C7H6O3	DB00936	Salicylic acid	-3.44	-3.44
C15H18N4O5	DB00305	Mitomycin	-3.437	-3.454
C29H41NO4	DB00921	Buprenorphine	-3.432	-3.432
C11H17NO	DB00379	Mexiletine	-3.431	-3.436
C10H21NO4	DB00419	Miglustat	-3.427	-5.474
C5H10N2O3	DB00130	L-Glutamine	-3.423	-3.423
C10H12ClNO2	DB00181	Baclofen	-3.422	-3.422
C27H34N2O7	DB00691	Moexipril	-3.421	-3.575
C20H34GdN5O10	DB00538	Gadoversetamide	-3.415	-5.289
C32H41NO2	DB00342	Terfenadine	-3.414	-3.417
C12H21NO8S	DB00273	Topiramate	-3.412	-3.422
C31H33N3O6S	DB00549	Zafirlukast	-3.411	-3.417
C21H28N2O5	DB00662	Trimethobenzamide	-3.409	-5.422
C8H10N4O2	DB00824	Enprofylline	-3.405	-3.464
C21H23ClFNO2	DB00502	Haloperidol	-3.405	-3.418
C16H19BrN2	DB00835	Brompheniramine	-3.404	-3.404
C6H13NO2	DB00513	Aminocaproic Acid	-3.401	-3.401
C14H18N2O3	DB00474	Methohexital	-3.4	-4.812
C14H19N5O4	DB00426	Famciclovir	-3.397	-3.397
C11H16N4O4	DB00380	Dexrazoxane	-3.392	-4.585
C6H9N3O2	DB00117	Histidine	-3.387	-3.821
C14H16N2O2	DB00292	Etomidate	-3.386	-3.397
C16H24N2O	DB00268	Ropinirole	-3.386	-3.387
C12H21N5O2S2	DB00585	Nizatidine	-3.379	-3.379
C14H18N4O3	DB00440	Trimethoprim	-3.377	-4.32
C17H19N3	DB00370	Mirtazapine	-3.374	-3.462
C19H21N5O4	DB00457	Prazosin	-3.372	-4.614
C19H27N5O4	DB00346	Alfuzosin	-3.366	-3.366
C4H8N2O3	DB00174	Asparagine	-3.359	-3.359
C2H5NO2	DB00551	Acetohydroxamic acid	-3.357	-3.36
C20H24ClN3S	DB00433	Prochlorperazine	-3.355	-3.964
C23H31NO7	DB00688	Mycophenolate mofetil	-3.352	-5.107
C12H15ClO3	DB00636	Clofibrate	-3.35	-3.35
C17H13ClN4	DB00404	Alprazolam	-3.35	-3.352
C14H15N3O5	DB00494	Entacapone	-3.348	-3.348
C59H84N18O14	DB00014	Goserelin	-3.348	-3.975
C22H23ClN2O2	DB00455	Loratadine	-3.34	-3.366
C16H28N2O4	DB00198	Oseltamivir	-3.34	-4.552
C25H27ClN2	DB00737	Meclizine	-3.34	-3.533
C16H16ClN3O3S	DB00808	Indapamide	-3.333	-3.336
C20H28N2O5S	DB00706	Tamsulosin	-3.327	-3.327
C5H5N3O	DB00339	Pyrazinamide	-3.325	-3.325
C8H9NO2	DB00316	Acetaminophen	-3.32	-3.321
C21H16ClF3N4O3	DB00398	Sorafenib	-3.32	-3.332
C6H13N3O3	DB00155	L-Citrulline	-3.319	-3.319
C21H43N5O7	DB00798	Gentamicin	-3.317	-4.93
C13H14N2O3	DB00849	Methylphenobarbital	-3.315	-4.491
C14H12O2	DB00676	Benzyl benzoate	-3.311	-3.311
C22H28O2	DB00294	Etonogestrel	-3.301	-3.301
C19H21N5O4	DB00457	Prazosin	-3.292	-3.384
C21H26O3	DB00459	Acitretin	-3.291	-3.294
C20H23NO4	DB00704	Naltrexone	-3.29	-5.021
C13H12F2N6O	DB00196	Fluconazole	-3.289	-3.289
C4H6O4S2	DB00566	Succimer	-3.288	-3.288
C7H15NO3	DB00583	Levocarnitine	-3.287	-3.287
C29H31N7O	DB00619	Imatinib	-3.286	-3.493
C10H8N6O	DB00885	Pemirolast	-3.279	-3.28
C11H18N2O3	DB00312	Pentobarbital	-3.279	-3.314
C19H24N2S	DB00392	Profenamine	-3.277	-3.279

C18H21NO3	DB00318	Codeine	-3.277	-4.821
C6H14N2O2	DB00123	L-Lysine	-3.268	-3.268
C17H23NO	DB00854	Levorphanol	-3.263	-3.268
C8H8N2O3S	DB00909	Zonisamide	-3.262	-3.264
C19H21N5O2	DB00670	Pirenzepine	-3.258	-3.899
C15H23N3O4S	DB00391	Sulpiride	-3.258	-3.258
C23H25F3N2OS	DB00875	Flupentixol	-3.253	-4.062
C11H16N2O3	DB00241	Butalbital	-3.244	-3.299
C6H10N6O	DB00851	Dacarbazine	-3.244	-3.277
C22H25N3O7S	DB00303	Ertapenem	-3.244	-4.745
C8H10N4O2	DB00201	Caffeine	-3.241	-3.241
C20H22N8O5	DB00563	Methotrexate	-3.232	-4.668
C11H10BrN5	DB00484	Brimonidine	-3.229	-3.278
C21H41N5O7	DB00955	Netilmicin	-3.228	-3.866
C6H14N4O2	DB00125	L-Arginine	-3.226	-3.226
C5H4N4O	DB00437	Allopurinol	-3.225	-3.328
C5H9N3	DB00272	Betazole	-3.224	-3.635
C24H29N5O3	DB00177	Valsartan	-3.223	-3.223
C15H11ClN2O2	DB00842	Oxazepam	-3.22	-3.22
C13H17N5O8S2	DB00355	Aztreonam	-3.216	-3.216
C21H21N	DB00434	Cyproheptadine	-3.212	-3.221
C13H22N4O3S	DB00863	Ranitidine	-3.21	-3.662
C6H9N3O2	DB00117	Histidine	-3.203	-3.659
C19H27N3O5S2	DB00204	Dofetilide	-3.202	-4.75
CH3O5P	DB00529	Foscarnet	-3.201	-3.207
C17H19NO3	DB00327	Hydromorphone	-3.198	-4.936
C5H12N2O2	DB00129	Ornithine	-3.195	-3.195
C18H13Cl4N3O	DB00239	Oxiconazole	-3.193	-3.306
C21H25ClN2O3	DB00341	Cetirizine	-3.193	-3.604
C43H55N5O7	DB00309	Vindesine	-3.192	-3.382
C9H8ClN5S	DB00697	Tizanidine	-3.192	-3.357
C19H22ClN5O	DB00656	Trazodone	-3.187	-3.605
C9H11Cl2N3O4S2	DB00232	Methyclothiazide	-3.169	-3.169
C6H9N3O3	DB00916	Metronidazole	-3.166	-3.166
C10H24N2O2	DB00330	Ethambutol	-3.164	-3.342
C24H30N2O2	DB00561	Doxapram	-3.163	-3.511
C17H20FN3O3	DB00487	Pefloxacin	-3.152	-5.611
C13H6Cl6O2	DB00756	Hexachlorophene	-3.148	-5.67
C10H7N3S	DB00730	Thiabendazole	-3.147	-3.147
C19H17Cl3N2S	DB00639	Butoconazole	-3.143	-3.522
C26H29N3O6	DB00622	Nicardipine	-3.14	-3.361
C8H16O2	DB00313	Valproic Acid	-3.138	-3.14
C23H32N6O4S	DB00862	Vardenafil	-3.134	-3.905
C23H32N6O4S	DB00862	Vardenafil	-3.131	-3.81
C16H14N2O3S	DB00580	Valdecocixib	-3.122	-3.122
C5H9NO3	DB00855	Aminolevulinic acid	-3.12	-3.819
C11H16N4O4	DB00380	Dexrazoxane	-3.113	-4.041
C2H7NS	DB00847	Cysteamine	-3.113	-3.136
C32H26N4O2	DB00872	Conivaptan	-3.111	-3.888
C21H31N5O2	DB00490	Buspirone	-3.111	-3.616
C29H33ClN2O2	DB00836	Loperamide	-3.111	-3.14
C18H26ClN3	DB00608	Chloroquine	-3.109	-3.145
C12H16F3N	DB00574	Fenfluramine	-3.107	-3.107
C9H11FN2O5	DB00322	Floxuridine	-3.1	-4.886
C28H27NO4S	DB00481	Raloxifene	-3.1	-5.562
C21H43N5O7	DB00798	Gentamicin	-3.098	-5.087
C7H6ClN3O4S2	DB00880	Chlorothiazide	-3.097	-3.41
C8H13N3O4S	DB00911	Tinidazole	-3.096	-3.096
C11H16N4O4	DB00380	Dexrazoxane	-3.095	-4.673
C15H10Cl2N2O2	DB00186	Lorazepam	-3.093	-3.093
C19H19N3O5S	DB00713	Oxacillin	-3.092	-3.092
C9H11NO2	DB00120	L-Phenylalanine	-3.086	-3.086
C9H10N4O2S2	DB00576	Sulfamethizole	-3.085	-3.101

C21H41N5O7	DB00955	Netilmicin	-3.083	-5.213
C16H24N2O	DB00935	Oxymetazoline	-3.08	-3.08
C18H13ClFN3	DB00683	Midazolam	-3.076	-3.288
C40H48I2N2O6	DB00416	Metocurine Iodide	-3.069	-3.069
C7H11NO3	DB00617	Paramethadione	-3.063	-3.063
C21H25NO	DB00245	Benzatropine	-3.062	-3.064
C9H8ClN5S	DB00697	Tizanidine	-3.057	-3.894
C20H23NS	DB00340	Metixene	-3.051	-3.051
C18H21NO3	DB00956	Hydrocodone	-3.046	-4.834
C33H34N6O6	DB00796	Candesartan cilexetil	-3.039	-3.195
C8H10N2O3S	DB00634	Sulfacetamide	-3.037	-3.055
C26H31Cl2N5O3	DB00251	Terconazole	-3.035	-4.192
CH5N3	DB00536	Guanidine	-3.035	-3.035
C18H25NO	DB00514	Dextromethorphan	-3.03	-3.034
C16H15F2N3O4S	DB00213	Pantoprazole	-3.027	-3.734
C15H13NO3	DB00465	Ketorolac	-3.024	-3.025
C46H62N4O11	DB00615	Rifabutin	-3.019	-3.228
C51H79NO13	DB00877	Sirolimus	-3.016	-3.018
C14H20GdN3O10	DB00789	Gadopentetic acid	-3.015	-5.192
C16H23NO2	DB00473	Hexylcaine	-3.01	-3.011
C20H15F3N4O3	DB00685	Trovafloxacin	-3.009	-4.905
C14H29NaO4S	DB00464	Sodium Tetradecyl Sulfate	-3.007	-3.007
C8H14O2S2	DB00166	Lipoic Acid	-3.006	-3.009
C22H28N6O3S	DB00705	Delavirdine	-3.006	-3.876
C8H12N2	DB00780	Phenelzine	-3.003	-3.358
C16H28N2O4	DB00198	Oseltamivir	-3	-3.082
C4H6O4	DB00139	Succinic acid	-2.998	-3.004
C18H14N4O5S	DB00795	Sulfasalazine	-2.998	-3.761
C10H15N5	DB00914	Phenformin	-2.993	-3.01
C21H29N3O	DB00280	Disopyramide	-2.991	-2.996
C3H7NO2S	DB00151	L-Cysteine	-2.989	-3.003
C10H15N	DB00191	Phentermine	-2.988	-2.989
C5H9Cl2N3O2	DB00262	Carmustine	-2.986	-2.986
C19H25NO	DB00504	Levallorphan	-2.979	-4.815
C17H12Cl2N4	DB00897	Triazolam	-2.976	-2.977
C18H22ClNO	DB00925	Phenoxybenzamine	-2.97	-3.344
C20H22ClN3O	DB00613	Amodiaquine	-2.97	-3.564
C16H16ClNO3	DB00800	Fenoldopam	-2.97	-4.958
C22H17ClN2	DB00257	Clotrimazole	-2.968	-3.367
C4H9NO3	DB00156	L-Threonine	-2.962	-2.962
C18H13ClFN3	DB00683	Midazolam	-2.953	-3.666
C24H30N2O2	DB00561	Doxapram	-2.952	-3.432
C14H9ClF3NO2	DB00625	Efavirenz	-2.944	-2.944
C8H15N7O2S3	DB00927	Famotidine	-2.935	-4.234
C22H28N2O2	DB00913	Anileridine	-2.934	-4.946
C14H21N3O3S	DB00839	Tolazamide	-2.914	-2.938
C22H29N3S2	DB00372	Thiethylperazine	-2.91	-3.519
C26H28N2	DB00568	Cinnarizine	-2.906	-2.994
C17H20FN3O3	DB00487	Pefloxacin	-2.905	-4.464
C23H31NO7	DB00688	Mycophenolate mofetil	-2.902	-4.61
C21H43N5O7	DB00798	Gentamicin	-2.9	-4.597
C17H21NO4	DB00907	Cocaine	-2.9	-2.957
C5H5N5	DB00173	Adenine	-2.898	-2.919
C12H13ClN4	DB00205	Pyrimethamine	-2.898	-3.634
C14H19NO2	DB00422	Methylphenidate	-2.897	-2.897
C17H19N3O3S	DB00736	Esomeprazole	-2.895	-4.291
C5H11NO4S	DB00659	Acamprosate	-2.892	-2.892
C10H20N2S4	DB00822	Disulfiram	-2.887	-2.887
C13H20N2O	DB00750	Prilocaine	-2.887	-4.257
C10H13ClN2O3S	DB00672	Chlorpropamide	-2.885	-2.892
C7H4ClNO2	DB00356	Chlorzoxazone	-2.883	-2.916
C6H5NO2	DB00627	Niacin	-2.881	-2.89
C6H9NO3	DB00347	Trimethadione	-2.875	-2.875

C19H23NO3	DB00234	Reboxetine	-2.874	-4.582
C21H25N	DB00857	Terbinafine	-2.869	-2.991
C12H24N2O4	DB00395	Carisoprodol	-2.862	-2.862
C18H16O3	DB00946	Phenprocoumon	-2.856	-4.357
C16H20N4O3S	DB00214	Torsemide	-2.853	-3.263
C16H25NO4	DB00187	Esmolol	-2.846	-2.848
C32H26N4O2	DB00872	Conivaptan	-2.846	-3.237
C18H13Cl4N3O	DB00239	Oxiconazole	-2.843	-3.882
C12H20N2O3S	DB00489	Sotalol	-2.836	-4.819
C11H21N	DB00657	Mecamylamine	-2.835	-2.835
C18H20N2S	DB00902	Methdilazine	-2.827	-2.827
C21H21ClN2O8	DB00618	Demeclocycline	-2.825	-5.338
C3H7NO3	DB00133	Serine	-2.823	-2.823
C7H10N2O2S	DB00389	Carbimazole	-2.82	-2.82
C12H13ClN4	DB00205	Pyrimethamine	-2.82	-3.606
C13H11N3O4S2	DB00469	Tenoxicam	-2.815	-2.816
C33H37N5O5	DB00320	Dihydroergotamine	-2.814	-4.54
C4H3FN2O2	DB00544	Fluorouracil	-2.814	-3.014
C18H21NO4	DB00497	Oxycodone	-2.806	-3.926
C14H14ClNS	DB00208	Ticlopidine	-2.802	-2.976
C21H23ClFN3O	DB00690	Flurazepam	-2.802	-2.814
C23H29ClFN3O4	DB00604	Cisapride	-2.798	-2.887
C5H11NO2S	DB00859	Penicillamine	-2.794	-2.808
C15H14F3N3O4S2	DB00436	Bendroflumethiazide	-2.792	-2.859
C21H41N5O7	DB00955	Netilmicin	-2.791	-5.241
C28H28O3	DB00210	Adapalene	-2.786	-2.786
C11H15NO	DB00830	Phenmetrazine	-2.783	-2.789
C22H46O	DB00632	Docosanol	-2.779	-2.779
C24H29NO3	DB00843	Donepezil	-2.772	-2.776
C46H56N4O10	DB00541	Vincristine	-2.768	-3.862
C17H21N	DB00865	Benzphetamine	-2.757	-2.797
C6H6Cl6	DB00431	Lindane	-2.745	-2.745
C21H19N3O3S	DB00276	Amsacrine	-2.74	-4.787
C14H20GdN3O10	DB00789	Gadopentetic acid	-2.739	-4.578
C14H12N6O	DB00922	Levosimendan	-2.732	-2.813
C21H26ClN3OS	DB00850	Perphenazine	-2.732	-4.702
C4H10N2	DB00592	Piperazine	-2.727	-2.741
C5H9N3	DB00272	Betazole	-2.727	-3.137
C6H13NO2	DB00149	L-Leucine	-2.723	-2.723
C19H22N2	DB00427	Tripolidine	-2.721	-2.724
C10H14N2	DB00184	Nicotine	-2.718	-2.743
C14H14ClNS	DB00208	Ticlopidine	-2.712	-3.522
C17H19N3O3S	DB00736	Esomeprazole	-2.707	-4.476
C26H29NO	DB00675	Tamoxifen	-2.706	-4.719
C17H17NO2	DB00714	Apomorphine	-2.704	-2.748
C46H62N4O11	DB00615	Rifabutin	-2.702	-3.421
C21H25ClN2O3	DB00341	Cetirizine	-2.696	-3.161
C5H9NO4	DB00142	Glutamic Acid	-2.693	-2.693
C13H14N2	DB00382	Tacrine	-2.69	-2.69
C18H27NO2	DB00645	Dyclonine	-2.689	-2.695
C17H20N2O2	DB00809	Tropicamide	-2.686	-5.244
C6H8N2O8	DB00883	Isosorbide dinitrate	-2.683	-2.683
C4H9N3O2	DB00148	Creatine	-2.683	-2.683
C5H14NO	DB00122	Choline	-2.681	-2.681
C23H25N5O5	DB00590	Doxazosin	-2.674	-2.804
C11H10BrN5	DB00484	Brimonidine	-2.669	-4.171
C20H22N2	DB00719	Azatadine	-2.666	-2.671
C8H17NO2	DB00230	Pregabalin	-2.657	-2.657
C24H33N3O4	DB00243	Ranolazine	-2.652	-4.506
C13H16N2	DB00633	Dexmedetomidine	-2.651	-3.438
C22H25N3O4S	DB00680	Moricizine	-2.649	-2.839
C7H9ClO	DB00189	Ethchlorvynol	-2.646	-2.646
C21H27NO4	DB00844	Nalbuphine	-2.646	-5.206

C8H8F3N3O4S2	DB00774	Hydroflumethiazide	-2.645	-2.691
C4H6N4O3S2	DB00819	Acetazolamide	-2.639	-2.894
C24H28O2	DB00307	Bexarotene	-2.637	-2.638
C11H12N4O3S	DB00664	Sulfametopyrazine	-2.632	-3.668
C9H15N5O3	DB00360	Sapropterin	-2.632	-4.95
C31H33F3N2O5S	DB00932	Tipranavir	-2.628	-3.56
C11H11N3O2S	DB00891	Sulfapyridine	-2.625	-2.783
C25H30N3	DB00406	Gentian violet cation	-2.622	-2.635
C17H19N3	DB00370	Mirtazapine	-2.615	-3.877
C17H21NO4	DB00907	Cocaine	-2.614	-4.033
C28H31FN4O	DB00637	Astemizole	-2.612	-3.126
C22H25N3O4S	DB00680	Moricizine	-2.612	-4.152
C21H21N	DB00735	Naftifine	-2.609	-3.839
C17H21NO3	DB00674	Galantamine	-2.605	-4.721
C22H19N3O4	DB00820	Tadalafil	-2.603	-2.603
C19H23NO3	DB00234	Reboxetine	-2.602	-2.636
C11H12N2S	DB00848	Levamisole	-2.6	-2.682
C19H19NOS	DB00920	Ketotifen	-2.59	-2.598
C22H30N6O4S	DB00203	Sildenafil	-2.588	-3.407
C9H11N2O5	DB00249	Idoxuridine	-2.586	-4.795
C5H9NO3	DB00855	Aminolevulinic acid	-2.585	-2.803
C20H23NO4	DB00704	Naltrexone	-2.584	-4.799
C10H21N3O	DB00711	Diethylcarbamazine	-2.578	-3.054
C3H7O4P	DB00828	Fosfomycin	-2.578	-2.831
C52H98N16O13	DB00803	Colistin	-2.56	-5.012
C21H24F3N3S	DB00831	Trifluoperazine	-2.558	-3.167
C26H31Cl2N5O3	DB00251	Terconazole	-2.557	-3.52
C23H25F3N2OS	DB00875	Flupentixol	-2.554	-4.075
C20H12O5	DB00693	Fluorescein	-2.54	-3.251
C3H7O4P	DB00828	Fosfomycin	-2.538	-3.163
C13H16N2	DB00633	Dexmedetomidine	-2.525	-3.014
C21H21NO2S	DB00799	Tazarotene	-2.523	-2.523
C45H54N4O8	DB00361	Vinorelbine	-2.516	-2.657
C21H24FN3O4	DB00218	Moxifloxacin	-2.513	-2.614
C19H22ClN5O	DB00656	Trazodone	-2.507	-2.91
C8H11NO3	DB00165	Pyridoxine	-2.501	-2.725
C21H32N6O3	DB00802	Alfentanil	-2.487	-2.554
C18H14N4O5S	DB00795	Sulfasalazine	-2.482	-2.771
C16H15N3	DB00751	Epinastine	-2.48	-4.124
C18H28N2O	DB00297	Bupivacaine	-2.471	-3.912
C11H16N4O4	DB00552	Pentostatin	-2.468	-4.202
C7H6ClN3O4S2	DB00880	Chlorothiazide	-2.467	-3.001
C29H35NO2	DB00834	Mifepristone	-2.465	-2.48
C29H38N4O10	DB00256	Lymecycline	-2.459	-3.588
C5H9NO2	DB00172	Proline	-2.456	-2.456
C10H16N2O3	DB00237	Butabarbital	-2.456	-4.136
C13H12O2	DB00600	Monobenzone	-2.454	-2.455
C14H12N6O	DB00922	Levosimendan	-2.453	-3.673
C7H10N2OS	DB00550	Propylthiouracil	-2.451	-4.12
C5H11NO2	DB00161	L-Valine	-2.45	-2.45
C13H19NO	DB00937	Diethylpropion	-2.444	-2.589
C6H8N2O2S	DB00259	Sulfanilamide	-2.443	-2.443
C17H22N4O	DB00805	Minaprine	-2.44	-3.624
C22H22FN3O2	DB00450	Droperidol	-2.43	-3.542
C8H12N2	DB00780	Phenelzine	-2.423	-3.43
C6H15N2O2	DB00411	Carbamoylcholine	-2.417	-2.417
C46H56N4O10	DB00541	Vincristine	-2.416	-2.741
C22H24N2O9	DB00595	Oxytetracycline	-2.413	-2.684
C21H29NO2	DB00611	Butorphanol	-2.413	-4.792
C19H16O4	DB00682	Warfarin	-2.412	-4.41
C10H15N3	DB00217	Bethanidine	-2.398	-2.398
C38H72N2O12	DB00207	Azithromycin	-2.398	-5.043
C10H12N4O3	DB00900	Didanosine	-2.397	-3.605

C21H25N	DB00857	Terbinafine	-2.389	-3.389
C12H21N	DB00478	Rimantadine	-2.387	-2.387
C9H13NO3	DB00668	Epinephrine	-2.361	-4.706
C9H11F2N3O4	DB00441	Gemcitabine	-2.355	-5.076
C20H24N2O2	DB00468	Quinine	-2.353	-4.63
C13H19NO	DB00937	Diethylpropion	-2.348	-3.255
C12H17N4OS	DB00152	Thiamine	-2.332	-4.382
C3H6N2O2	DB00260	Cycloserine	-2.329	-2.576
C46H56N4O10	DB00541	Vincristine	-2.327	-3.259
C4H7NO4	DB00128	Aspartic acid	-2.325	-2.325
C10H17NOS	DB00185	Cevimeline	-2.321	-2.323
C23H27FN4O2	DB00734	Risperidone	-2.318	-2.328
C3H6N2O2	DB00260	Cycloserine	-2.317	-2.955
C22H24N2O8	DB00759	Tetracycline	-2.313	-2.451
C19H21N5O2	DB00670	Pirenzepine	-2.297	-4.168
C17H21NO3	DB00867	Ritodrine	-2.295	-4.603
C19H27N5	DB00298	Dapiprazole	-2.295	-2.595
C10H10N4O2S	DB00359	Sulfadiazine	-2.293	-3.162
C18H22CINO	DB00925	Phenoxybenzamine	-2.292	-2.741
C4H6N2S	DB00763	Methimazole	-2.273	-2.273
C17H29GdN4O7	DB00597	Gadoteridol	-2.273	-2.304
C12H15N3O2S	DB00518	Albendazole	-2.272	-3.686
C19H20N2O3	DB00757	Dolasetron	-2.272	-3.191
C10H17N3O6S	DB00143	Glutathione	-2.27	-4.973
C3H2CIF5O	DB00753	Isoflurane	-2.27	-2.27
C32H45N3O4S	DB00220	Nelfinavir	-2.268	-4.5
C11H16N2O3	DB00306	Talbutal	-2.264	-3.704
C23H29CIFN3O4	DB00604	Cisapride	-2.261	-3.426
C13H24NO10P	DB00144	Phosphatidyl serine	-2.258	-4.542
C12H25NaO4S	DB00815	Sodium lauryl sulfate	-2.258	-2.258
C19H27NO	DB00652	Pentazocine	-2.257	-4.596
MgO4S	DB00653	Magnesium sulfate	-2.256	-2.256
C33H37N5O5	DB00320	Dihydroergotamine	-2.256	-4.442
C30H60I3N3O3	DB00483	Gallamine Triethiodide	-2.251	-2.251
C13H20N2O2	DB00721	Procaine	-2.239	-2.26
C9H11N	DB00752	Tranlycypromine	-2.227	-2.255
C14H20GdN3O10	DB00789	Gadopentetic acid	-2.22	-3.036
C5H8N4O3S2	DB00703	Methazolamide	-2.219	-2.454
C17H26N2O	DB00296	Ropivacaine	-2.217	-3.657
C14H21N3O3S	DB00839	Tolazamide	-2.214	-4.134
C20H24N2O2	DB00908	Quinidine	-2.2	-4.477
C33H40N2O9	DB00206	Reserpine	-2.194	-2.23
C9H9Cl2N3	DB00575	Clonidine	-2.194	-4.126
C19H27N5	DB00298	Dapiprazole	-2.191	-3.251
C18H26ClN3	DB00608	Chloroquine	-2.188	-3.864
C4H3FN2O2	DB00544	Fluorouracil	-2.171	-2.913
C20H22N8O5	DB00563	Methotrexate	-2.161	-4.622
C10H21N3O	DB00711	Diethylcarbamazine	-2.156	-2.508
C9H7Cl2N5	DB00555	Lamotrigine	-2.155	-3.975
C28H33ClN2	DB00354	Buclizine	-2.148	-2.963
C8H11Cl2N3O2	DB00791	Uracil mustard	-2.138	-4.07
C6H13NO2	DB00167	Isoleucine	-2.137	-2.137
C22H26F3N3OS	DB00623	Fluphenazine	-2.133	-4.103
C16H13N3O3	DB00643	Mebendazole	-2.132	-2.791
C52H88N10O15	DB00520	Casprofungin	-2.126	-4.718
C22H26N2O4S	DB00343	Diltiazem	-2.125	-4.221
C10H16N6S	DB00501	Cimetidine	-2.115	-2.668
C17H19N3O3S	DB00338	Omeprazole	-2.114	-3.825
C4H6CaO4	DB00258	Calcium acetate	-2.113	-2.116
C11H18N2O3	DB00312	Pentobarbital	-2.109	-3.797
C14H11NO5	DB00323	Tolcapone	-2.107	-4.662
C19H27N5	DB00298	Dapiprazole	-2.095	-2.966
C12H9N3O5S	DB00507	Nitazoxanide	-2.092	-4.276

C32H53N2O4	DB00728	Rocuronium	-2.092	-2.239
C5H11NO2S	DB00134	Methionine	-2.088	-2.088
C9H18N6	DB00488	Altretamine	-2.086	-2.134
C16H15N3	DB00751	Epinastine	-2.082	-2.12
C33H35N5O5	DB00696	Ergotamine	-2.079	-4.418
C18H30O2	DB00132	Alpha-Linolenic Acid	-2.051	-2.055
C19H24N2O3	DB00598	Labetalol	-2.033	-3.97
C10H16N6S	DB00501	Cimetidine	-2.029	-2.711
C13H22N4O3S	DB00863	Ranitidine	-2.002	-4.034
C66H75Cl2N9O24	DB00512	Vancomycin	-2.002	-4.285
C17H28N2O3	DB00892	Oxybuprocaine	-1.991	-3.977
C19H20N2O2	DB00812	Phenylbutazone	-1.991	-4.589
C22H24N2O8	DB00759	Tetracycline	-1.98	-4.31
C17H20N4S	DB00334	Olanzapine	-1.977	-3.635
C32H53N2O4	DB00728	Rocuronium	-1.974	-2.872
C11H17NO3	DB00816	Orciprenaline	-1.969	-4.18
C10H12N2	DB00797	Tolazoline	-1.967	-1.968
C24H34N4O5S	DB00222	Glimepiride	-1.961	-1.985
C22H29N3S2	DB00372	Thiethylperazine	-1.96	-4.304
C8H10N4O2	DB00824	Enprofylline	-1.958	-3.432
C19H20N2O3	DB00757	Dolasetron	-1.958	-2.099
C22H22N2O8	DB00931	Metacycline	-1.948	-2.243
C12H15N3O2S	DB00518	Albendazole	-1.946	-3.832
C25H27ClN2	DB00737	Meclizine	-1.92	-2.735
C26H28ClNO	DB00539	Toremifene	-1.917	-3.93
C17H19NO3	DB00327	Hydromorphone	-1.911	-4.014
C11H12N2O2S	DB00744	Zileuton	-1.909	-3.97
C3H2ClF5O	DB00228	Enflurane	-1.905	-1.905
C26H34FNO5	DB00439	Cerivastatin	-1.903	-3.84
C3H4O3	DB00119	Pyruvic acid	-1.899	-1.899
C19H29NO5	DB00449	Dipivefrin	-1.889	-4.551
C20H34GdN5O10	DB00538	Gadoversetamide	-1.888	-1.988
C45H54N4O8	DB00361	Vinorelbine	-1.883	-3.182
C3H5N3O9	DB00727	Nitroglycerin	-1.882	-1.882
C5H4N4O	DB00437	Allopurinol	-1.876	-3.055
C23H46N6O13	DB00452	Framycetin	-1.87	-2.556
C37H67NO13	DB00199	Erythromycin	-1.864	-4.508
C5H11Cl2N	DB00888	Mechlorethamine	-1.858	-1.923
C21H31N3O5	DB00722	Lisinopril	-1.854	-1.976
C22H28N2O	DB00813	Fentanyl	-1.85	-3.958
C10H10N4O2S	DB00359	Sulfadiazine	-1.847	-2.002
C24H26N6O3	DB00275	Olmesartan	-1.843	-1.941
C20H24ClN3S	DB00433	Prochlorperazine	-1.843	-4.186
C15H17FN4O3	DB00467	Enoxacin	-1.838	-4.473
C18H19ClN4	DB00363	Clozapine	-1.836	-3.705
C6H12N2O4S2	DB00138	Cystine	-1.835	-3.63
C10H16N6S	DB00501	Cimetidine	-1.83	-2.614
C11H11N3O2S	DB00891	Sulfapyridine	-1.828	-2.866
C26H37N5O2	DB00248	Cabergoline	-1.825	-2.058
C4H11N5	DB00331	Metformin	-1.822	-1.825
C8H12N2	DB00780	Phenelzine	-1.821	-2.601
C8H10NO6P	DB00114	Pyridoxal phosphate	-1.818	-4.317
C16H15F2N3O4S	DB00213	Pantoprazole	-1.818	-3.903
C6H9N3O2	DB00117	Histidine	-1.814	-3.534
C14H30N2O4	DB00202	Succinylcholine	-1.809	-1.809
C41H76N2O15	DB00778	Roxithromycin	-1.808	-4.447
C23H32N6O4S	DB00862	Vardenafil	-1.807	-3.565
C15H21NO2	DB00454	Meperidine	-1.803	-3.996
C21H23ClFN3O	DB00690	Flurazepam	-1.803	-4.1
C5H8N4O3S2	DB00703	Methazolamide	-1.8	-3.01
C21H43N5O7	DB00798	Gentamicin	-1.791	-3.301
C16H26N2O3	DB00807	Proparacaine	-1.79	-1.809
C72H95ClN14O14	DB00106	Abarelix	-1.781	-1.785

C16H14ClN3O	DB00475	Chlordiazepoxide	-1.766	-3.342
C8H11NO3	DB00368	Norepinephrine	-1.742	-3.837
C18H18ClN3O	DB00408	Loxapine	-1.741	-3.488
C11H12N2S	DB00848	Levamisole	-1.74	-2.952
C22H25N3O4S	DB00680	Moricizine	-1.736	-2.893
C52H98N16O13	DB00803	Colistin	-1.736	-3.955
C46H56N4O10	DB00541	Vincristine	-1.733	-3.435
C9H13NO2	DB00610	Metaraminol	-1.713	-4.122
C6H10N6O	DB00851	Dacarbazine	-1.709	-3.455
C22H28GdN3O11	DB00743	Gadobenidic acid	-1.701	-3.155
C23H24N2O4S	DB00876	Eprosartan	-1.698	-3.433
C20H28N2O5	DB00899	Remifentanyl	-1.697	-1.983
C26H28ClNO	DB00882	Clomifene	-1.692	-3.705
C17H21N	DB00865	Benzphetamine	-1.689	-3.302
C20H15F3N4O3	DB00685	Trovafloxacin	-1.68	-3.719
C3H7NO2	DB00160	L-Alanine	-1.679	-1.679
C11H11N3O2S	DB00891	Sulfapyridine	-1.679	-3.347
C9H16O4	DB00548	Azelaic acid	-1.654	-1.661
C21H41N5O7	DB00955	Netilmicin	-1.649	-4.058
C15H14F3N3O4S2	DB00436	Bendroflumethiazide	-1.632	-3.005
C7H9N2O	DB00733	Pralidoxime	-1.629	-1.854
C19H35NO2	DB00804	Dicyclomine	-1.616	-3.735
C16H26N2O3	DB00807	Proparacaine	-1.613	-3.652
C12H9N3O	DB00235	Milrinone	-1.593	-3.658
C27H36N2O4	DB00912	Repaglinide	-1.585	-4.123
C14H16ClN3O4S2	DB00606	Cyclothiazide	-1.58	-3.884
C21H24F3N3S	DB00831	Trifluoperazine	-1.563	-3.906
C13H20N2O2	DB00721	Procaine	-1.562	-3.549
C5H8N4O3S2	DB00703	Methazolamide	-1.56	-3.01
C14H22N2O	DB00281	Lidocaine	-1.545	-3.545
C32H52N4O4	DB00944	Demecarium	-1.539	-1.539
C16H13ClN2O	DB00579	Mazindol	-1.529	-4.144
C21H23ClFNO2	DB00502	Haloperidol	-1.528	-3.779
C9H13NO	DB00397	Phenylpropanolamine	-1.513	-3.923
C4H6N4O3S2	DB00819	Acetazolamide	-1.494	-2.913
C24H33N3O4	DB00243	Ranolazine	-1.484	-1.515
C19H17NOS	DB00525	Tolnaftate	-1.478	-1.478
C36H41N3O6	DB00528	Lercanidipine	-1.477	-3.265
C20H22ClN3O	DB00613	Amodiaquine	-1.471	-4.035
C10H15N5	DB00914	Phenformin	-1.461	-3.997
C10H24N2O2	DB00330	Ethambutol	-1.458	-2.258
C10H14N2	DB00184	Nicotine	-1.45	-3.358
C17H29GdN4O7	DB00597	Gadoteridol	-1.441	-3.926
C47H75NO17	DB00646	Nystatin	-1.431	-3.189
C66H83N17O13	DB00666	Nafarelin	-1.406	-2.232
C23H32N6O4S	DB00862	Vardenafil	-1.401	-3.066
C24H28N2O5	DB00542	Benazepril	-1.393	-1.864
C27H22Cl2N4	DB00845	Clofazimine	-1.37	-1.372
C7H8N4O2	DB00277	Theophylline	-1.363	-3.196
C2H5NO2	DB00145	Glycine	-1.363	-1.363
C11H17NO3	DB00723	Methoxamine	-1.361	-3.77
C52H98N16O13	DB00803	Colistin	-1.35	-3.758
C21H25ClN2O3	DB00341	Cetirizine	-1.349	-3.208
C10H11F3N2O5	DB00432	Trifluridine	-1.341	-2.535
C9H11N	DB00752	Tranlycypromine	-1.338	-3.147
C14H20GdN3O10	DB00789	Gadopentetic acid	-1.338	-1.576
C8H11NO3	DB00165	Pyridoxine	-1.337	-3.991
C2H6O	DB00898	Ethanol	-1.328	-1.328
C17H16ClN3O	DB00543	Amoxapine	-1.326	-3.576
C33H40N2O9	DB00206	Reserpine	-1.317	-2.991
C5H8N4O3S2	DB00703	Methazolamide	-1.315	-2.63
C9H9Cl2N3	DB00575	Clonidine	-1.304	-1.327
C16H16ClNO2S	DB00758	Clopidogrel	-1.297	-3.245

C29H31N7O	DB00619	Imatinib	-1.281	-3.784
C6H12CINO	DB00658	Sevelamer	-1.277	-1.279
C20H36N2O3S	DB00308	Ibutilide	-1.268	-3.63
C4H6N4O3S2	DB00819	Acetazolamide	-1.254	-2.599
C22H22N2O8	DB00931	Metacycline	-1.25	-3.516
C18H21NO3	DB00956	Hydrocodone	-1.241	-1.271
C10H15NO	DB00852	Pseudoephedrine	-1.211	-3.873
C22H24N2O9	DB00595	Oxytetracycline	-1.199	-3.515
C11H18N2O2S	DB00599	Thiopental	-1.183	-3.444
C5H5N5S	DB00352	Tioguanine	-1.17	-3.345
C4H6N4O3S2	DB00819	Acetazolamide	-1.167	-2.389
C26H28N2	DB00568	Cinnarizine	-1.164	-2.384
C12H21NO8S	DB00273	Topiramate	-1.154	-3.576
C15H18N4O5	DB00305	Mitomycin	-1.152	-3.29
C22H28GdN3O11	DB00743	Gadobenic acid	-1.143	-2.747
C8H6N4O5	DB00698	Nitrofurantoin	-1.122	-2.403
C7H4ClNO2	DB00356	Chlorzoxazone	-1.11	-2.832
C10H16N6S	DB00501	Cimetidine	-1.109	-3.615
C22H28GdN3O11	DB00743	Gadobenic acid	-1.101	-2.523
C31H33N3O6S	DB00549	Zafirlukast	-1.094	-3.755
C4H6N4O3S2	DB00819	Acetazolamide	-1.067	-3.205
C66H75Cl2N9O24	DB00512	Vancomycin	-1.056	-2.031
C7H9N2O	DB00733	Pralidoxime	-1.043	-1.725
C19H21N5O4	DB00457	Prazosin	-1.035	-3.336
C36H47N5O4	DB00224	Indinavir	-1.034	-1.425
C18H27NO2	DB00645	Dyclonine	-1.025	-3.731
C23H46N6O13	DB00452	Framycetin	-1.023	-2.848
C5H5N5	DB00173	Adenine	-1.022	-3.019
C14H16N2O2	DB00292	Etomidate	-1.012	-3.393
C20H25N3O2	DB00353	Methylethylmetrine	-1.011	-1.639
C12H19NO3	DB00871	Terbutaline	-1.011	-3.226
C8H8F3N3O4S2	DB00774	Hydroflumethiazide	-0.996	-2.606
C66H75Cl2N9O24	DB00512	Vancomycin	-0.988	-3.608
C9H13N2O2	DB00545	Pyridostigmine	-0.985	-0.985
C10H17N	DB00915	Amantadine	-0.98	-0.98
C10H16N2O4S3	DB00869	Dorzolamide	-0.974	-1.038
C18H37N5O9	DB00684	Tobramycin	-0.97	-2.554
C19H27N3O5S2	DB00204	Dofetilide	-0.965	-3.007
C29H39N5O8	DB00560	Tigecycline	-0.955	-3.606
C19H19NOS	DB00920	Ketotifen	-0.952	-3.527
C21H16ClF3N4O3	DB00398	Sorafenib	-0.933	-3.246
C14H13N3O4S2	DB00814	Meloxicam	-0.913	-3.082
C10H16N2O4S3	DB00869	Dorzolamide	-0.911	-2.323
C22H30N2O2S	DB00708	Sufentanil	-0.909	-0.948
C40H56O2	DB00137	Lutein	-0.909	-0.909
C21H41N5O7	DB00955	Netilmicin	-0.903	-2.825
C20H34GdN5O10	DB00538	Gadoversetamide	-0.877	-3.574
C16H14F3N3O2S	DB00448	Lansoprazole	-0.865	-2.898
C3H7NO2S	DB00151	L-Cysteine	-0.845	-3.064
C20H28N2O5	DB00899	Remifentanyl	-0.81	-1.378
C23H27FN4O2	DB00734	Risperidone	-0.787	-3.209
C46H58N4O9	DB00570	Vinblastine	-0.782	-2.807
C8H10N4O2	DB00824	Enprofylline	-0.772	-3.422
C25H27ClN2	DB00737	Meclizine	-0.771	-2.934
C24H34N4O5S	DB00222	Glimepiride	-0.771	-2.694
C8H10N2O3S	DB00634	Sulfacetamide	-0.768	-2.86
C25H30N3	DB00406	Gentian violet cation	-0.747	-3.027
C9H10N4O2S2	DB00576	Sulfamethizole	-0.73	-2.852
C5H11Cl2N	DB00888	Mechlorethamine	-0.709	-2.054
C9H13NO2	DB00388	Phenylephrine	-0.706	-3.367
C23H32N6O4S	DB00862	Vardenafil	-0.692	-3.408
C23H32N6O4S	DB00862	Vardenafil	-0.691	-1.555
C28H33ClN2	DB00354	Buclizine	-0.674	-2.836

C16H20N4O3S	DB00214	Torase mide	-0.671	-3.295
C36H41N3O6	DB00528	Lercanidipine	-0.642	-0.672
C20H34GdN5O10	DB00538	Gadoversetamide	-0.636	-2.862
C29H33CIN2O2	DB00836	Loperamide	-0.6	-2.39
C25H30N2O5	DB00881	Quinapril	-0.592	-1.466
C15H13N3O4S	DB00554	Piroxicam	-0.587	-0.592
C5H11NO2S	DB00859	Penicillamine	-0.578	-2.797
C29H35NO2	DB00834	Mifepristone	-0.544	-2.698
C22H22N2O8	DB00931	Metacycline	-0.518	-2.852
C4H6O4	DB00139	Succinic acid	-0.516	-3.185
C2H7NS	DB00847	Cysteamine	-0.515	-3.133
C45H54N4O8	DB00361	Vinorelbine	-0.494	-3.086
C5H4N4O	DB00437	Allopurinol	-0.487	-2.928
C41H42N4O8	DB00460	Verteporfin	-0.466	-0.466
C9H18N6	DB00488	Altretamine	-0.463	-1.968
C21H32N6O3	DB00802	Alfentanil	-0.423	-1.743
C10H13CIN2O3S	DB00672	Chlorpropamide	-0.415	-3.051
C21H21CIN2O8	DB00618	Demeclocycline	-0.379	-1.912
C26H28N2	DB00568	Cinnarizine	-0.358	-3.018
C4H10N2	DB00592	Piperazine	-0.355	-2.701
C3F8	DB00556	Perflutren	-0.35	-0.35
C16H15F2N3O4S	DB00213	Pantoprazole	-0.342	-2.034
C21H31N5O2	DB00490	Buspirone	-0.33	-0.66
C11H15NO	DB00830	Phenmetrazine	-0.326	-3.053
C22H30N2O2S	DB00708	Sufentanil	-0.301	-1.935
C28H30N2O2	DB00496	Darifenacin	-0.296	-0.298
C21H21CIN2O8	DB00618	Demeclocycline	-0.258	-2.662
C27H34N2O7	DB00691	Moexipril	-0.245	-1.119
C21H21N	DB00434	Cyproheptadine	-0.226	-2.701
C28H33CIN2	DB00354	Buclizine	-0.224	-0.417
C6H5NO2	DB00627	Niacin	-0.216	-2.664
C9H16O4	DB00548	Azelaic acid	-0.112	-2.71
C38H72N2O12	DB00207	Azithromycin	-0.09	-0.103
C17H19N3	DB00370	Mirtazapine	0.044	-2.431
C23H25N5O5	DB00590	Doxazosin	0.053	-2.163
C33H35N5O5	DB00696	Ergotamine	0.081	-0.784
C22H24N2O8	DB00254	Doxycycline	0.087	-2.435
C17H17CIN6O3	DB00402	Eszopiclone	0.107	-0.244
C41H76N2O15	DB00778	Roxithromycin	0.152	0.145
C22H25N3O4S	DB00680	Moricizine	0.173	-1.517
C17H29GdN4O7	DB00597	Gadoteridol	0.226	-1.881
C22H24N2O8	DB00759	Tetracycline	0.236	-2.164
CH3O5P	DB00529	Foscarnet	0.238	-2.449
C2H7NS	DB00847	Cysteamine	0.25	-1.933
C22H24N2O9	DB00595	Oxytetracycline	0.251	-2.127
C28H31FN4O	DB00637	Astemizole	0.274	-0.052
C15H12N2O2	DB00252	Phenytoin	0.346	-1.175
C12H18N2O3	DB00418	Secobarbital	0.432	-1.072
C33H34N6O6	DB00796	Candesartan cilexetil	0.614	-0.252
C11H16N2O3	DB00241	Butalbital	0.734	-0.707
C17H19NO3	DB00295	Morphine	0.771	-1.802
C24H32O4	DB00351	Megestrol acetate	0.865	0.865
C23H32N6O4S	DB00862	Vardenafil	0.967	-0.884
C53H72N2O12	DB00565	Cisatracurium	1.182	1.182
C45H54N4O8	DB00361	Vinorelbine	1.345	-0.09
C22H23CIN2O2	DB00455	Loratadine	1.669	-0.2
C43H55N5O7	DB00309	Vindesine	1.894	-0.666
C66H75Cl2N9O24	DB00512	Vancomycin	1.899	0.769
C70H92CIN17O14	DB00050	Cetorelix	1.981	1.976
C62H111N11O12	DB00091	Ciclosporin	2.637	2.637
C38H72N2O12	DB00207	Azithromycin	2.876	0.169
C33H38N4O6	DB00762	Irinotecan	2.976	2.974
C26H29N3O6	DB00622	Nicardipine	3.895	3.203

C46H58N4O9	DB00570	Vinblastine	4.289	3.421
C46H58N4O9	DB00570	Vinblastine	9.511	9.251

paronomycin with 6vw1, Table S11

Entry Name	PUBCHEM_COMPOUN	docking score	paronomycin with 6vw1, Table S11	
			glide gscore	
6vw1.1				
Conformer3D_CID_1655	165580		-7.692	-8.775
Conformer3D_CID_1655	165580		-7.333	-9.449
Conformer3D_CID_1655	165580		-7.181	-7.811
Conformer3D_CID_1655	165580		-7.113	-8.858
Conformer3D_CID_1655	165580		-7.059	-8.497
Conformer3D_CID_1655	165580		-6.533	-8.723
Conformer3D_CID_1655	165580		-6.038	-7.027
Conformer3D_CID_1655	165580		-5.947	-7.797
Conformer3D_CID_1655	165580		-4.637	-6.883
Conformer3D_CID_1655	165580		-4.53	-7.135
Conformer3D_CID_1655	165580		-3.955	-6.356

Paronomycin with 6y84, Table S12

Entry Name	PUBCHEM_COMPOUN	docking score	glide gscore	
6y84.1.1				
Conformer3D_CID_1655	165580		-9.553	-10.543
Conformer3D_CID_1655	165580		-9.424	-11.54
Conformer3D_CID_1655	165580		-8.115	-10.305
Conformer3D_CID_1655	165580		-7.473	-8.911
Conformer3D_CID_1655	165580		-6.544	-9.149
Conformer3D_CID_1655	165580		-6.475	-7.105
Conformer3D_CID_1655	165580		-6.196	-8.046
Conformer3D_CID_1655	165580		-6.05	-7.132
Conformer3D_CID_1655	165580		-5.57	-7.971
Conformer3D_CID_1655	165580		-4.278	-6.023
Conformer3D_CID_1655	165580		-1.77	-4.016

Figure S1: Forms of Paramomycin

