

Supporting Information for
The Impact of Introducing a Histidine into an
Apolar Cavity Site on Docking and Ligand Recognition

Matthew Merski & Brian K. Shoichet*

Dept. of Pharmaceutical Chemistry, University of California San Francisco

1700 4th St., San Francisco CA 94158-2550

To whom correspondence should be addressed: Brian Shoichet,

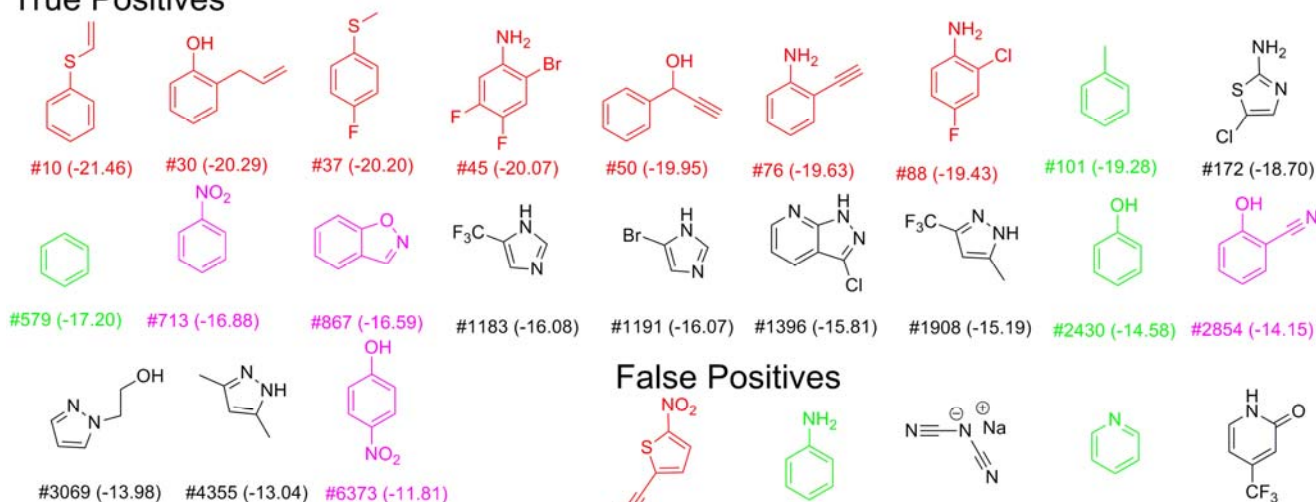
Dept. of Pharmaceutical Chemistry, University of California, San Francisco, 1700 4th St.

San Francisco, CA 94158-2330, email: shoichet@cgl.ucsf.edu

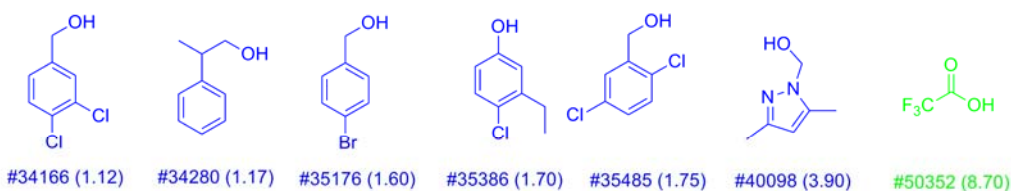
Contains the complete crystallographic table for protein ligand complex structures reported, 2D images of the molecules tested and their docking scores, graphical representations of the relationship between ΔT_m and binding affinity or docking rank, a truth table comparing the ability of molecular docking, a 1D chemotype and total polar surface area to predict ligands, as well as a list of the 10,000 molecules in the top of the docking ranked list with scores separated into individual terms (van der Waals, electrostatic interactions, polar and non-polar desolvation).

SI Figure 1

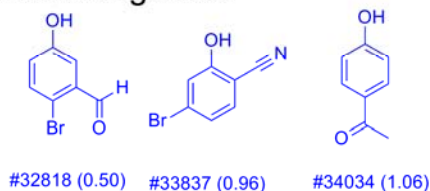
True Positives



True Negatives

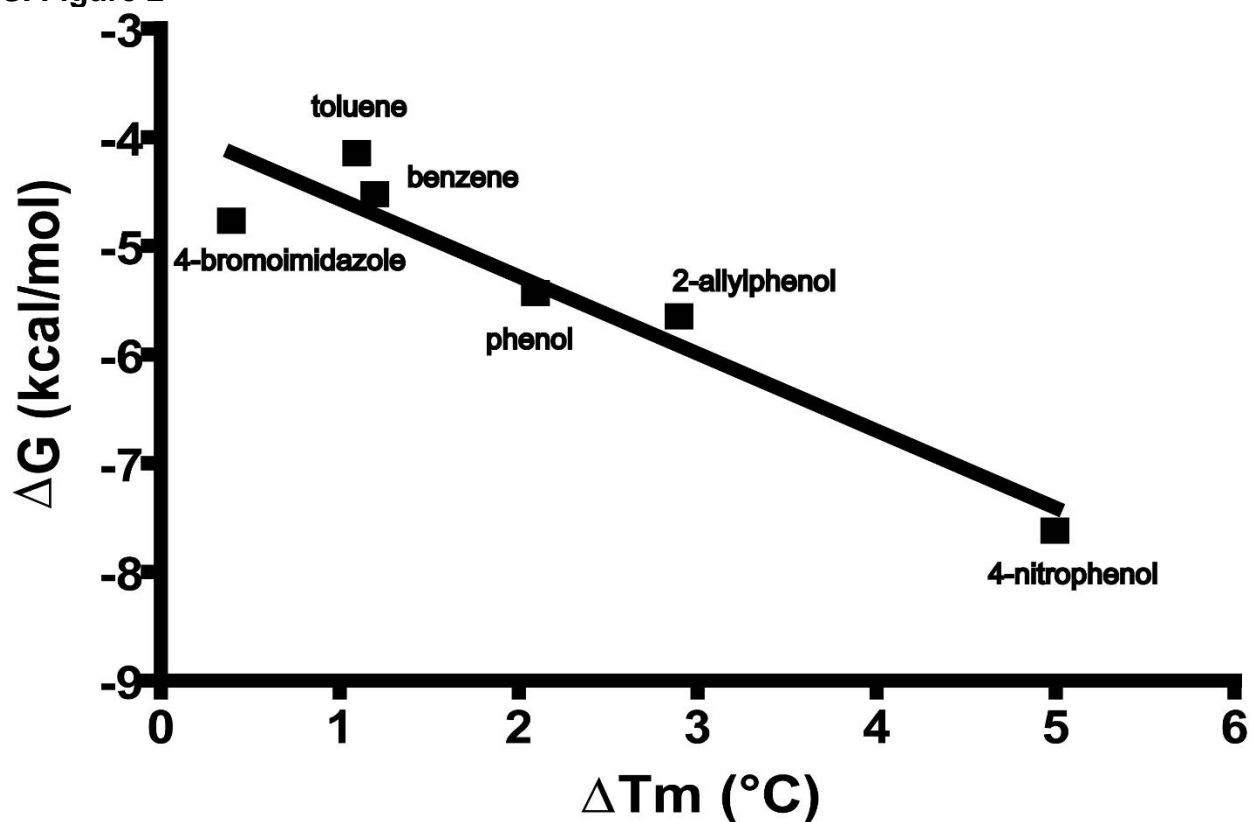


False Negatives



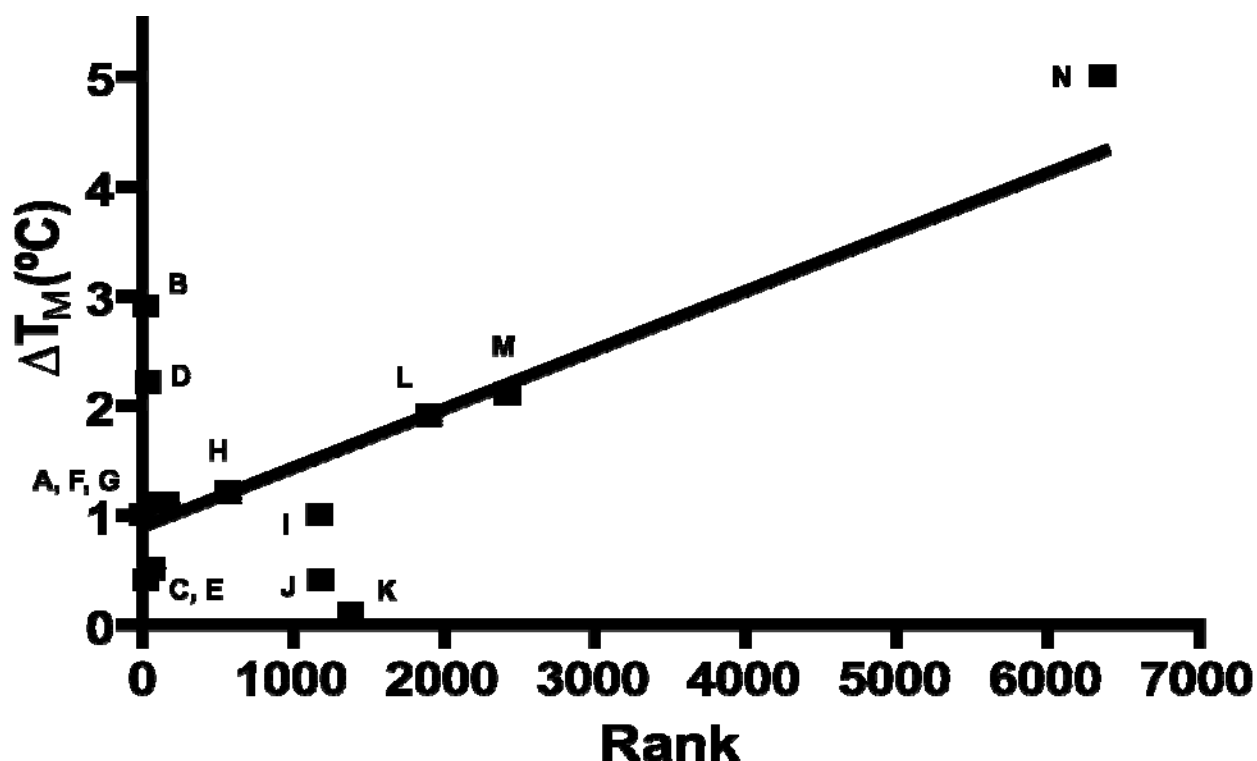
SI Figure 1: The molecules tested for L99A/M102H† binding reported here. The molecules are grouped into docking true positives (ligands ranked in the top 1% of the docking list), docking false positives (non-ligands ranked in the top 1% of the list), docking true negatives (non-ligands not present in the top 5% of the list) and docking false negatives (ligands not ranked in the top 5% of the list). Molecules are colored according to the reason they were chosen. Red molecules (high scoring set) scored in the top 100 of all molecules overall. Black molecules (dissimilar set) scored in the top 1% and had a low Tanimoto coefficient to the set of known cavity ligands. Violet molecules (previously known set) were known from a previous study on L99A/M102H†¹. Green molecules (*prima facie* set) were chosen due to high similarity to lysozyme cavity ligands that bind one or more of previously described model lysozyme cavities. Blue molecules (possible docking failures set) were chosen because they matched to 1D chemotype of discovered L99A/M102H† ligands. 2-mercaptoethanol, a ligand was ranked in the intermediate range between the true positives (1%) and false negatives (5%) and is not included on this list due to that ambiguity.

SI Figure 2



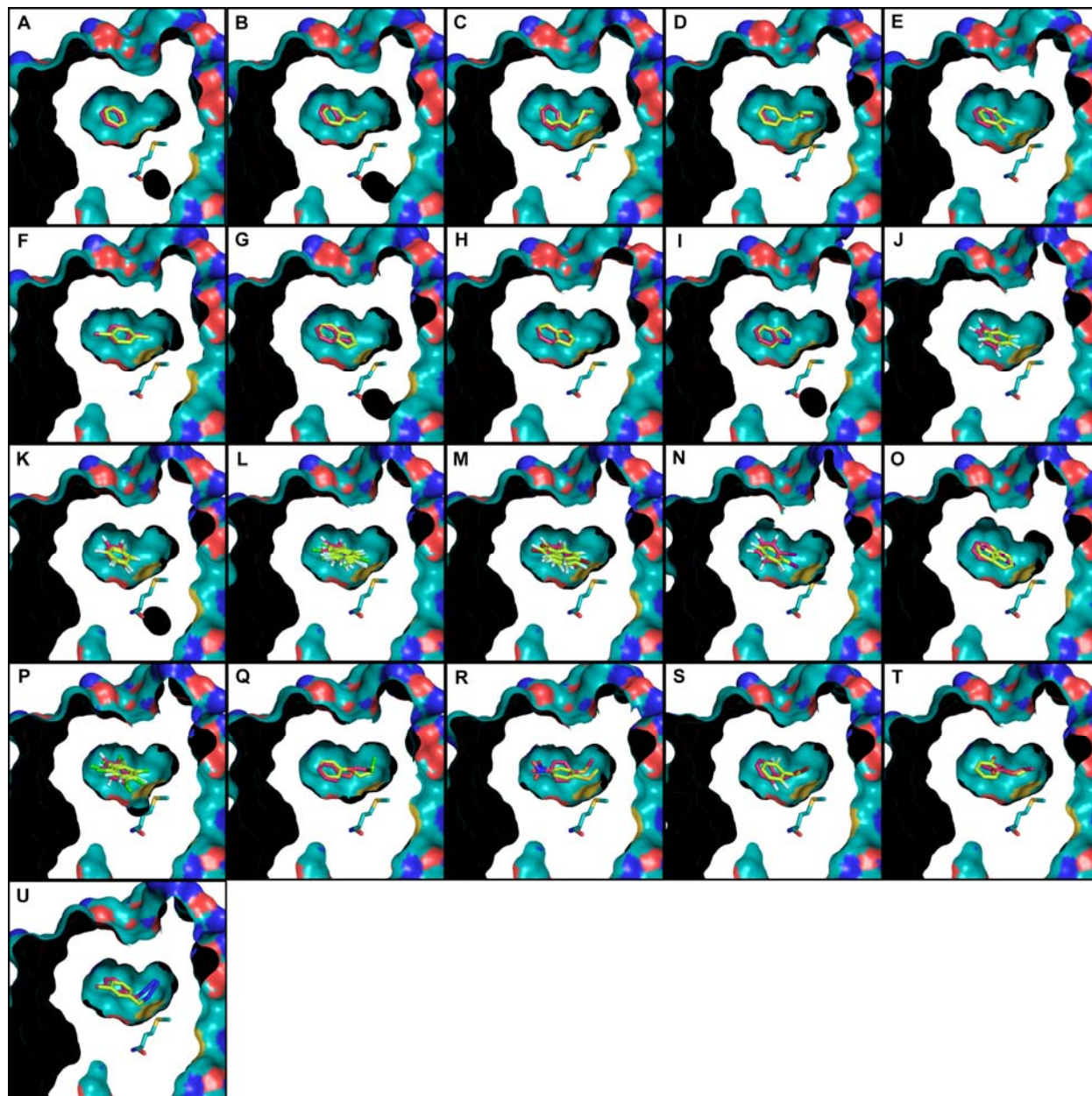
SI Figure 2: There is a good correlation between the ΔT_M (measured by CD, pH 5.4) and ΔG_{bind} (measured by ITC, 25 °C, pH 5.0) of ligands to the L99A/M102H† cavity ($R^2 = 0.897$, slope = $-0.71 \text{ kcal mol}^{-1} \text{ } ^\circ\text{C}^{-1}$).

SI Figure 3



SI Figure 3: An illustration of the dependence of docking rank with ΔT_M (measured by CD, pH 5.4). The fit line ($R^2 = 0.511$, slope = 5×10^{-4} ranks $^{\circ}\text{C}^{-1}$) shows that unlike SI Figure 2, which shows that the relationship between ΔT_M and ΔG_{bind} (measured by ITC, 25 $^{\circ}\text{C}$, pH 5.0), there is not a good correlation between docking rank and ΔT_M . The points correspond as follows: **A)** phenyl vinyl sulfide **B)** 2-allyl phenol **C)** 4-fluorothioanisole **D)** 1-phenyl-2-propyn-1-ol **E)** 2-ethynylaniline **F)** toluene **G)** 2-amino-5-chloro thiazole **H)** benzene **I)** 4-trifluoromethyl imidazole **J)** 4-bromoimidazole **K)** 3-chloro-1H-pyrazolo[3,4b] pyridine **L)** 3-methyl-5-(trifluoromethyl) pyrazole **M)** phenol **N)** 4-nitrophenol

SI Figure 4



SI Figure 4: Comparison of the crystallographic and DOCK generated poses of the L99A crystallographic ligands. In all cases oxygens are represented in red, nitrogens blue, fluorines white, iodine and bromine purple, and sulfurs yellow. A cut-away of the crystallographically determined protein structure (and surface) is shown with cyan carbons, the crystallographically determined ligand carbons are light yellow and the DOCK predicted poses are represented with magenta carbons. The side of the surface occupied entirely by the protein is in black. Met102 and the ligands are shown in a stick representation. The figure was rendered with PyMol. In all cases the ligand binding cavity is completely physically isolated from bulk solvent. Docking was performed

against PDB 181L². There were only minute changes in the binding site between the different crystal structures. Crystal structures with multiple ligand poses were all matched to the dock pose; RMSD values are given in ascending order in those cases.

A) PDB ID 181L², RMSD =0.583 Å **B)** PDB ID 1NHB², RMSD =0.822 Å **C)** PDB ID 186L², RMSD =1.086 Å **D)** PDB ID 184L², RMSD =0.779 Å **E)** PDB ID 188L², RMSD =1.812 Å **F)** PDB ID 187L², RMSD =0.847 Å **G)** PDB ID 183L², RMSD =1.026 Å **H)** PDB ID 182L², RMSD =0.286 Å **I)** PDB ID 185L², RMSD =0.344 Å **J)** PDB ID 3DMZ³, RMSD =1.472 Å **K)** PDB ID 3DN0³, RMSD =1.871/3.291 Å **L)** PDB ID 3DN1³, RMSD =1.341/2.099/2.454/3.054/3.476/3.854 Å **M)** PDB ID 3DN2³, RMSD =2.084/2.928/2.978 Å **N)** PDB ID 3DN3³, RMSD =1.153 Å **O)** PDB ID 3DN4³, RMSD =0.838/2.808 Å **P)** PDB ID 3DN6³, RMSD =1.017/4.552 Å **Q)** PDB ID 2RAY⁴, RMSD =0.749 Å **R)** PDB ID 2RAZ⁴, RMSD =1.486 Å **S)** PDB ID 2RB0⁴, RMSD =1.020 Å **T)** PDB ID 2RB1⁴, RMSD =1.946 Å **U)** PDB ID 2RB2⁴, RMSD =1.10 Å

SI Figure 5

		Docking	
		True	False
Ligand ???	Positive	21	5
	Negative	7	3

		1D Chemotype	
		True	False
Ligand ???	Positive	18	7
	Negative	5	6

		Polar Surface Area	
		True	False
Ligand ???	Positive	16	4
	Negative	8	8

SI Figure 5: Truth tables comparing various methods for ligand discovery in L99A/M102H†, from right to left, molecular docking (DOCK 3.6), a 1D chemotype (fewer than 10 non-hydrogen atoms, at least one polar atom, and neutral), and the polar surface area of the ligands (MollInspiration⁵, ligands had polar surface area between 26 and 46 Å²). Ligands were chosen prospectively by docking and retrospectively in the other two cases. Ligands are listed as true positives (a correctly predicted ligand), true negative (correctly predicted to not be a ligand), false positives (incorrectly predicted to be a ligand) and false negatives (incorrectly predicted to not be a ligand). Docking outperformed the 1D chemotyping method by virtue of the additional steric information contained in the receptor and the polar surface area method by correctly identifying the non-polar ligands. 36 ligands are listed in the truth table. The 37th ligand, 2-mercaptoethanol, found fortuitously by initial crystal screening and present in Table 3 of the main text has a DOCK rank of 12,241. This placed it in the intermediate range between the true positives (1%) and false negatives (5%) and is not included in the truth tables due to that ambiguity.

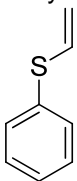
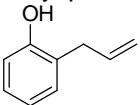
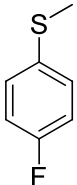
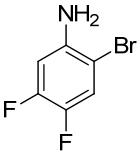
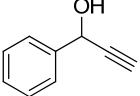
SI Table 1- XTAL data

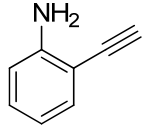
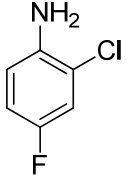
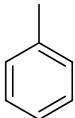
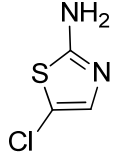

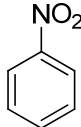
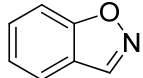
Complex	L99A/M102H†/benzene	L99A/M102H†/toluene	L99A/M102H†/phenol	L99A/M102H†/2-allyl phenol
PDB entry	4I7J	4I7K	4I7L	4I7M
Data Collection & Processing				
Crystals Used	1	1	1	1
Wavelength [Å]	1.116	1.116	1.116	1.116
Space Group	P2 ₁	P2 ₁	P2 ₁	P2 ₁
Unit Cell Parameters				
a, b, c [Å]	48.39, 75.58, 52.60	48.32, 75.55, 52.76	48.44, 75.37, 52.68	48.30, 75.09, 52.76
α, β, γ [°]	90.00, 93.28, 90.00	90.00, 93.22, 90.00	90.00, 93.31, 90.00	90.00, 93.08, 90.00
Matthews Coefficient[Å ³ /Da]	2.25	2.25	2.25	2.24
Solvent Content [%]	45.3	45.4	45.3	45.0
Diffraction Data				
Resolution Range [Å]	50-1.63 (1.73-1.63)	50-1.70 (1.80-1.70)	50-1.49 (1.58-1.49)	50-1.40 (1.48-1.40)
Unique Reflections	44,127 (7,216)	40,876 (6,592)	59,483 (9,634)	71,974 (10,932)
R(I)sym [%]	6.6 (36.4)	6.7 (37.7)	5.1 (35.5)	6.0 (78.0)
Completeness [%]	93.1 (94.4)	98.0 (98.2)	96.3 (96.7)	96.3 (90.8)
Redundancy	2.6 (2.5)	2.6 (2.5)	2.6 (2.5)	2.6 (2.5)
I/σ(I)	11.9 (2.6)	12.5 (2.8)	14.1 (2.7)	10.4 (1.3)
Refinement				
Resolution Range [Å]	48.3-1.67	48.2-1.72	48.4-1.52	43.1-1.48
Reflections Used (work/free)	40,933/1,636	39,514/1,570	56,080/2,247	60,991/2,437
Final R Values (work/free)[%]	20.48/23.93	16.79/20.05	16.10/18.08	17.43/19.81
Protein Residues	348	350	351	349
Ligand Atoms	12	28	14	20
Water Molecules	265	325	353	298
RMSDs				
Bonds[Å]	0.012	0.012	0.013	0.021
Angles[°]	1.4	1.5	1.4	1.8
Ramachandran plot: residues in:				
Favored (98%) regions [%]	98.9	98.9	99.5	99.2
Allowed (>99.8%) regions [%]	100.0	100.0	100.0	100.0
Mean B-Factor [Å²]				
Protein	12.8	14.1	13.4	17.5
Ligand	7.4	8.5	10.6	16.1
Water Molecules	19.7	23.7	24.4	27.1

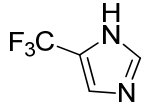
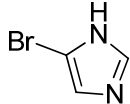

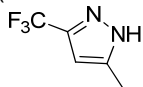
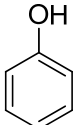
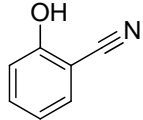
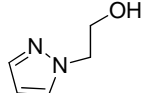
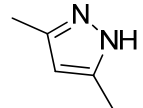
Complex	L99A/M102H†/ 1-phenyl-2-propyn-1-ol	L99A/M102H†/ 2-amino-5-chlorothiazole	L99A/M102H†/ 4-bromoimidazole	L99A/M102H†/ 4-trifluoromethyl imidazole
PDB entry	4I7N	4I7O	4I7P	4I7Q
Data Collection & Processing				
Crystals Used	1	1	1	1
Wavelength [Å]	1.116	1.116	1.116	1.116
Space Group	P2 ₁	P2 ₁	P2 ₁	P2 ₁
Unit Cell Parameters				
a, b, c [Å]	48.63, 75.14, 52.72	48.32, 75.34, 52.76	48.37, 75.40, 52.70	48.57, 75.31, 52.65
α, β, γ [°]	90.00, 93.18, 90.00	90.00, 93.22, 90.00	90.00, 93.17, 90.00	90.00, 93.28, 90.00
Matthews Coefficient[Å ³ /Da]	2.25	2.24	2.24	2.25
Solvent Content [%]	45.4	45.2	45.2	45.4
Diffraction Data				
Resolution Range [Å]	50-1.55 (1.64-1.55)	50-1.69 (1.79-1.69)	50-1.55 (1.65-1.55)	50-1.53 (1.62-1.53)
Unique Reflections	52,560 (7,397)	40,306 (6,526)	52,367 (8,523)	55,463 (8,676)
R(I)sym [%]	5.3 (42.9)	5.9 (40.1)	7.1 (43.6)	5.7 (38.8)
Completeness [%]	95.7 (83.6)	95.0 (95.1)	95.8 (96.7)	96.5 (93.3)
Redundancy	2.4 (1.8)	2.6 (2.4)	2.6 (2.5)	2.5 (2.4)
I/σ(I)	12.9 (1.9)	13.6 (2.5)	11.0 (2.5)	11.7 (2.4)
Refinement				
Resolution Range [Å]	48.6-1.58	48.2-1.73	48.3-1.60	48.5-1.58
Reflections Used (work/free)	50,322/2,006	37,583/1,499	48,060/1,918	50,441/2,033
Final R Values (work/free)[%]	17.47/20.17	16.84/19.40	17.94/20.42	18.84/21.32
Protein Residues	349	349	350	349
Ligand Atoms	20	14	12	18
Water Molecules	302	286	285	282
RMSDs				
Bonds[Å]	0.017	0.006	0.013	0.010
Angles[°]	1.6	1.0	1.4	1.3
Ramachandran plot: residues in:				
Favored (98%) regions [%]	99.5	99.2	99.2	99.4
Allowed (>99.8%) regions [%]	100.0	100.0	100.0	100.0
Mean B-Factor [Å²]				
Protein	14.7	15.3	13.5	14.3
Ligand	8.5	18.0	9.0	9.1
Water Molecules	25.3	25.3	22.0	24.2

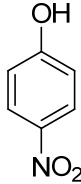
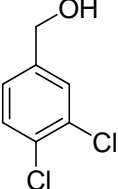
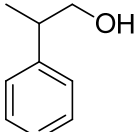
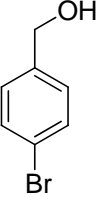
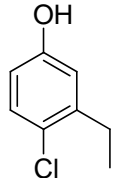
Complex	L99A/M102H†/ 2-(pyrazolo-1-yl) ethanol	L99A/M102H†/ 3-trifluoromethyl-5-methyl pyrazole	L99A/M102H†/ 2-bromo-5- hydroxybenzaldehyde
PDB entry	4I7R	4I7S	4I7T
Data Collection & Processing			
Crystals Used	1	1	1
Wavelength [Å]	1.116	1.116	1.116
Space Group	P2 ₁	P2 ₁	P2 ₁
Unit Cell Parameters			
a, b, c [Å]	48.59, 75.37, 52.63	48.58, 75.59, 52.60	48.06, 75.81, 52.71
α, β, γ [°]	90.00, 93.25, 90.00	90.00, 93.13, 90.00	90.00, 93.11, 90.00
Matthews Coefficient[Å ³ /Da]	2.25	2.26	2.24
Solvent Content [%]	45.4	45.5	45.2
Diffraction Data			
Resolution Range [Å]	50-1.48 (1.57-1.48)	50-1.64 (1.74-1.64)	50-1.50 (1.59-1.50)
Unique Reflections	58,809 (9,763)	45,870 (7,358)	56,323 (7,219)
R(I)sym [%]	4.6 (40.3)	6.0 (38.5)	5.5 (44.7)
Completeness [%]	93.5 (96.3)	98.6 (98.2)	92.7 (73.9)
Redundancy	2.7 (2.5)	2.5 (2.5)	2.5 (2.0)
I/σ(I)	15.8 (2.5)	12.8 (2.6)	13.9 (2.1)
Refinement			
Resolution Range [Å]	48.5-1.52	48.5-1.69	48.0-1.55
Reflections Used (work/free)	54,399/2,170	42,019/1,677	52,336/2,103
Final R Values (work/free)[%]	16.95/19.03	16.89/19.57	17.47/19.85
Protein Residues	349	349	349
Ligand Atoms	16	20	20
Water Molecules	335	355	320
RMSDs			
Bonds[Å]	0.010	0.014	0.021
Angles[°]	1.3	1.4	1.9
Ramachandran plot: residues in:			
Favored (98%) regions [%]	99.4	99.5	98.9
Allowed (>99.8%) regions [%]	100.0	100.0	100.0
Mean B-Factor [Å²]			
Protein	13.7	13.4	15.3
Ligand	12.5	11.4	15.0
Water Molecules	24.3	23.0	25.8

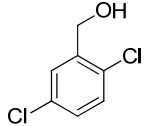
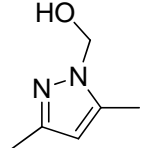
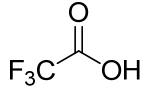
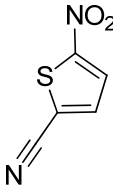
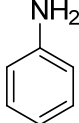
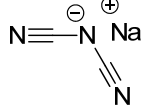

SI Table 2- DOCK Scores

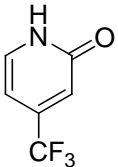
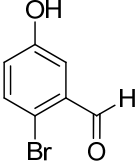
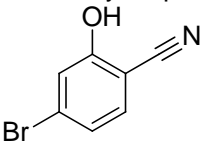
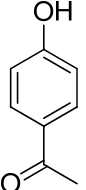
Docking True Positives	Rank	Electrostatics	VDW	Polar Desolvation	Non-Polar Desolvation	Total DOCK Score
phenyl vinyl sulfide 	10	0.2	-19.37	2.25	-4.55	-21.46
2-allyl phenol 	30	-0.87	-19.4	2.78	-2.8	-20.29
4-fluorothioanisole 	37	0.01	-18.24	2.24	-4.22	-20.2
2-bromo-4,5-difluoro aniline 	45	-3.46	-16.76	2.55	-2.39	-20.07
1-phenyl-2-propyn-1-ol 	50	-0.72	-20.06	3.35	-2.52	-19.95

2-ethynylaniline 	76	-1.95	-18.35	3.34	-2.67	-19.63
2-chloro-4-fluoroaniline 	88	-2.71	-16.86	2.38	-2.23	-19.43
toluene 	101	-0.91	-15.94	1.4	-3.84	-19.28
2-amino-5-chloro thiazole 	172	-4.35	-16.02	3.01	-1.34	-18.70
benzene 	579	-0.7	-14.48	1.34	-3.35	-17.2
nitrobenzene 	713	-2.56	-16.02	5.55	-3.85	-16.88
1,2-benzisoxazole 	867	-2.47	-17.42	6.19	-2.9	-16.59

4-trifluoromethyl imidazole 	1183	-4.96	-15.53	6.85	-2.43	-16.08
4-bromoimidazole 	1191	-4.48	-15.26	5.77	-2.09	-16.07
3-chloro-1H-pyrazolo[3,4b]pyridine 	1399	-1.88	-16.9	5.07	-2.1	-15.81
3-methyl-5-(trifluoromethyl) pyrazole 	1908	-0.77	-15.13	2.7	-1.98	-15.19
phenol 	2430	-3.01	-14.55	4.19	-1.21	-14.58
2-hydroxybenzonitrile 	2854	0.02	-18.31	5.63	-1.49	-14.15
2-(pyrazolo-1-yl) ethanol 	3069	-3.29	-15.86	4.81	0.35	-13.98
3,5-dimethyl pyrazole 	4355	-1.87	-13.58	4.1	-1.7	-13.04

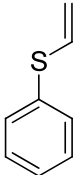
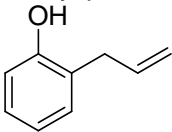
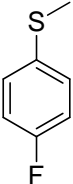
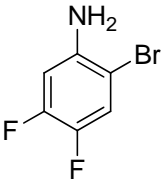
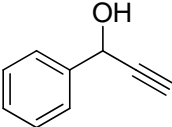
<p>4-nitrophenol</p> 	6373	-1.44	-14.19	5.45	-1.64	-11.81
Docking True Negatives						
<p>3,4-dichlorobenzyl alcohol</p> 	34166	-3.97	-0.01	3.69	1.4	1.12
<p>2-phenyl-1-propanol</p> 	34280	-1.57	-0.58	2.56	0.76	1.17
<p>3-bromobenzyl alcohol</p> 	35176	-0.72	-2.55	3.24	1.64	1.6
<p>4-chloro-3-ethyl phenol</p> 	35386	-1.06	-0.11	2.52	0.35	1.7

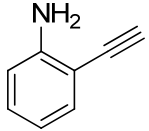
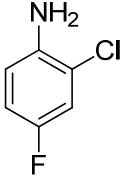
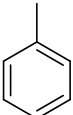
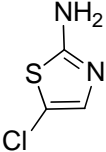

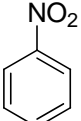
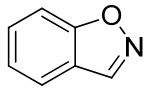
2,5-dichlorobenzyl alcohol 	35485	-1.83	-0.1	2.56	1.13	1.75
3,4-dimethylpyrazole-1-methanol 	40098	-0.29	-3.47	7.22	0.44	3.9
trifluoroacetic acid 	50352	-3.32	-12.51	25.72	-1.2	8.7
Docking False Positives						
5-nitrothiophene-2-carbonitrile 	19	-1.9	-20.27	4.84	-3.59	-20.93
aniline 	301	-1.76	-16.4	1.9	-1.81	-18.06
dicyanamide, sodium salt 	1482	-5.48	-10.07	4.81	-4.97	-15.71
pyridine 	1970	-1.22	-14.71	2.91	-2.06	-15.09

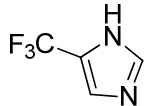
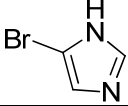
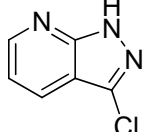
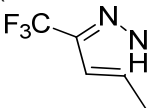
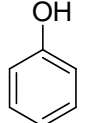
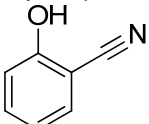
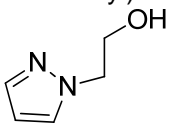
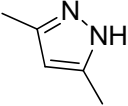
4-(trifluoromethyl) pyridin-2-ol 	2114	-4.8	-16.48	8.19	-1.83	-14.92
Docking False Negatives						
2-bromo-5-hydroxybenzaldehyde 	32818	-1.85	-2.08	5.83	-1.4	0.5
5-bromo-2-cyanophenol 	33837	-1.76	-2.22	4.73	0.21	0.96
4-hydroxyacetophenone 	34034	-2.23	-0.94	5.73	-1.5	1.06

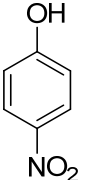
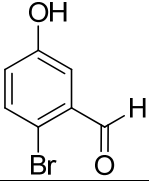
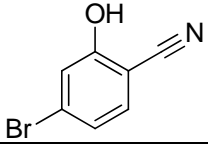
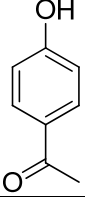
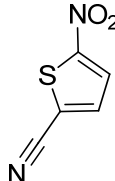
SI Table 2: The individual components of the DOCK scoring function⁴ (electrostatics, van der Waals interaction, polar and non-polar desolvation) shown for each of the tested molecules. This DOCK run used SEV desolvation on a set comprised of 650,000 purchasable small molecules with molecular weight less than 250 Daltons. 2-mercaptoethanol, a ligand was ranked in the intermediate range between the true positives (1%) and false negatives (5%) and is not included on this list due to that ambiguity.

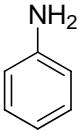
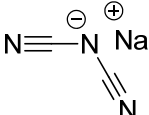

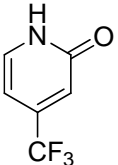
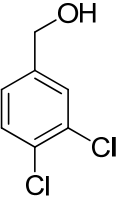
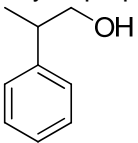
SI Table 3

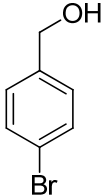
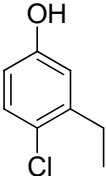
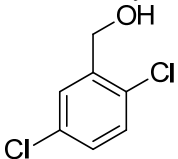
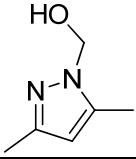
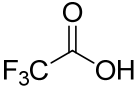
Ligands	Strd. Rank	Strd. Score	+0.4 e ⁻ Rank	+0.4 e ⁻ Score	+0.8 e ⁻ Rank	+0.8 e ⁻ Score	Scale VdW Rank	Scale VdW Score	Scale Elec. Rank	Scale Elec. Score	L99A Rank
phenyl vinyl sulfide 	10	-21.47	160	-20.66	1578	-19.91	36	-11.68	244	-19.59	3
2-allyl phenol 	30	-20.29	595	-18.9	2401	-18.81	218	-10.4	367	-19	59
4-fluorothioanisole 	37	-20.21	327	-19.72	1776	-19.58	98	-11	4022	-13.58	89
2-bromo-4,5-difluoro aniline 	45	-20.06	78	-21.49	268	-23.54	50	-11.5	60	-21.39	872
1-phenyl-2-propyn-1-ol 	50	-19.95	336	-19.68	765	-21.51	388	-9.86	196	-19.9	46

2-ethynylaniline 	76	-19.63	206	-20.36	972	-21	176	-10.55	90	-20.96	417
2-chloro-4-fluoroaniline 	88	-19.42	201	-20.39	670	-21.8	118	-10.82	2068	-15.69	262
toluene 	101	-19.29	367	-19.59	1543	-19.96	70	-11.27	287	-19.4	57
2-amino-5-chloro thiazole 	172	-18.7	728	-18.63	332	-23.13	1869	-7.95	380	-18.95	811
benzene 	579	-17.19	1452	-17.35	3688	-17.55	356	-9.94	990	-17.4	452
nitrobenzene 	713	-16.88	933	-18.16	1493	-20.04	1015	-8.8	1411	-16.66	436
1,2-benzisoxazole 	867	-16.6	1326	-175.51	2502	-18.71	2031	-7.81	1834	-16.03	1004

4-trifluoromethyl imidazole 	1183	-16.07	289	-19.89	163	-24.54	1331	-8.47	84	-21.02	2440
4-bromoimidazole 	1191	-16.06	451	-19.31	278	-23.46	1192	-8.6	428	-18.79	2640
3-chloro-1H-pyrazolo[3,4b]pyridine 	1399	-15.81	4437	-14.53	9360	-13.84	2859	-7.25	984	-17.41	536
3-methyl-5-(trifluoromethyl) pyrazole 	1908	-15.18	857	-18.33	797	-21.44	1539	-8.26	414	-18.85	3254
phenol 	2430	-14.58	1413	-17.39	1579	-19.91	1660	-8.14	2086	-15.67	1540
2-cyanophenol 	2854	-14.15	5043	-14.12	6821	-15.27	7900	-4.99	4468	-13.2	995
2-(pyrazolo-1-yl) ethanol 	3069	-13.99	2367	-16.26	1763	-19.59	4422	-6.38	1172	-17.04	6451
3,5-dimethyl pyrazole 	4355	-13.05	3585	-15.16	3364	-17.84	3845	-6.66	2252	-15.45	5132

<p>4-nitrophenol</p> 	6373	-11.82	7172	-12.82	8657	-14.22	8340	-4.83	5040	-12.74	6740
<p>2-bromo-5-hydroxybenzaldehyde</p> 	32818	0.5	34234	-0.15	31804	-3.44	30455	1.46	33422	5.14	23604
<p>5-bromo-2-hydroxybenzonitrile</p> 	33837	0.96	37376	1.41	39681	0.23	34323	2.53	40523	9.52	35078
<p>4-hydroxyacetophenone</p> 	34034	1.06	35061	0.26	37349	-0.83	32297	1.97	31678	4.02	26739
Non-Ligands											
<p>5-nitrothiophene-2-carbonitrile</p> 	19	-20.92	40	-22.17	309	-23.27	134	-10.71	48	-21.7	2852

aniline 	301	-18.07	446	-19.32	1010	-20.92	290	-10.13	168	-20.1	295
dicyanamide, sodium salt 	1482	-15.71	88	-21.34	33	-27.87	75	-11.21	1127	-17.12	3572
pyridine 	1970	-15.08	3145	-15.54	4504	-16.84	2153	-7.71	2142	-15.59	2187
4-(trifluoromethyl) pyridin-2-ol 	2114	-14.92	1208	-17.67	477	-22.44	3995	6.59	349	-19.06	4865
3,4-dichlorobenzyl alcohol 	34166	1.11	32567	-0.96	29103	-4.62	30449	1.46	25858	0.36	51574
2-phenyl-1-propanol 	34280	1.17	36096	0.77	34705	-2.09	30914	1.59	26561	0.78	43804

3-bromobenzyl alcohol 	35176	1.61	38320	1.85	38447	-0.33	35872	2.95	29275	2.53	26613
4-chloro-3-ethyl phenol 	35386	1.7	38242	1.81	40671	0.71	32063	1.9	44829	12.04	16211
2,5-dichlorobenzyl alcohol 	35485	1.76	37492	1.46	41098	0.91	32372	1.99	28177	1.82	25455
3,4-dimethylpyrazole-1-methanol 	40098	3.9	41547	3.37	43804	2.15	42659	4.8	39515	8.91	32895
trifluoroacetic acid 	50352	8.69	54698	9.43	63823	11.57	73744	13.77	34053	5.54	45263

SI Table 3: The ranks and scores of the tested molecules are listed to show the effect of modifying the docking scoring parameters on this set of molecules. The ranks are shown using the standard docking parameters (Strd.), adding +0.4 or +0.8 electrons to His102 (+0.4 e⁻ or +0.8 e⁻), scaling the van der Waals term by a factor of 0.5 (Scale VdW), scaling the electrostatics term by a factor of 2 (Scale Elec.), and docking to the L99A cavity using the standard parameters. 2-mercaptoethanol, a ligand was ranked in the intermediate range between the true positives (1%) and false negatives (5%) and is not included on this list due to that ambiguity.

SI Table 4- DOCK Rank List

Rank	SMILES	ZINC ID	DOCK Score	Electrostatics	VDW	Polar Desolv.	Non-Polar Desolv.
1	<chem>c1([nH]nc(n1)[N+](=O)[O-])[N+](=O)[O-]</chem>	C04405530	-28.47	-5.11	-21.46	3.6	-5.5
2	<chem>c1(nc(n2(nnc2n1)N)N)N</chem>	C16889989	-23.52	-9.59	-16.37	7.47	-5.02
3	<chem>c1ccc(c(c1)NC(=O)N=[N+]=[N-])F</chem>	C16941442	-22.48	-1.67	-24.27	3.57	-0.11
4	<chem>c1([nH]nc(n1)Br)[N+](=O)[O-]</chem>	C15446333	-22.07	-3.93	-17.11	2.56	-3.59
5	<chem>c1c(nc([n-]1)[N+](=O)[O-])[N+](=O)[O-]</chem>	C05425252	-22.05	-2.11	-18.34	3.4	-5
6	<chem>c1ccc(cc1)CN[N+](=O)[O-]</chem>	C01668645	-21.89	c-0.07	-22.58	4.12	-3.35
7	<chem>c1ccc(cc1)N=C=S</chem>	C00164500	-21.83	-0.06	-20.54	2.73	-3.97
8	<chem>c1ccc(cc1)COC(=O)Cl</chem>	C00388130	-21.52	0.02	-19.65	2.61	-4.5
9	<chem>c1cc(ccc1N=C=O)F</chem>	C00164841	-21.49	-0.86	-20.51	1.86	-1.98
10	<chem>C=CSc1ccccc1</chem>	C01671473	-21.46	0.2	-19.37	2.25	-4.55
11	<chem>c1ccc(cc1)CON=O</chem>	C04537786	-21.41	-0.37	-19.87	2.83	-4
12	<chem>c1cc(ccc1OC(=O)Cl)F</chem>	C00389521	-21.33	-0.94	-20.64	2.63	-2.37
13	<chem>c1ccc(cc1)CCS</chem>	C04271722	-21.26	-1.17	-16.92	1.42	-4.59
14	<chem>c1cc(c(c(c1N=C=O)F)F</chem>	C02539239	-21.2	-1.74	-20.05	2.55	-1.96
15	<chem>c1cc(c(c(c1F)F)NC(=S)N</chem>	C13657238	-21.2	-0.77	-20.53	2.54	-2.44
16	<chem>c1c(cc(c(c1F)N=C=O)F)F</chem>	C02580782	-21.12	0.19	-20.78	1.96	-2.49
17	<chem>c1cc(c(cc1F)N)Cl</chem>	C02575153	-21.08	-2.93	-17.71	1.8	-2.24
18	<chem>c1cc(c(cc1F)F)N=C=O</chem>	C00164769	-20.95	-1.39	-20.28	2.63	-1.91
19	<chem>c1cc(sc1C#N)[N+](=O)[O-]</chem>	C00076192	-20.93	-1.9	-20.27	4.84	-3.59
20	<chem>C/C=C/Cc1ccccc1O</chem>	C01868609	-20.85	-0.71	-19.18	2.55	-3.51
21	<chem>C/C=N/Cc1ccccc1</chem>	C16999032	-20.85	-0.19	-20.4	3.04	-3.31
22	<chem>c1ccc(cc1)N=C=O</chem>	C01620980	-20.61	-0.7	-19.98	2.01	-1.94
23	<chem>c1cc(c(cc1SC#N)F)N</chem>	C03886750	-20.56	-2.15	-19.61	3.41	-2.22
24	<chem>c1cnccc1N=C=S</chem>	C23584266	-20.54	-0.99	-20.38	3.34	-2.51
25	<chem>c1ccc(cc1)NC(=S)NN</chem>	C16739945	-20.51	-0.5	-22.1	4.26	-2.18
26	<chem>c1ccc(cc1)OC(=O)N=C=O</chem>	C02384737	-20.49	-0.24	-23.58	3.77	-0.44
27	<chem>c1cc(oc1)CN=C=S</chem>	C02146625	-20.44	-1.99	-19.3	3.26	-2.42
28	<chem>C#Cc1cc(c(cc1N)F)F</chem>	C16159017	-20.44	-2.93	-18.71	3.95	-2.74
29	<chem>c1(c(non1)/N=N/c2c(non2)N)N</chem>	C15636578	-20.3	-3.41	-21.46	5.04	-0.47
30	<chem>C=Cc1c1ccccc1O</chem>	C01576883	-20.29	-0.87	-19.4	2.78	-2.8
31	<chem>SCc1ccccc1</chem>	M1995A025	-20.26	-0.44	-17.63	1.82	-4.01
32	<chem>c1ccc(cc1)CSC#N</chem>	C01529490	-20.25	-0.88	-18.35	3.55	-4.57
33	<chem>c1ccc(cc1)C/C=N/O</chem>	C13520876	-20.25	-3.39	-19.89	5.17	-2.13
34	<chem>[H]/N=C(NC#N)/Nc1ccccc1</chem>	C19300262	-20.24	0.13	-22.75	8.42	-6.05
35	<chem>c1cc(ccc1CS)F</chem>	C00404004	-20.22	-1.31	-17.21	2.34	-4.04
36	<chem>c1cc(cc(c1)F)N=C=O</chem>	C02242675	-20.21	-1.51	-19.33	2.53	-1.9
37	<chem>CSc1ccc(cc1)F</chem>	C00403157	-20.2	0.01	-18.24	2.24	-4.22
38	<chem>c1c([nH]nc1[N+](=O)[O-])C(F)(F)F</chem>	C12396555	-20.2	-4.68	-16.7	4.15	-2.97
39	<chem>c1cc(cc(c1)F)NC(=S)N</chem>	C13658596	-20.19	-2.36	-18.09	2.67	-2.41
40	<chem>c1ccc(cc1)C#CC#N</chem>	C01696957	-20.16	-0.38	-18.04	3.04	-4.78
41	<chem>c1(nnc(s1)N)C(F)(F)F</chem>	C17045419	-20.14	-4.13	-16.56	1.42	-0.87
42	<chem>c1ccc(cc1)N=[N+]=[N-]</chem>	C13950915	-20.13	-0.24	-20.17	1.92	-1.63
43	<chem>c1c(ncn1)N[N+](=O)[O-]</chem>	C03860187	-20.11	-5.92	-18.6	6.66	-2.26
44	<chem>C=C=Cn1c(nnn1)N</chem>	C17105011	-20.11	-2.34	-18.92	3.61	-2.46
45	<chem>c1c(c(cc(c1F)Br)N</chem>	C02526707	-20.07	-3.46	-16.76	2.55	-2.39
46	<chem>c1cc(ccc1C(F)(F)F)N=C=O</chem>	C00164849	-20.06	-1.49	-18.11	1.99	-2.45
47	<chem>c1ccc(cc1)CSC#N</chem>	C32138416	-19.97	-1.02	-18.75	4.38	-4.59
48	<chem>c1ccc(cc1)C(C#N)(F)F</chem>	C08698399	-19.96	0.17	-18.53	2.69	-4.3
49	<chem>c1cc(c(c(c1N=C=O)F)F)F</chem>	C00152315	-19.95	-2.22	-19.17	3.98	-2.53
50	<chem>C#C[C@H](c1ccccc1)O</chem>	C01673125	-19.95	-0.72	-20.06	3.35	-2.52
51	<chem>c1cc(c(cc1F)F)CN=C=S</chem>	C31829483	-19.94	-2.11	-17.27	3.24	-3.8
52	<chem>c1cc(ncn1)N[N+](=O)[O-]</chem>	C06666632	-19.93	-0.32	-21.94	4.25	-1.92
53	<chem>COC(=O)C1ccccc1</chem>	C02526463	-19.88	0.11	-20.93	5.13	-4.19
54	<chem>c1c(nc([nH]1)Br)[N+](=O)[O-]</chem>	C05425250	-19.87	-1.52	-18.49	3.09	-2.65
55	<chem>c1cc2c(cc1Cl)nn[nH]2</chem>	C05425428	-19.85	-4.63	-17.48	3.91	-1.95
56	<chem>C#CCn1ncc(n1)[N+](=O)[O-]</chem>	C01067075	-19.84	-2.52	-20.32	6.19	-3.18
57	<chem>c1cc(ncn1)C(=N)C#N</chem>	C22995892	-19.82	-0.34	-22.59	6.1	-2.98
58	<chem>c1(c(c(nc(c1)F)F)F)F</chem>	C02539380	-19.81	0.17	-18.39	0.53	-2.12
59	<chem>c1c(nc(c1Br)N)F</chem>	C19616065	-19.81	-2.93	-18.01	2.74	-1.62
60	<chem>c1cc2c(cc1C#N)non2</chem>	C00161282	-19.78	-2.55	-19.21	4.71	-2.73
61	<chem>CCc1ccccc1</chem>	M1995A033	-19.78	-0.65	-15.97	1.3	-4.45
62	<chem>c1cnccc1N[N+](=O)[O-]</chem>	C00330820	-19.77	-2.06	-20.48	4.57	-1.79
63	<chem>Cc1ccc(c(n1)N)SC#N</chem>	C20413739	-19.77	-4.54	-18.43	5.21	-2.01
64	<chem>C=Cc1ccccc1</chem>	C02039882	-19.75	-1.07	-18.95	3.11	-2.84
65	<chem>c1ccc(cc1)NCN=O</chem>	C17300127	-19.75	-1.35	-21.05	4.57	-1.92
66	<chem>c1ccc(c(c1)N)Cl</chem>	C00164914	-19.72	-2.43	-17.12	2.02	-2.19
67	<chem>CCOC(=O)C(=O)Cl</chem>	C01639557	-19.72	-1.23	-17.9	1.96	-2.54
68	<chem>c1cc(sc1)/C=C/[N+](=O)[O-]</chem>	C00055258	-19.7	-1	-19.09	4.76	-4.36
69	<chem>c1ccc(cc1)CN=C=O</chem>	C01708235	-19.7	-0.98	-19.9	2.8	-1.62
70	<chem>c1c(ncn1)NN=O/[N+](=O)[O-]</chem>	C06524458	-19.7	-3.64	-17.74	3.8	-2.12
71	<chem>c1ccc(cc1)CCC#N</chem>	C01747831	-19.69	-1.21	-18.56	4.9	-4.82
72	<chem>c1nnc2n1nc(s2)N</chem>	C08617477	-19.67	-3.6	-19.95	5.92	-2.04
73	<chem>c1cc(c(cc1F)N)C#N</chem>	C16159342	-19.67	-2.24	-18.87	3.48	-2.05
74	<chem>c1cc(sc1C#N)Br</chem>	C02541509	-19.64	-1.02	-17.62	2.5	-3.5
75	<chem>c1c([n-]nc1[N+](=O)[O-])[N+](=O)[O-]</chem>	C04343199	-19.64	-4.43	-15.26	3.45	-3.4
76	<chem>C#Cc1ccccc1N</chem>	C02534489	-19.63	-1.95	-18.35	3.34	-2.67
77	<chem>c1c(ch(n1)[N+](=O)[O-])Cl</chem>	C02390477	-19.55	-1.84	-19.21	3.84	-2.33
78	<chem>c1([nH]nc([nH+]1)[O-])[N+](=O)[O-]</chem>	C05030609	-19.55	-3.48	-17.97	3.74	-1.84
79	<chem>c1ccc(cc1)CNO</chem>	C00389753	-19.53	-3.17	-18.8	3.01	-0.56
80	<chem>c1(nc(n1)C(F)(F)F)C(F)(F)F</chem>	C04803474	-19.52	-1.82	-15.91	1.2	-2.99
81	<chem>c1cc(ncc1N=C=O)Cl</chem>	C04287788	-19.51	-2.24	-19.56	3.09	-0.8
82	<chem>c1cc(nnc1N=C(N)N)Cl</chem>	C13608829	-19.5	-4.59	-20.08	7.09	-1.92
83	<chem>c1cc(c(cc1F)N)CBr</chem>	C16082895	-19.49	-2.23	-17.13	2.85	-2.97
84	<chem>C=CC1ccccc1</chem>	C01845718	-19.48	0.46	-19.12	2.85	-3.67
85	<chem>c1cc(ccc1O)SC#N</chem>	C00334839	-19.47	-1.9	-20.55	4.56	-1.58
86	<chem>c1cc(ncn1)C(=N)O/N</chem>	C12505213	-19.47	-4.2	-20.85	5.1	0.49

87	c1cc(ccc1N=C=O)Cl	C01707960	-19.45	-1.23	-19.07	1.55	-0.69
88	c1cc(c(cc1F)Cl)N	C00152883	-19.43	-2.71	-16.86	2.38	-2.23
89	c1cnccc1CCS	C04522278	-19.41	-1.72	-17.5	2.99	-3.18
90	c1ccc(cc1)[C@@H](C#C(F)(F)F)O	C15774487	-19.4	-0.82	-19.91	4.84	-3.51
91	c1cc(c(cc1F)N=C=O)F	C00152295	-19.39	0.26	-20.17	2.56	-2.04
92	c1cc(ccc1Cl)NN=O	C06536600	-19.39	-1.33	-21.17	4.82	-1.71
93	c1c(sc(n1)N)[N+](=O)[O-]	C08579229	-19.37	-5.69	-18.72	6.58	-1.55
94	c1cc(c(c(c1NC(=S)N)F)F)F	C13659124	-19.37	-1.02	-18.82	3.39	-2.92
95	c1cnn(c1)C(=NH2+)N	C04217344	-19.36	-3.84	-17.98	4.06	-1.59
96	c1c(nc(nc1F)F)FCl	C01845799	-19.3	-0.23	-17.87	0.57	-1.77
97	c1cc(c(cc1N)N)Cl	C00388158	-19.29	-2.84	-18.46	2.58	-0.57
98	c1csccl1C(F)(F)F	C15440554	-19.29	-1.59	-16.45	2.05	-3.31
99	C1CSP(S1)OCC(F)(F)F	C01579432	-19.28	1.53	-14.85	5.14	-11.11
100	CSc1ccccc1	C01688763	-19.28	0.2	-17.64	2.32	-4.16
101	Cc1ccccc1	M1995A023	-19.28	-0.91	-15.94	1.4	-3.84
102	c1(c(non1)N=[N+]=[N-])N	C12558738	-19.26	-2.9	-19.32	2.57	0.39
103	c1ccc(cc1)OC(=O)Cl	C00388419	-19.25	-0.42	-20.18	3.15	-1.8
104	c1ccc(cc1)OCCN[NH3+]	C19168146	-19.24	-3.77	-17.37	2.98	-1.07
105	CSc1ccccc1	M1995A026	-19.22	0.22	-17.6	2.3	-4.15
106	c1cc(c(cc1Cl)F)F	C00164831	-19.2	-0.89	-16.71	2.22	-3.22
107	c1ccc(c(c1)N=C=O)F	C00164839	-19.2	-0.57	-19.83	3.25	-2.05
108	Cc1c(non1)C(=N/O)N	C04342611	-19.2	-4.63	-18.88	3.19	1.11
109	c1cc(c(cc1F)N)CCl	C16082896	-19.19	-2.12	-17.19	2.99	-2.87
110	c1c(cc(cc1F)N)N=C=O	C02389320	-19.16	-1.16	-17.34	1.32	-1.99
111	[H]/N=C/(Nc1cnoc1)N(C(=NH2+))N	C26510250	-19.15	-2.2	-23.04	7.68	-1.6
112	CSc1nc([nH]n1)N=[N+]=[N-]	C17024990	-19.14	-4.89	-16.45	3.47	-1.26
113	c1(c(cc(nc1F)F)F)F	C01845797	-19.12	0.46	-17.45	0.68	-2.81
114	c1cc(c(nc1)N)Br	C19015172	-19.11	-2.47	-17.86	2.81	-1.6
115	c1nc([nH]n1)N/N=C(C#N)/[N+](=O)[O-]	C05005026	-19.1	-0.73	-19.14	5.01	-4.25
116	c1c(nc([nH]1)[N+](=O)[O-])Br	C26894018	-19.1	-1.76	-17.91	4.74	-4.17
117	c1cc(ncc1F)CBr	C14985908	-19.09	-1.56	-17.51	3.15	-3.17
118	c1c(csc1C#N)Br	C14988315	-19.08	-1.52	-17.3	3.19	-3.45
119	c1ccc(cc1)SC#N	C02037318	-19.07	-1.38	-19.56	3.51	-1.64
120	H]/N=C/c1cccc1	C01759569	-19.06	-2.11	-17.38	2.95	-2.53
121	C#Cc1ccccc1	M1995A028	-19.06	-0.11	-17.68	2.96	-4.23
122	c1cnccc1N=C=O	C12957599	-19.05	-1.46	-19.78	2.7	-0.51
123	c1c(c(nc(n1)N)N)C#N	C00393991	-19.04	-3.2	-19.65	4.64	-0.83
124	CC(=O)Oc1ccc(cc1)F	C00403164	-19.01	0.28	-19.96	5.01	-4.35
125	c1c(cc(c(c1F)N)F)F	C00406986	-19	-1.38	-17.18	1.51	-1.94
126	c1c(cncn1)I	C00967270	-19	-0.81	-17.68	2.19	-2.7
127	c1c(cncn1)Br	C00967317	-18.99	-0.85	-18.17	2.36	-2.32
128	c1cc(sc1Cl)Cl	C01690277	-18.99	-0.82	-15.34	0.67	-3.49
129	c1(nnc(s1)Cl)N	C17045344	-18.98	-3.66	-16.31	1.44	-0.45
130	c1ccc(c(c1)CCC#N)F	C31829539	-18.98	-1.39	-18.23	5.5	-4.86
131	c1c(cc(c(c1F)CC#N)F)F	C04290232	-18.97	-0.45	-19.5	4.71	-3.74
132	c1cnc(c1)SCC#N	C04244935	-18.96	-0.18	-20.38	5.07	-3.47
133	c1ccc(cc1)CC#N	C01666748	-18.95	-1.1	-19.06	5.44	-4.23
134	CCc1nc(on1)[N+](=O)[O-]	C27828798	-18.95	-0.39	-17.64	1.58	-2.5
135	Cc1ccc(cc1)N	C00164438	-18.94	-3.81	-15.44	2.69	-2.38
136	c1cc(cnc1)[N+](=O)[O-]	C02559924	-18.94	-3.14	-18.6	5.36	-2.56
137	C=Cn1c(nnn1)N	C04642610	-18.93	-2.94	-18.58	2.98	-0.39
138	c1c(cnccl1)F	C02547814	-18.92	-0.33	-17.67	1.54	-2.46
139	c1c(cc(c(c1N)N)F)F	C02571496	-18.92	-4.74	-16.83	3.08	-0.43
140	c1cnccc1C(=N)C#N/N	C16123684	-18.92	0.04	-21.1	5.04	-2.9
141	c1cc(cnc1)C=N/N	C00436681	-18.91	-3.52	-19.26	4.72	-0.85
142	c1csccl1CCl	C16124406	-18.91	-0.77	-16.56	1.97	-3.55
143	CSc1ccccc1N	C00391221	-18.9	-1.68	-17.23	2.61	-2.6
144	c1cc(cnc1)CBr	C11535817	-18.86	-0.79	-18.25	3.27	-3.09
145	c1cc(ccc1C(=N)N)C#N)Cl	C001715165	-18.84	-0.2	-18.94	2.92	-2.62
146	c1c(cc(c(c1F)F)N)N=C=O	C19737280	-18.84	-1.08	-18.19	2.46	-2.02
147	c1cc(c(cc1F)N)F	C00388527	-18.83	-2.75	-16.35	2.13	-1.86
148	c1cc2c(cc1C#N)n[nH]n2	C02524667	-18.83	-4.54	-19.54	6.59	-1.34
149	c1cc(nnc1C(=O)Cl)Cl	C19045534	-18.83	-2.54	-18.36	3.98	-1.92
150	c1cn(cn1)C(=O)Cl	C22011804	-18.83	-1.57	-18.4	3.57	-2.43
151	CC#Cc1ccccc1	M1995A037	-18.83	0.42	-17.66	3.43	-5.02
152	c1cc(cnc1)N=C=O	C04244934	-18.82	-0.91	-20.55	3.25	-0.6
153	c1ccc(cc1)NNC(=O)C(=O)N	C01599333	-18.81	-7.05	-17.52	5	0.75
154	Cc1ccccc1N	C01706910	-18.8	-3.34	-15.22	2.09	-2.32
155	CCOC(=O)C(C(F)F)F)F)F	C01847426	-18.79	-1.36	-15.02	1.66	-4.08
156	c1cc(c(cc1F)F)NC(=O)N	C00171226	-18.78	-1.92	-21.51	5.19	-0.54
157	c1c(nc(nc1F)F)N)Br	C03660073	-18.78	-4.01	-16.51	2.68	-0.94
158	c1cc(c(cc1F)N)[N+](=O)[O-]	C04416634	-18.78	-2.47	-17.66	3.82	-2.46
159	c1cc(c(nc1)N)I	C19735470	-18.78	-2.8	-16.97	2.94	-1.94
160	c1cc(cc1C#N)[N+](=O)[O-]	C00156982	-18.77	-2.3	-20.37	6.63	-2.72
161	Cc1ccc([nH]1)SC#N	C00334412	-18.77	-1.6	-17.46	3.05	-2.75
162	c1ccc(c(c1)CS)F	C00405148	-18.77	0.36	-17.82	2.72	-4.03
163	c1c(cc(c(c1N)Cl)F)F	C02504703	-18.75	-3.09	-17.37	2.14	-0.42
164	c1c2c([nH]c(=S)[nH]2)ncn1	C08100893	-18.75	-6.16	-18.6	7.93	-1.91
165	c1cc(cnc1)CCl	C00164815	-18.72	-0.72	-18.47	3.46	-2.99
166	c1cc(c(cc1F)N)N	C00152599	-18.71	-4.32	-17.3	3.28	-0.37
167	c1cnn2cncc2c1	C12357125	-18.71	-2.6	-17.43	5.74	-4.42
168	c1c(c(c(c1)Cl)F)F	C14982366	-18.71	-0.67	-17.71	2.18	-2.51
169	c1c(csc1C#N)[N+](=O)[O-]	C00334382	-18.7	-2.87	-18.81	6.47	-3.48
170	c1c(cnccl1)Br	C00336455	-18.7	-0.33	-17.37	1.54	-2.54
171	CSc1ccccc1	C01674080	-18.7	-0.01	-16.19	2.35	-4.85
172	c1c(sc(n1)N)Cl	C17354929	-18.7	-4.35	-16.02	3.01	-1.34
173	c1cc(c(nc1)N)Cl	C19737460	-18.69	-2.9	-17.57	3.24	-1.47
174	c1cc(ccc1NN)F	C00085251	-18.67	-2.04	-18.15	3.15	-1.63
175	COc1c(cc(cc1F)F)F	C02382169	-18.66	0.17	-18.3	2.22	-2.75
176	c1cncc(c1F)Cl	C02540648	-18.66	-2.33	-16.47	2.59	-2.45

177	c1cc(ncc1Cl)N	C19143849	-18.66	-3.34	-16.8	2.92	-1.44
178	c1c(cnc(c1)N)F	C19736832	-18.66	-3.39	-15.74	2.51	-2.04
179	c1ccc(c(c1)CCl)N	C20216992	-18.66	-1.68	-17.22	3.07	-2.82
180	COc1nc([nH]n1)N=[N+]=[N-]	C17024979	-18.65	-4.59	-19.62	3.81	1.75
181	c1([nH]nc(n1)[N+](=O)[O-])Cl	C05567031	-18.64	-4.81	-18.49	4.38	0.28
182	c1cc(cnc1)C(F)F	C08294933	-18.64	-2.57	-16.32	3.03	-2.78
183	c1cc(oc1)C=[NH2+]NO	C16082801	-18.63	-5.16	-18.89	4.85	0.57
184	c1ccc(c(c1)CC#N)F	C00406998	-18.62	-1.16	-19.34	6.15	-4.27
185	c1cc(ccc1CN=C=O)F	C02568124	-18.62	-1.67	-19	3.65	-1.59
186	c1ccn(c1)C(=O)O	C05521785	-18.62	-4.2	-17.92	4.83	-1.32
187	c1cc(c(c(c1)F)CBr)F	G2008A003	-18.61	0.51	-17.43	2.79	-4.49
188	c1ccc(c(c1)C=N/O)F	C02163529	-18.6	-3.24	-19.58	5.93	-1.7
189	Sc1ccccc1	S2001A005	-18.59	-0.07	-16.78	1.68	-3.42
190	c1cnccc1CBr	C02387257	-18.57	-0.96	-17.8	3.21	-3.03
191	C#Cc1cncnc1	C01387208	-18.56	-1.64	-17.95	3.83	-2.8
192	c1cc(sc1Cl)Br	C01840973	-18.56	-0.86	-14.83	0.69	-3.56
193	c1([nH]nc(n1)Br)Br	C04829562	-18.56	-3.61	-16.1	3.05	-1.91
194	c1c(ncc(n1)Br)NN=O	C06524494	-18.56	-2.86	-19.69	4.41	-0.44
195	c1nc(c2c(n1)[nH]n2)N	C03652180	-18.55	-4.59	-19.23	5.02	0.25
196	c1cc(oc1C#N)Br	C00097639	-18.54	-1.33	-17.71	3.28	-2.78
197	c1(c(non1)[N+](=O)[O-])N	C04087601	-18.54	-3.36	-17.34	3.4	-1.23
198	c1([nH+]c(=O)ss1)N	C08737721	-18.54	-2.64	-17.16	1.93	-0.67
199	Nc1ccc(F)cc1F	W2002A004	-18.54	-2.6	-16.72	2.67	-1.9
200	c1(=N([N+](=O)[O-])[nH]c(n1)[N-][N+](=O)[O-])	C13634238	-18.53	-1.4	-20.09	7.45	-4.48
201	c1c(cncn1)C	C30677788	-18.53	-1.4	-18.29	4.03	-2.87
202	lc1ccccc1	M1995A009	-18.53	-0.11	-15.62	1.41	-4.21
203	c1([nH]nnn1)c2n([nH]nn2)	C04257961	-18.52	-9.71	-17.31	6.84	1.65
204	c1c(c(cc(c1F)F)[N+](=O)[O-])N	C04329304	-18.51	-2.97	-17.06	4	-2.49
205	c1cc(c(cc1F)F)N	C00157573	-18.5	-2.46	-16.81	2.68	-1.9
206	CCc1ccccc1N	C01690957	-18.5	-1.65	-15.82	1.87	-2.91
207	c1cc(oc1C=O)[N+](=O)[O-]	C00152275	-18.48	-4.41	-17.31	5.41	-2.17
208	c1c(c(c(c(c1F)F)Br)N	C15443794	-18.48	-3.82	-15.81	3.57	-2.41
209	c1cnc(cn1)C(=N/O)N	C04270085	-18.47	-5.18	-20.6	5.49	1.81
210	c1cc(ccc1N=C(N)N)F	C05342293	-18.47	0.44	-21.35	4.83	-2.38
211	C/C=Nc1ccccc1	C17300129	-18.47	-0.55	-17.92	3.6	-3.6
212	c1cc(sc1)CN=C=O	C19730697	-18.47	-1.94	-18.76	3.15	-0.93
213	C=Cc1ccc(cc1)O	C00895826	-18.45	-0.92	-18.44	2.89	-1.99
214	C=Nc1ccccc1	C01682670	-18.45	-0.8	-18.49	3.81	-2.96
215	c1cc(sc1)CCl	C01845722	-18.45	-1.23	-15.73	2.16	-3.65
216	c1cc(ccc1N)F	C00013613	-18.44	-2.64	-16.67	2.69	-1.82
217	c1c(c(nc(n1)N)N)[N+](=O)[O-]	C04531688	-18.44	-3.19	-18.58	4.53	-1.2
218	Cc1ccc(cn1)N=C=O	C04716476	-18.44	-0.56	-20.07	3.22	-1.02
219	c1csc1C(=N/O)N	C04218335	-18.42	-4.68	-18.7	5.07	-0.1
220	CSc1ccc(cc1)N	C04244883	-18.42	-0.4	-18.36	2.87	-2.54
221	c1cc(c(cc1N)N)Br	C01715490	-18.41	-3.24	-17.04	2.55	-0.68
222	C=COc1c(C(C(F)F)F)F	C16125511	-18.41	0.6	-16.7	1.67	-3.98
223	Cc1cc(n[nH]1)C(F)F	C08700987	-18.4	-3.4	-16.72	4.11	-2.4
224	C=Cc1ccccc1	C00968269	-18.39	-0.57	-15.35	1.7	-4.19
225	c1c(cc(c(c1F)NN)F)F	C02384130	-18.39	-0.74	-18.31	2.29	-1.63
226	c1csc2c1sc(n2)S	C15945277	-18.39	-1.79	-18.6	4.45	-2.45
227	C=Cc1ccccc1	M1995A032	-18.39	-0.58	-15.33	1.71	-4.18
228	c1ccc(cc1)Oc2ccoc2	C16125361	-18.38	0.38	-19	4.28	-4.05
229	c1ccc2c(c1)[nH]c(n2)C#N	C00374942	-18.37	-3.07	-17.93	5.42	-2.79
230	c1cc(ccc1CC#N)F	C00388043	-18.37	-1.68	-19.28	6.89	-4.3
231	c1cc(cc(c1)F)C=C/[N+](=O)[O-]	C00103600	-18.36	-0.3	-18.45	5.43	-5.05
232	c1ccc(cc1)NN	C00388099	-18.36	-1.8	-17.48	2.56	-1.63
233	c1cc(ncc1Br)N	C19143844	-18.35	-3.13	-16.59	2.89	-1.52
234	Cc1ccc(cc1F)N=C=O	C02384731	-18.33	-0.52	-18.29	2.05	-1.56
235	c1ccc(cc1)C[NH+]=[N+]=[N-]	C04293814	-18.33	-0.35	-19.87	2.22	-0.33
236	c1c(cnc(n1)N)Cl	C01402616	-18.32	-1.67	-17.78	2.99	-1.86
237	C(=Nc1c(c(c(c1F)F)F)F)=O	C01995285	-18.32	-0.4	-15.48	1.12	-3.56
238	c1cc(cnc1)Cl	C02379647	-18.31	-0.78	-17.11	3.03	-3.46
239	c1cc(ccc1S)[S-]	C19683015	-18.31	-1.22	-15.01	1.47	-3.55
240	C=CCOc1ccccc1	C01680380	-18.3	-1.48	-15.3	2.51	-4.03
241	c1cc(sc1C(F)F)Cl	C15442288	-18.3	-1.24	-14.25	1.09	-3.89
242	c1cc(c(cc1F)F)NN	C00153133	-18.29	-0.75	-18.54	2.71	-1.7
243	c1cnccc1CCl	C00164896	-18.29	-0.87	-17.89	3.4	-2.93
244	c1c(c[nH]1)I	C02046962	-18.29	-3.73	-16.05	3.09	-1.6
245	Cc1([nH]nc(n1)N=[N+]=[N-])	C08383096	-18.29	-3.12	-17.02	2.97	-1.13
246	c1c(sc(n1)Cl)C#N	C01399115	-18.28	-1.04	-17.84	2.76	-2.17
247	c1c([nH+]cc2c1[nH]n2)	C05117686	-18.28	-4.63	-18.18	4.6	-0.06
248	c1csc1C=N/O	C00157006	-18.26	-3.28	-17.78	3.64	-0.83
249	CCc1ccsc1	C01995154	-18.26	-1.12	-14.85	1.33	-3.62
250	c1(=S)[nH]nc(n1)NN	C12958520	-18.24	-8.61	-16.1	7.45	-0.98
251	c1nc([nH]n1)/N=C(N)[O-]	C17328384	-18.24	-7.78	-17.4	7.27	-0.33
252	c1ccc2c(c1)non2	C00161248	-18.23	-2.35	-18.57	5.1	-2.41
253	c1cc(cnc1)CN=C=O	C19730700	-18.23	-1.57	-20.67	4.38	-0.36
254	C#Cc1ccc(cc1)N	C02534484	-18.22	-0.34	-18.76	3.48	-2.61
255	c1c(cnc(c1F)F)Br	C08698196	-18.22	-0.94	-17.06	2.29	-2.5
256	c1cnccc1Cl	C12958666	-18.22	-0.92	-16.86	2.97	-3.4
257	c1cc(ncc1[N+](=O)[O-])C#N	C14982543	-18.22	-2.59	-18.48	5.67	-2.82
258	C=Cc1ccsc1	C14983700	-18.22	-1.26	-15.23	1.69	-3.42
259	c1cc(c(cc1N)N)N	C00053658	-18.21	-4.63	-17.9	2.99	1.32
260	c1cc(oc1[N+](=O)[O-])Br	C01664806	-18.21	-2.14	-17.81	4.61	-2.88
261	c1([nH]nc(n1)Cl)Cl	C03882577	-18.21	-3.72	-15.39	2.76	-1.87
262	c1csc1N=C=O	C00158759	-18.2	-0.52	-18.58	2.1	-1.19
263	c1nc(c2c(n1)non2)N	C02272409	-18.2	-3.08	-19.59	5.54	-1.07
264	c1ccc(c(c1)N)N	C00004316	-18.19	-3.9	-16.46	2.51	-0.34
265	c1(nc(=S)ss1)N	C04710251	-18.19	-4.66	-14.21	3	-2.32
266	c1ccc(c(c1)N)NC#N	C19873054	-18.19	-1.35	-19.72	6.53	-3.65

267	c1c(cc(cc1F)F)N	C00164838	-18.18	-3.79	-15.03	2.46	-1.82
268	c1c(c(ncn1)N)C(=N)O/N	C04363312	-18.18	-6.11	-20.58	5.14	3.37
269	c1cc(c(cc1O)N)Cl	C00404165	-18.17	-2.91	-18.19	2.91	0.01
270	Cc1cc(ccc1N)F	C00406935	-18.17	-3.48	-15.16	2.84	-2.37
271	c1c(c(c(c(n1)F)F)C(F)F)F	C02513198	-18.16	-0.22	-17.22	2.59	-3.31
272	c1c(c(nc(n1)Cl)N)[N+](=O)[O-]	C04243102	-18.16	-3.86	-15.62	2.83	-1.51
273	c1cn(cn1)C#N	C08101017	-18.16	-2.23	-14.49	3.7	-5.13
274	c1cncc(c1Br)N	C14628887	-18.16	-3.78	-16.23	2.72	-0.87
275	c1ccc(cc1)/C=N/N	C01664869	-18.15	-2.98	-16.03	3.04	-2.19
276	c1ccc(c(c1)CN=C=O)F	C02389317	-18.15	0.24	-20.52	3.72	-1.58
277	c1cc(c(c(c1)F)CN=C=O)F	C15442300	-18.15	-0.26	-19.81	3.58	-1.65
278	c1cc(ccc1CC#N)N	C00152526	-18.14	-1.96	-19.59	6.03	-2.62
279	c1cc(ncc1Br)C#N	C00330869	-18.14	-1.62	-17.9	4.18	-2.79
280	c1cc(ncc1Cl)C#N	C02510866	-18.14	-1.3	-18.41	4.29	-2.71
281	C#C[C@H](c1cccc1)N	C32501211	-18.14	-0.44	-18.45	3.37	-2.62
282	Nc1cc(F)cc(F)c1	W2002A007	-18.13	-3.76	-15.03	2.47	-1.82
283	c1cc2c(n[nH]c2nc1)N	C00168464	-18.12	-5.9	-18.25	7.07	-1.05
284	c1cc(ccc1N)Cl	C00403225	-18.12	-0.77	-17.38	2.16	-2.13
285	c1cc(sc1)C(=[NH2+])NO	C13140013	-18.12	-5	-17.48	4.5	-0.14
286	c1c(c(cc(c1F)F)F)N	C00409371	-18.11	-3.14	-15.81	2.72	-1.88
287	CCc1cccnc1	C02034880	-18.11	-0.92	-16.89	2.77	-3.08
288	c1c[nH]c2c1cc(cn2)F	C14400996	-18.11	-2.83	-17.03	4.77	-2.95
289	c1c(cnc(c1Cl)F)F	C14982363	-18.11	-0.85	-17.16	2.3	-2.41
290	c1cc2c(c[nH]2)c(c1)F	C14983432	-18.11	-2.5	-17.69	4.39	-2.31
291	c1c(cnc(n1)N)CCl	C14989440	-18.11	-1.96	-18.3	4.62	-2.46
292	c1c(cncn1)C(F)F	C30714846	-18.11	-1.44	-16.68	2.61	-2.59
293	c1ccc(cc1)OC(=O)O	C05555526	-18.1	-1.43	-19.91	5.79	-2.55
294	C=Cn1ccnc1	C08294952	-18.1	-2.66	-16.9	4.77	-3.32
295	c1cc(cc(c1F)N	C00157619	-18.09	-3.23	-15.72	2.65	-1.79
296	CCc1cccs1	C02005192	-18.09	-1.28	-14.59	1.52	-3.74
297	c1ccc2c(c1)[nH]nn2	C00332008	-18.08	-3.96	-17.86	5.12	-1.39
298	c1c(cc(c1N)F)F	C02575075	-18.08	-2.92	-15.87	2.6	-1.88
299	c1cc(c(cc1F)F)CO	C00409278	-18.07	-1.61	-17.53	2.55	-1.47
300	c1c(c(nc(n1)F)F)Cl	C02540176	-18.06	-1.31	-17.68	2.71	-1.79
301	c1ccc(cc1)N	C17886255	-18.06	-1.76	-16.4	1.9	-1.81
302	Nc1ccccc1	Eliq_2GUN	-18.06	-1.89	-16.28	1.91	-1.8
303	c1cc(cnc1)Br	C00158591	-18.04	-0.34	-17.73	2.52	-2.49
304	c1ccc(cc1)C[N+](=O)[O-]	C01666770	-18.03	-0.92	-17.24	4.23	-4.1
305	c1cnccc1NN=O	C05464485	-18.03	-3.09	-17.96	3.57	-0.56
306	c1cc(ncc1Br)NN=O	C13213087	-18.03	-2.97	-19.01	5.71	-1.77
307	c1ccc(cc1)/C=C/C=O	C13523661	-18.02	-1.5	-17.42	4.87	-3.97
308	CCc1c(cncn1)F	C16158265	-18.02	-0.62	-16.99	2.52	-2.93
309	CC(=O)Nc1[nH+]cnc2n1nnc2	C20674155	-18.02	-6.83	-16.62	10.6	-5.16
310	c1cc(ccc1N)N	C08294962	-18.01	-2.8	-17.44	2.34	-0.1
311	c1c[nH]cc(c1=O)[N+](=O)[O-]	C08581558	-18.01	-5.09	-18.36	6.5	-1.06
312	c1c(c[nH]n1)[N+](=O)[O-]	C03852475	-18	-4.2	-17.48	4.95	-1.27
313	c1cc(cnc1)C(F)Cl	C03887768	-18	0.24	-18.06	2.89	-3.07
314	c1cncc(c1)CBr	C02387255	-17.99	-0.79	-17.45	3.38	-3.13
315	c1cc(sc1)CS	C00153137	-17.98	-1.38	-15.33	2.03	-3.3
316	c1ccc(cc1)NC#N	C01586445	-17.98	-3.12	-14.07	4.13	-4.91
317	c1c(c(nc(n1)Cl)N)C#N	C02169278	-17.98	-3.91	-16.71	3.81	-1.18
318	c1c(c(c(=O)[nH]n1)[O-])[N+](=O)[O-]	C09646749	-17.98	-3.46	-20.18	5.37	0.29
319	c1c(cnc(n1)N)Br	C00967319	-17.97	-1.84	-17.12	2.96	-1.96
320	Cc1ccc(cn1)C=C	C02040980	-17.97	-0.44	-17.37	3.26	-3.42
321	c1(c(non1)[n+][n-]c3c(n2)non3)N	C04017756	-17.97	-2.63	-18	3.79	-1.13
322	CCc1ccc(cc1)N	C12359032	-17.97	-1.52	-15.45	1.83	-2.83
323	c1c(c(c(c(n1)F)F)F)F	C14983574	-17.97	-1.22	-16.96	2.37	-2.17
324	c1(nc2n(n1)C(=O)C(=O)N2)N	C17005549	-17.97	-1.69	-22.03	6.89	-1.15
325	c1c(cnc(c1[N+](=O)[O-])N)F	C19616072	-17.97	-2.43	-18.08	4.13	-1.6
326	c1csc2c1scc2	C00165492	-17.96	-1.76	-15.71	3.19	-3.68
327	c1cscc1[N+](=O)[O-]	C00967491	-17.96	-2.18	-18	5.28	-3.05
328	c1cncc(c1F)Br	C02598963	-17.96	-2.35	-15.67	2.62	-2.57
329	Cc1ccc(cc1)N	C04774057	-17.96	-2.5	-15.3	2.01	-2.18
330	CCc1ccccc1	M1995A040	-17.96	-0.62	-13.49	1.22	-5.07
331	c1cc2c(cc1Cl)non2	C00161280	-17.95	-2.58	-17.19	2.94	-1.13
332	CCNC(=O)n1c(nnn1)N	C05456655	-17.95	-4.35	-18.65	4.25	0.8
333	c1cc(c(c(c1)F)Br)N	C12648832	-17.95	-2.58	-16.3	3.24	-2.33
334	C(=O)(C(F)F)Br	C04241560	-17.94	-0.22	-15.9	0.37	-2.19
335	c1nc(c(c(n1)F)Br)F	C14628950	-17.94	-1.86	-16.11	2.28	-2.26
336	c1(nnc(s1)N)N	C17002872	-17.94	-4.74	-16.33	2.65	0.48
337	c1ccc2c(c1)c[nH]n2	C16052862	-17.93	-2.04	-17.82	4.22	-2.29
338	c1cnccc1CN=C=O	C19730703	-17.93	-1.43	-20.69	4.45	-0.25
339	c1cc(c(c(c1)F)N=C=O)F	C00152291	-17.92	0.24	-20.16	4.11	-2.1
340	c1cc(c(cc1)F)F	C00164594	-17.92	-0.89	-14.71	2	-4.32
341	c1nc(nc(n1)N)N	C01445475	-17.92	-4.11	-16.56	4.77	-2.03
342	c1cncc(c1F)[N+](=O)[O-]	C02599078	-17.92	-3.18	-18.34	6.18	-2.57
343	c1c(c(c(c1F)F)N)[N+](=O)[O-]	C04269492	-17.92	-2.48	-15.26	2.39	-2.56
344	c1cncc(c1)N=C=O	C16677983	-17.92	-1.29	-18.79	3.65	-1.49
345	c1c(sc(n1)Cl)[N+](=O)[O-]	C32500065	-17.92	-2.1	-16	2.6	-2.41
346	c1cncc(c1Cl)N	C00331594	-17.91	-3.35	-16.56	2.76	-0.75
347	c1cc(cc(c1)F)CSC#N	C32138415	-17.91	-1.71	-16.11	4.5	-4.59
348	c1ccc(cc1)NC2=CC(=O)OC2	C00133694	-17.9	-1.32	-19.63	6.86	-3.81
349	c1ccc(c(c1)N)F	C00157599	-17.9	-2.06	-16.52	2.55	-1.87
350	c1cc(ncc1Cl)Cl	C00406964	-17.9	-1.38	-16.03	2.33	-2.81
351	c1c(cnc(c1F)N)F	C02510831	-17.9	-1.59	-17.34	2.27	-1.23
352	c1cc(cnc1)CNC(=S)N	C13545439	-17.9	0.26	-23.08	5.54	-0.62
353	c1ccc(c(c1)CC#N)N	C00389700	-17.89	-2.25	-18.53	5.63	-2.74
354	c1cc(oc1C#N)I	C28405036	-17.89	-1.59	-16.26	3.1	-3.13
355	c1c(cnc(c1F)C(F)F)F	C30714866	-17.89	-1.31	-15.64	1.88	-2.82
356	c1cc(sc1)Cl	C01648214	-17.88	-1.52	-14.92	1.55	-2.98

357	c1(c(c(nc(c1Cl)F)F)F)N	C02167052	-17.88	-4.08	-15.49	2.5	-0.81
358	c1cc(cnc1)N=C=S	C03132538	-17.88	-0.13	-18.69	3.51	-2.57
359	c1c(nc(s1)N)CCl	C04633527	-17.88	-2.36	-17.46	3.88	-1.93
360	c1ccc(cc1)/N=C/N	C15767277	-17.88	0.04	-20.02	4.66	-2.56
361	c1cc(ccc1C#N)C(F)F	C00164419	-17.87	-1.07	-16.93	3.74	-3.61
362	C(#N)c1c(non1)/C(=N/O)/N	C04342682	-17.87	-4.77	-16.39	3.32	-0.03
363	CCc1ccnc1	C08294961	-17.87	-1.34	-16.24	2.74	-3.03
364	c1cc(ccc1C#N)F	C00164613	-17.86	0.16	-17.9	3.51	-3.64
365	C#CCOc1ccccc1	C02169051	-17.86	-2.21	-17.54	3.77	-1.88
366	c1cc(cnc1)CNC(=O)C(=O)N	C04116536	-17.86	-2.73	-24.94	6.27	3.55
367	c1(nc(nn1C(=O)N)[N+](=O)[O-])N	C05071980	-17.86	-7.16	-17.39	4.81	1.88
368	COC(=O)Nc1ccc(cc1F)F	C06126169	-17.86	-0.61	-18.55	3.57	-2.26
369	c1cncn2c1nnc2	C01573373	-17.85	-3.17	-19.61	9.07	-4.15
370	c1cc(ccc1OC(F)F)F	C01847536	-17.85	0.22	-16.9	1.56	-2.72
371	c1ccn2c(c1)nnc2N	C08616242	-17.85	-3.76	-16.22	6.12	-3.99
372	c1cc(ccc1C=C/C(=O)Cl)F	C02574175	-17.84	-1.78	-18.18	3.94	-1.82
373	c1ncn(n1)C(=[NH2+])N	C06585615	-17.84	-5.21	-17.35	4.03	0.68
374	c1c(c(nc(c1F)N)F)N	C22006783	-17.84	-3.49	-17.04	3.79	-1.09
375	c1c(nc(c1)Br)C#N	C30678099	-17.84	-1.75	-18.32	3.68	-1.45
376	Nc1ccccc1F	W2002A003	-17.84	-2.25	-16.28	2.55	-1.86
377	c1c(nc[nH]1)I	C04244878	-17.83	-4.64	-15.99	5.22	-2.43
378	c1ccc(cc1)Oc2[nH]nnn2	C19910546	-17.83	-0.26	-22.71	5.64	-0.49
379	c1c(cc(cc1F)F)F	C00164868	-17.82	0	-15.33	0.98	-3.47
380	C=CCc1ccc(cc1O)F	C01562056	-17.82	-0.77	-19.34	3.16	-0.87
381	c1ccn(c1)CCl	C08294964	-17.82	-0.88	-17.51	3.6	-3.03
382	c1cc(c(cc1Cl)N)F	C00164833	-17.81	-1.47	-15.91	1.8	-2.24
383	c1cncnc1N[+](=O)[O-]	C01703180	-17.81	-3.06	-20.6	5.53	0.32
384	c1c(cc(c1N)Br)F	C01704162	-17.81	-3.08	-16.84	2.09	0.02
385	c1ccc(cc1)/C=C/C(=O)Cl	C01680031	-17.8	-1.45	-18.56	3.48	-1.27
386	Cc1ccc(cc1)C#N	C01696575	-17.8	0.08	-17.38	3.63	-4.14
387	CSc1cccs1	C00160928	-17.79	0.18	-16.61	2.1	-3.46
388	c1ccn(c1)CCS	C04522277	-17.79	-0.32	-16.83	2.74	-3.38
389	Cc1ccc(cc1N)N	C00388039	-17.78	-3.78	-15.93	2.64	-0.71
390	c1c([nH]nc1C(F)F)C(F)F	C01023256	-17.78	-3.41	-14.31	2.45	-2.52
391	c1cc(c(cc1NN)F)F	C02243112	-17.78	-2.54	-17.59	4.02	-1.67
392	c1ccn(c1)CCC#N	C01718831	-17.77	-1.64	-17.76	5.76	-4.14
393	c1cscc1Cl	C02168778	-17.76	-1.17	-15.23	1.54	-2.9
394	CCCN/C(=N/[N+](=O)[O-])/N	C25623935	-17.76	-5.36	-14.1	3.47	-1.77
395	c1cnc(c1N)Br	C19015182	-17.75	-2.46	-17.31	2.97	-0.96
396	c1cc(ccc1F)F	C00164664	-17.74	-0.31	-15.66	1.68	-3.45
397	c1cc(c(c1Cl)N)F	C02389922	-17.74	-2.16	-15.34	2.03	-2.27
398	COC(=O)CC=C=C	C15809774	-17.74	0.23	-18.49	4.29	-3.78
399	c1cc(cnc1)Cl	C00404335	-17.73	-0.5	-17.43	2.59	-2.39
400	c1(nc([nH]n1)N)C(F)F	C17173217	-17.73	-5.42	-16.03	5.44	-1.73
401	c1ccc(c1)C#N	C00157544	-17.72	-1.76	-17.95	3.98	-2
402	C#Cc1ccccc1	C02577202	-17.72	-0.58	-18.11	3.9	-2.94
403	c1nc([nH]1)I	C05204774	-17.72	-2.57	-16.3	3.25	-2.1
404	c1cc(ccc1NN)Cl	C00088600	-17.71	-1.97	-16.58	2.69	-1.85
405	c1ccc(cc1)/C=C/C#N	C01675000	-17.71	-0.66	-19.21	4.49	-2.33
406	c1cc(sc1)[N+](=O)[O-]	G2008A002	-17.71	-2.71	-17.89	6.13	-3.24
407	c1cc(cnc1)I	C00331802	-17.7	-0.51	-16.75	2.39	-2.82
408	c1cc(c(c1[N+](=O)[O-])F)F	C04255263	-17.7	-2.14	-16.76	3.71	-2.52
409	c1cc(nc(c1Cl)N)N	C19911452	-17.7	-3.25	-18.56	4.61	-0.5
410	C=CCc1ccccc1N	C00047330	-17.69	-1.43	-19.09	2.65	0.18
411	c1(nnn1C(=O)N)N	C05670121	-17.69	-5.19	-18.88	4.67	1.71
412	c1cc(cnc1)NN=O	C13212918	-17.69	-2.64	-19.77	5.42	-0.69
413	c1cc2cc[nH]c2nc1	C15442276	-17.69	-2.43	-17.61	5.29	-2.94
414	c1ccn(c1)CS	C04775643	-17.68	-1.27	-17.24	3.52	-2.69
415	C=CCOc1ccc(cc1)N	C00047331	-17.67	-0.24	-18.69	3.28	-2.02
416	c1cc(sc1)S	C02169156	-17.67	-1.47	-15.03	1.55	-2.71
417	c1c(c(nc(n1)N)N)CBr	C13283449	-17.67	-3.41	-17.41	4.81	-1.65
418	c1cc(c(cc1F)N)Br	C00403473	-17.66	-2.92	-17.04	1.77	0.52
419	c1c(nc(c1)Cl)C#N	C30678538	-17.66	-1.75	-18.31	3.81	-1.4
420	c1([nH]nc1n1)NN=O	C05567030	-17.65	-3.51	-22.66	5.36	3.16
421	c1cnc2c1cn[nH]2	C14985617	-17.64	-1.74	-19.52	4.66	-1.04
422	Cc1ccc(cc1)S	C19230140	-17.64	-0.01	-15.27	1.6	-3.96
423	Cc1c(ccc1N)F	W2004A010	-17.64	-3.45	-14.69	2.85	-2.35
424	c1c(cnc(c1F)F)Cl	C02525803	-17.63	-0.95	-17.91	2.42	-1.19
425	c1c(c(nc(n1)N)N)N	C08294936	-17.63	-5.62	-18.14	5.19	0.94
426	c1cc(sc1)CNO	C01698346	-17.62	-3.38	-17.25	2.9	0.11
427	c1cc2c(nc1)n[n-]n2	C05117290	-17.62	-5.93	-18.72	7.86	-0.83
428	c1cc(ncc1Br)N[+](=O)[O-]	C01020848	-17.61	-1.21	-19.44	6.49	-3.45
429	c1c(c(cc1F)N)Cl)N	C04334592	-17.61	-4.05	-15.08	2.19	-0.66
430	c1nc(n2c(n1)nnc2)N	C08618478	-17.61	-2.88	-17.49	7.73	-4.97
431	CCOc1ccccc1	C01599383	-17.6	-1.66	-14.79	2.45	-3.61
432	c1cc(c(cc1F)F)N=O	C16158150	-17.6	-0.52	-17.62	2.92	-2.38
433	c1ccc(cc1)C=NN	C17289008	-17.6	0.39	-18.68	2.86	-2.17
434	c1ccn(c1)N[+](=O)[O-]	C00085310	-17.59	-1.21	-20.86	7.48	-3
435	c1cc(c(nc1)Br)N	C00330809	-17.59	-3.31	-17.51	4.2	-0.97
436	C=CCOC(=O)Cl	C02033143	-17.59	-0.59	-16.28	1.86	-2.58
437	c1cc(c(nc1)N)CCl	C21984220	-17.59	-2.31	-17.46	4.3	-2.11
438	c1c(cc(cc1F)F)NN	C00404219	-17.58	-2.69	-15.99	2.81	-1.72
439	c1c(cc(cc1F)F)FCS	C04244671	-17.58	-1.12	-16.92	2.42	-1.96
440	c1cc(c(cc1N)N)C#N	C09371615	-17.58	-2.29	-19.61	4.7	-0.38
441	c1cc(c(cc1C#N)F)F	C00156995	-17.57	-0.87	-17.3	4.29	-3.69
442	c1cc(oc1C[N+](=O)[O-])[N+](=O)[O-]	C02506785	-17.57	-2.37	-18.15	7.09	-4.14
443	c1cc(c(cc1F)CS)F	C04244662	-17.57	0.53	-16.26	2.26	-4.1
444	c1cnc(c1F)Cl)F	C14982361	-17.57	-2.87	-16.18	3.87	-2.4
445	c1c(c(c(c1F)F)N)F	C00406982	-17.56	-2	-15.95	2.34	-1.96
446	CCOC(=O)C(=O)C(F)F	C02159467	-17.56	0.42	-16.95	1.97	-3

447	c1cc(c(cc1F)C#N)N	C02583740	-17.56	-2.11	-17.7	4.27	-2.03
448	c1c(c(nc(c1Cl)F)F)F	C02585567	-17.56	0.47	-18.7	2.28	-1.6
449	c1c[nH]c2c1cnnc2	C06862802	-17.56	-3.18	-17.58	5.85	-2.65
450	c1c(c[nH]c(=O)c1O)Cl	C00388202	-17.55	-3.7	-19.36	5.67	-0.16
451	c1ccc(cc1)C#CC=O	C01679343	-17.55	-1.92	-17.19	5.78	-4.23
452	c1ccc(cc1)Nc2[nH]nnc2	C01742045	-17.55	-0.78	-17.07	5.32	-5.03
453	Cc1c(n[nH]n1)[N+](=O)[O-]	C13410797	-17.55	-4.21	-16.66	4.85	-1.52
454	CSc1[nH]nc(n1)SC	C01603478	-17.54	-2.8	-16.66	4.46	-2.55
455	CC(=S)OCc1ccc1	C05225743	-17.54	-1.81	-17.15	4.71	-3.3
456	c1cc(ccc1/C=C/C=O)F	C21993071	-17.54	-1.83	-17.31	5.63	-4.04
457	c1cc(ccc1N)Br	C00013614	-17.53	-0.66	-16.78	2.12	-2.21
458	c1cc(c(c(c1F)N)N	C16158506	-17.53	-4.14	-16.12	3.12	-0.39
459	C=CCN/C=C/\C=CC=[NH+]1	C17378195	-17.53	1.15	-19.57	3.21	-2.32
460	c1cc(sc1)N=C=O	C00158753	-17.52	-0.33	-17.79	1.99	-1.38
461	c1cc(ccc1Cl)O)F	C02528619	-17.52	-2.4	-16.35	2.88	-1.66
462	c1cn[nH]c1[N+](=O)[O-]	C04692780	-17.52	-1.19	-18.33	4.12	-2.12
463	CNC(=O)n1c(nnn1)N	C05510474	-17.52	-8.19	-15.18	4.75	1.11
464	c1cc(cnc1)CCC#N	C08699947	-17.51	-1.2	-19.5	6.66	-3.46
465	C(=[NH2+])(N)SSC(=[NH2+])N	C12358898	-17.51	-4.38	-17.71	3.51	1.07
466	COC(=O)Cc1ccc1	C00388061	-17.5	-0.28	-17.69	4.96	-4.49
467	c1c(ccc1F)N	C08698158	-17.5	-3.91	-16.27	3.22	-0.55
468	c1c(nc[nH]1)[N+](=O)[O-]	C12358712	-17.5	-3.82	-17.18	6.44	-2.95
469	c1c(ccc1)F	C14400906	-17.5	-0.74	-15.3	1.44	-2.9
470	c1cc(ncc1)F	C14982824	-17.5	-1.32	-15.51	2.24	-2.91
471	c1c(nc(nc1F)N)F	C00967445	-17.49	-3.05	-15.98	2.8	-1.26
472	C=CCOC(=O)C(F)(F)F	C01577260	-17.49	-1.05	-15.07	1.74	-3.11
473	c1cc([nH]c1)[N+](=O)[O-]	C01561742	-17.48	-2.77	-17.88	6.29	-3.12
474	c1c(c[nH]1)CCl)Cl	C02552485	-17.48	-2.39	-16.37	4.07	-2.79
475	C/C(=C/C(=O)C(F)(F)Cl)[O-]	C04242400	-17.48	-5.42	-12.46	2.88	-2.48
476	c1ccc1CCC#N	C04716436	-17.48	-1.95	-18.96	6.83	-3.4
477	c1[n-]nc(n1)[N+](=O)[O-]	C18206667	-17.48	-4.59	-16.76	8.16	-4.29
478	c1cc(ncc1N=C=O)C(F)(F)F	C22010714	-17.48	-1.51	-18.31	3.65	-1.31
479	c1cc(sc1)[N+](=O)[O-]	C01680876	-17.47	-2.75	-17.81	6.3	-3.21
480	C#Cc1ccc1	C02526546	-17.47	-0.49	-16.4	2.86	-3.45
481	c1cc(sc1)C(F)(F)F	C02541355	-17.47	-2.31	-15.58	2.4	-1.99
482	c1cc(ncc1[N+](=O)[O-])Cl	C02564034	-17.47	-2.58	-15.76	3.78	-2.91
483	c1c(cc(c(c1N)[N+](=O)[O-])F)F	C04416633	-17.47	-2.85	-16.46	4.37	-2.53
484	c1ccc(cc1)/C(=N/O)/C#N	C05239373	-17.47	-1.61	-18.79	4.69	-1.75
485	c1c(nc(nc1F)F)F)F	C06090883	-17.47	0.18	-16.71	0.63	-1.57
486	c1cn2cnc2cn1	C12356946	-17.47	-2.43	-18.6	6.09	-2.52
487	Cc1ccc(c(c1N)Br	C08701094	-17.46	-2.7	-13.88	1.93	-2.82
488	c1ccc1Br	C00158596	-17.45	-0.86	-16.48	2.28	-2.39
489	C=NC1C=CCC=C1	C01764765	-17.45	-1.61	-16.44	2.97	-2.38
490	Cc1cncc1	C01852614	-17.45	-1.85	-16.82	3.6	-2.38
491	c1cc(c(cc1F)F)CS	C04244661	-17.45	-1.3	-17.31	2.57	-1.4
492	Cc1[n-]cc(n1)[N+](=O)[O-]	C18172810	-17.45	-2.35	-17.47	5.37	-3
493	Cc1c(ccc1F)N	C00407040	-17.44	-3.41	-14.52	2.85	-2.35
494	c1c(ccc1)Cl)[N+](=O)[O-]	C01420771	-17.44	-2.83	-16.4	4.29	-2.51
495	c1c(cnc(n1)F)Br	C04198784	-17.44	-1.05	-17.47	3.01	-1.93
496	C#CCNC(=O)n1ccnc1	C32628565	-17.44	-3.47	-18.67	7.63	-2.93
497	CC(=O)Oc1ccc(cc1F)F	C00152763	-17.43	1.41	-20.05	5.61	-4.4
498	c1ccc(cc1)N	C00334520	-17.43	-2.89	-15.84	2.52	-1.23
499	c1c(c(cc(c1F)F)N)N	C02600068	-17.42	-4.59	-16.88	4.47	-0.42
500	c1c(c(cc(c1F)F)F)C#N	C00389514	-17.41	1.4	-18.75	3.49	-3.54
501	C#Cc1ccc(cc1)Br	C02534482	-17.41	-0.09	-15.41	2.8	-4.7
502	c1cnc(cn1)CCS	C04802601	-17.41	-0.59	-18.36	3.48	-1.94
503	c1ccc(cc1)C(=N/C#N)N	C15889046	-17.41	0.37	-18.99	6.26	-5.05
504	c1c(c(ncn1)N)C#N	C00165356	-17.4	-2.27	-18.07	4.11	-1.18
505	c1c(c(cc(c1F)F)O)N	C02243122	-17.4	-5.37	-16.51	4.22	0.25
506	c1cc(cc(c1)N)N	C00164650	-17.39	-3.52	-16.35	2.59	-0.11
507	Cc1ncc(c(n1)N)C#N	C00165358	-17.39	-2.93	-17.29	4.04	-1.21
508	CSc1ccc(cc1)O	C00404129	-17.39	-0.05	-18.65	3.28	-1.96
509	CNC(=O)n1c(ncn1)N	C08628619	-17.39	-6.65	-15.32	6.2	-1.61
510	c1cc(ccc1N)OC(F)F	C00167204	-17.38	-3.43	-16.87	4.37	-1.45
511	c1nc(ncn1)C(=O)N)N	C17046277	-17.38	-5.83	-17.51	6.44	-0.47
512	c1cnc(c(n1)N)Cl	C01101989	-17.37	-3.42	-17.97	4.14	-0.12
513	c1cc(ccc1OC(F)F)Cl	C19735925	-17.37	-3.4	-14.06	3.52	-3.44
514	Cc1ccsc1	C01692445	-17.36	-0.63	-15.18	1.5	-3.05
515	c1c(cnc(c1F)N)Cl	C16158481	-17.36	-1.21	-17.49	2.85	-1.51
516	c1cc(ccc1C(F)(F)F)N	C00164442	-17.35	-2.32	-15.41	2.77	-2.39
517	c1cc(c(nc1)Cl)N	C00164466	-17.35	-3.54	-17.13	4.22	-0.9
518	c1c(c(=O)[nH]c(=O)[nH]1)SC#N	C03013979	-17.35	-3.6	-21.84	6.87	1.22
519	C(#N)Sc1c(non1)[N+](=O)[O-]	C04343705	-17.35	-1.51	-17.52	3.92	-2.24
520	c1cc(=O)occ1Cl	C21989740	-17.35	-1.56	-18.18	5.48	-3.09
521	c1c(cnc(c1F)F)F	C02585569	-17.34	-0.82	-16.98	2.56	-2.11
522	c1ccc(cc1)CSC(=[NH2+])N	C03874922	-17.34	-1.64	-15.97	2.9	-2.62
523	c1(c(ncn1)N)C(=O)NN	C03882149	-17.34	-5.77	-17.83	4.22	2.04
524	c1cc(c(cc1F)F)/C=C/C=O	C14982651	-17.34	-2.81	-15.39	5.05	-4.18
525	Fc1ccc1	M1995A008	-17.34	-1.11	-14.97	2.13	-3.39
526	c1c(cc(c(c1N)O)F)F	C02386500	-17.33	-4.46	-16.58	3.44	0.27
527	C#Cc1ccc(cc1)O	C02555301	-17.33	-0.29	-18.78	3.79	-2.05
528	c1ccc(c(c1)CC=O)F	C02581173	-17.33	-0.83	-18.48	3.84	-1.86
529	C(=C(C(F)(F)F)O)C(=O)C(F)(F)F	C12360020	-17.33	-5.05	-13.65	3.29	-1.92
530	CNc1nc(no1)[N+](=O)[O-]	C15782381	-17.33	-5.19	-16.23	5.62	-1.54
531	COC(=O)CNC1ncc1	C21795809	-17.33	-3.68	-15.94	4.43	-2.14
532	c1cc(ccc1CCC#N)F	C31829538	-17.33	-1.68	-17.06	6.29	-4.88
533	c1cnccc1Cl	C00402776	-17.32	-0.45	-16.93	2.35	-2.28
534	CCc1ccc1N	C02039219	-17.32	-1.58	-14.02	1.81	-3.53
535	c1cc(c(cc1F)O)N	C02567357	-17.32	-3.18	-17.98	3.58	0.26
536	C(=O)C(F)(F)Cl)C(F)(F)Cl	C04254804	-17.32	0.43	-15.18	0.29	-2.85

537	c1c2c(n[nH]c2ncn1)N	C13362450	-17.32	-3.63	-18.53	5.86	-1.01
538	c1c(cn(n1)[N+](=O)[O-])Br	C02390475	-17.31	-1.86	-18.3	3.73	-0.88
539	C(=O)(C(F)F)Cl)Br	C04329285	-17.31	-0.27	-15.41	0.46	-2.1
540	c1c(nc(s1)N)Br	C17044502	-17.31	-1.32	-16.5	1.91	-1.4
541	c1cc(c(c1)F)Cl)O	C21304466	-17.31	-1.93	-17.05	3.39	-1.72
542	c1ccc(cc1)CSC#N)F	C32138414	-17.31	-1.22	-16.05	4.57	-4.61
543	Cc1cccs1	C02034789	-17.3	-1.22	-14.57	1.66	-3.17
544	c1cc(c(cc1F)O)Cl	C02584351	-17.3	-0.59	-17.67	2.63	-1.67
545	c1cc(ccc1N=O)N=O	C04404450	-17.3	-2.23	-17.52	3.41	-0.97
546	c1c(cnc(c1N)Br)F	C02546107	-17.29	-3.87	-17.49	2.91	1.16
547	c1c(c(c(c1F)F)N)[N+](=O)[O-])F	C04416631	-17.29	-2.41	-15.28	2.97	-2.58
548	c1ccc(cc1)Sc2c[nH]cn2	C06188344	-17.29	-1.04	-16.2	4.79	-4.83
549	c1csc(n1)NC#N	C13638831	-17.29	-2.01	-17.51	6.14	-3.91
550	c1cc(ncc1C#N)Cl	C00166496	-17.28	-1.25	-17.68	4.31	-2.66
551	c1ccc2c(c1)c(on2)[O-]	C01681296	-17.28	-1.92	-17.19	5.26	-3.43
552	c1c(nc([nH]1)Cl)[N+](=O)[O-]	C05425251	-17.28	-1.7	-18.57	3.13	-0.14
553	c1ccc(cc1)OC=O	C08294965	-17.27	-0.13	-19.62	5.99	-3.51
554	c1cnc2c1cco2	C15444681	-17.27	-1.67	-17.77	4.5	-2.33
555	[H]N=C(N)Nc1cnoc1	C26510247	-17.27	-3.51	-19.8	6.77	-0.72
556	CSc1nc([nH]1)N	C17019767	-17.26	-3.76	-17.75	6.04	-1.79
557	C=CCOC(=O)OCC#N	C01733700	-17.25	-2.35	-17.01	5.28	-3.17
558	c1c(csn1)Br	C04344132	-17.25	-0.68	-16.63	2.02	-1.95
559	c1cnc1CN=C=S	C09239750	-17.25	-0.61	-17.77	3.5	-2.37
560	c1c(cnc(c1)C#N)Br	C00053986	-17.24	0.51	-19.35	3.76	-2.16
561	CCn1ccccc1	C01866964	-17.24	-1.38	-14.72	2.63	-3.76
562	c1cc(c(nc1)N=O)N=O	C05495396	-17.24	-2.53	-20.65	6.77	-0.83
563	c1cc(ncc1[N+](=O)[O-])N	C18810124	-17.24	-4.36	-17.27	5.92	-1.53
564	c1c(c(c(c1)F)F)N)F	C02386504	-17.23	-2.84	-16.81	2.94	-0.52
565	c1c(snn1)C(=O)Cl	C12428346	-17.23	-1.36	-17.79	3.03	-1.11
566	C[C@H]1C=C[C@@H]2COCC2=C1	C18529659	-17.23	-1.01	-14.83	1.87	-3.26
567	c1cc(ccc1O)Cl	C00001885	-17.22	-0.44	-17.71	2.49	-1.55
568	c1ccc2c(c1)c(no2)N	C00161908	-17.22	-3.75	-16.68	5.29	-2.08
569	C#Cc1ccncc1	C02506783	-17.22	-0.83	-17.44	3.83	-2.78
570	c1ccc(cc1)N=O	C04097291	-17.22	-1.82	-17.01	3.77	-2.16
571	c1cc(c(nc1))N	C04352695	-17.22	-3.71	-15.99	3.83	-1.35
572	c1([nH]nn1)C([N+](=O)[O-])(F)F	C04948492	-17.22	-4.1	-17.69	3.96	0.61
573	c1c(cn2c(n1)ncn2)Br	C20281956	-17.22	-3.05	-16.13	6.6	-4.64
574	c1c(c(c(c1F)F)N)F)F	C00388050	-17.21	-2.95	-14.15	1.84	-1.95
575	c1cc(oc1)/C=C/C#N	C01592389	-17.21	-0.99	-17.72	4.8	-3.31
576	c1cc(ccc1N=C=O)Br	C03861690	-17.21	-1.48	-17.02	1.51	-0.22
577	CC(=O)OCC1CCCC1	C00157134	-17.2	0.35	-17.73	4.87	-4.69
578	c1cc(c(c1)F)CC#N)F	C00409205	-17.2	0.01	-19.47	5.42	-3.16
579	c1ccccc1	E1992A001	-17.2	-0.7	-14.48	1.34	-3.35
580	c1cc(c(nc1)CBr)O	C00300814	-17.19	-1.62	-18.19	3.7	-1.07
581	c1cc(sc1)CC#N	C00388254	-17.19	-1.32	-17.94	5.65	-3.58
582	c1cc(c(c1F)N)F)F	C00409370	-17.19	-2.58	-15.4	2.71	-1.92
583	Cn1c(ncn1)[N+](=O)[O-]	C02760423	-17.19	-1.48	-15.67	4.59	-4.63
584	CC(=O)O[NH+]=c1/c-2no[n-]c2ncn1	C05624866	-17.19	-2.96	-18.25	7.68	-3.65
585	c1cc(oc1N=C=O)Br	C19505118	-17.19	-2.16	-16.89	1.96	-0.1
586	c1(c(no[nH]1)[O-])N(C(=O)N	C03894822	-17.18	-6.4	-17.27	5.35	1.14
587	Cc1c(ncn1)C(=[NH+]/N)/N	C04342582	-17.18	-6.21	-18.04	4.59	2.47
588	CC(=C1C(=O)CCC1=O)[O-]	C05855021	-17.18	-4.85	-16.17	5.73	-1.88
589	c1cc(c(cc1F)N)N)F	C00153197	-17.17	-0.56	-17.45	2.55	-1.71
590	c1cc(cc(c1)F)NN	C00164739	-17.17	-2.1	-16.89	3.46	-1.64
591	c1c2c([nH]c(n2)N)ncn1	C02382956	-17.17	-5.34	-18.18	8.53	-2.17
592	Cc1c(ncn1)C(=[NH+]/N)/N	C05380617	-17.17	0.32	-16.05	1.14	-2.59
593	c1cc(c(cc1F)F)CC#N	C00155244	-17.16	-1.71	-19.24	7.03	-3.24
594	c1cnc1[N+](=O)[O-]	C00332351	-17.16	-2.19	-16.8	4.4	-2.57
595	CCc1ccccc1	C08294956	-17.16	-1.04	-15.91	2.96	-3.17
596	c1cc(c(nc1)N)C#N	C19486678	-17.16	-2.22	-18.47	4.81	-1.27
597	c1cc(c(c1)F)N)F	C00159273	-17.15	-0.97	-16.73	2.48	-1.93
598	c1cc(cc(c1)F)CC#N	C00404417	-17.15	-1.22	-18.32	6.68	-4.29
599	C/C(=C/CC)/[N+](=O)[O-]	C01733879	-17.15	-1.51	-16.07	4.03	-3.6
600	CC(=O)OCC1CCCC1	C02149530	-17.15	-0.85	-18.85	5.73	-3.18
601	c1cc(nc(c1Br)N)N	C19862891	-17.15	-3.68	-17.44	4.57	-0.59
602	COCC(=O)Cc1ccsc1	C00156981	-17.14	-0.22	-18.14	4.92	-3.7
603	Cc1cc(nc1)N/C=N/O	C15906885	-17.14	-2.04	-19.29	5.99	-1.8
604	CCNc1ccc(cc1F)F	C19952389	-17.14	-1.65	-14.59	2.39	-3.29
605	Cc1c(nc(nc1F)F)F	C02025691	-17.13	-1.26	-16.16	2.12	-1.83
606	c1c(c(cnc1F)F)F	C02540460	-17.13	-0.84	-16.34	2.17	-2.11
607	C/C=C/C1ccc(cc1)O	C13526620	-17.13	-0.59	-16.79	2.77	-2.52
608	c1c(c(c(cn1)F)Cl)F	C14982370	-17.13	-0.31	-16.36	2.07	-2.53
609	c1nn2c(nnc2n1)N)N	C17141944	-17.13	-5.13	-18.94	11.26	-4.33
610	c1cc(ccc1N)NCC=O	C02556302	-17.12	-4.77	-18.75	6.41	-0.01
611	c1c(c(ncn1)Cl)F	C15444654	-17.12	-0.11	-17.53	2.78	-2.25
612	C#Cc1ccc(cn1)Br	C21981757	-17.12	-0.66	-17.58	4.57	-3.45
613	c1c(cnc1)C(Cl)[N+](=O)[O-]	C02569105	-17.11	-3.04	-17.91	6.75	-2.91
614	c1c(c(c(c1)F)F)Cl)F	C16159842	-17.11	-0.18	-16.74	2.14	-2.32
615	C/C(=C/O)/C(=O)C	C17129866	-17.11	-5.55	-15.29	5.23	-1.5
616	CCOC(=O)c1cc[nH]n1	C18161725	-17.11	-1.52	-18.47	5	-2.12
617	c1c(c(cnc1F)F)Cl	C21991290	-17.11	0.14	-16.96	2.01	-2.3
618	C#CCNc1ccccc1	C01737352	-17.1	-1.83	-14.11	2.47	-3.63
619	c1cnc1(c1Cl)F	C02598038	-17.1	-0.52	-16.91	2.68	-2.34
620	Cc1cnc1F	C02599065	-17.1	-1.6	-17.06	2.63	-1.06
621	c1c2c(c(ncn2)N)n[nH]1	C04822317	-17.1	-3.99	-18.79	5.64	0.04
622	c1c([nH]nc1C(F)F)C(=O)Cl	C12357635	-17.1	-6.43	-13.14	3.35	-0.88
623	c1ccc(cc1)N=C(N)N	C04276940	-17.09	0.77	-20.44	4.95	-2.37
624	c1([nH]nn1)C(F)F)F	C06523903	-17.09	-5.8	-14.62	3.52	-0.18
625	c1c(c(c(cn1)F)F)C(F)F)F	C16159826	-17.09	-1.53	-15.37	2.69	-2.87
626	c1cc(ncc1C(F)F)C(=O)Cl	C30715018	-17.09	-2.26	-14.73	3.04	-3.14

627	c1ccc(cc1)C(=O)[S-]	C05226314	-17.08	-3.75	-17.01	6.04	-2.36
628	c1ccc(c(c1)NC(=O)N)F	C00156334	-17.07	-3.07	-19.51	6.06	-0.55
629	c1cnoc1C(F)(F)Cl	C02540175	-17.07	-0.29	-16.78	2.71	-2.72
630	C=CCOC(=O)Cl	C02545380	-17.07	-0.41	-15.23	1.73	-3.15
631	c1ccnc(c1)CCCl	C12360602	-17.07	0.39	-16.59	2.84	-3.71
632	C=Cc1cnccn1	C00152334	-17.06	-2.19	-17.19	3.97	-1.65
633	CC(=O)Oc1cccc1	C00388064	-17.06	0.62	-18.97	5.59	-4.29
634	C=Cc1cncc1	C01769024	-17.06	-1.45	-15.92	3.09	-2.78
635	Cc1ccnc1	C08294958	-17.06	-1.44	-16.09	2.96	-2.5
636	CC(=O)c1c(no[n+][O-])N	C08727464	-17.06	-4.36	-16.66	5.49	-1.53
637	c1c(c(cc1F)F)O)C#N	C12359158	-17.06	-1.51	-18.61	4.67	-1.61
638	C(C)OC(=O)C(F)F	C16082642	-17.06	-1.13	-15.93	3.16	-3.16
639	c1(c(non1)N)/C(=N)O)/N	C18324333	-17.06	-5.11	-17.48	3.45	2.07
640	c1cnccc1	C00161788	-17.05	-0.92	-15.46	2.1	-2.78
641	c1cc(ncc1C#N)Br	C02559904	-17.05	-1.3	-17.25	4.22	-2.72
642	C(=O)C(F)Br)Cl	C04241563	-17.05	-0.11	-15.25	0.42	-2.11
643	c1cc(cnc1)N)N	C19074690	-17.05	-4.08	-17.08	3.88	0.23
644	c1ccc(cc1)COC(=O)N	C00157187	-17.04	0.07	-21.98	5.59	-0.72
645	c1cc(ccc1NC(=O)N)F	C00395190	-17.04	-3.01	-20.66	7.14	-0.51
646	c1ccnc(c1)NCC#N	C28294859	-17.04	-3.82	-17.35	6.47	-2.33
647	O=N(=O)c1cccc1	ntrbnz1	-17.04	-2.55	-16.06	5.44	-3.87
648	c1ccc(cc1)SC(=O)Cl	C00394908	-17.03	-1.15	-18.58	3.24	-0.54
649	c1cc(sc1N)S	C01095798	-17.03	-2.87	-15.33	2.34	-1.17
650	c1c(cnc1n)N)I	C01679675	-17.03	-1.08	-16.43	2.73	-2.26
651	c1c(c(c(c(c1F)F)F)F)F	L2009A001	-17.03	0.17	-15.68	2.03	-3.55
652	c1cc(c(cc1F)F)C#N	C00159425	-17.02	-0.05	-17.63	4.31	-3.66
653	c1c(ncc1n1)Cl)Cl	C01581403	-17.02	-1.53	-16.27	2.29	-1.51
654	c1cc(c(cc1F)CC=O)F	C02581082	-17.02	-0.54	-18.14	4.09	-2.43
655	C#CNc1cnc(n1)[N+](=O)[O-]	C08295833	-17.02	-3.72	-18.53	11.17	-5.94
656	c1ccnc(c1)CCC#N	C14987721	-17.02	-0.32	-18.53	5.45	-3.62
657	c1(nnc1n1)N)N	C16891524	-17.02	-5.98	-14.47	4.57	-1.14
658	Cc1c(cccn1)N	C00331888	-17.01	-3	-16.71	3.78	-1.07
659	C=Cn1cnan1	C01083359	-17.01	-3.01	-16.74	6.26	-3.52
660	c1ccc(cc1)[C@@H](C#CCO)O	C02347098	-17.01	-1.02	-21.29	5.9	-0.6
661	C#CCOC(=O)Cl	C02387284	-17.01	-0.58	-16.7	2.64	-2.37
662	c1(c([nH]nc1N)N)[N+](=O)[O-]	C04624940	-17.01	-4.49	-18.94	5.96	0.45
663	c1ccc(cc1)Nc2nns2	C00401042	-17	-0.71	-19.75	2.34	1.12
664	c1ccc(cc1)CN=C=S	C01529592	-17	-0.01	-15.45	2.21	-3.75
665	CNc1ccc(cc1)F	C01847398	-17	-2.38	-14.61	2.61	-2.62
666	C#Cc1cccs1	C02576039	-17	-0.53	-16.38	3.49	-3.58
667	c1c(sc1n)Br	C04198797	-17	-1.11	-16.84	2.68	-1.73
668	c1c(cc(c(c1F)N)F)N	C04334615	-17	-1.66	-17.77	2.67	-0.24
669	Cc1cc([nH]n1)[N+](=O)[O-]	C18166915	-17	-0.67	-17.3	3.63	-2.65
670	c1ccc(c(c1)F)I	C00164528	-16.99	1.04	-16.38	2.58	-4.24
671	C/C=C/c1ccncc1	C25489416	-16.99	-1.68	-14.89	3.04	-3.46
672	c1cc(c(cc1F)N)O	C02555148	-16.98	-3.37	-17.08	3.19	0.28
673	c1ccn(c1)CCBr	C02556775	-16.97	-0.99	-13.97	2.29	-4.31
674	c1c(c(nc(=S)[nH]1)N)C#N	C00169893	-16.96	-3.61	-16.5	3.86	-0.72
675	c1ccc(cc1)COC=O	C01530244	-16.96	0.34	-21.12	7.75	-3.93
676	c1nc(c(c1)F)F)F	C02546080	-16.96	-1.58	-15.88	2.39	-1.89
677	c1cc(c(cc1N)F)Cl	C02572861	-16.96	-3.51	-14.65	3.28	-2.09
678	c1cc(ncc1)C#N	C30677683	-16.96	-1.98	-15.8	3.97	-3.15
679	Cc1ccnc(n1)NC#N	C01693055	-16.95	-2.8	-14.8	5.97	-5.31
680	c1cc(ccc1CC=O)F	C02581175	-16.95	-1.12	-18.95	5.05	-1.93
681	c1c([nH]c2c1cc(cn2)C#N	C06643342	-16.95	-0.85	-18.79	5.83	-3.14
682	c1cc(c2c1F)cn[nH]2)F	C14986073	-16.95	-1.37	-16.8	3.59	-2.37
683	c1cc(ccc1N)S	C19850183	-16.95	-3.25	-15.16	3.21	-1.75
684	c1ccc(c(c1)O)Cl	C00402767	-16.94	-1.11	-17.21	3.07	-1.68
685	C=CC1=CSSN1	C01624249	-16.94	-1.48	-16.94	3	-1.51
686	CSs1[nH]ncc1	C03165681	-16.94	-3.06	-15.98	4.24	-2.15
687	c1c(c([nH]1)[N+](=O)[O-])Cl	C04086103	-16.94	-1.36	-17.19	3.91	-2.3
688	Cc1ccc(c(c1)N)C#N	C04272117	-16.94	-2.42	-15.84	3.83	-2.52
689	c1cc(c(cc1F)F)C)N	C19267642	-16.94	0.29	-18.52	2.68	-1.39
690	c1cscc1CC#N	C00157111	-16.93	-1.2	-17.92	5.63	-3.44
691	c1cc(c(cc1F)CC#N)F	C00409204	-16.93	-1.28	-18.28	5.86	-3.23
692	Cc1ccc(s1)C#N	C01756772	-16.93	-0.35	-16.57	3.56	-3.56
693	c1cnc(nc1)N/C=N/O	C15934902	-16.93	-3.86	-17.7	7.09	-2.46
694	c1cncc1Br	C20358092	-16.93	-1.19	-16.95	3.45	-2.26
695	C#Cc1cc(cc1N)F)F	C21987735	-16.93	-2.71	-15.4	3.95	-2.76
696	c1c(cnc(c1F)N)OC(F)F)F	C30677975	-16.93	-1.37	-17.46	2.89	-1
697	CC(=O)c1ccc(s1)C#N	C00128854	-16.92	-0.95	-17.14	4.58	-3.4
698	c1ccc(cc1)c2nc[nH]n2	C02027091	-16.92	0.62	-19.92	6.29	-3.91
699	c1ccc(cc1)ON	C00391872	-16.91	-0.77	-17.6	3.11	-1.64
700	c1ccc(cc1)OC(F)F	C01559023	-16.91	-3.13	-14.6	3.92	-3.1
701	c1c(ncnc1)F)F	C02529895	-16.91	-0.19	-16.27	1.71	-2.16
702	c1cc(c(cc1C#N)F)Br	C14989287	-16.91	-1.69	-14.83	3.69	-4.09
703	c1c(ncnc1)Cl)F	C15444568	-16.91	-0.69	-16.5	2.48	-2.2
704	C=CCOC(=O)C(F)F)Cl	C16159461	-16.91	0	-14.93	1.43	-3.41
705	c1(c(non1)N)C(=O)N	C05670118	-16.9	-5.19	-17.43	3.67	2.05
706	c1ccc(cc1)S(=O)(=O)N=C([NH-])\N+](=O)[O-]	C16939446	-16.9	1.98	-21.5	6.05	-3.43
707	c1cnc(nc1N)N	C01661391	-16.89	-4.75	-16.45	4.83	-0.52
708	c1c(c(c(nc1F)F)F)F	C02585566	-16.89	-0.29	-16.78	2.24	-2.06
709	c12c(nc3c(n1)n[n+](n3)[O-])no[nH]2	C06862763	-16.89	-4.21	-16.72	4.59	-0.55
710	c1cnc(cn1)SC#N	C00331847	-16.88	-1.28	-20.28	6.02	-1.34
711	COc1ccc(cc1)F	C00404414	-16.88	-2.56	-13.98	2.56	-2.91
712	c1cc(c(cc1Cl)F)N	C00409384	-16.88	-0.82	-16.25	2.36	-2.17
713	c1ccc(cc1)[N+](=O)[O-]	C00896426	-16.88	-2.56	-16.02	5.55	-3.85
714	c1cc(cc1C=O)Cl	C02584625	-16.88	-0.86	-16.96	3.12	-2.19
715	C(=O)C(C(F)F)Cl)F)F)Cl	C14611410	-16.88	-0.06	-14.66	0.59	-2.75
716	c1c(cnc(n1)Cl)Cl	C21298678	-16.88	-1.41	-15.76	2.59	-2.29

717	c1cc(c(cc1N)N)F	C00404027	-16.87	-2.89	-16.96	3.16	-0.18
718	c1n2c(n1)sc(n2)S	C06554273	-16.87	-2.64	-18.71	6.51	-2.03
719	Cc1ccc(c(n1)N)C#N	C22011470	-16.87	-2.81	-16.96	4.68	-1.79
720	c1c(c[nH]1)Br	C00967315	-16.86	-3.41	-15.58	3.39	-1.25
721	c1cnoc1C(=O)Cl	C02170053	-16.86	0.95	-18.94	2.99	-1.86
722	c1cc(cc1)Br	C02558994	-16.86	-1.6	-15.25	2.35	-2.36
723	c1cnc(n1)CS	C08100931	-16.86	-1.66	-18.05	4.12	-1.27
724	c1cc(ncc1F)C=O	C08698202	-16.86	-3.46	-14.86	3.34	-1.89
725	c1c(c(cnc1F))F	C21987582	-16.86	0.51	-16.23	1.67	-2.81
726	c1ccc2c(c1)con2	C00154777	-16.85	-1.95	-17.9	6.04	-3.04
727	c1c(cc(cc1F)F)O	C00406989	-16.85	-2.51	-15.46	2.46	-1.34
728	c1(=O)c(nnc1[nH]1)[O-][N+](=O)[O-]	C05530560	-16.85	-4.96	-16.81	5.15	-0.23
729	COC(=O)/C=C/N=[N+]=[N-]	C05760459	-16.85	-2.05	-17.76	5.32	-2.37
730	CCOCc1cccc1N	C13346819	-16.85	-2.19	-15.01	2.96	-2.61
731	Cc1ccc(cc1)/C=N/O	C17303025	-16.85	-2	-17.01	4.37	-2.21
732	Cc1ccc(c(n1)N)Br	C19798390	-16.85	-3.32	-14.75	3.28	-2.06
733	CSc1nc(sn1)Cl	C22112817	-16.85	-1.59	-15.54	2.43	-2.14
734	c1c(cnc(n1)C(F)(F)F)Cl	C26440922	-16.85	-1.65	-15.63	3.14	-2.71
735	Cc1cncnc1	C00967366	-16.84	-1.42	-15.95	2.96	-2.42
736	c1ccc(cc1)CC(=O)[S-]	C02041149	-16.84	-2.46	-17.74	3.85	-0.5
737	CCOCc1cn[nH]n1	C05502177	-16.84	-3.4	-16.65	3.56	-0.35
738	c1(nc(nc1)C(=O)N)N	C17353821	-16.84	-7.68	-16.91	7.92	-0.17
739	c1cc(c(cc1C(=O)N=C=S)F)F	C21968391	-16.84	1.59	-19.71	4.48	-3.19
740	c1ccc(c(c1)NN)F	C00153109	-16.83	-0.36	-17.67	2.86	-1.67
741	c1c(ncc(n1)Br)N	C01420726	-16.83	-3.77	-16.95	4.09	-0.2
742	c1c(c(cc(c1F)F)F)CC#N	C04290231	-16.83	-1.67	-18.43	7.07	-3.8
743	c1cc(ncc1F)NN=O	C06536603	-16.83	-3.61	-18.65	5.17	0.25
744	c1(nc(nc(n1)F)F)F	C01669280	-16.82	0.15	-15.79	0.5	-1.69
745	c1cc([nH]c1)CCC#N	C01868300	-16.82	-2.03	-17.33	5.81	-3.26
746	c1ccc(cc1)CS	C03873647	-16.82	-0.88	-17.38	1.8	-0.35
747	c1c(cnc(c1)F)C#N	C12471972	-16.82	0.03	-17.91	3.46	-2.41
748	c1cnc(nc1)NC#N	C13638829	-16.82	-2.28	-15.83	6.16	-4.87
749	c1cncnc1/C(=N/O)/N	C15828512	-16.82	-5.35	-16.67	4.63	0.57
750	c1c(ncc(n1)Br)Cl	C30678093	-16.82	-1.75	-15.71	2.22	-1.58
751	c1c(c[nH]1)[N+](=O)[O-]	C01049761	-16.81	-4.24	-17.65	6.4	-1.32
752	COC1C=CC=CC=C1	C01710633	-16.81	1.09	-16.7	2.06	-3.27
753	c1c(c(n2c(n1)ncn2)N)C#N	C04342642	-16.81	-1.77	-18.74	7.27	-3.56
754	Cc1csc(n1)NN=O	C06523538	-16.81	-4.33	-14.63	3.28	-1.13
755	c1cc(nnc1C#N)Cl	C21299079	-16.81	-1.96	-19.04	6.08	-1.89
756	c1c(c(c(cn1)F)Br)F	C30678558	-16.81	0.2	-16.57	2.03	-2.47
757	c1cc(sc1)CCO	C00391955	-16.8	-2.65	-15.67	2.7	-1.19
758	C=CCC1C=CC(=O)C=C1	C01565456	-16.8	-0.36	-18.94	2.7	-0.2
759	c1c(cnc(n1)N)N	C01590037	-16.8	-3.93	-17.67	4.7	0.11
760	c1c(cnc(c1O)Cl)F	C02384091	-16.8	-1.5	-18.17	3.3	-0.43
761	c1c(cnc(c1)C#N	C02524724	-16.8	-0.69	-16.58	3.22	-2.74
762	c1(c(noc1[N+](=O)[O-])[O-])[N+](=O)[O-]	C04565377	-16.8	-4.64	-16.41	3.43	0.82
763	c1c(sc(n1)N)SC#N	C08294946	-16.8	-2.49	-18.33	5.3	-1.28
764	c1cc2nccn2c(c1)F	C14982821	-16.8	-2.78	-16.17	5.79	-3.64
765	Cc1cccn1	C00967365	-16.79	-1.38	-16	3.14	-2.55
766	C=C(CSC#N)Br	C01674057	-16.79	-1.15	-16.16	3.69	-3.17
767	c1cncc(c1Br)F	C02598039	-16.79	-0.65	-16.33	2.61	-2.42
768	C1C=CC(=C1)CC#N	C12358645	-16.79	-1.33	-16.76	5.17	-3.86
769	c1cc(c(cc1C#N)N)F	C14989290	-16.79	-0.9	-17.43	3.69	-2.15
770	c1c(c(nc(=S)[nH]1)N)[N+](=O)[O-]	C17289250	-16.79	-3.52	-15.36	3.16	-1.07
771	Cc1cncnc1[S-]	C26438568	-16.79	-1.63	-14.49	1.82	-2.49
772	c1ccc(cc1)COC(=S)S	C01562479	-16.78	-2.91	-19.55	4.71	0.96
773	C#Cc1ccccc1	C01680639	-16.78	-0.1	-17.62	2.96	-2.03
774	c1cnc(c1C(F)(F)F)F	C02511158	-16.78	-0.25	-16.86	3.17	-2.84
775	c1c(cc(c(c1F)CO)F)F	C04290165	-16.78	-0.3	-17.91	2.79	-1.36
776	c1c(nc([nH]1)Br)Br	C15020990	-16.78	-3.82	-15.6	4.61	-1.98
777	c1cc2c(cc1Cl)onc2[O-]	C15923721	-16.78	-4.35	-14.94	4.24	-1.72
778	c1cncnc1Br	C26439052	-16.78	-1.37	-17.71	3.96	-1.66
779	c1cc(c(cc1Cl)N)Cl	C00154585	-16.77	-3.33	-12.44	1.54	-2.54
780	c1cc(c(cc1N)F)F	C00388528	-16.77	-3.63	-15.33	4	-1.82
781	c1c[nH]c2c1cnc2	C02040901	-16.77	-1.57	-18.1	5.02	-2.12
782	CC#CCOC(=O)Cl	C02564822	-16.77	0.16	-17.77	2.9	-2.05
783	c1c2c([nH]n1)CSC2	C03848620	-16.77	-3.12	-17.49	5.77	-1.93
784	CNc1ccc(cc1F)F	C00167002	-16.76	-0.66	-16.06	2.59	-2.64
785	c1cc(cc(c1)F)CN=C=O	C02389319	-16.76	-2	-16.65	3.6	-1.71
786	c1cc(oc1C=O)C(F)(F)F	C05177782	-16.76	-3.64	-13.64	3.55	-3.04
787	CSc1ncc(cn1)F	C30677905	-16.76	0.45	-17.88	3.2	-2.54
788	c1cc(ncc1C#N)C(F)(F)F	C00154407	-16.75	-1.19	-17.3	4.9	-3.16
789	c1c2c(nc[nH]2)ncn1	C00391913	-16.75	-2.83	-18.73	7.36	-2.56
790	c1c(cn(c1C#N)O)Cl	C01764092	-16.75	-2.81	-16.96	4.71	-1.68
791	c1ccn(c1)CCO	C02556833	-16.75	-2.62	-16.26	3.22	-1.09
792	c1ccc(c1)C(=O)Cl	C02582853	-16.75	-1.11	-17.24	3.73	-2.14
793	C=C/c1cncn1	C15776679	-16.75	-3.45	-15.1	6	-4.2
794	c1ccc2c(c1)cco2	C01591814	-16.74	-1.86	-15.34	4.05	-3.6
795	c1c[nH]c2c1cnc2	C02040902	-16.74	-1.5	-18.15	5.04	-2.14
796	CCc1cncnc1	C08294967	-16.74	-1.22	-14.56	2.69	-3.65
797	c1cc([nH+]cc1N)N	C19015166	-16.74	-3.36	-17.64	3.8	0.46
798	c1cnn(c1)CCCl	C01393361	-16.73	-1.58	-15.84	3.59	-2.89
799	c1c(c(c(cn1)F)N)F	C02386531	-16.73	-2.31	-16.1	2.26	-0.58
800	c1c2c([nH]pn2)ncn1	C05567619	-16.73	-1.31	-18.4	3.41	-0.43
801	CNC(=O)Oc1ccc(cc1)F	C00399265	-16.72	-0.33	-21.71	5.66	-0.34
802	C/C=C/Cl)SC#N	C01673783	-16.72	-0.99	-16.12	3.54	-3.15
803	c1c(c(c(c(c1F)F)N)N	C02574886	-16.72	-5	-16.27	5.02	-0.47
804	c1cc(sc1)CSC(=[NH2+])N	C17289425	-16.72	-1.11	-16.59	2.95	-1.97
805	CC(=O)N/C(=N/[N+](=O)[O-])/N	C06562790	-16.71	-5.26	-17.11	3.74	1.91
806	Cc1ccc(c(c1)N)N	C00331686	-16.7	-4.01	-14.46	2.56	-0.8

807	c1ccc(cc1)COC(=O)C(=O)N	C01707303	-16.7	-2.21	-18.48	5.97	-1.98
808	c1c2cn[nH]c2ncc1Br	C02547938	-16.7	-0.73	-18.09	4.41	-2.29
809	c1cc2c(c(c1)F)non2	C02576406	-16.7	-2.67	-17.79	5.62	-1.87
810	C1c2c(noc2N)CS1	C07951901	-16.7	-3.91	-17.11	4.77	-0.44
811	c1cncnc1Cl	C20358090	-16.7	-1.24	-16.76	3.5	-2.2
812	c1cc(cc1N=C=O)ClF	C00164881	-16.69	-2.2	-15.29	2.06	-1.27
813	c1cc(sc1C(F)F)Br	C15442476	-16.69	-1.18	-12.58	1.09	-4.02
814	c1cc(oc1)CC(=O)ON=O	C20231630	-16.69	2.9	-22.99	7.09	-3.68
815	c2cc1ccccc1o2	M1995A029	-16.69	-1.63	-15.52	4.06	-3.6
816	c1c(cc(c(c1F)C#N)F)F	C00164883	-16.68	1.49	-18.6	3.93	-3.5
817	c1cn2cncc2cn1	C01601710	-16.68	-2.75	-18.96	5.7	-0.67
818	CCOC(=O)C(=C)F	C02525415	-16.68	-0.76	-16.61	3.47	-2.78
819	c1c(c(nc(n1)Cl)N)Br	C04198794	-16.68	-4.16	-13.98	2.86	-1.39
820	CCOc1nc(c(nn1)F)[O-]	C04522035	-16.68	-3.2	-18.91	4.22	1.21
821	Cc1c2c(c[nH]2)n[nH]1	C13119669	-16.68	-2.21	-19.2	5.09	-0.35
822	CC(=O)c1c[nH]cn1	C16696762	-16.68	-4.99	-16.41	6.78	-2.06
823	CC(=O)Oc1ccc2c(c1)nsn2	C00258314	-16.67	-2.61	-17.8	6.57	-2.84
824	CNC(=O)Oc1ccccc1N	C01716745	-16.67	-1.27	-21.75	6.86	-0.52
825	c1ccccc1Br	C02141003	-16.67	-1.95	-14.66	2.27	-2.32
826	c12c(nc(c(n1)NO)[O-])non2	C05753647	-16.67	-1.09	-21.34	5.3	0.46
827	c1ccc(cc1)/C(=[NH+])N)/N	C15889049	-16.67	-1.18	-17.95	4.03	-1.56
828	c1c(c(sc1Cl)C#N)N	C16696879	-16.67	-2.92	-15.28	3.33	-1.8
829	c1cc(oc1)CN=C=O	C02390452	-16.66	-1.68	-18.54	3.91	-0.35
830	C(=O)(C(F)F)NOC(=O)C(F)F	C04240915	-16.66	-0.88	-16.04	3.06	-2.81
831	c1cc(cnc1)/C=C/C=O	C04773466	-16.66	-1.94	-18.04	5.95	-2.63
832	c1cc(ncc1Cl)C(F)F	C15440742	-16.66	-0.95	-15.3	2.9	-3.32
833	c1csc(n1)N=C=O	C22001992	-16.66	-0.84	-17.91	2.92	-0.82
834	c1ccc(cc1)CNC=O	C01733926	-16.65	0.66	-21.07	5.81	-2.05
835	C=CCNc1ccccc1F	C19737073	-16.65	-2.06	-13.22	2.32	-3.69
836	Cc1ccccc1F	C02599054	-16.64	-1.82	-15.36	2.98	-2.43
837	c1cc(c(c(c1)F)N)O	C16158906	-16.64	-3.51	-16.67	3.32	0.22
838	c1c(c(c(c(n1)F)F)Br)F	C16159837	-16.64	-0.08	-16.26	2.1	-2.41
839	COC(=O)c1c(non1)N	C02473576	-16.63	-1.36	-17.7	3.24	-0.81
840	c1c([nH]nc1C(F)F)C2CC2	C04243650	-16.63	-3.23	-14.78	4.52	-3.15
841	c1c(c(c(cn1)Cl)Cl)F	C14982617	-16.63	-1.09	-14.51	1.75	-2.78
842	COc1ccccc1	C00403175	-16.62	-1.92	-16.79	3.62	-1.52
843	C=COCCOC=C	C05157944	-16.62	-1.06	-16.09	2.65	-2.12
844	c1cc2cnccn2c1	C05771137	-16.62	-2.15	-17.86	4.34	-0.96
845	c1ccc(c(c1)N=[N+]=[N-])F	C12505595	-16.62	0.43	-18.27	2.92	-1.69
846	c1cc2c(cc1Br)non2	C00158675	-16.61	-2.54	-16.13	2.74	-0.68
847	Cn1ccccc1	C01692446	-16.61	-1.69	-14.85	2.92	-3
848	CSc1ccc(cc1F)F	C02511091	-16.61	-0.15	-18.01	3.3	-1.75
849	c1c(c(nc(c1F)F)F)C#N	C02540462	-16.61	1.32	-19.64	3.95	-2.25
850	c1cc2c(ccc2)cc1N=C=O	C02548443	-16.61	-2.12	-16	3.61	-2.09
851	c1c2c([nH]n1)CCCC2	C08078164	-16.61	-3.19	-15.37	4.49	-2.53
852	c1cc(ncc1F)N	C19735097	-16.61	-3.14	-16.62	4.29	-1.14
853	c1ccc(c(c1)N)Sc2[nH]ncn2	C19845536	-16.61	-2.98	-16.68	5.84	-2.81
854	c1c(c(c(cn1)Cl)F)Cl	C26893241	-16.61	-0.77	-14.83	1.85	-2.86
855	Cc1c(cncn1)N	C01562392	-16.6	-3.77	-16.55	4.56	-0.83
856	CC(C=O)ON[N+](=O)[O-]	C01732519	-16.6	-2.26	-15.63	4.41	-3.12
857	c1cc(oc1)CNC(=O)C(=O)N	C03072973	-16.6	-3.58	-21.22	5.64	2.57
858	c1c(sc(n1)N)Br	C04624087	-16.6	-4.47	-16.97	3.04	1.79
859	C#CCSc1[nH]ncn1	C14608578	-16.6	-1.12	-18.9	7.12	-3.69
860	c1cc2cn[nH]c2c(c1)F	C14985760	-16.6	-1.86	-17.21	4.86	-2.39
861	c1csc(n1)N/C=N/O	C15934906	-16.6	-2.63	-18.66	5.81	-1.12
862	c1cc(c(c(c1CC=O)F)F)F	C21984093	-16.6	-3.5	-14.87	5.57	-3.8
863	CNc1ccccc1	M2007002_	-16.6	-1.98	-14.07	2.02	-2.58
864	CC(=O)Oc1ccc(nc1)Cl	C00335980	-16.59	-0.55	-18.39	5.74	-3.39
865	CNc1ccccc1	C00901343	-16.59	-2.03	-14	2.01	-2.57
866	C1C=NN=C1Br	C00967346	-16.59	-2.03	-16.01	2.62	-1.16
867	c1ccc2c(c1)cno2	C04521187	-16.59	-2.47	-17.42	6.19	-2.9
868	CNc1ccccc1	C05141034	-16.59	-2.41	-16.48	3.55	-1.25
869	c1cc(cc(c1)F)C(=O)N=C=O	C19408029	-16.59	1.27	-19.91	3.23	-1.17
870	c1ccc(c(c1)N)O	C00157526	-16.58	-2.98	-16.88	3.01	0.27
871	Cc1cc(n[nH]1)C#N	C32005330	-16.58	-3.31	-16.32	4.63	-1.58
872	c1cnc(nc1Cl)N	C00967348	-16.57	-2.59	-16.07	4.02	-1.93
873	c1ccc(cc1)C(=O)F	C01847403	-16.57	-2.18	-14.91	3.71	-3.19
874	C=COCC(=O)C(F)F	C02242722	-16.57	-0.4	-15.32	1.88	-2.72
875	c1([nH]nnn1)/N=N/c2[nH]nnn2	C06862759	-16.57	-0.62	-21.58	6.92	-1.29
876	Cc1ccc(nc1)N[N+](=O)[O-]	C13214339	-16.57	-1.53	-18.76	7.19	-3.47
877	C1CS/C(=N)C#N)N1	C14982514	-16.57	-1.72	-16.23	4.33	-2.96
878	c1c(c(c(cn1)F)F)F	C14983676	-16.57	-0.43	-16.51	2.57	-2.2
879	c1cc(cc(c1O)F)F	C00164811	-16.56	-3.39	-15.74	3.86	-1.29
880	c1cc(cc(c1)F)O	C00164911	-16.56	-2.88	-15.57	3.16	-1.27
881	c1nnc2n1[C@@H](N=N2)[N+](=O)[O-]	C04343691	-16.56	-1.47	-18.2	6.86	-3.74
882	Cc1cnc(s1)N	C08652421	-16.56	-3.57	-15.21	3.83	-1.62
883	c1cc2nccn2cc1F	C18555974	-16.56	-2.66	-15.08	4.9	-3.71
884	c1cc([nH+]c(c1)N)N	C19075726	-16.56	-3.73	-16.51	3.79	-0.11
885	c1cc(nnc1Cl)Cl	C01685243	-16.55	-2.08	-16.92	4.45	-2.01
886	CSc1ccccc1O	C01701825	-16.55	-0.51	-17.81	3.79	-2.02
887	c1cnc(cn1)I	C02245235	-16.55	-1.21	-17.47	3.47	-1.35
888	c1ccc(cc1)[C@@H](CC)O	C02555240	-16.55	-0.77	-16.2	3.06	-2.64
889	c1c(c(nc(n1)NN)N)F	C09189735	-16.55	-3.3	-16.97	4.26	-0.54
890	c2cc1ccccc1[nH]2	M1995A031	-16.55	-1.24	-15.83	3.87	-3.35
891	Cn1ccccc1	M2007003_	-16.55	-1.7	-14.78	2.92	-2.99
892	c1cc(c(cc1Cl)N)C#N	C00395567	-16.54	-2.71	-14.68	3.25	-2.39
893	C1C/C(=C/[O-])C(=O)C1	C01235150	-16.54	-5.22	-14.9	5.44	-1.86
894	c1cc(ccc1N)Br)N	C01438949	-16.54	-3.57	-14.63	2.4	-0.73
895	c1ccc(cc1)CC=O	C01699889	-16.54	-2.28	-15.28	5.3	-4.29
896	c1ccc(cc1)C(=O)N=C=O	C01766603	-16.54	1.65	-20.65	3.56	-1.11

897	C=CCSCC=C	M1995A014	-16.54	-0.44	-13.46	1.41	-4.05
898	c2ccc1oncc1c2	isooxzl	-16.54	-2.5	-17.34	6.19	-2.9
899	c1cc(c(cc1F)F)NC=O	C00399097	-16.53	-0.13	-20.31	5.36	-1.45
900	CCO[P@](=O)(O)[S-]	C02017442	-16.53	-1.72	-13.21	5.42	-7.02
901	c1cc(c(c(c1F)N)C#N	C16159792	-16.53	-1.61	-16.67	3.84	-2.09
902	c1cc(ccc1N)Oc2nccs2	C16677891	-16.53	-0.8	-18.87	5.02	-1.88
903	c1noc2ccccc12	M1995A018	-16.53	-2.43	-17.4	6.19	-2.89
904	c1cc(cnc1)C=O	C00158588	-16.52	-2.05	-17.95	5.3	-1.81
905	c1cnc(cc1Br)F	C02526716	-16.52	-1.23	-15.92	3	-2.36
906	c1ccc2c(c1)cc[nH]2	C14516984	-16.52	-1.24	-15.79	3.87	-3.35
907	c1(c(c(c(c1F)F)C)F)F	L200A002_	-16.52	0.53	-13.58	0.5	-3.96
908	c1cc(ccc1CO)F	C00157464	-16.51	-1.29	-17.47	3.55	-1.31
909	c1csc2c1nn(c2)N	C00334093	-16.51	-4.14	-18.15	7.09	-1.31
910	c1cc(cc(c1)F)C#N	C00407069	-16.51	0.41	-17.33	4.05	-3.64
911	CSc1nc(sn1)N	C08652418	-16.51	-3.44	-16.03	4.11	-1.14
912	[H]/N=C(N)/N1CCCC1=O	C22521270	-16.51	-3.1	-17.61	5.73	-1.53
913	c1cncoc1C(F)F	C00166563	-16.5	0.24	-16.57	2.65	-2.81
914	c1c(cc(c(c1O)N)F)F	C02243350	-16.5	-2.58	-17.06	2.97	0.17
915	CCc1ccc[nH]1	C02528141	-16.5	-1.3	-14.83	2.5	-2.87
916	c1c2c(nc(n1)[S-])n[nH]n2	C05763113	-16.5	-3.96	-16.83	6.13	-0.3
917	c1cncoc1CF	C15042152	-16.5	-2.05	-15.73	3.79	-2.51
918	c1cc(c(c1F)OCC#N)F	C15442721	-16.5	0.17	-19.93	6.87	-3.62
919	Cc1ccc(c(c1)N)F	C00388035	-16.49	-2.3	-14.32	2.5	-2.36
920	c1c[nH]nc1	C01027316	-16.49	-3.93	-16.17	5.16	-1.55
921	c1ccc(cc1)C[C@H]2CO2	C01673126	-16.49	-1.62	-15.38	3.72	-3.22
922	c1(nc([nH]n1)N)C(=O)NN	C16971468	-16.49	-7.59	-16.64	6.47	1.27
923	c1c(ncn1)CC)Br	C02569104	-16.48	-2.68	-14.92	4.02	-2.9
924	c1cc(c(cc1F)Br)N	C00159787	-16.47	-2.84	-16.56	2.39	0.53
925	c1cc(cnc1)CC#N	C00391916	-16.47	-1.35	-19.65	7.42	-2.9
926	C(C)N(C#N)N=O	C05495985	-16.47	0.92	-17.49	2.75	-2.64
927	c1c(cnc(c1F)NN)F	C16158485	-16.47	-2.09	-16.14	2.9	-1.14
928	C=CCNc1nnns1	C32603397	-16.47	-1.48	-19.39	5.63	-1.23
929	c1cc(c(cc1F)O)F	C00409280	-16.46	-1.67	-16.52	3.07	-1.34
930	Cc1c(ncn1)N	C01731583	-16.46	-3.64	-16.98	4.46	-0.3
931	c1ccc(cc1)P2(=O)OCCO2	C01737302	-16.46	-10.3	-6.71	1.7	-1.15
932	c1ccc(cc1)C(=O)Cl	C02041164	-16.46	-0.44	-15.82	3.36	-3.55
933	c1cc(c(cc1C#N)F)Cl	C02512522	-16.46	-1.56	-16.31	3.79	-2.38
934	CSc1cccs1	S2001A003	-16.46	-0.64	-14.48	2.16	-3.5
935	c1c(c(ncn1)N)N	C00967391	-16.45	-4.9	-16.63	4.7	0.38
936	c1cc(oc1)CCL	C01587710	-16.45	-0.77	-15.72	2.99	-2.95
937	Cc1ccncc1	C02026722	-16.45	-1.94	-16.07	3.91	-2.35
938	c1cnc(cn1)[C][NH+]=[N+]=[N-]	C05045522	-16.45	-1.2	-20.97	4.75	0.97
939	c1c(c(oc1[N+](=O)[O-])N)N[N+](=O)[O-]	C05641452	-16.45	-5.16	-17.14	5.36	0.48
940	C/C(=C/C(=O)C(F)F)/[O-]	C12358633	-16.45	-3.24	-14.3	3.16	-2.07
941	c1(c(ncn1)N)C(=N/O)/Cl	C13844192	-16.45	-3.47	-18.18	4.07	1.13
942	c1cc(cnc1)CF	C15042156	-16.45	-1.64	-15.96	3.79	-2.65
943	CCc1cccnc1F	C21981766	-16.45	-1.03	-17.06	4.67	-3.02
944	c1ccc(c(c1)N)Br	C00404305	-16.44	-2.6	-16.88	1.97	1.08
945	c1cc2cn[nH]c2nc1	C03852638	-16.44	-1.42	-19.02	5.81	-1.82
946	c1cc(c(cc1F)N+)(=O)[O-]N	C04261952	-16.44	-2.29	-17.09	5.41	-2.47
947	c1cnc(c1)Br	C00158586	-16.43	-0.66	-17.02	3.73	-2.49
948	c1cc(ccc1N=C=S)F	C00167224	-16.43	0.89	-15.43	2.1	-4
949	c1c(c(nc(c1F)F)F)F	C00409383	-16.43	0.66	-17.58	2.53	-2.05
950	COC(=O)c1c(ncn1)[N+](=O)[O-]	C01295934	-16.43	-0.37	-15.87	2.88	-3.08
951	c1cc(c(c1F)NN)F	C02243111	-16.43	-0.51	-17.66	3.34	-1.61
952	c1(ncn1N)[S-]C(F)F	C04237615	-16.43	-4.13	-15.43	4.66	-1.53
953	Cc1c(cccn1)F	C14982837	-16.43	-0.16	-16.75	3.07	-2.59
954	c1c(n[nH]c1C2CC2)C#N	C32005406	-16.43	-4.17	-14.1	4.6	-2.75
955	c1ccc(c(c1)F)F	C00164418	-16.42	-1.62	-15.03	3.63	-3.4
956	c1cc(c(nc1)F)C(F)F	C02540646	-16.42	-3.35	-15.99	5.24	-2.32
957	C(=O)(C(F)F)C(F)F)Cl	C03875510	-16.42	0.27	-14.73	0.51	-2.47
958	c1cc(cnc1)C(=O)N=[N+]=[N-]	C15784782	-16.42	1.5	-22.54	3.81	0.81
959	c1c(cnc(n1)C#N)Cl	C00336445	-16.41	0.51	-18.84	3.99	-2.07
960	c1(c(c(nc(c1F)F)F)F)N	C01085205	-16.41	-3.56	-15.01	2.6	-0.44
961	CCc1ccc(cc1)O	C01690956	-16.41	-0.82	-15.99	2.63	-2.23
962	c1ccc2c(c1)N2	C20230945	-16.41	-3.81	-15.41	4.93	-2.12
963	C=Cc1ccc(cc1)N	C01673648	-16.4	-0.75	-15.31	2.22	-2.56
964	c1ccc(cc1)OCCC#N	C01700385	-16.4	-1.85	-15.84	5.33	-4.04
965	c1cn2c(cn1)nnn2	C01701960	-16.4	-3.19	-20.01	7.44	-0.63
966	CC(=C)OC(=O)Cl	C02384739	-16.4	-0.76	-15.67	2.21	-2.17
967	c1cc(c(c(c1)F)F)CS	C04244660	-16.4	-1.06	-15.51	4.26	-4.09
968	c1cc(cnc1)/C=N/O	C04758522	-16.4	-3.9	-18.85	6.6	-0.26
969	c1ccc(cc1)CNC(=S)N	C05850155	-16.4	-1.4	-21.51	3.62	2.88
970	Cc1ncc(cn1)C#N	C14593177	-16.4	-0.74	-17.44	4.05	-2.27
971	c1cc(cnc1)/C=N/O	C19730699	-16.4	-1.55	-19	4.56	-0.41
972	c1cc(oc1)CS	C00388704	-16.39	-1	-15.68	2.89	-2.6
973	c1cc2c([nH]c(=S)[nH]2)nc1	C04786354	-16.39	-2.3	-17.79	5.78	-2.08
974	C(=C(C(F)F)F)(O-))C(=O)C(F)F	C12410248	-16.39	0.72	-18.95	4.3	-2.47
975	c1nnc(n1N)SCC#N	C22201976	-16.39	-3.19	-19.31	8.91	-2.79
976	c1csc2n1cc(n2)Cl	C00124263	-16.38	-1.34	-18.19	6.77	-3.62
977	c1ccc2c(c1)CC2=O	C01728837	-16.38	-1.9	-15.49	4.63	-3.62
978	#CCn1cnc(c1Cl)Cl	C02543584	-16.38	-2.41	-15.12	5.83	-4.67
979	Cc1ccc(cc1O)F	C02568100	-16.38	-1.18	-16.35	3.07	-1.92
980	c1cnc(cc1F)F	C02599002	-16.38	-1.8	-15.6	3.07	-2.05
981	c1cc(ccc1CNC=O)F	C03097781	-16.38	0.16	-20.68	6.22	-2.08
982	C[C@H](c1ccc(cc1F)F)O	C12506480	-16.38	-1.18	-15.62	2.67	-2.24
983	c1cc(c(cc1F)F)C(=O)N=C=S	C21964249	-16.38	2.86	-21.23	5.2	-3.21
984	c1cc(ccc1C#N)Cl	C00157255	-16.37	-0.71	-17.09	3.27	-1.84
985	C[C@H](c1ccccc1)O	C00896626	-16.37	-0.98	-15.75	2.47	-2.1
986	COC(=O)C(C(C(F)F)F)F	C01847517	-16.37	1.4	-14.82	2.05	-5.01

987	c1cc2c(nc1)nc[nH]2	C04003201	-16.37	-2.95	-17.9	7.21	-2.72
988	c1c(c(cc1F)F)O	C04262384	-16.37	-1.94	-16.37	3.02	-1.07
989	c1ccc(cc1)NC(=O)Cl	C06864539	-16.37	-0.45	-20.28	4.21	0.15
990	c1cc(cc1)F)CSC(=NH2+)N	C07715600	-16.37	-1.65	-15.46	3.41	-2.68
991	c1cnc(c1)Br	C08698473	-16.37	-2.67	-16.1	3.62	-1.22
992	c1cc(ncc1Cl)NN	C08729997	-16.37	-4.36	-14.54	3.82	-1.29
993	c1c2c(ncnc2[nH]n1)N	C13542589	-16.37	-4.7	-17.08	6.27	-0.85
994	c1csc(n1)CN=C=O	C22861654	-16.37	-2.44	-18.81	4.49	0.4
995	c1ccc(cc1)OC(=O)NN	C00079243	-16.36	0.22	-22.46	6.67	-0.8
996	c1c(ccc1Cl)Cl	C00404352	-16.36	-0.35	-14.59	1.36	-2.79
997	c1nnc(n1)N	C01685262	-16.36	-2.15	-15.73	4.1	-2.58
998	CCc1ccccc1O	C01706027	-16.36	-1	-15.56	2.61	-2.41
999	c1cc(sc1)N	C01708748	-16.36	-2.92	-14.41	2.11	-1.15
1000	c1c(c(n[nH]1)[N+](=O)[O-])[N+](=O)[O-]	C05248441	-16.36	-1.86	-17.19	5.38	-2.69
1001	c1cnc(c1[N+](=O)[O-])N	C14982118	-16.36	-3.16	-16.91	4.73	-1.02
1002	CN(c1[nH]nn1)[N+](=O)[O-]	C25627715	-16.36	-5.24	-16.11	6.76	-1.77
1003	CNC(=O)Oc1ccc(cc1)N	C01716763	-16.35	-0.22	-22.8	7.05	-0.37
1004	c1cc(cc(c1)F)/C=C/C(=O)Cl	C02574174	-16.35	-1.77	-16.7	3.94	-1.82
1005	Cc1ccc(c1)Cl	C02599020	-16.35	-0.17	-15.78	2.55	-2.96
1006	C=C(c1ccccc1)N=[N+]=[N-]	C05369766	-16.35	-0.62	-15.6	1.88	-2.02
1007	c1cnc(nc1)NN=O	C06584933	-16.35	-1.16	-19.34	5.96	-1.8
1008	COC(=O)C(F)Br	C14628562	-16.35	-1.41	-14.31	1.77	-2.4
1009	c1ccc(cc1)C2c(nsn2)O	C16125338	-16.35	-3.93	-16.73	4.34	-0.04
1010	c1cc2c(cc1N)n[nH]n2	C19626986	-16.35	-6.81	-18.24	8.15	0.55
1011	Cc1ccc(cc1)OC(=O)Cl	C00389522	-16.34	-1.05	-16.32	3.1	-2.07
1012	c1c[nH]cc(c1=O)Cl	C02599072	-16.34	-2.56	-17.04	3.51	-0.26
1013	c1c(cnc(c1N)N)F	C21981774	-16.34	-5.47	-17.34	6.19	0.28
1014	CCOC(=O)[C@H](F)Br	C04255720	-16.33	-0.69	-15.71	3.07	-3
1015	c1c(c(non1Cl)[N+](=O)[O-])	C14982438	-16.33	-1.99	-15.58	3.85	-2.61
1016	c1cc(nnc1N/C=N/O)Cl	C15906878	-16.33	-3.23	-22.1	10.52	-1.51
1017	c1cc(c(c1N)F)F	C00164526	-16.32	-3.26	-16.03	4.87	-1.91
1018	c1ccc(cc1)N(C#N)N	C01704255	-16.32	-1.76	-14.15	3.97	-4.38
1019	C1=CC=CC(C=C1)C#N	C02556987	-16.32	0.37	-18.03	5.11	-3.77
1020	Cc1cncnc1N	C02582043	-16.32	-4.26	-14.82	3.66	-0.89
1021	Cc1cc(sc1)N=C=O	C04200662	-16.32	-0.21	-16.1	1.82	-1.83
1022	C/C(=C/C(=O)C(F)F)[O-]	C04243025	-16.32	-5.52	-14.44	5.58	-1.93
1023	c1cc(ncc1)N	C19143839	-16.32	-2.6	-14.55	2.72	-1.89
1024	C#Cc1cc(cnc1)Cl	C22013250	-16.32	0.31	-16.48	3.22	-3.38
1025	N#Cc1ccccc1	benznlrl	-16.32	0.77	-17.36	3.85	-3.58
1026	c1csc1CCO	C00391956	-16.31	-2.34	-15.61	2.69	-1.05
1027	c1ccc2c(c1)CC(C2)N=C=S	C02243801	-16.31	-1.48	-12.02	1.93	-4.74
1028	c1cc(c(c1F)N)I	C02389393	-16.31	-3.22	-15.25	1.59	0.56
1029	c1c(cnc(c1F)Br)F	C02513193	-16.31	0.07	-17.7	2.1	-0.77
1030	c1c(cnc(n1)N)C#N	C02559851	-16.31	-0.25	-19.08	4.76	-1.74
1031	c1cnn(c1)C#C#N	C02584631	-16.31	-2.19	-17.62	6.25	-2.75
1032	CC(=S)Nc1ccccc1	C20130858	-16.31	-1.37	-17.49	6.73	-4.17
1033	c1cnc(c1C#N)N	C20357578	-16.31	-2.85	-17.84	4.9	-0.52
1034	c1cc(=O)occ1I	C21989738	-16.31	-1.54	-16.22	5.03	-3.59
1035	Cc1ccc(cc1)SC#N	C01095293	-16.3	-1.09	-16.69	3.38	-1.91
1036	c1cc2c(cc1N)non2	C01504263	-16.3	-4.16	-17.9	6.54	-0.78
1037	CC(=C)C(=O)OC=C	C01665002	-16.3	0.92	-17.72	3.81	-3.3
1038	Cc1c(nc(nc1F)F)N	C02025696	-16.3	-4.71	-15.55	4.97	-1
1039	c1cc2c(cc1F)cn[nH]2	C12359144	-16.3	-1.71	-16.2	3.95	-2.34
1040	c1c(c(cc(c1F)F)F)CO	C00403442	-16.29	-1.63	-16.11	2.97	-1.52
1041	CCc1ccccc1	C00967178	-16.29	-0.84	-14.39	2.66	-3.73
1042	c1cc(sc1)CCN=C=O	C02169322	-16.29	-0.98	-16.4	2.47	-1.38
1043	COC(=O)C(=O)C(F)F	C02577560	-16.29	-0.54	-15.74	2.25	-2.26
1044	C(=O)C(F)F)C(F)F)Br	C04242004	-16.29	0.18	-14.35	0.45	-2.56
1045	Cc1c(c[nH]n1)I	C15022021	-16.29	-4.22	-13.39	3.34	-2.02
1046	Cc1cc(cnc1)F	C02384097	-16.28	-1.55	-16.26	2.65	-1.12
1047	CO/C(=N/c1ccccc1)/O	C16157438	-16.28	-2.48	-21.29	7.28	0.2
1048	C1Cc2c(sc(n2)N)C1	C17126087	-16.28	-2.91	-14.67	3.75	-2.45
1049	c1ccc(cc1)CN[NH3+]	C19166973	-16.28	1.01	-18.61	2.66	-1.34
1050	c1cc(ccc1CN)N	C19171876	-16.28	0.62	-18.51	2.98	-1.37
1051	c1cc(c(nc1)CC)N	C21985290	-16.28	-2.11	-17.57	4.93	-1.52
1052	c1cc(c(cc1O)Cl)N	C00395500	-16.27	-3.99	-15.34	3.11	-0.03
1053	CCOC(=O)n1ccccc1	C01634244	-16.27	0.83	-17.47	4.01	-3.64
1054	c1cnc(c1F)F	C02599070	-16.27	-1.97	-15.17	3.05	-2.17
1055	Cc1cc(c(cc1N)F)F	C12359155	-16.27	-4.1	-15.31	3.96	-0.82
1056	CCOC(=O)C(F)F)Br	C01845846	-16.26	-0.85	-13.78	1.53	-3.16
1057	c1cc(c(c1N)N)F	C02526225	-16.26	-3.87	-16.42	4.47	-0.43
1058	Cc1c(cncn1)Cl	C14982422	-16.26	-0.79	-15.19	2.41	-2.69
1059	c1c(cnc(n1)Br)F	C14989449	-16.26	-0.06	-17.03	2.81	-1.98
1060	c1ccc(cc1)[C@H](CS)O	C32625176	-16.26	-0.71	-16.14	2.83	-2.25
1061	COC(=O)Nc1ccc(cc1)F	C00243830	-16.25	-0.25	-19.07	5.23	-2.16
1062	c1ccc(cc1)C#N	C00899417	-16.25	1.04	-17.58	3.86	-3.57
1063	c1cnc(c1N)N	C01724764	-16.25	-4.45	-17.39	4.67	0.92
1064	c1csc1C(=O)Cl	C02504558	-16.25	-1.79	-15.31	3.62	-2.76
1065	c1ccc(c(c1)NC(=O)NN)F	C02509220	-16.25	-3.45	-17.88	5.79	-0.7
1066	c1cc(ccc1C=NN)[N+](=O)[O-]	C13542678	-16.25	-2.82	-16.97	6.15	-2.61
1067	CN(C)C1nc[nH]n1)N	C17024975	-16.25	-3.67	-17.16	7.97	-3.39
1068	COC(=O)C=CCBr	C17353061	-16.25	-1.89	-14.52	3.23	-3.07
1069	c1cnc(c1)NN	C00404420	-16.24	-2.78	-16.74	4.4	-1.12
1070	Cc1ccccc1O	C00901022	-16.24	-1.65	-15.51	2.72	-1.8
1071	c1c(nc(nc1F)N)N	C01083705	-16.24	-4.7	-15.79	4.7	-0.45
1072	C(C(F)F)F)OC(=O)C(F)F)F	C01847450	-16.24	-1.85	-12.37	2.38	-4.41
1073	c1c(cnc(c1F)C#N)F	C02510830	-16.24	1.07	-19.07	4.17	-2.41
1074	C1[C]C@@H](OC1)CN=C=S	C03882601	-16.24	-0.26	-17.39	3.09	-1.67
1075	c1cc(ccc1N)O	C04623758	-16.24	-2.53	-17.43	3.28	0.45
1076	c1cc2c[nH]nc2cc1C#N	C05086226	-16.24	-0.14	-18.98	5.48	-2.59

1077	COC(=O)/C=C/N=[N+]=[N-]	C06379516	-16.24	-0.06	-16.74	2.78	-2.22
1078	c1c(con1)[N+](=O)[O-]	C15782467	-16.24	-1.36	-17.39	4.51	-1.99
1079	Cc1ccc(s1)/C=N/N	C16982515	-16.24	-1.12	-16.44	3.24	-1.92
1080	c1cc(nnc1N)Cl	C00967320	-16.23	-4.23	-17.22	5.87	-0.64
1081	c1ccc(cc1)OCCON	C01673093	-16.23	-1.76	-17.68	4.86	-1.66
1082	c1c(c(nc(n1)Cl)N)F	C01718953	-16.23	-3.59	-14.78	3.07	-0.93
1083	c1c(ncnc1)Cl	C02513831	-16.23	-0.85	-17.84	2.38	0.08
1084	C(C(F)(F)F)OC(=O)Cl	C04290611	-16.23	-0.87	-14.89	2.27	-2.73
1085	c1cc(cnc1)N	C00967327	-16.22	-2.48	-16.68	3.45	-0.5
1086	c12c([nH]c(=O)[nH]1)nc3c(n2)non3	C00972772	-16.22	-3.61	-16.59	4.88	-0.9
1087	CC(=O)Oc1ccc(cc1)O	C01679468	-16.22	0.02	-20.66	6.5	-2.08
1088	c1ccc(cc1)C@H](C=O)O	C06116374	-16.22	-3.27	-17.26	6.5	-2.19
1089	c1cc(ncc1F)C#N	C12359109	-16.22	-0.32	-18.12	4.59	-2.36
1090	CC(=O)OCc1cccnc1	C13281461	-16.22	-0.12	-18.56	5.85	-3.39
1091	c1c[nH]c2c1c(ccn2)F	C14984908	-16.22	-2.08	-16.53	5.35	-2.95
1092	c1ccc(cc1)C(=O)N=C=S	C01652069	-16.21	2.26	-20.41	4.99	-3.05
1093	c1c[nH]cc1[N+](=O)[O-]	C02527916	-16.21	-4.27	-17.69	8.11	-2.35
1094	c1[nH]c(=S)nc(n1)N	C02566991	-16.21	-0.7	-17.66	4.13	-1.98
1095	c1(nc([n-]n1)N[N+](=O)[O-])C(=O)N	C08661649	-16.21	-6.94	-19.86	6.47	4.12
1096	c1cc(ccc1C=O)F	C00157154	-16.2	-2.2	-15.8	4.99	-3.18
1097	c1cc(cnc1)Cl	C02008821	-16.2	-2.48	-16.23	3.65	-1.12
1098	C#CCOC(=O)Cl	C02562433	-16.2	-1.74	-14.96	2.66	-2.16
1099	c1cc(nnc1[S-])Cl	C08616233	-16.2	-2.27	-16.93	4.63	-1.63
1100	c1cc(nc(c1Cl)N)Cl	C19907216	-16.2	-3.92	-13.6	3.12	-1.79
1101	CCNc1cc(ccc1F)F	C19907910	-16.2	-2.12	-12.83	2.04	-3.3
1102	c1ccc(cc1)NC(=O)N	C00391870	-16.19	-3.29	-19.52	7.07	-0.45
1103	c1c(sc(n1)Br)[N+](=O)[O-]	C01081253	-16.19	-1.95	-14.26	2.49	-2.47
1104	COC1=CCC=CC1	C01840966	-16.19	0.3	-15.34	1.86	-3.01
1105	C#Cc1cccc(c1)N	C02560531	-16.19	-0.23	-16.85	3.58	-2.69
1106	c1cc(c(c(c1CO)F)F)F	C02575077	-16.19	-2.32	-16.25	3.89	-1.5
1107	c1c(c(cc(c1F)N)F)N	C04334614	-16.19	-1.34	-17.07	2.45	-0.23
1108	C(#N)N=C(N)N	C05112486	-16.19	-5.16	-13.11	4.24	-2.17
1109	c1cc(ccc1N=O)Cl	C05328624	-16.19	-1.55	-16.65	2.27	-0.27
1110	c1c[nH]nc1/C=N/O	C05613512	-16.19	-5.63	-17.21	4.78	1.87
1111	c1c[nH]c2c1cc(cn2)Cl	C06643319	-16.19	-0.72	-16.63	4.43	-3.27
1112	c1cnc(cc1F)N	C15444651	-16.19	-3.15	-15.82	3.88	-1.11
1113	c1(c(nc(c1F)F)F)[N+](=O)[O-]	C16159845	-16.19	-0.08	-14.65	1.22	-2.67
1114	c1c(c[nH]1)C(F)F	C32911377	-16.19	-4.27	-15.45	5.04	-1.52
1115	c1cnn(c1)C(F)F	C02538923	-16.18	-3.11	-14.76	3.61	-1.91
1116	C1COC(=O)/C=C/N=[N+]=[N-]	C17175261	-16.18	-0.72	-19.53	4.74	-0.68
1117	c1ccc(cc1)Cl)N	C00047986	-16.17	-1.12	-14.97	2.11	-2.19
1118	c1c(c(c(c(c1F)F)F)F)N	C00388049	-16.17	-3.64	-14.69	4.05	-1.89
1119	c1ccc2c(c1)C(C@H)2C#N	C02140854	-16.17	0.27	-16.91	5.11	-4.63
1120	c1cnc(c(c1)N+)(=O)[O-]	C02583405	-16.17	-3.04	-15.46	5.12	-2.79
1121	c1cc(ncc1F)C(F)F	C16159702	-16.17	-0.78	-15.47	3.07	-2.99
1122	c1cc(c(cc1Cl)F)O	C00389569	-16.16	-0.72	-16.93	3.08	-1.59
1123	c1cc(c(c(c1)F)F)N	C00409208	-16.16	-2.8	-15.53	4.04	-1.87
1124	c1c(c([nH]1))N+)(=O)[O-]Br	C01049759	-16.16	0.71	-17.89	3.29	-2.27
1125	c1nc([nH]n1)N=N/c2[nH]jncn2	C05045644	-16.16	0.75	-18.13	6.18	-4.96
1126	CN(C(=O)NCCCl)N=O	C05542262	-16.16	-2.25	-17.18	3.92	-0.65
1127	c1ccc(cc1)NC=O	C13550498	-16.16	-3.21	-19.91	6.84	0.12
1128	c1cnc(c1)N	C13952160	-16.16	-2.6	-15.75	3.33	-1.13
1129	Cc1csc(n1)N=C(N)N	C19419052	-16.16	-3.14	-18.45	7.56	-2.13
1130	C=C(C=O)OCc1ccccc1	C21998761	-16.16	1.28	-21.42	8.45	-4.48
1131	COC(=O)Cc1cccs1	C00153594	-16.15	-0.33	-17.19	5.21	-3.85
1132	c1cc(cc1C=O)Br	C00155120	-16.15	-0.92	-16.05	3.13	-2.31
1133	CSc1ccsc1	C00161206	-16.15	-0.98	-14.11	2.31	-3.38
1134	C=CCn1cccn1	C00399151	-16.15	-1.52	-17.38	4.21	-1.45
1135	c1ccc(c(c1)/C=C/C(=O)Cl)F	C02521287	-16.15	-0.16	-19.14	4.94	-1.78
1136	c1nc2n(n1)[C@H](N=N2)[N+](=O)[O-]	C04593311	-16.15	-0.45	-17.72	5.04	-3.02
1137	c1cncn1C(=O)Cl	C12359655	-16.15	-2.95	-16.14	4.61	-1.67
1138	C/N=[NH+]/Cc1ccccc1	C17021521	-16.15	-0.84	-17.09	2.8	-1.03
1139	c1cc(ccc1O)F	C00164463	-16.14	-2.86	-14.83	2.81	-1.26
1140	c1cncn(c1)N(N=O)O	C04365544	-16.14	-2.39	-19.39	5.89	-0.24
1141	C(/C(=C(Cl)Cl)N)C=S	C08665400	-16.14	0.66	-15.47	1.39	-2.72
1142	c1cn(cn1)C(=O)C(F)F	C01081150	-16.13	0.29	-17.15	3.43	-2.71
1143	c1cnc(cc1[N+](=O)[O-])F	C02526706	-16.13	-2.53	-15.42	4.34	-2.53
1144	Cc1ccc(cc1N)O	C04293750	-16.13	-3.55	-15.92	3.48	-0.14
1145	c1ccc2c(c1)c([nH][nH+])2)N	C13682782	-16.13	-4.89	-16.67	7.07	-1.65
1146	c1cc(ncc1F)CO	C14985906	-16.13	-1.74	-17.56	3.33	-0.15
1147	c1cc(cnc1)C=NN	C17148270	-16.13	0.04	-19.2	3.9	-0.87
1148	C1Cc2c(nc([nH]2)Cl)C1	C22126196	-16.13	-1.93	-17.11	5.88	-2.97
1149	CCc1cnc(nc1)N	C25490304	-16.13	-2.37	-15.85	4.63	-2.54
1150	C1C=Cc2ccccc21	M1995A038	-16.13	-1.23	-12.73	2.53	-4.7
1151	Cc1c(non1)C(=O)C	C00153433	-16.12	-2.54	-14.48	2.67	-1.77
1152	C#C[C@H](c1ccccc1)O	C02038031	-16.12	-0.94	-15.98	3.35	-2.55
1153	c1cc(ncc1F)Cl	C02384133	-16.12	-1.04	-16.96	2.62	-0.74
1154	COCOc1ccccc1	C03163258	-16.12	0	-16.22	3.09	-2.99
1155	c1cc(c(cc1C#N)O)F	C12471672	-16.12	-1.6	-17.91	4.92	-1.53
1156	CSCc1ccccc1	C13218299	-16.12	-0.66	-16.14	4.23	-3.54
1157	c1ccc2c(c1)[nH]c([nH+])2)N	C16889973	-16.12	-4.06	-15.66	6.53	-2.92
1158	CNN=Cc1ccccc1	C17021523	-16.12	0.18	-16.33	3.2	-3.17
1159	c1cc(ccc1/C=C/C#N)N	C19075641	-16.12	-2.88	-15.3	5.1	-3.04
1160	Cc1ccc(cn1)F	C02384095	-16.11	-1.63	-16.38	2.96	-1.05
1161	C=Cn1c(nnn1)[O-]	C03844473	-16.11	-2.97	-17.65	4.06	0.45
1162	c1c(snn1)Cl	C04090397	-16.11	-1.15	-16.51	2.63	-1.08
1163	CO/N=C(/c1c(non1)N)N	C04729052	-16.11	-2.24	-17.48	3.08	0.53
1164	c1cnc(c1)/N=N/O	C05159622	-16.11	-0.92	-19.54	5.83	-1.48
1165	COC(=O)Cc1ccncc1	C08294949	-16.11	-0.57	-19.04	6.57	-3.07
1166	c1c(cnc(c1N)F)Br	C08698195	-16.11	-1.55	-16.78	3.16	-0.94

1167	c1cc(c(c(c1F))N	C26892772	-16.11	-3.16	-13.77	3.52	-2.7
1168	c1cc(c(c(c1N)Br)F)F	C31829582	-16.11	-3.29	-15.6	5.12	-2.34
1169	Cc1cccc(c1)N	C03861040	-16.1	-3.29	-12.65	2.07	-2.22
1170	c1c(con1)Br	C04235230	-16.1	-0.65	-16.31	2.71	-1.85
1171	CCSC(=N-)C(F)(F)F	C04620656	-16.1	-2.79	-13.88	2.04	-1.47
1172	c1cc(c(nc1)N)F	C19616068	-16.1	-1.56	-16.95	3.72	-1.31
1173	c1c(ncn1)C=O	C00154066	-16.09	-2.56	-18.01	6.18	-1.7
1174	c1ccnc(c1)Cl	C00404334	-16.09	-0.59	-16.86	3.78	-2.42
1175	CCOC1cccs1	C01586926	-16.09	-1.61	-16.3	2.33	-0.52
1176	CO(=O)Cc1cccc1N	C02540630	-16.09	-1.64	-17.64	6.13	-2.93
1177	c1c(c(n[nH]1)C(=O)Cl)Cl	C05941977	-16.09	1.01	-18.95	3.34	-1.49
1178	c1cncc2c1[nH+]c[nH]2	C15042100	-16.09	-4.33	-16.92	7.09	-1.92
1179	CO(=O)c1cn[nH]n1	C16052238	-16.09	-2.74	-18.07	4.85	-0.14
1180	c1cc(cc(c1)F)CC#N	C16159619	-16.09	-1.43	-15.87	6.09	-4.88
1181	c1cnn(c1N)C(=O)N	C01659964	-16.08	-3.54	-18.98	5.21	1.23
1182	c1cnoc1C(F)(F)F	C02568253	-16.08	-1.91	-14.77	2.9	-2.31
1183	c1c(nc[nH]1)C(F)(F)F	C08698428	-16.08	-4.96	-15.53	6.85	-2.43
1184	Cc1cc(on1)CBr	C12370186	-16.08	-1.65	-15.43	4.13	-3.13
1185	CO(=O)CNC1cccc1	C21799249	-16.08	-2.86	-15.97	5.84	-3.09
1186	c1cc2c(cc1O)non2	C00161315	-16.07	-3.05	-17.98	5.2	-0.25
1187	Cc1ccc(cc1F)N	C00164593	-16.07	-2.26	-14.34	2.78	-2.25
1188	C(CBr)OC(=O)Cl	C02242592	-16.07	-0.21	-16.05	2.89	-2.7
1189	c1cnccc1F	C02525804	-16.07	-1.35	-15.17	2.56	-2.11
1190	c1cc(ccc1N)SC(F)F	C02572376	-16.07	-0.56	-16.48	3.7	-2.73
1191	c1c(nc[nH]1)Br	C08294972	-16.07	-4.48	-15.26	5.77	-2.09
1192	CO(=O)c1c(cccn1)N	C14982149	-16.07	-3.51	-17.34	6	-1.21
1193	C=CCOC(=O)C(F)(F)Br	C16082658	-16.07	-0.86	-13.05	1.39	-3.55
1194	c1c(ccc1Cl)O	C00164486	-16.06	-0.8	-17.93	2.97	-0.3
1195	c1ccc2c(c1)[nH](c2)NC#N	C00394716	-16.06	-8.02	-6.78	4.92	-6.18
1196	c1cc(c(nc1)F)Br	C02526710	-16.06	-0.44	-17.76	4.58	-2.44
1197	C1CCC(=CC1)CC#N	C03860303	-16.06	-1.47	-14.71	4.48	-4.36
1198	CCOC(=O)/C=Cl	C04975987	-16.06	-0.46	-15.53	3.45	-3.52
1199	c1c(sc(n1)NN=O)[N+](=O)[O-]	C06524518	-16.06	-3.05	-18.82	4.64	1.16
1200	c1cc2c(cc1F)nc(o2)N	C08614802	-16.06	-4.06	-15.25	3.27	-0.03
1201	c1cc(c(cc1O)N)F	C11919363	-16.06	-2.66	-17.13	3.34	0.39
1202	c1cncc(c1)/C(=N/O)N	C12505254	-16.06	-4.11	-17.5	5.21	0.34
1203	c1c2c([nH](c2)NO)ncn1	C17174545	-16.06	-8.27	-16.56	9.86	-1.09
1204	c1[nH]nc(n1)N[N+](=O)[O-]	C18082053	-16.06	-5.22	-17.99	10.45	-3.31
1205	C[NH2+]NCC1cccc1	C19167414	-16.06	-1.76	-14.72	2.46	-2.04
1206	c1cc2c(cc1F)[nH]cn2	C32497100	-16.06	-4.32	-14.89	6.44	-3.29
1207	CN(c1cnns1)N	C32911288	-16.06	-3.87	-18.45	6.29	-0.04
1208	c1cc(cc(c1Cl)F)NN	C01494959	-16.05	-0.42	-16.19	2.48	-1.92
1209	c1cc(nnc1N)Br	C02382954	-16.05	-4.17	-16.92	5.75	-0.72
1210	c1cc(sc1CC)Cl	C02539266	-16.05	-2.07	-11.87	2.04	-4.15
1211	CC1=CCCC(=O)O1	C04529437	-16.05	-1.32	-16.4	4.98	-3.31
1212	C=CCn1nc(n1)N	C17105010	-16.05	-3.48	-16.86	6.48	-2.18
1213	c1cc(cc(c1F)N)Sc2[nH]ncn2	C19869340	-16.05	-3.4	-15.9	6.12	-2.87
1214	c1c(c(ncn1)Cl)Cl	C22009763	-16.05	-1.22	-14.66	2.43	-2.6
1215	c1(c(c(c(c1F)Br)F)F)F	L2009A003	-16.05	0.44	-12.88	0.43	-4.04
1216	c1cc(c(cc1N)Cl)N	C00388453	-16.04	-3.32	-14.51	2.39	-0.6
1217	Cc1ccc2c(c1)[nH]n2	C00406978	-16.04	-5.43	-13.86	5.04	-1.79
1218	c1c(nc(s1)N)C(F)(F)F	C00967258	-16.04	-3.23	-16.18	4.67	-1.31
1219	c1c(cnc(n1)NN)C#N	C01391058	-16.04	-1.6	-18.04	5.33	-1.73
1220	c1cc(sc1)/C=C/C(=O)Cl	C02379211	-16.04	-1.54	-17.1	3.3	-0.69
1221	CNc1ccc(cc1)N	C04262606	-16.04	-2.91	-14.64	2.44	-0.94
1222	C(=O)(C(=O)C(F)(F)C(F)(F)F)	C04265862	-16.04	0.68	-15.69	1.02	-2.05
1223	C=C/N=N/Nc1cccc1	C17109761	-16.04	1.14	-17.53	3.46	-3.11
1224	c1cc(ncc1Cl)F	C01596028	-16.03	-0.73	-17.51	2.86	-0.64
1225	c1cc(ncc1[N+](=O)[O-])F	C01628309	-16.03	-2.09	-16.9	4.13	-1.18
1226	C[C@H](c1cccc1F)O	C02560496	-16.03	-1.02	-16.23	3.38	-2.15
1227	C[C@H](c1ccccc1)O	C06037199	-16.03	-1.23	-15.71	2.22	-1.32
1228	C=Cc1cn[nH]1	C13284960	-16.03	-5.05	-14.25	5.86	-2.59
1229	c1cnccc1C(=O)N=[N+]=[N-]	C15784784	-16.03	1.2	-21.8	3.67	0.9
1230	c1cncc(c1CC)N	C21985286	-16.03	-2.04	-17.48	4.84	-1.36
1231	c1ccc(cc1)NC(=S)C#N	C00155222	-16.02	-3.43	-14.49	5.63	-3.73
1232	c1cc(c(cc1Cl)O)Cl	C00388512	-16.02	-2.57	-13.73	2.31	-2.02
1233	COc1cccc1	C02242715	-16.02	-1.03	-15.92	3.18	-2.24
1234	C[C@H](c1cccn1)O	C02383113	-16.02	-1.69	-17.4	3.84	-0.76
1235	CO(=O)C(=C(F)F)F	C02555202	-16.02	-1.21	-14.65	2.04	-2.2
1236	CC(=O)/C=C/c1cccn1	C15838226	-16.02	-2.57	-15.83	5.8	-3.42
1237	c1cc(ccc1CC#N)O	C00164447	-16.01	-1.62	-19.76	7.43	-2.06
1238	c1c(cc(nc1F)F)F	C02585568	-16.01	-0.12	-16.31	2.46	-2.03
1239	c1(nnc(s1)NN)N	C17173590	-16.01	-4.29	-16.58	4	0.85
1240	c1nc(c2c(n1)sn2)N	C01674122	-16	-3.33	-17.14	4.64	-0.16
1241	c1ccc(cc1)/C=C/[N+](=O)[O-]	C01700197	-16	-0.22	-15.58	4.78	-4.97
1242	[C@@H](C(=O)Br)C(F)(F)F	C02524526	-16	-0.33	-15.69	2.39	-2.37
1243	c1cncc(cc1F)Cl	C02525818	-16	-0.58	-15.62	2.68	-2.47
1244	c1cc(c(c1F)CC#N)F	C04290230	-16	-0.04	-18.29	6.05	-3.72
1245	c1c(ncn1[N+](=O)[O-])[N+](=O)[O-]	C05323064	-16	-2.64	-14.67	5.68	-4.37
1246	c1[nH]nc(n1)Cl	C05380440	-16	-2.34	-15.25	3.31	-1.73
1247	c1c(cn1)CC(F)F	C12397692	-16	-2.51	-17.09	4.4	-0.81
1248	c1c(ncs1)CBr	C20358139	-16	-1.19	-16.07	3.49	-2.23
1249	c1cc(cc(c1Cl)N)Br	C02567820	-15.99	-3.37	-11.47	1.5	-2.65
1250	c1cn(nc1N)CC(F)F	C12395178	-15.99	-2.35	-17.3	5.21	-1.54
1251	c1cc(nc(c1[N+](=O)[O-])N)Cl	C18996093	-15.99	-3.11	-14.39	3.79	-2.27
1252	C1C2c(n[nH]c2C#N)C1	C24408467	-15.99	-2.35	-15.92	4.65	-2.38
1253	(C(=C(F)F)OC(F)F)F	C04290222	-15.99	-0.25	-14.6	0.66	-1.59
1254	c1ccc2c(c1)nsn2	C00151237	-15.98	-2.33	-16.48	4.69	-1.86
1255	c1cnccc1CC#N	C00409321	-15.98	-1.17	-19.5	7.5	-2.82
1256	c1cnc([nH]1)[N+](=O)[O-]	C01481980	-15.98	-3.75	-17.29	8.8	-3.74

1257	c1cc(oc1)[N+](=O)[O-]	C01689931	-15.98	-2.71	-17.76	6.78	-2.29
1258	c1c2c(nc(n1)N)CCC2	C18531251	-15.98	-5.25	-15.42	7.88	-3.19
1259	c1ccc(c(c1)CO)F	C00164568	-15.97	0.22	-17.86	3.13	-1.46
1260	COc1ccsc1	C00389817	-15.97	-1.76	-14.72	2.63	-2.13
1261	C=CC(=O)OCC#C	C01766085	-15.97	-0.42	-17.05	4.71	-3.21
1262	c1ccc(c(c1)N)[N+](=O)[O-]	C03860642	-15.97	-1.92	-17.41	5.79	-2.42
1263	C=CCOn1ccnc1	C04002507	-15.97	-1.5	-15.25	4.24	-3.46
1264	c1c(c(ncn1)N)[N+](=O)[O-]	C04114388	-15.97	-2.29	-18.54	4	0.87
1265	c1cn2c(n1)NCC2	C11920166	-15.97	-2.85	-16.94	6.59	-2.78
1266	c1cc(ccc1OCCO)F	C15014797	-15.97	-3.56	-15.99	4.66	-1.08
1267	c1cn(cn1)C(=O)OCC#N	C21991421	-15.97	-3.74	-16.35	7.17	-3.04
1268	c1cc(c(cc1O)O)Cl	C00404336	-15.96	-1.32	-18.85	3.7	0.52
1269	c1c(ncnc1N)N	C00967323	-15.96	-3.77	-16.71	4.52	0
1270	c1cnn(c1)[N+](=O)[O-]	C02146824	-15.96	-2.49	-18.07	6.52	-1.92
1271	c1c(cc(c1F)N)F	C02243351	-15.96	-1.26	-17.96	2.93	0.34
1272	c1cc(c(cc1C#N)F)N	C02516094	-15.96	-0.58	-18.01	4.68	-2.04
1273	CCOOC(=O)N[N+](=O)[O-]	C04507511	-15.96	-4.94	-14.52	2.96	0.53
1274	c1cc(ccc1NN=O)[N+](=O)[O-]	C08656046	-15.96	-3.52	-16.19	6.09	-2.34
1275	c1cnc2c1np[nH]2	C08667498	-15.96	-3.72	-16.16	3.82	0.11
1276	C#Cc1cnc(cn1)Br	C30678103	-15.96	-0.86	-17.87	4.88	-2.11
1277	c1cc(sc1)C(=O)c2[nH]ccn2	C00146169	-15.95	0.47	-19.72	6.57	-3.27
1278	c1c(cnc1)Cl	C02510623	-15.95	-1.2	-15.52	2.77	-2
1279	CC1=CSCC(=O)N1	C03846685	-15.95	-2.25	-16.64	4.35	-1.41
1280	c1cc(cc(c1)F)CS	C04244654	-15.95	-1.63	-15.9	2.5	-0.92
1281	c1c(cn(n1)N)[N+](=O)[O-]	C04294111	-15.95	-3.18	-18.71	6.78	-0.84
1282	c1cc(c(c1)N)C(F)(F)F	C19735913	-15.95	-2.37	-15.11	3.47	-1.94
1283	c1c(ncs1)CS	C31890176	-15.95	-1.99	-15.77	3.7	-1.9
1284	COC(=O)C=C(F)C(F)(F)F	C02031428	-15.94	-0.91	-14.42	2.35	-2.95
1285	CC1=CC(=O)CCC1	C03860608	-15.94	-0.69	-15.25	3.34	-3.34
1286	C(=O)C(F)C(F)Cl	C04329286	-15.94	-0.14	-14.76	0.52	-1.55
1287	C1CCC(=CC1)/C=C/C#N	C05103577	-15.94	-0.13	-17.36	3.68	-2.13
1288	c1c(c(ncn1)N)C(=S)N	C05580303	-15.94	-2.98	-15.53	3.13	-0.56
1289	c1cc(ncc1NN=O)Cl	C06536611	-15.94	-4.51	-17.11	4.37	1.32
1290	c1c(cnc1Br)N=C=O	C12370808	-15.94	-1.12	-15.68	1.82	-0.95
1291	c1nncn1N[N+](=O)[O-]	C15767158	-15.94	-1.01	-18.76	6.77	-2.94
1292	COC(=O)CNC(=O)N1ccnc1	C26189414	-15.94	-5.31	-15.13	7.09	-2.6
1293	c1c(c2cncnc2[nH]1)Cl	C33359058	-15.94	-4.63	-14.38	6.15	-3.08
1294	c1cc(ccc1C=N/O)F	C00153662	-15.93	-1.29	-18.33	5.52	-1.82
1295	c1cc(ccc1CON)F	C00168568	-15.93	0.93	-18.33	3.28	-1.8
1296	Cc1ccc(c(c1)F)N	C00389592	-15.93	-0.44	-15.76	2.54	-2.27
1297	c1cc([nH]c1)C(=O)Cl	C01683282	-15.93	-2.57	-16.05	4.7	-2.01
1298	C#CC(=O)c1cccc1	C01725590	-15.93	0.01	-18.27	6.43	-4.1
1299	C#Cc1cccn1	C02390334	-15.93	-0.71	-17.73	5.41	-2.91
1300	Cc1ccc(nc1)F	C04255973	-15.93	-1.73	-15.89	4.18	-2.49
1301	c1c(cnc(c1N)N)Cl	C18995692	-15.93	-5.72	-13.69	3.5	-0.02
1302	c1cc(ncc1[N+](=O)[O-])Br	C00331610	-15.92	-2.35	-14.24	3.69	-3.02
1303	c1cc(c(cc1F)Cl)O	C00388394	-15.92	0.29	-17.35	2.81	-1.68
1304	Cc1ccc(cc1)O	C00897142	-15.92	-1.57	-15.48	2.8	-1.66
1305	C(#N)/C=C(C#N)F	C01606792	-15.92	-0.19	-14.73	2.96	-3.95
1306	C/C=C/Cc1ccc(cc1)O	C01866906	-15.92	-0.8	-17.69	2.73	-0.15
1307	COC(=O)Nc1ccc(cc1)N	C02243618	-15.92	-0.49	-22.79	5.92	1.44
1308	c1ccc(cc1)CNC(=O)O	C11535717	-15.92	-1.23	-21.88	5.2	1.98
1309	c1cc(c(cc1Cl)N)N	C00388066	-15.91	-4.71	-13.31	2.74	-0.62
1310	CC(=O)SCC=C	C01611273	-15.91	-0.48	-15.25	2.68	-2.86
1311	c1cc(cnc1)CN=C=S	C02528215	-15.91	-0.45	-16.51	3.63	-2.58
1312	c1[nH]c(c(n1)N)[N+](=O)[O-]	C12957904	-15.91	-3.51	-17.84	7.66	-2.22
1313	C(=[NH+])N(N)N)/C(=[NH+])N)/N	C13856292	-15.91	-4.69	-17.4	3.38	2.79
1314	c12c([nH]c(=O)[nH]1)non2	C16382880	-15.91	-7.87	-18.35	8.49	1.81
1315	c1c(cnc(c1[O-])F)Cl	C21981949	-15.91	-1.36	-18.11	3.85	-0.29
1316	c1ccc(cc1)CSC(F)F	C32627719	-15.91	-2.66	-10.69	2.61	-5.17
1317	Cc1ccc(nc1)Cl	C00152326	-15.9	-0.82	-15.52	3.39	-2.94
1318	c1ccc(c(c1)O)F	C00164476	-15.9	-2.53	-15.93	3.9	-1.34
1319	c1cc2c(noc2nc1)N	C00168472	-15.9	-3.86	-18.85	6.54	0.26
1320	c1csc(n1)NN=O	C06585052	-15.9	-1.97	-18.24	5.09	-0.77
1321	c1cnc(nc1)CCl	C11887620	-15.9	-0.17	-17.87	4.56	-2.43
1322	c1c(nc(n1)N)C(F)(F)F	C21994014	-15.9	-0.28	-19.04	4.79	-1.37
1323	c1ccc(cc1)CNC(=O)N	C00157440	-15.89	0.07	-21.92	6.38	-0.42
1324	CC(=O)n1ccnc1	C00388370	-15.89	-2.95	-17.39	6.99	-2.54
1325	C#CCOc1c(c(nc(c1F)F)F)F	C02483190	-15.89	0.14	-15.5	2.74	-3.27
1326	c1cc(c(c(c1)F)Cl)N	C02513560	-15.89	-2.68	-16.65	3.29	0.16
1327	Cc1cnn(c1)CCl	C02536482	-15.89	-2.02	-15.32	4.37	-2.91
1328	c1cn(cn1)CCCl	C02569851	-15.89	-0.77	-15.77	4.58	-3.93
1329	c1cc(cc(c1)Br)N	C03861310	-15.89	-1.41	-14.29	2.08	-2.27
1330	c1c(ncs1)Br	C04198774	-15.89	-2.1	-15.61	3.5	-1.67
1331	Cc1cc(on1)CCl	C04218850	-15.89	-1.67	-15.55	4.36	-3.03
1332	Cc1ccc(cn1)C#N	C00166514	-15.88	0.12	-17.59	4.46	-2.86
1333	CCOc1cccn1	C00331682	-15.88	-1.9	-15.81	3.6	-1.77
1334	C1CC=C(C1)CC#N	C02242643	-15.88	-1.38	-15.12	4.58	-3.96
1335	CSc1nc(sn1)[S-]	C02569840	-15.88	-2.61	-15.57	4	-1.72
1336	CC(=O)N/C(=N/C#N)N	C05430946	-15.88	-5.09	-16.32	5.52	0
1337	[H]N=C(N)/N/C(=N)c1cccn1)/N	C12524107	-15.88	-1.36	-20.51	9.88	-3.88
1338	c1ccc(c(c1)O)O	C13512214	-15.88	-3.35	-16.58	3.77	0.28
1339	c1cnc(c(c1F)F)F	C14983673	-15.88	-2.01	-16.27	4.51	-2.11
1340	c1cc(cnc1)NN	C19737047	-15.88	-2.34	-18.42	5.17	-0.29
1341	CNc1cccn1	C25494514	-15.88	-2.9	-15.65	4.43	-1.76
1342	c1cc(c(cc1N)F)Br	C00338968	-15.87	0.35	-17.2	3.22	-2.25
1343	c1ccc(cc1)C=O	C00895145	-15.87	-1.66	-16.04	4.98	-3.14
1344	CCc1nnc(n1)N	C02023573	-15.87	-1.42	-16.81	4.13	-1.77
1345	Cc1cnn(c1)[N+](=O)[O-]	C02390474	-15.87	-2.75	-17.19	5.83	-1.77
1346	c1c(c(c(c(n1)N)F)C(F)(F)F)F	C02513195	-15.87	-0.66	-16.48	3.13	-1.86

1347	c1cc(c(c1F)F)NBr	C02513894	-15.87	-2.91	-15.33	2.41	-0.04
1348	c1cc(c(c1F)Br)O	C02524482	-15.87	-1.6	-16.62	4.1	-1.76
1349	Cc1cnccc1Cl	C02578098	-15.87	-1.86	-13.45	2.29	-2.85
1350	c1cnc(c(c1Cl)Cl)F	C14982615	-15.87	-2.85	-13.92	3.61	-2.71
1351	CCOC(=O)C=CCF	C17285154	-15.87	-0.73	-15.12	3.39	-3.41
1352	c1cc(sc1)CC=O	C19729366	-15.87	-2.5	-15.27	4.94	-3.05
1353	c1cc(cnc1)Nc2ncccn2	C21995867	-15.87	0.69	-18.55	6.21	-4.22
1354	c1c2c(cnn1)n[nH]n2	C26506608	-15.87	-5.94	-17.83	6.99	0.9
1355	c1ccc(cc1)NCC#N	C01683664	-15.86	-3.44	-14.27	4.8	-2.95
1356	CC(=S)Nc1ccc(cc1)F	C09086570	-15.86	-1.57	-17.01	6.64	-3.92
1357	c1cnccc1NN	C11919487	-15.86	-1.82	-17.73	3.94	-0.25
1358	c1cc(ccc1C#N)N	C00152697	-15.85	0.22	-18.73	4.62	-1.97
1359	c1cc(c(c1F)C#N)N	C00153053	-15.85	-2	-17.52	5.69	-2.02
1360	c1cc(c(cc1F)O)Br	C00389860	-15.85	-1.06	-17.76	2.48	0.5
1361	Cc1cnccn1	C01661081	-15.85	-1.92	-16.57	3.81	-1.16
1362	c1cc(ccc1C(=O)Cl)F[N+](=O)[O-]	C02243158	-15.85	-3.35	-15.64	4.98	-1.84
1363	c1csccl1CBr	C02513314	-15.85	-1.23	-16.45	1.81	0.02
1364	c1c(ncs1)CCl	C02566814	-15.85	-1.21	-16.26	3.74	-2.11
1365	c1c(ncnc1Cl)[N+](=O)[O-]	C02599046	-15.85	-1.06	-14.9	3.05	-2.93
1366	c1ccnc(c1)OCC#N	C02703484	-15.85	-1.43	-18.06	5.28	-1.64
1367	C=CCNC(=O)C(F)(F)F	C03100061	-15.85	-0.84	-16.94	3.25	-1.32
1368	c1(c(nc2c(n1)non2)Cl)N	C03121914	-15.85	-6.8	-15.82	5.55	1.21
1369	C(CO[N+](=O)[O-])CO[N+](=O)[O-]	C04743754	-15.85	-0.49	-14.4	3.52	-4.48
1370	c1c(ncnc1)BrBr	C15022219	-15.85	-1.73	-14.61	2.16	-1.67
1371	c1ccc(c(c1)Cl)Cl	M2007001_	-15.85	-1.77	-12.36	2.32	-4.05
1372	COc(=O)C(=O)Cl	C02242601	-15.84	-1.57	-14.67	2.19	-1.8
1373	c1cc(c(cc1O)F)N	C02555149	-15.84	-2.85	-17.07	3.67	0.41
1374	c1cc2cn[nH]c2cc1Cl	C04878475	-15.84	0.08	-16.78	3.62	-2.76
1375	c1nc([nH]n1)N=C(C(F)(F)F)[O-]	C05510755	-15.84	0.93	-20.59	5.8	-1.97
1376	c1cc(cnc1)/C=C/[N+](=O)[O-]	C13227015	-15.84	-0.35	-18.04	6.19	-3.64
1377	CSc1ccc(cc1)C(F)(F)F	C19615578	-15.84	-0.07	-13.16	2.31	-4.91
1378	Cc1ccc(c(c1)O)N	C00388270	-15.83	-3.45	-15.29	3.03	-0.13
1379	c1ccc(cc1)CCN=C=O	C02384722	-15.83	-0.37	-15.85	2.42	-2.03
1380	c1[nH](cnn1)[S-]	C04084758	-15.83	-3.26	-14.92	3.67	-1.32
1381	C(#N)C(C(=C(F)F)F)F	C16082619	-15.83	0.25	-14.98	1.47	-2.57
1382	Cc1ccc(c1N)F	C16158148	-15.83	-3.15	-12.86	2.59	-2.41
1383	c1c(c(nc1)N)Cl	C31176453	-15.83	-1.53	-16.58	4.23	-1.94
1384	c1ccc2c(c1)[nH]cn2	C00331902	-15.82	-3.19	-15.76	6.36	-3.23
1385	c1ccn(c1)N	C02169662	-15.82	-2.43	-14.43	2.72	-1.68
1386	C1(=NSC(=NS1)Cl)Cl	C04887163	-15.82	-1	-17.09	1.06	1.22
1387	c1c(scn1)[N+](=O)[O-]	C12471766	-15.82	-1.99	-17.75	5.85	-1.94
1388	c1c(cnc1F)NNCl	C16158741	-15.82	-2.93	-14.25	2.75	-1.39
1389	c1c(c(nc1)F)F	C30718802	-15.82	-1.08	-16.29	3.04	-1.49
1390	c1ccc(cc1)NCC#N	G2008A001	-15.82	-3.62	-14.04	4.8	-2.95
1391	c1cc(c(nc1)F)[N+](=O)[O-]	C02383998	-15.81	-3.87	-17.74	8.32	-2.52
1392	c1cc(c(c1)F)C=O	C02539337	-15.81	-2.58	-16	5.99	-3.21
1393	c1ccc(nc1)FCl	C02598988	-15.81	-2.74	-15.28	4.6	-2.39
1394	c1c(ncn1)[S-]Cl	C04228198	-15.81	-1.31	-15.34	2.65	-1.82
1395	Cc1csc(n1)N	C05438431	-15.81	-2.53	-15.29	3.45	-1.44
1396	c1ccc(cc1)N(N=O)O	C12358639	-15.81	-3.64	-13.46	3.47	-2.18
1397	[H]/N=C\1/C(=C(C#N)/N)/NC=N1	C13217433	-15.81	-6.77	-15.87	7.37	-0.54
1398	CCc1cnc(nc1)F	C22016529	-15.81	-1.67	-16.59	4.98	-2.52
1399	c1cc2c([nH]nc2Cl)nc1	C22054899	-15.81	-1.88	-16.9	5.07	-2.1
1400	c1ccc(nc1)NCl	C00331618	-15.8	-3.63	-15.73	4.25	-0.69
1401	c1nc([n-]n1)n2cnnc2	C01300688	-15.8	-4.91	-16.96	11.62	-5.54
1402	c1ccc(c(c1)/C(=N/O)/N)N	C04912395	-15.8	-4.08	-18.4	6.31	0.37
1403	c1c(cc(c1F)Cl)F	C16158244	-15.8	0.46	-18.03	3.39	-1.62
1404	c1cc(ncc1C#N)F	C19616136	-15.8	0.19	-18.48	4.76	-2.28
1405	c1c(cnc1)F[N+](=O)[O-]	C21981786	-15.8	0.21	-16.04	2.61	-2.58
1406	c1c(c[nH]c1C=O)Br	C00337448	-15.79	-1.83	-16.45	4.49	-2
1407	c1ccn2ccnc2c1	C00409233	-15.79	-2.27	-16.46	6.78	-3.84
1408	c1ccc(c1)CN=C=S	C02168970	-15.79	-0.24	-15.34	3.55	-3.76
1409	c1cc(ccc1[C@@H]2CO2)F	C02584571	-15.79	-2.43	-14.54	3.89	-2.72
1410	c1ccc(nc1)F	C02599022	-15.79	-0.67	-16.12	3.07	-2.07
1411	COc(=O)Nc1cccc1F	C06126171	-15.79	-0.43	-17.89	4.73	-2.21
1412	Cc1ccc(nc1)NN=O	C13212916	-15.79	-4.73	-15.8	6.55	-1.81
1413	CCOC(=O)n1c(ncn1)N	C16980639	-15.79	-2.01	-16.78	5.96	-2.95
1414	Oc1cccc(Cl)c1	W2002A002	-15.79	-1.02	-15.91	2.74	-1.61
1415	C(c1nc(s1)Cl)Cl	C01574839	-15.78	-0.68	-15.43	2.29	-1.96
1416	COc(=O)CNC(=O)C(F)(F)F	C01726312	-15.78	-1.83	-17.26	4.27	-0.96
1417	Cc1cnc(c1)N	C01757519	-15.78	-3.63	-16.17	4.26	-0.25
1418	COc1cccnc1	C05329533	-15.78	-0.86	-17.54	4.3	-1.66
1419	Cc1ccc(c1)N	C08294948	-15.78	-2.57	-15.99	3.68	-0.89
1420	C[C@H](c1ccc(cc1)F)O	C12506430	-15.78	-1.22	-15.58	3.21	-2.19
1421	c1cnc(c(c1)F)F	C14982368	-15.78	-1.45	-16.22	4.2	-2.3
1422	C(=C([N+](=O)[O-])[N+](=O)[O-])N)NN	C19333183	-15.78	-5.7	-18.71	9.88	-1.26
1423	c1c(nc(c1)Br)C=O	C30678070	-15.78	-4.38	-15.54	3.85	0.29
1424	COc1cccc1	M1995A024	-15.78	-2.03	-13.4	2.53	-2.89
1425	c1ccc2c(c1)OCO2	C00164507	-15.77	-1.63	-16.28	4.36	-2.23
1426	c1cc(sc1C=O)Cl	C00165421	-15.77	-1	-16.84	4.94	-2.87
1427	c1c(cnc1)NCl	C00166669	-15.77	-4.08	-13.17	2.77	-1.28
1428	c1ccc(cc1)Oc2c(non2)N	C01295948	-15.77	-0.39	-19.99	5.91	-1.3
1429	CCOC(=O)[C@H](F)Cl	C02168354	-15.77	-0.63	-15.71	3.49	-2.91
1430	c1c([nH]nc1O)C(F)(F)F	C03073602	-15.77	-2.99	-18.61	4.55	1.28
1431	c1(nc(s1)N)N	C03896990	-15.77	-5.77	-15.57	5.58	-0.01
1432	c1cc(sc1C(F)F)F	C05769898	-15.77	-2.81	-15.61	2.97	-0.31
1433	C=C(C(=O)Cl)C(F)(F)F	C21982551	-15.77	-1.65	-15.22	3.58	-2.48
1434	c1cc(c(c1)F)O	C26896238	-15.77	-1.8	-14.59	2.87	-2.24
1435	Cc1ccc(o1)C#N	C00403421	-15.76	-0.43	-16.58	4.11	-2.86
1436	c1c(ncn1)N	C01593931	-15.76	-4.47	-15.18	4.25	-0.35

1437	Cc1ccc1	C01666987	-15.76	-1.4	-14.45	2.55	-2.46
1438	Cc1ccc(cc1F)NN	C02243288	-15.76	-1.26	-15.59	3.09	-2
1439	C1C[C@H]2[C@H](CCC2=C1)O	C02519601	-15.76	-0.71	-15.87	2.88	-2.05
1440	c1cc(ncc1F)Br	C02559898	-15.76	-1.04	-17.06	2.57	-0.23
1441	c1c(ncnc1F)N	C03098198	-15.76	-3.26	-15.91	4.22	-0.82
1442	c1c(c(c(n1)F)C=O)F	C04208906	-15.76	-1.79	-16.67	4.63	-1.93
1443	C=C(CSC(=[NH2+])N)Cl	C05606573	-15.76	-2.06	-14.94	2.54	-1.31
1444	c1c(c(nc(nH+1)N)N)O	C13829353	-15.76	-4.22	-18.11	4.99	1.59
1445	c1c(noc1C(F)F)C(F)F	C16125565	-15.76	-0.66	-13.93	2	-3.16
1446	c1cc(c(cc1O)F)Cl	C00409351	-15.75	-0.54	-16.97	3.34	-1.57
1447	C#Cc1ccc(c1)O	C02149788	-15.75	-0.86	-16.94	4.14	-2.1
1448	Cc1cnsc1	C02563976	-15.75	-1.82	-15.3	3.21	-1.83
1449	c1c(c(c(c1F)F)C(=O)Cl)F	C02585572	-15.75	0.06	-15.68	2.93	-3.05
1450	CCOn1ccnc1	C04023723	-15.75	-1.3	-15.75	4.33	-3.03
1451	c1cc(cc(c1)F)OCC(=O)Cl	C09245895	-15.75	-3.06	-13.15	4.74	-4.27
1452	c1cc(oc1)CNC(=S)NN	C13685440	-15.75	0.03	-18.69	3.8	-0.89
1453	c1cc2cn[nH]c2cc1F	C14984745	-15.75	-0.43	-16.92	4.01	-2.42
1454	C/C(=C)C([N+](=O)[O-])	C16968746	-15.75	-1.4	-16.22	5.46	-3.61
1455	C/[NH+]=C/c1ccccc1	C18101893	-15.75	-1.43	-14.48	2.86	-2.69
1456	c1cc(oc1C)Br	C20077988	-15.75	-1.3	-13.86	2.92	-3.51
1457	c1cc(nc(c1)F)CCl	C21985780	-15.75	-0.35	-17.52	5.14	-3.02
1458	c1csc(n1)CCl	C22861495	-15.75	-0.27	-16.63	3.53	-2.38
1459	COc1ccc(c1)F	C00388393	-15.74	-0.19	-15.22	2.59	-2.92
1460	c1cc(cc(c1)Cl)O	C00404329	-15.74	-1.06	-15.82	2.75	-1.6
1461	c1c(cnc1F)O	C02384047	-15.74	-3.36	-15.92	3.09	0.45
1462	c1cc(c(nc1)Cl)F	C02384113	-15.74	-2.45	-15.25	4.4	-2.44
1463	c1c[nH+]ccc1/C(=N/O)/N	C13130175	-15.74	-4.39	-19.06	7.2	0.5
1464	CC(=O)OCc1ccncc1	C13232422	-15.74	-1.11	-17.13	5.83	-3.33
1465	c1cc(oc1)C(=O)Nc2[n-]nnn2	C13306638	-15.74	-1.4	-19.41	6.96	-1.9
1466	c1cc(=O)occ1[N+](=O)[O-]	C18810132	-15.74	-1.02	-17.48	5.99	-3.22
1467	c1cnn(c1)C(=S)N	C01393570	-15.73	-3.3	-17.82	7.17	-1.77
1468	c1c(cc(c1F)F)O	C02584330	-15.73	-4.15	-14.2	3.95	-1.32
1469	c1c(c(nc(n1)F)N)F	C03129093	-15.73	-3.46	-16.43	3.48	0.68
1470	C/C=C/n1ccccc1	C05480262	-15.73	-1.89	-14.2	2.52	-2.15
1471	CNC(=O)Nc1ccc(cc1F)F	C12762527	-15.73	-0.39	-18.76	5.2	-1.77
1472	COC(=O)C@H(C(=O)C(=O)OC)O	C14496485	-15.73	-2.47	-16.89	5.06	-1.42
1473	c1cc(ccc1NCC#N)F	C20051929	-15.73	-2.54	-16.53	6.36	-3.03
1474	c1cc(cc(c1F)F)NC(=[NH2+])N	C20857747	-15.73	0.35	-21.12	7.3	-2.26
1475	CC(=O)Oc1ccc(c(c1F)F)F	C21986553	-15.73	1.35	-20.12	7.5	-4.46
1476	c1c(nc[nH]1)CC(F)F	C30714975	-15.73	-3.54	-15	5.7	-2.88
1477	c1cc2cn[nH]c2c(c1)N	C00112557	-15.72	-3.4	-15.83	4.31	-0.8
1478	CC(=O)OCc1ccc1	C00388413	-15.72	-0.33	-17.72	5.63	-3.3
1479	CSC(=[NH2+])NCC=C	C04276941	-15.72	-1.21	-14.94	2.43	-2.01
1480	c1cc(sc1)C(=O)N=C=O	C19408027	-15.72	1.28	-20.66	3.83	-0.18
1481	CCc1cnccn1	C04262348	-15.71	-1.41	-16.18	3.64	-1.77
1482	C(#N)NC#N	C05225679	-15.71	-5.48	-10.07	4.81	-4.97
1483	Cc1cc(sn1)Br	C15042087	-15.71	-0.3	-15.08	2.25	-2.59
1484	C=CC/C(=[NH+])N/N	C15937651	-15.71	-3.64	-14.93	3.16	-0.31
1485	c1ccc2c(c1)cc([nH]2)S	C18032180	-15.71	-1.17	-13.61	2.49	-3.41
1486	c1cc(cc(c1)O)N	C00157527	-15.7	-3.26	-16.34	3.42	0.46
1487	CCc1cc[nH]c1	C01561739	-15.7	-1.81	-15.7	2.45	-0.64
1488	c1cc(c(cc1CC#N)F)N	C02243166	-15.7	-2.37	-17.73	7.1	-2.7
1489	Cc1ccc(cc1F)C#N	C02526234	-15.7	-0.96	-15.92	3.9	-2.73
1490	CO/C=C/c1ccccc1	C02567999	-15.7	0.59	-17.77	3.01	-1.52
1491	c1cc(oc1)c2cc(no2)C=O	C05177628	-15.7	-0.03	-18.3	5.36	-2.74
1492	c1c(c([nH]1)N)N+([O-])[O-]	C08101022	-15.7	-5.42	-16.19	6.27	-0.37
1493	C/C(=C)C/COC	C16970512	-15.7	-1.23	-13.71	1.67	-2.44
1494	Cc1ccc(c(n1)N)N+([O-])[O-]	C19798352	-15.7	-2.53	-16.52	5.35	-2.01
1495	c1csc(n1)N=C=S	C20153799	-15.7	-0.44	-16.44	3.94	-2.76
1496	c1ccc(cc1)CON	C00155377	-15.69	1.53	-18.51	3.09	-1.8
1497	c1cnc(nc1[N+](=O)[O-])N	C01574113	-15.69	-3.43	-16.55	7.02	-2.73
1498	c1cc(cnc1)F	C01680674	-15.69	-1.8	-14.6	2.85	-2.13
1499	c1cc(oc1)C(=O)Cl	C01846582	-15.69	-2.35	-16.11	5.35	-2.58
1500	c1ccc(cc1)/C=N/O	C04528806	-15.69	-2.73	-16.44	5.1	-1.62
1501	CCc1ccccc1	C08294957	-15.69	-0.89	-13.85	2.85	-3.8
1502	c1c(cnc1N)N	C13230016	-15.69	-4.05	-16.86	4.09	1.13
1503	CNc1c(c[nH]1)N+([O-])[O-]	C04002765	-15.68	-3.23	-17.11	5.97	-1.31
1504	CCC(=O)CC(=O)C	C04877757	-15.68	-1.53	-15.33	3.56	-2.39
1505	c1c[nH]cc(c1=O)Br	C08698540	-15.68	-2.98	-15.82	3.51	-0.38
1506	c1ccc(cc1)[C@H](C#C)C(F)F	C15774485	-15.68	-0.73	-16.09	4.73	-3.6
1507	c1ccc1N=C=O	C19507274	-15.68	0.05	-18.07	2.96	-0.62
1508	c1cnc(cc1[N+](=O)[O-])N	C19851305	-15.68	-4.01	-15.75	5.67	-1.59
1509	c1cc2c(cc1N)CC2	C22013192	-15.68	-1.95	-14.71	3.66	-2.68
1510	c1ccc(cc1)NN=C(C#N)C#N	C00039770	-15.67	-1.88	-15.5	3.76	-2.05
1511	c1ccc2c(c1)cc(o2)C#N	C00122171	-15.67	-1.59	-16.26	4.37	-2.2
1512	c1cc(c(cc1F)F)O	C00164410	-15.67	-2.38	-15.26	3.28	-1.31
1513	c1cc(ncc1N)F	C00335086	-15.67	-3.11	-17.09	4.94	-0.42
1514	CCOc1cnsc1	C01391701	-15.67	-0.76	-17.2	3.34	-1.04
1515	c1c(cnc(n1)Cl)Br	C01529074	-15.67	0.84	-16.59	2.45	-2.38
1516	COC(=O)C(F)F	C02003941	-15.67	-1.48	-13.71	1.85	-2.33
1517	c1c(c(nc(c1F)N)N)F	C02529882	-15.67	-2.9	-17.15	2.8	1.58
1518	c1c[nH]nc1C(F)F	C04243565	-15.67	-1.3	-15.53	2.67	-1.51
1519	c1cnc(cc1F)Br	C14982262	-15.67	-0.69	-15.07	2.63	-2.54
1520	c1ccc(cc1)C(=O)N=[N+]=[N-]	C15784780	-15.67	2	-20.66	3.55	-0.57
1521	c1cnn(c1)C#N	C22016511	-15.67	-2.17	-14.55	5.22	-4.17
1522	c1c(cc(c1O)Cl)F	C00389677	-15.66	-0.54	-17.34	2.67	-0.44
1523	c1cc(ccc1C#N)N+([O-])[O-]	C01680884	-15.66	-1.78	-15.53	5.74	-4.09
1524	c1nc(c(c1)F)N	C01693119	-15.66	-4.81	-16.38	4.96	0.57
1525	c1ccc(cc1)CCN=C=S	C02022074	-15.66	-1.89	-16.06	1.77	0.52
1526	c1ccn2c(c1)[nH]c2=O	C02654018	-15.66	-4.92	-17.34	8.65	-2.05

1527	Cc1cc(sn1)Cl	C15042084	-15.66	-0.18	-15.18	2.17	-2.47
1528	c1(n[nH]c(=O)s1)N	C17173601	-15.66	-6.43	-14.78	4.22	1.33
1529	c1ccc(cc1N)N)O	C00388490	-15.65	-3.46	-17.7	3.54	1.96
1530	Cc1ccc(cc1)OCC=O	C02559106	-15.65	-0.52	-18.73	4.84	-1.24
1531	CC(=O)O/N=C/C(=O)C(=O)N)N	C04529889	-15.65	-1.19	-20.42	7.31	-1.36
1532	c1c2cn[nH]c2nc(n1)N	C13362452	-15.65	-3.3	-17.53	6.36	-1.17
1533	c1cnccc1CC=O	C13551730	-15.65	-2.96	-16.51	6.09	-2.27
1534	c1cc(=O)ccc1C(=O)Cl	C16124716	-15.65	0.55	-19.16	5.92	-2.96
1535	c1cc(ccc1N)I	C00013615	-15.64	-0.55	-14.41	1.93	-2.61
1536	c1c(c(c(c1Br)N)F)F	C00056705	-15.64	-3.29	-13.97	2.2	-0.58
1537	c1cc(cc(c1)F)N=C=S	C00167163	-15.64	-2.15	-12.16	2.69	-4.01
1538	c1csc(n1)Br	C01592420	-15.64	-1.8	-15.09	3.06	-1.8
1539	c1nc([nH]n1)SCC#N	C05373230	-15.64	-4.07	-17.55	5.86	0.12
1540	Cn1ccnc1N	C13354637	-15.64	-3.24	-15.66	5.55	-2.29
1541	c1cnc(cn1)/N=N/O	C16940934	-15.64	-1.75	-19.43	5.59	-0.05
1542	c1ccc(c(c1)/C=C/C(=O)F	C21304314	-15.64	-1.27	-15.62	5.42	-4.16
1543	c1c(c(cc(c1F)F)Br)O	C00389788	-15.63	-1.09	-17.22	2.69	0
1544	c1c(c(cc(c1N)F)F)N	C01598771	-15.63	-2.94	-15.68	3.22	-0.24
1545	c1ccc(c(c1)/C=C/[N+](=O)[O-])O	C01688684	-15.63	0.13	-21.48	6.19	-0.47
1546	Cc1nnc(s1)N	C08615005	-15.63	-3	-15.49	3.51	-0.65
1547	c1cc(ncc1C(F)F)NN=O	C13213559	-15.63	-0.66	-19.04	6.05	-1.98
1548	c1cncc2c1[nH]cc2N	C14985667	-15.63	-3.1	-16.78	4.79	-0.53
1549	C1(=C(C(C1=O)(F)F)F)F	C16159297	-15.63	-0.01	-14.79	1.38	-2.2
1550	c1ccc2c(c1)C=O	C21985379	-15.63	-0.67	-16.63	3.28	-1.6
1551	c1c(cnc2c1nc([nH]2)Cl)N	C00217087	-15.62	-3.94	-16.33	5.58	-0.93
1552	c1cc(cc(c1)O)N=C=S	C00336175	-15.62	-0.82	-19.91	3.89	1.22
1553	c1cc(c(c(c1C#N)F)F)F	C00389524	-15.62	-1.26	-16.73	5.93	-3.55
1554	CCOc1ccc(cc1)F	C00393902	-15.62	-1.93	-14.51	2.36	-1.54
1555	Cc1ccc(cc1O)N	C00394645	-15.62	-2.47	-16.27	3.31	-0.19
1556	Cc1cccc(c1)O	C00897141	-15.62	-1.58	-15.27	2.86	-1.63
1557	C(#N)c1c(non1)N	C01063089	-15.62	-4.43	-13.88	3.03	-0.34
1558	[H]/N=C1/CSC(=N1)N	C12359944	-15.62	-5.16	-15.57	5.21	-0.1
1559	c1ccc(cc1)OCCO	G2008A005	-15.62	-3.19	-16.19	4.81	-1.06
1560	Oc1ccc(F)cc1F	W2002A006	-15.62	-2.37	-15.23	3.28	-1.31
1561	c1cc2n(c1)CC=C2	C01570201	-15.61	-1.78	-17.35	4.07	-0.55
1562	c1c(cnc(c1)Br)O	C02566952	-15.61	-0.78	-17.39	2.93	-0.38
1563	c1cc(c(c(c1CS)F)F	C04244664	-15.61	-0.9	-16.85	3.6	-1.45
1564	c1c(ncs1)C(=O)Cl	C16124686	-15.61	-2.67	-16.28	4.88	-1.54
1565	c1c(cc(nc1F)Br)F	C21987574	-15.61	0.53	-15.69	2.1	-2.56
1566	CCc1cccc1	M1995A012	-15.61	-0.38	-14.6	2.41	-3.05
1567	c1cc(ccc1NN)Br	C00088596	-15.6	-1.88	-14.5	2.69	-1.91
1568	c1cc(oc1C(=O)N)Br	C01664804	-15.6	-3.34	-16.26	4.07	-0.07
1569	CC(=O)c1cnns1	C12650588	-15.6	-2.56	-16.85	5.03	-1.22
1570	c1cc(ccc1C=O)F)F	C00164803	-15.59	-3.23	-14.05	4.9	-3.21
1571	c1cc(ccc1O)cc2cnns2)F	C01388230	-15.59	-0.74	-17.4	3.58	-1.03
1572	CC/C=C/OCC=C	C01653150	-15.59	-0.85	-14.69	1.83	-1.87
1573	c1c(nns1)C(=O)Cl	C02513224	-15.59	-2.76	-15.98	4.16	-1
1574	CCNc1cnccn1	C21511135	-15.59	-0.5	-17.93	4.08	-1.23
1575	COc1cccc1	C00389547	-15.58	-1.75	-14.07	2.47	-2.23
1576	c1cc(nnc1[N+](=O)[O-])Cl	C00967197	-15.58	-1.61	-21.54	9.95	-2.38
1577	c1cc(ccc1[N+](=O)[O-])Cl	C03860273	-15.58	-1.5	-13.39	3.53	-4.22
1578	c1c(c(n[nH]1)N)Cl	C04244022	-15.58	-3.19	-16.09	3.95	-0.25
1579	C(=O)C(C(F)F)F)F)Cl	C05178388	-15.58	-0.1	-13.82	0.66	-2.33
1580	Cn1cncc1[N+](=O)[O-]	C08294935	-15.58	-1.74	-15.99	6.11	-3.96
1581	c1c(cncn1)C#N	C08698486	-15.58	0.75	-18.26	4.11	-2.18
1582	c1cncc1Br	C30677654	-15.58	-1.98	-15.72	3.98	-1.87
1583	CC(=O)Oc1ccnc1	C00388199	-15.57	-0.01	-18.72	6.19	-3.03
1584	c1ccc(cc1)CO	C00895302	-15.57	-0.96	-17.53	4.19	-1.27
1585	[H]/N=C(/c1cnccn1)\OC	C05320081	-15.57	-2.04	-20.29	5.23	1.53
1586	c1cnc(cn1)/C(=[NH+])N)N	C06244369	-15.57	-4.5	-19.97	4.87	4.02
1587	C(=O)C(C(F)F)F	C16159156	-15.57	-0.59	-14.03	1.09	-2.05
1588	c1cc(ccc1S)F)N	C20247140	-15.57	-1.07	-16.33	3.71	-1.88
1589	c1c(nc(c1Cl)F)Br	C21981946	-15.57	-1.15	-13.52	1.96	-2.86
1590	c1c(nc(nc1)Cl)N	C01101988	-15.56	-1.62	-17.65	3.89	-0.17
1591	c1ccc(cc1)/C=C/C=O	C01532777	-15.56	-3.28	-14.09	5.91	-4.1
1592	Cc1cnc(nc1F)F	C01582389	-15.56	-2.42	-16.11	4.87	-1.9
1593	Cc1cc(no1)C(=O)Cl	C02159744	-15.56	-1	-16.02	3.79	-2.34
1594	c1cc(ccc1C#N)N)Cl	C02566106	-15.56	-0.94	-15.49	3.37	-2.51
1595	c1cncc(c1[N+](=O)[O-])[O-]	C14982956	-15.56	-2.91	-17.22	5.65	-1.08
1596	c1cc(sc1)C=O	C00158751	-15.55	-1.35	-16.2	4.43	-2.43
1597	c1c(ccc1Br)N	C00331807	-15.55	-0.94	-16.57	2.92	-0.96
1598	C#Cc1ccc(cc1)[N+](=O)[O-]	C01433114	-15.55	-0.86	-14.8	4.84	-4.73
1599	c1cc(ccc1F)N+](=O)[O-]	C01690401	-15.55	-2.38	-14.23	4.97	-3.91
1600	CNC(=O)n1cncc1	C01727047	-15.55	-4.12	-14.92	5.24	-1.75
1601	c1cc(ccc1Cl)O)N	C02389348	-15.55	-3.93	-14.67	3.08	-0.02
1602	c1nc(c2c(n[nH]c2n1)C#N)N	C03852596	-15.55	-1.96	-16.66	4.08	-1
1603	[H]/N=C1/N=C(CS1)[S-]	C08628604	-15.55	-3.09	-14.2	3.15	-1.42
1604	c1c(ncs1)CCCl	C19092526	-15.55	0.78	-16.42	2.98	-2.9
1605	CC(=O)c1cnccn1	C26899027	-15.55	-0.04	-18.88	5.57	-2.21
1606	c1cc(nc(c1)F)NCC(=O)C(F)F)F	C01392500	-15.54	-1.44	-17.34	5.32	-2.09
1607	c1csc(n1)Cl	C01676248	-15.54	-1.91	-14.98	3.06	-1.71
1608	c1c(c(cc(c1F)O)F)N	C02243352	-15.54	-4.52	-14.78	3.47	0.3
1609	c1c(c(nc(n1)Br)N)C#N	C02555749	-15.54	-4.27	-13.79	3.76	-1.23
1610	c1cc(ccc1NC(=S)C#N)F	C06512096	-15.54	-4.5	-15.03	7.73	-3.73
1611	c1cc(ncc1C=O)F	C08698168	-15.54	-2.73	-16.87	5.82	-1.76
1612	c1cnc2c(n1)[nH]c(=S)[nH]2	C13283495	-15.54	-3.55	-19.01	8.43	-1.4
1613	c1(c(c(nc(c1Cl)F)F)F)O	C16082820	-15.54	-1.89	-16.18	2.75	-0.22
1614	c1cc(ccc1F)OCC#N	C19425892	-15.54	-3.71	-14.27	5.89	-3.45
1615	c1cc(ccc1CNC(=O)N)F	C00103941	-15.53	-0.19	-21.57	6.69	-0.46
1616	COc1cnccn1	C00334489	-15.53	-1.91	-17.11	3.6	-0.11

1617	C=CCOC(=O)C=C	C01577261	-15.53	-0.47	-15.9	4.03	-3.19
1618	C[C@H](c1cccc(c1)F)O	C02560497	-15.53	-0.95	-15.39	3	-2.19
1619	c1cncc(c1C=O)F	C04208893	-15.53	-1.16	-16.17	3.66	-1.86
1620	c1ccc2c(c1)CCO2	C06661321	-15.53	-1.27	-14.35	3.29	-3.19
1621	c1cc([nH]c1)/C=N/O	C08618515	-15.53	-3.58	-17.3	5.63	-0.28
1622	Cc1c[nH]ccc1=O	C14982930	-15.53	-2.22	-16.42	3.65	-0.54
1623	[H]/N=C(\C)/Oc1cccc1	C16978057	-15.53	0.58	-18.62	3.9	-1.38
1624	C1c2c(n[nH]c2N)CS1	C26506273	-15.53	-4.17	-17.29	6.96	-1.02
1625	c1cc(c2c(c1)non2)N	C00158119	-15.52	-2.53	-16.71	4.65	-0.93
1626	c1c(cc(c1F)O)F	C00389659	-15.52	-0.01	-16.71	2.59	-1.39
1627	CC(=O)c1cccnc1	C01587582	-15.52	0.57	-18.73	4.97	-2.33
1628	c1ccc(cc1)OCF	C01765109	-15.52	-2.48	-15.12	3.47	-1.39
1629	CCc1cccc1	C02037726	-15.52	-0.37	-14.52	2.42	-3.05
1630	CSc1nnc(n1N)C(F)F	C02536954	-15.52	-3.31	-16.25	6.56	-2.51
1631	c1cc(c(c1F)CS)F	C04244663	-15.52	0.4	-17.53	2.94	-1.33
1632	Cc1ccc(cc1)C	M1995A036	-15.52	-1.01	-11.63	1.5	-4.38
1633	Cc1cc(ccc1N)O	C00388268	-15.51	-4.39	-14.39	3.44	-0.17
1634	c1cc(ncc1Br)F	C00403389	-15.51	-0.75	-17.35	2.78	-0.18
1635	c1cc(c(cc1F)C#N)F	C00407108	-15.51	1.74	-17.97	4.38	-3.66
1636	c1c(c[nH]c1)Cl	C01049758	-15.51	-3.23	-14.48	3.4	-1.2
1637	C=COc(=O)Cl	C02242591	-15.51	-0.33	-14.89	1.92	-2.21
1638	c1cncc(c1[N+](=O)[O-])F	C02526725	-15.51	-2.69	-17.05	5.44	-1.21
1639	c1c(cc(c1F)C=O)F	C04290144	-15.51	-1.31	-15.42	3.99	-2.76
1640	CCC(=O)C=C/C	C12359419	-15.51	-1.24	-14.38	3.35	-3.24
1641	c1(c(c(c(nc1F)F)F)Cl)F	C16159839	-15.51	0	-13.81	0.59	-2.29
1642	C#CCSc1nc([nH]c1)N	C17045223	-15.51	-2.76	-16.92	7.48	-3.32
1643	c1cnn2c1nnc(c2N)C#N	C00250355	-15.5	-4.53	-16.1	6.4	-1.27
1644	c1cc(c(cc1N))N	C00334515	-15.5	-3.72	-12.82	2.17	-1.13
1645	c1cc(cc1C(=O)N)N+([=O])[O-]	C01042801	-15.5	-5.77	-15.63	5.69	0.21
1646	c1cc(cc1C(=O)N)N=C=S	C02528075	-15.5	-1.25	-19.14	6.5	-1.61
1647	c1cc(c(c1F)N)F	C12359240	-15.5	-1.65	-15.71	2.24	-0.37
1648	c1c(c(=O)[nH]c(n1)N)Br	C16698778	-15.5	-2.4	-18.39	4.22	1.07
1649	c1cc(c(cc1O)Br)N	C19872883	-15.5	-3.95	-16.17	4.72	-0.1
1650	c1c(nc(c(n1)Br)N)Cl	C32915138	-15.5	-4.75	-13.66	3.47	-0.56
1651	c1ccn(c1)C(=O)N	C01674962	-15.49	-2.74	-18.17	6.36	-0.94
1652	Cc1ccc(c(c1F)NN	C02546166	-15.49	-0.13	-16.65	3.33	-2.04
1653	c1cc(cnc1)CNC=O	C08701028	-15.49	0.76	-22.46	6.97	-0.77
1654	c1ccn(c1)CCBr	C12360598	-15.49	0.42	-14.81	2.73	-3.82
1655	C#Cc1cccoc1	C12957855	-15.49	-1.1	-15.65	4.06	-2.79
1656	Cc1cc(nc1)CBr	C00158681	-15.48	-1.11	-15.17	3.91	-3.1
1657	c1cnc(nc1)N	C00967472	-15.48	-2.68	-15.79	4.44	-1.46
1658	c1ccnc(c1)SC(=NH2+)N	C01615476	-15.48	-0.68	-18.25	4.95	-1.5
1659	c1cnoc1CCl	C04200425	-15.48	-1.42	-15.65	4.12	-2.53
1660	c1cn(cn1)CCO	C08294942	-15.48	-3.36	-16.58	5.22	-0.76
1661	c1c(ccc1F)C=O	C08698169	-15.48	-2.69	-16.59	5.67	-1.86
1662	CCOCn1ccnc1	C16677898	-15.48	-1.62	-16.96	5.72	-2.61
1663	CNC(=O)c1c(nsn1)N	C17163636	-15.48	-3.68	-17.49	4.12	1.57
1664	C1CCC=CC1	M1995A013	-15.48	-0.23	-12.16	0.4	-3.49
1665	Cc1cc(nc1)CCl	C00166026	-15.47	-1.09	-15.5	4.13	-3.02
1666	Cc1cc(ccc1O)F	C00389593	-15.47	-0.75	-15.69	2.8	-1.83
1667	c1c(c(=O)[nH]c(=O)[nH]1)CCl	C01670523	-15.47	-3.09	-19.09	6.51	0.21
1668	c1c(cc(=O)O)Cl	C01760795	-15.47	-1.91	-15.95	4.82	-2.43
1669	c1c(ncs1)C=O	C02566818	-15.47	-2.45	-16.75	4.73	-1
1670	c1(c(c(c(c1F)F)F)[N+](=O)[O-])N	C05510640	-15.47	-2.97	-12.37	2.48	-2.61
1671	CCSc1[nH]nnc1	C05654998	-15.47	-2.76	-13.41	3.62	-2.93
1672	CCc1cnc(s1)N	C12481760	-15.47	-1.32	-15.99	3.68	-1.84
1673	c1cnc(c(c1F)O)N	C21981850	-15.47	-4.97	-16.32	4.86	0.95
1674	Oc1ccccc1	phenol	-15.47	-2.03	-15.02	2.77	-1.2
1675	COC(=O)c1c(ncn1)N	C00108965	-15.46	-3.45	-17.33	5.82	-0.49
1676	c1cc(ccc1C(=O)ON)[N+](=O)[O-]	C01732516	-15.46	-2.1	-15.96	5.91	-3.31
1677	c1cc2c(cc1F)[nH]c(=S)[nH]2	C09927090	-15.46	-3.32	-13.44	3.97	-2.67
1678	c1cc(cnc1)NC(=O)N	C13538945	-15.46	-2.93	-20.72	7.38	0.82
1679	Cc1cc([nH]c1)Cl	C17058591	-15.46	-1.44	-15.18	2.73	-1.57
1680	c1c[nH]c(c1N)N	C19075780	-15.46	-4.38	-16.32	4.13	1.1
1681	c1cncc(c1N)[N+](=O)[O-]	C19798391	-15.46	-2.29	-18.08	5.86	-0.94
1682	c1cn(cn1)CCS	C20437221	-15.46	-0.86	-15.8	4.84	-3.63
1683	c1c(snn1)[S-]	C22016682	-15.46	-1.67	-16.07	3.1	-0.82
1684	COC(=O)c1ccc(c(c1N)F)F	C31829484	-15.46	-3.29	-13.64	3.89	-2.43
1685	CCSCC=C	M1995A005	-15.46	-0.02	-13.17	1.33	-3.6
1686	C1CS[P@](O1)OCC(F)(F)F	C05459485	-15.45	0.65	-16.03	6.56	-6.63
1687	CNc1c(non1)[O-]	C05699251	-15.45	-3.03	-17.76	4.22	1.12
1688	CCNc1nccs1	C20556872	-15.45	-1.75	-15.82	4.22	-2.09
1689	c1ccn(c1)CC#N	C00164491	-15.44	-1.42	-19.03	7.98	-2.96
1690	c1ccc2c(c1)CC2=O	C00897152	-15.44	-1.27	-14.09	3.9	-3.98
1691	Cc1c(non1)[N+](=O)[O-]	C01295932	-15.44	-0.15	-16.25	3.13	-2.18
1692	c1cc(ncc1C(F)(F)F)C#N	C01463603	-15.44	-2.15	-14.9	4.65	-3.03
1693	C(#N)/C(=C(\C#N)\Cl)/F	C01606791	-15.44	-0.57	-13.97	2.67	-3.26
1694	CCSCC=C	C02166476	-15.44	-0.04	-13.13	1.33	-3.59
1695	CSc1cccc(c1)F	C02511053	-15.44	-0.2	-16.35	2.34	-1.22
1696	Cc1ccc(c(c1)N)C	C03860836	-15.44	-3.27	-11.47	2.14	-2.84
1697	CN(c1cnccn1)N	C04038296	-15.44	-1.96	-17.05	4.42	-0.85
1698	c1c(non1)c2nnnn2O	C04728868	-15.44	-3.12	-18.2	4.77	1.12
1699	c1cc(ccc1N=C(N)N)Cl	C05003398	-15.44	0.69	-18.02	4.51	-2.63
1700	c1ccc(cc1)Nc2cn[nH]n2	C05072484	-15.44	-1.1	-16.03	3.8	-2.1
1701	c1[nH]c(c(n1)C(=O)N)N=[N+]=[N-]	C16952133	-15.44	-3.98	-20.94	7.78	1.71
1702	c1cc2c([nH]c(n2)N)nc1	C17060146	-15.44	-4.86	-17.59	9.21	-2.2
1703	c1c(snn1)/C=N/O	C17129871	-15.44	-5.06	-17.99	6.72	0.88
1704	c1c(cc(c1F)F)F	C00404224	-15.43	-3.2	-14.77	4.45	-1.92
1705	Cc1ccc(cn1)Br	C00966674	-15.43	-0.23	-14.69	2.53	-3.04
1706	c1ccc(cc1)OCCO	C01577061	-15.43	-3	-16.16	4.8	-1.08

1707	C#CCn1ccc(n1)C(F)F	C02556148	-15.43	-3.09	-15.68	7	-3.65
1708	Cc1cc(cnc1)F	C02598989	-15.43	-1.85	-13.59	2.62	-2.62
1709	c1c(c[nH+]cc1[O-])[N+](=O)[O-]	C14982959	-15.43	-4.47	-15.78	5.17	-0.35
1710	c1cc(oc1CBr)[N+](=O)[O-]	C00120684	-15.42	-1.44	-16.88	6.43	-3.53
1711	c1cc(c(c1)F)F)CO	C00409277	-15.42	-1.67	-16.18	3.88	-1.46
1712	COc1ccccc1	C00897131	-15.42	-1.77	-13.3	2.54	-2.89
1713	Cc1ccoc1	C01580392	-15.42	-1.11	-14.42	2.46	-2.35
1714	c1cc(ccc1N)NCC#N	C01848391	-15.42	-2.97	-16.28	5.19	-1.35
1715	C/C=C/C=C#N	C02584527	-15.42	-0.93	-14.78	3.88	-3.59
1716	CSSSC	C04097550	-15.42	-0.87	-11.77	1.82	-4.6
1717	CC(=O)/C=C/(c1ccccc1)N	C06262272	-15.42	-1.68	-15.31	4.9	-3.32
1718	c1csc(n1)NC(=[NH2+])N=C(N)N	C20459028	-15.42	-2.23	-19.44	9.42	-3.16
1719	CCOC(=O)C=[N+]=[N-]	C04521365	-15.41	-1.74	-15.97	4.05	-1.74
1720	Cc1nc(cs1)C(=O)Cl	C12370153	-15.41	-2.16	-15.58	4.48	-2.15
1721	c1cncc(c1Cl)C=O	C14982474	-15.41	-2.53	-14.7	3.96	-2.13
1722	c1c(nc(s1)N)N	C15863137	-15.41	-5.06	-14.95	4.14	0.45
1723	CC(=O)c1c[nH]nc1	C16696740	-15.41	-3.42	-16.83	5.88	-1.05
1724	C/C(=C)Br/COC	C16970519	-15.41	-1.23	-13.48	1.77	-2.48
1725	c1c(cnc(c1)Br)N	C19943157	-15.41	-3.5	-16.35	4.4	0.04
1726	Cc1ccc(cc1)NN	C00153114	-15.4	-1.36	-14.71	2.64	-1.96
1727	c1ccc(c(c1)N)OC(F)F	C00528010	-15.4	-1.39	-16.66	4.28	-1.63
1728	Cc1ccc(cc1)FO	C02512465	-15.4	-2	-15.01	3.28	-1.67
1729	Cc1ccncc1/C(=N/O)N	C04269154	-15.4	-2.53	-17.48	4.96	-0.35
1730	c1(c(n[O+])1[O-])[N+](=O)[O-]C(=O)N	C04903937	-15.4	-0.75	-16.56	3.48	-1.57
1731	c1cc(ccc1C(=[NH2+])NO)F	C12649842	-15.4	-2.97	-16.03	4.51	-0.9
1732	c1ccc2c(c1)non2	C00161256	-15.39	-3.43	-13.7	4.66	-2.93
1733	Cn1cnc1[N+](=O)[O-]	C01564459	-15.39	-3.82	-14.86	8.62	-5.34
1734	c1c(nc(nc1)F)F	C01845800	-15.39	-0.77	-15.8	2.53	-1.35
1735	c1(c(nc2c(n1)non2)[O-])N	C03163100	-15.39	-3	-19.07	6	0.67
1736	c1cc(oc1)/C=C/C=N/O	C03200730	-15.39	-3.12	-19.5	8.39	-1.16
1737	c1ccnc(c1)CCC(=O)Cl	C04204053	-15.39	-2.36	-13.37	3.87	-3.53
1738	c1ccc2c(c1)nc(o2)N	C08581625	-15.39	-4.21	-15.71	4.45	0.07
1739	c1c(c(cc(c1)F)F)N	C19615643	-15.39	0.21	-16.59	3.26	-2.27
1740	C/C(=C)C(F)(F)F/[N+](=O)[O-]	C22221040	-15.39	-0.27	-14.25	2.51	-3.38
1741	[H]/N=C/1/C=C/C@H(S1)CC	C31861623	-15.39	-1.75	-14.81	3.31	-2.13
1742	Oc1ccccc1	W2002A005	-15.39	-2.02	-14.95	2.77	-1.19
1743	Cc1cc(ccc1)N	C00388337	-15.38	-4.31	-12.84	2.51	-0.75
1744	C1C(=NO)CSS1	C05181011	-15.38	-2.77	-14.56	3.4	-1.45
1745	c1ccnc(c1)NC(=S)N	C05594482	-15.38	0.05	-18.22	4.73	-1.94
1746	c1cc(sc1)CCC=O	C19682802	-15.38	-1.55	-15.45	5.24	-3.62
1747	c1cc(ccc1)OS	C19735431	-15.38	-0.82	-17.32	4.02	-1.25
1748	CCc1ccc[nH+]c1N	C21985770	-15.38	-0.9	-16.14	3.89	-2.22
1749	c1cc(sc1/C=N/O)Cl	C00112364	-15.37	-2.87	-16.59	5.45	-1.36
1750	c1c(c(cs1)N)N	C02170007	-15.37	-3.87	-14.58	2.54	0.54
1751	CCC/C(=C/C(=O)C(F)F)/[O-]	C04023573	-15.37	-2.1	-12.34	2.32	-3.25
1752	C=CCOCCI	C04203522	-15.37	-0.49	-14.15	1.79	-2.52
1753	c1(nc(sn1)Br)N	C06720865	-15.37	-2.28	-14.53	2.67	-1.22
1754	Cn1cc(nc1)CCl	C08614783	-15.37	-1.09	-16.03	5.51	-3.77
1755	Cc1c(cncn1)O	C14982946	-15.37	-2.19	-17.01	4.15	-0.32
1756	c1cc(nn2c1ncc2)F	C18555988	-15.37	-3.59	-15.13	5.76	-2.4
1757	c1cc(ccc1c2cc(no2)CC(=O)[O-])F	C20270419	-15.37	0.02	-18.82	7.31	-3.89
1758	Cc1cc(co1)C(F)F	C26506528	-15.37	-0.94	-13.94	2.8	-3.29
1759	C[C@H](c1ccc(cc1)F)O	C00388214	-15.36	-1.09	-15.13	3.04	-2.18
1760	c1ccc(cc1)NNC=O	C01711848	-15.36	-0.55	-18.96	5.89	-1.74
1761	C#CCOc1ccc(cc1)N	C09239338	-15.36	-0.53	-16.65	4.25	-2.43
1762	CN/C(=N/C#N)/N=[N+]=[N-]	C17024863	-15.36	-3.01	-15.32	5.54	-2.57
1763	c1cc(c(nc1)N)[N+](=O)[O-]	C19596908	-15.36	-2.24	-18.25	6.57	-1.44
1764	[C@H-]1C(=[NH+])C(=CN1)Br	C28617731	-15.36	-0.65	-18.48	5.5	-1.72
1765	c1c(c(nnc1)Cl)N	C01688662	-15.35	-4.61	-15.06	4.79	-0.46
1766	Cc1cc[nH]c1	C02034399	-15.35	-1.83	-13.85	2.64	-2.31
1767	C(COC(=O)c1c(non1)N)O	C02288990	-15.35	-3.88	-17.82	5.33	1.03
1768	c1cc(cc(c1)F)OC(F)F	C02560217	-15.35	-0.35	-13.55	1.8	-3.25
1769	c1c(cc(c(c1[N+](=O)[O-])N)F)F	C03876123	-15.35	-2.2	-13.49	2.87	-2.53
1770	[C@]1(C)(O1)(F)F(C(F)F)F	C04266015	-15.35	0.05	-13.46	0.5	-2.43
1771	Cc1c(c[nH]1)Br	C05424919	-15.35	-4.09	-13.33	3.7	-1.63
1772	c1c2c([nH]c(=O)[nH]2)ncn1	C13548121	-15.35	-5.09	-18.18	6.35	1.58
1773	c1cc(oc1)N=C=O	C19502690	-15.35	-0.13	-18.13	2.72	0.19
1774	c1cc(cnc1)CC=O	C19729368	-15.35	-2.53	-16.98	6.54	-2.39
1775	CC(=O)Nc1ccc(cc1)F	C00151118	-15.34	-1.46	-15.73	4.65	-2.8
1776	Cc1ccnc(c1)F	C00403519	-15.34	-1.46	-15.64	4.22	-2.46
1777	CC(=O)OCc1cccn1	C01665465	-15.34	-0.31	-18.07	6.47	-3.43
1778	c1c(ncnc1)Cl	C01675006	-15.34	-2.97	-14.86	3.8	-1.31
1779	c1cc(c(cc1SC#N)O)O	C01680025	-15.34	-1.82	-20.32	5.75	1.05
1780	c1ccc(cc1)OP(O)O	C01755749	-15.34	-2.2	-19.32	7.93	-1.76
1781	c1(c(c(c(c1)F)S)F)F	C02022402	-15.34	-0.22	-12.7	0.55	-2.96
1782	c1cnnc(n1)NN=O	C06585043	-15.34	-3.81	-17.99	7.66	-1.2
1783	C(=C/[N+](=O)[O-])C(F)F	C16889905	-15.34	1.68	-16.98	2.99	-3.03
1784	c1cc(nc(c1)F)N	C19616089	-15.34	-3.92	-15.93	5.49	-0.97
1785	Cc1cc[nH]c1	W2002A001	-15.34	-1.86	-13.84	2.65	-2.3
1786	COc1cc(cc(c1)F)F	C00409323	-15.33	-0.07	-14.27	1.97	-2.96
1787	c1enn2c1c(nnc2)[O-]	C00501376	-15.33	-3.18	-17.84	6.62	-0.92
1788	c1cnnc1N	C01593930	-15.33	-2.54	-16	4.2	-1
1789	CCOC(=O)C(F)Cl	C01691290	-15.33	-1.06	-12.75	1.56	-3.07
1790	c1cc(sc1)C(=O)Cl	C02141006	-15.33	2.02	-18.3	3.87	-2.92
1791	c1cncc(c1)C(F)F	C02578102	-15.33	-2.8	-14.18	4.5	-2.85
1792	c1cc(c(c1NC(=O)N)F)F	C19398959	-15.33	-2.3	-20.39	7.9	-0.54
1793	c1c(c(ncn1)N)F	C26466410	-15.33	-3.63	-15.1	4.54	-1.14
1794	C(#N)c1c(n[nH]1)Cl	C02566328	-15.32	-5.07	-13.54	3.62	-0.33
1795	c1c(non1)c2c(non2)N	C02566776	-15.32	-1.63	-17.72	4.07	-0.05
1796	Cc1cc(sc1)C#N	C04290335	-15.32	-0.24	-15.03	3.42	-3.47

1797	c1cc(nc(c1C=O)F)F	C14982658	-15.32	-1.47	-16.52	4.37	-1.7
1798	c1ccc(c(c1)N)I	C00157582	-15.31	-2.27	-15.93	1.8	1.09
1799	c1cc([nH]c1C=O)[N+](=O)[O-]	C01681946	-15.31	-4.07	-17.13	8.73	-2.84
1800	Cc1cnc(cn1)C#N	C02528733	-15.31	-0.9	-18.03	5.16	-1.54
1801	c1ccc(cc1)c2cc(cn2)[O-]	C02774749	-15.31	-3.78	-14.1	5.36	-2.79
1802	c1cc(sc1)C(=O)C=O	C04204386	-15.31	-0.37	-19.33	7.61	-3.22
1803	CCOC(=O)C@H](F)I	C04255779	-15.31	-0.79	-13.72	2.56	-3.36
1804	CC(=O)N(C)N=O	C04742492	-15.31	-2.02	-15.46	2.84	-0.68
1805	c1c(cnc(n1)Br)Br	C08698478	-15.31	-1.62	-13.59	2.39	-2.49
1806	c1cn2cc(cnc2n1)Br	C16125217	-15.31	-2.22	-16.09	7.65	-4.66
1807	c1cnc(cc1Cl)N	C19735878	-15.31	-2.03	-15.48	3.6	-1.41
1808	c1cc(ccc1Cl)Cl	C00388507	-15.3	-0.69	-15.04	1.08	-0.65
1809	COC(=O)Cct1cccnc1	C00393945	-15.3	-0.22	-18.51	6.58	-3.16
1810	c1(c(nc(c(n1)F)F)N)N	C01655762	-15.3	-5.9	-17.7	6.13	2.17
1811	CNC(=O)Oc1cccnc1	C01716719	-15.3	0.33	-21.01	7.4	-2.03
1812	c1cc(c(nc1)Br)F	C02598979	-15.3	0.49	-17.71	4.45	-2.53
1813	c1c(c(n[nH]1)N)Br	C04240086	-15.3	-4.37	-14.7	4.18	-0.41
1814	Cc1ccnc(n1)N	C00404289	-15.29	-2.88	-14.91	4.58	-2.07
1815	COC(=O)Cct1ccc(cc1)N	C01494999	-15.29	-1.62	-16.35	5.56	-2.88
1816	COCc1cccnc1	C01586379	-15.29	-0.51	-14.12	2.53	-3.2
1817	Cc1c(ccc1F)O	C01732032	-15.29	-1.78	-16.52	3.22	-0.21
1818	c1c(c(nc(n1)N)N)C=O	C01748627	-15.29	-6.61	-14.34	6.21	-0.56
1819	CC(=O)Oc1ccc(c1)F	C02512236	-15.29	-0.86	-16.19	6.12	-4.36
1820	[C@]1(C(O1)(F)F)(C(F)F)F	C04266020	-15.29	0.33	-13.54	0.49	-2.58
1821	C(#N)C1=NC(=S)N=C1[NH-]	C05500160	-15.29	-3.12	-16.01	4.24	-0.39
1822	c1ccc1C=N/O	C15219920	-15.29	-3.45	-16.22	4.61	-0.24
1823	c1c[nH+]ccc1N	C19075724	-15.29	-2.4	-16.04	3.51	-0.36
1824	c1c(c(cc(c1F)Cl)F)N	C20286525	-15.29	0.47	-16.85	3.29	-2.19
1825	CC(=O)c1ncc(s1)Cl	C22007391	-15.29	-0.6	-15.15	2.74	-2.28
1826	c1cc(ncc1N)Br	C01427060	-15.28	-3.17	-15.49	4.15	-0.77
1827	COC(=O)C#CBr	C01635685	-15.28	-0.96	-15.46	2.72	-1.57
1828	c1cc(ccc1Cl)N[N+](=O)[O-]	C03852415	-15.28	-2.23	-13.83	3.6	-2.82
1829	CC(=O)Nn1cnc2c(c1=O)cn[nH]2	C05479373	-15.28	-3.11	-22.51	11.68	-1.34
1830	c1cc(ccc1N)F)N	C05479668	-15.28	-2.93	-17.08	3.03	1.7
1831	c1ccnc(c1)/C=C/C#N)/N	C12348960	-15.28	-2.43	-18	7.16	-2.01
1832	c1c(n[nH]n1)S	C12405203	-15.28	-4.04	-14.67	3.03	0.4
1833	Cc1[n-]c(nn1)Cl	C14982426	-15.28	-3.56	-14.15	4.35	-1.92
1834	c1ccc(cc1)OC(C(=C(F)F)F)(F)F	C15441996	-15.28	-0.79	-12.26	2.16	-4.4
1835	c1nnc(n1)C(=O)N	C01727048	-15.27	-4.39	-17.18	5.15	1.15
1836	CCOC(=O)N(CC=C)N=O	C05412145	-15.27	0.58	-17.91	3.68	-1.62
1837	c1cc(ccc1c2cc(no2)CC[NH3+])Cl	C20270381	-15.27	-0.07	-10.41	-0.58	-4.22
1838	c1[nH]nc(n1)C(=O)Nn2cnc2	C01064775	-15.26	-0.33	-21.76	9.47	-2.65
1839	C=C(C[N+](=O)[O-])CCl	C01678154	-15.26	-0.43	-15.69	3.99	-3.12
1840	c1cn2cnc2cn1	C01695126	-15.26	-2.44	-19.81	8.24	-1.25
1841	Cc1cccnc1CN=C=O	C02568120	-15.26	-1.37	-14.4	2.76	-2.25
1842	c1cc(oc1)CC=O	C02581181	-15.26	-2.17	-16.6	5.23	-1.72
1843	[H]/N=C\1/n(ccs1)C	C12504702	-15.26	-2.14	-15.29	4.27	-2.1
1844	c1ccc(cc1)CC(=O)NO	C16887669	-15.26	-4.23	-15	3.99	-0.02
1845	c1cscnc1C=O	C00158756	-15.25	-1.57	-16.81	5.45	-2.31
1846	c1cc(cnc1)C(=O)Cl	C02539499	-15.25	-2.51	-14.11	3.59	-2.21
1847	C#Cc1ccc(cc1)C#N	C02541504	-15.25	-0.76	-14.13	4.23	-4.59
1848	C(C(=O)C(C(F)F)F)Br	C04242005	-15.25	-0.59	-14.44	2.75	-2.98
1849	C(F)F(F)SSC(F)F)F	C04329251	-15.25	-0.23	-12.32	0.57	-3.27
1850	c1ccc(cc1/C=N/O)Cl	C04582531	-15.25	-3.76	-15.3	4.18	-0.37
1851	COC(=O)Nc1ccc(cc1F)Cl	C06126168	-15.25	0.94	-19.13	3.49	-0.56
1852	c1c(cc(c2c1[nH]nc2)F)F	C14983967	-15.25	-1.3	-14.42	2.91	-2.44
1853	CCOC1c(ccc1F)F	C16159347	-15.25	0.89	-16.76	4.45	-3.84
1854	c1c2c(no1)CCCC2	C16951353	-15.25	-0.56	-15.47	3.95	-3.17
1855	CSc1cnc(s1)N	C16952003	-15.25	-5.35	-11.12	3	-1.79
1856	C[C@]([H])C=C[C@H]2COCC2=C1	C18529661	-15.25	-1.65	-12.1	1.76	-3.26
1857	CC(=C)C(=O)Cl	C02040191	-15.24	-1.44	-14.51	2.93	-2.22
1858	COc1c(cc(cc1F)O)F	C02527841	-15.24	0.16	-18.7	4.13	-0.84
1859	C1C=CC(=C1)CO	C12358631	-15.24	-2.28	-14.71	2.88	-1.13
1860	CNc1ccc(cc1)C(F)F)F	C12956268	-15.24	-0.62	-14.11	2.63	-3.15
1861	c1([nH]c(=O)[nH]n1)C(F)F)F	C14608573	-15.24	-2.93	-16.46	4.22	-0.07
1862	c1cc(c(nc1)C(F)F)F)F	C15442281	-15.24	-3.1	-14.66	5.45	-2.93
1863	c1(c(ncc(=O)[nH]1)Br)[O-]	C18106308	-15.24	-2.78	-17.34	3.49	1.39
1864	c1(nc2n(n1)[C@]([H])(N=N2)N)N	C19798284	-15.24	-3.03	-19.4	6.83	0.36
1865	COC(=O)C(=O)Ct1cccsc1	C32007764	-15.24	1.2	-17.17	4.93	-4.2
1866	COC(=O)c1cnoc1N	C00258212	-15.23	-0.9	-18.63	4.51	-0.21
1867	c1cc(c(nc1)C#N)N	C01433329	-15.23	-3.08	-17.84	6.36	-0.67
1868	CCc1ccc(c1)O	C01648289	-15.23	-1.13	-14.63	2.74	-2.21
1869	Cc1cscn1	C01675771	-15.23	-1.75	-14.96	3.22	-1.74
1870	c1c(cc(c(c1F)N)Cl)F	C02512350	-15.23	-2.69	-13.42	1.34	-0.47
1871	c1c(nc(nc1F)F)N	C02565586	-15.23	-4.56	-15.13	4.88	-0.42
1872	C=CCO/N=C/c1c(non1)N)N	C04181337	-15.23	-0.55	-17.76	2.85	0.22
1873	Cc1c(c(n[nH]1)N)Cl	C12356776	-15.23	-4.14	-14.66	4.23	-0.67
1874	c1ccnc(c1)CF	C15042159	-15.23	-1.85	-14.99	4.27	-2.66
1875	Cc1ccc(ncc1N)F	C16159661	-15.23	-4.24	-15.21	5.04	-0.82
1876	c1c(c(c(nn1)[O-])N)[N+](=O)[O-]	C26506582	-15.23	-3.4	-18.01	5.07	1.1
1877	Cc1cccnc1F	C00403518	-15.22	-1.56	-15.86	4.65	-2.46
1878	CC(=O)OC/C=C/Cl	C01681467	-15.22	-0.87	-16.47	3.96	-1.84
1879	c1ccc2c(c1)COC2	C02040452	-15.22	-1.14	-13.91	2.73	-2.9
1880	c1cc(ccc1N)N[N+](=O)[O-]	C04044869	-15.22	-2.18	-18.55	6.29	-0.78
1881	Cc1ccc(c(c1N)N)[N+](=O)[O-]	C04520851	-15.22	-2.02	-15.44	5.14	-2.9
1882	c1cc(oc1)C=N/O	C08579610	-15.22	-4.3	-17.28	6.55	-0.2
1883	c1c(nc(s1)Cl)Cl	C08939671	-15.22	-1.28	-14.86	2.96	-2.04
1884	c1ccc2c(c1)nc(s2)C#N	C12360442	-15.22	-1.47	-15.08	4.74	-3.42
1885	c1ccc(cc1)N=[N+]=[N-]	M1995A010	-15.22	0.58	-15.88	1.78	-1.7
1886	CCc1[nH]c(cn1)C=O	C00164927	-15.21	-2.54	-16.9	6.06	-1.84

1887	c1cc(c(cc1O)O)Br	C00404317	-15.21	-1.21	-18.06	3.62	0.43
1888	c1cncc(c1Cl)CO	C01585512	-15.21	-3.13	-15.12	3.55	-0.52
1889	Cc1ccc(s1)C	C01690407	-15.21	-0.93	-12.4	1.9	-3.78
1890	c1cc(c(cc1N)O)Cl	C02567235	-15.21	-0.5	-18.28	3.58	-0.01
1891	C1C(=O)NC=CS1	C03846684	-15.21	-2.99	-16.13	4.81	-0.89
1892	c1ccc(cc1)SC(=NH2+)N	C04203785	-15.21	-0.14	-16.33	3.35	-2.09
1893	Cc1c(c([n-]n1)[N+](=O)[O-])[N+](=O)[O-]	C05296576	-15.21	-3.44	-13.81	5.04	-3
1894	c1cc(c(c(c1F)N)Cl)F	C12359296	-15.21	-2.34	-14.63	2.2	-0.44
1895	c1c(cnc1Br)[N+](=O)[O-]	C14982289	-15.21	-1.34	-13.79	2.95	-3.03
1896	c1(nc(sn1)Cl)N	C17061322	-15.21	-3.24	-15.06	4.24	-1.14
1897	C(CCl)n1nc(nn1)N	C17104993	-15.21	-5.29	-13.94	6.01	-1.99
1898	c1c(cnc1N)Cl)N	C21981912	-15.21	-4.49	-17.95	6.45	0.78
1899	[H]/N=C1/C=C2CCCC2S1	C31861595	-15.21	-1.97	-14.81	4.05	-2.48
1900	c1cnnc(c1Cl)Cl	C01699062	-15.2	-2.92	-14.76	4.49	-2
1901	c1cc(nc(c1)Cl)F	C02149727	-15.2	-1.02	-16.6	4.81	-2.39
1902	C(#N)C(C(#N)(F)F)F	C02576929	-15.2	-0.16	-14.57	2	-2.47
1903	c1cc(cnc1)/C(=N/N)N	C02580892	-15.2	-2.94	-20	4.45	3.28
1904	c1cnc(cc1Br)N	C19862889	-15.2	-2.08	-15.21	3.59	-1.51
1905	c1cc(ccc1NC(=O)N)Cl	C00097935	-15.19	-2.54	-18.78	6.82	-0.69
1906	CCOC(=O)CCS	C00409355	-15.19	-1.34	-13.65	2.84	-3.03
1907	Cc1ccc(c(c1)N)I	C02570685	-15.19	-2.77	-10.97	1.75	-3.2
1908	Cc1cc(n[nH]1)(C(F)F)F	C04693290	-15.19	-0.77	-15.13	2.7	-1.98
1909	C=CCO1c1ccnc1N	C19093139	-15.19	-1.26	-15.61	3.57	-1.9
1910	Cc1cc(n[nH]1)C=O	C20357649	-15.19	-2.23	-15.68	4.72	-2.01
1911	c1ccc(c(c1)C=O)N	C04202514	-15.18	-4.92	-14.12	5.49	-1.63
1912	CCn1ccnc1	C08294979	-15.18	-2.18	-14.41	4.8	-3.39
1913	C=C(Cl=O)Cl)F	C08698303	-15.18	-1.6	-14.4	2.59	-1.77
1914	c1c(cc(c(c1O)F)F)F	C00389682	-15.17	-1.24	-15.89	3.29	-1.33
1915	c1nc(c(c(n1)N)SC#N)N	C01036822	-15.17	-2.63	-18.03	6.21	-0.72
1916	c1cnc(cn1)NN	C01402333	-15.17	-3.11	-17.26	4.89	0.7
1917	c1csc2c1nns2	C01632266	-15.17	-2.94	-17.93	5.11	0.58
1918	c1ccc(c(c1)c2nc([nH]n2)N)N	C06658084	-15.17	-0.12	-19.53	6.72	-2.24
1919	c1(mnc(n1)NN)C(F)F	C12336363	-15.17	-5.14	-15.95	7.36	-1.44
1920	[H]/N=C1/NC(SS1)(Cl)Cl	C17173602	-15.17	-0.36	-13.31	0.77	-2.26
1921	C1C[C@H]2[C@H](C)C2=C1O	C25695669	-15.17	-1.89	-14.47	3.04	-1.85
1922	c1c(cnc1F)CO	C01573930	-15.16	-1.55	-17.76	4.11	0.03
1923	Cc1cc([nH]1)C	C01574400	-15.16	-0.96	-14.1	2.71	-2.82
1924	c1cc(ccc1[N+](=O)[O-])F	C01706157	-15.16	-1.05	-13.94	3.72	-3.89
1925	CCOC1cncnc1	C02560521	-15.16	-1.98	-16.42	3.67	-0.42
1926	c1cc(cc(c1)F)NNC(=O)N	C02569462	-15.16	-1.76	-19.5	6.45	-0.34
1927	c1csc2c1csc2	C05605232	-15.16	-1.22	-16.96	3	0.01
1928	c1cnc(cc1C(F)F)F	C19616126	-15.16	0.76	-16.46	3.3	-2.76
1929	CNc1nccs1	C19872627	-15.16	-2.57	-15.92	4.76	-1.43
1930	C=Cc1cnc1	C00389820	-15.15	-1.28	-14.7	4.7	-3.88
1931	c1c(c(nc(n1)N)N)F	C01574355	-15.15	-3.92	-17.45	3.76	2.47
1932	CNC(=O)C1c(non1)N	C06679794	-15.15	-5.9	-14.21	3.8	1.16
1933	c1csc(n1)N	C08579603	-15.15	-3.79	-14.46	3.65	-0.55
1934	c1cc(sc1)CNN	C19263370	-15.15	-0.64	-16.36	2.58	-0.73
1935	c1cc(c(c(c1)F)CO)F	C00409199	-15.14	-2.93	-15.17	4.35	-1.39
1936	c1cc(cc(c1)N)CC#N	C02507095	-15.14	-1.46	-17.06	5.99	-2.62
1937	c1c([nH]c2c1cc(cn2)N	C06643328	-15.14	-1.6	-18.05	5.72	-1.2
1938	Cc1cc(cs1)Cl	C21986910	-15.14	-0.83	-12.33	1.63	-3.6
1939	c1ccc(c(c1)CO)O	C00002054	-15.13	-2.36	-17.62	4.15	0.7
1940	Cc1ccsc1C	C01845895	-15.13	-1.41	-11.94	1.85	-3.63
1941	c1(c(c(c(c(c1F)F)F)F)N)N	C02022416	-15.13	-1.41	-13.91	1.88	-1.68
1942	Cl(=O)(C(F)F)Cl)F	C05178392	-15.13	-0.26	-13.72	1.08	-2.24
1943	Cc1nc(n(n1)C)N	C17024968	-15.13	-5.84	-13.52	6.59	-2.36
1944	c1c(c(n[nH]c1=S)[S-])N	C17426315	-15.13	-5.69	-15.04	5.3	0.29
1945	c1c(cnc(c1Cl)N)C#N	C20218632	-15.13	-0.53	-17.41	4.57	-1.76
1946	c1c(cnc(n1)Cl)Cl	C22005578	-15.13	-1.65	-13.11	2.35	-2.73
1947	c1c(ccon1)CN=[N+]=[N-]	C26547916	-15.13	-0.53	-19.49	4.33	0.57
1948	Cc1c(cccn1)O	C00153239	-15.12	-1.57	-16.98	3.97	-0.54
1949	c1ccc(c(c1)CC=O)O	C06095286	-15.12	-0.59	-19.53	4.93	0.06
1950	c1cc(ccc1C(=O)N=C=O)F	C06661885	-15.12	1.45	-18.48	3.08	-1.17
1951	c1(c([nH+]nc(=S)[nH]1)[O-])[O-]	C09354658	-15.12	-6.15	-18.13	6.35	2.81
1952	C/C=C/C=CO	C13546463	-15.12	-2.85	-13.71	2.39	-0.95
1953	[H]/N=C/(c1cncnc1N)N	C20272756	-15.12	-5.1	-16.6	6.49	0.1
1954	c1c(cnc(n1)NN)Cl	C26441083	-15.12	-3.35	-14.66	4.46	-1.56
1955	c1cc(ncc1O)Cl	C00335761	-15.11	-1.18	-17.74	4.04	-0.23
1956	c1ccn2cccc2c1	C02040898	-15.11	-1.99	-15.37	3.83	-1.58
1957	c1cnoc1C(=O)N	C02565041	-15.11	-3.04	-17.8	4.91	0.82
1958	c1cc(c(cc1F)N)N	C02584360	-15.11	-3.02	-14.97	2.29	0.59
1959	Cc1cc(no1)C(F)F	C04137189	-15.11	-1.13	-15.06	3.91	-2.84
1960	c1nnc2n1C(=O)CS2	C09024413	-15.11	-0.08	-19.96	7.95	-3.03
1961	Cc1cccc(n1)N	C19075790	-15.11	-3.3	-13.83	3.56	-1.53
1962	c1c(cnc(c1Cl)N)O	C21981818	-15.11	-3.69	-18.02	5.89	0.71
1963	c1c([nH+]cc(c1)O)O	C21988285	-15.11	-0.46	-16.32	2.37	-0.7
1964	Cc1c(cccn1)[S-]	C26438572	-15.11	-0.62	-13.73	1.83	-2.59
1965	c1[nH]c2c([nH+]1)CCC2	C26441246	-15.11	-2.42	-17	7.35	-3.04
1966	C=Cc1cncn1	C00051189	-15.1	-2.65	-14.37	5.61	-3.69
1967	c1ccc(cc1)SCC#N	C02163480	-15.1	-0.49	-15.45	5.48	-4.64
1968	c1cc(ncc1)NN=O	C13213266	-15.1	-2.77	-15.78	5.55	-2.1
1969	c1cc(mnc1Cl)I	C20358093	-15.1	-2.27	-14.44	4.06	-2.45
1970	c1ccncc1	C00895354	-15.09	-1.22	-14.71	2.91	-2.06
1971	c1cnc(cn1)N	C00967322	-15.09	-3.7	-15.78	4.17	0.22
1972	Cn1c(=O)c([nH]c1=O)Br	C01592762	-15.09	-2.46	-16.13	3.36	0.14
1973	c1ccsc1	C01597767	-15.09	-1.12	-12.86	1.43	-2.54
1974	CC[C@@H]([N+](=O)[O-])Cl	C02034489	-15.09	-0.64	-14.39	2.74	-2.8
1975	CCOC(=C(F)F)F	C02572592	-15.09	-0.47	-13.95	1.34	-2
1976	C[C@H]1C(=O)N=C(S1)N	C05527921	-15.09	-2.71	-15.11	3.14	-0.4

1977	c1cc([nH]c1)c2cccnc2	C13208435	-15.09	0.99	-17.69	4.76	-3.16
1978	c1cc(ncc1N)CS	C21985586	-15.09	-1.47	-17.75	5.21	-1.08
1979	c1c(cc(c(c1F)N)Br)F	C00152682	-15.08	-2.87	-13.51	1.34	-0.04
1980	c1cc(ccc1C#N)O	C00388759	-15.08	0.43	-18.76	4.65	-1.4
1981	Cn1c(ncn1)N	C01067758	-15.08	-3.19	-15.6	6.13	-2.43
1982	C1CS[P@@](O1)OCC(F)(F)F	C01579433	-15.08	-1.52	-12.19	5.45	-6.82
1983	c1cc(=O)oc(c1)Cl	C02548333	-15.08	-1.36	-17.29	6.73	-3.16
1984	c1cc(cnc1)/C=C/C=O	C12360000	-15.08	-3.48	-16.78	7.93	-2.74
1985	Cc1c(noc1N)N	C15784487	-15.08	-4.55	-16.84	5.26	1.04
1986	CCNc1ccc(c(c1F)F)F	C19907714	-15.08	-2.47	-13.55	4.26	-3.32
1987	CSc1ccncc1	C00330923	-15.07	-0.6	-17.6	3.2	-0.07
1988	c1c(nns1)C(=O)N	C01718901	-15.07	-3.09	-18.8	5.18	1.64
1989	c1(c(c(c(c1F)F)F)F)F)N	C02022414	-15.07	-3.46	-11.71	2.08	-1.97
1990	C=C(C(=O)OCC(F)(F)F)F	C02525787	-15.07	-0.18	-15.65	3.91	-3.15
1991	C[C@@H](CO[NH](=O)[O-])O[N+](=O)[O-]	C05735208	-15.07	-0.5	-14.17	3.92	-4.32
1992	COc1c2c([nH]n1)nncc2	C18272284	-15.07	-3.39	-17.07	4.82	0.57
1993	c1cc(ncc1C(F)F)F)N	C19735095	-15.07	-4.34	-13.4	4.38	-1.72
1994	c1ccc(cc1)O[P@@H](=O)N	C20230606	-15.07	-1.37	-19.28	6.84	-1.26
1995	c1cc(c(cc1F)C(=O)N=C=S)F	C21968788	-15.07	1.45	-18.98	5.7	-3.23
1996	C1Cc2c(n[nH]c2N)C1	C26506268	-15.07	-4.03	-16.29	6.54	-1.29
1997	c1cnc(n2c1nccn2)N	C26894647	-15.07	-2.29	-16.88	7.04	-2.94
1998	C[C@H](c1ccoc1)O	C01403558	-15.06	-2.62	-15.37	3.51	-0.59
1999	CCCc1ccccc1O	C01692499	-15.06	0.14	-14.75	2.56	-3.02
2000	C#CCOC(=O)C(=O)N=[N-]	C05940572	-15.06	-0.45	-17.78	4.67	-1.51
2001	Cc1cn[nH]c1[N+](=O)[O-]	C09356400	-15.06	1.02	-17.79	4.06	-2.35
2002	Cc1c(c(on1)[O-])[N+](=O)[O-]	C11804032	-15.06	-5.92	-13.22	5.33	-1.25
2003	c1cncnc1	Elig_2GUP	-15.06	-1.11	-14.8	2.9	-2.06
2004	CNc1ncccn1	C00330858	-15.05	-1.26	-15.95	4.61	-2.45
2005	C/C=C/C(=O)Cl	C02242606	-15.05	-1.33	-14.14	2.9	-2.49
2006	c1nc(nm1C(=O)N)N	C04633181	-15.05	-6.7	-15.43	7.38	-0.31
2007	c1cc(oc1[N+](=O)[O-])[N+](=O)[O-]	C04722185	-15.05	-2.07	-17.48	7.32	-2.82
2008	Cc1ncc(c(n1)N)C(S)N	C05579929	-15.05	-3.32	-14.36	3.22	-0.6
2009	c1c(cnc(c1N)Br)Cl	C15441993	-15.05	-4.06	-12.42	2.77	-1.34
2010	Cc1cccc(c1F)N	C15442933	-15.05	-2.18	-13.18	2.65	-2.34
2011	c1cnc(c1)SN	C15858165	-15.05	-3.48	-14.6	4.02	-0.99
2012	COc1=C(C(C1F)F)F)F)F	C16082643	-15.05	-1.45	-12.56	1.46	-2.5
2013	c1cc(c(nc1)N)O	C19015386	-15.05	-3.38	-16.65	4.08	0.9
2014	c1cncnc1C#N	C00331641	-15.04	0.2	-17.26	4.17	-2.15
2015	c1cc(ncc1Cl)[N+](=O)[O-]	C01580803	-15.04	-2.41	-14.59	5.76	-3.8
2016	c1cc(ccc1[S-])I	C02382815	-15.04	-0.88	-10.81	0.96	-4.31
2017	c1c(sc(n1)Cl)C(=O)Cl	C12370742	-15.04	-1.04	-16.78	2.36	0.42
2018	c1cc2nncn2cc1Br	C16124908	-15.04	-2.97	-16.54	6.8	-2.33
2019	c1cc(sc1CC#N)Cl	C19411203	-15.04	-2.64	-14.64	6.32	-4.08
2020	C/C(=C/C#N)/CCl	C22054708	-15.04	-1.61	-14.82	4.76	-3.37
2021	c1c(cnc(n1)N)C=O	C00249481	-15.03	-4.52	-15.99	6.77	-1.28
2022	c1cc(cnc1)C#N	C00331637	-15.03	0.71	-18.02	4.57	-2.3
2023	COc(=O)Nc1ccncc1	C00406333	-15.03	0.08	-19.75	5.49	-0.85
2024	c1c(nc(n1)Cl)Cl	C02141061	-15.03	-1.23	-14.97	2.61	-1.42
2025	c1cc(c(c(c1F)C=O)O	C02572868	-15.03	-2.44	-15.75	5.28	-2.12
2026	c1c(cnc(c1N)F)Cl	C08698192	-15.03	-1.31	-17.8	3.24	0.84
2027	c1ccc(c(c1)C(F)(F)F)N	C12358767	-15.03	-1.09	-15.32	2.43	-1.05
2028	CC(=O)OBr	C14989404	-15.03	-1.04	-14.69	3.1	-2.4
2029	CC(=O)c1c(ccs1)N	C00159898	-15.02	-2.42	-15.68	4.75	-1.67
2030	COc1ccccc1	C00393924	-15.02	-1.33	-15.01	3.37	-2.04
2031	Cc1cccc(n1)F	C00403520	-15.02	-0.69	-16.35	4.58	-2.55
2032	CCOc1nccs1	C01850626	-15.02	-2.07	-15.39	3.25	-0.81
2033	C=C(CCO)Br	C02530726	-15.02	-2.4	-14.15	2.17	-0.64
2034	c1cc(ccc1CO)N	C04271989	-15.02	-1.76	-17.47	3.83	0.38
2035	c1(ncc(s1)[S-])[S-]	C05425387	-15.02	-4.81	-14.86	6.22	-1.57
2036	Cc1ccc(c(c1)O)F	C00403180	-15.01	-1.74	-15.24	3.74	-1.77
2037	CSCc1ccco1	C00409334	-15.01	-0.3	-14.84	3.58	-3.44
2038	c1nc([nH]n1)NN=C(C#N)C#N	C03165161	-15.01	-2.11	-18.77	9.54	-3.67
2039	C(c1nc(on1)C(F)(F)Cl	C12362081	-15.01	1.51	-17.46	2.47	-1.53
2040	c1cc(nn2c1nnc2)Cl	C00240318	-15	-3.46	-15.15	6.95	-3.34
2041	c1cc(ccc1OC(=S)Cl)F	C00389825	-15	0.2	-16.55	1.92	-0.57
2042	c1c(c(nc(n1)Cl)N)N	C01677559	-15	-6.46	-14.88	5.73	0.62
2043	CCc1ccc(o1)C	C01995224	-15	-0.84	-13.25	2.73	-3.65
2044	C1C(=O)C(=CN=C1Cl)Cl	C02386405	-15	-2.49	-14.85	3.01	-0.66
2045	c1cc(c(cc1C#N)F)C(F)(F)F	C02560174	-15	-0.48	-14.74	4.34	-4.13
2046	C#CCn1cncn1	C03207447	-15	-2.4	-17.68	7.06	-1.99
2047	Cc1c(non1)C#N	C04343170	-15	-0.33	-15.46	2.53	-1.73
2048	c1cc(sc1)C(=O)N=[N+]=[N-]	C15784786	-15	1.66	-20.87	3.9	0.3
2049	CCCCO[N+](=O)[O-]	C16054440	-15	0.92	-13.54	1.59	-3.97
2050	Cc1nc(sn1)Cl	C19770067	-15	-0.13	-15.46	2.14	-1.56
2051	c1cc(sc1)SCC#N	C20078165	-15	-0.1	-15.44	4.52	-3.98
2052	c1c(c(ncn1)C(F)(F)F)N	C26461821	-15	-2.47	-16.71	5.43	-1.25
2053	c1ccc(c(c1)Nc2nccnc2)N)F	C00073736	-14.99	-0.47	-13.93	5.64	-6.24
2054	c1cc(ncc1N)C(F)(F)F	C00154421	-14.99	-2.62	-16.11	4.96	-1.21
2055	c1cc(c(cc1Cl)N)O	C00404323	-14.99	-1.12	-16.54	2.76	-0.08
2056	CC(=O)Oc1ccc(cc1)Cl	C00823280	-14.99	-0.49	-17.32	4.83	-2.01
2057	C/(C(=C/Cl)/Cl)SC#N	C01639296	-14.99	-0.54	-16.84	4.24	-1.84
2058	CCCC(=O)C(=O)C	C01663926	-14.99	-0.44	-13.68	2.26	-3.23
2059	c1cc(ccc1N)SC#N	C01757899	-14.99	-0.34	-16.44	3.96	-2.17
2060	Cc1ccsn1	C02031401	-14.99	-1.28	-15.29	3.55	-1.97
2061	C=Cc1cccc(c1)N	C02566109	-14.99	-0.14	-14.62	2.35	-2.58
2062	C=C(CSC(=NH2+))[S-]Cl	C05426445	-14.99	-0.56	-17.06	1.76	0.87
2063	c1cnc(cc1C#N)F	C12359106	-14.99	-0.55	-17.13	4.82	-2.12
2064	CCc1c(cccn1)O	C15951910	-14.99	-1.25	-16.52	3.88	-1.1
2065	c1cc(c(cc1O)N)N	C00388397	-14.98	-3.01	-18.69	4.21	2.52
2066	c1ccc(cc1)CCO	C00895934	-14.98	-1.22	-14.19	2.49	-2.06

2067	COc1c(ccc(c1F)F)F	C02382167	-14.98	0.05	-16.5	4.2	-2.74
2068	c1(c(n[nH]n1)N)C(=O)NN	C04878416	-14.98	-6.5	-17.51	5.71	3.33
2069	COc1nc(sn1)N	C17045321	-14.98	-4.07	-16.37	4	1.45
2070	c1c(nc(c1Br)N)O	C21981813	-14.98	-3.55	-17.9	5.88	0.59
2071	C1CC(=O)NN=C1C(=O)Cl	C32016271	-14.98	-1.96	-17.44	4.8	-0.37
2072	c1cc2c(cc[nH]2)cc1F	C00388684	-14.97	-1.4	-14.6	4.44	-3.41
2073	COc1c(c(c(c1F)F)F)F	C01583745	-14.97	0.04	-12.73	1.55	-3.84
2074	c1c(nc(n1)Cl)[N+](=O)[O-]	C01607263	-14.97	0.11	-17.73	2.74	-0.08
2075	c1ncncn1	C01718513	-14.97	-0.86	-14.76	3.5	-2.85
2076	c1nc(c(c(n1)N)[N+](=O)[O-])N	C04087396	-14.97	-0.76	-17.8	4.3	-0.71
2077	c1c(cnc(n1)[O-])[N+](=O)[O-]	C17174457	-14.97	-3.05	-18.58	4.71	1.96
2078	COC(=O)Cn1cncn1	C19993817	-14.97	-3.25	-16.78	6.36	-1.3
2079	CCc1[nH]cc(n1)Br	C22001002	-14.97	-2.04	-14.78	4.28	-2.42
2080	c1cnc2cncn2c1	C00389493	-14.96	-3.62	-17.4	10.55	-4.5
2081	COC(=O)/C=C/C=C	C02004075	-14.96	-1.05	-15.66	3.99	-2.24
2082	c1cc(c(cc1F)O)O	C02244021	-14.96	-3.47	-16.25	4.46	0.3
2083	Cc1[nH]cc(n1)I	C02583967	-14.96	-3.88	-13.82	5.09	-2.35
2084	C(OC(=O)Cl)Cl	C04521315	-14.96	-1.63	-14.22	2.88	-1.98
2085	c1ccc(cc1)COC(=O)N	C32914677	-14.96	-0.49	-17.15	4.63	-1.95
2086	c1cc2c(cc[nH]2)c(c1)F	C00403104	-14.95	-1.78	-14.99	5.24	-3.24
2087	CCSc1cccc1	C01674079	-14.95	-0.94	-11.4	2.22	-4.84
2088	C=CCOC=C	C01693372	-14.95	-0.3	-14.5	1.99	-2.14
2089	Cc1ccc(nc1)NC(=S)N	C05553560	-14.95	0.5	-17.58	4.56	-2.42
2090	c1ccc(cc1)N)F	C12649839	-14.95	-1.73	-12.13	1.64	-2.73
2091	Cc1ccc(c(c1)N)CC#N	C16678028	-14.95	-3.62	-13.83	5.74	-3.24
2092	CSc1nnc(s1)N	C18252372	-14.95	-2.92	-13.91	2.65	-0.77
2093	c1csc1C[NH2+]N	C19399364	-14.95	1	-18	2.67	-0.62
2094	CCc1ccc(cc1)S	C19735107	-14.95	-1.04	-10.77	1.44	-4.58
2095	Cc1ccc(o1)CN=C=O	C22861425	-14.95	-1.39	-16.84	4.16	-0.88
2096	C1CC(=O)N(C1)CCN=C=O	C32005302	-14.95	-2.33	-19.18	6.91	-0.35
2097	CCc1cc(ccc1O)F	C02539743	-14.94	-1.1	-14.17	2.74	-2.42
2098	Cc1cncnc1Cl	C02599069	-14.94	-1.68	-12.96	2.57	-2.86
2099	c1cc(ccc1N)Sc2[nH]nnc2	C19845532	-14.94	-3.21	-15.58	6.64	-2.79
2100	c1c(c(cnc1Cl)Br)N	C29786621	-14.94	-4.14	-13.23	3.71	-1.27
2101	Cc1ccc(cc1)I	M1995A021	-14.94	-0.23	-11.28	1.3	-4.73
2102	c1ccc(cc1)NCl	C01556464	-14.93	-2.32	-14.47	1.9	-0.03
2103	c1cc(c2nncn2c1)N	C01705761	-14.93	-3.45	-17.1	8.43	-2.81
2104	Cc1c([n+](on1)[O-])C(=O)N	C01761229	-14.93	-4.08	-16.4	5.33	0.22
2105	C=CCOC(C(F)F)F	C01997107	-14.93	-0.81	-13.99	2.65	-2.79
2106	c1ccc(cc1)F)N	C02506896	-14.93	-3.09	-16.31	4.99	-0.52
2107	c1c(c([n-]n1)C(F)F)F)N(=O)[O-]	C04243631	-14.93	-2.18	-15.32	4.47	-1.9
2108	c1nnc2n1[C@H](N=N2)[N+](=O)[O-]	C04343693	-14.93	0.05	-17.66	6.67	-3.95
2109	Cn1c(nnn1)N(C)N=O	C05052880	-14.93	-0.91	-15.97	3.97	-2.02
2110	c1c(scn1)CCO	C14766019	-14.93	-2.77	-16.37	4.02	0.19
2111	Cc1cncn1)N	C16124478	-14.93	-2.47	-16.47	4.33	-0.31
2112	c1ccc(cc1)OS	C19597470	-14.93	-1.58	-17.06	5.09	-1.39
2113	C(O)c1cccc1	W2004A007	-14.93	-1.22	-14.14	2.5	-2.07
2114	c1c[nH]c(=O)cc1C(F)F)F	C00132769	-14.92	-4.8	-16.48	8.19	-1.83
2115	c1cc(ccc1C#N)Br	C00164599	-14.92	-1.14	-15.6	3.19	-1.37
2116	c1cc(ccc1)Cl)N=C=O	C01707959	-14.92	-2.2	-14.19	2.18	-0.72
2117	c1cc(c(cc1C#N)F)O	C02558778	-14.92	-0.65	-17.99	5.2	-1.47
2118	CC(=C)C(=O)OCC#C	C02563333	-14.92	0.65	-16.31	4.47	-3.74
2119	c1cc(ncc1C(F)F)F)F	C03880144	-14.92	-1.37	-14.25	3.09	-2.39
2120	c1cnc([nH]1)NN	C08628559	-14.92	-4.1	-15.99	6.38	-1.21
2121	c1c(csn1)C=O	C20443581	-14.92	-2.05	-16.72	5.12	-1.27
2122	c1ccc(cc1)CNC(=S)C(=O)N	C20522688	-14.92	-2.83	-17.2	6.23	-1.12
2123	Fc1ccc(cc1)CCO	W2004A006	-14.92	-1.67	-14.06	2.91	-2.09
2124	CC(=S)Nc1cccc1	C00337295	-14.91	-0.9	-16.57	6.39	-3.83
2125	c1cc(c(c(c1)Cl)F)N	C00403487	-14.91	-1.07	-14.89	3.28	-2.22
2126	CC(=O)c1ccc1	C00410301	-14.91	-0.83	-15.63	4.59	-3.05
2127	c1cnc(c1)CCBr	C00807146	-14.91	-1.8	-13.58	3.48	-3.01
2128	C=CCOC(=O)CCl	C01677158	-14.91	-1.13	-14.77	4.25	-3.26
2129	C#Cc1ccc(cc1)C=O	C02548316	-14.91	0.51	-17.43	6.04	-4.01
2130	c1c(nc(n1)Cl)NN=O	C06524481	-14.91	-1.74	-17.98	5.14	-0.33
2131	CNc1cncn1	C14987933	-14.91	-2.14	-16.46	4.24	-0.55
2132	[H]N=c1[nH]c(cs1)O	C16969925	-14.91	-4.7	-15.3	3.43	1.65
2133	c1ccc(cc1)COC(=O)CO	C00395587	-14.9	-0.17	-19.83	7.75	-2.64
2134	c12c([nH]c(=O)c(=O)[nH]1)non2	C01235037	-14.9	0.71	-20.42	4.7	0.11
2135	Cc1ccc(o1)[N+](=O)[O-]	C01693511	-14.9	-2.44	-17.16	6.29	-1.59
2136	C[C@H](c1cccc1)O	C02539887	-14.9	-1.52	-15.93	3.26	-0.71
2137	c1cnc1C(=S)N	C02565045	-14.9	-2.69	-18.15	6.98	-1.03
2138	CCn1cc(n1)C=O	C04255822	-14.9	-2.71	-16.09	6.24	-2.34
2139	CC/C=C/C(=O)Cl	C04269657	-14.9	-1.14	-15.19	2.69	-1.26
2140	C=Cn1nc(nn1)N	C05853295	-14.9	-3.44	-16.57	5.77	-0.66
2141	c1c(cnc2c1nc[n-]2)C#N	C08417966	-14.9	-1.66	-18.36	8.05	-2.93
2142	c1cc(=O)[nH]cc1Cl	C08698076	-14.9	-2.2	-18.35	7.04	-1.39
2143	CC(=O)c1ccns1	C12650017	-14.9	-2.21	-14.78	4.01	-1.92
2144	c1cc2c(cc1C#N)nsn2	C30714676	-14.9	-2.85	-14.75	4.79	-2.09
2145	c1c(n2c(cn1)nnn2)N	C01585670	-14.89	-4.35	-18.31	7.24	0.53
2146	C(#N)c1c(c(c(c1F)F)F)F	C01845698	-14.89	1.33	-13.94	2.3	-4.59
2147	Cc1cp[nH]n1	C03957206	-14.89	-1.92	-15.35	2.4	-0.03
2148	c1ccc(nc(c1)F)F	C16159557	-14.89	0.31	-16.28	3.82	-2.75
2149	c1cnc(c1)/C=N)N	C17174158	-14.89	-2.53	-15.54	4.53	-1.35
2150	c1cnc(n1)CCCl	C19089269	-14.89	0.11	-16.19	5.11	-3.92
2151	c1cc(sc1)CNC(=O)N	C00090725	-14.88	0.36	-21.63	6.14	0.24
2152	c1cnc2c1sc2	C00334174	-14.88	-2.09	-16.59	3.65	0.16
2153	CCOCn1cncn1	C05905381	-14.88	-2.27	-17.14	4.63	-0.1
2154	c1c(cnc(n1)C(F)F)F)Br	C26440925	-14.88	-1.65	-13.4	2.97	-2.8
2155	c1c(c(cc(c1O)F)F)N	C00168054	-14.87	-2.81	-16.23	3.81	0.36
2156	c1ccc(cc1)NO	C00901466	-14.87	-3.24	-16.71	6	-0.91

2157	c1cc(ncc1C(F)(F)F)N[N+](=O)[O-]	C01231988	-14.87	-1.9	-16.18	6.89	-3.69
2158	c1cscc1Br	C01626895	-14.87	-1.16	-15.33	1.48	0.13
2159	C=COC(=O)CCI	C02507818	-14.87	-2.1	-14.3	4.4	-2.88
2160	[H]/N=C\1/n(ccs1)CC	C04105137	-14.87	-1.84	-14.3	4.06	-2.79
2161	COC(=O)Nc1ccc(c(c1)F)F	C05526236	-14.87	-0.58	-19.29	7.21	-2.22
2162	c1cc(ncc1)Cl	C08764173	-14.87	-2.7	-16.12	5.62	-1.67
2163	c1cc(=O)[nH]cc1Br	C08772776	-14.87	-2.09	-18.24	6.93	-1.47
2164	CCCc1nc([nH]n1)N	C13639955	-14.87	-3.02	-14.56	5.13	-2.41
2165	CCSSSS	C14590161	-14.87	0.63	-11.25	1.6	-5.86
2166	CNN=Cc1cccnc1	C17062281	-14.87	-0.2	-16.95	4.14	-1.85
2167	c1cncc(c1C(F)(F)F)[O-]	C19616318	-14.87	0.14	-17.11	3.08	-0.98
2168	Cc1cnc(nc1)F	C22016534	-14.87	-2.06	-16.29	5.43	-1.94
2169	Cc1ncc(cn1)N	C01644845	-14.86	-3.43	-15.76	4.63	-0.29
2170	c1cc(ncc1C#N)NN=O	C13213275	-14.86	-3.24	-18.06	8.06	-1.63
2171	Cc1ccc(o1)CCI	C20077984	-14.86	-1.1	-13.46	3.28	-3.58
2172	CCNC(=O)c1c(non1)N	C01295889	-14.85	-0.27	-17.89	3.27	0.04
2173	COC1c(cc(c1)F)Nf	C02527833	-14.85	0.21	-18.11	4.46	-1.41
2174	C1COC=C1C(=O)C(F)(F)F	C02568770	-14.85	-0.89	-15.4	3.68	-2.24
2175	c1cc(ncc1O)Br	C02599016	-14.85	-3.28	-15.47	4.1	-0.19
2176	CN(C(=O)NC(=O)N)C(=O)N=O	C04887722	-14.85	-0.84	-19.86	5.9	-0.05
2177	CC(=O)O/C=C\O/C(=O)C	C05029577	-14.85	-1.02	-17.43	7.21	-3.61
2178	c1c(ncc(=O)[nH]1)Br	C06732065	-14.85	-2.51	-18.32	6.11	-0.12
2179	c1c(c(cnc1Cl)[N+](=O)[O-])N	C15021890	-14.85	-3.79	-14.45	4.69	-1.3
2180	CCc1ccc(o1)[N+](=O)[O-]	C15784475	-14.85	-1.53	-15.75	5.98	-3.55
2181	Cc1nc(cs1)C(=O)C	C15855283	-14.85	-1.43	-15.6	4.51	-2.33
2182	c1cc2c(cc1F)CCO2	C16159654	-14.85	-1.31	-13.21	2.93	-3.27
2183	CSc1ccccc1F	C00404215	-14.84	0.09	-17.78	4.04	-1.2
2184	Cc1cc(=O)n(c(n1)N)N	C00497576	-14.84	-6.86	-14.29	7.21	-0.9
2185	c1c(nc2n1CCC2)Cl	C00497776	-14.84	-0.39	-17.31	6.45	-3.58
2186	Cn1cncnc1	C01095289	-14.84	-0.67	-14.76	4.07	-3.48
2187	C=CCCCO	C01845660	-14.84	-2.72	-12.95	1.98	-1.14
2188	c1cc(ccc1OCC)Cl	C02242619	-14.84	1.01	-18.06	2.74	-0.53
2189	c1cc(sc1C(=O)N)Cl	C02753342	-14.84	-2.51	-16.16	4.47	-0.65
2190	COnc1cnc1	C05285697	-14.84	-1.54	-15.63	4.62	-2.29
2191	c1cc(ncc1C#N)I	C12471965	-14.84	-1.83	-13.9	3.97	-3.08
2192	c1cc(cc(c1)Cl)NC(=S)NN	C13685566	-14.84	-1.04	-14.85	3.82	-2.78
2193	[H]/N=C(N)NNC(=O)C(F)(F)F	C20157005	-14.84	-0.82	-19.51	5.75	-0.26
2194	c1c[nH+]ccc1ON	C21985253	-14.84	-1.5	-17.32	4.24	-0.25
2195	Oc1c(cccc1)O	G2005A001	-14.84	-3.2	-16.49	4.57	0.28
2196	c1cc(c(nc1)I)O	C00160343	-14.83	-1.37	-17.14	4.44	-0.76
2197	CC(=O)c1cccnc1	C01607046	-14.83	-2.44	-16.84	5.46	-1.01
2198	c1cnc(cc1)Cl	C02526715	-14.83	-1.06	-16.29	3.05	-0.54
2199	C(=N/O)Nc1nnc(s1)C(F)(F)F	C04300298	-14.83	-2.89	-19.04	8.57	-1.47
2200	COC(=O)O/N=C/c1c(non1)N)N	C04843969	-14.83	-0.91	-17.15	4.49	-1.26
2201	COCc1cn[nH]n1	C05502939	-14.83	-3.31	-15.64	3.69	0.42
2202	c1cn2c(n1)NCCC2	C11920167	-14.83	-1.11	-16.35	6.05	-3.42
2203	CCO[N+](=O)[O-]	C16893044	-14.83	-1.02	-13.12	1.98	-2.67
2204	c1cc(ccc1N)Oc2[nH]nn2	C19090679	-14.83	-1.03	-22.05	7.01	1.23
2205	c1cc(ccc1F)COF	C00409279	-14.82	-0.02	-16.4	3.08	-1.48
2206	c1c(csc1[N+](=O)[O-])C#N	C00143162	-14.81	-1.78	-16.52	7.01	-3.51
2207	c1cc(oc1)/C=C/C(=O)Cl	C02568191	-14.81	0.29	-15.89	4.18	-3.39
2208	c1ccc2c(c1)C[C@H]2O	C03107553	-14.81	-1.69	-14.82	3.5	-1.81
2209	c1ccc(cc1)CCCN=O	C05773267	-14.81	-3.04	-15.8	4.09	-0.06
2210	c1c(c[nH]1)CCCl	C19089888	-14.81	-0.67	-16	4.06	-2.19
2211	c1cc(ccc1CCO)F	C00388332	-14.8	-1.71	-13.89	2.89	-2.1
2212	c1cc(cc(c1)N)C#N	C00388409	-14.8	-0.09	-16.72	4.08	-2.07
2213	CC(=O)Oc1ccccc1F	C02567799	-14.8	1.79	-19.31	7.09	-4.36
2214	COc1cnc(nc1)N	C03123156	-14.8	-2.87	-15.16	4.23	-0.99
2215	c1(nnc(o1)C(F)(F)F)C(F)(F)F	C04329254	-14.8	0.6	-17.15	1.32	0.43
2216	Cc1ccoc1C	C05239577	-14.8	-0.93	-13.73	2.81	-2.94
2217	CSc1nc([nH]n1)Cl	C06425446	-14.8	-3.81	-16.28	3.75	1.54
2218	Cc1ccc(o1)C(F)(F)F	C15442277	-14.8	-2.24	-12.11	2.92	-3.37
2219	c1c(nns1)C(=O)N=[N+]=[N-]	C17173515	-14.8	-1.6	-19.35	3.99	2.15
2220	c1(c(nsn1)N)C(=O)NN	C17322776	-14.8	-5.36	-17.69	5.29	2.95
2221	c1ccc2c(c1)ccs2	C01679161	-14.79	-1.48	-12.02	3.09	-4.38
2222	C/C(=C/(C#N)\[N+](=O)[O-])/N	C16951772	-14.79	-2.15	-15.58	3.3	-0.36
2223	Cc1ccsc1N=C=O	C19503704	-14.79	-1.22	-13.93	2.19	-1.83
2224	c1cnccc1C=O	C20441048	-14.79	-2.7	-18.17	7.06	-0.98
2225	COC(=O)[C@@H]1C[C@H]1[N+](=O)[O-]	C32627893	-14.79	-1.2	-16.65	6.1	-3.04
2226	c1cc(ccc1F)F(=O)Cl	C02140809	-14.78	-1.28	-15.54	4.06	-2.02
2227	c1ccc2c(c1)C[C@@H]2C#N	C02140856	-14.78	-1.45	-13.89	5.19	-4.63
2228	CCCON=O	C04262304	-14.78	-0.61	-13.23	1.91	-2.85
2229	c1(nnc(n1)N)N	C04558148	-14.78	-3.44	-17.64	4.44	1.86
2230	c1c(nc[nH]1)Cl	C04771902	-14.78	-3.16	-14.16	4.49	-1.96
2231	CC(=O)CCC(=O)C=C	C05283399	-14.78	0.17	-17.71	4.58	-1.82
2232	c1c(c([nH]1)C(=O)Cl)Br	C12357572	-14.78	1.03	-17.51	3.23	-1.53
2233	c1c(cnc(c1)N)Cl	C19230138	-14.78	-0.43	-14.98	2.51	-1.89
2234	c1(nnc(s1)Cl)C(F)(F)F	C21304390	-14.78	-1.76	-13.7	2.54	-1.87
2235	c1nc(nc(n1)N)N	C22126365	-14.78	-3.57	-16.41	7.2	-2
2236	c1cc(ccc1)F)CO	C00388395	-14.77	-1.22	-16.07	3.82	-1.3
2237	COc1ccc(c(c1)F)F	C00409288	-14.77	-2.2	-12.81	3.2	-2.95
2238	C1=CC(=O)C=CC1=O	C00895247	-14.77	-0.04	-17	4.3	-2.04
2239	Cn1cnc1Br	C01437392	-14.77	-0.76	-15.06	4.26	-3.2
2240	C=CCOCC=C	C01683669	-14.77	-0.36	-13.43	1.59	-2.57
2241	C=Cc1ccccc1	C01769022	-14.77	-1.42	-13.66	3.41	-3.1
2242	COC(=O)CCN=C=O	C02569575	-14.77	-0.41	-17.81	3.92	-1.48
2243	c1ccc2c(c1)cc([nH]2)C#N	C03123101	-14.77	-0.99	-16.36	3.65	-0.88
2244	c1c([nH]c(=O)[nH]c1=O)N=C=S	C03218501	-14.77	-1.35	-19.95	6.64	-0.11
2245	c1(nc2[nH]nc(n2)N)N	C05388813	-14.77	-3.12	-20.5	5.79	3.06
2246	c1c(cnc2c(n1)ncn2)N	C18556069	-14.77	-3.77	-18.77	10.26	-2.49

2247	Cc1ccsc1CCI	C20077986	-14.77	-0.6	-12.22	2.19	-4.15
2248	C1=C2[C@H](N=CN=C2N=N1)N	C20230332	-14.77	-1.68	-18.38	4.03	1.25
2249	C1CCC(C1)SC#N	C30714930	-14.77	0.22	-14.08	2.73	-3.64
2250	c1ccc(c(c1)CON)F	C00168989	-14.76	2.84	-18.89	3.17	-1.88
2251	Cc1ccc([nH]1)C	C01673420	-14.76	-1.18	-13.61	2.69	-2.66
2252	C1C[C@H](CC=C1)C(=O)Cl	C02560420	-14.76	0.13	-13.22	2.07	-3.74
2253	CC1=CC(=O)CC(=O)O1	C04273393	-14.76	-2.57	-15.49	5.91	-2.61
2254	CCOC(=O)N(C)N=O	C04403799	-14.76	-1.02	-16.54	3.42	-0.62
2255	CCOC(=O)c1c[nH]cn1	C13281753	-14.76	-0.66	-18.21	6.99	-2.88
2256	Cn1cccc/c1=N/N	C17109865	-14.76	-2.17	-14.33	4.1	-2.36
2257	c1ccc(c(c1)Cn2c(ccn2)N)F	C19392567	-14.76	1.92	-18.28	5.52	-3.92
2258	c1cnc(nc1)CC#N	C31829581	-14.76	-0.81	-19.1	7.44	-2.29
2259	c2cc1ccccc1s2	M1995A030	-14.76	-1.65	-11.81	3.08	-4.37
2260	c1csc1/C=C/[N+](=O)[O-]	C00101093	-14.75	0.92	-16.41	4.92	-4.18
2261	C(CO)NC(=O)c1c(non1)N	C02491560	-14.75	-5.59	-17.54	4.96	3.41
2262	Cc1cc(ccc1O)N)F	C02540120	-14.75	-3	-14.8	3.3	-0.24
2263	COC(=O)C(=[N+]=[N-])C(F)(F)F	C04268757	-14.75	0.46	-16.74	2.76	-1.22
2264	c1cnn(c1)C(=O)CCI	C04992598	-14.75	-2.81	-15.05	5.23	-2.12
2265	C(CO)C(=C(F)F)F	C08698326	-14.75	-2.79	-13.69	2.1	-0.38
2266	COc1cc(cnc1)N	C14982096	-14.75	-2.04	-16.95	4.18	0.05
2267	c1cc(=O)[nH]c(c1)Cl	C00388230	-14.74	-1.28	-18.04	6	-1.41
2268	c1cc(cc1CC)[N+](=O)[O-]	C01621103	-14.74	-3.17	-16.92	6.69	-1.33
2269	C=C(C(=O)OCC(C(F)(F)F)(F)F)F	C02573961	-14.74	0.09	-13.49	3.68	-5.01
2270	C(C(=O)Cl)(Cl)Cl	C04261781	-14.74	0.43	-14.75	1.78	-2.2
2271	Cn1c(ccn1)[N+](=O)[O-]	C06072268	-14.74	1.83	-17.98	4.3	-2.88
2272	c1ccc(c(c1)C)N)F	C19171896	-14.74	0.76	-18.47	4.33	-1.37
2273	c1nnc(s1)SCC#N	C19847667	-14.74	-1.86	-17.56	6.53	-1.84
2274	c1ccc2c(c1)csn2	C26479250	-14.74	-1.78	-14.67	4.91	-3.21
2275	c1(c(nc(nc1)F)C(F)(F)F)F	C02540464	-14.73	0.37	-12.87	0.71	-2.94
2276	c1csc(n1)C(=O)CBr	C04277256	-14.73	0.91	-17.77	4.37	-2.24
2277	CS/C(=C/C(=O)C(F)(F)F)/[O-]	C04521881	-14.73	-1.33	-14.12	2.32	-1.59
2278	Cc1c(c(n[nH]1)C#N)N	C04878135	-14.73	-1.95	-16.9	4.2	-0.08
2279	c1cc(cc(c1)F)N=[N+]=[N-]	C12505577	-14.73	0.13	-15.63	2.5	-1.73
2280	c1ccc2c(c1)C/C2=N/O	C13407686	-14.73	-4.15	-13.32	4.73	-2
2281	c1(c(nc([nH]1)Cl)[N+](=O)[O-])Cl	C17042366	-14.73	-2.35	-12.22	3.02	-3.18
2282	c1cc(c(nc1)Br)O	C00157191	-14.72	-1.44	-17.77	4.9	-0.41
2283	Cc1ccc(cc1N)Cl	C00157612	-14.72	-3.96	-10.24	2.18	-2.69
2284	c1cc(ccc1C#N)N=C=O	C00159625	-14.72	-2.26	-14.28	3.97	-2.15
2285	c1cc(c(cc1N=C=O)Cl)Cl	C01707972	-14.72	-2.24	-11.74	1.74	-2.49
2286	CCC(=O)SCC=C	C01850438	-14.72	-0.43	-15.68	2.6	-1.21
2287	C/C=C/C=C/C(=O)Cl	C02507466	-14.72	0.33	-14.49	2.99	-3.55
2288	c1cc(c(cc1N=C=O)C(F)(F)F)F	C02568131	-14.72	-2.77	-11.76	2.75	-2.94
2289	c1ccc(c(c1)C(=N/O)/N)O	C06322753	-14.72	-3.84	-17.75	5.97	0.89
2290	Cc1ccc(nc1)C#N	C15903639	-14.72	-0.83	-16.49	5.41	-2.82
2291	c1ccc(sc1CCl)Br	C20077998	-14.72	-1.57	-11.07	2.14	-4.22
2292	c1c(cc(c(c1)F)Cl)F)N	C22011423	-14.72	0.22	-17.77	4.99	-2.16
2293	c1cc(c(cc1CO)F)F	C00164814	-14.71	-2.16	-15.92	4.68	-1.32
2294	Cc1ccc(cc1)OC(F)F	C00167171	-14.71	1.08	-17.72	3.94	-2
2295	c1cc(c(cc1Cl)O)O	C00388291	-14.71	-2.15	-16.68	4.13	-0.01
2296	CC(=[N+]=[N-])C	C01575618	-14.71	-1.91	-14.89	5.19	-3.1
2297	C=C(C)C#N	C01759957	-14.71	-2.18	-13.73	3.25	-2.05
2298	COC(=O)C(F)(F)F	C02040619	-14.71	-1.72	-13.18	2.13	-1.94
2299	c1c(cc(c(c1O)Br)F)F	C02575683	-14.71	-0.6	-16.72	2.6	0.01
2300	c1cc(c(cc1N)C#N)N	C05200429	-14.71	-3.02	-15.54	4.27	-0.41
2301	COc1cccnc1	C13213189	-14.71	-0.85	-15.8	3.82	-1.89
2302	c1cnc(c1Br)O	C14982272	-14.71	-0.32	-17.4	3.31	-0.29
2303	c1cc(c(c(c1)F)C(F)(F)F)N	C16158162	-14.71	-2.48	-13.65	3.98	-2.57
2304	c1cc(ncc1C#N)N	C19441342	-14.71	-3.71	-15.73	6.06	-1.33
2305	CCNc1ccc(cn1)Cl	C20547374	-14.71	-3.51	-11.06	2.69	-2.83
2306	c1cc(c(cc1CC#N)F)F	C00155245	-14.7	-1.71	-18.3	8.59	-3.28
2307	COc1ccncc1	C00330918	-14.7	-2.74	-14	3.52	-1.48
2308	c1c(cc(c(c1)F)F)C#N	C00389548	-14.7	0.25	-15.02	3.66	-3.59
2309	c1ccc(c(c1)NC(=O)N2N=N2)F	C00401684	-14.7	0.17	-17.87	3.7	-0.7
2310	c1ccc(c(c1)/C=C/C(=O)O	C01704590	-14.7	0.08	-21.14	6.48	-0.12
2311	c1cc(c(cc1N)CBr)F	C02243179	-14.7	-0.63	-14.41	3.15	-2.81
2312	c1(=O)[nH]c(=O)ss1	C05339603	-14.7	0.4	-17.23	2.24	-0.12
2313	c1cc(ncc1Cl)I	C08698214	-14.7	-1.48	-11.95	1.99	-3.27
2314	Cc1ccc(c(c1)F)N)F	C12359260	-14.7	-2.75	-13.72	2.48	-0.71
2315	C#CCn1ccc1C=O	C20154855	-14.7	-0.97	-16.03	6.17	-3.88
2316	c1c(cnc(c1)F)C(F)(F)F	C30714979	-14.7	-1.06	-13.41	2.71	-2.94
2317	CC(=N)C1CCCC1C	C32601425	-14.7	0.11	-14.35	3.25	-3.72
2318	c1cc(ccc1CNC(=S)N)F	C00069387	-14.69	-1.67	-19.33	9.21	-2.9
2319	COC(=C)C=C	C01753295	-14.69	-1.21	-13.22	1.78	-2.04
2320	C#CC[C@H](c1ccccc1)O	C02390319	-14.69	-0.65	-14.54	3.63	-3.14
2321	c1c(ccc1C=O)Br	C02567282	-14.69	-1.51	-16.53	6	-2.65
2322	c1c(nc(s1)C=O)Br	C04198752	-14.69	-3.98	-13.44	4.25	-1.51
2323	c1cnc2nccn2c1	C12350100	-14.69	-2.7	-18.28	10.57	-4.29
2324	c1c(c(=O)nc([nH]1)N)C#N	C17039866	-14.69	-1.79	-20.19	6.05	1.24
2325	CNc1ccc(cc1)F)F	C20050277	-14.69	-3.7	-13.05	4.72	-2.66
2326	c1c(cc(cc1)F)C#N	C00156994	-14.68	0.68	-14.47	2.8	-3.69
2327	c1ccc(cc1)OC(=O)N	C00404454	-14.68	0.43	-20.95	6.24	-0.4
2328	Cn1cc(nc1)Br	C01095271	-14.68	-2.33	-14.65	5.66	-3.36
2329	c1cc(c(cc1OC(F)(F)O)F)F	C02527816	-14.68	-1.47	-14.74	2.79	-1.25
2330	c1c(ncc1)F)F	C02529896	-14.68	-1.25	-15.1	2.61	-0.95
2331	C=CCCC(=O)Cl	C02569933	-14.68	-0.72	-15.09	2.56	-1.44
2332	CSc1nccs1	C02570798	-14.68	-0.87	-14.94	3.12	-1.99
2333	c1ccc(cc1)/C=C/C=N/O	C12370146	-14.68	-2.22	-17.48	5.21	-0.19
2334	c1nnc(n1)N)N	C17878181	-14.68	-4.8	-16.21	8.13	-1.79
2335	c1cc(cc(c1)F)NC(=NH2+)N	C26423539	-14.68	0.59	-20.11	7.33	-2.48
2336	c1cnc2c(c1)cnn2	C00391481	-14.67	-3.37	-18.01	8.9	-2.18

2337	C1CC(=C1)CCO	C01767928	-14.67	-1.23	-14.04	1.99	-1.38
2338	c1ccc2c(c1)cc([nH]2)O	C02020050	-14.67	-3.57	-14.51	4.06	-0.66
2339	c1c(cn(n1))[N+](=O)[O-]][N+](=O)[O-]	C04291308	-14.67	-1.57	-14.75	4.12	-2.47
2340	CCSC(=S)N	C05598930	-14.67	-2.36	-14.37	0.99	1.08
2341	C1CC1c2nc(on2)CCl	C12803975	-14.67	-0.49	-16.31	4.65	-2.52
2342	c1c(scn1)C(=O)Cl	C26899047	-14.67	-1.9	-15.79	4.67	-1.65
2343	c1cc(cc(c1))N	C00013616	-14.66	-1.18	-12.71	1.91	-2.68
2344	c1c(c(c(c1F)F)F)C#N	C00389594	-14.66	1.44	-15.61	3.64	-4.13
2345	c1cn(cn1)CCC#N	C02387555	-14.66	-2.32	-16.72	8.37	-4
2346	c1c(cnc(c1Cl)F)Cl	C02525820	-14.66	-0.99	-15.24	2.1	-0.53
2347	c1c(c(=O)[nH]c1=O)[nH]1)NN=O	C04692071	-14.66	-4.69	-20.38	7.15	3.26
2348	C(#N)[NH+]=C([S-])[S-]	C05178345	-14.66	-5.29	-12.46	4.41	-1.32
2349	C(CN=[N+]=[N-])N=[N+]=[N-]	C05178766	-14.66	0.27	-17.25	1.79	0.53
2350	c1c(c(nc(n1)Cl)[O-])[N+](=O)[O-]	C05286129	-14.66	-0.47	-18.01	2.51	1.31
2351	CSCc1csc(n1)N	C17061540	-14.66	-1.6	-14.46	3.79	-2.4
2352	c1c(c([nH]1)C=N)O[N+](=O)[O-]	C01043046	-14.65	-4.12	-16.4	5.22	0.65
2353	c1ccc2c(c1)oc(=O)o2	C01090559	-14.65	-2.17	-14.98	6.23	-3.73
2354	CC(=O)SCCC=C	C01682812	-14.65	-0.63	-15.45	2.66	-1.23
2355	CCSCC#C	C02168531	-14.65	-0.59	-13.15	2.69	-3.59
2356	COC(=O)C(=C)CBr	C02539421	-14.65	-2.03	-12.81	3.14	-2.95
2357	c1cn(nc1[N+](=O)[O-])CO	C02552533	-14.65	-5.18	-16.97	7.75	-0.24
2358	C1C(=O)N=C(S1)N	C03860694	-14.65	-2.49	-16.03	3.85	0.01
2359	C(=O)(C(F)F)BrF	C04334582	-14.65	-0.44	-13.56	1.08	-1.73
2360	C/C=C/[C@H](c1ccccc1)O	C08579442	-14.65	-3.97	-11	3.4	-3.09
2361	c1cc(ncc1Br)NN	C08700532	-14.65	-4.42	-12.64	3.78	-1.37
2362	c1c([nH]c2c1c(=O)cc[nH]2	C12956316	-14.65	-4.09	-16.05	6.24	-0.76
2363	c1c(csc1[N+](=O)[O-])Br	C15782966	-14.65	-1.82	-13.42	4.31	-3.72
2364	Fc1c(c(c(c1F)F)F)F	M1995A007	-14.65	0.74	-12.48	0.71	-3.61
2365	C1CON=C1[N+](=O)[O-]	C01584492	-14.64	-0.63	-16.54	4.93	-2.41
2366	Cc1c(cnc1N)C	C02524881	-14.64	-3.67	-14.21	5.01	-1.77
2367	c1cc2c([nH]nc2cc1N	C04353646	-14.64	-5.29	-16.75	8.12	-0.72
2368	c1c(mns1)Br	C04946437	-14.64	-2.78	-14.86	4.14	-1.14
2369	C1CCC(=CC1)C#CC#N	C05382457	-14.64	-0.14	-14.69	2.61	-2.41
2370	c12[nH]nc(n1nc(n2)[O-])[N+](=O)[O-]	C06320734	-14.64	-1.14	-17.55	7.26	-3.21
2371	c1c([nH]cc1=O)N	C08672849	-14.64	-2.76	-17.21	3.93	1.41
2372	CCNc1ccccc1	C12358766	-14.64	-1.61	-11.58	1.78	-3.24
2373	c1cnc([nH]c1=O)N	C14419854	-14.64	-4.76	-17.32	7.98	-0.54
2374	C1=C(C(=O)[C@@H]2[C@H](C1=O)O2)O	C18177957	-14.64	-2.11	-18.54	5.16	0.85
2375	C(CC)c1ccccc1N	W2004A011	-14.64	-0.51	-12.33	1.78	-3.58
2376	c1cc(c2c(c1)[nH]n2)N	C00372332	-14.63	-5.06	-14.87	5.02	0.29
2377	c1cc(cnc1)CNC(=O)N	C00389733	-14.63	0.44	-23.37	7.37	0.93
2378	c1cc(ccc1NC=O)Cl	C00409833	-14.63	-1.85	-17.47	7.02	-2.33
2379	CC(=O)c1c(cccn1)N	C01420799	-14.63	2.18	-19.71	4.3	-1.41
2380	CC(=CCOC(=O)C)C	C02039792	-14.63	-0.12	-16.4	4.03	-2.15
2381	[C@H](OC(=O)Cl)Cl	C02242593	-14.63	0.75	-15.39	2.62	-2.61
2382	Cc1ccsc1Cl	C02504556	-14.63	-0.04	-12.85	1.74	-3.47
2383	c1cnccc1C=N/O	C04501411	-14.63	-3.09	-17.22	5.88	-0.2
2384	c1cnccc1NC(=S)N	C05594608	-14.63	-0.38	-18.23	4.47	-0.49
2385	c1cc(oc1)/C(=C)C(=O)C(F)F/[O-]	C05942173	-14.63	-0.78	-16.27	5.24	-2.82
2386	c1c(csc1C=N)O)Br	C13115191	-14.63	-3.34	-13.67	3.76	-1.37
2387	CC(=O)CCC=C	C01867148	-14.62	-0.3	-14.7	3.5	-3.12
2388	CC(=O)O/C=C/C=C	C02039494	-14.62	-0.24	-14.96	4.12	-3.54
2389	CCOC(=O)[C@@H](F)I	C02379348	-14.62	-0.02	-13.75	2.54	-3.4
2390	c1cc(sc1)C(=O)CCl	C02383794	-14.62	-1.54	-14.7	5.19	-3.57
2391	C(C(C(F)F)F)F)OC(F)F	C02560089	-14.62	-0.89	-12.57	2.85	-4.02
2392	Cc1c(cno1)I	C04277305	-14.62	-0.74	-13.53	2.48	-2.82
2393	C(C(=O)N)O/N=C(/c1c(non1)N)N	C04418887	-14.62	-3.53	-22.38	8.55	2.74
2394	Cc1cccn1C	C04689168	-14.62	-1.86	-12.51	3.16	-3.42
2395	C1=C(C(=O)NC1=O)Br	C13379821	-14.62	-1.5	-17.43	4.13	0.18
2396	c1cc(sc1)C#N	C00388338	-14.61	-1.66	-13.7	3.74	-2.99
2397	c1cncnc1	C00895216	-14.61	-1.62	-14.89	3.82	-1.92
2398	C=CC(=O)OC=C	C01680391	-14.61	-1.16	-14.71	3.98	-2.73
2399	c1cc(nnc1)C(=O)N	C01700271	-14.61	-3.4	-19.23	6.43	1.58
2400	CSc1nncn1N	C01942635	-14.61	-4.27	-13.93	5.9	-2.31
2401	Cc1ccc(cc1)NC	C02034345	-14.61	-0.02	-16.82	2.11	0.12
2402	c1cc(c(cc1N=C=S)F)F	C02555887	-14.61	0.6	-14.12	2.91	-4
2403	c1c(mns1)C=O	C02577969	-14.61	-2.77	-15.9	4.53	-0.48
2404	c1c(nc(o1)N)C(F)F	C04198753	-14.61	-3.64	-17.16	4.97	1.21
2405	c1ccc(c(c1)N=O)N=O	C05733483	-14.61	-2.39	-19.37	8.3	-1.14
2406	COc1cc(cnc1)O	C06643313	-14.61	-2.26	-17.25	4.27	0.62
2407	c1cc(cnc1)NC(=O)NN	C13281615	-14.61	-4.14	-18.41	7.17	0.78
2408	CCc1ccc(cn1)O	C15781951	-14.61	-1.65	-15.81	3.82	-0.98
2409	c1c(csc1CCl)Br	C20475277	-14.61	-0.65	-11.91	2.09	-4.14
2410	c1cc(sc1)CNC(=S)NN	C00039523	-14.6	-0.1	-20.41	8.04	-2.12
2411	[C@H](c1ccncc1)O	C00391918	-14.6	-1.85	-15.95	3.92	-0.72
2412	c1cc([nH]c1)C#N	C01868299	-14.6	-3.1	-13.86	4.46	-2.1
2413	c1cc(oc1)C(=O)CC#N	C02619065	-14.6	-2.45	-15.53	6.72	-3.34
2414	Cc1cc([nH]1)C(F)F	C04243651	-14.6	-3.14	-14.69	5.16	-1.93
2415	C(=O)(C(F)F)C(F)F	C04262093	-14.6	0.32	-13.79	0.88	-2.01
2416	c1ccc(cc1)N/C=C/O	C16978948	-14.6	-1.92	-17	7.78	-3.46
2417	Cc1nc2c(s1)ccs2	C22002134	-14.6	-1.11	-15.99	5.55	-3.05
2418	c1cc(nc1[N+](=O)[O-])F	C31176462	-14.6	-3.52	-14.81	6.24	-2.52
2419	CCOC(=O)C(F)F	C01755719	-14.59	-0.76	-13.02	1.87	-2.68
2420	c1cc(c(c(c1NN)F)F)F	C02243115	-14.59	-0.87	-16.51	4.52	-1.72
2421	c1ccc2c(c1)c(no2)[O-]	C03588816	-14.59	-2.46	-18.45	6.12	0.21
2422	c1cn(nc1N)C(F)F	C12397775	-14.59	-3.11	-14.93	4.25	-0.79
2423	C#Cc1c(cc(cn1)Cl)N	C32914748	-14.59	-3.76	-15.18	6.11	-1.76
2424	c1cc(oc1C(=O)Cl)[N+](=O)[O-]	C01621102	-14.58	-1.52	-14.92	4.57	-2.71
2425	c1c(cc(c(c1F)N)F)C#N	C01719547	-14.58	0.22	-16.11	3.43	-2.12
2426	CCC1=CCC(=O)O1	C01721525	-14.58	-0.88	-15.47	5.26	-3.49

2427	CSSSCC=C	C01850544	-14.58	-0.29	-13.72	1.8	-2.37
2428	CSCC=C	C02015871	-14.58	-0.23	-12.86	1.48	-2.97
2429	c1cc(nc(c1F)F)F	C02585565	-14.58	-1.79	-15.5	4.76	-2.05
2430	c1ccc(cc1)O	C05133329	-14.58	-3.01	-14.55	4.19	-1.21
2431	c1cc(=O)[nH]c(c1)Br	C08698198	-14.58	-1.23	-18.04	6.13	-1.45
2432	c1c(ncnc1O)N	C14982076	-14.58	-4.28	-16.42	4.41	1.71
2433	c1cn(cn1)C(=O)N	C15880087	-14.58	-4.55	-17.01	7.55	-0.56
2434	c1cn(cn1)CCBr	C19414770	-14.58	-0.71	-14.3	4.48	-4.05
2435	c1c(cnc(c1N)N)N	C21985591	-14.58	-5.52	-18.06	7.02	1.98
2436	c1csc2n1cc(n2)CBr	C00078823	-14.57	-2.19	-15.05	6.94	-4.27
2437	c1cc2c(cc1C#N)nns2	C00171442	-14.57	-2.16	-16.17	6.49	-2.73
2438	CCOC(=O)[C@H](C)F	C02379402	-14.57	-0.58	-14.83	3.86	-3.02
2439	c1(c(c(nc(c1F)F)F)F)O	C10157846	-14.57	-1.62	-15.68	2.74	-0.01
2440	c1cn2cncc2c(=O)[nH]1	C17025297	-14.57	-4.03	-18.73	10.33	-2.14
2441	CC(=O)c1cccc1	C00157401	-14.56	-1.8	-15.39	4.95	-2.32
2442	Cc1c(non1)C(=O)CBr	C01295929	-14.56	2.98	-17.72	2.54	-2.36
2443	c1ccnc(c1)F	C01680673	-14.56	-1.61	-15.38	4.43	-2
2444	c1cc(c(cc1N)F)O	C02567358	-14.56	-2.94	-16.42	4.34	0.46
2445	Cc1nccn1	C02582016	-14.56	-0.51	-16.08	4.08	-2.06
2446	C=CCSc1[nH]ncn1	C05517733	-14.56	-2.11	-16.97	3.65	0.87
2447	c1cc(cc1)N)C=O	C19702477	-14.56	-4.86	-15.78	6.98	-0.9
2448	c1cc(nc(c1[+])=O)[O-]N)Br	C21985743	-14.56	-3.04	-13.17	3.81	-2.16
2449	Cc1c[nH]nc1C	C00967493	-14.55	-2.49	-14.67	4.22	-1.6
2450	Cc1ccc(o1)C	C01693339	-14.55	-0.94	-13.44	2.89	-3.06
2451	Cc1c(non1)C(=O)NN	C01761224	-14.55	-2.72	-16.86	4.02	1.01
2452	c1cc(sc1)C=C/C#N	C02164362	-14.55	-1.47	-15.26	3.94	-1.76
2453	Cc1[nH]cc(n1)Br	C02529806	-14.55	-1.73	-14.78	3.98	-2.02
2454	c1cc(=O)[nH]cc1I	C02559902	-14.55	-2	-16.43	5.8	-1.92
2455	Cc1c(cccn1)Cl	C02598976	-14.55	-1.85	-12.46	2.66	-2.9
2456	c1cc(c(nc1)F)F	C02598987	-14.55	-1.62	-16.08	5.19	-2.05
2457	CSc1[n-]nc(n1)C(F)F	C06425444	-14.55	-3.02	-12.72	3.62	-2.44
2458	c1ccc(cc1)OC(=S)N	C06575458	-14.55	-0.71	-18.44	3.19	1.41
2459	c1cc(ncc1N)I	C12359488	-14.55	-1.63	-15.44	3.76	-1.24
2460	c1cnoc1C=O	C15020993	-14.55	-1.59	-16.13	4.48	-1.31
2461	C(#N)C(=N/O)/c1c(non1)N	C15221727	-14.55	-1.9	-19.08	5.01	1.43
2462	c1cc(c(c1c1N)F)FBr	C15444572	-14.55	-1.08	-15.28	4.1	-2.29
2463	c1nc(sn1)N	C16977388	-14.55	-4.15	-14.31	4.55	-0.63
2464	Cc1cc(ccc1F)O	C00389596	-14.54	-0.54	-15.16	2.9	-1.75
2465	c1ccc(cc1)OC[C@H]2CO2	C01462351	-14.54	-2.76	-14.31	4.88	-2.34
2466	c1ccc(cc1)Cc2ccc[nH]2	C01574588	-14.54	0.29	-17.52	3.43	-0.74
2467	COc(=O)Sc1ccc(cc1)F	C01604544	-14.54	-0.58	-16.08	4.07	-1.95
2468	c1ccc(cc1)[C@H](CBr)O	C04071989	-14.54	-1.32	-13.45	2.92	-2.69
2469	c1nc2n(n1)[C@H](N=N2)[N+](=O)[O-]	C04593310	-14.54	-2.66	-14.49	5.21	-2.61
2470	C(CCl)N(C(=O)N)N=O	C04705960	-14.54	-3.53	-15.14	3.48	0.64
2471	C=COCC=C	C05157937	-14.54	-0.02	-14.93	3	-2.59
2472	c1[nH]nc(n1)Br	C06119231	-14.54	-5.31	-15.03	7.85	-2.05
2473	Cc1nc(sn1)N	C08652409	-14.54	-5.26	-14.54	5.97	-0.71
2474	Cc1ccc(cn1)NN	C21298527	-14.54	-1.99	-17.36	5.5	-0.69
2475	c1c[nH]c2c1nnc2	C21298867	-14.54	-4.84	-16.7	8.87	-1.87
2476	c1c(cc(cc1F)F)C(=O)N=C=S	C21963792	-14.54	2.56	-17.25	3.37	-3.21
2477	c1cc(c(nc1)Cl)O	C00164485	-14.53	-1.58	-17.67	5.03	-0.31
2478	CC(=C)C(=O)OCC=C	C01561515	-14.53	-0.62	-15.06	3.69	-2.54
2479	CCNC(=O)OCC=C	C01682119	-14.53	-1.77	-15.85	4.25	-1.15
2480	CC(=O)OCC=C	C01683665	-14.53	-0.32	-15.4	3.94	-2.76
2481	c1cc(c(cc1CBr)F)N	C02243165	-14.53	-1.8	-16.26	3.01	0.52
2482	c1cc(nnc1N)N	C02551261	-14.53	-3.97	-17.81	6.64	0.61
2483	Cn1nc(n1)[N+](=O)[O-]	C02755199	-14.53	-4.32	-15.32	10.02	-4.91
2484	c1c2nncn2cnc1Cl	C12505138	-14.53	0.17	-18.86	8.79	-4.63
2485	c1cnn(c1N)CCC#N	C26545198	-14.53	-3.05	-17.43	7.88	-1.93
2486	CCOC(=O)Cl	C02034866	-14.52	-0.68	-13.72	2	-2.12
2487	c1c(ccn1)CCO	C02559654	-14.52	-2.69	-16.42	4.46	0.13
2488	COc(=O)C1ccc(cc1)F	C02570118	-14.52	-1.06	-16.56	5.69	-2.6
2489	Cc1cncc(n1)Cl	C04287800	-14.52	-0.7	-15.87	3.58	-1.53
2490	Cc1cc(c(s1)C#N)N	C15442537	-14.52	-1.98	-15.37	4.79	-1.96
2491	C=CC[C@H](CC)O	C31829554	-14.52	-1.54	-13.91	2.32	-1.4
2492	COc(=O)c1cc[nH]n1	C32445539	-14.52	-1.78	-16.7	5.34	-1.39
2493	c1cnccc1C=O	C00157163	-14.51	-2.07	-16.43	5.76	-1.77
2494	CC/C=C/CCO	C01531144	-14.51	-1.96	-13.3	1.91	-1.16
2495	c1c(sc(n1)[O-])[N+](=O)[O-]	C01603230	-14.51	-3.22	-18.96	7.27	0.39
2496	C[C@H](CO[N+](=O)[O-])[O-][N+](=O)[O-]	C04743757	-14.51	-0.15	-13.95	3.92	-4.34
2497	c1nc([n-]n1)NC2=CC(=O)CCC2	C06062900	-14.51	0.79	-18.1	7.88	-5.08
2498	CNC(=O)n1cnc(n1)N	C16981303	-14.51	-5.72	-13.93	6.76	-1.63
2499	c1cc(nc(c1)Br)N	C19735573	-14.51	-2.01	-15.55	4.63	-1.59
2500	CCOC(=O)CCl	C20231543	-14.51	-0.24	-13.15	2.77	-3.89
2501	Cc1cc(no1)C(=O)C	C32501215	-14.51	-0.62	-15.79	4.41	-2.52
2502	c1csc1CO	C00158760	-14.5	-1.21	-16.17	3.33	-0.45
2503	c1csc(c1C#N)N	C00159971	-14.5	-2.96	-15.32	5	-1.23
2504	Cc1nccs1	C02510297	-14.5	-1.73	-14.16	3.22	-1.84
2505	c1cnc(n1)CCO	C02566780	-14.5	-5.46	-16.28	5.98	1.25
2506	C=CC(=O)OCCF	C02584299	-14.5	-0.61	-16.14	5.1	-2.86
2507	C=CCNC(=S)N	C03875768	-14.5	-2.72	-14.48	3.05	-0.35
2508	[H]/N=C/(c1c(non1)N)OC	C05248327	-14.5	0.42	-19.77	3.54	1.31
2509	Cc1cccnc1C	C08294963	-14.5	-0.38	-14.41	3.27	-2.99
2510	c1([nH]c(=O)n1)N)N	C17105082	-14.5	-4.61	-16.34	5.93	0.52
2511	c1cc(cc(c1)Nc2nccs2)N	C19432130	-14.5	0.47	-18.08	5.53	-2.42
2512	c1csc(c1C=O)C=O	C00160395	-14.49	-2.27	-16.71	6.7	-2.2
2513	c1c(c(c(c1F)F)[O-])F	C00406984	-14.49	-1.55	-14.41	3.09	-1.62
2514	COc(=O)c1ccno1	C02381208	-14.49	-0.64	-15.92	4.18	-2.1
2515	c1c(c(cc(c1F)N)F)C#N	C02556403	-14.49	1.22	-18.41	4.81	-2.1
2516	C/C=C/C(=O)N=C=S	C04253936	-14.49	-0.49	-16.28	4.13	-1.85

2517	C/C=C(C(=O)OC=C	C13380325	-14.49	1.16	-15.88	3.56	-3.33
2518	C(c1[nH]c(nn1)[S-])S	C16754627	-14.49	-2.67	-16.15	5.99	-1.66
2519	c1ccc(cc1)OC(=O)N=C=S	C22006795	-14.49	0.34	-18.81	6.5	-2.51
2520	Oc1c(cccc1)CCC	W2004A003	-14.49	-0.86	-13.14	2.54	-3.03
2521	c1cc(ccc1C=O)C#N	C00156750	-14.48	-0.89	-17.28	7.05	-3.35
2522	c1cc(ccc1C=O)Cl	C00896325	-14.48	-0.27	-15.42	4.69	-3.49
2523	Cc1ccc(s1)O	C01701785	-14.48	-4.32	-14.34	3.14	1.04
2524	C(CN=C=S)C(=O)Cl	C01755319	-14.48	0.7	-18.55	2.38	0.99
2525	c1cc(cnc1)C(=O)NO	C02558618	-14.48	-6.05	-18.41	8.14	1.85
2526	CCCCSC(=NH2+)N	C04582268	-14.48	-2.43	-12.67	2.37	-1.75
2527	c1c2c([nH]n1)nc([nH]c2=O	C13298313	-14.48	-3.55	-19.95	9.68	-0.67
2528	c1c(cnc1)O	C14400981	-14.48	-1.03	-15.49	2.82	-0.78
2529	Cc1c(n[nH]n1)C(=O)C	C16265729	-14.48	-3.09	-15.11	4.22	-0.51
2530	c1cnc(c1C(F)F)F	C00077224	-14.47	0.68	-16.62	2.88	-1.41
2531	CC(=C)C[N+](=O)[O-]	C01575619	-14.47	-1.17	-15.32	3.38	-1.36
2532	CC(=C)CC#N	C01669345	-14.47	-0.3	-14.57	2.81	-2.4
2533	Cc1cc(cnc1F)C#N	C02384025	-14.47	-0.42	-15.58	4.33	-2.8
2534	c1csc(n1)CC#N	C04228173	-14.47	-2.65	-16.58	6.99	-2.23
2535	c1cc(sc1)C=N/O	C04582794	-14.47	-3.66	-15.51	5.53	-0.83
2536	c1cc2c(cc1O)n[nH]n2	C06567234	-14.47	-5.52	-18.23	8.18	1.09
2537	c1cc(sc1C=N)OBr	C12359046	-14.47	-1.82	-18.3	4.43	1.22
2538	Cc1cc(on1)C(F)F	C12398509	-14.47	0.81	-15.29	2.85	-2.84
2539	c1ccc(c(c1)N)N=[N+]=[N-]	C20495219	-14.47	-1.89	-15.61	3.29	-0.26
2540	c1cc(c(cc1O)Cl)F	C00164535	-14.46	-3.67	-12.47	3.29	-1.61
2541	Cc1ccnnc1	C01603717	-14.46	-2.13	-16.06	5.38	-1.65
2542	c1ccc(cc1)OCC#N	C01681319	-14.46	-0.4	-16.59	6	-3.47
2543	C(=O)C(=C(Cl)Cl)Cl	C02038399	-14.46	-1.37	-13.24	2.59	-2.44
2544	c1c(cncn1)CO	C02511464	-14.46	-3.73	-17.7	5.09	1.88
2545	c1cc(sc1)CNC(=S)N	C13535068	-14.46	-1.89	-18.9	8.54	-2.21
2546	c1cnc2c(n1)[nH]cn2	C15895404	-14.46	-4.08	-18.78	10.43	-2.03
2547	Cn1cncnc1=O	C00330833	-14.45	-3.11	-17.45	8.29	-2.18
2548	c1cc(ccc1C#N)NN	C00396173	-14.45	-0.54	-17.12	5.02	-1.8
2549	Cc1ccc(cc1)OC(=O)C	C00409286	-14.45	-0.17	-15.12	5.68	-4.84
2550	C1=CC(=CO)C=C1	C05133089	-14.45	-1.04	-13.98	3.21	-2.65
2551	c1cc2c(cc1)noc2nc1[O-]	C05636149	-14.45	-5.84	-17.05	7.17	1.27
2552	c1cc(c(c1)F)O	C16159287	-14.45	-3.12	-15.73	4.13	0.27
2553	c1cc(sc1)CO	C00157467	-14.44	-1.29	-16.09	3.59	-0.65
2554	Cc1c(snn1)Cl	C01391101	-14.44	-0.34	-15.28	2.7	-1.53
2555	Cc1cc(cnc1)C=C	C01435983	-14.44	0.27	-14.32	3.02	-3.4
2556	CC(C)CCO[N+](=O)[O-]	C02034832	-14.44	0.47	-14.29	1.45	-2.06
2557	C=CCOCc1ccccc1	C02555302	-14.44	1.2	-13.78	2.58	-4.44
2558	c1(nnc(n1N)[S-])C(F)Cl	C04294112	-14.44	-5.49	-10.58	3.69	-2.07
2559	C#CCSC(=NH2+)N	C04627434	-14.44	-0.88	-15.51	2.94	-0.99
2560	C(=C(N=O)Cl)(NO)Cl	C05178359	-14.44	-7.96	-14.37	6.95	0.94
2561	c1c(ncn1)Cl)C#N	C05784094	-14.44	-1.44	-16.77	4.27	-0.5
2562	C=Cc1c(ccc1)C=O	C06665692	-14.44	0.32	-17.15	5.25	-2.87
2563	c1cc2c(c[nH]c2nc1)Cl	C08729948	-14.44	-4.22	-11.84	4.81	-3.18
2564	CN/C(=NC#N)[S-]	C12243856	-14.44	-5.75	-13.05	7.58	-3.22
2565	c1cc(nnc1C(F)F)Cl	C19616299	-14.44	-2.72	-14.12	4.86	-2.46
2566	CCc1cc(n[nH]1)C(F)F	C26547615	-14.44	-3.78	-12.58	4.93	-3.01
2567	c1cc(ccc1CNC(=S)NN)F	C00103927	-14.43	0.12	-20.27	8.51	-2.79
2568	c1cc(ccc1SC#N)Br	C01597251	-14.43	-1.87	-14.81	3.29	-1.04
2569	c1cnc(nc1)Cl	C01676249	-14.43	-2.49	-15.16	5.08	-1.86
2570	c1ccc(c(c1)[N+](=O)[O-])F	C01682934	-14.43	-3.19	-15.21	7.81	-3.84
2571	c1c(cncn1)F	C01845840	-14.43	-0.73	-15.68	2.56	-0.59
2572	c1csc2c1C(=O)CC2	C02345435	-14.43	-0.64	-16.61	6.19	-3.37
2573	c1cnc(c1Cl)Cl	C02386413	-14.43	-2.27	-14.34	2.26	-0.07
2574	c1cnc([nH]1)I	C02531019	-14.43	-1.52	-15.56	4.44	-1.79
2575	c1c(c[nH]c(=O)c1F)Br	C08698166	-14.43	-2.27	-18.58	7.94	-1.53
2576	c1(c(n[nH]n1)Cl)C(=O)N=[N+]=[N-]	C13764156	-14.43	0.08	-21.72	4.39	2.82
2577	c1c(n[nH]c1N)C(F)F	C18217802	-14.43	-5.01	-15.56	6.7	-0.56
2578	c1csc2n1cc(n2)CCl	C20272873	-14.43	-2.28	-15.24	7.31	-4.22
2579	c1c(csc1Br)C=O	C20282211	-14.43	-0.28	-14.65	3.42	-2.92
2580	C/C(=NH+)C#N)/NC	C21984054	-14.43	-1.81	-13.64	3.8	-2.78
2581	c1c(c(n[nH]1)C=O)Cl	C01494998	-14.42	-1	-16.14	3.65	-0.92
2582	c1c(cnc(n1)NN)Br	C01495002	-14.42	-2.69	-13.56	3.52	-1.7
2583	CC(=O)NCCc1cncn1	C01601708	-14.42	-0.91	-22.76	7.49	1.76
2584	Cn1cnc1Cl	C01845610	-14.42	-2.11	-13.33	4.11	-3.08
2585	c1cc(c(c1F)O)F)Cl	C02381671	-14.42	-1.78	-16.06	3.8	-0.38
2586	C(=O)(C(=O)F)C(F)F	C02525507	-14.42	-0.11	-14.79	1.66	-1.19
2587	c1cnc([nH]1)Br	C02577854	-14.42	-2.65	-14.61	4.55	-1.71
2588	c1cc(ccc1N=O)Br	C03850578	-14.42	-1.48	-15.35	2.2	0.22
2589	c1ccc(cc1)NC(=S)C(=O)N	C04358287	-14.42	-4.51	-14.46	5.47	-0.92
2590	c1c(c(cc1F)Cl)F)C#N	C19615480	-14.42	-0.52	-13.02	3.18	-4.06
2591	c1cnc1C=O	C20417648	-14.42	-1.71	-16.56	5.03	-1.17
2592	c1cc2nncn2cc1Cl	C22995851	-14.42	-2.33	-14.7	7.2	-4.59
2593	c1ccc(cc1)Cn2c(nnn2)N	C00247141	-14.41	0.06	-19.36	8.57	-3.68
2594	c1ccc(c(c1)NC=O)O	C00393914	-14.41	-2.32	-19.12	6.99	0.05
2595	c1cc(ccc1F)NC=O	C01685769	-14.41	-2.83	-15.96	6.44	-2.07
2596	CCOC(=O)Cl	C01689384	-14.41	-1.17	-13.29	3.32	-3.26
2597	c1cc(ccc1C(F)F)O	C01847459	-14.41	-1.23	-15.16	2.98	-1
2598	C(OC(=O)OCC)Cl	C02511045	-14.41	-2.05	-14.49	4.68	-2.55
2599	c1(c(non1)Oc2c(non2)[N+](=O)[O-])[N+](=O)[O-]	C04343708	-14.41	-0.44	-13.29	0.73	-1.4
2600	CC=C=CCO	C04658605	-14.41	-1.51	-13.44	1.79	-1.25
2601	CC(=O)CC(=O)C	C04720638	-14.41	-2.71	-13.84	3.94	-1.8
2602	c1cnc(nc1)NN	C17748851	-14.41	-1.48	-17.15	5.7	-1.48
2603	c1csc(n1)NCC(=O)N	C20559709	-14.41	-5.13	-17.51	7.28	0.96
2604	c1cc([nH+])c(c1[O-])F)Br	C21982774	-14.41	-1.37	-17.32	4.57	-0.3
2605	Cc1ccc(cc1)NC=O	C00337958	-14.4	-1.93	-17.16	7.17	-2.48
2606	c1cc(c(cc1F)Br)O	C00409324	-14.4	-0.34	-17.38	2.77	0.55

2607	CCOCc1ccco1	C01668234	-14.4	-0.61	-14.97	3.75	-2.56
2608	CC(=O)OCC(=O)Cl	C02019437	-14.4	0.55	-16.99	4.78	-2.74
2609	c1cc(oc1C(=O)Cl)Br	C02574178	-14.4	-1.66	-16.14	4.11	-0.71
2610	c1cnc2nc(cn2c1)N	C03218662	-14.4	-3.27	-18.29	10.46	-3.3
2611	c1cc2c(c[nH]2)c(c1)O	C04204272	-14.4	-2.54	-16.92	5.22	-0.16
2612	C/C=C/SSC	C05371734	-14.4	-0.97	-13.76	1.62	-1.3
2613	Cn1cnc(n1)N	C13451776	-14.4	-3.55	-15.47	7.07	-2.45
2614	c1cnc(c(=O)c1)N[N+](=O)[O-]	C15767170	-14.4	-0.3	-22.15	10.59	-2.55
2615	CCc1cc(=O)[nH]nc1	C17108646	-14.4	-2.93	-17.12	6.77	-1.12
2616	CCN/C=C/1C=CC=[NH+]	C17378191	-14.4	1.1	-16.77	3.19	-1.92
2617	c1c(cnc(c1)[N+](=O)[O-])N)C#N	C21981864	-14.4	-1.95	-16.47	5.87	-1.85
2618	COC(=O)OCC(=O)Cl	C22002285	-14.4	-2.61	-14.49	5.21	-2.51
2619	c1cnc(cn1)C(=O)N	C00002005	-14.39	-4.94	-17.44	6.42	1.59
2620	c1cc(sc1)C(=O)N	C00153111	-14.39	-3.21	-16.93	5.94	-0.19
2621	c1cc(occ1C#N)C#N	C00391934	-14.39	-1.84	-14.52	5.9	-3.93
2622	CCC(=O)COC(=O)C	C00393908	-14.39	0.76	-18.14	6.5	-3.5
2623	Cc1cnoc1	C02529291	-14.39	-1.5	-14.55	3.58	-1.91
2624	C(C(F)(F)F)OC([C@@H](F)Cl)(F)F	C02560093	-14.39	-1.31	-13.13	2.91	-2.86
2625	c1c(c(cs1)C(=O)N)N	C04344037	-14.39	-5.45	-15.73	4.45	2.34
2626	c1(c(nH)n1)N)C(=S)N	C04878413	-14.39	-3.54	-18.95	6.6	1.51
2627	CCOC(=O)C(=N)N)C	C05046670	-14.39	-2.98	-13.68	3.76	-1.5
2628	c1cc(nc1Sc2[nH]ncn2)N	C19869342	-14.39	-3.49	-16.13	7.27	-2.04
2629	c1c(c(cs1)C=O)C=O	C22003342	-14.39	-2.7	-17.65	8.02	-2.07
2630	CS1cc(nnc1)N	C30678126	-14.39	-1.9	-17.8	6.42	-1.11
2631	C=COCCOC=C	C01603457	-14.38	-0.34	-16.26	4.11	-1.9
2632	c1[nH]c2c(n1)CCCC2	C01734290	-14.38	-2.75	-13.64	5.31	-3.3
2633	CC(=O)C(=O)C(=O)C	C01754507	-14.38	0.62	-17.62	4.52	-1.9
2634	CCSC(=O)Cl	C02033138	-14.38	-1.02	-13.04	2.01	-2.33
2635	c1cc2c(cc1F)OC(O2)(F)F	C02560205	-14.38	0.27	-15.71	2.78	-1.73
2636	c1cc(occ1OCC#N)F	C02580715	-14.38	-0.6	-17.16	6.88	-3.51
2637	Cc1c[nH]c(n1)Cl	C04771953	-14.38	-2.96	-14.07	4.64	-1.99
2638	[H]/N=c1/n(nnn1C=C)C	C04984238	-14.38	-3.87	-12.08	3.73	-2.15
2639	Cc1c([nH+][nH]c1)N)C	C16769947	-14.38	-3.64	-14.53	4.55	-0.75
2640	CCc1ccc(cn1)Br	C21304087	-14.38	-2.01	-11.02	2.37	-3.72
2641	Cc1ccccc1C	M1995A034	-14.38	-0.93	-10.78	1.62	-4.29
2642	c1cc(ccc1N)OC(F)(F)F	C00081472	-14.37	-0.13	-15.22	2.53	-1.54
2643	CC(=O)NC/C(=C)Cl/Cl	C01674053	-14.37	-0.52	-19.66	5.18	0.63
2644	c1ccc(cc1)C(=O)C(F)(F)F	C01675545	-14.37	1.68	-15.05	3.01	-4.01
2645	CCOC(=O)CN=C=S	C02014870	-14.37	-1.36	-15.88	5.1	-2.23
2646	[C@]1(C(O1)(F)F)(C(F)(F)F)Br	C16082669	-14.37	-0.11	-13.19	0.36	-1.43
2647	CO/C=C/C=C	C16893178	-14.37	-1.73	-12.63	2.21	-2.22
2648	Cc1c(csn1)N	C26461281	-14.37	-2.71	-15.71	4.49	-0.44
2649	c1cc(cnc1)CO	C00001799	-14.36	-1.38	-17.81	4.72	0.11
2650	c1cnc(cn1)F	C01585904	-14.36	-4.11	-15.57	5.84	-0.52
2651	c1(nnc(s1)Br)N	C04468797	-14.36	-4.69	-14.2	4.94	-0.4
2652	c1c(c(=O)[nH]cn1)Br	C05425261	-14.36	-2.29	-17.82	3.63	2.13
2653	c1cnc([nH]1)CCl	C01494936	-14.35	-1.55	-16.13	5.35	-2.01
2654	C=NNc1ccccc1	C01692376	-14.35	-2.44	-15.53	4.1	-0.48
2655	CN(C(=O)NCCF)N=O	C04921203	-14.35	-2.3	-16.44	4.23	0.15
2656	Cn1c(nnn1)C(F)(F)F	C05053144	-14.35	-1.07	-15.52	5.06	-2.83
2657	[C@H](C(F)(F)Br)(OC(F)(F)F)F	C08698310	-14.35	0.12	-13.94	1.53	-2.06
2658	c1cc(c(cc1SC(F)(F)F)N)Cl	C15442354	-14.35	-2.66	-10.06	1.73	-3.35
2659	c1ccc(cc1)Cc2nnc(n2)N	C16952811	-14.35	-1.47	-12.86	4.44	-4.46
2660	CCNc1ccc(c[nH+]1)C	C21503152	-14.35	-3	-11.51	3.14	-2.98
2661	Cc1ccc(c(c1)N)O	C00388269	-14.34	-3.27	-13.99	3.06	-0.14
2662	c1cc(nn2c1nnn2)Cl	C01435441	-14.34	-4.12	-17.95	8.77	-1.04
2663	C=CC[C@H](C=C)O	C01674838	-14.34	-0.66	-14.23	1.68	-1.14
2664	CCOC(=O)C(=O)N	C01679740	-14.34	-3.69	-15.55	4.78	0.12
2665	c1cscc1I	C02015848	-14.34	-0.64	-15.13	1.25	0.19
2666	C(CF)OC(=O)Cl	C02040572	-14.34	-0.97	-14.51	3.43	-2.29
2667	COc1nccs1	C02381581	-14.34	-0.92	-16.68	3.35	-0.09
2668	COc1cc(no1)Cl	C03882970	-14.34	0.83	-15.98	2.5	-1.69
2669	Cc1cc[nH]n1	C04701702	-14.34	-2.82	-14.47	4.15	-1.2
2670	Cn1ccc(c1)[N+](=O)[O-]	C04753651	-14.34	-2.99	-15.55	7.89	-3.68
2671	c1c([nH]nc1NN)N	C04772536	-14.34	-5.24	-16.1	5.8	1.19
2672	CC/C=C/CO	C05224689	-14.34	-2.02	-13.72	2.1	-0.71
2673	C1C(=CC(=O)CS1)O	C05385876	-14.34	-6.28	-16.23	7.92	0.25
2674	C#CCN1C(=O)CSC1=O	C06295348	-14.34	1.35	-19.54	6.01	-2.16
2675	c1c(cnc(c1N)N)Br	C18995568	-14.34	-0.52	-17	3.42	-0.23
2676	c1cc(cc(c1)F)CNC	C19171905	-14.34	0.63	-16.46	2.85	-1.37
2677	c1nc(on1)CCl	C20282418	-14.34	-1.9	-15.51	4.25	-1.17
2678	Cc1cnc(cn1)Br	C20358077	-14.34	-0.86	-15.25	3.47	-1.69
2679	c1ccc(c(c1)C#N)F	C00164450	-14.33	0.43	-16.69	5.56	-3.63
2680	c1cc2nnnn2cc1O	C01597528	-14.33	-5.45	-18.46	9.6	-0.02
2681	c1c(c(=O)[nH]c(=O)[nH]1)N=C=S	C01598890	-14.33	-2.54	-21.9	9.7	0.42
2682	CCOC(=O)C(=O)C	C01679741	-14.33	-0.77	-14.6	3.73	-2.69
2683	C=C(C(=O)OCC(C(F)F)(F)F)F	C02383137	-14.33	-0.04	-13.98	4.32	-4.63
2684	c1c(c[nH]1)C#N	C02389916	-14.33	-4.74	-14.81	6.32	-1.1
2685	c1cc(ccc1NC(=O)C(=O)N)F	C04525690	-14.33	-2.13	-19.17	5.16	1.82
2686	Cn1nc(nn1)C(F)(F)F	C05053143	-14.33	-2.39	-13.97	4.73	-2.69
2687	C/C=N/n1cncn1	C05282697	-14.33	-3.61	-15.04	7.96	-3.64
2688	c1c(sc(n1)C=O)Br	C15022153	-14.33	-1.26	-14.8	3.37	-1.64
2689	c1c(nc(s1)CS)Br	C15442514	-14.33	-1.69	-13.87	3.66	-2.42
2690	c1([nH]c(=S)[nH]n1)N	C16955814	-14.33	-4.7	-14.85	6.57	-1.35
2691	C1CCC(C1)CN=C=O	C19502816	-14.33	-0.92	-13.87	1.82	-1.36
2692	c1cc([nH]c1C(=O)Cl)[N+](=O)[O-]	C20248576	-14.33	-2.69	-12.06	3.74	-3.32
2693	Cc1cc(n(n1)C)N	C00152286	-14.32	-5.05	-13.15	5.21	-1.33
2694	c1ccc(c(c1)CNC(=O)N)F	C01383313	-14.32	0.31	-21.62	7.43	-0.44
2695	c1c(cc(c(c1F)C=O)F)O	C03880149	-14.32	-0.97	-18.61	5.99	-0.73
2696	Cc1c(c([nH]1)C(F)(F)F)N	C04244014	-14.32	-3.13	-13.73	3.1	-0.56

2697	C/C=C(C(=O)Cl	C13380326	-14.32	-1.87	-12.9	2.88	-2.43
2698	c1cnc(c(c1Cl)O)N	C21981844	-14.32	-4.53	-14.22	4.02	0.41
2699	c1cc(sc1)Br	C01673392	-14.31	-0.42	-15.7	1.6	0.2
2700	C/C=C(\C)/[N+](=O)[O-]	C02037572	-14.31	-1.53	-14.94	5.33	-3.17
2701	COC(=O)C(=C)C(F)F	C02539782	-14.31	-1.34	-14.33	4.21	-2.84
2702	c1cc(c(c1)Br)N	C02574362	-14.31	-2.04	-14.79	2.04	0.48
2703	COC(=O)c1c(c[nH]n1)Cl	C04243785	-14.31	0.4	-17.65	4.59	-1.64
2704	CCNn1cnc1	C05312200	-14.31	-1.24	-16.53	6.35	-2.89
2705	Cc1c(c(on1)N)Cl	C12336381	-14.31	-3.78	-13.82	3.36	-0.08
2706	CC(=O)Nc1[nH]ccn1	C13354633	-14.31	-4.93	-13.65	6.46	-2.19
2707	c1cc(=O)cc1Br	C21989743	-14.31	-0.89	-16.74	6.47	-3.15
2708	c1ccc(cc1)[C@@H]2CO2	C00901251	-14.3	-1.89	-13.37	3.65	-2.68
2709	CN(C(=O)OC)[N+](=O)[O-]	C01646520	-14.3	-1.98	-14.9	3.94	-1.36
2710	C(C#N)Sc1nc(nH)n1N	C02241721	-14.3	-1.91	-17.85	7.8	-2.33
2711	c1c2c(ncn1)nc(nH)2Cl	C04430278	-14.3	-4.95	-18.24	7.37	1.52
2712	[C@H](C(=O)Br)(C(F)F)F	C16125632	-14.3	0.14	-14.37	2.33	-2.4
2713	Cc1cnc(n1)[N+](=O)[O-]	C00967455	-14.29	-2.96	-15.34	6.37	-2.36
2714	c1cc(nc(c1)F)NN	C01387409	-14.29	-3.31	-15.64	5.64	-0.98
2715	c1c(cncn1)C(=O)Cl	C02511468	-14.29	0.34	-17.69	3.14	-0.08
2716	c1(c(=O)[nH]c(n1)[O-])N	C05425207	-14.29	-2.74	-19.26	4.88	2.83
2717	c1c(cc(nc1F)F)NN	C16159843	-14.29	-2.53	-16.92	5.31	-0.15
2718	c1cnc(c(c1F)F)F	C21987576	-14.29	0.66	-15.87	3.8	-2.88
2719	Cn1c(=O)cn[nH]c1=O	C01689468	-14.28	-2.1	-19.32	5.59	1.56
2720	COC(=O)CNC=S	C01755266	-14.28	-0.97	-17.08	5.29	-1.53
2721	c1(c(c(c(nc1F)F)F)Br)F	C02545334	-14.28	-0.07	-13.24	0.54	-1.51
2722	Cc1cc([nH]n1)N	C03886974	-14.28	-3.83	-14.63	4.47	-0.29
2723	c1cc2nccn2nc1	C05117297	-14.28	-3.36	-16.35	7.85	-2.42
2724	C=CCC(=O)c1cccc1	C05606416	-14.28	0.21	-14.89	5.24	-4.85
2725	Cc1cc(cs1)CCl	C19754921	-14.28	-0.96	-11.33	2.19	-4.18
2726	c1c(nc(cn1)Br)Cl	C32914877	-14.28	-1.26	-14.09	2.54	-1.48
2727	c1ccc(c(c1)CO)N	C00331680	-14.27	-1.56	-16.65	3.88	0.05
2728	C[C@H]1C(=S)C=CO1	C00396117	-14.27	-1.1	-13.26	2.57	-2.48
2729	CC(=O)n1cccc1	C00400012	-14.27	-2.2	-14.89	5.73	-2.91
2730	c1c(c(c2nnnn2n1)N)Cl	C01713793	-14.27	-4.36	-17.03	6.6	0.53
2731	c1cc(c(cc1F)C=O)O	C02572869	-14.27	-3.47	-14.06	5.36	-2.1
2732	CC1=COCCO1	C05217915	-14.27	-1.29	-14.68	3.2	-1.5
2733	Cn1cc[nH+]c1	C06165925	-14.27	-1.96	-14.72	5.11	-2.7
2734	c1c(c2c([nH]cn2)nn1)N	C08616408	-14.27	-3.55	-18.91	8.57	-0.38
2735	C=CCC(=O)Cl	C13380327	-14.27	-0.87	-13.96	2.83	-2.27
2736	Cc1c(ccc(n1)N)F	C21297356	-14.27	-4.28	-13.02	4.52	-1.48
2737	Cc1cccc1S	C21303045	-14.27	-1.21	-10.93	1.75	-3.88
2738	Cc1c[nH]nc1C(F)F	C00066375	-14.26	-0.42	-14.62	2.72	-1.94
2739	COC(=O)C(=O)CBr	C01606708	-14.26	-1.1	-14.37	3.72	-2.51
2740	C=CC[NH+]=C=S	C01687017	-14.26	0.33	-14.08	1.46	-1.96
2741	COc1ccc(cn1)F	C02384083	-14.26	-1.19	-14.67	2.7	-1.1
2742	CCSc1nnc(n1N)C(F)F	C02536950	-14.26	-2.73	-13.3	4.81	-3.04
2743	CNc1nnns1	C03844498	-14.26	-2.8	-16.96	5.61	-0.11
2744	c1c(c(n[nH]1)/C=N/O)Cl	C04262682	-14.26	-3.94	-14.68	3.65	0.71
2745	c1cc(oc1)CNC(=S)N	C00116470	-14.25	-1.49	-20.33	9.11	-1.54
2746	CC(=O)c1ccc[nH]1	C00153027	-14.25	-1.92	-15.14	5.04	-2.24
2747	c1cc(oc1CBr)C(F)F	C00161832	-14.25	-2.71	-12.51	3.25	-2.28
2748	CC(=O)c1ccc(oc1)[N+](=O)[O-]	C00334121	-14.25	-1.12	-14.89	4.57	-2.81
2749	c1cc(oc1)CNC=O	C01529539	-14.25	-1.96	-18.52	6.4	-0.18
2750	CC(=O)OCCC=C	C01601431	-14.25	-0.18	-14.52	3.79	-3.34
2751	c1cc([nH]c1)C(=O)CCC#N	C01615151	-14.25	-2.92	-14.85	6.75	-3.23
2752	c1nnc2n1ncs2	C01657453	-14.25	-2.79	-18.56	9.83	-2.72
2753	c1cc([nH]1)CCO	C01721467	-14.25	-4.19	-15.48	3.62	1.8
2754	c1cnc(cn1)C(=O)C=[N+]=[N-]	C03882905	-14.25	-1.49	-18.46	5.65	0.06
2755	c1c2c([nH]c1=O)CCC2	C04342676	-14.25	-1.45	-17.88	6.57	-1.49
2756	CCOc1ccc(cn1)N	C04352765	-14.25	-2.24	-15.99	4.11	-0.13
2757	C1CC(C1)CS	C17013832	-14.25	-0.16	-11.04	0.65	-3.7
2758	c1cc(nc(c1))N	C19735875	-14.25	-1.95	-14.55	4.23	-1.97
2759	c1cncnc1CNC=O	C23993720	-14.25	0.19	-21.61	7.79	-0.62
2760	c1c[nH]nc1C(F)F	C26547607	-14.25	-3.82	-15.01	5.94	-1.36
2761	Cc1c(sc1)C	C00407027	-14.24	-1.38	-14.27	3.61	-2.19
2762	c1cnc(c1)C(=O)N	C01482000	-14.24	-3.54	-17.57	5.78	1.09
2763	CC1=CCC(=O)O1	C01596395	-14.24	-1.27	-15.4	5.33	-2.9
2764	CCOC(=O)CBr	C01648257	-14.24	-1.28	-13.97	3.91	-2.89
2765	C=CCOCOC=O	C01705956	-14.24	-2.84	-16.26	6.77	-1.91
2766	Cc1ncc(c(n1)N)CCl	C01719385	-14.24	-4.05	-12.83	4.66	-2.02
2767	c1cc2c(cc[nH]2)nc1	C02040899	-14.24	-4	-14.7	6.55	-2.1
2768	Cc1c(n[nH]1)[O-][N+](=O)[O-]	C03894821	-14.24	0.16	-16.49	5.69	-3.6
2769	c1c(oc1Br)CCl	C04198765	-14.24	-2.35	-15.1	3.87	-0.67
2770	c1cc2cn[nH]c2c(c1)O	C14985814	-14.24	-2.77	-16.36	5.16	-0.28
2771	c1cc(oc1)C(=O)CCCl	C32005846	-14.24	-1.62	-13.28	4.18	-3.52
2772	c1ccc2c(c1)c([nH]2)O	C00153260	-14.23	-5.16	-15.29	5.11	1.11
2773	COC(=O)c1cncnc1	C01713427	-14.23	0.93	-16.91	4.2	-2.46
2774	c1c(c[nH]1)CCO	C02549368	-14.23	-3.18	-16.87	4.96	0.86
2775	c1cc(ncc1O)F	C02572509	-14.23	-3.44	-15.38	4.53	0.06
2776	C1(SC(S1)(F)F)F	C05019030	-14.23	0.04	-12.4	0.12	-1.99
2777	c1c([nH]cn1)C(=O)N	C05116852	-14.23	-5.61	-17.8	8.37	0.81
2778	c1cnc([nH]1)C(=O)N	C05117662	-14.23	-4.73	-17	6.24	1.26
2779	CNC(=S)N(C)N=O	C05412909	-14.23	-2.33	-15.62	2.53	1.19
2780	c1[nH]cc1C#N	C05426226	-14.23	-5.21	-13.95	6.36	-1.42
2781	COC(=O)/C=C/Br	C13379807	-14.23	-0.86	-15.17	4.23	-2.43
2782	c1c(cc(nc1F)F)N	C16159832	-14.23	-4.34	-14.94	5.27	-0.22
2783	c1c(cnc(c1[N+](=O)[O-])N)Cl	C19015102	-14.23	-1.74	-13.77	3.44	-2.16
2784	c1cc(c(cc1Cl)N)OC(F)F	C21984714	-14.23	-3.75	-10.84	2.43	-2.07
2785	c1c(cc(cc1F)Cl)N	C00732130	-14.22	-3	-11.14	2.13	-2.21
2786	c1nc(c(c(n1)N)N)N	C00967361	-14.22	-2.96	-17.32	4.99	1.07

2787	c1ccc(c(c1)CONC(=O)N)F	C01398290	-14.22	-3.63	-18.73	9.44	-1.3
2788	CSCCC(=O)Cl	C02522844	-14.22	0.62	-14.35	2.42	-2.91
2789	c1cc(ccc1/C=C/C=O)F	C02580761	-14.22	-3.76	-12.96	6.67	-4.16
2790	C(=C(C#N)C#N)/C=[N+](O)\[O-]	C12378683	-14.22	-7	-15.71	9.87	-1.37
2791	Cc1ccc(o1)CC#N	C12957816	-14.22	-1.88	-15.6	6.75	-3.49
2792	Cc1cc(no1)N	C16981047	-14.22	-2.99	-14.65	4.68	-1.26
2793	CC(=O)NCCc1ccccc1	C00061519	-14.21	0.54	-17.84	5.74	-2.65
2794	c1cc(c(cc1NC(=O)N)F)F	C00137453	-14.21	-4	-19.2	9.53	-0.54
2795	CCn1c(ccn1)N	C00154804	-14.21	-2.48	-14.81	4.67	-1.6
2796	Cc1ccc(cn1)O	C00331651	-14.21	-2.2	-15.66	4.02	-0.36
2797	CC(=O)c1ccsc1	C00334460	-14.21	0.82	-17.54	5.43	-2.91
2798	c1ccc(cc1)Cn2c(ccn2)N	C00807913	-14.21	0.85	-16.77	5.48	-3.77
2799	c1cc(c([nH+]c1)[O-])	C00967325	-14.21	-2.53	-15.45	3.8	-0.03
2800	c1c(c(n1)C(=O)N)N)C#N	C01754746	-14.21	-1.71	-19.62	5.83	1.29
2801	c12c(non1)Nc3c(non3)N2	C02273571	-14.21	0.36	-16.79	3.62	-1.41
2802	c1ccc(cc1)SC2=NN=CC2	C05286402	-14.21	1.72	-15.81	3.79	-3.91
2803	c1cc(sc1)/C=N/N	C05896834	-14.21	-2.75	-17.33	3.47	2.39
2804	[H]/N=C(/C)\SCCCC	C17023706	-14.21	-2.18	-10.38	1.31	-2.96
2805	c1cc(nc(c1)Cl)N	C19735874	-14.21	-1.45	-15.97	4.74	-1.53
2806	c1c(cnc(c1)[O-])BrCl	C21981892	-14.21	-3.01	-13.12	2.74	-0.82
2807	c1[nH]c2c(n1)c(ccn2)N	C00000882	-14.2	-3.9	-16.28	7.59	-1.62
2808	c1ccc(c(c1)C(=O)N)N	C00152578	-14.2	-2.82	-17.16	5.29	0.5
2809	c1cc(c2cn[nH]c2c1)N	C00169219	-14.2	-4.18	-13.95	4.73	-0.79
2810	c1cc(cc(c1)F)/C=C/C#N	C01624968	-14.2	-0.63	-16.38	5.71	-2.9
2811	COc1ccc(cc1)N=C=O	C01683477	-14.2	-1.24	-14.3	2.58	-1.24
2812	Cc1ccn1	C01683906	-14.2	-1.29	-14.49	3.65	-2.07
2813	C(#CS)c1nc(sn1)N(C(F)F)F	C04984696	-14.2	0.73	-18.1	5.46	-2.29
2814	c1c(cnc(c1)Br)O)F	C08698129	-14.2	0.63	-18.33	3.01	0.49
2815	Cc1c(cno1)[N+](=O)[O-]	C15782469	-14.2	-0.24	-15.21	3.75	-2.51
2816	C=CC[C@H](c1ccc1)O	C00403957	-14.19	-0.87	-14.42	3.02	-1.92
2817	CCc1ccnccn1	C02509971	-14.19	-1.37	-13.93	3.5	-2.39
2818	Cc1ccc(c1)NC(=S)N	C08577652	-14.19	-1.12	-12.88	3.09	-3.28
2819	c1ccc(cc1)c2ccn[nH]2	C09238252	-14.19	-0.42	-14.71	4.21	-3.28
2820	c1([nH]c(=S)[nH]1)C(=O)NN	C10150814	-14.19	-5.81	-16.71	6.94	1.39
2821	c1c[nH]c(cc1Sc2nc[nH]n2)N	C20370869	-14.19	-2.95	-17.35	7.57	-1.46
2822	c1cnc(nc1)l	C21298949	-14.19	0.08	-16.65	4.64	-2.25
2823	c1cnc(cc1F)NN	C21987580	-14.19	-2.21	-15.52	4.66	-1.12
2824	CCOc1ccccc1F	C00393901	-14.18	-1.7	-13.06	4.23	-3.66
2825	c1cnc(nc1)Br	C01569572	-14.18	-2.36	-14.76	4.94	-2
2826	Cc1c([nH]c(=S)[nH]1)	C02511422	-14.18	-2.49	-15.05	4.85	-1.49
2827	c1c(cn(n1)CC#N)Cl	C02537511	-14.18	-3.19	-17.57	9.29	-2.7
2828	c1c(cnc2c1[nH]cn2)Br	C13635304	-14.18	-5.66	-15.89	10.39	-3.03
2829	c1cc(ccc1Cn2c(ccn2)N)F	C14988456	-14.18	0.09	-16.39	5.93	-3.82
2830	c1ccc(c(c1)/C(=C/C=O)\[O-])O	C15442675	-14.18	-4.84	-15.51	8.02	-1.85
2831	Cn1c(nnn1)N	C16890072	-14.18	-3.89	-15.79	6.34	-0.83
2832	c1c(nnc(n1)Cl)Cl	C22005360	-14.18	1.17	-14.64	0.99	-1.7
2833	c1cc(c(cc1F)F)NC(=S)NN	C00039569	-14.17	0.33	-19.1	7.28	-2.68
2834	c1ccc(c(c1)O)Br	C00388200	-14.17	-0.58	-17.61	2.95	1.06
2835	c1ccc(c(c1)/C=C/C/[N+](=O)[O-])F	C01688697	-14.17	-0.45	-17.21	5.87	-2.38
2836	c1cncnc1CCl	C04343312	-14.17	-0.91	-15.29	4.4	-2.36
2837	CCO[C@H](H)C=CCCO1	C05809849	-14.17	-1.39	-13.04	2.88	-2.61
2838	c1cc(oc1)C(=O)N=[N+]=[N-]	C15784358	-14.17	1.33	-20.96	4.48	0.98
2839	c1ccc(cc1)/C=C\NC=O	C17175561	-14.17	0.83	-17.08	5.68	-3.6
2840	c1cncnc1CO	C00158595	-14.16	-1.57	-17.28	4.56	0.13
2841	c1csccl1C#N	C00165405	-14.16	0.42	-15.9	4.11	-2.79
2842	c1c(sc(n1)Cl)C=N/O	C01386795	-14.16	-2.98	-17.24	6.18	-0.12
2843	c1cc(ccc1NC(=O)C(F)F)F	C01572856	-14.16	-3.36	-13	4.43	-2.23
2844	c1cc(oc1)C#N	C01668241	-14.16	-2.18	-14.1	4.4	-2.29
2845	C1=CC(=O)C=CC1=NO	C01669666	-14.16	-6.61	-15.49	7.91	0.03
2846	CN(C)NC(=S)C(F)F	C05599631	-14.16	-1.15	-13.21	2.38	-2.18
2847	c1(nnnn1O)c2nnnn2O	C05670122	-14.16	-2.71	-17.41	6.04	-0.09
2848	Cc1c(non1)[O-]	C05721361	-14.16	-2.65	-15.04	4.09	-0.57
2849	c1cc(c(=O)[nH]c1)Br	C08698110	-14.16	-0.84	-18.23	4.44	0.48
2850	C=CSc1ncccn1	C15043173	-14.16	0.17	-16.57	5.11	-2.87
2851	c1cc(c(c(c1)Br)F)N	C16159705	-14.16	-1.32	-13.74	3.21	-2.31
2852	c1cc(oc1)C(=O)CCl	C32005474	-14.16	1.14	-17.95	5.54	-2.89
2853	Cc1cncnc1[N+](=O)[O-]	C00332952	-14.15	0.35	-15.89	4.42	-3.03
2854	c1ccc(c(c1)C#N)O	C00388252	-14.15	0.02	-18.31	5.63	-1.49
2855	Cn1cccn1	C01845529	-14.15	-2.14	-14.75	4.44	-1.69
2856	c1c(nc[nH]1)C(=S)N	C02559873	-14.15	-5.15	-17.34	9.5	-1.17
2857	Cc1cc(no1)C=O	C03880794	-14.15	-1.37	-15.5	4.56	-1.84
2858	c1cc(c(c2c1[nH]cn2)F)F	C04243027	-14.15	-2.5	-14.77	6.33	-3.21
2859	Cc1ncc(c(n1)N)CS	C04362801	-14.15	-3.98	-12.96	4.47	-1.68
2860	Cc1[nH]ccp1	C05722977	-14.15	-1.9	-14.92	2.98	-0.31
2861	c1c(cncnc1)N	C06643306	-14.15	-0.52	-15.05	2.78	-1.36
2862	CC(OCC(F)F)F)F)F	C08698362	-14.15	-0.75	-13.57	2.35	-2.18
2863	c1c(sc(n1)N)C#N	C08698529	-14.15	-0.55	-17.86	5.28	-1.02
2864	c1c(=O)n(c(=O)[nH]n1)N	C16382953	-14.15	-3.11	-19.04	6.1	1.9
2865	c1(nnc(o1)[S-])C(F)F	C16957733	-14.15	-3.16	-15.29	2.92	1.38
2866	c1cc(c(cc1F)Cl)N=C=O	C19509523	-14.15	0.18	-14.21	2.15	-2.27
2867	c1cnc(nc1)C(F)F	C21297509	-14.15	-3.45	-14.28	5.94	-2.35
2868	Cc1cncnc1N	C21300847	-14.15	-4.64	-15.78	7	-0.73
2869	c1ccc(c(c1)N)Oc2cncn2	C22141877	-14.15	-1.73	-17.09	5.35	-0.68
2870	c1cc(nc(c1[N+](=O)[O-])N)N	C22198856	-14.15	-2.52	-18.79	7.74	-0.58
2871	CC(C)c1cc(n[nH]1)C#N	C32005421	-14.15	-2.73	-13.34	4.46	-2.54
2872	c1cn2ccsc2n1	C00330640	-14.14	-1.83	-18.61	6.8	-0.51
2873	COc(=O)C(=C)Cl	C01664994	-14.14	-1.47	-13.8	3.48	-2.35
2874	C=CC(=O)OCC(F)F)F	C01664997	-14.14	-0.09	-14.76	3.79	-3.08
2875	CC(=C)COc(=O)C	C01845661	-14.14	-0.38	-15.49	4.06	-2.33
2876	c1cc([nH]c1)C(=O)C(F)F	C02508541	-14.14	1.57	-17.36	4.23	-2.59

2877	c1cnc(c1[N+](=O)[O-])Cl	C02566376	-14.14	-0.37	-15.48	4.54	-2.83
2878	COC(=O)Nc1cccc(c1)F	C03206929	-14.14	0.1	-18.87	6.84	-2.21
2879	c1cc(ccc1C#N)NN=O	C06535244	-14.14	-3.97	-12.99	5.01	-2.19
2880	C/C(=C/CSC(=NH2+)N)/Cl	C13693447	-14.14	-0.57	-14.78	3.24	-2.03
2881	C1CN=C(N1)SCC#N	C16808311	-14.14	-1.58	-16.14	4.41	-0.83
2882	c1cc(c(cc1F)F)[N+](=O)[O-]	C00164453	-14.13	-2.13	-13.15	5.06	-3.9
2883	C1CN2C(=CSC2=N1)N	C00274793	-14.13	-3.53	-14.66	4.68	-0.62
2884	c1c(csn1)C#N	C01618092	-14.13	-2.06	-14.41	4.23	-1.88
2885	CC(=O)Oc1ccc(cc1)[N+](=O)[O-]	C01641045	-14.13	-1.33	-14.77	6.8	-4.83
2886	c1c(c[nH]c1C=O)I	C02519474	-14.13	-5.56	-13.24	4.35	0.32
2887	c1csc(c1)CC(=O)Cl	C02574167	-14.13	0.94	-18.3	3.86	-0.63
2888	c1ccc(c(c1)OCC#N)F	C02685693	-14.13	-2.39	-14.05	6.37	-4.06
2889	c1ccc(cc1)/C=N/N=C(N)N	C04342962	-14.13	-0.71	-16.94	6.68	-3.16
2890	C1CCC(=CC1)CCO	C04684325	-14.13	-2.17	-15.1	1.96	1.18
2891	C/C=C/Cc1ccccc1O	C08580485	-14.13	-0.67	-16.15	2.87	-0.17
2892	Cc1csc(n1)CCl	C11764196	-14.13	-0.62	-14.37	3.67	-2.8
2893	C(#N)c1c(c(n1)Cl)Cl	C15443044	-14.13	-1.78	-11.47	1.77	-2.65
2894	COc1nc([nH]n1)N	C17024988	-14.13	-5.54	-15.51	5.98	0.93
2895	c1cc2c(cc1Br)nn[nH]2	C19859472	-14.13	-1.17	-16.61	5.36	-1.72
2896	c1cc(c(cc1N)Cl)F	C00157622	-14.12	0.15	-15.32	3.29	-2.23
2897	Cc1c(ccc1O)N	C00407044	-14.12	-3.52	-13.57	3.33	-0.36
2898	c12c([nH]n1)Nc3c(non3)N2	C01194591	-14.12	-7.11	-13.45	7	-0.56
2899	CC(=O)OCC(=C)Cl	C01681466	-14.12	0.44	-15.77	4.42	-3.21
2900	CCCCN=C=S	C01845901	-14.12	-0.6	-15.15	1.14	0.49
2901	Cc1cc(cnc1)O	C01871320	-14.12	-2.27	-15.25	3.79	-0.38
2902	Cn1cncn1	C02034214	-14.12	-2.97	-14.41	5.93	-2.67
2903	c1cc(oc1)C(=O)CBr	C02525565	-14.12	1.22	-17.3	4.96	-2.99
2904	c1cc(oc1)C(=O)N	C03848454	-14.12	-3.48	-17.23	6.06	0.52
2905	c1ccc(cc1)CCN=[N+]=[N-]	C04748468	-14.12	-0.34	-15.28	1.9	-0.39
2906	CC(=O)c1cc[nH]1	C05386998	-14.12	-3.77	-17.1	6.3	0.45
2907	c1cc(c(c1F)N)[N+](=O)[O-]	C05784415	-14.12	-2.04	-16.45	4.88	-0.51
2908	C1Cc2c([nH]nc2C(F)(F)F)C1	C05799093	-14.12	-3.03	-11.65	3.41	-2.86
2909	c1cc(sc1)/C=C/C=O	C05843463	-14.12	-1.98	-17.75	6.53	-0.92
2910	c1nc(c(c1)Cl)F)Cl	C08698232	-14.12	-0.5	-13.01	1.95	-2.56
2911	c1cc(c(cc1O)O)F	C16158134	-14.12	-3.45	-15.95	4.33	0.95
2912	CCn1cc(cc1N)C	C16162964	-14.12	-2.93	-11.18	3.35	-3.36
2913	c1(c(nsn1)N)C(=O)N	C17163632	-14.12	-3.55	-18	4.58	2.85
2914	CCNc1cccnc1	C19884497	-14.12	-2.33	-13.68	3.82	-1.92
2915	[C@H-](C(=[NH2+]N)N)C(C(F)F)(F)F	C20518719	-14.12	-5.49	-15.02	7.24	-0.85
2916	C=C1CCCC1=O	C21982782	-14.12	-0.97	-14.16	3.85	-2.83
2917	CCc1ccc(C)cc1	M1995A043	-14.12	-0.68	-9.8	1.34	-4.99
2918	c1cc(cnc1)C(=O)N	C00005878	-14.11	-3.61	-17.29	6.45	0.35
2919	c1c(cnc1)Cl)N	C00332989	-14.11	-0.99	-17.38	2.95	1.31
2920	COc1cncn1	C00409287	-14.11	-0.52	-17.8	3.85	0.36
2921	c1cc(oc1)C(=O)C(=O)N	C01707277	-14.11	-1.43	-18.73	6.36	-0.31
2922	c1c(c(nc(=S)[nH]1)N)N	C02164504	-14.11	-5.85	-15.11	5.78	1.07
2923	C[C@H](C(=O)Br)Br	C02242574	-14.11	0.41	-13.95	1.9	-2.47
2924	c1cc(ccc1)/C=N/O)O	C04578804	-14.11	-0.99	-18.91	5.41	0.39
2925	Cc1c(c1=O)c2ccccc2	C06068885	-14.11	-0.29	-19.42	6.64	-1.04
2926	c1c(nsc1Cl)[O-]	C09226750	-14.11	-2.1	-16.75	5.19	-0.46
2927	COc1cnc(c1)N	C15635457	-14.11	-1.74	-16.52	5.61	-1.47
2928	c1(nc(n1)O)N	C16931802	-14.11	-3.02	-16.41	4.06	1.25
2929	c1cncnc1C[NH3+]	C20417407	-14.11	-2.27	-17.98	5.45	0.68
2930	CSc1ccc(nc1)Br	C21953220	-14.11	-0.64	-13.32	3.11	-3.27
2931	c1cc(c(c1)F)C(=N)O)F	C00075251	-14.1	-2.04	-16.72	6.33	-1.67
2932	C[C@H](c1ccc1)O	C00164797	-14.1	-1.73	-14.76	3.09	-0.7
2933	Cc1c[nH]n1	C00897288	-14.1	-2.15	-14.69	3.91	-1.17
2934	c1c(cnn2c1nnc2)N	C01730469	-14.1	-3.67	-19.92	11.01	-1.52
2935	c1[n-]c(c1n1)[N+](=O)[O-][N+](=O)[O-]	C04468969	-14.1	-5.31	-15.44	10.98	-4.33
2936	C/C(=C)Cl)CO	C05104107	-14.1	-3.32	-12.84	2.56	-0.51
2937	Cc1ccc(c1)F)O	C21300193	-14.1	-1.9	-14.14	3.73	-1.79
2938	C1CC(C1)C(=O)N=C=S	C22148233	-14.1	-0.26	-15.24	3.78	-2.39
2939	c1cc2c(cc1N=C=O)CCO2	C00158514	-14.09	-1.6	-13.85	3.01	-1.66
2940	c1cc(ccc1C(F)(F)F)Br	C00164872	-14.09	-1	-12.59	1.44	-1.93
2941	c1ccc(c(c1)C(F)(F)F)O	C00164884	-14.09	-2.25	-14.55	3.75	-1.04
2942	c1cc(ccc1NN)SC#N	C00393806	-14.09	-1.14	-15.67	4.73	-2.01
2943	C=CC(=O)OCC=C	C01632702	-14.09	1.4	-15.15	3.48	-3.83
2944	CSC(=O)C(=O)SC	C01757821	-14.09	-1.03	-15.8	3.11	-0.37
2945	c1cc(c(cc1Br)F)N=C=O	C02568114	-14.09	-2.02	-13.68	2.19	-0.58
2946	Cc1[n-]nc(n1)C(F)(F)F	C03883866	-14.09	-4.78	-12.79	5.63	-2.14
2947	c1c(nc[nH]1)CCl	C15894707	-14.09	-4.41	-12.75	5.63	-2.56
2948	c1cc(ccc1NN)O	C19386006	-14.09	-1.88	-18.79	5.93	0.64
2949	c1cnc([nH]1)C=O	C01069165	-14.08	-2.51	-16.16	5.41	-0.81
2950	c1(=O)c(nnc([nH]1)[O-])I	C01078850	-14.08	-1.21	-17.24	3.38	0.99
2951	c1cnc(nc1N)Cl	C01595944	-14.08	-4.83	-13.48	5.08	-0.85
2952	Cc1c(c[nH]n1)N	C04244016	-14.08	-3.72	-14.89	4.21	0.32
2953	CSC1=NCCCS1	C04284607	-14.08	1.13	-15.31	2.36	-2.26
2954	C(C(=S)N)C(=S)N	C05410038	-14.08	-2.36	-14.57	2.96	-0.12
2955	CCOc1ccc(=O)[nH]n1	C17014098	-14.08	-3.22	-17.3	5.76	0.69
2956	CC(=O)c1cncn1C	C19091704	-14.08	1.26	-17.02	4.39	-2.71
2957	c1ccc(c(c1)NCC#N)F	C20052436	-14.08	-3.6	-13.5	6.05	-3.04
2958	c1cc(c(cc1Br)N)N	C00158488	-14.07	-0.82	-15.09	2.68	-0.84
2959	c1cc(ncc1Br)Cl	C00404153	-14.07	-1.4	-15.37	2.25	0.45
2960	c1cc2c(cc1N=C=O)OCO2	C02387324	-14.07	-2.23	-14.39	3.35	-0.8
2961	c1ccc(c(c1)OC(F)(F)F)F	C02560216	-14.07	1.53	-15.54	3.26	-3.32
2962	c1cc(c(cc1F)F)C(=N)O)N	C04365212	-14.07	-3.8	-15.41	6.18	-1.03
2963	C1CN=C(N1)N=[N+]=[N-]	C04722293	-14.07	-0.74	-16.99	2.94	0.72
2964	c1cc(c(=O)[nH]c1)N	C08698104	-14.07	-4.82	-16.73	5.04	2.45
2965	Cc1csc(n1)Cl	C12505746	-14.07	-0.64	-14.33	3.08	-2.18
2966	CCN1CCCC1=O	C14684426	-14.07	-2.24	-13.67	2.81	-0.97

2967	C[C@@H]1CC(=NO1)[N+](=O)[O-]	C15783913	-14.07	0.31	-16.28	4.89	-3
2968	Cc1cc(on1)N/C=N/O	C15934904	-14.07	-2.4	-19.76	8.56	-0.47
2969	c1c(c(=O)nc([nH]1)N)O	C17378517	-14.07	-6.82	-18.29	10.13	0.91
2970	c1cc(ccc1NC(=S)C(=O)N)Cl	C20478536	-14.07	-6.15	-13.08	6.4	-1.24
2971	CCC(=O)N=C=S	C22149244	-14.07	-1.5	-14.94	3.76	-1.4
2972	c1cc(c(cc1Br)N)O	C00078184	-14.06	-1.09	-15.52	2.73	-0.18
2973	c1c(c(cc(c1O)Cl)F)N	C00167400	-14.06	-0.13	-17.14	3.28	-0.07
2974	c1ccoc1C#N	C01581465	-14.06	-2.68	-14.12	4.99	-2.24
2975	CCOC(=O)CSC#N	C01591776	-14.06	-1.6	-14.3	4.83	-2.99
2976	CC1=CCCO1	C02039526	-14.06	-0.5	-13.44	1.99	-2.11
2977	c1ccc(cc1)NCC(F)(F)F	C02040769	-14.06	-1.58	-13.36	2.3	-1.41
2978	c1nc(c(c(n1)N)N=O)N	C04558794	-14.06	-3.14	-16.14	4.8	0.42
2979	CCc1nc([nH]n1)N	C06820881	-14.06	-2.07	-15.26	5.23	-1.95
2980	C(=[NH+]/N)(C(=[NH+]/N)[S-])/N	C13409865	-14.06	-3.37	-16.13	3.3	2.14
2981	c1c(nc(s1)C(=O)C(F)F)F	C20438837	-14.06	-4.44	-12.66	4.93	-1.89
2982	C#CCOc1cccn1	C21993371	-14.06	-0.29	-18.69	6.19	-1.28
2983	c1ccc(c(c1)C=N/O)N	C00330045	-14.05	-4.39	-13.09	3.84	-0.41
2984	c1cnc2c1C(=O)OC2	C01592491	-14.05	-2.26	-16.45	6.96	-2.29
2985	c1cc(ccc1NCC#N)O	C02023082	-14.05	-2.88	-16.9	6.49	-0.77
2986	c1cnn(n1)CCO	C02513898	-14.05	-4.51	-15.97	5.05	1.38
2987	Cc1cc(cnc1)C	C08294960	-14.05	-0.57	-13.3	2.89	-3.07
2988	c1c(c([nH]c(=O)c1Cl)Cl	C08672844	-14.05	-4.31	-15.86	7.92	-1.8
2989	c1c([nH]cn1)CCCl	C13283532	-14.05	-0.58	-16.05	5.71	-3.13
2990	C/C=C/C(=O)OC	C13380319	-14.05	-1.03	-14	3.56	-2.58
2991	CC(=O)Oc1ccc(=O)[nH]c1	C17105134	-14.05	-2.74	-19.99	10.65	-1.97
2992	Cc1c(c([nH]n1)Cl	C17946022	-14.05	-5.08	-12.23	4.76	-1.5
2993	c1cc(oc1)CCO	C19729362	-14.05	-2.81	-15.37	4.53	-0.4
2994	c1c2c(=O)[nH]cnn2cn1	C22013543	-14.05	-3.7	-18.92	10.68	-2.11
2995	c1cscc1SCCO	C01598574	-14.04	-3.92	-11.98	3.18	-1.32
2996	C(CC)OC(=O)Cl	C02031641	-14.04	0.07	-14.67	3.09	-2.53
2997	c1(nc(sn1)Cl)Cl	C04254807	-14.04	-2.13	-14.86	1.67	1.28
2998	C1=CC(C=C1)CO	C05133144	-14.04	-1.83	-13.74	2.45	-0.92
2999	c1cc(cnc1)NC(=S)N	C05161968	-14.04	0.04	-19.09	5.38	-0.38
3000	CC(=O)c1cscn1	C06357117	-14.04	-2.13	-16.38	4.86	-0.39
3001	c1cnc(c1)[N+](=O)[O-]	C08294941	-14.04	-3.28	-16.11	8.78	-3.43
3002	Cc1c(n2c(nn1)nnn2)[O-]	C08834353	-14.04	-4.75	-17.49	8.18	0.02
3003	COc(=O)C=C1	C14556351	-14.04	-0.41	-14.46	3.61	-2.78
3004	c1cnc(c1N)C(F)F	C19735127	-14.04	-3.44	-13.44	4.08	-1.25
3005	c1cc(c(c(c1)O)N)N	C00389621	-14.03	-3.75	-15.42	3.53	1.6
3006	c1cc(ccc1CCC#N)O	C01635610	-14.03	-2.19	-15.73	6.54	-2.64
3007	c1[nH]c(c(n1)Cl)Cl	C01728337	-14.03	-3.33	-13.56	5.13	-2.27
3008	c1c(cn[nH]1)C=O	C02738050	-14.03	-4.36	-15.23	6.1	-0.55
3009	C1=CC(=O)C=C1O	C04521345	-14.03	-4.11	-15.21	5.53	-0.24
3010	Cc1cc(cnc1)N	C08698082	-14.03	-1.21	-15.37	3.52	-0.97
3011	Cc1ccc(c(c1F)N)Cl	C12359282	-14.03	-2.53	-13.47	2.08	-0.11
3012	c1c(c([nH]n1)N)C(=O)N	C17039868	-14.03	-5.6	-17.68	6.8	2.45
3013	c1ccc(cc1)OC2cnns2	C01388237	-14.02	-0.5	-16.93	3.89	-0.47
3014	COc1=CC=CCC1	C01841394	-14.02	-1.2	-13.82	1.96	-0.96
3015	C(C(F)F)O[C@@H](F)Cl	C02389410	-14.02	-0.3	-14.27	2.49	-1.93
3016	C=CCOC([C@@H](F)Cl)(F)F	C02579135	-14.02	-0.91	-13.18	2.13	-2.06
3017	CCSC(=[NH2+])N	C03806245	-14.02	-2.18	-13.46	2.12	-0.5
3018	C=CCSC(=[NH2+])N	C05193890	-14.02	-2.43	-15.15	2.14	1.42
3019	c1cc(=S)[nH]nc1	C06512974	-14.02	-2.71	-15.71	5.7	-1.3
3020	C(=C(C(F)F)[O-])C(=O)C(F)F	C08700988	-14.02	-5.71	-14.48	8.28	-2.12
3021	c1cnn(n1)CCC#N	C12505453	-14.02	-1	-17.84	6.47	-1.65
3022	c1(c(nc([nH]c1=O)N)N)Cl	C17158224	-14.02	-4.33	-16.52	4.78	2.06
3023	c1cc(c(nc1)N)OC(F)F	C20483737	-14.02	-1.38	-17.43	5.67	-0.88
3024	Cc1cnc(c1F)N	C21981826	-14.02	-3.04	-13.35	3.98	-1.61
3025	CC(=O)c1ncc(s1)Br	C22007396	-14.02	-0.39	-14	2.74	-2.37
3026	c1cc(ncc1NN)Cl	C22200171	-14.02	-2.54	-16.9	5.93	-0.52
3027	CCCc1cccs1	C01631214	-14.01	-0.68	-13.97	1.41	-0.77
3028	Cc1ccc(c(c1)O)C	C01641024	-14.01	-2.29	-12.16	2.76	-2.31
3029	c1cnn(c1N)N	C02023828	-14.01	-4.37	-17.17	6.52	1.01
3030	c1cnc(cn1)C(=O)Cl	C02569383	-14.01	-3.34	-14.32	4.67	-1.02
3031	c1cc2n(c1)CCC2	C04914414	-14.01	-0.39	-16.28	3.32	-0.66
3032	C1C2=CC=NC2=NC=C1O	C06643323	-14.01	-2.76	-16.52	5.92	-0.65
3033	Cc1c2cccnc2[nH]n1	C12336552	-14.01	-1.75	-16.1	6.08	-2.25
3034	Cc1cc[nH+][cc1][O-]	C13511085	-14.01	-2.35	-15.16	3.89	-0.4
3035	Cc1cncnc1Cl	C14982420	-14.01	-0.94	-13.75	3.39	-2.7
3036	c1c(onc2c1[nH]nn2)Br	C19857217	-14.01	-1.36	-19.66	8.27	-1.26
3037	c1cc(ccc1OC(=O)N)Cl	C32603035	-14.01	-1.22	-18.96	6.92	-0.75
3038	Cc1ccc(nn1)N	C00153000	-14	-3.33	-16.08	6.21	-0.8
3039	Cc1c(c(on1)C)N	C00158485	-14	-2.77	-14.51	4.33	-1.05
3040	c1cc(c(nc1)Cl)Cl	C00333069	-14	-2.45	-12.66	3.88	-2.77
3041	Cc1nn2cnn2s1	C01657454	-14	-2.99	-17.07	9.13	-3.07
3042	Cn1cc(nc1)I	C02382639	-14	-2.24	-13.17	5.13	-3.72
3043	Cc1cc(on1)C	C02504362	-14	-1.78	-13.76	4.08	-2.54
3044	c1cc(c(cc1Cl)O)Br	C02512340	-14	-3.4	-12.68	4.18	-2.11
3045	c1c(cc(cc1F)Cl)O	C02584280	-14	-3.06	-11.52	2.27	-1.69
3046	c1c2c([nH]n1)ncnc2Cl	C03865628	-14	-2.62	-13.4	4.1	-2.09
3047	c1cc(c(nc1)c2ccco2)N	C04244134	-14	-2.6	-15.17	5.89	-2.11
3048	c1cc(cnc1)C(=S)N	C05842709	-14	-2.18	-15.87	2.93	1.12
3049	CCc1cc(n[nH]1)N	C12359712	-14	-2.33	-15.07	4.37	-0.97
3050	c1nc(nc(n1)Cl)Cl	C12650759	-14	-0.18	-13.77	2.72	-2.76
3051	c1cc(c(nc1)NN)F	C16158483	-14	-1.7	-15.19	4	-1.11
3052	c1cnc(cc1N)Cl	C19015383	-14	-4.03	-13.28	4.04	-0.73
3053	Cc1cnn(c1N)C	C19090099	-14	-3.06	-14.21	4.8	-1.54
3054	c1cnc(cc1C#N)N	C19424559	-14	-0.99	-16.78	5.09	-1.33
3055	c1cc(nc(c1C#N)N)C(F)F	C26461729	-14	-4.05	-12.69	4.81	-2.07
3056	C1Cc2c(sc(n2)Br)C1	C31772066	-14	-0.36	-13.92	3.61	-3.33

3057	C(CO)n1c(nnn1)N	C01564350	-13.99	-5.89	-16.75	7.51	1.14
3058	c1cc2c(nc1)CCC2	C01846564	-13.99	-0.28	-13.83	3.63	-3.51
3059	c1cc(oc1)CSC=O	C01850318	-13.99	-0.23	-18.1	6.97	-2.63
3060	c1cc(sc1)F	C02578015	-13.99	-1.43	-13.58	2.02	-1
3061	Cc1cc(on1)C(=O)Cl	C12370184	-13.99	1.41	-15.87	2.73	-2.26
3062	C[C@H](c1ccc(c(c1)F)F)O	C12506427	-13.99	-1.28	-14.78	4.27	-2.2
3063	c1cc(c(cc1N)F)C#N	C16125829	-13.99	-0.09	-17.97	6.08	-2
3064	[H]/N=C(N)/[NH+]=C/c1cccs1	C16430445	-13.99	-0.99	-14.68	4.14	-2.46
3065	c1cc(cnc1)CN/C(=[NH+]/N)/[S-]	C18202848	-13.99	1.83	-18.75	3.9	-0.97
3066	[H]/N=c/1/n(nnn1CCO)C	C32107231	-13.99	-4.66	-14.58	5.44	-0.19
3067	#Cc1ncc(cn1)Br	C32911350	-13.99	1.45	-18.3	5.66	-2.79
3068	CNc1ccc(cc1)O	C00388191	-13.98	-2.6	-14.37	3.34	-0.35
3069	c1cnn(c1)CCO	C01671842	-13.98	-3.29	-15.86	4.81	0.35
3070	CCNc1nncs1	C01680369	-13.98	-2.85	-15.1	5.42	-1.46
3071	c1cn(nc1[N+](=O)[O-])CCl	C02536477	-13.98	-3.68	-15.7	9.09	-3.69
3072	Cc1c(snn1)C(=O)Cl	C02555783	-13.98	1	-16.01	2.6	-1.57
3073	c1c(nc(nc1F)N)NN	C02565662	-13.98	-1.98	-16.81	5.21	-0.39
3074	CCC(=C(C)C(=O)C(F)F)[O-]	C04430787	-13.98	0.27	-13.89	2.7	-3.06
3075	CO/N=C/c1cccnc1	C05496351	-13.98	0.22	-16.86	4.75	-2.09
3076	COc1c(non1)O	C05794883	-13.98	-1.76	-17.47	4.04	1.21
3077	Cn1c(nnn1)NC#N	C06494464	-13.98	-4.46	-14.93	9.16	-3.75
3078	C(#N)C(F)FBr	C08698276	-13.98	-0.28	-12.62	1.06	-2.13
3079	c1c(oc(=O)oc1)ClCl	C01760794	-13.97	-1.08	-12.47	1.79	-2.22
3080	c1c([nH]nc1O)C(F)F	C04262653	-13.97	-3.51	-15.47	3.14	1.86
3081	CCC(=O)CC(=O)C(=O)OC	C05052153	-13.97	1.85	-19.41	4.97	-1.38
3082	C1CNC(=S)NC1	C06661066	-13.97	-2.13	-14.33	2.67	-0.18
3083	[C@H](C(=O)Cl)FCl	C16159206	-13.97	0.05	-14.27	2.15	-1.89
3084	c1c2c(cc(c1F)Cl)n[nH]n2	C00152702	-13.96	-3.45	-15.41	3.31	1.59
3085	c1cc(ncc1Br)[N+](=O)[O-]	C00331611	-13.96	-2.2	-13.46	5.56	-3.86
3086	c1ccc(cc1)CC=O	C00895323	-13.96	0.77	-15.59	4.53	-3.68
3087	c1cc([nH]c1)C(=O)CCl	C01574410	-13.96	-2.32	-14.69	5.76	-2.71
3088	c1cc(c(cc1C#N)N)O	C01704673	-13.96	-0.74	-17.9	4.66	0.03
3089	c1ccc(cc1)C(=O)CF	C02040597	-13.96	0.2	-17.22	6.89	-3.84
3090	c1c[nH]c(cc1=O)F	C02599000	-13.96	-2.47	-16.15	4.6	0.07
3091	C1CC=C[C@H](C1)O	C04744355	-13.96	-1.53	-13.23	1.88	-1.09
3092	c1cnc(cn1)C#N	C00164542	-13.95	-2.95	-15.48	5.56	-1.08
3093	CCOC1ccncc1F	C00331921	-13.95	-1.18	-14.75	4.25	-2.26
3094	c1cc(c(c(c1)O)N)O	C01680023	-13.95	-3.7	-16.29	3.78	2.26
3095	c1cc(c(cc1Br)N)F	C02243118	-13.95	-1.4	-14.95	1.78	0.63
3096	CCc1cc(no1)N	C05341526	-13.95	-1.18	-15.33	4.42	-1.87
3097	c1c(nc(cn1)N)C#N	C08698476	-13.95	-3.77	-16.33	6.2	-0.05
3098	c1[nH]nc(n1)C(=O)N	C11612727	-13.95	-5.54	-16.3	4.78	3.11
3099	C1=CN=N[C@H]1C=O	C14808558	-13.95	-3.94	-15.99	6.51	-0.53
3100	c1cc(c(=O)oc1)Cl	C21989733	-13.95	-2.36	-17.39	8.85	-3.04
3101	c1c2c(cnn1)nc[n-]2	C26506602	-13.95	-4.45	-18.67	10.17	-0.99
3102	c1cc(c(cc1O)Br)O	C00388415	-13.94	-1.24	-16.87	3.78	0.39
3103	c1cc(cc(c1)O)C#N	C00388758	-13.94	-0.31	-16.97	4.85	-1.51
3104	C=CC(=O)OC(C(F)F)C(F)F	C01841395	-13.94	-1.72	-11.09	3.5	-4.64
3105	Cc1cc(cnc1)Cl	C02599045	-13.94	0.25	-13.55	2.3	-2.93
3106	Cc1csc(=O)[nH]1	C04204717	-13.94	-2.42	-16.32	5.56	-0.75
3107	c1nc(no1)/C(=N)O/N	C05670167	-13.94	-5.05	-19.08	7.62	2.57
3108	c1ccc(cc1)C/C(=N)O/N	C12505212	-13.94	-1.93	-15.94	5.19	-1.26
3109	c1cc(cnc1)CN[NH3+]	C20283463	-13.94	1.69	-18.97	3.4	-0.06
3110	Cc1cccc(=O)oc1	C22004979	-13.94	-1.66	-17.06	8.07	-3.3
3111	CCNC(=O)n1ccnc1	C32628661	-13.94	-3.48	-15.86	7.91	-2.51
3112	c1ccc(cc1)O)O	C00002028	-13.93	-3.04	-16.06	4.16	1.01
3113	CC(=O)c1cc[nH]c1	C00153020	-13.93	-3.74	-16.52	8.54	-2.22
3114	c1c(c(nen1)N)C(=O)N	C00332913	-13.93	-2.68	-18.45	6	1.2
3115	Cc1c[nH]nc1C#N	C01423208	-13.93	-0.65	-15.52	3.81	-1.57
3116	c1cc2nenn2[nH]c1=O	C01590753	-13.93	-2.31	-19.04	6.94	0.48
3117	CSc1ccnnc1	C01605910	-13.93	-0.98	-17.71	5.26	-0.5
3118	Cc1ccnnc1	C01627093	-13.93	-1.66	-16.39	5.88	-1.76
3119	c1nc(no1)C(F)F	C02022421	-13.93	-3.51	-15.44	5.57	-0.54
3120	C=CCOCC(F)F	C02039481	-13.93	0.2	-14.5	2.86	-2.49
3121	C(C(C(F)F)F)OC(=O)C(F)F	C02566530	-13.93	0.65	-15.38	4.45	-3.65
3122	Cc1nc(cs1)C=O	C04198756	-13.93	-1.38	-15.31	4.4	-1.64
3123	C1CC=COC1	C04726938	-13.93	-0.69	-12.73	1.53	-2.04
3124	Cc1[nH]nc(n1)N[N+](=O)[O-]	C04952531	-13.93	-4.47	-18.14	7.18	1.5
3125	CCP(=S)(O)O	C06424831	-13.93	-0.67	-14.66	6.97	-5.57
3126	c1cnccc1CON	C14986311	-13.93	0.74	-18.48	4.2	-0.4
3127	c1c(c(c(cn1)Cl)N)C(F)F	C16158616	-13.93	-0.21	-14.3	2.37	-1.79
3128	c1ccc2c(c1)nnn2[O-]	C00058261	-13.92	-5.24	-15.57	7.09	-0.19
3129	c1ccc(c(c1)C=O)O	C00896073	-13.92	-2.97	-15.14	5.27	-1.08
3130	COCCCN=C=S	C02164238	-13.92	-0.94	-14.14	2.53	-1.36
3131	#Cc1ccc(cc1)CO	C02548215	-13.92	0.19	-16.52	4.61	-2.2
3132	c1c(sc(n1)N)C=O	C02577861	-13.92	-4.71	-15.21	6.39	-0.4
3133	c1cc(c(c(c1C#N)F)F)F	C04290229	-13.92	-2.42	-17.32	9.6	-3.77
3134	CC1=CCC[C@H]1O	C05179827	-13.92	-0.6	-13.46	1.8	-1.66
3135	c1nnc(n1)CCl	C05522105	-13.92	-2.94	-16.09	5.93	-0.82
3136	C=C[C@H](CBr)O	C06129901	-13.92	-0.64	-13.69	1.8	-1.38
3137	c1c(c([nH]c(=S)N1)[O-])C#N	C12395137	-13.92	-3.07	-17.09	4.98	1.26
3138	[C@H](C(F)F)F)OC(F)F	C14611408	-13.92	-0.09	-13.94	1.88	-1.77
3139	c1c(cncc1N)C#N	C21984988	-13.92	0.25	-19.04	5.63	-0.76
3140	c1c(c(cc(c1N)N)N)N	C00391939	-13.91	-4.46	-15.52	3.37	2.7
3141	c1cc(c(cc1N)O)N	C00394997	-13.91	-3.65	-17.33	3.47	3.61
3142	c1cc(c(cc1N)Cl)O	C00396100	-13.91	-2.23	-15.06	3.46	-0.07
3143	c1cc(ccc1CO)C#N	C00403449	-13.91	-0.55	-16.82	5.05	-1.59
3144	CCSC=C	C01581199	-13.91	-0.54	-11.68	1.2	-2.89
3145	c1nc(c2c(n1)[nH]c(n2)Cl)N	C01595876	-13.91	-3.05	-14.29	4.86	-1.44
3146	c1cc(n(c1)O)C#N	C01755382	-13.91	-3.23	-15.29	5.66	-1.05

3147	C=CCn1cnc(n1)[N+](=O)[O-]	C02315323	-13.91	-2.94	-14.56	9.54	-5.94
3148	C=CC(=O)OC(C(F)F)F(C(F)F)F	C02564824	-13.91	-1.74	-10.77	3.53	-4.93
3149	Cc1csc(n1)[S-]	C02569756	-13.91	-1.16	-14.34	3.39	-1.79
3150	Cc1nc(cs1)Br	C04198751	-13.91	-1.5	-13.63	3.51	-2.29
3151	CN1C(=O)N=NC1=O	C04529566	-13.91	-1.23	-17.39	2.41	2.3
3152	CSc1ccc(c(c1)F)Br	C12471941	-13.91	-0.82	-10.66	2.23	-4.65
3153	c1ccnc(c1)NO	C16954563	-13.91	-2.43	-17.59	6.52	-0.4
3154	CCc1cc(n[nH]1)C(F)F	C26547610	-13.91	-3.79	-12.81	5.17	-2.49
3155	c1(c(c(c(c1F)F)F)F)F	L2009A004	-13.91	0.36	-10.25	0.41	-4.42
3156	Cn1cccc1C=O	C00130187	-13.9	-3.01	-13	4.86	-2.77
3157	CCC(=O)OC=C	C00391909	-13.9	-0.82	-13.75	3.6	-2.94
3158	c1ccc(c(c1)C=N)O	C00500289	-13.9	-3.25	-14.52	4.15	-0.29
3159	C=CCn1ccc(=O)[nH]c1=O	C01644934	-13.9	-2.11	-21.48	9.53	0.16
3160	CO/C=C/C=C	C01648514	-13.9	-1.59	-12.3	2.16	-2.16
3161	C=CCNc1nc(ns1)N	C02026821	-13.9	-2.55	-14.27	4.84	-1.91
3162	C=CCn1cnc1[N+](=O)[O-]	C02285055	-13.9	-3.08	-13.21	8.56	-6.16
3163	c1(nc(sn1)Cl)Br	C04241473	-13.9	-2.21	-15.12	1.58	1.85
3164	Cc1c(c(on1)N)[N+](=O)[O-]	C04284533	-13.9	-4.82	-12.96	4.15	-0.28
3165	C(=O)(C(F)F)FCl	C04521880	-13.9	-0.08	-12.98	0.84	-1.68
3166	C/C=C/Cl)SC#N	C05046667	-13.9	1.1	-15.89	3.9	-3.02
3167	c1cc(ncc1O)I	C14982916	-13.9	-1.1	-15.8	3.67	-0.67
3168	C(=O)(C@H)(C(F)F)F(Cl)Br	C16159140	-13.9	0.52	-12.18	0.54	-2.77
3169	c1c[nH]c2c1cc(nc2)N	C18551745	-13.9	-5.44	-12.91	5.65	-1.21
3170	Cn1c(ccc1[N+](=O)[O-])C(=O)Cl	C20248573	-13.9	-0.89	-12.3	3.49	-4.21
3171	Cc1cc(cs1)CS	C20515421	-13.9	-0.91	-11.26	2.16	-3.9
3172	c1(nc(c1)Br)C(F)F	C21304395	-13.9	-1.6	-12.9	2.53	-1.94
3173	c1cc(=O)cc1I	C21989745	-13.9	-0.81	-15.95	6.39	-3.53
3174	CN1C(=O)C=CC1=O	C01688138	-13.89	-2.5	-16.44	5.95	-0.89
3175	Cc1c(=O)nc(c(=O)[nH]n1)C	C01689048	-13.89	-3.03	-15.52	4.67	-0.01
3176	C/C=C/C=CO	C02041062	-13.89	-2.12	-13.12	2.53	-1.18
3177	CCc1[nH]cc([nH]1)C	C04555707	-13.89	-1.75	-14.74	5.1	-2.5
3178	CC(=O)n1cccn1	C05383527	-13.89	0.58	-17.78	5.02	-1.72
3179	c1(c(non1)Cl)C(=N)O)/N	C05749057	-13.89	-2.71	-16.16	4.08	0.91
3180	c1cc2nncn2cc1Br	C12471957	-13.89	-2.28	-13.99	7.07	-4.68
3181	CNNC(=O)C(=O)n1ccnc1	C13207718	-13.89	-3.84	-14.69	4.94	-3.63
3182	Cc1cnc(c1)Br	C15021818	-13.89	-0.78	-15.06	3.56	-1.61
3183	c1[nH]c(nc1)NC(=S)N	C17328386	-13.89	-4.04	-18.8	12.29	-3.34
3184	c1cc(c(c(c1)F)F)C#N	C00409196	-13.88	-0.63	-16.09	6.51	-3.68
3185	c1cc(c(c(c1)N)O)F	C02243214	-13.88	-3.45	-15.77	5.29	0.04
3186	COc(=O)C(O)F	C04977188	-13.88	-3.21	-13.99	4.07	-0.76
3187	CCOC(=O)n1cnc(n1)N	C16980642	-13.88	-0.51	-15.56	5.33	-3.15
3188	Cn1c(=O)ccc(n1)[O-]	C17744645	-13.88	-2.96	-17.32	6.43	-0.04
3189	Cc1c(cns1)C=O	C20443682	-13.88	-2.92	-13.97	4.94	-1.93
3190	C1C(=CC(=O)O)Br	C30677957	-13.88	-0.81	-15.71	4.99	-2.36
3191	c1c(c(=O)[nH]nc1Cl)N	C30678129	-13.88	-1.34	-19.28	5.48	1.26
3192	c1ccc2c(c1)nco2	C00404297	-13.87	-2.27	-16.66	5.98	-0.91
3193	COc1cc(c(cc1F)F)F	C00405260	-13.87	-2.53	-11.63	2.9	-2.61
3194	CN(C=C)OC	C01623512	-13.87	-0.89	-13.19	2.04	-1.84
3195	c1cc(ncc1)F	C02384112	-13.87	-0.76	-15.58	2.59	-0.12
3196	Cc1c(cno1)C(=O)Cl	C02524899	-13.87	1.46	-15.9	3.01	-2.45
3197	C/C=C/C(F)F)F)O	C02555216	-13.87	-3.78	-13.09	3.34	-0.34
3198	c1cnc([nH]1)Cl	C02577855	-13.87	-2.04	-14.76	4.59	-1.66
3199	c1nnc(s1)Br	C04277253	-13.87	-0.65	-17.04	4.79	-0.97
3200	CCSC/C(=[NH+])N)/N	C05003077	-13.87	-3.66	-12.94	3.4	-0.67
3201	CC/C=C/OCC=C	C17146901	-13.87	0.1	-12.17	1.66	-3.46
3202	c1ccc2c(c1)ncs2	C00019726	-13.86	-2.38	-13.68	5.11	-2.91
3203	c1ccc(cc1)NC(=O)NN	C00157484	-13.86	-3.94	-17.75	8.45	-0.61
3204	CCCc1ccc1	C01668229	-13.86	-0.92	-13.49	2.33	-1.78
3205	c1c2c([nH]c(S)[nH]2)nc(n1)N	C01693117	-13.86	-5.83	-14.75	8.92	-2.2
3206	c1cc(c(cc1N)Br)F	C02510756	-13.86	0.23	-14.99	3.23	-2.32
3207	C=CC[C@H](C=C)O	C02568007	-13.86	-0.56	-13.36	1.43	-1.37
3208	c1cnc(c1C=O)N	C02583497	-13.86	-5.9	-14.14	6.41	-0.23
3209	CC/C(=C/C(=O)C(F)F)/[O-]	C04262607	-13.86	-0.97	-13.07	2.97	-2.79
3210	Cn1c(c(cn1)[N+](=O)[O-])N	C04728771	-13.86	-4.9	-14.25	6.85	-1.56
3211	c1cnncc1C#N	C12359491	-13.86	-0.17	-17.97	5.73	-1.44
3212	c1cc(cc(c1)F)C(=N)O)/Cl	C13367399	-13.86	-0.74	-14.96	3.84	-1.99
3213	c1ccc(c(c1)F)SCC#N	C19847576	-13.86	-0.3	-16.65	7.75	-4.67
3214	CC(=O)c1nccs1	C00164484	-13.85	0.9	-17.44	4.35	-1.66
3215	COc(=O)Nc1ccsc1	C00336546	-13.85	0.56	-18.02	5.01	-1.39
3216	c1(c(c(c(c1F)F)F)F)F)O	C01583742	-13.85	-2.27	-11.92	2.5	-2.15
3217	CC(=O)Oc1cccc1O	C01688153	-13.85	0.02	-18.97	7.64	-2.53
3218	C=CC(=O)OC/C=C/Cl	C01871135	-13.85	-0.37	-13.6	3.79	-3.68
3219	c1(=O)c(ncc([nH]1)[O-])F	C02272459	-13.85	-2.82	-16.79	3.86	1.9
3220	CCC(=C)C(=O)Cl	C02541518	-13.85	-1.04	-14.22	2.87	-1.46
3221	CCOC(=O)[C@H](C#C)O	C02556928	-13.85	-4.03	-12.71	4.41	-1.52
3222	C=CCNC(=O)C(C(F)F)F	C03165303	-13.85	-0.99	-14.94	3.96	-1.89
3223	c1cc(cnc1)NC(=O)C=N	C05581138	-13.85	-4.15	-21.35	10.75	0.92
3224	CCO[C@H]1C=CCO1	C05840128	-13.85	-0.09	-13.97	2.85	-2.64
3225	c1c[nH]c(cc1=O)Cl	C08672866	-13.85	-3.73	-13.89	4.06	-0.29
3226	c1c(nc[nH]1)C(C(F)F)F)F	C13230019	-13.85	-2.54	-12.29	4.1	-3.11
3227	CCc1[nH]c(=O)ccn1	C16998009	-13.85	-2.79	-17.18	7.88	-1.76
3228	c1c(c(nc1F)F)Br	C21990775	-13.85	0.37	-13.9	2.04	-2.36
3229	c1ccc2c(c1)NC(N2)S	C22013613	-13.85	-2.48	-13.71	3.78	-1.44
3230	c1cc(c(c(c1F)O)F)F	C00389657	-13.84	-1.44	-15.41	4.36	-1.35
3231	c1c[nH]c(nc1=O)NN	C01188491	-13.84	-3.7	-17.93	8.22	-0.43
3232	CCCC(=O)C(F)F)Cl	C01675526	-13.84	-0.61	-13.13	1.97	-2.06
3233	C1(=O)C(C(C(=O)N1)(F)F)F)F	C01728889	-13.84	-0.04	-17.18	3.15	0.23
3234	c1nnc(n1)CCC#N	C12505747	-13.84	-0.77	-17.21	8.13	-3.99
3235	c1c(ccnc1[N+](=O)[O-])N	C14982119	-13.84	-1.84	-16.3	5.22	-0.91
3236	c1c(scn1)N	C16696910	-13.84	-3.55	-14.23	3.79	0.15

3327	c1c(c[nH]1)C(=O)N	C12398963	-13.77	-4.44	-18.12	7.15	1.64
3328	CN/C(=N)C1CCCC1/NN	C17023479	-13.77	2.06	-18.33	5.65	-3.15
3329	c1c(c(nn1CC(F)F)N)Cl	C20348912	-13.77	-4.5	-12.81	5.4	-1.86
3330	c1nc(no1)C(=O)Cl	C20357967	-13.77	-3.62	-16.48	6.36	-0.03
3331	c1ccc(c(c1)CC(=O)Cl)F	C02513824	-13.76	-1.76	-12.66	4.84	-4.18
3332	c1c(c(ns1)C(=O)NN)N	C04784130	-13.76	-4.08	-17.38	5.26	2.45
3333	c1ccc(c1N=[N+]=[N-])C=O	C08383144	-13.76	0.7	-19.1	5.23	-0.59
3334	c1cc(c(=O)[nH]c1)[N+](=O)[O-]	C08698093	-13.76	-3.65	-17.51	7.64	-0.23
3335	Cc1[nH]c(=O)c(cn1)Br	C16082606	-13.76	-2.55	-15.56	3.74	0.61
3336	c1cc(nc(c1Cl)[O-])Cl	C16123752	-13.76	-2.53	-15.65	6.27	-1.84
3337	c1cc(c(c(c1)N)N)N	C00087438	-13.75	-2.72	-15.07	3.01	1.03
3338	c1cc2c(nc1)COC2=O	C00335085	-13.75	-2.4	-15.85	6.86	-2.36
3339	c1cc(c(c(c1O)F)F)F	C00389597	-13.75	-2.22	-15.62	5.36	-1.26
3340	c1cc(c(cc1F)O)C=O	C02510730	-13.75	-3.72	-14.3	6.43	-2.16
3341	c1cc(c(nc1)F)CO	C02598033	-13.75	-2.49	-17.09	4.77	1.05
3342	CCc1cc[nH]n1	C03593983	-13.75	-1.67	-16.21	3.71	0.41
3343	C=C(/C#N)Cl)Cl	C12405131	-13.75	-1.28	-12.63	2.74	-2.59
3344	c1cc(ccc1c2nc(no2)CCC[NH3+])F	C19682255	-13.75	0.98	-11.92	-0.82	-2
3345	Cn1cc(cn1)S	C20476949	-13.75	-2.33	-13.75	4.31	-1.99
3346	c1c(cnc(c1O)N)F	C21981857	-13.75	-4.08	-17.4	7	0.73
3347	c1cncnc1NN	C25491315	-13.75	-1.85	-16.92	6.07	-1.04
3348	c1cc(c(c(c1)F)O)F	C00388530	-13.74	-2.33	-14.52	4.38	-1.27
3349	Cc1c(non1)N	C01295959	-13.74	-2.83	-14.84	4.18	-0.25
3350	CC(=O)C1CCCC1	C01700205	-13.74	-1.12	-13.52	5.28	-4.38
3351	COO(=O)C1CCCC1F	C02570115	-13.74	-0.41	-16.67	5.87	-2.54
3352	c1ccc(c(c1)CSC(=[NH2+])N)F	C04377625	-13.74	-0.47	-14.72	4.08	-2.64
3353	c1(nc(on1)C(F)F)C(=NO)/N	C05510674	-13.74	-2.2	-15.98	3.52	0.92
3354	CCCc1nc(on1)CCl	C12505493	-13.74	0.49	-15.98	4.13	-2.38
3355	c1cc(ccc1N)N=[N+]=[N-]	C12956370	-13.74	-0.61	-15.91	2.78	0
3356	c1cncnc1NC(=O)N	C13538948	-13.74	-3.52	-19.12	7.95	0.94
3357	C=C=CCCCO	C15809780	-13.74	-0.98	-14.33	2.79	-1.22
3358	CSc1ccccc1	C15880094	-13.74	0.44	-14.45	3.25	-2.98
3359	c1cncnc1CN[NH3+]	C19169056	-13.74	1.51	-18.59	3.3	0.04
3360	CCCCN/C(=N)[N+](=O)[O-]/N	C19943825	-13.74	-4.65	-10.22	3.51	-2.38
3361	Cc1coanc1C=O	C20443655	-13.74	-2.05	-14.89	4.83	-1.63
3362	Cc1nc(sn1)C=O	C20443854	-13.74	-4.06	-13.25	4.41	-0.83
3363	CNc1ncc(cn1)C#N	C21953250	-13.74	-1.69	-14.53	5.35	-2.86
3364	Cc1c(c(no1)N)Cl	C22129881	-13.74	-2.36	-14.11	4.25	-1.51
3365	c1c2nncn2c3nncn3n1	C26471499	-13.74	-1.65	-14.81	8.68	-5.96
3366	CN1CC(=O)N=C1N	C00967189	-13.73	-2.82	-15.28	5.5	-1.13
3367	C=CC(=O)Cl	C01609475	-13.73	-1.63	-13.55	3.21	1.75
3368	Cc1c(ccc(n1)F)N	C02383956	-13.73	-4.36	-15.2	5.33	0.5
3369	C(=N/N=C(N)S)C(F)F	C05409951	-13.73	-1.9	-14.89	3.79	-0.74
3370	c1cc(c(=O)[nH]c1)C(F)F	C08698400	-13.73	-3.01	-16	5.1	0.17
3371	Cn1cc(cn1)CCl	C12398537	-13.73	-0.99	-14.95	4.82	-2.61
3372	c1cn(cn1)C=O	C14516302	-13.73	-3.3	-15.72	7.45	-2.17
3373	C(=C/N)C(=O)C(F)F	C16158775	-13.73	-3.49	-15.19	5.81	-0.86
3374	c1c(c(nc(n1)Cl)[O-])F	C17004699	-13.73	-1.8	-17.01	3.94	1.13
3375	Cc1[nH]cc(c(=O)n1)C#N	C17378342	-13.73	-2.44	-17.39	5.32	0.78
3376	C/C(=C(C(=O)C(F)F)Cl)/[O-]	C18167146	-13.73	1.12	-14.85	2.26	-2.26
3377	c1nc2n(n1)CCCN2	C20216425	-13.73	-3.4	-14.45	7.42	-3.31
3378	c1cc(ncc1[N+](=O)[O-])C=O	C21985566	-13.73	-5.33	-10.91	4.8	-2.28
3379	CN1C(=O)C=CC1(F)F	C21997047	-13.73	-2.54	-15.91	6.07	-1.35
3380	c1cc(c(cc1S)O)O	C26479313	-13.73	-2.32	-16.64	5.06	0.17
3381	Cc1nc(cs1)CS	C31890180	-13.73	-0.9	-14.08	3.8	-2.54
3382	CC(=O)c1ccc1	C00334128	-13.72	-2.16	-16.4	7.18	-2.33
3383	c1ccc(c(c1)CCO)N	C00406951	-13.72	-2.09	-13.94	2.83	-0.53
3384	c1c(c(c(nn1)Cl)Cl)N	C00967451	-13.72	-4.04	-14.44	5.16	-0.4
3385	Cn1c(cn1)N	C01390247	-13.72	-2.53	-15.27	4.88	-0.8
3386	c1cc(ccc1C=O)N	C01677280	-13.72	-3.41	-14.46	5.68	-1.52
3387	c1cnc([nH]1)N[N+](=O)[O-]	C01742154	-13.72	-4.33	-15.45	8.82	-2.77
3388	C/C=C/c1ccc1O	C02140904	-13.72	0.1	-16.71	3.03	-0.14
3389	CC(=C)[C@@H](CC=C)O	C02169052	-13.72	-1.15	-13.97	1.62	-0.21
3390	c1c(c(cn1)[O-])C#N	C02382604	-13.72	-0.67	-18.55	4.91	0.59
3391	c1cnc(cn1)F	C02506842	-13.72	-2.07	-15.06	4.09	-0.68
3392	c1c(c(c(nc1F)F)C(F)F)F	C02513199	-13.72	1.48	-14.1	2.24	-3.34
3393	c1ccc(c(c1)NC(=O)C=N)O	C04900984	-13.72	-3.71	-20.03	9.34	0.69
3394	CC/C=N/C	C04946289	-13.72	-0.92	-13.82	2.42	-1.4
3395	C=CCC(=O)c1ccc1	C05283033	-13.72	0.95	-17.24	4.65	-2.08
3396	Cc1c(nc(n1)C)O	C05401452	-13.72	-3.76	-13.56	5.44	-1.83
3397	C(CSC(=C(F)F)F)O	C08983558	-13.72	-2.46	-12.99	2.29	-0.56
3398	Cc1c([nH]c(S)[nH]1)C	C15892418	-13.72	-2.66	-13.76	4.68	-1.98
3399	[C@@]1(C(O1)F)F(C(F)F)Br	C16082668	-13.72	-0.03	-12.57	0.35	-1.48
3400	c1cnc(c1)CO	C00158585	-13.71	-0.31	-17.36	4.11	-0.15
3401	c1ccc(cc1)N(C=S)O	C01582369	-13.71	-1.61	-17.62	4.81	0.71
3402	CCOC(=O)C=C(C=O)C	C02144785	-13.71	-0.62	-14.67	4.87	-3.3
3403	c1c2c(c(ncn2)[O-])[nH]n1	C11592630	-13.71	-2.46	-18.83	5.45	2.12
3404	Cc1cc(no1)C#N	C12370156	-13.71	-0.9	-15.24	4.84	-2.41
3405	c1cnc(c1)CC(F)F	C12395930	-13.71	0.52	-17.35	5.76	-2.63
3406	c1c(c(cc(c1F)F)O)C=O	C16158091	-13.71	-4.6	-14.03	6.1	-1.19
3407	CCc1[nH]c(cn1)Cl	C20358066	-13.71	-4.41	-13.32	6.52	-2.51
3408	CCNc1nccc1	C21013773	-13.71	-1.3	-13.88	4.59	-3.11
3409	c1c(=O)n(c2nncn2n1)N	C26443341	-13.71	-3.9	-15.2	7.93	-2.55
3410	c1c(cn1)C(F)F	C26510661	-13.71	-2.82	-15.46	4.85	-0.28
3411	c1cc(c2nccn2c1)F	C26894738	-13.71	-2.65	-16.03	8.86	-3.9
3412	Cc1c(cccc1O)O	C00154621	-13.7	-1.71	-16.03	3.76	0.27
3413	C(#N)c1c(c(nc(c1F)F)F)F	C00389641	-13.7	0.54	-14.01	1.91	-2.15
3414	Cc1c(non1)C(=O)N	C01273612	-13.7	-2.16	-15.9	3.39	0.98
3415	c1ccc(cc1)SC(=O)NN	C01704240	-13.7	-0.26	-18.41	6.17	-1.2
3416	CC1=CC(=O)CC1	C02035915	-13.7	-1.57	-14.57	5.28	-2.83

3417	C/C=C(C)/C(=O)C	C02036684	-13.7	-0.52	-13.51	3.41	-3.07
3418	c1csc1N	C02510647	-13.7	-2.53	-14.3	2.09	1.03
3419	c1cc(c(cc1Cl)F)C#N	C02512515	-13.7	-1.37	-14.06	4.08	-2.36
3420	c1c(ncs1)C(=S)N	C02527456	-13.7	-3.27	-17.29	7.57	-0.71
3421	CCOC(=O)C(CO)(F)F	C02559538	-13.7	-1.43	-16.03	4.48	-0.72
3422	CCOC(=O)CS	C03860449	-13.7	-1.3	-14.04	4.08	-2.44
3423	c1cc2c(cc1N)[nH]cn2	C04692941	-13.7	-5.68	-13.61	7.22	-1.63
3424	Cc1c2c(ncn1)[nH]n2	C05544348	-13.7	-1.03	-17.78	6.36	-1.26
3425	C1[C@@H](OC1)CN=C=O	C11802365	-13.7	-0.95	-16.84	3.61	0.48
3426	c1cc([nH]c1C(=O)N)Br	C13379819	-13.7	-2.81	-16.39	5.32	0.19
3427	C1=CN=C[C@@H](C1=O)[O-]	C13521874	-13.7	-3.18	-16.68	4.43	1.72
3428	c1c(nc(s1)[N+](=O)[O-])[N+](=O)[O-]	C15784321	-13.7	-2.63	-18.01	10.97	-4.03
3429	C[NH+](Cc1ccccc1)N	C19167200	-13.7	-2.2	-11.3	1.81	-2
3430	Cc1c(nns1)C=O	C20443830	-13.7	-3.12	-13.98	4.34	-0.93
3431	c1c(cnc(c1Cl)[N+](=O)[O-])Cl	C26459716	-13.7	-2.35	-12.23	4.93	-4.04
3432	CC(=O)CSc1ccccc1N	C32698055	-13.7	-2.65	-14.65	6.83	-3.24
3433	CCCOCC(=O)Cl	C01586736	-13.69	-0.86	-12.96	1.71	-1.57
3434	c1cn(c(=O)[nH]c1=O)CC=O	C01701740	-13.69	-2.8	-20.85	9.45	0.51
3435	c1(c(c(c(c1F)F)F)N)F)N	C01704671	-13.69	-3.43	-12.62	2.71	-0.36
3436	c1cc(cc(c1F)NC(=O)N	C02031132	-13.69	-4.16	-17.78	8.78	-0.53
3437	c1cc(c(c1O)OC(F)F	C02560137	-13.69	0.47	-18.76	4.82	-0.21
3438	Cc1ccc(c(c1F)O)F	C02574955	-13.69	-2.07	-15.25	4.36	-0.72
3439	COC(=O)C=C(F)F	C03880140	-13.69	-0.48	-14.58	3.54	-2.17
3440	C1C=CC@H1N=O)Cl	C05004376	-13.69	-1.26	-12.37	1.55	-1.61
3441	CC(=NOCC#C)C	C05377860	-13.69	-0.03	-15.88	4.64	-2.42
3442	c1c(c(nc1Cl)Cl)[O-]	C05425248	-13.69	-4.48	-15.59	5.32	1.05
3443	COC(=O)Cc1[nH]c(n1)[N+](=O)[O-]	C05510987	-13.69	-4.67	-16.85	12.44	-4.61
3444	Cc1c[nH+]c[nH]1	C08283845	-13.69	-2.9	-14.06	5.29	-2.01
3445	Cc1nc(on1)CCl	C12463251	-13.69	-1.47	-15.73	4.55	-1.03
3446	C=CC/C(=N/O)/N	C15937655	-13.69	-3.58	-14.51	4.07	0.33
3447	CCOC1ccc(n1)N	C16677890	-13.69	-3.22	-16.57	5.98	0.12
3448	c1(nc(s1)S(=O)(=O)[NH-])N	C16969869	-13.69	-5.01	-19.28	6.76	3.84
3449	c1c2c(nc(n1)[O-])snn2	C17328366	-13.69	-2.21	-19.78	4.89	3.42
3450	Cc1csc(n1)/C(=N/O)/C#N	C17837217	-13.69	-0.26	-19.66	6.56	-0.34
3451	Cc1c([nH]c1N)C(F)F	C26511518	-13.69	-4.09	-15.5	6.82	-0.92
3452	c1ccc2c(c1)c(=O)c2=O	C00158295	-13.68	-2.32	-13.75	5.47	-3.1
3453	CS1ccc(cc1)Cl	C00161046	-13.68	-0.17	-14.88	1.91	-0.54
3454	COC(=O)Nn1cnc1	C01437193	-13.68	-1.66	-18.62	8.43	-1.84
3455	c1ncc(n1)CCO	C01442884	-13.68	-2.6	-17.7	4.46	2.17
3456	CCO/C=C/Br	C01613352	-13.68	-1.11	-11.71	1.57	-2.42
3457	C[C@H](C(=O)Cl)Cl	C02242618	-13.68	-0.37	-13.21	2.22	-2.33
3458	COC(=O)C(=C)F	C02525784	-13.68	-1.27	-13.88	3.53	-2.06
3459	CC#CCOC(=O)C	C02555299	-13.68	0.9	-15.96	4.92	-3.54
3460	c1cc(cc(c1)OC(=S)Cl)[N+](=O)[O-]	C02576025	-13.68	-3.19	-11.79	6.01	-4.72
3461	CC(=O)N/[NH+]=C/c1c(ncn1)N)N	C04837426	-13.68	-3.03	-21.68	8.81	2.22
3462	c1(c([n+](on1)[O-])N)C(=O)N	C05002537	-13.68	-5.21	-18.39	8.83	1.1
3463	c1cn(cn1)C(=O)CCl	C05729244	-13.68	-3.04	-15.17	7.64	-3.11
3464	CCN1C(=O)C(=O)NC1=O	C06496934	-13.68	-1.1	-18.36	4.63	1.14
3465	Cc1ccc(nc1)NN	C06755403	-13.68	-3.73	-12.76	4.19	-1.39
3466	c1cc(=O)[nH]cc1[N+](=O)[O-]	C08580643	-13.68	-2.39	-17.52	5.67	0.56
3467	[C@@H](C(F)F)Br)OC(F)F)F	C08698311	-13.68	-0.25	-12.88	1.49	-2.05
3468	C(=O)c1c(snn1)Cl	C15021036	-13.68	0.46	-16.01	2.76	-0.89
3469	COC(=O)/C=C/N	C21297651	-13.68	-3.15	-15.39	5.38	-0.53
3470	c1c(c(ncn1)N)C=O	C26894937	-13.68	-5.01	-15.87	8.02	-0.82
3471	c1cc(cc(c1)F)CC#N	C00157125	-13.67	-1.51	-17.54	8.59	-3.22
3472	CC(=O)c1cccs1	C00157402	-13.67	1.41	-16.67	4.64	-3.05
3473	C=COCC(=O)c1ccccc1O	C00394054	-13.67	-0.16	-17.83	5.87	-1.55
3474	C[C@@H](c1ccccc1)O	C01403557	-13.67	-1.36	-15.21	3.45	-0.55
3475	CCOC1cnc1	C01574034	-13.67	-0.7	-16.74	4.06	-0.3
3476	c1cnc(nc1F)F	C01575075	-13.67	-2.25	-15.31	5.32	-1.42
3477	c1c[nH]cc1CCO	C01728760	-13.67	-3.76	-15.55	3.98	1.66
3478	CCOC(=O)COC(=O)C	C01736012	-13.67	1.01	-17.12	5.83	-3.39
3479	c1cc(c(cc1N)F)C(F)F	C02556414	-13.67	-2.1	-13.27	4.09	-2.4
3480	Cc1c(=O)nc(c(=S)[nH]n1)N	C02581674	-13.67	-4.84	-14.27	5.63	-0.19
3481	Cc1cc(sn1)N	C04240488	-13.67	-2.73	-14.63	4.19	-0.49
3482	[H]N=C(CC)/SC	C04353471	-13.67	-0.92	-12.19	1.35	-1.9
3483	C=Cn1ccc1C=O	C05377628	-13.67	0.31	-17.47	5.62	-2.13
3484	c1ccn2cc(nc2c1)S	C13207463	-13.67	-1.95	-14.97	7.04	-3.79
3485	c1cc(cnc1)CNC(=O)C(F)F	C13208170	-13.67	0.45	-20.41	7.8	-1.51
3486	Cc1cn(cn1)C	C13282287	-13.67	-2.07	-13.67	5.37	-3.31
3487	Cc1c(c(sn1)N)Br	C15042090	-13.67	-3.52	-12.46	3.2	-0.89
3488	C=CCOC1cnc1	C15894714	-13.67	-2.26	-12.17	3.38	-2.62
3489	[C@H](C(=O)Cl)(F)Cl	C16159204	-13.67	0.21	-14.13	2.15	-1.9
3490	C(c1c(=O)[nH]c(=O)[nH]n1)F	C17379051	-13.67	-3.88	-17.15	6.12	1.25
3491	COCc1ccc(nc1)Cl	C19385596	-13.67	-2.23	-13.19	3.92	-2.17
3492	Cc1n2cnc2s1	C33359219	-13.67	-1.21	-15.35	6.68	-3.78
3493	COC(=O)Cc1ccccc1O	C00397535	-13.66	-0.02	-18.13	6.93	-2.44
3494	c1cnc(c1)N	C01737540	-13.66	-3.15	-15.89	6.12	-0.75
3495	c1ccc(c(c1)C(=O)Cl)F	C02022413	-13.66	1.23	-16.83	5.59	-3.66
3496	C[C@H](C(=O)C)Cl	C02038108	-13.66	-0.66	-13.17	2.58	-2.41
3497	C[C@@H](C(=O)Cl)Br	C02043872	-13.66	1.24	-14.57	2.07	-2.4
3498	c1cc(ccc1CCO)N	C04013051	-13.66	-2.19	-14.19	3.09	-0.38
3499	Cc1c[nH]c(n1)Br	C04352759	-13.66	-2.06	-14.33	4.7	-1.97
3500	C(C(=O)Cl)I	C05226702	-13.66	0.25	-14.3	2.66	-2.27
3501	C1CCC(=CC1)CO	C05409961	-13.66	-1.68	-12.81	2.37	-1.55
3502	C1C[C@H](CC=C1)C(=O)Cl	C08100892	-13.66	-0.03	-11.87	1.97	-3.74
3503	C1C(=CC(=O)O)I	C15444545	-13.66	-0.82	-14.87	4.73	-2.7
3504	C/C(=C/C(=O)C)/N	C16001389	-13.66	-3.03	-14.02	4.5	-1.11
3505	CCOC(=O)C=CCBr	C17353063	-13.66	-0.97	-11.85	3.02	-3.86
3506	C1=C/C(=C/C(=O)N/C=C1	C19729367	-13.66	-1.26	-16.64	6.72	-2.47

3507	c1cc(c(cc1N)O)Br	C19872881	-13.66	-2.43	-17.71	6.59	-0.1
3508	c1ccc(cc1)COC(=O)NO	C00389485	-13.65	-0.62	-20.61	8.36	-0.78
3509	c1cc(ccc1O)Br	C00404316	-13.65	-0.56	-16.72	2.44	1.19
3510	c1ccc2c(c1)CC(C@H)2O	C00901097	-13.65	-1.58	-12.77	3	-2.3
3511	COC(=O)c1c(c[nH]n1)[N+](=O)[O-]	C01075965	-13.65	-3.06	-16.21	7.52	-1.89
3512	C(=C)SC#N)C(=O)N	C01604241	-13.65	-2.67	-19.47	8.25	0.24
3513	C1C[C@H]2C(=C1)CC(=O)O2	C01616151	-13.65	-1.21	-14.39	5.22	-3.28
3514	CCCc1cc[nH]n1	C03636498	-13.65	-1.83	-12.75	3.3	-2.37
3515	CC(=O)CC(=O)c1ccccc1	C04262604	-13.65	-0.64	-17.1	5.31	-1.21
3516	c1c(n[nH]n1)CN=[N+]=[N-]	C05544994	-13.65	-2.44	-18.26	4.74	2.31
3517	c1ccc(c(c1)c2nc[nH]n2)N	C06896574	-13.65	-0.63	-19.28	9.16	-2.89
3518	c1cc(oc1C=O)c2cncnc2	C20216282	-13.65	-0.17	-16.27	5.91	-3.12
3519	C(COC(=O)CS)O	C20231604	-13.65	-3.64	-16.52	6.5	0.02
3520	c1csc(c1N)C(=O)NN	C00080615	-13.64	-4.87	-16.72	6.63	1.31
3521	COC1cc(=O)[nH]nc1	C00337136	-13.64	-2.96	-17.41	6.24	0.5
3522	CCOC(=O)CCBr	C01583936	-13.64	-0.03	-12.95	2.87	-3.53
3523	Cc1ncc(cn1)Cl	C01644846	-13.64	-0.79	-15.51	2.5	0.16
3524	CC(=O)OCCSC#N	C01661159	-13.64	-1.27	-15.14	5.79	-3.02
3525	c1c(ncnc1Cl)Cl	C01670096	-13.64	0.07	-13.41	2.23	-2.53
3526	c1c(c(c2nncn2n1)N)Cl	C01674219	-13.64	-5.02	-14.56	5.8	0.15
3527	CC(=O)NCC(=O)c1c(non1)N	C02227534	-13.64	-3.32	-19.49	6.52	2.65
3528	CCOC(=O)[C@H]2C(=O)C	C03848375	-13.64	-2.45	-13.27	4.78	-2.7
3529	C=CCN(CC=C)N=O	C04783263	-13.64	-1.08	-14.13	3.21	-1.65
3530	c1ccc(cc1)/C=C/C=N/O	C12370145	-13.64	-2.71	-15.45	4.48	0.03
3531	Cn1nc(nn1)N	C16954943	-13.64	-4.74	-15.24	7.17	-0.83
3532	C=C/C=C=N/Nc1ccccc1	C17324211	-13.64	-1.13	-12.56	4.11	-4.05
3533	CSCSC	C01621620	-13.63	-1.11	-11.08	1.38	-2.83
3534	c1ccc(cc1)/C=C\2/C(=O)OC=N2	C01707320	-13.63	-0.6	-16.47	7.27	-3.83
3535	C=C1CCC(=O)O1	C02015886	-13.63	-1.01	-15.51	5.72	-2.83
3536	Cc1ccc(s1)Cl	C02382622	-13.63	-0.29	-14.57	1.58	-0.34
3537	c1c(c(c(c1F)Br)F)O	C02541323	-13.63	0.44	-16.9	2.72	0.12
3538	c1cc2c(cc1N)COC2	C02559710	-13.63	-1.75	-13.97	3.23	-1.14
3539	CCOC(=C)C	C02563426	-13.63	-0.29	-13.46	1.54	-1.43
3540	COC(=O)[C@H]2C(=O)C(=O)OC2O	C04099934	-13.63	1.9	-20.11	5.8	-1.22
3541	c1cc(ncc1Br)C=O	C04208988	-13.63	-0.83	-13.7	3.09	-2.2
3542	CN(C(=O)NCC(F)F)N=O	C04804439	-13.63	-1.73	-14.23	3.12	-0.8
3543	C1CC=CC(=O)C1	C05188148	-13.63	-1.95	-14.52	4.21	-1.38
3544	c1c(ncnc1Cl)NN	C08615712	-13.63	-2.4	-14.46	4.42	-1.19
3545	c1cc(ccc1)/C=C/C(=O)C(F)F/[O-]F	C18161714	-13.63	-2.96	-10.03	4.35	-4.98
3546	c1ccnc(c1)[C@H]2CO2	C19730640	-13.63	-2.42	-13.96	4.08	-1.33
3547	Cn1ccnc1F	C22001040	-13.63	-2.08	-14.88	5.67	-2.34
3548	c1ncc(c1Cl)O	C02583363	-13.62	-1.12	-17.26	3.44	1.32
3549	CN(C=C)N=O	C04984176	-13.62	-1.63	-13.96	3.28	-1.32
3550	CCOC1ccccc1	C05114909	-13.62	-2.62	-12.13	3.33	-2.19
3551	Cc1cc(cnc1)C#N	C08294945	-13.62	0.25	-15.06	4.05	-2.86
3552	c1cc(ncc1Cl)C=O	C08698212	-13.62	-0.85	-15.55	3.14	-0.36
3553	c1cc(c(c1)Br)F)O	C16158469	-13.62	-1.46	-14.73	4.31	-1.74
3554	COC(=O)c1c[nH]nc1	C19722105	-13.62	-2.01	-17.2	6.86	-1.27
3555	C=C[C@H]1C(=C)CCCO1	C21990741	-13.62	0.58	-12.84	1.8	-3.16
3556	c1cc(c(cc1O)F)C#N	C00161696	-13.61	0.12	-18.1	5.81	-1.44
3557	CCOC1ccccc1N	C00331030	-13.61	-2.04	-14.61	3.64	-0.6
3558	Cc1c(s)[nH]c(=O)[nH]n1	C01237630	-13.61	-2.58	-15.52	4.59	-0.1
3559	c1nc(c(c2n1nnn2)N)Cl	C01599810	-13.61	-4.15	-14.28	4.6	0.22
3560	CCOC(=O)[C@H](F)Cl	C02168353	-13.61	-1.31	-12.87	3.43	-2.86
3561	c1cc(cnc1)CNc2[nH]ncn2	C03954464	-13.61	-0.7	-15.4	6.37	-3.88
3562	CCOC(=O)[C@H](C)S	C04802714	-13.61	-1.2	-12.53	3.11	-2.99
3563	c1ccc(c(c1)C(=[NH2+])NO)F	C06251708	-13.61	-3.44	-18.04	7.03	0.84
3564	c1c[nH]nc1C(=O)N	C14684055	-13.61	-4.44	-18.44	7.69	1.58
3565	C(=C)C#N)C=C/C#N	C16927505	-13.61	-1.5	-15.43	6.36	-3.05
3566	Cc1c(scc1C)Cl	C19754919	-13.61	-1.05	-10.21	2.25	-4.61
3567	C1CCC(C1)NCC#N	C20037012	-13.61	-1.61	-14.14	4.26	-2.12
3568	c1cnc(cn1)CNC=O	C01601709	-13.6	-3.26	-19.49	7.59	1.55
3569	C#CCNC(=O)NCCCl	C01673738	-13.6	-1.74	-17.25	6.51	-1.11
3570	c1ccnc(c1)c2csnn2	C03844531	-13.6	-2.88	-14	5.46	-2.17
3571	c1cnc(c1)F	C04352657	-13.6	0.39	-16.21	2.35	-0.13
3572	c1[nH]c(c(n1)[N+](=O)[O-])Cl	C06645761	-13.6	-2.53	-15.61	7.69	-3.15
3573	Cc1c(=O)nc([nH]n1)N	C09171147	-13.6	-4.01	-17.33	5.98	1.77
3574	C1C=CC(=C1)C=O	C12358630	-13.6	-1.5	-15.82	6.46	-2.73
3575	Cc1c(nno1)C(=O)Cl	C16124705	-13.6	1.05	-16.67	3.35	-1.33
3576	c1c(cnc2c1[nH]cn2)N	C18544363	-13.6	-4.81	-15.89	8.22	-1.12
3577	c1c(cn1)C(F)F)Br	C26510703	-13.6	-0.93	-14.76	4.24	-2.14
3578	c1cc(ccc1NC(=S)N)F	C00064840	-13.59	-1.51	-19.07	9.71	-2.71
3579	Cc1cc(ccc1F)N	C00394668	-13.59	-0.5	-13.58	2.81	-2.32
3580	c1nc(c(c1n)Cl)N	C00967452	-13.59	-5.1	-13.09	4.49	0.11
3581	c1cc([nH]c1)C=O	C01069171	-13.59	-2.29	-16.69	6.48	-1.49
3582	c1cc(nnc1NN)Cl	C01225177	-13.59	-5.21	-14.77	6.84	-0.45
3583	c1c(ocn1Cl)CCO	C01608228	-13.59	-2.59	-14.26	3.77	-0.52
3584	CCCC/C=C/C#N	C01729045	-13.59	0.01	-15.12	4.02	-2.49
3585	c1c[nH]c(=S)nc1	C02008823	-13.59	-2.26	-14.91	5.01	-1.42
3586	C(=O)(C(=O)N)C(F)F)F	C02525295	-13.59	-3.11	-15.13	3.65	1.01
3587	c1c(c(nno1)N)C#N	C04289162	-13.59	-2.47	-15.42	5.42	-1.12
3588	CC(=O)O/C=C/OC(=O)C	C05431797	-13.59	0.33	-17.67	7.32	-3.57
3589	Cc1ccc(nc1)C	C08294955	-13.59	-1.37	-12.15	3.05	-3.12
3590	CC(=O)[C@H]1[C@H](O1)c2ccccc2	C13213324	-13.59	0.06	-18.91	7.38	-2.12
3591	C/C(=C)Br)C#N	C16138636	-13.59	-0.31	-13.06	2.56	-2.78
3592	C1C[NH+](=C)S1N	C17744492	-13.59	-1.71	-14.4	2.68	-0.15
3593	c1cc(c(c1CC(=O)F)F)N	C21985471	-13.59	-3.75	-13.71	6.01	-2.13
3594	c1c(c(c(c1F)F)NN)F)F	C00035750	-13.58	-0.85	-13.22	2.13	-1.65
3595	Cc1[nH]cc(n1)C=O	C00164636	-13.58	-2.03	-16.78	6.52	-1.29
3596	Cc1cc(no1)C(=O)N	C00401316	-13.58	-2.36	-17.16	5.59	0.37

3597	c1cc(ncc1O)C=O	C01716571	-13.58	-3.8	-14.99	4.87	0.34
3598	c1cssc1=S	C01846561	-13.58	-2.6	-14.99	8.35	-4.34
3599	Cn1cncc1C(=O)Cl	C02509362	-13.58	0.71	-17	5.51	-2.81
3600	CC(=O)SCC#N	C02555811	-13.58	-0.96	-15.12	4.77	-2.28
3601	c1ccc(c(c1)c2ccno2)F	C02578084	-13.58	-0.02	-15.98	4.64	-2.22
3602	c1c[nH]cc(c1=O)F	C02599064	-13.58	-1.61	-16.08	4.03	0.08
3603	c1cc2c(nc1)nc(o2)[S-]	C03884046	-13.58	-3.27	-17.49	7.85	-0.67
3604	C[C@@H]1Cn2c(=O)[nH]nc2S1	C04761200	-13.58	-0.59	-18.59	7.2	-1.59
3605	c1ccc2c(c1)nc(o2)NN	C05011791	-13.58	-5.66	-13.77	5.7	0.16
3606	COC(=O)Nc1c(c(c(c1F)F)F)F	C06126161	-13.58	1.27	-16	4.23	-3.09
3607	c1cc(nnc1[O-])Cl	C08616208	-13.58	-4.83	-16.52	6.22	1.55
3608	Cc1ccccc1/C(=N/O)/N	C13477352	-13.58	-3.51	-14.72	6.17	-1.53
3609	c1cnccc1C(=S)N	C00154867	-13.57	-3.51	-17.81	9.26	-1.52
3610	Cn1ccc(=N)cc1	C00330933	-13.57	-3.57	-16.4	8.38	-1.98
3611	c1cc(sc1[N+](=O)[O-])Br	C01103311	-13.57	-1.75	-14.89	3.2	-0.12
3612	C=CC(=O)OCCCl	C01561511	-13.57	-0.79	-14.16	4.63	-3.26
3613	c1cc(sc1)I	C01587822	-13.57	-0.56	-14.73	1.46	0.26
3614	c1cc([nH]c1)C(=O)Cl	C01674530	-13.57	-1.44	-13.75	4.8	-3.19
3615	c1cccc(=O)cc1	C02034873	-13.57	-1.99	-16.77	8.28	-3.09
3616	c1cc(cc(c1)F)CN=C=S	C02528111	-13.57	-0.43	-12.31	2.94	-3.77
3617	CCOC1cccc(c1)F	C02568102	-13.57	-1.47	-13.02	2.47	-1.55
3618	c1cc(sc1)CN=C=S	C02582030	-13.57	-1.88	-15.44	2.42	1.32
3619	CCOC(=O)[C@@H](F)Br	C02584260	-13.57	-1.39	-12.25	3.01	-2.93
3620	C1CCC(=CC1)NC=O	C06691800	-13.57	-1.79	-16.67	5.09	-0.19
3621	CO/C=C/C(F)F	C08698287	-13.57	-2.05	-13.32	3.94	-2.14
3622	C(/C(=N/O)/C(F)F)F)Br	C14628464	-13.57	-1.85	-14.2	3.45	-0.95
3623	c1c(csn1)N	C20417334	-13.57	-2.54	-15.06	3.95	0.08
3624	c1cc(cnc1)CC(F)F	C30714905	-13.57	-2.09	-12.25	4.13	-3.36
3625	CC(=C)OC(=O)C	C00154688	-13.56	-0.54	-14.12	4.1	-3
3626	c1c(cncc1Br)C#N	C00161484	-13.56	-0.89	-13.04	3.18	-2.81
3627	CCc1ccc(cc1)O	C00404411	-13.56	-0.92	-16.19	3.7	-0.14
3628	CCc1c(ccc1)O	C01665466	-13.56	-1.1	-14.51	3.77	-1.73
3629	C=C(CN=C=S)Br	C01697477	-13.56	0.77	-17.59	2.26	0.99
3630	CCOC(=O)N(C)Cl	C01748985	-13.56	-1.14	-12.46	2.15	-2.11
3631	c1cc(ncc1C(F)F)Cl	C02168608	-13.56	-1.87	-12.54	2.61	-1.76
3632	Cc1ccc(cc1)OCC#N	C02170125	-13.56	1.15	-18.71	6.07	-2.07
3633	c1cc(c(c1N)F)F	C02243354	-13.56	-3.25	-16.21	5.51	0.4
3634	COCCC(=O)Cl	C02574132	-13.56	-1.05	-13.93	2.67	-1.24
3635	COC(=O)CCS	C03860879	-13.56	-0.49	-13.85	3.1	-2.31
3636	COC(=N)C(C(C(C(F)F)F)F)F	C04627537	-13.56	-1.04	-12.33	2.2	-2.4
3637	c1cnccc1CCO	C08294937	-13.56	-1.7	-14.9	3.7	-0.66
3638	c1cc2c(cc1F)nc([nH]2)NN	C14987849	-13.56	-6.29	-10.45	5.79	-2.62
3639	CCc1csc(n1)N	C15015336	-13.56	0.47	-15.99	3.65	-1.7
3640	Cc1ncc(c(n1)N)N	C25491251	-13.56	-5.91	-15.65	7.44	0.55
3641	c1ccc(c(c1)N)OC(F)F	C00163283	-13.55	-2.58	-12.63	2.35	-0.68
3642	c1ccnc(c1)C#N	C00404339	-13.55	0.13	-17.35	5.94	-2.27
3643	c1cc(c(cc1O)Cl)O	C00404794	-13.55	-1.58	-16.25	3.81	0.48
3644	CCSC(=O)C(F)F	C01569573	-13.55	-0.95	-11.71	1.94	-2.83
3645	CCC(=O)c1ccc(o1)[N+](=O)[O-]	C01583723	-13.55	-0.66	-13.69	4.35	-3.54
3646	CNC(=O)Oc1cccc(c1)N	C01716721	-13.55	-0.75	-19.5	7.11	-0.42
3647	C[C@H](C(=O)Cl)Br	C01847220	-13.55	0.47	-13.72	2.1	-2.4
3648	Cc1cc(cnc1F)Cl	C02384024	-13.55	-0.52	-14.98	2.79	-0.84
3649	c1c(cnc(c1F)F)C(F)F	C02540285	-13.55	0.49	-13.66	2.42	-2.81
3650	c1cc2c(cc1F)[nH]c(=O)[nH]2	C02547617	-13.55	-3.4	-14.7	5.78	-1.23
3651	C(C(=O)Br)Br	C03860232	-13.55	0.17	-14.63	2.89	-1.99
3652	CCOC(=O)C(=C/C(=O)C)/[O-]	C03861646	-13.55	0.85	-15.82	4.1	-2.67
3653	C1C=C[C@H]2[C@H]1C(=O)C2	C05046474	-13.55	-0.67	-12.62	3.05	-3.3
3654	c1ccc2c(c1)[nH]c(=S)o2	C12341569	-13.55	-1.64	-15.77	5.08	-1.21
3655	c1cc(ncc1Br)CO	C12370891	-13.55	-3.45	-12.71	3.11	-0.5
3656	c1cc2c(cc1Cl)nncc2	C16431183	-13.55	-2.44	-12.49	4.38	-3
3657	c1ccc(c(c1)COCC(F)F)F	C19272316	-13.55	-3.14	-13.37	5.9	-2.94
3658	c1cc(c(cc1F)F)NCC#N	C20053279	-13.55	-2.91	-14.41	6.85	-3.09
3659	c1cc(nnc1N)I	C20357599	-13.55	-3.53	-15.49	6.51	-1.05
3660	COc1cc(no1)N	C21298963	-13.55	-1.9	-15.82	5.18	-1.01
3661	c1cc(nc(c1N)N)Cl	C22116128	-13.55	-5.64	-14.57	6.54	0.11
3662	C1COCC=C1	C32152383	-13.55	-0.69	-12.84	1.68	-1.7
3663	CC(=O)NCC1ccnc1	C00160564	-13.54	0.02	-18.93	6.76	-1.39
3664	Cc1ncc(c(n1)N)Br	C00392459	-13.54	-3.57	-15.11	3.05	2.08
3665	COC(=O)c1[n-]nc(n1)[N+](=O)[O-]	C01574152	-13.54	-2.23	-12.36	4.96	-3.91
3666	CCOC(=O)C=C	C01586528	-13.54	-0.47	-14.23	3.94	-2.77
3667	c1ccn2c(c1)nnn2	C01587624	-13.54	-3.2	-19.03	10.63	-1.93
3668	C=C[C@H](CB)O	C01997856	-13.54	-1.22	-13.9	2.39	-0.81
3669	CCOC(=O)CC(=O)Cl	C02242607	-13.54	-2.51	-14.6	6.98	-3.41
3670	COC(=O)C(C(=O)F)F	C02516002	-13.54	-0.07	-12.77	2.22	-2.92
3671	C=C[C@H]1CCCCC1=O	C05496344	-13.54	2.32	-15.32	3.29	-3.82
3672	COc1ccc(nc1)N	C14982095	-13.54	-2.4	-15.49	4.92	-0.57
3673	CCOC(=O)c1c(mns1)N	C15221690	-13.54	-1.6	-14.19	3.54	-1.29
3674	c1c/c(=N/O)/[nH]cc1C(F)F	C16383544	-13.54	-6.34	-10.46	4.59	-1.32
3675	CC(=O)c1[nH]ccn1	C16696747	-13.54	-1	-16.12	5.18	-1.6
3676	[H]/N=C/1NCC(=NN1)N	C17045389	-13.54	-7.88	-15.41	10.5	-0.74
3677	CN(c1ccc(cc1)Cl)N	C32105957	-13.54	-1.53	-12.09	2.83	-2.76
3678	CN(C)C(=O)c1ccc(o1)Cl	C32904163	-13.54	-0.91	-14.19	4	-2.44
3679	CN(c1ccccc1)N	C00388434	-13.53	-0.83	-13.12	2.82	-2.4
3680	c1ccn(c(=O)c1)CC#N	C00536182	-13.53	-2.28	-20.23	12.01	-3.04
3681	c1cc2c([nH]c(n2)CC#N)nc1	C01304619	-13.53	-5.82	-17.52	12.75	-2.94
3682	CCOC(=O)CCCl	C01648267	-13.53	-0.64	-12.46	2.94	-3.38
3683	CC(=O)NCC1cccs1	C02016200	-13.53	-0.17	-16.9	5.59	-2.06
3684	C/C=C(/C)C=O	C02039911	-13.53	-1.3	-14.1	4.25	-2.38
3685	Cn1cc(cn1)N	C02552486	-13.53	-2.78	-14.9	4.3	-0.14
3686	C1C=CCC1=O	C02569653	-13.53	-0.73	-13.53	3.09	-2.36

3687	C1CCC(=CC1)C[N+](=O)[O-]	C04285346	-13.53	0.49	-16.58	3.36	-0.79
3688	CCOc1nc(ns1)N	C04290485	-13.53	-2.75	-15.61	4.71	0.12
3689	c1cc(ccc1OC(F)(F)F)Cl	C05225638	-13.53	0.16	-12.96	1.31	-2.03
3690	CcN1cnc(n1)N	C05957038	-13.53	-2.01	-15.17	6.89	-3.24
3691	c1cc(=O)[nH]cc1F	C08698071	-13.53	-2.45	-15.93	3.93	0.92
3692	Cc1[nH]c(n1)C=O	C12956226	-13.53	-5.21	-12.54	5.46	-1.25
3693	Cn1cnc1C=O	C20443586	-13.53	-3.26	-15.12	7.3	-2.45
3694	[H]/N=C(/C)\SC(C)C	C22309033	-13.53	-2.08	-10.87	1.87	-2.45
3695	c1ccc2c(c1)nns2	C00031178	-13.52	-2.82	-17.01	6.13	0.18
3696	c1cc(oc1C=O)I	C00065135	-13.52	-0.58	-15.34	3.13	-0.72
3697	c1cc2c(nc1)n(nn2)O	C00396136	-13.52	-5.85	-16.18	8.29	0.22
3698	CC(C)O[N+](=O)[O-]	C01569571	-13.52	-1.37	-11.03	2.01	-3.14
3699	CCCCOC=C	C01586529	-13.52	-0.13	-13.33	1.57	-1.64
3700	C1=CC(=NNC(=O)N)C=C1	C01700518	-13.52	-5.14	-13.67	5.18	0.11
3701	C1[C@H](C=C1)CO	C02032015	-13.52	-0.77	-14.04	2.19	-0.9
3702	CN(C)C(=O)n1ccnc1	C02450819	-13.52	-1.96	-16.59	7.75	-2.73
3703	c1cncnc1CO	C02511466	-13.52	-4.19	-15.36	4.33	1.7
3704	CCCO[P@H](=O)C=C=C	C05431490	-13.52	2.69	-19.51	5.8	-2.5
3705	CcN1cccn1	C06125795	-13.52	-0.42	-14.9	4.25	-2.45
3706	C1Cc2c(noc2N)C1	C06855320	-13.52	-3.3	-16.41	5.02	1.18
3707	Cc1cc([nH]1)C(=O)N	C10342264	-13.52	-4.31	-17.44	7.09	1.14
3708	c1c(ccc1)O	C13208871	-13.52	-3.64	-16.44	4.35	2.2
3709	Cc1ccc(s1)[C@@H]2CO2	C19271536	-13.52	-1.74	-14.12	4.89	-2.55
3710	C(#N)c1nc([nH]n1)N	C19802969	-13.52	-5.35	-16.53	9.73	-1.37
3711	c1cn2c(cc1Br)ncn2	C30677876	-13.52	-3.74	-10.99	5.47	-4.27
3712	C/C(=C/C(=O)C)Cl/[O-]	C01995229	-13.51	0.68	-14.52	2.38	-2.04
3713	CNc1ccccc1F	C02243024	-13.51	-1.05	-12.44	2.61	-2.63
3714	c1cc(ccc1CC(F)(F)F)N	C02540430	-13.51	-1.6	-11.86	3.05	-3.1
3715	c1cc(ccc1N)OCC#N	C03338693	-13.51	-1.12	-16.98	6.43	-1.84
3716	c1cc(ccc1CSC(=[NH2+])N)F	C04013946	-13.51	-1.09	-12.82	3.11	-2.71
3717	c1cc(ccc1Cl)FCS	C04244669	-13.51	0.15	-11.49	2.27	-4.45
3718	c1nnc(s1)[N+](=O)[O-]	C05105421	-13.51	-1.94	-18.18	7.67	-1.06
3719	c1onn(c1)C(=O)C(F)F	C05705288	-13.51	-2	-14.04	4.61	-2.07
3720	c1cnc(cc1Cl)O	C12359529	-13.51	-2.1	-16.1	3.82	0.87
3721	c1ccc(cc1)CNC(=S)NN	C13684764	-13.51	0.08	-20.83	9.99	-2.76
3722	[C@@H](C(F)F)(OC(F)F)F	C16082612	-13.51	-0.15	-13.69	1.96	-1.64
3723	C/C(=C/C(=O)C)Nc1[nH]cnn1	C16134370	-13.51	-0.44	-18.28	10.44	-5.22
3724	c1cnc2c(n1)c([nH]n2)N	C16982871	-13.51	-2.39	-19.09	7.52	0.46
3725	COC(=O)/C=C/c1ccc(cc1)F	C00567266	-13.5	-1.03	-14.54	4.69	-2.62
3726	c1cc(c(c1)Cl)N)N	C01588400	-13.5	-3.44	-11.82	2.52	-0.76
3727	C=CCOCC#N	C01640805	-13.5	-1.01	-14.88	4.28	-1.89
3728	c1ccc(cc1)C(=O)ON	C01732511	-13.5	1.92	-17.66	5.06	-2.83
3729	Cn1cc(cn1)I	C02547891	-13.5	0.83	-15.14	3.51	-2.69
3730	c1cc(ccc1/C=N)N)F	C05893819	-13.5	-2.04	-15.88	3.18	1.24
3731	Cc1ccccc1C	C08294959	-13.5	-1.67	-12.02	3.1	-2.91
3732	c1cc(nc(c1)[N+](=O)[O-])[O-]Cl	C13301916	-13.5	-3.82	-14.63	5.6	-0.64
3733	c1cc(c(cc1N)Br)O	C14628846	-13.5	-2.03	-14.69	3.38	-0.16
3734	c1cc(c(c1)F)[N+](=O)[O-]N	C16158504	-13.5	-2.24	-15.88	7.03	-2.4
3735	C1CCC(=CC1)/C=N/O	C16952893	-13.5	-1.58	-14.4	4.26	-1.78
3736	c1csc2c1[C@@H](CC2)O	C19727103	-13.5	-1.06	-15.81	4.95	-1.58
3737	Cc1cc(ccc1O)O	C00388086	-13.49	-3	-14.66	3.83	0.35
3738	C=CCOC(=O)OCC=C	C01562404	-13.49	-0.77	-11.98	3.1	-3.83
3739	Cc1cc(n(c1)O)C#N	C01755384	-13.49	-0.58	-16.89	5.3	-1.31
3740	[H]/N=C(/C)\CCl)OC	C04613656	-13.49	-2.29	-13.43	2.24	-0.01
3741	CCO[C@H]1C=CC(=O)O1	C05316553	-13.49	-2	-16.12	7.15	-2.51
3742	COC(=O)CSc1[nH]cnc1	C05660255	-13.49	-1.97	-14.79	5.87	-2.61
3743	CCOC(=O)N(CCF)N=O	C05665076	-13.49	-1.95	-13.23	3.28	-1.58
3744	c1c(cnc(c1O)Cl)Br	C14400912	-13.49	-2.94	-12.86	3.08	-0.77
3745	c1cc(c(cc1C)N)F	C19385524	-13.49	0.21	-16.81	4.49	-1.39
3746	c1nnc(n1)CCBr	C19414595	-13.49	0.1	-14.57	5.03	-4.05
3747	c1(nc(nc(n1)N)N)N	C00897751	-13.48	-2.68	-14.76	5.42	-1.46
3748	c1cnn(c1N)Cc2ccsc2	C04206193	-13.48	0.34	-16.08	5.22	-2.97
3749	c1(nnc(s1)Cl)Cl	C05215421	-13.48	-1.14	-15.02	2.56	0.12
3750	c1nnc(s1)[S-]	C05226028	-13.48	-1.61	-15.99	4.77	-0.64
3751	c12c(nc(nc1n[nH]n2)F)N	C05479749	-13.48	-4.3	-17.13	7.29	0.67
3752	Cc1cnc([nH]c1=O)N	C17322277	-13.48	-3.33	-16.53	5.36	1.02
3753	c1nc(nn1CCO)N	C19088805	-13.48	-4.44	-15.53	6.95	-0.45
3754	c1cc(sc1C)N)Cl	C19410224	-13.48	-0.38	-13.61	1.73	-1.22
3755	c1cnncc(c1N)C#N	C19854097	-13.48	-3.01	-18.54	7.93	0.14
3756	c1ccc2c(c1)nnn2C#N	C00406327	-13.47	1.51	-15.57	5.3	-4.72
3757	CCOCc1ccccc1	C01586382	-13.47	-0.41	-14.83	2.47	-0.7
3758	c1cnc(cn1)CON	C01722640	-13.47	0.92	-19.82	4.62	0.81
3759	COc1ccc(cc1F)F	C02539389	-13.47	1.83	-15.91	3.56	-2.96
3760	C1(=O)C(C(=O)NC(=O)N1)(F)F	C03040745	-13.47	0.18	-19.72	4.69	1.36
3761	c1cc2c(cc1Cl)con2	C06414093	-13.47	-1.67	-13.19	4.85	-3.45
3762	COC(=O)Cn1ccnc1	C08377783	-13.47	-2.82	-15.16	6.39	-1.89
3763	c1cnc(c1)OC#N	C12958642	-13.47	0.78	-19.98	5.07	0.66
3764	c1ccc(c(c1)/C=C)C=O)O	C13547077	-13.47	-2.35	-15.13	5.93	-1.92
3765	CSc1c(nc(=O)[nH]n1)[O-]	C20829009	-13.47	-2.75	-17.79	6.01	1.06
3766	C/C=C/[N+](=O)[O-]	C21304285	-13.47	-1.55	-14.29	5.15	-2.78
3767	[C@H](c1ccccc1N)O	C21985758	-13.47	-1.79	-17.12	5.25	0.2
3768	c1c(cnc(c1Cl)C)C#N	C22995864	-13.47	-1.28	-12.59	3.41	-3.01
3769	CC(=O)Nc1ccccc1F	C00126905	-13.46	-1.05	-15.28	5.61	-2.75
3770	c1cc(ccc1CO)O	C00388762	-13.46	-1.13	-17.87	4.59	0.95
3771	c1cc(ccc1NC=O)O	C00410172	-13.46	-1.34	-20.73	8.41	0.19
3772	CC(=O)Oc1ccc(cc1)C=O	C01672089	-13.46	-1.03	-16.51	8.17	-4.09
3773	C1CC1N=C=S	C02168469	-13.46	-0.57	-12.45	1.74	-2.18
3774	c1csc(c1Cl)C=O	C02383503	-13.46	-1.91	-14.97	3.87	-0.44
3775	CC(=O)C1=CCCC1	C02569899	-13.46	-0.9	-13.03	3.88	-3.41
3776	c1cc(c(cc1SC#N)Cl)N	C03886711	-13.46	-1.71	-14.87	3.16	-0.05

3777	c1cc(ccc1O)O	C05133378	-13.46	-0.86	-17.24	3.67	0.97
3778	c1ccc(c(c1)C)C2cccs2N	C32008179	-13.46	-1.01	-11.06	3.21	-4.6
3779	C1CC[NH+](C1)CC(=O)Cl	C32016244	-13.46	-0.95	-14.11	3.12	-1.53
3780	c1cc(cc(c1)F)CON	C00168990	-13.45	1.33	-16.41	3.45	-1.81
3781	c1cncc2c1[nH]c(n2)C(F)(F)F	C00549515	-13.45	-4.24	-12.23	5.19	-2.17
3782	CC(=C)COC(=O)C=C	C01608909	-13.45	-0.67	-14.12	3.88	-2.55
3783	C(C#N)c1c(c(c(c1F)F)F)F	C01612151	-13.45	-0.88	-13.41	5.7	-4.86
3784	CCOC(=O)[C@H](C)F	C01674837	-13.45	-0.73	-13.56	3.86	-3.03
3785	C=CC(=O)Oc1ccccc1	C01850915	-13.45	-0.2	-14.32	5.8	-4.73
3786	c1ccc2c(c1)c(c[nH]2)F	C02529146	-13.45	-1.13	-13.85	4.94	-3.41
3787	CC(=C)CCC#N	C02557576	-13.45	-0.77	-14.11	4.07	-2.65
3788	c1c(scn1)C=O	C02577851	-13.45	-2.64	-15.79	6.16	-1.18
3789	c1cc(c(nc1)C=O)F	C04208890	-13.45	-3.16	-15.26	6.82	-1.85
3790	c1nncn1n2cnnc2	C04843822	-13.45	-0.94	-19.04	9.73	-3.19
3791	[H]N=C/c1ccccc1O	C04921497	-13.45	-2.85	-14.01	4.1	-0.69
3792	c1cnc(c1)N	C14982080	-13.45	0.12	-15.08	3.42	-1.91
3793	c1cc(nnc1C(=O)N)Cl	C16123717	-13.45	-3.81	-15.39	5	0.75
3794	Cc1cncnc1C=O	C20443751	-13.45	1.53	-16.73	3.95	-2.2
3795	CC(=O)c1cncnc1	C00163730	-13.44	-2.48	-14.86	5.14	-1.24
3796	C[C@H]1C(=O)C=C(O)1C	C00164379	-13.44	-1.24	-14.86	4.74	-2.08
3797	Cc1cccc(=O)[nH]1	C00164932	-13.44	-2.59	-17.25	7.96	-1.56
3798	Cc1cc(nc(n1)F)F	C01582390	-13.44	-1.34	-14.9	4.69	-1.89
3799	c1cc(cc(c1)N=C=O)C(F)(F)F	C02040817	-13.44	-2	-11.35	2.32	-2.41
3800	C=C(C(=O)OC(C(F)(F)F)C(F)(F)F)F	C02243173	-13.44	-0.62	-11.2	3.56	-5.18
3801	C(C(=O)c1c(nofn+1)[O-])NBr	C03165401	-13.44	-0.31	-15.87	4.98	-2.24
3802	C1(=[N+]=[N-])C(=O)NC(=O)N=C1[O-]	C04071678	-13.44	0.29	-20.66	4.66	2.27
3803	c1c(nns1)N	C04945770	-13.44	-3.25	-14.93	4.56	0.18
3804	CNC(=[NH2+])SC	C06590260	-13.44	-3.14	-12.46	2.24	-0.08
3805	C/C=C/C(=O)OCC=C	C08612885	-13.44	-1.33	-11.86	3.46	-3.71
3806	CCCCON=O	C20230701	-13.44	0.22	-12.12	1.96	-3.5
3807	COC(=O)CCBr	C01666985	-13.43	0.06	-13.81	3.06	-2.74
3808	CCC(=O)OCC#C	C01995101	-13.43	-0.08	-14.28	4.32	-3.4
3809	CCCC(=O)Cl	C02040974	-13.43	-0.61	-12.86	2.56	-2.52
3810	c1c(c[nH]1)c2c[nH]nc2	C03306620	-13.43	-8.01	-11.46	6.76	-0.72
3811	C1=C([C@H](N=N1)C=O)Br	C04262629	-13.43	-5.46	-13.51	6.53	-0.98
3812	c1c(c([nH]1)C(=N)O)N)Br	C04277649	-13.43	-4.65	-15.2	5.18	1.24
3813	C1C=CCOC1	C04411091	-13.43	-0.67	-14.04	2.47	-1.2
3814	c1([n-]nnc1)NC(=[NH2+])N[N+](=O)[O-]	C05395785	-13.43	-9.39	-20.79	16.25	0.49
3815	CC/C=C/[N+](=O)[O-]	C05761952	-13.43	-1.44	-14.79	4.59	-1.79
3816	Cc1c(cco1)Br	C12370514	-13.43	-1.61	-11.39	2.47	-2.9
3817	CCOC(=O)C=CBr	C12405145	-13.43	-0.79	-13.56	4.03	-3.1
3818	CCOC(=O)CC[N+](=O)[O-]	C14614148	-13.43	-0.42	-14.18	4.37	-3.2
3819	c1ccc1C[NH2+]N	C19275663	-13.43	-1.23	-16.18	3.84	0.14
3820	Cc1cc(ccc1F)OC(=O)Cl	C19615523	-13.43	-2.37	-9.14	2.77	-4.69
3821	CNc1ccc(cn1)N	C22141615	-13.43	-2.35	-15.64	4.85	-0.29
3822	c1cc(ncc1N)C#N	C00403997	-13.42	-0.46	-18.79	6.53	-0.7
3823	C(COC(=O)Cl)CCl	C01845910	-13.42	1.34	-14.14	2.6	-3.22
3824	c1cc(c(cc1Cl)N)OC(F)F	C02529872	-13.42	-1.55	-13.82	3.9	-1.95
3825	CCOC(=O)[C@@]([C](F)(F)F)(F)Cl	C02530824	-13.42	-0.78	-10.56	1.65	-3.74
3826	Cn1cc(c(n1)N)Br	C02567054	-13.42	-3.02	-13.86	4.62	-1.17
3827	Cc1c(cco1)C=O	C04208885	-13.42	-2.91	-12.88	4.65	-2.28
3828	c1c(c([nH]1)C(F)F)Cl	C04243628	-13.42	-0.73	-14.44	2.42	-0.67
3829	c1c(cc(cc1F)F)CS	C04244665	-13.42	-1.32	-12.86	2.21	-1.45
3830	c1c[nH]nc1CCCl	C05386997	-13.42	-2.74	-15.36	3.96	0.71
3831	CC(=O)O[C@]([C@H]1CC(=O)C=C1	C05663725	-13.42	0.72	-18.48	5.89	-1.55
3832	c1c[nH]c(=O)cc1F	C14982909	-13.42	-2.98	-15.18	3.87	0.88
3833	c1cc(c(c1NC(=O)C(F)F)F)F	C00063065	-13.41	-3.2	-10.19	3.29	-3.31
3834	Cn1cc(cn1)[N+](=O)[O-]	C02038197	-13.41	-2.75	-14.88	6.61	-2.4
3835	c1c(cc(c1F)O)F)N	C02243353	-13.41	-3.32	-14.9	4.47	0.35
3836	CCNc1ccc(cc1)F	C04206095	-13.41	-2.69	-12.66	2.34	-0.41
3837	Cc1c(nc[n1])[N+](=O)[O-]	C04343025	-13.41	-1.01	-15.53	6.44	-3.31
3838	C1C(=O)N(C(=O)S1)CCCl	C11804308	-13.41	1.06	-17.08	4.86	-2.25
3839	c1ccc(c(c1)OCC#N)F	C19485220	-13.41	-3.87	-14.76	8.67	-3.45
3840	c1cc(c(c1NC(=S)NN)F)F	C20426677	-13.41	-0.97	-19.48	9.71	-2.67
3841	c1cnc1C#N	C22009492	-13.41	-3.64	-13.98	5.92	-1.72
3842	c1cc(c(cc1[C@@]([C@H]2CO2)F)F	C22165566	-13.41	-3.01	-12.19	4.55	-2.77
3843	C1CCc2c(c([nH]2)C#N)C1	C24732293	-13.41	-2.42	-12.35	4.07	-2.71
3844	Cc1ncc(c(n1)Cl)F	C26466426	-13.41	-0.98	-12.7	2.69	-2.42
3845	CCCc1cc([nH]1)C(F)F	C26547613	-13.41	-3.55	-9.75	3.02	-3.13
3846	c1nc(c(c1N)C=O)N	C01556563	-13.4	-4.07	-15.08	5.89	-0.14
3847	CC(=O)OC=C	C01586656	-13.4	-1.79	-13.22	4	-2.39
3848	COC(=O)C(=C)Br	C01608900	-13.4	0.37	-15.89	3.5	-1.38
3849	C(CO)C(C(F)F)F	C02573965	-13.4	-2.99	-11.99	2.24	-0.66
3850	C[C@H](CN=[N+]=[N-])OC(=O)C(F)F	C04984156	-13.4	-1.37	-13.24	3.68	-2.48
3851	c1cc(nnc1nnc2)[O-]	C06753419	-13.4	-3.69	-15.68	7.81	-1.85
3852	c1c(oc1Br)CO	C08614800	-13.4	-2.65	-14.03	3.8	-0.52
3853	c1c([nH]c(=O)c1[N+](=O)[O-])F	C08698153	-13.4	-2.46	-16.66	5	0.73
3854	c1ccc(cc1)NC(=O)N2N=N2	C00401686	-13.39	0.45	-18.28	4.55	-0.11
3855	COC(=O)c1c([nH]1)Cl	C01235058	-13.39	0.1	-18.02	5.09	-0.56
3856	c1c(c(nc1)Cl)Cl[N+](=O)[O-]	C02023569	-13.39	-1.04	-12.09	2.36	-2.62
3857	CCOCC=C	C02034774	-13.39	-0.46	-12.19	1.45	-2.2
3858	C1CCC(C1)N=C=O	C02389322	-13.39	0.46	-14.27	1.59	-1.17
3859	c1c(c[n1])CC#N)Br	C02537512	-13.39	-3.55	-16.27	9.23	-2.8
3860	c1c(cc(c1CO)F)F	C02575068	-13.39	-3.2	-11.49	2.8	-1.5
3861	C=CCOC([C@]([C](F)F)F)F	C02584542	-13.39	0.05	-12.24	2.45	-3.64
3862	c1cc(c(cc1O)[N+](=O)[O-])N	C04262549	-13.39	-3.21	-16.24	6.34	-0.27
3863	c1cc(c(c1F)C=O)F	C04290142	-13.39	-2.59	-13.05	5.01	-2.75
3864	CC(=O)Oc1ccno1	C12359057	-13.39	0.2	-17.92	7.49	-3.16
3865	CC(=O)Oc1c(ccs1)N	C16124417	-13.39	-1.65	-16.18	6.41	-1.97
3866	c1cnc(cc1C(F)F)F)NN	C16159621	-13.39	0.06	-15.49	3.75	-1.71

3867	C[C@H](c1cccs1)Cl	C32005545	-13.39	-1.22	-10.25	2.18	-4.1
3868	c1c(c(nH)1)C(F)(F)C(F)(F)F	C01585877	-13.38	-3.47	-12.93	6.27	-3.25
3869	CC(=O)C(=O)OC	C01692440	-13.38	-0.92	-14.39	3.87	-1.94
3870	c1ccc(cc1)[C@H](C#CCO)O	C01726269	-13.38	-1.22	-17.41	5.88	-0.63
3871	COc1ccc(cc1)N	C04556034	-13.38	-2.53	-12.7	3.09	-1.24
3872	C[C@H]([N+](=O)[O-])Br	C04683080	-13.38	-0.44	-13.64	3.02	-2.32
3873	CC1cnc(nc1N)N	C12344009	-13.38	-2.4	-13.81	4.53	-1.71
3874	Cc1ccoc1N=C=O	C12370517	-13.38	-0.56	-15.33	2.88	-0.38
3875	c1cc(c(cc1F)OCC#N)F	C15442719	-13.38	-3.81	-13.25	7.17	-3.5
3876	c1c(csc1CC#N)Br	C16123657	-13.38	-1.35	-13.91	6	-4.12
3877	c1cnc(c(=O)[nH]1)N	C17061495	-13.38	-3.46	-18.28	7.36	0.99
3878	CCOC(=O)/C(=N[O-])/C#N	C18204413	-13.38	-7.2	-11.8	6.59	-0.97
3879	CCOCCCl	C19415016	-13.38	-0.84	-12.02	2.17	-2.69
3880	CCNc1ccc(cn1)N	C19952780	-13.38	-3.64	-13.38	4.51	-0.85
3881	c1cc(c(cc1N)O)O	C00006364	-13.37	-2.27	-18.2	5.12	1.97
3882	c1cnc(nc1C(F)F)F	C01023366	-13.37	-0.21	-15.4	4.42	-2.17
3883	COc(=O)CCN=C=S	C02390114	-13.37	0.68	-15.17	3.11	-1.99
3884	c1c(nc(c1Br)F)Cl	C02539939	-13.37	-1.07	-11.51	2.06	-2.84
3885	CSC(=O)Cl	C04537766	-13.37	-1.25	-13.98	2.27	-0.41
3886	c1cn(cn1)O	C05286604	-13.37	-4.35	-12.9	4.79	-0.91
3887	c1c(c(cc(c1F)F)O)O	C06091087	-13.37	-2.04	-16.97	4.94	0.71
3888	c1c(c(nH)n1)N	C12397092	-13.37	-3.17	-15.94	4.17	1.56
3889	C1CSC(=N1)N[N+](=O)[O-]	C14983373	-13.37	-1.37	-15.48	5.12	-1.64
3890	c1cc(c(c1C#N)F)F	C16159963	-13.37	-0.69	-17.5	6.9	-2.09
3891	Cc1cnccc1CCl	C16948467	-13.37	-1.1	-12.33	3.42	-3.36
3892	c1nc(nc1)C=O	C20443630	-13.37	-3.26	-16.68	6.86	-0.29
3893	C1CSC[C@@H]1S	C20476693	-13.37	0.48	-12.81	1.94	-2.98
3894	Cc1ccc(cc1O)C#N	C22114923	-13.37	-2.36	-14.82	5.79	-1.98
3895	c1cc(ccc1CO)Cl	C00157482	-13.36	-2.47	-12.53	3.21	-1.56
3896	CCOC(=O)OCC	C00388482	-13.36	-0.6	-13.19	3.35	-2.92
3897	c1csc(n1)[N+](=O)[O-]	C01582750	-13.36	-2.88	-18.18	8.26	-0.57
3898	c1cnc2c1cnnc2	C01606663	-13.36	-2.6	-17.28	6.75	-0.22
3899	C1C=CC(C=C1)CO	C01669156	-13.36	-1.13	-13.13	2.29	-1.39
3900	c1cnccc1N	C08294943	-13.36	-3.13	-16.46	5.91	0.33
3901	C(/C=C/C)C#N	C19430709	-13.36	-1.89	-14.56	5.95	-2.87
3902	c1(nc([nH]n1)N)C(F)F	C19485644	-13.36	-5.52	-15.56	9.5	-1.78
3903	c1cc(ccc1CN=C=O)O	C19730727	-13.36	-1.35	-18.4	5.74	0.65
3904	c1c(oc(n1)N)[N+](=O)[O-]	C19772587	-13.36	-5.32	-17.92	8.26	1.62
3905	Cc1ccnc1C(=O)C	C30678451	-13.36	2.02	-16.57	4.33	-3.14
3906	C[C@H]([C@H]1C#CC(=O)F)O	C32005742	-13.36	-3.75	-10.36	3.29	-2.54
3907	c1cc(c(c1)O)Cl	C32188351	-13.36	-2.99	-15.95	5.74	-0.15
3908	c1cc(nnc1)N	C01621830	-13.35	-3.16	-15.9	6.08	-0.37
3909	Cc1ccc(c1)F	C02243235	-13.35	-1.68	-15.29	3.8	-0.18
3910	C=CCN(C(=O)N)N=O	C04706150	-13.35	-3.43	-14.88	4	0.96
3911	Cc1c(sc(n1)N)C	C08627583	-13.35	-3.2	-11.95	3.72	-1.92
3912	C(n1c(=O)[nH]c(n1)[N+](=O)[O-])O	C16136400	-13.35	-2.91	-16.85	6.13	0.27
3913	COc(=O)Nc1ccc(c1)N	C19815651	-13.35	0.18	-19.99	6.99	-0.53
3914	c1cc(oc1)C(=S)N	C00159594	-13.34	-2.62	-17.44	8.16	-1.43
3915	c1ccc(cc1)Nc2ccccc2	C00343387	-13.34	1.53	-13.94	4.33	-5.25
3916	Cc1cccc(c1)C#N	C01674308	-13.34	-0.72	-12.2	3.69	-4.12
3917	C=C(=O)OCC(C(F)F)F	C01847515	-13.34	0.45	-12.98	3.61	-4.43
3918	COc(=O)C1ccc(c1)F	C02506532	-13.34	-0.25	-16.24	5.74	-2.6
3919	COc1c(cccc1F)F	C02512335	-13.34	-2.2	-12.73	4.52	-2.93
3920	CC(=CC#N)C	C02557575	-13.34	-0.69	-14.54	4.35	-2.46
3921	c1c(cn1)CCO)Cl	C04290901	-13.34	-2.91	-13.89	3.85	-0.39
3922	C1CC1C(=O)C(F)F	C08700957	-13.34	-0.45	-12.38	2.38	-2.89
3923	CCO/C=C/Br	C12359516	-13.34	-1.05	-12.58	2.64	-2.34
3924	c1c(c(c(n1)N)Cl)N	C13284947	-13.34	-3.22	-15.7	4.93	0.66
3925	c1cnc(cc1C(F)F)F	C19616079	-13.34	0.31	-15.83	3.93	-1.75
3926	Cc1ncc(o1)C=O	C20443735	-13.34	-2.34	-16.55	5.53	0.02
3927	c1ccc(c1)CCO)O	C00406927	-13.33	-2.26	-14.83	3.72	0.03
3928	Cn1cc(nc1)[N+](=O)[O-]	C01063081	-13.33	-3.47	-16.77	11.18	-4.27
3929	c1c2c(ncnc2on1)N	C01295887	-13.33	-1.76	-18.47	6.84	0.05
3930	COc1ccc(c1)F	C02382629	-13.33	-2.57	-13.02	3.55	-1.29
3931	Cn1cc(c1)N)Cl	C02537812	-13.33	-3.08	-13.89	4.69	-1.05
3932	C=CCn1c(nnn1)[S-]	C02556298	-13.33	-1.88	-15.66	5.39	-1.18
3933	Cc1ccn(n1)C(=O)N	C02566285	-13.33	-4.24	-14.76	5.79	-0.12
3934	CNc1cccc(c1)F	C02583443	-13.33	-1.9	-11.5	2.71	-2.63
3935	CON/C=N/O	C04002012	-13.33	-3.49	-12.51	3.74	-1.07
3936	c1c(cn1)CCO)[N+](=O)[O-]	C04290899	-13.33	-3.5	-15.94	6.53	-0.41
3937	c1ccc(cc1)C(=O)NO	C04701351	-13.33	-1.67	-17.6	4.39	1.55
3938	c1cc(occ1/C=N/O)Br	C06888997	-13.33	-4.06	-13.54	4.14	0.12
3939	CN/C=C/C(=O)C(F)F	C12668624	-13.33	-2.47	-13.46	4.46	-1.87
3940	CNC(=O)Nc1cccc1F	C00039688	-13.32	-0.13	-17.76	6.31	-1.74
3941	c1cc(cnc1)CCO	C00161624	-13.32	-2.13	-14.6	3.91	-0.5
3942	c1ccc(c1)NC(=S)NN)F	C00166666	-13.32	0.9	-19.49	7.86	-2.6
3943	c1cc(c(c1)F)F	C00409209	-13.32	-2	-15.02	5.09	-1.39
3944	c1c([n-]nc1[N+](=O)[O-])C(=O)N	C01083683	-13.32	-4.15	-15.46	5.88	0.41
3945	Cc1ccc(cc1O)N	C01669677	-13.32	-2.67	-13.68	3.25	-0.22
3946	c1ccc(c1)C=O	C01729594	-13.32	-2.52	-15.66	7.74	-2.88
3947	CCOC(=O)OCC=C	C02564164	-13.32	-0.63	-13.57	3.28	-2.39
3948	c1cc2cc[nH]c2c(c1)F	C02572395	-13.32	-1.65	-14.97	3.98	-0.68
3949	Cn1ccnc1Cl	C02577856	-13.32	-1.52	-13.85	4.83	-2.78
3950	CCCc1ccno1	C02643992	-13.32	-1.06	-12.36	3.27	-3.17
3951	c1c(cc(c1F)Br)F	C04290728	-13.32	0.43	-17.28	3.38	0.15
3952	C1C=C[C@H]([C@H]1N=O)Cl	C05004379	-13.32	-1.77	-11.97	2.22	-1.8
3953	c1cc(c2c1)C(F)cc[nH]2)F	C08698088	-13.32	-0.42	-14.14	4.72	-3.48
3954	c1cc2c(ncnn2c1)N	C08764136	-13.32	-3.57	-14.05	6.62	-2.32
3955	c1cc(oc1)CCC(=O)Cl	C20252760	-13.32	-1.08	-12.69	3.88	-3.44
3956	c1cnccc1CC(F)F	C30714911	-13.32	-0.92	-13.23	4.11	-3.28

3957	c1cc(cc(c1)C)C#N	C00404318	-13.31	-1.04	-12.06	3.77	-3.98
3958	c1cc(oc1CO)[N+](=O)[O-]	C01081206	-13.31	-3.49	-17.5	7.95	-0.28
3959	c1cc(ncc1C(F)(F)F)N	C01390093	-13.31	-4.87	-11.06	4.26	-1.63
3960	C1=CC2C=CC1O2	C01433325	-13.31	-1.11	-13.1	2.8	-1.9
3961	C1=CC(=O)C=CC1=NCl	C01555531	-13.31	1.02	-15.76	3.99	-2.55
3962	C1[C@@H]2C=C[C@H]2CC1=O	C01570417	-13.31	-0.53	-12.47	2.88	-3.18
3963	Cc1c(ncn1)Cl	C01672435	-13.31	-1.34	-14.13	3.76	-1.6
3964	COc1ccncc1	C01733140	-13.31	-3.27	-14.32	3.64	0.64
3965	Cc1c(cnn1C)N=C=S	C02537535	-13.31	-0.14	-15.26	4.88	-2.79
3966	c1c(cc(c1O)F)CBr	C02539974	-13.31	-2.45	-13.13	4.61	-2.34
3967	C[C@H](C#N)Oc1cccc1	C11834606	-13.31	-2.92	-13.46	5.1	-2.04
3968	Cc1nc[nH]n1	C12398213	-13.31	-3.27	-14.26	5.99	-1.77
3969	CC(=O)OCCSC(F)(F)F	C12618875	-13.31	-0.36	-13.4	4.18	-3.73
3970	Cc1c(cccn1)[N+](=O)[O-]	C13208028	-13.31	-1.24	-14.23	5.09	-2.94
3971	c1(nnc(s1)[S-])N	C16382868	-13.31	-2.83	-15.99	5.54	-0.03
3972	c1cnc2c(n1)[nH]c(=O)[nH]2	C16931073	-13.31	-0.78	-19.47	6.94	0.01
3973	c1cc(nc(c1F)C(F)F)F	C30714852	-13.31	-1.85	-13.63	5.04	-2.87
3974	CCSSCC	M1995A004	-13.31	-0.34	-10.22	1.62	-4.36
3975	CC(=O)Oc1cccc(c1)O	C00002029	-13.3	-1.32	-16.48	6.65	-2.15
3976	c1cc(oc1C=N/O)Br	C00375251	-13.3	-1.56	-17.35	7.19	-1.58
3977	c1cc(ccc1NC(=O)N2N=N2)F	C00401685	-13.3	0.23	-17.48	4.63	-0.68
3978	c1ccc(c(c1)O)I	C00409257	-13.3	-0.43	-16.58	2.6	1.11
3979	CC(=C)C(=O)C	C01608904	-13.3	-0.98	-13.67	3.67	-2.33
3980	c1cc([nH]c1)/C=C/O	C02519586	-13.3	-2.56	-14.78	6.66	-2.62
3981	c1ccc(cc1)CCON	C03635304	-13.3	-0.16	-13.47	2.71	-2.38
3982	c1c(n[nH]n1)CO	C03861563	-13.3	-4.42	-15.09	5.87	0.34
3983	CCOC(=O)[C@H](C(F)(F)F)O	C04255845	-13.3	-2.17	-13.25	3.58	-1.46
3984	CCc1c(c([nH]n1)N)C	C04953860	-13.3	-2.3	-14.33	4.72	-1.38
3985	C=C([C@H](CO)O)Cl	C05426447	-13.3	-4.56	-13.99	3.36	1.89
3986	Cn1c(cnc1[N+](=O)[O-])[N+](=O)[O-]	C05460184	-13.3	0.5	-15.28	3.46	-1.98
3987	CCOC(=O)C(=S)N	C05828397	-13.3	-2.75	-13.86	3.1	0.2
3988	c1cc(cnc1)[C@H](CC)O	C08764125	-13.3	-1.44	-14.94	4.4	-1.33
3989	c1ccc2c(c1)[nH]c(n2)/N=N/O	C13211981	-13.3	-3.96	-15.82	9.29	-2.8
3990	c1cc2c(cc1C#N)cn[nH]2	C14985966	-13.3	-0.92	-15.49	5.7	-2.59
3991	c1c(c([nH]n1)N)C#N	C18217608	-13.3	-5.12	-15.08	7.19	-0.29
3992	COc(=O)Cc1cncs1	C20272676	-13.3	-0.92	-16.82	6.9	-2.46
3993	c1c(cnc1)Cl)N	C20357595	-13.3	-4.48	-15.83	7.16	-0.15
3994	CCc1ccc[nH+]c1N	C21985766	-13.3	-0.78	-13.4	3.71	-2.82
3995	c1cc2c(cc1N)cn[nH]2	C00152290	-13.29	-2.22	-14.97	4.56	-0.65
3996	Cc1ccc(nn1)Cl	C00152979	-13.29	-1.4	-15.28	5.54	-2.15
3997	c1cc(cc(c1)OC(F)(F)F)N	C00164780	-13.29	-0.39	-13.71	2.49	-1.68
3998	C1C2c2([nH]nc2O)C1	C00270745	-13.29	-4.46	-15.85	5.63	1.39
3999	COc(=O)CCc1cccc1	C00396313	-13.29	-0.91	-14.38	4.06	-2.07
4000	CC(=O)C(=O)C	C01532732	-13.29	-1	-13.54	2.64	-1.39
4001	Cc1ccc[nH]1	C01574399	-13.29	-0.95	-14.62	2.67	-0.39
4002	CCOC(=O)C	C01592691	-13.29	-0.83	-11.69	2.01	-2.78
4003	c1c(cnc1)Cl)O	C02524877	-13.29	0.47	-18.62	4.05	0.81
4004	CCc1c(c([nH]n1)C)C	C03848382	-13.29	-1.85	-12.98	4.2	-2.65
4005	c1cc(cc(c1)F)/C=N/O	C04582791	-13.29	-2	-15.98	5.72	-1.03
4006	COc(=O)c1c(c[nH]n1)N	C05686979	-13.29	-0.77	-16.99	4.36	0.11
4007	c1c(c(=O)[nH]c(n1)N)CCS	C08627353	-13.29	-3.46	-15.29	5.16	0.3
4008	c1nc(c(c1)[O-])N(C(F)F)F	C11919801	-13.29	-5.8	-15.03	7.96	-0.42
4009	Cc1cncccc1Br	C13283752	-13.29	-1.83	-10.83	2.29	-2.93
4010	Cc1cncnc1Cl	C15444620	-13.29	-2.41	-14.31	5.54	-2.1
4011	c1cc(c(cc1F)F)[C@@H]2CO2	C19256620	-13.29	-1.57	-11.56	2.64	-2.8
4012	c1c(cnc1)NN)I	C19872654	-13.29	-2.56	-12.84	4.27	-2.16
4013	COc1ccc2c(c1)non2	C00161239	-13.28	-3.32	-13.29	5.34	-2.01
4014	c1cc(ncc1)Cl)Br	C00330764	-13.28	-1.31	-14.79	2.29	0.53
4015	c12c(sc(c1O)s1)sc(=O)s2	C01044327	-13.28	-0.42	-11.15	1.54	-3.25
4016	c1c(nns1)C(=O)NO	C01403330	-13.28	-4.8	-17.61	7.71	1.42
4017	CCOC(=O)CCl	C01648258	-13.28	-0.96	-13.84	4.35	-2.83
4018	CCCCC(=O)Cl	C01850951	-13.28	-0.6	-12.17	2.65	-3.16
4019	C/C=C1/CCOC1=O	C02034939	-13.28	-1.11	-15.54	6.37	-2.99
4020	C1[C@H]([C@@H]1F)C(=O)Cl	C02540316	-13.28	0.29	-13.62	2.68	-2.63
4021	C/C(=N)Nc1[nH]ncn1/[N+](=O)[O-]	C04401865	-13.28	-1.78	-13.09	6.24	-4.65
4022	C#CCO/N=C/c1c(non1)N)N	C04418888	-13.28	-1.14	-15.74	3.93	-0.33
4023	C1C=C[C@H]([C@H]1N=O)Cl	C05004375	-13.28	-1.48	-12.3	2.17	-1.68
4024	CNn1cncn1	C05353904	-13.28	-1.49	-16.48	6.9	-2.21
4025	c1[nH]c(c1n1)[N+](=O)[O-]S	C08615692	-13.28	-4.14	-15.84	9.52	-2.82
4026	Cc1cnc(nc1)Cl	C14982419	-13.28	-2.02	-13.53	4.61	-2.35
4027	Cc1ccc(o1)N=C=O	C20252600	-13.28	-1.72	-14.01	2.76	-0.31
4028	C1CCC(C1)SCC#N	C32667676	-13.28	-0.45	-13.28	4.92	-4.47
4029	CC(=O)/C=C/c1cccc1	C00154592	-13.27	0.75	-15.56	5.04	-3.5
4030	CSc1cncn1	C00156980	-13.27	-0.9	-14.27	3.52	-1.62
4031	CCCC(=O)C(F)(F)F	C01675527	-13.27	-0.71	-12.04	2.49	-3
4032	CCOC(=O)CN=C=O	C01693377	-13.27	-1.68	-17.06	5.58	-0.11
4033	c1(c(c(=O)c(=O)c(=O)c1=O)[O-])O	C03861035	-13.27	-4.61	-14.38	6.44	-0.72
4034	Cc1c(c([nH]1)[N+](=O)[O-])Cl	C04243745	-13.27	-1.17	-12.25	3.13	-2.97
4035	c1[nH]c(c1n1)Br)Cl	C04771900	-13.27	-3.43	-12.54	5.05	-2.35
4036	c1ccc(cc1)CN/C(=N)C#N)N	C05840054	-13.27	2.53	-15.68	5.22	-5.34
4037	Cn1cnc1C#C	C06553981	-13.27	-0.98	-14.81	6.15	-3.63
4038	C1C(=O)N(C(=O)S1)CCC#N	C08804380	-13.27	0.26	-19.02	7.63	-2.14
4039	Cc1cccnc1CCl	C14807832	-13.27	0.41	-13.73	3.55	-3.5
4040	c1cnc(cc1F)C#N	C14982526	-13.27	0.42	-15.92	4.57	-2.34
4041	c1cc(ncc1O)C#N	C14984854	-13.27	-0.39	-18.82	6.05	-0.12
4042	C/C=C/C=C/C=N/O	C15274129	-13.27	-1.07	-14.41	3.69	-1.48
4043	c1cc(c(c1)Br)N)O	C16125294	-13.27	-2.83	-12.95	2.74	-0.23
4044	Cn1c(nnc1S)N	C18043370	-13.27	-4.03	-14.45	7.52	-2.32
4045	c1cc(cc(c1)F)Cn2c(ccn2)N	C19090082	-13.27	0.62	-15.36	5.3	-3.83
4046	c1cnc(cc1Cl)CCl	C21985727	-13.27	-1.74	-10.98	2.89	-3.45

4047	C#CCOC1cncc(n1)Cl	C26515734	-13.27	-1.47	-14.54	3.85	-1.11
4048	c1cnc(c1)C(=O)N	C00388048	-13.26	-4.21	-15.3	6.01	0.24
4049	C=CC(=O)OCc1ccco1	C01608911	-13.26	1.79	-16.8	5.46	-3.71
4050	c1cc(sc1N)SN	C01737341	-13.26	-1.35	-14.91	3.02	-0.02
4051	CO/N=C/(c1c(non1)N)Cl	C02272193	-13.26	0.86	-17	3.59	-0.72
4052	c1ccc(cc1)N/C(=N/[N+](=O)[O-])/N	C06578372	-13.26	0.18	-14.32	4.62	-3.74
4053	Cc1ccc(s1)[N+](=O)[O-]	C15784486	-13.26	-2.38	-12.88	5.86	-3.85
4054	C/C=C/CNc1ccccc1	C17322283	-13.26	-0.65	-9.91	1.65	-4.35
4055	CC(=O)c1cc(ccc1N)F	C21298704	-13.26	-2.52	-12.52	3.99	-2.21
4056	Cc1c(cc(c1F)F)C#N)F	C21299376	-13.26	1.82	-14.2	3.36	-4.23
4057	COC(=O)Cc1ccc(cc1)O	C00395674	-13.25	-1.29	-16.39	6.73	-2.3
4058	C[C@H](C(=O)C)Br	C02031007	-13.25	-1.13	-12.25	2.55	-2.42
4059	Cc1ccc(cc1)CC#N	C02242671	-13.25	-1.89	-14.56	5.62	-2.42
4060	c1c(c(cc(c1Br)F)F)N	C02580921	-13.25	-0.24	-15.31	2.21	0.09
4061	C1CCN(C1)/C(=N/O)/N	C04203681	-13.25	-4.33	-14.36	6.43	-0.98
4062	CCCC(=N)N)N	C04203854	-13.25	-2.66	-13.01	2.96	-0.54
4063	CC(=O)C(=NH+)N)N	C04203887	-13.25	-4.28	-15.33	3.55	2.82
4064	Cc1cc(sc1)C=O	C04208894	-13.25	-1.54	-13.79	5.02	-2.93
4065	c1cc(cnc1)NC(=O)C(F)F)F	C13208177	-13.25	-3.38	-12.8	4.63	-1.7
4066	C/C=C/C=CO	C13546467	-13.25	-2.03	-12.84	2.57	-0.96
4067	c1c(ccc1O)C(=O)N=[N+]=[N-]	C13764320	-13.25	1	-21.57	4.34	2.99
4068	Cc1cc2cc[nH]c2nc1	C14401061	-13.25	-1.25	-13.87	5.26	-3.38
4069	c1[nH]c(c(n1)C(=S)N)N	C16955122	-13.25	-6.47	-15.55	9.07	-0.3
4070	c1c(nc(s1)N)C(=O)N	C17005372	-13.25	-2.2	-17.27	4.73	1.5
4071	c1c2c(n[nH]1)nnnc2[O-]	C17025473	-13.25	-4.22	-18.58	6.73	2.82
4072	C/(C=C)Br)Br)N	C17299574	-13.25	-0.01	-13.63	1.05	-0.66
4073	COc1cc(cnc1)Cl	C19872631	-13.25	-2.45	-11.5	2.66	-1.96
4074	C1CC(=C[C@H]1O)Br	C21994683	-13.25	-1.45	-13.7	2.89	-0.99
4075	c1cc(c(c1O)N)C#N	C26422640	-13.25	-4.56	-15.31	6.51	0.11
4076	CC(=O)n1cc(c(=O)[nH]c1=O)F	C00007886	-13.24	0.28	-18.14	5.09	-0.47
4077	c1ccc(c1)CCO)F	C00407056	-13.24	0.02	-14.75	3.57	-2.08
4078	c1cc(c(cc1Br)F)O	C00409378	-13.24	-0.77	-16.16	3.04	0.65
4079	C/C=C/C(=O)OC=C	C01680772	-13.24	-0.73	-12.75	3.68	-3.44
4080	CC(=O)c1cc(ccc1F)F	C01995083	-13.24	0.78	-17.55	5.84	-2.31
4081	COC(=O)C(C(F)F)F)F	C02040697	-13.24	-1.39	-11.2	2	-2.66
4082	c1cnn2c(nnc2n1)N	C02289036	-13.24	-5.2	-18.11	13.47	-3.4
4083	Cn1ccccc1C(=O)Cl	C02389443	-13.24	1.7	-16.8	4.94	-3.07
4084	c1cc2c([nH]c(=O)[nH]2)nc1	C11919566	-13.24	-7.38	-18.2	10.86	1.47
4085	c1cc2c(c1[nH]c2nc1)N	C14984902	-13.24	-1.23	-15.76	5.04	-1.29
4086	C1CSC/C1=N/O	C15022738	-13.24	-1.66	-14.66	3.78	-0.7
4087	c1cnc(c1)C(=O)N=[N+]=[N-]	C15785118	-13.24	1.49	-20.57	4.98	0.85
4088	Cc1cc(nc1)F)F	C16054434	-13.24	-1.77	-13.87	4.73	-2.33
4089	Cc1cnc(n1)N)C	C16887557	-13.24	-2.66	-13.89	5.13	-1.82
4090	Cc1cnc(c1)CCl	C21985734	-13.24	-1.46	-11.68	3.49	-3.59
4091	c1cc(ccc1/C=C/[N+](=O)[O-])F	C00101337	-13.23	-0.55	-15.67	5.41	-2.42
4092	Cc1c(noc1)N)C	C00164496	-13.23	-3.53	-14.1	4.59	-0.19
4093	c1cncccc1C(=O)Cl	C01586817	-13.23	1.72	-16.11	3.34	-2.19
4094	c1cnn2cnncc2c1N	C01674220	-13.23	-3.97	-17.75	8.43	0.06
4095	c1cc(noc1)C(=O)CCl	C01713556	-13.23	-1.62	-14.54	5.85	-2.91
4096	C(CBr)C(=O)Cl	C02242609	-13.23	-1.57	-11.42	2.33	-2.57
4097	C1CC1C(=O)Cl	C02242630	-13.23	0.35	-13.59	2.56	-2.55
4098	C/C=C(C)C(=O)Cl	C02570159	-13.23	-0.05	-13.18	2.88	-2.87
4099	CCN(C(=O)N)N=O	C04804054	-13.23	-1.53	-16.32	3.54	1.08
4100	COc1cncn1	C05526523	-13.23	-3.21	-14.76	4.85	-0.11
4101	[H]/N=c1/[nH+]c(ss1)N	C05783684	-13.23	-5.99	-15.37	5.58	2.55
4102	c1cc(c(cc1Br)O)F	C06091818	-13.23	-1.1	-15.53	2.79	0.6
4103	c1cc2c(c1)F(c[nH]2)N	C06855063	-13.23	-4.4	-15.64	8.36	-1.55
4104	Cc1ccc(=O)[nH]c1	C08698077	-13.23	-2.81	-15.79	4.7	0.67
4105	C/C=C/C=C=O	C13540492	-13.23	-1.1	-13.97	4.67	-2.83
4106	c1c(cnc(=O)[nH]1)Cl	C15721423	-13.23	-2.61	-17.05	4.14	2.29
4107	C=CCc1ccccc1	C19801720	-13.23	0.02	-12.7	3.08	-3.62
4108	c1c(c(nn1CC(F)F)N)Br	C20348914	-13.23	-4.49	-12.14	5.33	-1.94
4109	c1cc(ncc1O)C(F)F)F	C01529156	-13.22	-1.27	-15.96	4.66	-0.65
4110	c1cc(ccc1NO)Cl	C01659910	-13.22	-4.13	-14.24	4.04	1.11
4111	C1[C@H](C=C1)CC=O	C01709947	-13.22	-0.77	-14.75	3.49	-1.19
4112	c1c(c(n1)CO)Cl	C02538866	-13.22	-2.48	-15.71	4.41	0.55
4113	CSc1nc(sn1)NN	C16928839	-13.22	-1.14	-16.52	5.02	-0.57
4114	CSc1cccc(c1)O	C29753674	-13.22	-0.27	-15.58	4.67	-2.04
4115	c1cc(c(cc1NN)Cl)F	C00153199	-13.21	-2.49	-12.31	3.5	-1.91
4116	c1ccc(c1)C=O)F	C00157161	-13.21	-2.26	-15.48	7.69	-3.16
4117	COC(=O)C(C)Cl	C01641200	-13.21	-0.64	-13.2	3.16	-2.53
4118	COC(=O)CSC#N	C01672999	-13.21	-0.21	-15.59	5.16	-2.57
4119	Cc1nc(cs1)C(=O)N	C02559290	-13.21	-2.91	-16.66	5.84	0.51
4120	Cn1c(c(cn1)Cl)C=O	C02565634	-13.21	-0.13	-14.88	3.72	-1.93
4121	c1cc(sc1)Cn2c(ccn2)N	C03399149	-13.21	0.23	-15.32	4.98	-3.1
4122	c1cncoc1CC#N	C04206813	-13.21	-1.92	-17.15	8.29	-2.42
4123	CCN(C(=O)OCC)N=O	C04536311	-13.21	-1.86	-13.66	3.42	-1.11
4124	c1c[nH]c(=O)cc1Br	C05037781	-13.21	-4.84	-14.72	7.91	-1.56
4125	COc1cncn1	C05285605	-13.21	-1.95	-15.29	5.82	-1.8
4126	Cc1cnn2c(c1)nncc2N	C08616270	-13.21	-5.13	-9.14	5.62	-4.56
4127	Cc1c(ccc(c1F)C)N)F	C12359161	-13.21	-1.92	-12.32	4.2	-3.18
4128	Cn1c(c2c(n1)CCC2)N	C12504958	-13.21	-4.05	-12.63	5.78	-2.32
4129	c1cc(c(c1O)C=O)F)F	C15444596	-13.21	-1.26	-14.8	5.02	-2.16
4130	CCn1cncn1[N+](=O)[O-]	C15782793	-13.21	-2.66	-14.18	8.83	-5.2
4131	c1([n+](=O)[O-])c(n1)N)N	C20330021	-13.21	-5.49	-19.08	11.94	-0.58
4132	c1cc2c(cc1)Fns2	C00071450	-13.2	-2.7	-14.84	3.43	0.91
4133	c1cc(c(cc1Br)F)N	C00152960	-13.2	-0.75	-15.49	2.34	0.7
4134	C[C@H](c1cncn1)O	C00391917	-13.2	-2.15	-14.2	3.91	-0.75
4135	CC(=O)Sc1ccccc1	C00406910	-13.2	-0.75	-16.05	4.46	-0.85
4136	Cc1c(c(nc1F)F)F)F	C00409327	-13.2	-1.44	-11.28	1.94	-2.42

4137	c1(c(snn1C)C(=O)N	C01417140	-13.2	0.5	-18.35	3.38	1.26
4138	CCO[C@H]1C(=O)C(=O)C(=O)O1	C01653813	-13.2	0.38	-17.6	5	-0.98
4139	c1cc(ccc1CCC)O	C01765697	-13.2	-0.97	-15.7	3.01	0.46
4140	C[C@H](CC=C)O	C02003063	-13.2	-0.71	-14.22	1.48	0.24
4141	c1cc(cc(c1)O)/C=C/[N+](=O)[O-]	C02244055	-13.2	-1.07	-17.77	6.02	-0.39
4142	c1c(c(cc(c1F)Br)F)N	C02575681	-13.2	0.62	-16.31	2.32	0.16
4143	C1CC(=COC)C=O	C03884197	-13.2	-1.33	-16.13	6.11	-1.85
4144	CN(C=O)N=O	C04726478	-13.2	-1.68	-13.59	2.9	-0.83
4145	c1c(c(=O)[nH]cn1)I	C05294982	-13.2	-3.89	-15.68	8.27	-1.9
4146	C[C@H]1C(=O)N=C(S1)N	C05529024	-13.2	-1.38	-14.56	3.16	-0.42
4147	c1cc(c(n1))	C12958172	-13.2	-1.82	-14.49	3.49	-0.37
4148	COC(=O)C=C	C17061970	-13.2	-4.29	-14.99	6.44	-0.37
4149	c1cc(c(c(c1F)C#N)F)F	C00155264	-13.19	1.86	-17.75	6.17	-3.47
4150	C1CCC(C1)N=C=S	C00167186	-13.19	0.25	-11.57	1.27	-3.13
4151	c1ccn2c(c1)ncn2	C01657314	-13.19	-2.91	-17.41	7.99	-0.86
4152	CCC[N+](=O)[O-]	C01693429	-13.19	-1.02	-13.16	3.39	-2.41
4153	C/C=C(C)/[C@H](C)O	C01730154	-13.19	-1.15	-12.83	1.98	-1.19
4154	C1CSCS1	C01733027	-13.19	-0.77	-11.87	2.3	-2.85
4155	CSc1nc(ns1)N	C02569836	-13.19	-3.05	-13.98	5.22	-1.38
4156	CC(=C)C(=O)OCCF	C02584300	-13.19	-1.54	-13.14	4.91	-3.41
4157	c1cc(oc1)C=O	C03861345	-13.19	-2.04	-16.25	7.23	-2.13
4158	c1cc2c(c(c1)F)nc[nH]2	C05479669	-13.19	-3.41	-15.06	8.58	-3.29
4159	c1ccn(c1)SC/C(=N/O)/N	C08552692	-13.19	0.34	-21.93	6.07	2.33
4160	C/C(=NH+)(C#N)/N	C12480368	-13.19	-5.18	-12.7	7.09	-2.4
4161	c1c(cnc2c1nc[nH]2)O	C18544047	-13.19	-4.21	-16.75	8.27	-0.5
4162	C[C@H](c1ccc1)Cl	C32005370	-13.19	-1.23	-11.46	2.91	-3.41
4163	COC1cccc1	C00391193	-13.18	-0.71	-15.02	3.65	-1.09
4164	CN1C(=O)C(=O)C(=O)NC1=O	C01760254	-13.18	-0.3	-18.26	5.1	0.27
4165	c1c(c(n1)CC=O)Cl	C02537470	-13.18	-3.03	-15.04	7.03	-2.15
4166	c1ncn(c1)C(=O)n2cncn2	C02584455	-13.18	-1.33	-17.06	6.81	-1.6
4167	c1ccc(cc1)OCCS	C04522230	-13.18	-2.25	-12.81	2.03	-0.15
4168	c1c(ncn1)O	C04566580	-13.18	-3.64	-14.79	3.95	1.29
4169	c1cc2c(cc1Cl)cn[nH]2	C04876880	-13.18	-0.98	-13.08	3.58	-2.7
4170	c1ccc(cc1C)F(F)F	C08764120	-13.18	-3	-11.03	3.34	-2.5
4171	c1cc2ncnnc2cc1Br	C12471795	-13.18	-3.59	-10.76	5.28	-4.1
4172	c1cc(oc1C(=S)N)Br	C12810442	-13.18	-2.31	-14.79	5.92	-2.01
4173	c1[nH]c(nn1)N/C(=NH+)[c2[n-]cnn2	C16981432	-13.18	0.46	-15.59	8.16	-6.22
4174	C(#N)/C=C(\C#N)/F	C17174232	-13.18	-0.03	-14.02	3.12	-2.26
4175	c1c2c([nH]n1)C=CC2=O	C20216475	-13.18	-4.56	-14.53	7.77	-1.86
4176	c1ccc2c(c1)[nH]c(n2)Cl	C00152282	-13.17	-2.9	-15.88	4.88	0.73
4177	c1cc(c(cc1C#N)O)O	C00157092	-13.17	-1.3	-18.22	6.24	0.11
4178	c1cc(oc1)CNC(=O)N	C00162619	-13.17	-0.14	-20.83	6.87	0.93
4179	c1cc(ccc1NC=O)F	C00394988	-13.17	-2.85	-16.71	7.27	-0.88
4180	c1cccnc1)I	C00404222	-13.17	-0.66	-16.27	3.32	0.44
4181	CC[C@H](c1ccc1)O	C01481898	-13.17	-1.14	-11.56	2.32	-2.78
4182	Cc1cc(on1)N	C01604212	-13.17	-3.65	-14.28	4.4	0.35
4183	c1cncn1	C01692439	-13.17	-1.54	-14.6	3.69	-0.72
4184	c1cc(sc1C(=O)Cl)Cl	C02168777	-13.17	-0.91	-14.52	2.38	-0.13
4185	C1(=S)C(=S)SC(=S)S1	C02382900	-13.17	-0.45	-9.03	0.53	-4.22
4186	C=CC(=O)OCC(C(F)F)F	C02584317	-13.17	0.3	-15.1	5.71	-4.07
4187	C[C@@H](C(=O)Cl)Cl	C04262242	-13.17	0.03	-13.09	2.21	-2.32
4188	c1cccnc1)CN[NH3+]	C19172755	-13.17	-1.24	-15.68	3.83	-0.39
4189	CC(=O)C1ccsc1	C20252681	-13.17	-1.43	-13.61	5.51	-3.64
4190	c1cc(cc2c1cc[nH]2)F	C00163312	-13.16	-3.65	-9.94	3.85	-3.42
4191	CCOC(=O)C=C	C00403287	-13.16	-0.34	-15.66	4.88	-2.04
4192	c1cc2[nH]cnc2c(=O)c1	C01566204	-13.16	-2.6	-18.52	7.77	0.18
4193	COC(=O)CBr	C01641052	-13.16	-0.88	-14.2	4.1	-2.19
4194	c1cc(cc(c1)OC(F)F)N	C02560125	-13.16	0.48	-16.68	4.56	-1.51
4195	C(CCl)[N+](=O)[O-]	C05113366	-13.16	0.12	-13.96	2.99	-2.31
4196	CC[C@H](C)ON=O	C06129972	-13.16	-1.06	-11.81	2.49	-2.78
4197	c1nnc(s1)NC(=S)N	C06599630	-13.16	-4.03	-16.17	7.36	-0.32
4198	c1c[nH]c2c1c(=O)nc[nH]2	C08638189	-13.16	-4.68	-16.24	7.22	0.55
4199	CCc1nnc(s1)N	C17744087	-13.16	-1.93	-15.72	5.71	-1.22
4200	c1(=O)c(n[nH]c(=O)[nH]1)NN	C18189881	-13.16	-4.64	-18.66	6.98	3.16
4201	c1cc2c(c(c1)F)c(no2)N	C19869410	-13.16	-4.96	-13.06	7.1	-2.23
4202	c1csc(n1)NCC(F)F	C21799605	-13.16	-3.16	-11.09	3.53	-2.44
4203	C=Cn1cnn1	C22000920	-13.16	-2.6	-17.39	8.6	-1.78
4204	c1csc(n1)C(=O)N	C22113384	-13.16	-3.47	-17.26	6.4	1.16
4205	Cc1ccc(o1)c2cc[nH]n2	C32501645	-13.16	1.22	-17.44	5.82	-2.76
4206	c1c(onc2c1[nH]nc2)Br	C32915118	-13.16	-0.23	-15.9	4.45	-1.49
4207	c1cc(ncc1C=O)Cl	C00169497	-13.15	-1.62	-14.81	5.49	-2.21
4208	Cc1ccc(c1N)O	C00389589	-13.15	-4.17	-11.82	3.09	-0.25
4209	c1cc(c2cn[nH]c2c1N)F	C01404079	-13.15	-3.97	-13.02	4.65	-0.81
4210	C/C=C(\C=O)/Cl	C02043284	-13.15	-1.81	-14.79	5.68	-2.24
4211	Cc1ccc(c(c1)F)C#N	C02243215	-13.15	1.81	-17.21	4.98	-2.74
4212	Cc1ccc(c(c1)F)CC#N	C02243232	-13.15	-0.2	-14.49	6.35	-4.8
4213	c1cc(c(nc1)[N+](=O)[O-])F	C02598978	-13.15	-3.88	-16.04	10.23	-3.46
4214	C1C(=NC(=[NH2+])S1)N	C08649581	-13.15	-5.65	-15.58	8.13	-0.05
4215	c1cc(c(=O)[nH]c1)[O-]	C12243851	-13.15	-4.2	-18.01	8.76	0.29
4216	[H]/N=C(\CCl)/OCC	C17300981	-13.15	-1.74	-13.79	2.54	-0.15
4217	Cc1c([nH]c(=S)nn1)[O-]	C18153959	-13.15	-2.05	-16.16	5.82	-0.75
4218	CC(=O)C(=O)[C@H](S)[S-]	C20231292	-13.15	0.13	-14.37	2.96	-1.87
4219	c1c(oc(n1)N)C(F)F	C20357591	-13.15	-3.26	-16.36	5.32	1.15
4220	COC1ccsn1	C26506541	-13.15	-0.48	-16.25	3.8	-0.22
4221	c1cc(cc(c1)F)C=O	C00157155	-13.14	-2.59	-13.93	6.56	-3.18
4222	c1ccc(cc1)OC(F)F	C00167127	-13.14	-0.25	-12.78	2.05	-2.15
4223	c1ccc(c(c1)N+)(=O)[O-]Cl	C00331636	-13.14	-2.74	-12.8	6.5	-4.1
4224	CC(C)SC(=[NH2+])N	C03806248	-13.14	-1.75	-12.2	1.89	-1.08
4225	c1c([nH]c(=O)[nH]c1=O)NN=O	C04768985	-13.14	-3.36	-19.97	6.91	3.27
4226	c1c2c(c(n1)N)n[n-]n2	C13518221	-13.14	-4.49	-19.04	8.68	1.72

4227	[C@H](C(F)F)(OC(F)F)F	C16082613	-13.14	-0.07	-13.37	1.97	-1.66
4228	c1(c(nsn1)Cl)O	C16124756	-13.14	-2.3	-16.58	3.01	2.73
4229	Cc1cc(O)[nH]nc1	C17108644	-13.14	-3.4	-16.53	7.21	-0.41
4230	CC(=O)Cc1ccccc1F	C01840990	-13.13	-1.39	-13.39	6.05	-4.41
4231	c1cc(O)CCl)C=O	C01995255	-13.13	-1.23	-16.68	8.09	-3.3
4232	c1ccc(cc1)[C@H](CCl)O	C02555239	-13.13	-1.12	-12.4	3.07	-2.69
4233	C/C=C/C(=O)OCC#N	C04933464	-13.13	-0.31	-16.02	6.9	-3.71
4234	CCOC1CCnc1	C06387813	-13.13	-0.11	-14.2	3.47	-2.3
4235	c1csc(n1)NC(=S)[S-]	C06585049	-13.13	-2.04	-16.62	4.21	1.32
4236	c1cc(Cc1)N)F)C#N	C08700947	-13.13	-0.69	-16.06	5.72	-2.1
4237	C(#N)c1(c(nc(nn1)N=[N+]=[N-])N	C13304197	-13.13	-4.88	-12.33	3.87	0.2
4238	c1cc(O)C2COc2)F	C15442913	-13.13	-1.59	-12.71	5.32	-4.14
4239	c1cc(O)C(F)C/C(=N/O)/N	C16082805	-13.13	-2.4	-14.2	4.74	-1.27
4240	c1c(ncnc1Cl)CCl	C26510543	-13.13	-2.08	-11.63	3.7	-3.12
4241	C1C[C@H](C=C1)O	C01640968	-13.12	-1.52	-12.87	1.92	-0.64
4242	CC(C)C(=O)C(=O)C	C01663923	-13.12	-0.54	-12.34	2.35	-2.59
4243	c1cc(O)C(c1F)C#N)F)O	C02243358	-13.12	1.43	-19.07	5.99	-1.48
4244	c1cc(O)C(=O)C=O	C02560445	-13.12	-1.35	-12.96	1.36	-0.17
4245	c1cc(O)C(F)CC(=O)Cl)F	C02574154	-13.12	-2.5	-12.59	4.13	-2.16
4246	CC(C)C(=O)C(=O)C	C12953124	-13.12	-1.75	-13.02	4.53	-2.88
4247	CC(C)C(=O)C(=O)OCC	C13525876	-13.12	0.54	-13.87	3.2	-2.99
4248	c1c(sc(n1)C(F)F)C=O	C20445797	-13.12	-3.46	-12.78	5.21	-2.09
4249	c1cnccc1NN	C26459841	-13.12	-3	-18.16	7.53	0.51
4250	CC(=O)CCC(=O)Cl	C32016229	-13.12	-0.76	-13.98	4.06	-2.44
4251	SCCC1CCCC1	M1995A045	-13.12	-0.99	-8.94	2.02	-5.21
4252	c1c(O)CC(F)F)CC#N	C00164759	-13.11	-2.11	-14.72	7.01	-3.29
4253	C/C=C/C)C=O	C01577193	-13.11	-1.55	-13.72	4.55	-2.39
4254	CCC(=O)C(=O)CC	C01602516	-13.11	-0.33	-12.25	2.17	-2.7
4255	Cc1cnnc1N)N	C01672563	-13.11	-3.67	-16.45	6.02	0.99
4256	CCN(C1CCCC1)N	C01845872	-13.11	-3.59	-8.72	2.38	-3.17
4257	CC(=O)OCC(=O)C=C	C02510854	-13.11	0.41	-17.06	6.9	-3.37
4258	c1cc(O)C(F)C=O)F	C02539346	-13.11	-1.26	-14.52	5.92	-3.25
4259	[H]N=C\1/N=C(SCS1)N	C05624795	-13.11	-0.41	-15.69	3.15	-0.17
4260	CCc1c(O)[nH]1)C	C05634178	-13.11	-1.78	-12.6	3.49	-2.23
4261	C/(C=C/C(F)F)F)O	C08698332	-13.11	-4.07	-14.01	5.31	-0.34
4262	c1cn(O)CC#N	C12360633	-13.11	-2.11	-17.34	9.7	-3.35
4263	c1cc(O)C(=O)C=N/O	C15446206	-13.11	2.06	-20.41	6	-0.76
4264	C/(C=N/O)/N)Br	C16082757	-13.11	-4.14	-12.7	2.87	0.86
4265	c1cc(O)C(N)F)I	C19616304	-13.11	0.4	-14.92	4.02	-2.6
4266	C=COCC(=O)c1ccccc1	C00395557	-13.1	3.05	-15.85	4.32	-4.63
4267	COc1cc(O)CC(F)F	C02584353	-13.1	1.77	-15.09	3.19	-2.97
4268	[H]N=C/(CC1)SCC	C04352967	-13.1	-1.05	-13.81	1.52	0.23
4269	c1cc(O)C(c1Cl)O)N	C04520808	-13.1	-3.53	-12.64	3.24	-0.17
4270	Cc1ccc2c1n[nH]n2	C05116315	-13.1	-5.33	-10.91	5.06	-1.92
4271	c1cc(O)C(O)C(F)F)F	C05177786	-13.1	-3.52	-13.71	4.85	-0.71
4272	c1ccc2c1c1c[nH]2)C#N	C05544212	-13.1	-1.61	-13.67	4.79	-2.61
4273	c1(c([nH]c(=O)[nH]c1=O)N)Cl	C06239834	-13.1	-4.68	-19.2	9.22	1.56
4274	c1c(O)C(=O)[N+](=O)[O-])F)Cl	C15442494	-13.1	-2.17	-12.38	4.33	-2.88
4275	c1nnc(n1N)[S-]	C16979488	-13.1	-5.02	-14.39	8.24	-1.92
4276	c1nc(c2c(n1)sn2)NN	C17352058	-13.1	-2	-16.03	5.03	-0.1
4277	Cn1cncc1CCI	C19090588	-13.1	-0.6	-14.12	5.28	-3.65
4278	c1cc(O)C(c1F)C)N)F	C19171894	-13.1	3.32	-18.43	3.41	-1.4
4279	C1CC[NH2+][C@H](C1)Br	C26893210	-13.1	0.14	-12.68	0.94	-1.5
4280	c1cc(O)C(=O)O	C00156709	-13.09	-2.52	-15.63	6.02	-0.96
4281	CC(=O)SCc1ccco1	C00409294	-13.09	-1.94	-12.25	4.43	-3.33
4282	c1c(O)C(n1)N)N)Cl	C00967252	-13.09	-4.32	-14.72	5.16	0.79
4283	c1cnc(O)CCO	C01435984	-13.09	-3.16	-15.43	4.62	0.88
4284	CCOC(=O)[C@H](C(=O)C)F	C01614535	-13.09	-1.18	-12.64	3.59	-2.86
4285	CCC(=O)C(F)F)F	C01675401	-13.09	-0.26	-13.11	2.71	-2.43
4286	Cc1ccoc1	C01683907	-13.09	-1.48	-13.98	4.03	-1.66
4287	COCC(=O)C1=NCCOC1=O	C04042532	-13.09	1.61	-19.4	6.63	-1.92
4288	C1CCC(C1)S	C04501358	-13.09	0.41	-11.11	0.76	-3.16
4289	C/(C=C/C)NC(=S)N	C05500579	-13.09	-1.47	-17.38	2.99	2.76
4290	[C@H](C(F)F)(F)C(F)Cl)O	C08698375	-13.09	-1.72	-12.8	2.16	-0.73
4291	COCC(=O)C(=N+)(O)[O-])[N+](=O)[O-]	C15771887	-13.09	0.73	-17.4	6.4	-2.82
4292	c1cnc(O)C(F)F)C#N	C16159523	-13.09	0.41	-15.28	4.84	-3.06
4293	c1c(O)C(c(n1)[N+](=O)[O-])N)N	C19117694	-13.09	-3.46	-15.5	5.52	0.35
4294	CCOC=C(=O)Cl	C21987137	-13.09	0.17	-14.42	3.38	-2.21
4295	C1C2c(O)C2C#N)C1	C24445897	-13.09	2.11	-16.88	4.86	-3.18
4296	c1c(O)C(n1)NO)Cl	C26441010	-13.09	-4.19	-15.34	7.31	-0.87
4297	c1cscc1C(=S)N	C00161840	-13.08	-2.85	-17.87	9.67	-2.04
4298	Cc1cccn1)C	C00967363	-13.08	-2.17	-13.43	4.8	-2.28
4299	c1cc2c(O)cc1N	C01389542	-13.08	-2.29	-13.45	4.59	-1.93
4300	c1(c([nH]n1)N)C(=O)N	C01653220	-13.08	-6.96	-16.87	5.41	5.35
4301	CN1C=NN(C=N1)C	C01720059	-13.08	-2.17	-13.65	6.17	-3.43
4302	C(CCl)C(=O)Cl	C01736653	-13.08	0.18	-13.3	2.44	-2.4
4303	CC(C)CO[N+](=O)[O-]	C02034837	-13.08	-0.88	-11.92	1.61	-1.88
4304	c1cscc1C(=O)N	C02548216	-13.08	-2.14	-17.79	7.05	-0.21
4305	Cc1ccc(O)C(F)F	C04208889	-13.08	-1.4	-15.13	3.8	-0.36
4306	Cc1c([nH]cn1)C=O	C04807266	-13.08	-3.28	-14.35	6.35	-1.79
4307	CN=C(=O)C(C(F)F)F)Cl	C04865168	-13.08	-2.68	-13.77	5.32	-1.95
4308	c1cc(O)C(=O)C([N+](=O)[O-])[O-]	C06829185	-13.08	-0.7	-18.64	7.96	-1.71
4309	c1nc(O)C(F)F)N	C12395192	-13.08	-0.72	-17.57	8.33	-3.11
4310	[H]N=C(NC#N)Nc1ccc(O)C1	C13116101	-13.08	-1.21	-10.03	4.09	-5.94
4311	COCC(=O)COc1ccco1)F	C20297595	-13.08	-2.15	-12.71	5.92	-4.15
4312	c1cc(O)C1=NN(C(=S)N)F	C00069512	-13.07	-1.68	-18.42	9.91	-2.88
4313	c1c(O)C(Cc1N)O)N	C00403311	-13.07	-5.66	-15.98	4.49	4.08
4314	CC(=O)C(Cl)Cl	C01675518	-13.07	-1.4	-12.34	3.01	-2.34
4315	c1c(O)C([nH]c(O)Oc1=O)Br	C01760207	-13.07	-1.42	-16.24	5.83	-1.24
4316	c1c(nc2nncn2c1[O-])[O-]	C02327305	-13.07	-8.85	-14.99	9.98	0.79

4317	Cc1cc(cc(c1)F)N	C02555193	-13.07	-2.68	-10.75	2.67	-2.33
4318	CCc1ccc(=O)N(N)[O-]	C04054152	-13.07	-2.73	-11.37	4.74	-3.72
4319	c1ccc(c(c1)/C(=O)N)/N)Cl	C12504600	-13.07	-3.64	-13.74	5.73	-1.41
4320	C(=N)N(H)+C(=O)N(N)C(F)F	C17328624	-13.07	-4.89	-14.55	7.81	-1.44
4321	COCC1nc(no1)CCl	C19092519	-13.07	-2.57	-14.86	4.9	-0.54
4322	c1c(ccn1)NC=O	C22000930	-13.07	-3.28	-18.11	8.53	-0.21
4323	c1ccc2c(c1)c([nH]2)N	C00530874	-13.06	-2.68	-12.27	3.72	-1.84
4324	Cc1c(ccn1)N)N	C01688414	-13.06	-3.68	-16.27	4.61	2.28
4325	CCOC(=O)C(=O)CBr	C01752920	-13.06	1.27	-13.51	2.93	-3.75
4326	C(CC(=C(F)F)F)CO	C02530956	-13.06	-3.61	-11.79	3.1	-0.76
4327	c1ccc(cc1)COCC=O	C02556950	-13.06	1.29	-16.34	5.18	-3.18
4328	C1C=C(CS1)C=O	C03346456	-13.06	-1.17	-15.97	6.68	-2.61
4329	CN1CCSC1=[NH2+]	C03865408	-13.06	-1.57	-13.72	4.04	-1.8
4330	c1c2c([nH]n1)CCC2	C05013003	-13.06	-2.83	-16.19	5.05	0.91
4331	c1cc(c(cc2c1non2)N)Cl	C12243770	-13.06	-1.84	-12.43	2.67	-1.46
4332	Cc1c(=O)nc(=O)[nH]n1)N	C16249017	-13.06	-2.73	-16.81	5.11	1.37
4333	C1C(=C(C(=O)O1)Cl)[O-]	C18183478	-13.06	-1.39	-15.02	5.17	-1.8
4334	c1ccc(cc1)N(=[O-])[O-]O	C19691768	-13.06	-1.23	-17.53	6.02	-0.32
4335	c1c(c(c(c1)F)F)F)N)N	C21304442	-13.06	-1.36	-14.52	4.56	-1.74
4336	C/C(=C/C([NH2+]CC=C)/Br	C26504236	-13.06	-1.34	-10.16	0.96	-2.53
4337	c1(c(nc2c(n1)non2)N)N	C01082675	-13.05	-9.01	-15.42	11.23	0.15
4338	CC(=CC#N)C	C01756010	-13.05	-1.75	-13.25	4.17	-2.22
4339	c1cc(cc1CO)F)N	C02243164	-13.05	-2.08	-15.56	4.28	0.31
4340	Cn1cc(=O)N=C=S	C02537532	-13.05	-0.67	-14.58	4.67	-2.48
4341	COc1[nH]c(=O)s1	C03650785	-13.05	-2.86	-16.41	3.46	2.77
4342	Cc1c2c(c(n1)N)N(=[O-])[O-]	C04067459	-13.05	-5.62	-10.16	4.27	-1.53
4343	C([C@H](C)O)N(=[O-])[O-]N(=[O-])	C04212632	-13.05	-1.55	-14.47	5.17	-2.19
4344	CCOC(=O)NNC(=O)O	C04962795	-13.05	-6.31	-15.38	6.17	2.47
4345	Cc1c([n+](on1)[O-])[N+](=O)[O-]	C05064025	-13.05	-1.62	-16.66	7.63	-2.4
4346	C=Cn1cc(=O)Br	C05495164	-13.05	-0.87	-14.81	3.88	-1.24
4347	c1c(c([nH]c(=O)c1)Cl)Br	C15684480	-13.05	-4.64	-14.3	7.77	-1.88
4348	c1(c(c(c1)N)F)F)F)Cl)F	C16159831	-13.05	-2.81	-10.81	2.1	-1.54
4349	Cc1c(scc1/C=C/[N+](=O)[O-])C	C20921170	-13.05	-1.6	-11.13	4.93	-5.24
4350	c1c(ncn1)Cl)CF	C26466628	-13.05	-2.54	-11.71	4.05	-2.85
4351	CNC(=S)Nc1ccc(cc1)F	C00088789	-13.04	-0.65	-15.93	7.11	-3.57
4352	C/C(=O)N)/c1cc([nH]c1	C00153021	-13.04	-3.21	-14.45	5.2	-0.58
4353	c1c(cc(cc1)F)F)C=O	C00164753	-13.04	-1.74	-12.76	4.68	-3.22
4354	c1cc(cc(c1)Br)O	C00388034	-13.04	-1.18	-15.76	2.74	1.15
4355	Cc1cc([nH]1)C	C00594608	-13.04	-1.87	-13.58	4.1	-1.7
4356	CSCC(Cl)	C01592634	-13.04	0.56	-11.83	1.24	-3.01
4357	C=CN=C=O	C02509860	-13.04	-0.84	-12.44	1.61	-1.37
4358	c1c(cc(c(c1)C#N)F)F)F	C02575065	-13.04	2.06	-15.34	3.79	-3.55
4359	c1([nH]nc(n1)N)N	C04118774	-13.04	-5.49	-14.59	8.59	-1.55
4360	CC(C)CON=O	C04261994	-13.04	-0.73	-11.52	1.95	-2.74
4361	c1(nc2c(n1)nc2[N+](=O)[O-])N)N	C04558145	-13.04	0.95	-13.94	6.52	-6.58
4362	c1nc([nH]1)CCl	C06062898	-13.04	-2.73	-16.14	4.91	0.92
4363	c1cc(c(cc1)F)/C(=O)N)F	C06453252	-13.04	-4.68	-14.09	5.44	0.29
4364	c1c(=O)n2c(n1)sc(n2)[S-]	C06523955	-13.04	-3.78	-17.96	7.88	0.82
4365	Cc1[nH]c([nH+])1	C08283844	-13.04	-2.06	-14.51	5.18	-1.64
4366	C=CCn1cnc(n1)I	C08295365	-13.04	-1.76	-12.76	5.81	-4.33
4367	C/C(=O)N)/c1ccc(=O)1	C12866695	-13.04	-4.15	-12.56	4.39	-0.71
4368	c1cc(oc1)CCC=O	C13546592	-13.04	-1.18	-15.02	6.06	-2.89
4369	CC(=O)O/C(=C(C(F)F)F)F)F	C14628477	-13.04	-1.42	-12.57	4.34	-3.38
4370	CCNc1cnc(n1)Cl	C16124192	-13.04	-3.57	-11.36	3.3	-1.41
4371	c1cc(c(nc1)N)C=N/O	C19735473	-13.04	-5.17	-14.77	6.54	0.35
4372	C#CCNc1ccc(s1	C19875410	-13.04	-0.47	-12.77	2.95	-2.75
4373	c1c(noc1N)C(F)F	C26512576	-13.04	-3.76	-15.34	5.92	0.15
4374	c1cc2c(cc1CO)non2	C00158674	-13.03	-4.29	-14.21	5.75	-0.28
4375	CCn1cccc1=O	C00397642	-13.03	-1.88	-16.71	8.77	-3.2
4376	CN1C2=CC=CCN2N=N1	C01598330	-13.03	0.74	-15.18	3.97	-2.57
4377	CCOC(=O)N=C=O	C01711364	-13.03	-0.99	-15.91	2.47	1.4
4378	C1=CC=CC(C=C1)NC(=O)N	C01727544	-13.03	0.1	-21.8	6.23	2.44
4379	c1(c(non1)N)c2nc(on2)C(F)F	C02271911	-13.03	-0.56	-15.47	3.13	-0.12
4380	Cn1ccc(n1)[N+](=O)[O-]	C04293945	-13.03	-3.76	-15.25	9.15	-3.17
4381	Cc1cnc([nH]c1=O	C05545258	-13.03	-4.07	-17.47	8.22	0.29
4382	Cc1[nH]c2c(n1)ccc2	C06369911	-13.03	-2.1	-15.4	7.08	-2.62
4383	C1=C/C(=C)N)C(=O)C=C1	C06661478	-13.03	-1.5	-15.25	3.77	-0.05
4384	c1cc2c([nH]c(=O)oc2=O)nc1	C11919575	-13.03	2.19	-20.61	7.16	-1.76
4385	c1cc(nc(c1)F)C#N	C12359444	-13.03	-0.38	-17.44	7.02	-2.24
4386	c1cc(oc1CN=O)[N+](=O)[O-]	C13828133	-13.03	-1.71	-15.95	5.51	-0.89
4387	c1ccn(c(=O)c1)C[C@H]2CO2	C19258978	-13.03	-2.88	-15.87	7.81	-2.09
4388	CNc1cc(c1)F)F	C20044972	-13.03	-2.21	-10.49	2.37	-2.69
4389	Cc1csc(n1)C	C00150863	-13.02	-0.96	-13.14	3.4	-2.31
4390	c1cc(nnc1)CO	C00158628	-13.02	-1.68	-17.84	5.86	0.64
4391	c1cc(ccc1C(=O)C=O)F	C01595133	-13.02	1.37	-19.53	9.03	-3.89
4392	Cc1c(sc(n1)[S-])C	C02384954	-13.02	-1.17	-12.61	3.17	-2.41
4393	c1c(c(n1)CC=O)[N+](=O)[O-]	C02537471	-13.02	-3.78	-17.05	10.1	-2.29
4394	CCOCCBr	C04283933	-13.02	-0.59	-11.59	2	-2.85
4395	CC(=CC)S	C05138189	-13.02	-0.25	-13.12	1.01	-0.66
4396	[C@H](C)C(F)F)OC(F)F)F	C08698271	-13.02	0.2	-13.3	1.81	-1.74
4397	[H]/N=C([C@H](C#N)Cl)C(F)F	C16158417	-13.02	-1.02	-13.35	2.18	-0.83
4398	C/C=C/C(=O)N	C17299624	-13.02	-3.18	-16.03	5.74	0.45
4399	c1ccn(c1)CCl	C26422555	-13.02	-1.18	-9.33	2.19	-4.7
4400	c1cc(nnc1)N)F	C30678112	-13.02	-3.97	-16.6	7.81	-0.25
4401	C1[C@H](NCS1)C(=O)Cl	C32016247	-13.02	0.7	-17.14	4.09	-0.66
4402	CCOC(=S)C(=O)N	C33359018	-13.02	-4.04	-14.97	6.02	-0.02
4403	c1c(c(cc1)F)C)N)N	C00152701	-13.01	0.32	-16.29	3.76	-0.8
4404	c1cc2c(cc1N)oc(=O)[nH]2	C00347252	-13.01	-5.68	-14.62	7.25	0.04
4405	CCOC(=O)c1cncnc1N	C00408009	-13.01	-0.66	-13.68	3.81	-2.48
4406	COCCOC(=O)CCCl	C01597354	-13.01	0.94	-16.98	4.08	-1.04

4407	CCC(=O)C(=O)C	C01683666	-13.01	-0.48	-12.84	2.42	-2.11
4408	CCc1ccc(O)C(=O)C	C01707723	-13.01	-1.26	-12.41	4.26	-3.61
4409	COCCC=C	C01769413	-13.01	0.03	-13.35	1.31	-1.01
4410	C=CC(C=C)O	C01845568	-13.01	-0.61	-13.81	1.47	-0.06
4411	CCSc1nnn1N	C02554082	-13.01	-0.91	-14.86	5.73	-2.97
4412	c1c([nH]nc1N)C2CC2	C04674333	-13.01	-3.49	-14.75	6.56	-1.33
4413	CCOC(=O)c1cnnc1N	C04889229	-13.01	-5.64	-19.87	10.39	2.13
4414	COC(=O)c1cnsc1	C12650022	-13.01	-1.48	-13.34	3.89	-2.07
4415	c1cn(cn1)C(=O)C(=O)NN	C13207717	-13.01	2.02	-20.98	5.6	0.35
4416	c1csc(n1)C#N	C14982559	-13.01	-1.53	-14.56	4.77	-1.68
4417	c1c(c(c(c1F)F)[N+](=O)[O-])N)F	C15440474	-13.01	-2.34	-12.07	3.98	-2.58
4418	c1c(ncn(c1B)F)N	C16159755	-13.01	0.48	-17.34	4.76	-0.91
4419	c1cc2nnn2cc1N	C18555997	-13.01	-3.61	-16.13	9.3	-2.56
4420	C=C(CO)C1CCOC1	C21997324	-13.01	-0.18	-16.63	4.77	-0.96
4421	c1ccc2c(c1)[nH]c(n2)CF	C26466829	-13.01	-4.47	-13.27	8.01	-3.28
4422	CC(=O)CSc1nnn1N	C32698059	-13.01	-3.42	-16.07	9.51	-3.02
4423	c1cc(ccc1OC(=S)Cl)Cl	C00403296	-13	0.12	-14.92	1.66	0.14
4424	c1cc(c(cc1OC(F)F)F)N)N	C02243191	-13	-0.41	-15.39	3.01	-0.21
4425	c1cc(c(cc1C#N)F)[N+](=O)[O-]	C02540647	-13	-2.72	-13.15	6.98	-4.11
4426	CC(=O)NCC1CCC(c1)F	C02562036	-13	0.46	-16.83	6.07	-2.7
4427	c1(nc(c1)N(c(=O)n1)Cl)Cl)O	C04217607	-13	-0.18	-15.6	3.5	-0.73
4428	c1[n-c(n1)C#N	C04218567	-13	-4.29	-14.25	7.53	-1.98
4429	c1nc(c(n1)N)C#N	C05020384	-13	-3.42	-16.91	8.23	-0.9
4430	CC1=NN=C(C1)OC	C05285841	-13	-2.46	-14.32	4.07	-0.29
4431	C(n1nc(nn1)C(F)F)F[N+](=O)[O-]	C05369174	-13	-2.29	-15.09	7.02	-2.64
4432	c1cc(c(c1)Nc2nc(cnn2)[O-])O	C08738204	-13	2.39	-20.53	6.6	-1.46
4433	CCOC(=O)C=C(Cl)C	C13380320	-13	-0.79	-12.45	3.5	-3.27
4434	COCC/C=C(Cl)Cl	C16997518	-13	-1.11	-10.91	1.9	-2.88
4435	CCn1ncc(n1)N	C19088830	-13	-2.05	-15.5	4.97	-0.42
4436	C=CCNC#C	C19735309	-13	-0.37	-13.13	2.06	-1.56
4437	Cn1c(c(n1)C#N)N	C00169364	-12.99	-2.99	-16.33	6.31	-0.94
4438	C=CNC(=O)C(C(F)F)F)F)F)F)F	C01730429	-12.99	0.41	-13.69	2.84	-2.55
4439	COC(=O)C(C(F)F)F)C(F)F)F)F	C02040737	-12.99	-0.39	-12.07	4	-4.53
4440	c1(c(=O)[nH]c(O)[nH]n1)C(F)F)F	C02479684	-12.99	-3.58	-15.92	5.45	1.06
4441	c1nnn1CCO	C02507132	-12.99	-5.59	-15.66	7.98	0.27
4442	CNc1c(nof[n+][O-])[N+](=O)[O-]	C04087617	-12.99	-3.25	-12.91	5.61	-2.44
4443	C1[C@H]([C@@H]([C@H]1)C)C=O	C05031331	-12.99	-1.27	-14.55	4.05	-1.23
4444	[H]N=C(/C/Nc1ccccc1)C#N	C05590893	-12.99	-4.37	-9.94	3.6	-2.28
4445	C[C@H]1CON=C1[N+](=O)[O-]	C15784735	-12.99	-0.34	-14.61	4.49	-2.53
4446	OCCc1ccccc1	M1995A044	-12.99	-1.48	-12.54	3.31	-2.28
4447	c1ccc(cc1)CONC(=O)N	C00084002	-12.98	-3.23	-18.86	10.39	-1.28
4448	c1cc(c(cc1F)[N+](=O)[O-])F	C00164551	-12.98	-1.83	-14.61	5.79	-2.33
4449	C=C[C@H]([C@@H]([C@H]1)C)O)O	C00389839	-12.98	-1.43	-14.11	2.1	0.45
4450	CC(=CC1c1ccccc1)O)C	C01600125	-12.98	-0.36	-15.17	2.97	-0.42
4451	COC(=O)CCCl	C01696146	-12.98	-0.51	-14.15	3.13	-1.46
4452	c1ccc(cc1)O)C1	C01846601	-12.98	-2.28	-16.26	8.25	-2.68
4453	Cc1ccc(O)SC	C01850677	-12.98	-0.71	-11.81	2.93	-3.39
4454	CCC[C@H]([C@@H]([C@H]1)C)O	C02037591	-12.98	-1.17	-11.39	1.19	-1.61
4455	CCOC(=O)C(=O)C(C)C	C02534762	-12.98	0.21	-12.5	3.1	-3.78
4456	CCn1ccc(n1)N	C02558418	-12.98	-1.71	-15.09	5.32	-1.5
4457	c1ccc2c(c1)c(n[nH]2)Cl	C03852548	-12.98	2.41	-18.56	6	-2.83
4458	c1cnnc1)CCO	C03861008	-12.98	-3.35	-13.22	4.09	-0.5
4459	c1c[nH]nc1C2CC2	C04291288	-12.98	-1.98	-13.13	4.46	-2.33
4460	C1[C@H]([C@@H]([C@H]1)C)C=O	C04429377	-12.98	-1.77	-11.68	4.81	-4.34
4461	CCOC(=O)C=C(C)C	C05324772	-12.98	-0.6	-12.41	3.83	-3.8
4462	Cc1ccc(cc1)[N+](=O)[O-]	C06276125	-12.98	-3	-11.95	5.04	-3.09
4463	c1cc(oc1)C=C[N+](=O)[O-]	C12370918	-12.98	-0.25	-17.08	8.32	-3.98
4464	Cn1cnnc1[N+](=O)[O-]	C13207526	-12.98	-2.6	-14.65	8.84	-4.57
4465	CCCc1nccc1	C00164546	-12.97	-0.9	-11.91	2.88	-3.04
4466	Cc1cnnc1C	C00967364	-12.97	-1.33	-13.98	4.5	-2.16
4467	c1cc(ccc1)C=C(C)O)O	C01529484	-12.97	-2.51	-15.32	4.78	0.08
4468	C=CCOC(=S)S	C01602466	-12.97	-0.74	-13.75	3.85	-2.32
4469	c1c(ncs1)CON	C01704689	-12.97	-2.73	-14.32	3.9	0.18
4470	C1CC=C(C1)C(=O)N	C01706729	-12.97	-1.6	-16.15	5.46	-0.68
4471	c1csc(=S)s1	C01845530	-12.97	-2.25	-13.26	5.77	-3.23
4472	CO[C@H]([C@@H]([C@H]1)C)C=C1	C02143306	-12.97	-0.94	-13.12	1.6	-0.51
4473	C=Cc1ccc(cc1)C#N	C02571926	-12.97	-1.25	-12.84	3.68	-2.56
4474	C1Cn2c(nnn2)N1	C03590965	-12.97	-3.81	-17.17	8.98	-0.98
4475	CCOC([C@H]([C(F)F)F)F)F)F)F	C04266049	-12.97	-0.82	-11.37	2.51	-3.29
4476	COC(=O)[C@H]([C@@H]([C(F)F)F)O	C04269247	-12.97	-1.86	-14.22	3.85	-0.74
4477	C1CCC(=O)C=CC1	C04528558	-12.97	-1	-12.61	3.85	-3.21
4478	C1=CC2C=CC=C2CN2C=C1	C05282709	-12.97	-1.57	-9.46	2.67	-4.61
4479	Cc1cnoc1C	C05783285	-12.97	-1.34	-13.54	3.78	-1.86
4480	CC(=O)NNC(=S)N	C06602474	-12.97	-0.98	-17.33	5	0.34
4481	C1CO[C@H]1Cl	C14983076	-12.97	-0.47	-11.74	1.77	-2.53
4482	Cc1c(ccc(c1F)N)N	C16677972	-12.97	-4.42	-10.91	3.13	-0.77
4483	c1cm(cn1)CCC=O	C28628432	-12.97	-2.25	-16.58	9.15	-3.29
4484	C1COC=C1C(=O)C(F)F)Cl	C32628531	-12.97	-1.44	-12.3	3.34	-2.56
4485	c1cc(sc1)C(=O)CC#N	C00047508	-12.96	0.74	-19.71	9.47	-3.46
4486	Cc1csc(n1)CC#N	C00164976	-12.96	-1.45	-15.98	7.17	-2.71
4487	CCCOC(C)C#N	C01641037	-12.96	-1.4	-12.97	4.08	-2.66
4488	c1ccc(cc1)CC(C=O)Cl	C01641183	-12.96	-1.94	-12.95	3.12	-1.19
4489	c1ccn2cnnc2c1	C01695118	-12.96	-3.12	-18	9.89	-1.72
4490	Cc1c(c(ncn1)N)N	C01711127	-12.96	-2.24	-15.56	5.01	-0.18
4491	C/C=C/Sc1cccc1	C01721964	-12.96	0.38	-14.43	2.22	-1.13
4492	CC(=C)CC(=O)C	C02038441	-12.96	-1.27	-11.89	3.06	-2.85
4493	C#CCN=C=S	C02528120	-12.96	-1.51	-12.21	2.55	-1.79
4494	c1(c(c(nnc1N)N)N)N	C04342670	-12.96	-6.32	-18.62	7.31	4.67
4495	Cc1[nH]c2nnc(n2n1)N	C05721316	-12.96	-4.65	-16.35	12.45	-4.4
4496	c1cc(nnc1F)F	C06093471	-12.96	-1.41	-15.49	5.54	-1.6

4497	#CCn1cnc(n1)l	C08295369	-12.96	-3.3	-12.74	7.4	-4.31
4498	c1cc(cnc1)/C=C/2/C(=O)NC(=O)N2	C12934220	-12.96	1.21	-21.3	7.33	-0.2
4499	CCCC/C=C/C=O	C13544962	-12.96	-0.95	-12.52	4.12	-3.61
4500	C=CCNC(=S)S	C13562440	-12.96	-1.96	-15.04	6	-1.96
4501	c1c(c(ncn1)Cl)l	C21299825	-12.96	-1.2	-11.17	2.38	-2.96
4502	c1c(cnc(c1F)N)C(F)F	C21304412	-12.96	-2.53	-11.91	3.28	-1.81
4503	CCn1cncn1	C21985098	-12.96	-1.39	-13.99	5.81	-3.39
4504	c1c(cc(nc1F)F)C#N	C21985261	-12.96	-0.21	-14.75	4.07	-2.07
4505	c1cc(ncc1)[N+](=O)[O-]CCl	C21985582	-12.96	-3.27	-11.54	5.4	-3.55
4506	c1c(csc1/C=C/N)OCl	C00140134	-12.95	-3.91	-13.16	3.3	0.82
4507	C[C@H](c1c(ccc1F)F)O	C00403102	-12.95	-0.11	-14.89	4.17	-2.12
4508	CC(=O)SCC	C01606268	-12.95	0.01	-12.36	2.47	-3.07
4509	CC1csnn1	C01611441	-12.95	-1.25	-15.41	4.9	-1.19
4510	CC1=CC(=O)NC1=O	C01676456	-12.95	-1.75	-17.33	5.17	0.96
4511	CC(=C)CCl	C01683469	-12.95	-0.68	-10.53	1.13	-2.86
4512	c1cc(nc(c1)Br)F	C02384085	-12.95	-1	-16.61	4.74	-0.08
4513	C(CBr)/C(=N/O)N	C02547087	-12.95	-2.32	-15.16	4.18	0.35
4514	CCO[C@H]1[C@H](C=C)O1C	C04897479	-12.95	0.2	-12.1	2.26	-3.32
4515	c1cc(c(cc1)S)O	C05133255	-12.95	-2.75	-15.67	4.78	0.7
4516	C=C(CNC(=S)N)Br	C05600792	-12.95	-1.67	-17.67	3.12	3.27
4517	Cc1ccc(c(=O)[nH]1)Br	C08698092	-12.95	-1.83	-15.51	4.42	-0.02
4518	c1cc(sc1CO)Cl	C08727655	-12.95	-2.56	-12.79	3.34	-0.94
4519	c1c(ncc(n1)Br)O	C12356940	-12.95	-2.05	-16.89	4.08	1.91
4520	c1cc(=O)[nH]cc1C#N	C12471683	-12.95	-2.87	-18.53	9.8	-1.35
4521	CC(C)/C=C/C=O	C17284647	-12.95	-0.66	-13.41	3.9	-2.78
4522	c1c(c(cnc1Cl)N)N	C19800990	-12.95	-6.1	-14.53	6.93	0.76
4523	C1COC(=CO1)C[NH3+]	C32629230	-12.95	-1.96	-15.94	4.15	0.81
4524	c1c(c(cc(c1O)N)O)N	C00156887	-12.94	-3.89	-17.45	4.39	4.01
4525	c1scs(c1N)C(=O)N	C00159923	-12.94	-4.64	-15.5	5.91	1.29
4526	c1(c([nH]c(=O)[nH]c1=O)N)Br	C00967243	-12.94	-5	-18.52	9.09	1.49
4527	Cc1c(nc([nH]1)C	C00967285	-12.94	-2.25	-13.32	5.18	-2.55
4528	C=CC(=O)OCCBr	C01561510	-12.94	0.41	-14.52	4.55	-3.38
4529	CSCCSC	C01690291	-12.94	0.96	-11.98	1.59	-3.5
4530	c1ccc(cc1)NCCF	C01724315	-12.94	-0.98	-14.17	2.57	-0.35
4531	c1c(ncs1)C(=O)N	C02046868	-12.94	-4.14	-17.13	6.17	2.17
4532	COC(=O)N=C=O	C02384736	-12.94	-1.6	-14.63	2.71	0.59
4533	Cn1ccc(n1)N	C02565745	-12.94	-2.31	-15.4	5.44	-0.66
4534	c1cc(=O)[nH]cc1C(F)Cl	C03181206	-12.94	-1.07	-15.92	6.12	-2.08
4535	c1csc(n1)C(=O)Cl	C04277255	-12.94	1.22	-18.33	5.69	-1.52
4536	[C@](C(F)(F)Cl)(OC(F)(F)F)F)Cl	C04329298	-12.94	-0.21	-10.57	0.15	-2.32
4537	C=C(C([NH+]=C(N)[S-])Cl	C05600793	-12.94	-1.98	-16.88	3.19	2.72
4538	C/C(=N/O)C(=O)C	C12358749	-12.94	-3.48	-14.59	4.95	0.17
4539	Cc1c(scc1N)C	C14000036	-12.94	-1.98	-11.4	2.53	-2.09
4540	Cn1cncn1	C16977393	-12.94	-3.63	-16	9.62	-2.94
4541	c1cc(ccc1[N+](=O)[O-])ON	C20159946	-12.94	-1.17	-15.18	5.42	-2.01
4542	C=Cn1cc(cn1)l	C29865927	-12.94	-0.86	-12.4	3.75	-3.43
4543	CC(=O)c1cccc1F	C00157320	-12.93	1.2	-18.04	7.66	-3.75
4544	c1cc(nc(c1)F)F	C00388533	-12.93	-1.68	-15.01	5.62	-1.85
4545	Cn1c(c(cn1)Br)N	C01027574	-12.93	-3.7	-12.06	4.26	-1.43
4546	CCO/C=C/C#N	C01641626	-12.93	-0.36	-14.63	4.21	-2.15
4547	Cc1ccc(cc1)[n+][2cc(on2)][O-]	C01668375	-12.93	-1.32	-14.56	7.96	-5
4548	CC/C=C(C)C=O	C01699996	-12.93	-1.12	-14.45	4.28	-1.63
4549	CCOc1ccc(c(c1)F)N	C02382631	-12.93	-2.56	-11.74	3.42	-2.06
4550	c1cc2c(ccc2)cc1C#N	C02548356	-12.93	-2.23	-11.75	4.92	-3.87
4551	Cc1cc(ns1)[O-]	C03128500	-12.93	-3.13	-15.81	4.72	1.28
4552	C(#N)c1c(non1)C#N	C04343214	-12.93	-1.17	-12.62	2.34	-1.49
4553	CCn1nc(nn1)N	C06226239	-12.93	-1.92	-14.73	5.27	-1.55
4554	COC(=O)c1ccc(nn1)[O-]	C07996961	-12.93	-1.42	-16.61	5.57	-0.47
4555	c1c(cc(c(c1F)O)F)Cl	C12359198	-12.93	-0.82	-14.25	2.5	-0.37
4556	Cc1cc(on1)C=O	C12370185	-12.93	-1.57	-14.38	4.79	-1.78
4557	c1cc(ncc1)CO	C14455323	-12.93	-1.92	-17.71	4.6	2.1
4558	c1c(nc(s1)Cl)CCl	C15444540	-12.93	-1.99	-12.03	3.7	-2.61
4559	C#C/C=C/CO	C17299191	-12.93	-3.01	-12.81	3.24	-0.34
4560	c1cnc(cc1C#N)Cl	C00154100	-12.92	-2.05	-12.7	4.38	-2.55
4561	CC(=O)c1ccc(nc1)Cl	C00161835	-12.92	-1.52	-13.74	4.94	-2.59
4562	Cc1cncn1C	C00404377	-12.92	-1.17	-14.03	3.96	-1.68
4563	CC(=O)OCC1=C(C=O)C=O	C01568569	-12.92	-0.42	-20.29	9.46	-1.67
4564	c1cnc(c1)N=C=S	C01737031	-12.92	-2.39	-14.97	4.29	0.15
4565	C1CC(=CC(=O)C1)[O-]	C03860300	-12.92	-3.84	-15.18	6.9	-0.8
4566	CC1=CC(=O)NON1	C04499552	-12.92	-3.08	-17.69	7.4	0.45
4567	Cc1cc(n2c(n1)nn2)[O-]	C13154290	-12.92	-1.92	-15.28	6.06	-1.78
4568	c1cc(ccc1O)OC(F)F	C00162805	-12.91	-0.3	-14.8	2.79	-0.6
4569	CSc1[nH]ccn1	C01671795	-12.91	-2.4	-15.5	4.46	0.54
4570	C=CCN(C(=O)O)OCC=C	C01716734	-12.91	1.02	-16.79	5.07	-2.2
4571	c1cc(c(cc1N)CC#N)F	C02243245	-12.91	-1.24	-15.83	6.8	-2.63
4572	c1cc(cc(c1)O)CC#N	C02507096	-12.91	-1.97	-17.69	7.38	-0.63
4573	c1cc2c(c(c1)F)C@H(C2)O	C03847714	-12.91	-0.65	-14.46	4.02	-1.83
4574	CC(=O)CC(=O)C(=O)O	C03882590	-12.91	-4.27	-10.94	4.29	-1.98
4575	c1cc(c(c(c1O)N)[N+](=O)[O-]	C04272219	-12.91	-3.75	-14.76	5.89	-0.29
4576	c1c2c(nc[nH]2)nc(n1)[S-]	C12955987	-12.91	-0.13	-17.95	7.25	-2.08
4577	Cc1[n-]c2cnc2n1	C13216414	-12.91	-4.03	-13.98	6.88	-1.78
4578	Cc1cn2ccsc2n1	C15980479	-12.91	-1.48	-14.76	7.05	-3.72
4579	c1cc2c(cc1F)nc2	C16159802	-12.91	-2.35	-14.95	5.44	-1.04
4580	c1nc([nH]n1)N	C16889962	-12.91	-4.42	-13.7	6.78	-1.57
4581	c1(c([nH]c(=S)nn1)[O-])C(=O)NN	C17380711	-12.91	-5.46	-17.01	5.73	3.83
4582	c1cc(cnc1)OCC(F)F	C20282571	-12.91	-3.34	-11.26	4.41	-2.72
4583	Cc1ccc(o1)C@H(C2CO	C22176510	-12.91	-1.77	-15.3	6	-1.84
4584	c1cc(sc1)CC(=O)NN	C00262467	-12.9	-4.87	-15.64	8.36	-0.74
4585	c1c(sc(n1)Cl)C=O	C01392611	-12.9	-3.03	-12.78	4.52	-1.62
4586	c1c[nH]c2c1SCC2=O	C01601586	-12.9	-1.87	-15.04	6.21	-2.21

4587	CC(=O)SC	C02004049	-12.9	-1.03	-12.82	2.73	-1.77
4588	CCOC(=O)[C@@H](C(F)(F)F)F	C02525720	-12.9	-0.85	-12.71	3.97	-3.31
4589	C[C@@H](C(=O)C(F)(F)F)Br	C04329275	-12.9	1.16	-13.62	2.37	-2.81
4590	c1cc2c([nH]c2nc1)Br	C05763894	-12.9	-4.64	-10.77	5.77	-3.26
4591	C/C=C(Br)/CO	C12416533	-12.9	-3.21	-13.57	2.69	1.19
4592	C(#N)c1c([n]-[n]1)N	C19414036	-12.9	-4.62	-15.63	6.38	0.98
4593	c1ccc2c(c1)NCN2	C22000610	-12.9	-2.3	-12.85	3.83	-1.58
4594	Cc1ccc(cn1)CC#N	C32628157	-12.9	-1.86	-15.28	7.72	-3.47
4595	Cn1ccc(n1)C(F)(F)F	C00160136	-12.89	-3.1	-12.81	5.56	-2.54
4596	c1c(cc(cc1F)F)CO	C00164758	-12.89	-2.82	-12.17	3.43	-1.32
4597	c1cc(c(c(c1F)CO)F)F	C00396155	-12.89	-3.1	-12.77	4.41	-1.44
4598	C=CCSCC=C	C01531083	-12.89	-0.05	-12.72	1.41	-1.53
4599	c1cc(ccc1CCCl)N	C01674982	-12.89	-1.77	-13.78	2.15	0.51
4600	CC1=NCSC1	C02038687	-12.89	-1.14	-13.66	2.9	-0.99
4601	c1cnc(c(n1)Cl)Cl	C02168474	-12.89	-1.64	-14.21	4.37	-1.42
4602	c1cc(c(cc1O)F)Br	C02510139	-12.89	1.01	-17.83	3.27	0.67
4603	CCCCN=C=O	C02516945	-12.89	-0.99	-13.61	1.73	-0.02
4604	CO/C=C/C(F)(F)F	C02525274	-12.89	-1.25	-11.85	2.18	-1.97
4605	Cc1cnn(c1)CC#N	C02537501	-12.89	-2.77	-16.56	9.29	-2.85
4606	C/N=C/[C@H]([N+](=O)[O-])\SC	C04002668	-12.89	0.46	-15.69	3.88	-1.54
4607	CN(C(=O)N)N=O	C04202501	-12.89	-2.78	-15.49	3.54	1.84
4608	CC[C@@]1(C(=O)O1)Br	C05104211	-12.89	-0.66	-11.81	1.89	-2.31
4609	C[C@H]([N+](=O)[O-])Cl	C05735423	-12.89	-0.7	-13.06	3.15	-2.28
4610	CC[C@H](C)N(N=O)O	C05758836	-12.89	-1.19	-14.1	2.96	-0.55
4611	c1[nH]c(=O)c(c(n1)N)[N+](=O)[O-]	C08764094	-12.89	-1.27	-18.7	5.63	1.44
4612	CN/C(=N/[N+](=O)[O-])/N	C20220203	-12.89	-4.93	-16.47	9.57	-1.06
4613	c1cc(c(c1F)C#N)F	C00164372	-12.88	2.03	-17.97	6.7	-3.64
4614	c1c(nns1)C(=O)NN	C01605005	-12.88	-3.93	-16.45	5.86	1.64
4615	c1nc2c(ncnc2nn1)N	C01667963	-12.88	-3.1	-15.71	7.24	-1.31
4616	C=C[C@H](CBr)O	C01997857	-12.88	-0.61	-13.49	2.16	-0.94
4617	c1cc(ccc1)OCC#N	C02023211	-12.88	-1.32	-15.27	6.35	-2.63
4618	c1cc(ccc1N)OCCO	C02030291	-12.88	-2.89	-15.95	5.38	0.58
4619	c1cccc1C=C(C#N)C#N	C02381297	-12.88	2.14	-20.16	8.85	-3.71
4620	c1cc(c(cc1F)OC(F)F)N	C02537714	-12.88	-1.31	-15.99	5.27	-0.86
4621	Cc1nc([nH]n1)N	C02566399	-12.88	-5.46	-13.92	7.97	-1.46
4622	Cc1c(cnn1C)N	C02578432	-12.88	-2.28	-14.51	4.54	-0.62
4623	Cc1ccc(cc1O)O	C04530928	-12.88	-1.01	-16.38	4.1	0.4
4624	C(c1[nH]c(=O)[nH]n1)S	C12558729	-12.88	-3.09	-17.34	7.36	0.19
4625	Cc1nc([nH]n1)NC(=O)C	C15081339	-12.88	-7.76	-10.49	7.49	-2.11
4626	CC(=O)/C=C/N	C17823645	-12.88	-2.96	-13.75	4.44	-0.61
4627	c1cc(c(c1n)F)Cl	C19615464	-12.88	-2.26	-14.94	4.48	-0.16
4628	CC1=C(C(=O)CO1)O	C00404230	-12.87	-2.72	-16.29	5.46	0.68
4629	c1c2c(=O)[nH]c(nc2ncn1)[O-]	C00525630	-12.87	-3.34	-14.84	5.26	0.06
4630	Cc1c(c([n]-[n]1)Cl)[N+](=O)[O-]	C01225148	-12.87	-3.48	-13.87	6.49	-2
4631	CC(C)C(=O)c1ccc(c1)[N+](=O)[O-]	C01583727	-12.87	-0.93	-12.08	4.14	-4
4632	c1c(cnc(c1F)Cl)Br	C02524878	-12.87	-0.79	-13.83	1.81	-0.05
4633	c1cc(c(c1)N)F	C03880145	-12.87	-2.62	-12.64	1.85	0.54
4634	CC[C@H](C#CC(F)F)O	C05468414	-12.87	0.17	-13.72	2.23	-1.56
4635	Cc1c(cco1)N=C=O	C12370513	-12.87	-1.45	-13.35	2.95	-1.02
4636	c1cc(c(nc1C=O)N)[N+](=O)[O-]	C21985817	-12.87	-5.44	-11.41	5.42	-1.44
4637	c1c(ncnc1)N	C25494510	-12.87	-0.24	-15.68	4.76	-1.72
4638	CCOc1cc(ncn1)Cl	C00730496	-12.86	-1.15	-13.2	2.76	-1.27
4639	CC(=O)On1cc(c(=O)[nH]c1=O)F	C01083182	-12.86	-2.19	-17.73	9.64	-2.58
4640	[C@@H]1(C(=O)NC(=O)S1)Br	C01399352	-12.86	1.54	-17.93	3.46	0.07
4641	COC(=O)c1ccncc1N	C01403568	-12.86	-4.03	-11.68	4.03	-1.18
4642	C/C=C/c1ccccn1	C01457684	-12.86	-0.5	-11.82	3.31	-3.85
4643	c1cscn1	C01484626	-12.86	-1.51	-13.21	3.08	-1.21
4644	CCSc1nc([nH]n1)N	C01939756	-12.86	-3.98	-15.29	8.85	-2.43
4645	CCCCCC[N+](=O)[O-]	C02031533	-12.86	-0.08	-11.96	3.38	-4.19
4646	C(C(=O)C(F)F)Br	C02579119	-12.86	-0.26	-13.47	3.26	-2.4
4647	C[C@H](COC)N=C=S	C03276934	-12.86	-0.23	-14.14	2.83	-1.32
4648	C=CC[C@H](C(F)F)O	C08698315	-12.86	-1.17	-12.43	1.91	-1.18
4649	Cn1cnc1/C=N/O	C13957014	-12.86	-3.51	-15.25	6.89	-0.98
4650	C(C(F)F)OC(F)F	C14611418	-12.86	-0.01	-13.32	2.16	-1.7
4651	[H]N=C(\C)/SCC	C16022350	-12.86	-0.72	-12.08	1.79	-1.85
4652	Cc1cnc(=O)[nH]1	C16953338	-12.86	-2.89	-17.59	7.78	-0.15
4653	c1c(c(=O)nc([nH]1)N)[N+](=O)[O-]	C17003686	-12.86	-2.04	-17.17	5.87	0.49
4654	c1c(c(=O)[nH]cn1)O	C17378546	-12.86	-4.31	-16.31	4.99	2.77
4655	C1C=C[C@H]2[C@H]1CC2=O	C19230142	-12.86	-0.69	-12.8	3.91	-3.27
4656	[C@H-](C(=NH2+)N)C(F)(F)F	C19482198	-12.86	-6.54	-13.79	7.76	-0.28
4657	c1cc(ncn1)[N+](=O)[O-]CBr	C21985583	-12.86	-3.2	-11.19	5.19	-3.65
4658	c1ccn(c1)C(=O)Cl	C01557054	-12.85	-2.09	-12.93	4.65	-2.47
4659	COC(=O)C=C	C01608901	-12.85	-1.2	-13.75	4.09	-2
4660	C#CCSCCO	C01708308	-12.85	-2.18	-12.98	3.35	-1.05
4661	CSCCCN=C=S	C01850039	-12.85	-0.81	-15.57	2.57	0.97
4662	C=CCOC(=O)CC#N	C02019683	-12.85	-3.05	-15.59	8.88	-3.09
4663	c1c(ncn1C(F)F)[N+](=O)[O-]	C05268974	-12.85	-2.18	-16.72	10.34	-4.29
4664	c1c([nH]nc1)NC=O	C05386258	-12.85	-2.93	-17.99	8.39	-0.32
4665	Cc1cncnc1[N+](=O)[O-]	C08294978	-12.85	-2.78	-12.34	5.14	-2.87
4666	c1ccc2c(c1)[nH]c(=O)O2	C08801890	-12.85	-3.33	-15.83	7.9	-1.59
4667	c1cc(=O)[nH]cc1N	C11757519	-12.85	-3.22	-17.64	5.28	2.72
4668	c1cc(c(c1)Br)N	C15021415	-12.85	-3.45	-11.03	2.49	-0.86
4669	c1cc(ncc1[N+](=O)[O-])CS	C21985585	-12.85	-3.17	-11.72	5.3	-3.26
4670	Cc1cnc(c1)CCl	C22016720	-12.85	-1.58	-12.75	4.36	-2.88
4671	C1[C@H]([N-]1)C(=O)Cl	C32016248	-12.85	1.77	-17.06	3.08	-0.65
4672	CCcn1c(ccn1)N	C00801646	-12.84	-2.26	-12.83	4.47	-2.23
4673	Cn1cnc1C=O	C01069169	-12.84	-3.29	-12.89	5.34	-1.99
4674	Cc1ccc(cc1)OCC=C	C01615713	-12.84	-1.52	-12.27	2.52	-1.57
4675	C/C=C/c1ccc(cc1)O	C01696959	-12.84	-0.57	-15.1	2.87	-0.04
4676	COCOC(=O)Cl	C01845909	-12.84	1.6	-16.1	3.22	-1.56

4677	c1ccc(c(c1)N)SC(F)F	C03440473	-12.84	-0.66	-15.72	3.68	-0.14
4678	c1c(c(n[nH]1)C(F)F)Br	C04243643	-12.84	-0.84	-14.38	2.45	-0.06
4679	COC(=O)Nc1cnccc1	C05141052	-12.84	-0.67	-17.51	6.04	-0.7
4680	Cc1c(=O)[nH]nnc1	C05285765	-12.84	-0.63	-17.97	4.29	1.46
4681	CC[C@H](C(F)F)O	C08698395	-12.84	-1.89	-12.19	1.92	-0.68
4682	CSc1ncc(cn1)C=N/O	C13957177	-12.84	-0.31	-18.65	7.02	-0.89
4683	c1ccc(c1)NCCS	C17325846	-12.84	-1.63	-9.87	2.06	-3.4
4684	CCc1ccc(nc1)C	C00967331	-12.83	-1.17	-11.12	3	-3.54
4685	c1ccc(cc1)C2=N[C@H]2C=O	C01557438	-12.83	2.15	-17.82	4.33	-1.5
4686	CCCSC(=O)C	C01850875	-12.83	-0.99	-11.48	2.65	-3
4687	C1C(=O)C=C(S1)C(F)F	C02559552	-12.83	-0.13	-13	3.16	-2.87
4688	c1c(oc1[O-])CCl	C03131391	-12.83	-2.94	-16.24	5.6	0.75
4689	c1c(nns1)/C=N/O	C04265462	-12.83	-4	-18.26	8.4	1.03
4690	C(=C/(C(=O)C(F)F)C(F)F)\O	C04579483	-12.83	-4.1	-15.34	7.85	-1.24
4691	COC(=O)CCC(=O)C=[N+]=[N-]	C04791964	-12.83	-2.09	-14.77	6.29	-2.26
4692	C(COCc1c(non1)N)N=[N+]=[N-]	C05368997	-12.83	-3.94	-17.36	6.42	2.05
4693	c1([nH]nc1)C1N	C05567036	-12.83	-3.02	-16.33	3.88	2.64
4694	c1cc(c(c2c1non2)[O-])O	C06224229	-12.83	-3.31	-16.01	5.49	1
4695	Cc1nc(cnn1)N=[N+]=[N-]	C08383094	-12.83	-1.33	-15.31	3.65	0.17
4696	c1csc(c1)Br	C12959127	-12.83	-0.15	-11.3	2.08	-3.46
4697	Cc1ccc(cn1)I	C14983205	-12.83	-0.26	-11.54	2.39	-3.43
4698	C=CCNc1nccs1	C19737071	-12.83	-0.62	-13.58	3.99	-2.61
4699	CC/C=C(\C)/[N+](=O)[O-]	C21304258	-12.83	-1.04	-12.8	4.75	-3.74
4700	Cc1ccc(s1)CN=C=O	C22861884	-12.83	-1.29	-13.24	3.35	-1.66
4701	CC(O)c1cc(n[nH]1)C(F)F	C26547624	-12.83	-4.09	-10.64	4.87	-2.97
4702	CCOCc1c[nH]nc1N	C30677777	-12.83	-3.12	-15.48	6.27	-0.5
4703	CSc1ncc(s1)N	C32914948	-12.83	-0.72	-16.89	5.44	-0.67
4704	Cc1c(c(n[nH]1)C)N	C00039481	-12.82	-2.06	-14.86	4.29	-0.18
4705	CC(=O)C=C(N)SC	C00273377	-12.82	-3.9	-14.47	6.99	-1.44
4706	CCOC(=O)c1c(non1)N	C01052721	-12.82	-2.1	-12.22	3.03	-1.54
4707	C=C(C#N)C(F)F	C01755904	-12.82	-3.09	-12.68	5.44	-2.49
4708	c1cncc1N	C02168333	-12.82	-2.93	-13.95	4.7	-0.64
4709	c1cncc(c1C=O)O	C02244273	-12.82	-3.72	-15.58	5.69	0.79
4710	c1ccc(nc1)COF	C02384040	-12.82	-2.02	-17.53	5.48	1.25
4711	Cc1ccc(o1)C(=O)Cl	C02521277	-12.82	-1.92	-11.93	3.9	-2.87
4712	C(/C=C/C(F)F)Br	C02526364	-12.82	-2.04	-13.1	3.07	-0.75
4713	c1c(cn(n1)CC#N)[N+](=O)[O-]	C02537510	-12.82	-3.89	-18.96	12.88	-2.85
4714	c1cc(c(c1C#N)F)O	C02562249	-12.82	-1.11	-17.36	7.16	-1.51
4715	CCOC(=O)SC(=[NH2+])N	C04642969	-12.82	-2.73	-16.48	5.23	1.17
4716	c1nc(c(n1)C(=O)NO)N	C04809156	-12.82	-5.17	-19.31	8.28	3.39
4717	CCOC/C=C\COC	C05808185	-12.82	-1.34	-12.84	2.45	-1.09
4718	COC(=O)CC(=O)C(F)F	C05996866	-12.82	1.79	-16.49	6.48	-4.6
4719	c1ccc(cc1)N2NC(=O)SN2	C06475547	-12.82	-3.02	-11.91	4.02	-1.92
4720	c1cc(c(nc1)CO)F	C12370202	-12.82	-0.24	-17.94	5.39	-0.03
4721	COCCn1cc[nH+]c1	C14608646	-12.82	-2.07	-12.6	4.63	-2.78
4722	c1nc([nH]n1)SCC#N	C19847558	-12.82	-3.12	-15.24	8.79	-3.25
4723	c1cncc(c1)C(=O)NN	C00010573	-12.81	-3.24	-16.7	6.85	0.29
4724	c1cc(oc1)C(=O)CC#N	C00157314	-12.81	0.87	-20.18	9.28	-2.78
4725	Cc1ccc(c(c1F)F)O	C02382373	-12.81	-1.9	-15.42	5.17	-0.66
4726	c1c(sc1)Br)C=O	C02510761	-12.81	-3.21	-12.41	4.52	-1.71
4727	CC(=O)CCCCl	C02556912	-12.81	-0.63	-12.68	4.23	-3.73
4728	c1ccc(sc1C(=O)N)Br	C02750706	-12.81	-2.69	-13.84	4.45	-0.73
4729	C(SC(F)F)FCI	C04531691	-12.81	-1.36	-11.84	2.03	-1.64
4730	CO/C(=N)/[NH+](=O)[O-]/[NH-]	C04901330	-12.81	-2.12	-17.19	4.34	2.16
4731	c1[nH]c(c(n1)C#N)N	C08628646	-12.81	-5.71	-15.19	9.21	-1.12
4732	CCNc1nc(nn1)N	C09601303	-12.81	-3.49	-12.34	4.94	-1.92
4733	CC(=O)c1cnsc1	C12650585	-12.81	-2.45	-14.31	5.7	-1.76
4734	Cc1c(=O)[nH]ccn1	C14491607	-12.81	-4.3	-16.94	8.66	-0.23
4735	c1ccc([nH]c(=O)c1)N	C14982071	-12.81	-3.43	-16.62	5.15	2.09
4736	COC1=C(C(C1(F)F)F)OC	C16082663	-12.81	-2.75	-10.43	2.5	-2.14
4737	C1C(=NNC(=O)S1)CCl	C20216358	-12.81	-1.92	-18.51	8.59	-0.96
4738	c1cc(c(oc1N)F)Sc2[nH]ncn2	C20474968	-12.81	-1.77	-16.23	8.01	-2.83
4739	Cc1nc(c(s1)CCl	C22861726	-12.81	-1.27	-12.22	3.66	-2.98
4740	CCC1=C(C(=O)CC1)O	C25695693	-12.81	-1.83	-15.05	5.39	-1.33
4741	c1cc(sc1)C(=S)N	C00166060	-12.8	-1.94	-17.04	8.28	-2.1
4742	CCC(=O)C(C(F)F)F	C01675403	-12.8	-0.57	-11.72	2.46	-2.97
4743	CCOCCI	C02507815	-12.8	-1.16	-11.37	1.81	-2.09
4744	CNC(=O)N(C)N=O	C03793045	-12.8	-2.82	-14.46	3.75	0.73
4745	C(C(=O)Cl)Br	C04521278	-12.8	0.15	-14.18	3.14	-1.91
4746	CC[C@H](C)S	C04775629	-12.8	-0.18	-10.66	0.78	-2.73
4747	CC(=C)/C=N/O	C13508699	-12.8	-4.17	-12.75	4.43	-0.3
4748	C1C=CC[C@H]2[C@H]1O2	C17022497	-12.8	-0.93	-12.87	2.77	-1.77
4749	C1=C2C(=NC(=S)N=C2[O-])N=N1	C18151915	-12.8	-3.73	-15.36	6.58	-0.29
4750	Cc1[nH]cc(c1)C(=O)C	C22000856	-12.8	-4.49	-13.86	7.53	-1.99
4751	CC(C)C(=O)N=C=S	C22143666	-12.8	-0.74	-13.79	3.56	-1.83
4752	COc1ccc(cc1)C#N	C00159092	-12.79	-1.01	-13.02	4.26	-3.02
4753	c1cc(ccc1)C(=O)CCl	C01703019	-12.79	0.85	-18.14	8.72	-4.21
4754	CCOC(=O)C(F)F	C02040590	-12.79	-0.66	-14.04	4.48	-2.57
4755	c1cncc(c1C#N)Cl	C02547813	-12.79	-3.13	-11.3	4.24	-2.6
4756	c1c([nH]nc1)C(F)F	C02559437	-12.79	-2.62	-13.59	5.6	-2.08
4757	CC(=O)c1cc(oc1)[N+](=O)[O-]	C04180505	-12.79	0.06	-14.02	2.94	-1.77
4758	CN(C(=O)C)OC	C04291205	-12.79	-1.26	-13.98	3.46	-1.01
4759	c1ncn(n1)C[C@H]2CO2	C11919571	-12.79	-3.55	-14.22	7.24	-2.25
4760	COCC1CCCC1N	C13346815	-12.79	-1.04	-12.94	3.01	-1.82
4761	CCO/C=C\C	C16892512	-12.79	-0.55	-11.46	1.67	-2.46
4762	c1c2c(ncn1)nc([nH]2)CO	C17311339	-12.79	-4.37	-15.63	6.94	0.26
4763	CSc1[nH]c(=O)c(c1)N	C17315889	-12.79	-1.82	-17.13	6.04	0.13
4764	C(=C([NH+](=O)[O-])[N+](=O)[O-])(N)N	C19324383	-12.79	-6.24	-17.13	11.93	-1.36
4765	c1cc(oc1)c2cc(n[nH]2)C(F)F	C26547627	-12.79	0.62	-17.48	6.83	-2.77
4766	c1cc(oc1)CC[N+](=O)[O-]	C01733890	-12.78	-0.27	-13.58	4.44	-3.38

4767	c1cc(ccc1[C@@H]2CO2)Cl	C02571277	-12.78	-2.36	-14.26	3.48	0.36
4768	C=CCN1C(=O)C(=O)NC1=O	C02647845	-12.78	-0.81	-16.43	4.51	-0.06
4769	C=C(c1cccnc1)NNC=O	C03250374	-12.78	1.16	-19.96	7.17	-1.15
4770	c1ccc(cc1)C(=O)C=[N+]=[N-]	C04536622	-12.78	1.76	-19.39	6.45	-1.6
4771	c1ccc(cc1)C2=NCOC2=O	C04726942	-12.78	-1.32	-20.38	5.57	3.34
4772	C1(C(OC1(F)F)F)F	C05187447	-12.78	0.01	-10.83	0.38	-2.35
4773	c1ccn2c(c1)nc2N	C05386220	-12.78	-2.9	-13.96	6.84	-2.77
4774	c1ccc(c(c1)NCCO)F	C13517039	-12.78	-3.21	-13.38	4.35	-0.54
4775	c1cc2c(c(c1)F)c(n[nH]2)O	C14983441	-12.78	-5.77	-14.73	6.67	1.05
4776	C/C=C(Cl)O	C16343299	-12.78	-2.68	-12.33	2.18	0.05
4777	C/C=N/CC(F)F	C19795290	-12.78	-2.35	-12.42	3.4	-1.41
4778	c1cc(c(cc1C=O)N)F	C21981687	-12.78	-3.95	-13.07	5.85	-1.61
4779	CCc1cc(ncn1)Cl	C26420701	-12.78	-1.73	-10.87	3.14	-3.33
4780	CCc1c(c[nH]n1)N	C26545509	-12.78	-2.21	-15.86	5.51	-0.22
4781	c1cc(cc1)C2=CC(=O)CC2	C32005602	-12.78	0.7	-15.51	5.79	-3.76
4782	Cn1c(cc(=O)[nH]c1=O)N	C00154763	-12.77	-5.97	-17.4	9.96	0.63
4783	Cc1cccnc1Cl	C00403383	-12.77	-0.63	-13	3.74	-2.87
4784	CCC[C@H](C=C)O	C01575584	-12.77	-0.32	-12.63	1.44	-1.26
4785	c1cc(oc1)/C=C/C=O	C01577145	-12.77	-2.87	-14.88	7.79	-2.81
4786	CCn1c(=O)cn[nH]c1=O	C01757767	-12.77	0.74	-18.52	5.23	-0.22
4787	Cc1ccc(cc1)SOC	C01849780	-12.77	-1.45	-14.85	3.32	0.21
4788	CC(=O)c1ccsc1	C02573578	-12.77	-1.72	-13.07	5.64	-3.63
4789	CCOC(=O)CSC(F)F	C02646155	-12.77	-0.62	-12.85	4.28	-3.58
4790	c1c(c(c(n1)Cl)Cl)[O-]	C03014162	-12.77	-1.54	-15.47	5.55	-1.31
4791	c1(c(c(c(c1F)F)F)F)N=O	C03847087	-12.77	-0.51	-10.22	1.04	-3.09
4792	c1c[nH]c(=O)cc1C=O	C04202749	-12.77	-4.83	-15.57	8.52	-0.9
4793	CC(=Nn1cnnc1)C	C05225643	-12.77	-2.39	-14.55	7.95	-3.78
4794	CN1C(=O)C(=O)N(C1=O)C	C05965946	-12.77	-0.4	-16.78	4.76	-0.35
4795	CCn1cc(n1)[N+](=O)[O-]	C15782786	-12.77	-3.43	-14.8	10.42	-4.95
4796	c1ann2n1NC(=O)CC2	C18558879	-12.77	-2.51	-15.23	6.05	-1.08
4797	Cn1ccc(n1)N	C19088827	-12.77	-3.42	-15.02	5.18	0.49
4798	c1ccnc(c1)CCC=O	C19682804	-12.77	-3.72	-11.95	5.96	-3.06
4799	C1CC(=CC(=O)C1)Cl	C20160223	-12.77	-0.3	-13.88	4.57	-3.16
4800	C/C=C/CSC	C20231229	-12.77	-0.74	-10.03	1.48	-3.48
4801	CNC(=O)c1ccccc1	C20282841	-12.77	-2.56	-16.14	6.8	-0.87
4802	c1c(c[nH]c(=O)c1N)Cl	C21981960	-12.77	-3.59	-19.26	9.23	0.85
4803	CC(=O)C(=O)N(C)OC	C21986919	-12.77	-1.4	-13.44	4.14	-2.08
4804	c1ccc(cc1)C(=S)N	C00049654	-12.76	-1.37	-17.67	9.12	-2.85
4805	Cc1[nH]c2cccc2n1	C00164607	-12.76	-3.07	-12.97	6.42	-3.14
4806	COc1ccc(cc1)C#C	C00984394	-12.76	0.04	-12.64	3.5	-3.66
4807	c1c(sc(n1)Cl)CC#N	C01387125	-12.76	-2.49	-15.28	7.75	-2.74
4808	c12c([nH]c1=O)nc1ann2[O-]	C01666582	-12.76	-1.29	-19.41	6.32	1.61
4809	CC(=O)C1=CCCCC1	C03860149	-12.76	1.81	-14.54	3.8	-3.83
4810	C=C[C@]P@[H](=O)[O-]	C03958468	-12.76	-5.79	-13.34	6.97	-0.61
4811	c1(c(snn1)NN=O)C(=O)N	C05836055	-12.76	-2.22	-16.06	2.8	2.73
4812	C1CC(=C(C1)[O-])C(=O)C(F)F	C12394856	-12.76	-2.92	-13.15	5.99	-2.68
4813	c1ccc(cc1)SCN=[N+]=[N-]	C12956364	-12.76	-0.78	-13.05	2.59	-1.52
4814	Cc1cc(cnc1)CCl	C15021787	-12.76	-0.42	-12.11	3.34	-3.57
4815	c1nnc(s1)N	C17744119	-12.76	-4.62	-14.11	5.86	0.1
4816	COc(=O)c1c(cno1)Br	C26547711	-12.76	0.82	-14.18	3.1	-2.49
4817	c1ccc2c(c1)CCN2	C00967454	-12.75	-1.37	-10.8	2.34	-2.92
4818	CC(=O)CC(=C)C	C01631227	-12.75	-1.11	-13.02	3.04	-1.65
4819	COc(=O)CCC(=O)Cl	C01712453	-12.75	-0.98	-13.23	3.95	-2.49
4820	c1cc(c(cc1)F)CO	C02512516	-12.75	-1.13	-14.44	2.34	0.48
4821	CCOCCCl	C02522731	-12.75	-0.59	-11.65	2.24	-2.75
4822	Cc1c(non1)C(=O)C(=N[O-])/Br	C03164846	-12.75	-3.25	-12.73	3.45	-0.22
4823	CC(=O)NCC1CCCC1	C05260754	-12.75	-2.67	-15.91	7.13	-1.29
4824	c1c[nH]c(=O)c2c1sc2	C16972315	-12.75	-2.66	-15.25	5.2	-0.04
4825	C=CCCC(=O)Cl	C21997308	-12.75	-0.57	-11.78	3.23	-3.63
4826	Cc1ccc(c(c1)N)C(=O)N	C00153352	-12.74	-2.82	-15.31	5.32	0.06
4827	c1ccc(cc1)COC(=O)NN	C00403316	-12.74	0.07	-17.56	5.78	-1.04
4828	CC(=O)C=C	C01574309	-12.74	-0.83	-13.18	3.75	-2.48
4829	C(CBr)C(=O)N	C01664836	-12.74	-4.7	-13.08	4.79	0.25
4830	c1ccc(c1)CO	C02037862	-12.74	-1.76	-15.3	4.18	0.14
4831	CO[C@H]1CCC=C1	C02143305	-12.74	-0.32	-13.54	1.62	-0.51
4832	CC(=O)N=C=S	C02386803	-12.74	-1.28	-14.74	3.95	-0.67
4833	c1ccc(c(c1)NC(=O)C(=O)N)F	C03072950	-12.74	-1.86	-18.13	5.43	1.83
4834	c1cc(ncc1S)S	C03130114	-12.74	-1.86	-16.59	4.79	0.91
4835	CCn1ccc(n1)C	C09426710	-12.74	-1.06	-13.49	4.67	-2.86
4836	C/C(=NN)/c1ccco1	C17047406	-12.74	-2.96	-12.37	3.9	-1.31
4837	C(=N(O))(N)/C(=N(O)N	C18119586	-12.74	-6.49	-14.81	4.41	4.15
4838	c1cc2nncn2nc1N	C18555647	-12.74	-4.42	-16.19	9.83	-1.96
4839	c1ccn(c(=O)c1)CCBr	C19416026	-12.74	-1.6	-15.66	8.29	-3.77
4840	CCOC1ccnc(c1)F	C21982022	-12.74	-0.14	-14.58	4.22	-2.25
4841	C=CCN(CC=C)C=O	C00394527	-12.73	-0.12	-14.52	5.03	-3.13
4842	c1(c(nsc1)Cl)Cl)N	C01064136	-12.73	-3.05	-13.26	1.47	2.1
4843	CC(=O)OCC#C	C01845917	-12.73	0.05	-14.68	4.63	-2.73
4844	Cc1ccc(cc1)N=C=O	C01845938	-12.73	0.12	-13.69	1.95	-1.11
4845	C#CCOCC#C	C02029723	-12.73	-0.1	-14.62	4.49	-2.5
4846	CCc1cnc(n1)Cl	C02569912	-12.73	-1.95	-12.08	4.21	-2.91
4847	C(/C(=N)/N)(Cl)Cl	C04203874	-12.73	-3.02	-12.26	2.77	-0.22
4848	c1cc(cnc1)c2cc[nH]2	C09238272	-12.73	-0.84	-15.08	5.14	-1.95
4849	c1cc(ncc1C(=O)N)C#N	C15772047	-12.73	-3.27	-17.36	7.76	0.14
4850	COc(=O)Cn1ccnc1	C20362220	-12.73	-0.73	-17.33	9.17	-3.85
4851	c1cc(oc1)CO	C01648266	-12.72	-2.71	-14.68	4.61	0.06
4852	C=Nc1ccc(cc1)Cl	C01654174	-12.72	1.61	-17.11	3.56	-0.79
4853	C1C=C[C@H]2[C@@H]1C(=O)C2	C01669121	-12.72	-0.68	-12.57	3.74	-3.21
4854	CCOC(=O)C(=O)CBr	C01691048	-12.72	-0.12	-12.86	3.57	-3.32
4855	C=C1COCCO1	C01708305	-12.72	-0.33	-14.13	2.79	-1.05
4856	Cn1cncn1N	C03194504	-12.72	-4.39	-14.4	9.15	-3.08

4857	c1cc(ccc1N(N=O)O)Cl	C05046692	-12.72	-0.36	-14.4	2.48	-0.45
4858	CC(=O)c1cnc([nH]1)Cl	C12647654	-12.72	1.76	-17.98	5.3	-1.81
4859	[C@@H](C(F)(F)F)(OC(F)(F)Cl)Cl	C14628419	-12.72	0.09	-11.6	1.27	-2.47
4860	Cn1cnc1C=O	C00158990	-12.71	-2.86	-15.34	7.95	-2.46
4861	[H]/N=Nc1ccc(cc1)Br	C00409254	-12.71	-1.84	-13.97	1.87	1.23
4862	C1(=O)C(=O)NC(=O)N=C1[O-]	C01631379	-12.71	0.27	-19.93	5.69	1.26
4863	Cc1c(c[n1]C)N	C02388744	-12.71	-2.75	-13.94	4.7	-0.73
4864	c1cc(c(c1O)F)F)O	C02525459	-12.71	-4.14	-15.65	6.19	0.89
4865	Cc1c(=O)[nH]c(=O)[nH]c1F	C02559882	-12.71	-2.05	-16.37	5.11	0.6
4866	c1cnc(cc1)F	C02598036	-12.71	-1.28	-14.24	2.81	0.01
4867	c1(=O)c(n[nH]c(=O)[nH]1)SC(F)F	C03068995	-12.71	-0.33	-18.95	5.74	0.83
4868	c1cc(c(c1)F)N=O)F	C04576633	-12.71	-2.82	-15.2	6.76	-1.45
4869	Cc1ccnc(c1)NN=O	C13213092	-12.71	-4.22	-12.96	6.3	-1.84
4870	c1cnc(cn1)CN[NH3+]	C19271336	-12.71	-1.6	-16.64	4.25	1.27
4871	c1cc(cc(c1)F)NCC#N	C20051118	-12.71	-4.07	-12.04	6.43	-3.03
4872	c1cc(oc1)/C=C/C(=O)/[O-]	C26515316	-12.71	1.89	-18.96	6.67	-2.31
4873	c1cc(oc1)/C=C/I	C30677960	-12.71	0.37	-12.24	2.91	-3.75
4874	c1cc(ccc1/C=C/[N+](=O)[O-])O	C00039663	-12.7	-1.18	-14.85	6.11	-2.78
4875	CSc1ccc(cc1N)Cl	C00159318	-12.7	-2.75	-13.14	2.33	0.86
4876	C1C(=S)NC(=O)S1	C01469722	-12.7	0.42	-16.42	4.25	-0.94
4877	CC(=O)c1cccnc1	C01655483	-12.7	2.34	-17	4.58	-2.63
4878	CC(=O)ONC(=O)C(=O)N	C01686534	-12.7	-1.65	-18.66	7.35	0.26
4879	CCO/C=C/C	C01693281	-12.7	-0.63	-11.35	1.8	-2.52
4880	CC/C=C/CC=C=O	C01999333	-12.7	-0.47	-12.53	4.03	-3.73
4881	COCOCBr	C02244257	-12.7	-1.19	-12.71	2.82	-1.62
4882	c1cc(ccc1CNC(=O)N)N	C02512909	-12.7	-0.12	-20.75	6.91	1.26
4883	CC(=O)CC1=C(C)C=C1	C02519746	-12.7	-1.33	-11.63	4.4	-4.14
4884	C=C(C)C(N+)(=O)[O-]	C02557054	-12.7	-0.22	-14.78	3.67	-1.37
4885	c1c(cc(cc1F)Br)F)N	C02560292	-12.7	-0.02	-16.56	3.66	0.22
4886	C#CCCC(=O)Cl	C02574131	-12.7	-0.62	-13.12	4.6	-3.56
4887	C=C[C@H](c1cccnc1)O	C02575264	-12.7	-3.13	-9.15	2.31	-2.73
4888	c1cc(c(cc1O)Br)F	C02580752	-12.7	0.14	-16.73	3.27	0.62
4889	Cc1c(nc2nncn2n1)[O-]	C03888383	-12.7	-0.93	-15.24	6.58	-3.11
4890	CCO/N=C/c1c(ncn1)N)N	C04091469	-12.7	-1.32	-14.75	2.85	0.52
4891	C1=C=CCON1	C05493277	-12.7	-1.35	-13.36	2.42	-0.41
4892	c1cc(oc1)/C=C/C(=O)N=[N+]=[N-]	C15022779	-12.7	0.24	-17.16	4.3	-0.08
4893	c1cn(cn1)S(=O)=O	C15767161	-12.7	-2.46	-17.61	7.23	0.14
4894	c1cn2cc(nc2n1)Br	C20358109	-12.7	0.01	-14.95	5.04	-2.8
4895	COC(=O)[C@H](c1cccnc1)O	C00391162	-12.69	-0.7	-13.89	4.62	-2.73
4896	c1cc(ccc1CN=C=S)F	C01841066	-12.69	-1.33	-10.18	2.63	-3.82
4897	c1cc(ccc1F)C(=O)Cl)F	C02539281	-12.69	0.89	-15.66	4.07	-2
4898	c1cc2c(cc1N)OC(O2)(F)F	C02556425	-12.69	-0.54	-15.43	4.4	-1.13
4899	COC(=O)Cl	C03860600	-12.69	-1.45	-12	2.18	-1.42
4900	C=C/C=C/C=O	C04758198	-12.69	-1.35	-14.05	4.91	-2.2
4901	c1n([nH]n1)CC(=O)C(=O)S	C04879756	-12.69	-3.78	-14.94	6.13	-0.1
4902	c1cncnc1C(=O)/C=N/O	C04900709	-12.69	-3.78	-16.84	8.93	-1
4903	C1CC(=O)NC1	C14684428	-12.69	-4.41	-12.36	2.61	1.47
4904	c1c(cc(cc1F)F)CCO	C16698356	-12.69	-0.73	-12.8	3	-2.16
4905	c1nnc(n1)CO	C01504277	-12.68	-4.79	-15.47	6	1.58
4906	CCOC(=O)C(=C(C)F)F)F	C01668037	-12.68	0.42	-12.52	3.49	-4.07
4907	Cc1cncnc1=O	C01733139	-12.68	-2.39	-17.64	8.22	-0.87
4908	c1cc(c(cc1Br)O)O	C02018046	-12.68	-0.7	-15.95	4.07	-0.11
4909	Cc1ccc(cc1)F)Br	C02384010	-12.68	1.25	-15.3	4.35	-2.97
4910	c1c(cn(n1)C(F)F)N+](=O)[O-]	C02534800	-12.68	-0.58	-14.84	5.31	-2.57
4911	CCn1ccc(n1)[N+](=O)[O-]	C02537792	-12.68	-1.46	-16.34	8.94	-3.81
4912	Cc1nnc(s1)[S-]	C04528607	-12.68	-2.52	-13.61	4.71	-1.26
4913	C#CCO[C@H](H)1CCCO1	C04529398	-12.68	-0.88	-12.47	3.83	-3.16
4914	C/C(=N/c1[nH]ncn1)/O	C05431543	-12.68	-5.72	-13.79	9.33	-2.5
4915	c1(c(ncn1)N)c2nncn2[O-]	C06452769	-12.68	-3.15	-16.82	5.15	2.14
4916	c1(c(n[s1]Cl)S	C06523907	-12.68	-1.87	-14.44	1.68	1.96
4917	c1ccc(c(c1)/C=N/O)O	C06661419	-12.68	-3.72	-14.32	5.06	0.29
4918	c1cc(oc1CO)Br	C08727831	-12.68	-2.76	-13.62	4.24	-0.53
4919	c1cnc(c(c1Cl)C#N	C14628929	-12.68	-2.49	-11.91	4.29	-2.57
4920	CCn1c(c(cn1)C)N	C19091012	-12.68	-3.14	-11.99	4.62	-2.17
4921	Cc1cc(s1)C=O	C20443687	-12.68	-1.86	-13.82	4.78	-1.77
4922	CCOC(=O)OCCl	C21989293	-12.68	-2.42	-11.57	4.01	-2.7
4923	C[C@@H](c1cccnc1)O	C00393774	-12.67	-1.26	-14.49	3.84	-0.76
4924	CCCC(=O)OC	C00404765	-12.67	-0.38	-13.17	3.62	-2.73
4925	Cc1ccc(cc1)O)Br	C01583783	-12.67	-1.92	-14.43	2.82	0.86
4926	COC(=O)c1csnn1	C01632276	-12.67	1.06	-18.14	5.67	-1.26
4927	[H]/N=C/1\CC(=NN1C(=O)N)C	C01659742	-12.67	-3.99	-16.35	5.17	2.51
4928	COCCl	C01699870	-12.67	0.36	-13.02	1.85	-1.86
4929	CCCCO=C	C01845732	-12.67	-0.35	-12.46	1.62	-1.48
4930	Cc1ccc(cc1)CC=O	C01851033	-12.67	-1.57	-13.84	4.34	-1.6
4931	c1cnc(c1)OC(=O)C(F)F)F	C02557083	-12.67	-0.28	-14.55	5.34	-3.17
4932	C1CC1C(=N)NN	C04202550	-12.67	-2.32	-13.11	3.23	-0.47
4933	CC(C)C/C(=C/C(=O)C(F)F)F/[O-]	C04430782	-12.67	-1.49	-9.98	2.23	-3.43
4934	C(c1c(nc[n+]1)[O-])[N+](=O)[O-])O	C04481279	-12.67	0.67	-18.75	6.55	-1.14
4935	c1cnc2nc(nn2c1)N	C04487619	-12.67	-1.41	-18.51	11.1	-3.85
4936	c1c(c[nH]1)N	C05784074	-12.67	-3.2	-14.01	3.8	0.74
4937	COCc1ccnc(c1)N	C06643273	-12.67	-2.99	-13.07	4.04	-0.65
4938	Cc1nc(cs1)C(F)F)F	C08614797	-12.67	-2.33	-11.87	4.22	-2.69
4939	C/C(=C/[N+](=O)[O-])/C(=O)OC	C08655546	-12.67	0.62	-14.02	3.9	-3.16
4940	COC(=O)c1ccc(cc1)C=O	C08728864	-12.67	0.28	-16.04	5.47	-2.39
4941	c1c(c(c[nH]c1=O)Cl)[O-]	C13831809	-12.67	-2.15	-17.99	4.51	2.96
4942	Cc1ncc(cn1)O	C14982942	-12.67	-1.27	-15.94	4.29	0.24
4943	Cc1cc(nc1)C=O	C20443769	-12.67	-1.79	-14.68	5.31	-1.51
4944	C1[C@@H](OC1)CBr	C00158846	-12.66	0.14	-12.74	2.32	-2.39
4945	Cc1cn(cn1)CC=C	C01672433	-12.66	-2.17	-13.46	4.77	-1.79
4946	CCOC/C=C/C	C01765538	-12.66	-0.17	-13.05	1.5	-0.94

4947	c1cnsc1	C01847600	-12.66	-1.09	-13.37	3.27	-1.46
4948	Cn1c(=O)cc(s1)Cl	C02002061	-12.66	-0.16	-16.02	5.43	-1.9
4949	c1ccc2c(c1)oc(=S)o2	C02518996	-12.66	1.54	-17.78	7.46	-3.88
4950	CCCC(=C)C(=O)Cl	C02541519	-12.66	-1.33	-12.6	2.83	-1.56
4951	CNc1cc(nc(n1)F)F	C03129092	-12.66	-1.85	-14.01	4.52	-1.32
4952	CC(=O)CC(=O)COC	C04353401	-12.66	-2.92	-15.18	7.01	-1.57
4953	CN1cncc1C=O	C04384378	-12.66	-2.59	-14.33	7.42	-3.15
4954	CC[C@H](c1ccccc1F)O	C15442977	-12.66	-1.22	-11.88	3.26	-2.82
4955	c1c(c(c[nH]c1=O)F)Br	C15684419	-12.66	-0.24	-16.51	3.34	0.75
4956	CCC(=O)[C@H](C#N)Cl	C21982974	-12.66	0.23	-13.99	3.96	-2.86
4957	C[C@H](c1cccc1)Cl	C32005372	-12.66	-1.14	-11.06	2.98	-3.44
4958	COc1ccc(cc1)O	C00001684	-12.65	-2.51	-13.06	3.57	-0.65
4959	COC(=O)CCc1ccccc1O	C00153017	-12.65	-1.48	-15.46	4.95	-0.66
4960	CCC(=O)n1cncc1	C00901601	-12.65	-3.02	-13.1	6.7	-3.22
4961	C(CCl)SC#N	C01734841	-12.65	0.42	-14.16	3.75	-2.66
4962	CCc1ccc(o1)C=O	C02243037	-12.65	-1.41	-15.3	7.41	-3.36
4963	c1c(cc(c1N=C=S)F)F	C02506744	-12.65	-0.02	-13.81	3.14	-1.95
4964	CC(C)OC(=O)CBr	C02539275	-12.65	-1.65	-11.46	3.88	-3.43
4965	CC(=O)NCCc1ccco1	C03279385	-12.65	-0.09	-17.48	6.26	-1.34
4966	C1=C(N=NC1=O)N	C04582838	-12.65	-4.34	-15.52	4.98	2.24
4967	C1CC=C[C@H](C1)CC#N	C04706407	-12.65	-0.91	-14.54	4.8	-2
4968	CC(=NOC=C)C	C05377858	-12.65	-0.15	-13.94	3.69	-2.26
4969	CSC(=S)N	C06425141	-12.65	-1.52	-13.32	1.1	1.1
4970	Cc1ccc[nH]c1=O	C08580061	-12.65	-1.57	-16.28	4.76	0.44
4971	C(C(=O)C(F)F)F	C16158475	-12.65	-0.16	-12.55	2.84	-2.78
4972	c1cc(ccc1C/C(=N/O)/N)F	C16957726	-12.65	-2.59	-16.62	7.81	-1.25
4973	c1cc(ccc1)CCC=O	C19682806	-12.65	-0.82	-16.19	7.31	-2.95
4974	CN(C)C=C/[N+](=O)[O-]	C19735116	-12.65	-2.2	-14.75	7.18	-2.87
4975	c1cc(c(c(c1O-))C#N)F	C26522326	-12.65	1.16	-17.82	5.55	-1.55
4976	c1cc(ccc1N)NC(=S)N	C00569446	-12.64	-2.12	-19.49	9.96	-0.98
4977	c1cc(cc(c1)NC=O)N	C01566598	-12.64	-1.39	-18.19	7.41	-0.47
4978	CC(=O)C(C(F)F)(F)F	C01675519	-12.64	-1.09	-12.03	2.89	-2.4
4979	CC(=O)OCBr	C01846487	-12.64	-1.42	-13.16	4.2	-2.26
4980	CSC(=O)c1ccco1	C01850674	-12.64	-0.56	-13.82	4.45	-2.71
4981	CC#C[C@H](C)O	C02508066	-12.64	-2.58	-12.03	2.81	-0.84
4982	CN1c(c(cn1)N=O)N	C04285550	-12.64	-4.45	-15.16	7.59	-0.62
4983	Cc1c(non1)/N=N/c2c(non2)C	C04460104	-12.64	-0.64	-13.03	3.93	-2.91
4984	c1c(c(cnc1Cl)F)Br	C08698173	-12.64	0.8	-12.15	1.62	-2.91
4985	c1c(=O)nc([nH]n1)NN	C16955996	-12.64	-5.06	-16.48	6.55	2.35
4986	c1cc(oc1)[C@H]2CO2	C19730639	-12.64	-1.67	-14.99	5.39	-1.37
4987	CCC(C(=O)OCC)(F)F	C31176451	-12.64	-0.39	-10.99	2.42	-3.68
4988	C=CCNC(=O)n1cncc1	C32628636	-12.64	-2.83	-14.37	7.57	-3.02
4989	c1cc(c(nc1)C(=O)N)O	C00156997	-12.63	-7.07	-14.25	7.39	1.3
4990	c1ccn(c(=O)c1)CCC#N	C01606328	-12.63	-2.34	-19.7	11.44	-2.03
4991	CC(=O)C(=C)COCO	C01636251	-12.63	-3.37	-15.31	6.1	-0.04
4992	COC([C@H](F)Cl)F	C02040626	-12.63	-1.45	-11.75	2.21	-1.63
4993	c1cc(c(nc1)F)I	C02384102	-12.63	-0.38	-16.43	4.31	-0.13
4994	C=Cc1ccc(cc1)CO	C02566080	-12.63	-1.07	-15.52	3.52	0.44
4995	CCNc1cccc(c1)F	C19772292	-12.63	-2.84	-9.16	2.6	-3.24
4996	c12c(n[nH]n1)C(=O)N=NC2=O	C19798253	-12.63	-5.87	-18.76	5.81	6.19
4997	c1c(nc(s1)[O-])O	C00967383	-12.62	-5.58	-15.25	5.93	2.27
4998	C1CC(=O)C=C1Cl	C02004732	-12.62	-0.45	-15.83	4.22	-0.57
4999	C/C=C/COC(=O)C	C02168392	-12.62	0.17	-13.16	3.81	-3.44
5000	Cc1cc(=O)n([nH]1)C	C03199631	-12.62	-3.83	-13.85	4.86	0.21
5001	Cc1c(c[nH]n1)C=O	C04243451	-12.62	-2.58	-15.17	6.14	-1.01
5002	Cc1cnccc1C#N	C05420335	-12.62	-2.57	-11.36	3.99	-2.68
5003	c1c(nc(s1)N)CSC(=[NH2+])N	C08617634	-12.62	-2.08	-14.22	3.79	-1.62
5004	c1nnnn1c2nnc(s2)S	C11690073	-12.62	-4.34	-12.45	5.18	-1.02
5005	c1cc(nc(c1Br)F)Cl	C12359471	-12.62	-2.36	-13.83	3.54	0.03
5006	c1c(cc(c2c1[nH]nc2Cl)F)F	C14983965	-12.62	-0.53	-12.44	3.14	-2.79
5007	CCO/C(=C/C(=O)C(F)F)/N	C15442533	-12.62	-3.52	-12.63	4.3	-0.77
5008	c1cc(c(cc1C(F)F)F)O	C16159595	-12.62	-6.03	-9.64	3.66	-0.3
5009	c1(nnc(o1)N)C(F)F	C16382873	-12.62	-4.99	-15.1	4.53	2.94
5010	Cn1c(cnn1)C=O	C20443600	-12.62	-4.04	-15.57	7.63	-0.65
5011	c1c(c([nH+](c1Cl)F)[O-])	C21981948	-12.62	-6.15	-12.36	6.14	-0.24
5012	CC[C@H](CC#C)O	C21991298	-12.62	-0.39	-13.24	3.02	-2.02
5013	CC1=CC(=NNC1)C	C21992753	-12.62	-1.62	-12.52	3.29	-1.77
5014	COc1cnc(cn1)Cl	C33359456	-12.62	-1.52	-13.83	2.74	-0.02
5015	c1csc1S(=O)(=O)N	C00967207	-12.61	-1.07	-19.65	6.85	1.25
5016	Cn1c[nH]c1=S	C01187543	-12.61	-1.48	-13.79	4.95	-2.29
5017	C1C=CCC1CO	C01435886	-12.61	-1.37	-12.47	2.13	-0.91
5018	c1c(=O)[nH](c(=O)[nH]c1F)	C01607275	-12.61	-1.45	-17.78	5.52	1.11
5019	CCOCC(=C)Br	C01639892	-12.61	-0.42	-14.19	2.26	-0.26
5020	CC(=O)C=C/C	C01693783	-12.61	-1.88	-13.28	4.19	-1.64
5021	c1c(cc(cc1O)F)[N+](=O)[O-]	C01701564	-12.61	-2.87	-12.49	4.56	-1.81
5022	Cn1cccc1C#N	C02584072	-12.61	-1.53	-12.35	4.49	-3.23
5023	c1ccc2c(c1)[C@H]2O	C03107554	-12.61	-2.18	-12.39	3.59	-1.63
5024	c1c(cc(c1F)C#N)F	C12359184	-12.61	1.02	-14.44	3.67	-2.85
5025	c1cc(ccc1)F)OCCON	C19727751	-12.61	-2.18	-13.84	5.11	-1.69
5026	CCC(=O)Oc1cccnc1	C22129873	-12.61	-0.93	-13.9	5.86	-3.63
5027	CNc1ccc(cc1F)N	C26515334	-12.61	-2	-13.53	3.89	-0.97
5028	c1tsc1N)CO	C30678144	-12.61	-3.55	-16.22	6.1	1.07
5029	C(CBr)C(=O)N=C=O	C32501080	-12.61	1.61	-17.45	2.95	0.27
5030	c1c([nH]c(=O)[nH]c1=O)N)N	C01666585	-12.6	-5.41	-19.25	8.63	3.44
5031	CC1=C(OCC1)C	C01707813	-12.6	-0.47	-13.41	2.11	-0.83
5032	C#Cc1ccc(s1)C#C	C02541494	-12.6	-0.43	-12.32	3.8	-4.66
5033	Cc1cc(ccc1N)SC#N	C03164873	-12.6	-1.14	-12.64	3.91	-2.72
5034	c1cc(ccc1[P@@H](=O)[O-])Cl	C03165596	-12.6	-4.47	-14.32	7.73	-1.53
5035	C(OCC)Cl	C04202480	-12.6	-1.4	-11.81	1.86	-1.25
5036	CCNC(=O)c1cnccn1	C05472106	-12.6	0.71	-19.25	6.2	-0.26

5037	c1ccc(cc1)OCC(=S)N	C05647051	-12.6	-3.07	-14.19	3.88	0.78
5038	c1(c(non1)[N+](=O)[O-])c2[nH]nnn2	C06452771	-12.6	-5.71	-10.21	4.66	-1.34
5039	C=C[S@](=O)c1cccc1	C08294950	-12.6	-3.64	-15.06	8.99	-2.9
5040	c1c(nc(s1)N)C#N	C12320990	-12.6	-0.64	-16.87	5.94	-1.03
5041	Cc1c2c(nc[nH]2)ncn1	C14593164	-12.6	-1.76	-15.11	7.28	-3
5042	c1cscc1[C@@H](C#N)N	C21950033	-12.6	0.22	-16.54	4.8	-1.08
5043	CCc1[n-]c2cnc2n1	C26439583	-12.6	-4.76	-13.12	7.58	-2.3
5044	[H]/N=C\1/C=C(C(S1)C)C	C31861601	-12.6	-0.97	-13.21	3.6	-2.02
5045	Cc1c(ccc1N)N	C00388289	-12.59	-2.71	-11.73	2.73	-0.88
5046	c1cnc2c1csc2	C00966806	-12.59	-1.62	-14.88	3.68	0.23
5047	c1c(c(=O)[nH]c(=O)[nH]1)Br	C00967318	-12.59	-4.87	-16.89	8.82	0.34
5048	C1CCC(=O)C1	C00967469	-12.59	-1.19	-13.73	3.35	-1.01
5049	Cn1cc(n1)CCl	C01610364	-12.59	-1	-14.2	5.13	-2.52
5050	c1cnc(c(n1)C(=O)N)N	C01719389	-12.59	-3.14	-18.67	5.61	3.61
5051	CCn1cc(cn1)N	C02554028	-12.59	-0.48	-15.29	4.08	-0.91
5052	c1c(c(c(nn1)NN)N)Cl	C08616364	-12.59	-5.08	-14.12	5.77	0.82
5053	c1cc2c(cc1O)[nH]cn2	C18543204	-12.59	-4.08	-14.51	7.04	-1.04
5054	CCc1ccc(s1)[N+](=O)[O-]	C32602823	-12.59	-2.18	-11.25	5.3	-4.46
5055	CC(C)I	M1995A003	-12.59	0.49	-10.81	0.69	-2.96
5056	c1c(c(c(c1F)F)Br)N)F	C00056691	-12.58	-3.06	-10.96	1.99	-0.54
5057	c1c(cc(c1F)N)F)Br	C00159313	-12.58	-0.52	-13.51	1.33	0.12
5058	c1c(cncn1)C(=O)N	C00334399	-12.58	-2.88	-18.35	6.7	1.94
5059	c1cnc(c1)NC=O	C00388697	-12.58	-1.98	-18.51	9.77	-1.86
5060	COCC(=O)Cc1ccccn1	C00404445	-12.58	0.05	-16.68	7.4	-3.34
5061	C(C(=O)C(F)F)Cl	C02382176	-12.58	-0.11	-13.93	3.66	-2.2
5062	c1cnc(c1)CC=O	C02537468	-12.58	-1.23	-17.32	7.48	-1.51
5063	C/C=C/CC(=O)OC	C02556897	-12.58	0.1	-14.37	3.83	-2.14
5064	CC(=O)CC=O	C05114132	-12.58	-5.04	-13.25	5.64	0.07
5065	c1cncsc1C=O	C06119181	-12.58	-1.65	-16.25	6.59	-1.27
5066	Cc1nc2n(n1)C(=O)C(=N2)[O-]	C06816747	-12.58	-1.07	-18.65	6.39	0.75
5067	c1c(nc[nH]1)N	C12958660	-12.58	-3.04	-14.08	5.33	-0.8
5068	c1cc(c2ccccc2c1)O	C14982888	-12.58	-1.86	-14.49	5.23	-1.47
5069	c1ccc(cc1)CNC(=S)NO	C15783302	-12.58	-0.32	-22.45	12.13	-1.93
5070	C1NNC(=N)N)1)N	C16778243	-12.58	-3.34	-13.37	4.38	-0.26
5071	c1c(c(c(cn1)Cl)N)Cl	C19419098	-12.58	0.26	-13.74	2.28	-1.38
5072	Cc1cnc(c(c1F)O)N	C21981848	-12.58	-1.59	-16.21	4.82	0.41
5073	CC(=O)OCOC(=O)C	C00409289	-12.57	-0.38	-16.14	6.74	-2.79
5074	c1cc(cc(c1)N)C=O	C01655484	-12.57	-3.77	-12.51	5.28	-1.57
5075	CCCOC(=O)C=C	C01665004	-12.57	0.65	-13.82	4	-3.41
5076	c1cc(c(c(c1F)NN)F)F	C01678677	-12.57	-1.37	-16.64	3.67	1.78
5077	COCC1CCSC1	C02166996	-12.57	-1.08	-11.86	2.1	-1.73
5078	Cc1ccnc(c1)N)F	C02526738	-12.57	-3.8	-12.91	5	-0.86
5079	Cc1cc(cc(c1)F)O	C02527808	-12.57	-1.71	-12.06	3.03	-1.83
5080	c1cc2c(cc1F)C(OC2(F)F)(F)F	C02540395	-12.57	-3.01	-9.8	3.47	-3.23
5081	CC(C=C)C(=O)Cl	C02574130	-12.57	0.13	-14.01	2.67	-1.36
5082	c1cc(c(cc1CCO)F)F	C04255270	-12.57	-2.3	-12.22	4.05	-2.09
5083	C(#N)C(=NO)C#N	C05500529	-12.57	-4.44	-12.31	3.72	0.47
5084	c1cnc(nc1)C=O	C15022141	-12.57	-3.22	-15.33	7.27	-1.29
5085	c1c(cnc(n1)N)CO	C26894820	-12.57	-2.54	-18	7.28	0.69
5086	c1ccc(cc1)CC(=O)NN	C00080757	-12.56	-5.81	-13.26	7.91	-1.4
5087	Cc1cccc(c1)OC(=O)NC	C00135179	-12.56	-0.86	-15.78	6.55	-2.47
5088	Cc1c(c(c(c1F)N)F)F	C00155915	-12.56	-0.74	-11.64	1.93	-2.11
5089	c1cc(c(c(c1)F)O)O	C00164683	-12.56	-2.09	-16.22	5.49	0.25
5090	COCC(=O)n1cccc1	C00396077	-12.56	-1.28	-12.69	4.27	-2.86
5091	CCSCC	C01529401	-12.56	-0.55	-10.15	1.23	-3.08
5092	Cc1csc(n1)NN	C01588808	-12.56	-3.72	-12.51	4.36	-0.69
5093	C=C(C#N)Cl	C01603500	-12.56	-2.41	-12.11	4.08	-2.12
5094	C1CC(C1)C(=O)Cl	C01609476	-12.56	0.93	-13	2.47	-2.97
5095	C/(C=C/Br)NC(=O)C(F)F	C01673955	-12.56	-0.96	-14.58	3.55	-0.57
5096	CCC(=O)OCC=C	C01683670	-12.56	-0.19	-12.48	3.52	-3.41
5097	c1ccc(cc1)OC#N	C02004401	-12.56	-0.63	-13.91	2.52	-0.54
5098	C(#CC#N)C#N	C02039983	-12.56	-1.33	-11.79	2.79	-2.23
5099	c1cc(sc1)CC(=O)Cl	C02141010	-12.56	-2.51	-13.61	4	-0.45
5100	c1cnc(cn1)CO	C02383124	-12.56	-0.88	-18.01	5.02	1.31
5101	c1c[nH]c2c1c(cc2F)F	C02572575	-12.56	-2.61	-10.04	3.59	-3.5
5102	C1[C@H](C)C=C1)C=O	C03875686	-12.56	-0.96	-12	3.61	-3.2
5103	c1c[nH]nc1N	C04674340	-12.56	-3.75	-13.76	4.89	0.06
5104	CC(=O)NCc1ccncc1	C11535644	-12.56	-0.91	-17.03	6.69	-1.32
5105	C1CSc2n1c(nn2)N	C11919854	-12.56	-2.68	-17.76	10.81	-2.93
5106	c1ccc2c(c1)[nH]c(=O)[nH]2	C18115182	-12.56	-2.19	-15.37	6.19	-1.19
5107	c1ccc(cc1)NC(=O)NO	C00161805	-12.55	-3.76	-18.63	10.41	-0.57
5108	Cc1c[nH]c(S)nn1[S-]	C01239139	-12.55	-2.75	-13.89	6.24	-2.15
5109	CCOC(=C(C(F)F)C(F)F)F	C01826977	-12.55	-0.96	-9.01	2.19	-4.77
5110	c1cc(cc(c1)O)CCl	C02034015	-12.55	-1.42	-15.23	3.5	0.6
5111	C[C@H]1CCCS1	C02039244	-12.55	0.18	-11.3	1.97	-3.39
5112	COCC1c(ccc1O)O	C02146972	-12.55	-1.28	-17.5	5.95	0.28
5113	CCOnc1cc(cn1)N	C02537624	-12.55	-2.22	-15.32	4.17	0.82
5114	C/C=C(C)/C=N/O	C04783426	-12.55	-1.16	-14.63	3.47	-0.24
5115	CCCOC(=O)CCS	C04802679	-12.55	1.2	-12.81	2.74	-3.68
5116	c1[nH]c2c(n1)c(cnc2)Cl	C04807217	-12.55	-4.38	-13.05	7.72	-2.84
5117	Cc1ccc(=O)[nH]n1	C08603112	-12.55	-1.95	-17.25	7.09	-0.43
5118	c1cc(c(cc1CO)N)F	C12336788	-12.55	-2.78	-14.1	4.07	0.26
5119	C=C1CC(C1)C(=O)Cl	C16124713	-12.55	-0.5	-11.74	2.92	-3.23
5120	c1cc(c(c(c1N)N)F)Br	C16125748	-12.55	-1.08	-14.26	3.68	-0.88
5121	c1cc(c(cc1Br)O)N	C20357555	-12.55	-1.92	-15.2	4.7	-0.13
5122	c1cc2c(c1)c(=O)[nH]2	C00150793	-12.54	-1.89	-13.36	5.23	-2.52
5123	CCOC(=C)OCC	C00391146	-12.54	-0.68	-12.45	2.25	-1.66
5124	C[C@H]1C[C@@H](C=C1)OC(=O)C	C01095300	-12.54	0.13	-15.22	4.43	-1.88
5125	CCOC(F)F)F	C01845822	-12.54	-0.81	-11.76	1.18	-1.14
5126	Cc1ccc(cc1N)C#N	C02526462	-12.54	-1.47	-12.58	4.07	-2.57

5127	c1cc(sc1)[P@H](=O)O	C06513153	-12.54	-3.43	-17.03	7.6	0.32
5128	C[C@H]1CON=C1[N+](=O)[O-]	C15784737	-12.54	1.44	-16	4.63	-2.61
5129	c1cncc(c1C(F)F)F	C16159519	-12.54	-1.98	-10.23	2.74	-3.06
5130	CC(=O)Nn1c(nnn1)N	C16955107	-12.54	-4.43	-15.54	7.82	-0.39
5131	c1cc(nnc1)C#N	C26460099	-12.54	-3.28	-15.06	7.42	-1.62
5132	c1c[nH]nc1CC#N	C26898483	-12.54	-2.15	-17.63	8.79	-1.55
5133	CC[C@H](c1ccncc1)O	C32914835	-12.54	-1.73	-13.5	3.97	-1.28
5134	c1cc(c(nc1))F	C01443090	-12.53	0.43	-16.93	4.07	-0.1
5135	c12c(nc(nc1n[nH]n2)N)N	C01666567	-12.53	-5.41	-15.62	7.87	0.63
5136	CN[P@H]Cc1cccc1	C01691054	-12.53	-1.75	-9.48	1.71	-3.01
5137	CCOc1ccc(cc1)Cl	C01693308	-12.53	0.75	-14.52	2.05	-0.8
5138	CCN=C=S	C01736702	-12.53	-0.08	-12.43	1.43	-1.45
5139	COC(=O)[C@H](C(F)F)F	C01847473	-12.53	-0.39	-13.9	4.37	-2.61
5140	c1cnc(cc1Cl)Cl	C02012914	-12.53	-1.96	-10.47	2.54	-2.65
5141	c1csc(c1)/C=C/C(=O)Cl	C02513848	-12.53	1.01	-13.36	3.68	-3.86
5142	Cc1cnc(c1)O	C02537613	-12.53	-2.57	-15.49	5.11	0.43
5143	c1cc(cc1C=O)SC(F)F	C02643974	-12.53	-0.31	-15.76	5.5	-1.96
5144	c1cnccc1c2ccn[nH]2	C09238267	-12.53	-1.22	-14.6	5.13	-1.83
5145	c1c(cnc(=O)[nH]1)l	C12958973	-12.53	-1.39	-16.6	3.81	1.64
5146	CC(1=NNC(=O)/C1=N)O	C17058625	-12.53	-4.42	-16.57	6.2	2.26
5147	Cc1cc2cccc2o1	M1995A039	-12.53	-1.21	-11.19	4.15	-4.28
5148	c1cc(c(cc1F)Nc2nccn(n2)N)F	C00089563	-12.52	-0.58	-10.73	5.15	-6.35
5149	c1cc(c(cc1C#N)Cl)F	C00152696	-12.52	-1.68	-12.31	3.87	-2.41
5150	Cc1c(c(on1)N)C#N	C00168736	-12.52	-4.39	-13.01	4.75	0.12
5151	c1ccc(cc1)/C=C/NC=O	C01611408	-12.52	-2.8	-16.54	7.43	-0.6
5152	CC(=C(=O)Cl)C	C02140825	-12.52	0.01	-13.91	2.63	-1.26
5153	c1cc(oc1)/C=C/C=O	C06096965	-12.52	-0.06	-16.26	6.54	-2.73
5154	c1(c(c(c(c1F)F)F)F)O)N	C10157948	-12.52	-4.99	-11.83	4.11	0.19
5155	c1ccc(c1C=O)Br	C12370772	-12.52	-1.86	-14.05	5.63	-2.25
5156	CC(=O)c1cnc([nH]1)Br	C12647614	-12.52	-2.22	-13.74	5.45	-2.01
5157	c1ccc(c1)N)SCC#N	C19431015	-12.52	-0.9	-14.38	5.9	-3.15
5158	c1nc(c(n1C#N)Cl)Cl	C00160929	-12.51	-4.07	-14.57	10.17	-4.05
5159	CSct1nccn1	C00967360	-12.51	-3.27	-13.63	5.95	-1.57
5160	c1c(=O)[nH]c(=O)n(n1)CCC#N	C01584613	-12.51	-1.49	-19.75	8.76	-0.04
5161	CCCCOC(=O)Cl	C01586311	-12.51	-0.98	-11.59	1.72	-1.66
5162	c1cc2c([nH]nc2O)nc1	C01715820	-12.51	-4.35	-17.32	7.99	1.18
5163	CCCCSC(=O)C	C01736013	-12.51	-0.68	-13.43	2.51	-0.91
5164	c1cc(c(cc1C=O)F)O	C02566026	-12.51	-3.47	-13.66	5.63	-1.02
5165	C(CS)CCl	C04501375	-12.51	0	-11.53	1.86	-2.84
5166	c1cc(sc1)/C=C/CO	C05181090	-12.51	-1.12	-15.68	3.04	1.25
5167	c1c(c(c(S)[nH]1)l)S-])N	C08616365	-12.51	-4.02	-14.23	5.45	0.29
5168	c1cc(sc1CO)Br	C08727737	-12.51	-2.72	-12.14	3.39	-1.03
5169	c1c2c(cc(c1F)F)nc[nH]2	C11535703	-12.51	-3.59	-12.54	6.81	-3.19
5170	c1cc(c(cc1F)N)C(F)F	C12359261	-12.51	-3.23	-9.56	1.94	-1.66
5171	C1C[C@H](COC1)CCl	C14987965	-12.51	-0.67	-11.13	1.94	-2.65
5172	C1COC(=CO1)C(=O)Cl	C31772028	-12.51	2.1	-18.43	5.76	-1.94
5173	c1cc(oc1)/C=C/[N+](=O)[O-]	C00055261	-12.5	-0.02	-14.36	5.51	-3.63
5174	c1cc([nH]c1)C(=O)N	C00331859	-12.5	-3.64	-17.4	7.91	0.63
5175	CNc1cccc(c1)N	C00395228	-12.5	-0.47	-16.59	2.72	1.84
5176	CC(=O)OC1=CCCC1	C00397582	-12.5	-0.28	-14.76	4.52	-1.99
5177	c1c(ocnc1(O))C(=O)N	C01601705	-12.5	-4.98	-17.8	8.26	2.02
5178	C(C=C(Cl)Cl)O	C01634330	-12.5	-2.09	-13.76	2.06	1.28
5179	CC(=C)C(=O)OCC(F)F	C01665001	-12.5	-1.33	-10.98	3.49	-3.67
5180	Cc1c[nH]cc1C#N	C05378563	-12.5	-4.91	-12.51	6.5	-1.58
5181	CCOC(=O)/C=N/O	C14455584	-12.5	-4.82	-13.86	6.14	0.05
5182	CCNc1cc(ncn1)Cl	C15021259	-12.5	-0.52	-12.46	3.3	-2.82
5183	C[C@H](C(=O)Cl)N	C20216998	-12.5	-2.04	-12.8	2.14	0.19
5184	c1nc(sn1)C=O	C20443625	-12.5	-2.95	-16.61	7.66	-0.59
5185	C1C(=O)SCC(=O)S1	C01558011	-12.49	1.18	-16.65	4.62	-1.64
5186	CC(=O)c1cccn1C	C01561741	-12.49	1.47	-15.63	4.97	-3.3
5187	CC(=C)[C@H](CC=C)O	C02169054	-12.49	-0.87	-12.93	1.6	-0.29
5188	C/C=C/C(=O)OCC(F)F	C02525291	-12.49	-1.6	-10.48	3.41	-3.82
5189	c1c[nH]c(=O)cc1Cl	C02598079	-12.49	-4.44	-14.72	8.13	-1.46
5190	CC(C)CCON=O	C03830220	-12.49	-0.05	-11.03	1.82	-3.24
5191	Cc1c([nH]cn1)l	C04352766	-12.49	-3.3	-12.13	5.7	-2.76
5192	C/C=C/C(=O)O	C05082921	-12.49	0.06	-12.19	3.39	-0.76
5193	CCCCN=[N+]=[N-]	C05352785	-12.49	-0.32	-12.89	1.19	-3.46
5194	CC/C=C/CO	C06661425	-12.49	-2.19	-11.72	2.14	-0.72
5195	C(=O)([C@H](C(F)F)(F)Cl)Br	C16159138	-12.49	-0.25	-10.15	0.65	-2.74
5196	c1cc(cc(c1)OC(F)F)Cl)N	C16159191	-12.49	-1.66	-11.28	2.52	-2.07
5197	C(C(F)F)OC([C@H](F)Cl)(F)F	C16159415	-12.49	-1.5	-11.05	2.87	-2.8
5198	CC(=O)C=CC(=O)C	C17146014	-12.49	-2.01	-15.09	8.18	-3.57
5199	C1C(=O)N/C(=C/C#N)/S1	C18217617	-12.49	-2.4	-16.98	8.15	-1.26
5200	COC(=O)Nc1cccc(c1)N	C19815594	-12.49	0.16	-19.39	7.22	-0.48
5201	CCC(=O)[C@H](C)Br	C19843047	-12.49	0.53	-12.27	2.42	-3.17
5202	c1ccc2c1C(=O)CC2	C20216470	-12.49	-0.69	-16.79	7.73	-2.74
5203	c1c(snn1)C=O	C20443605	-12.49	-2.48	-16.55	7.18	-0.63
5204	C/C=C/OC(=O)CCl	C21986546	-12.49	1.54	-15.09	4.63	-3.57
5205	C[C@H](C(=O)n1ccnc1)Cl	C28166230	-12.49	-0.27	-13.84	4.66	-3.04
5206	c1ccc(cc1)[C@H](CS)O	C32625175	-12.49	-0.91	-11.99	2.78	-2.37
5207	CC(=O)c1ccc(s1)Cl	C00035873	-12.48	-0.41	-14.69	3.1	-0.48
5208	Cc1ccc(=O)[nH]c1=O	C00399538	-12.48	-2.65	-18.38	9.58	-1.02
5209	CSct1c(ncn1)N	C01559181	-12.48	-1.7	-13.02	3.68	-1.43
5210	C[C@H](C(=O)OCC(=C)Cl)O	C01641211	-12.48	-0.77	-14.29	4.41	-1.83
5211	CCOC(=O)[C@H](C)[N+](=O)[O-]	C01691713	-12.48	-1.16	-14.13	6.29	-3.49
5212	C[C@H](C#N)OC(=O)C	C02045170	-12.48	-1.76	-12.88	4.88	-2.72
5213	COC(C(F)F)F	C02242932	-12.48	-1.4	-10.86	1.19	-1.41
5214	c1cc(c(c1F)O)Cl)F	C02382102	-12.48	-0.97	-14.72	3.66	-0.44
5215	Cc1ccc(cc1F)CC#N	C02382216	-12.48	-2.37	-14.05	6.87	-2.93
5216	c1ccc(c(nc1)F)O	C02526745	-12.48	-1.61	-16.81	5.81	0.12

5217	CN(CCC)N=O	C04403988	-12.48	-0.07	-14.63	3.44	-1.21
5218	CC(=O)OC(=C)C#N	C04521097	-12.48	-1.29	-15.89	8.02	-3.31
5219	C[C@H]1C(=O)CCS1	C05227203	-12.48	-0.89	-12.02	3.12	-2.69
5220	Cc1cc(n1)N(+)=O][O-]	C12395839	-12.48	-0.96	-14.85	6.4	-3.07
5221	Cc1cc(ncc1F)N	C19615667	-12.48	-3.87	-11.39	4.39	-1.61
5222	c1c(cnc(n1)N)O	C21298001	-12.48	-5.15	-15.14	7.23	0.57
5223	Cc1c(cc(n1)Br)Cl	C21993119	-12.48	-0.54	-10.03	1.42	-3.33
5224	C[C@H]1C[C@H]1C(=O)N=C=S	C22141578	-12.48	-0.27	-13.29	3.73	-2.64
5225	Cc1[nH]cc(n1)C(F)(F)F	C31176470	-12.48	0.78	-15.73	4.78	-2.3
5226	c1cc(c2c(c1)[nH]cn2)N	C00112552	-12.47	-3.73	-13.08	5.99	-1.65
5227	c1c(c(n[nH]1)C(=O)N)N	C01072662	-12.47	-3.51	-19.27	6.18	4.12
5228	CC(C)COC(=O)C=C	C01577264	-12.47	0.3	-12.65	3.74	-3.86
5229	COC(=O)C=C/CBr	C01708353	-12.47	-1.2	-12.64	4.55	-3.18
5230	C(CO)C#Cl	C03164239	-12.47	-3.08	-12.95	2.34	1.22
5231	c1cc(ncc1C(=O)Cl)F	C04208891	-12.47	-1.04	-13.02	3.8	-2.21
5232	c1c(cc1[N+](=O)[O-])[N+](=O)[O-]	C04404088	-12.47	-2.22	-13.2	6.68	-3.73
5233	c1c(nc[nH]1)F	C04771528	-12.47	-3.45	-12.43	4.98	-1.56
5234	C[C@H]1CC[C@H](O)1C	C05225617	-12.47	0.03	-11.56	1.55	-2.5
5235	CCCc1ccc(n1)O	C05311252	-12.47	-1.71	-12.88	3.73	-1.61
5236	CC(=O)Cc1ccncc1	C08294938	-12.47	-1.8	-14.5	6.79	-2.97
5237	c1cc2c(c1)[nH]ncc2c1	C08584258	-12.47	-3.88	-15.73	9.47	-2.33
5238	CO/C=C/OC	C13410577	-12.47	-1.18	-13.09	2.46	-0.65
5239	CC(C(=O)NCCO)(F)F	C14628935	-12.47	-3.61	-14.99	4.8	1.32
5240	C[C@H](N+)(=O)[O-]Br	C16968743	-12.47	-0.87	-12.12	2.88	-2.36
5241	C1=NC(=O)N=C2C1=NN=N2	C17173524	-12.47	-5.78	-18.79	8.05	4.04
5242	C1CC=C(C(=O)C)1O	C18056386	-12.47	-1.9	-15.27	5.94	-1.24
5243	c1cc(n[nH]c1=O)[O-]	C18181713	-12.47	-4.26	-15.94	6.49	1.23
5244	c1cnc(c(c1N)[N+](=O)[O-])N	C19802592	-12.47	-1.39	-16.96	6.08	-0.2
5245	Cc1ccc(cc1)NC(=S)C(=O)N	C20367814	-12.47	-5.61	-12.3	6.8	-1.36
5246	c1cc(c(c1)F)NCC#N)F	C20476380	-12.47	-1.56	-12.74	4.77	-2.93
5247	C(CO)/C=C/CO	C22060201	-12.47	-3.33	-15.72	5.23	1.35
5248	CC1=CN[C@H](C=C1)O	C22060901	-12.47	-1.28	-16.85	4.79	0.87
5249	C[C@H](c1ccc(cc1)N)O	C00404059	-12.46	-2.18	-12.81	3.03	-0.5
5250	Cc1cccc1CO	C00896724	-12.46	-1.33	-12.63	3.38	-1.88
5251	c1cc(ccc1OC(=N)N2+))N)Cl	C01670681	-12.46	0.04	-19.04	3.34	3.2
5252	c1(c(c(nc(c1)F)F)F)F)F)N	C02579295	-12.46	-1.59	-13.38	2.72	-0.22
5253	Cc1ccc2c(c1)CC2=O	C03847808	-12.46	-1.94	-10.98	4.64	-4.18
5254	c1ccc(cc1)OC(=S)Cl	C03861662	-12.46	0.68	-15.58	2.44	0
5255	c1ccc(cc1)NC(=S)N	C03875720	-12.46	-2.66	-15.49	4.22	1.47
5256	c1cc(ncc1Br)C(F)(F)F	C04244987	-12.46	-1.03	-12.81	2.79	-1.4
5257	c1(c(nc(nc1N)N)N)[N+](=O)[O-]	C04852051	-12.46	-2.35	-14.36	4.63	-0.38
5258	c1ccc2c(c1)nc(s2)N	C12341454	-12.46	-1.17	-14.48	5.59	-2.4
5259	CCC/C=C/ICO	C12358736	-12.46	-1.21	-12.23	2.11	-1.14
5260	COc1ccc(n1)N=O	C13213121	-12.46	-2.05	-16.27	5.34	0.53
5261	Cc1c[nH]c2c1cccn2	C14984918	-12.46	-3.62	-10.86	5.3	-3.28
5262	C(=N/O)C(=O)C=N/O	C16980630	-12.46	-7.25	-16.85	9.72	1.91
5263	c1cc(c(cc1C#N)F)C1[NH3+]	C19502678	-12.46	-0.87	-14.88	5.1	-1.81
5264	c1cc(cc(c1)O)CN=C=O	C19730729	-12.46	-1.51	-17.17	5.69	0.52
5265	CN(c1cc[nH+]cc1)N	C19735433	-12.46	1.08	-16.31	3.96	-1.19
5266	c1ccc(cc1)CNCC(F)(F)F	C19807542	-12.46	-0.83	-11.25	2.99	-3.37
5267	c1ccc(c(c1)CC(=O)N)F	C33029051	-12.46	-2.17	-17.69	8.77	-1.37
5268	CCc1ccccc1C	M1995A041	-12.46	-0.67	-8.38	1.42	-4.82
5269	c1ccc(cc1)NC(=O)C(F)(F)F	C00170161	-12.45	-2.89	-12.12	4.22	-1.66
5270	c1cc(c(cc1)F)C(F)(F)F)N	C01706171	-12.45	-1.81	-11.87	2.81	-1.57
5271	CC(=C)CCO	C01712065	-12.45	-1.8	-11.97	1.88	-0.56
5272	Cc1nc(nc1)CCl	C01731419	-12.45	-0.59	-15.68	4.72	-0.9
5273	COCCOC(=C(F)F)F	C02530850	-12.45	-0.82	-10.14	1.45	-2.94
5274	CCC(=O)OC/C=C/C	C03074855	-12.45	-0.18	-13.72	3.49	-2.04
5275	c1csc2n1cc(n2)CO	C04262675	-12.45	-3.11	-15.69	7.45	-1.1
5276	c1c(n[nH]n1)CO	C04343262	-12.45	-3.37	-15.75	4.49	2.17
5277	c1cnc2c(c1)cn[nH]2	C04771835	-12.45	-2.74	-11.86	4.4	-2.25
5278	c1ccc(cc1)C[C@H](C)C2nc[nH]n2)O	C05487491	-12.45	-1.68	-18.47	5.28	2.42
5279	C1CCN(C1)C(=S)N	C05566863	-12.45	-0.66	-15.96	2.79	1.37
5280	CC1=C(CCCCC1=O	C05767016	-12.45	-0.78	-12.97	4.63	-3.33
5281	c1cc(cc1)/C(=C/C(=O)C(F)(F)F)/O	C12358666	-12.45	-0.33	-12.5	3.8	-3.43
5282	Cn1ccc(n1)Cl	C12370914	-12.45	-0.6	-15.02	5.13	-1.95
5283	COC(=O)COCc1cccc1	C26515754	-12.45	-1.4	-16.78	8.85	-3.13
5284	CNC(=O)c1cn[nH]c1N	C29865936	-12.45	-7.13	-15.23	8.5	1.41
5285	C(c1nnc(s1)N)Cl	C32500431	-12.45	-2.1	-16.9	7.62	-1.07
5286	CC(=O)c1ccccc1N	C00164490	-12.44	-1.71	-12.6	4.22	-2.36
5287	Cn1cccc1=O	C00331653	-12.44	-2.24	-16.45	8.72	-2.48
5288	COC(=O)COC1cccc1	C00409231	-12.44	-3.04	-11.81	6.61	-4.2
5289	C(OC(C(F)(F)F)C(F)(F)F)F	C01530810	-12.44	-0.53	-12.73	4.4	-3.58
5290	CC(C)OC(=O)C=C	C01665003	-12.44	-1.28	-11.88	3.96	-3.25
5291	CC(=C)OC	C02041033	-12.44	-0.64	-11.82	1.59	-1.58
5292	CC(=O)CCn1cncn1	C02555552	-12.44	-2.27	-12.69	6.56	-4.03
5293	CCN1C(=O)CC(=O)NC1=O	C04085830	-12.44	0.78	-18.55	5.63	-0.3
5294	Cn1c(=S)[nH][nH]c1=S	C05783563	-12.44	-2.41	-13.79	5.83	-2.07
5295	c1ccc(c(c1)Nc2nccn2)F	C06665761	-12.44	0.96	-13.7	5.91	-5.61
5296	c1c(cnc(n1)O)Br	C12360026	-12.44	-1.17	-17.55	4.06	2.21
5297	c1c(c(n1)CO)Br	C12394771	-12.44	-2.6	-14.78	4.4	0.54
5298	C/C=C/CC#N	C13526271	-12.44	-1.02	-12.7	4.27	-3
5299	Cn1cc(nc1N)O	C14246971	-12.44	-5.05	-15.76	7.46	0.92
5300	c1(c(non1)N)N=Nc2c(non2)N)N	C15938951	-12.44	-2.02	-18.16	7.18	0.56
5301	c1cc(ncc1Br)CC#N	C21993125	-12.44	-3.63	-13.75	8.4	-3.46
5302	Cc1c(c(c(n1)C)N)N	C26896001	-12.44	-5.27	-14.47	7.12	0.17
5303	c1cc2nccn2cc1Cl	C00170151	-12.43	-2.89	-10.26	4.79	-4.07
5304	c1cc(cnc1)NC=O	C00392672	-12.43	-1.71	-18.31	7.34	0.26
5305	Cc1c(ccc1=O)O	C01293553	-12.43	-3.65	-16.53	8.84	-1.09
5306	Cn1c(=O)c(c[nH]c1=O)F	C01571650	-12.43	-4.17	-17.33	9.61	-0.54

5307	c1ccc(cc1)CC(=O)C=O	C01577749	-12.43	-0.7	-20.03	10.27	-1.97
5308	CCOC(=O)C(C(C(F)(F)F)(F)F)(F)F	C01666909	-12.43	2.02	-11.16	1.67	-4.95
5309	C1C=CCC1O	C01721045	-12.43	-2.03	-11.92	1.99	-0.46
5310	CC[C@@H](C=C)O	C02034403	-12.43	-0.18	-12.49	1.22	-0.98
5311	c1cc(c(c1)Cl)OF	C02382268	-12.43	-0.3	-15.81	3.67	0.02
5312	CCOC1ccc(c1)F	C02567870	-12.43	-1.81	-11.99	3.46	-2.09
5313	C1CNn2c(nnn2)N1	C03163359	-12.43	-3.34	-17.34	8.46	-0.22
5314	c1c(=O)[nH]c(nc1F)N	C05037825	-12.43	-5.41	-17.23	10.67	-0.45
5315	CCOc1nccc(n1)[O-]	C05285461	-12.43	-3.22	-15.04	5.68	0.16
5316	Cc1c[nH]c([nH+])C	C05425079	-12.43	-3.44	-13.06	6.16	-2.09
5317	[H]N=C(N(C)C)Cl	C05508944	-12.43	-1.79	-12.62	1.93	0.05
5318	c1cc(oc1)c2cccc2	C05843207	-12.43	1.09	-16.28	4.81	-2.05
5319	C1CSC(=NC1=O)N	C12651529	-12.43	-1.99	-15.17	5	-0.28
5320	c1c(nc(s1)Cl)CO	C15444551	-12.43	-2.36	-13.42	3.13	0.22
5321	CCc1ccc(s1)CC#N	C19440060	-12.43	-2.23	-11.27	5.89	-4.81
5322	c1cc(c(nc1CBr)N)[N+](=O)[O-]	C21985814	-12.43	-3.8	-12.15	6.11	-2.59
5323	C=CC(=O)OCCC#N	C01561512	-12.42	-1.94	-14.96	7.65	-3.17
5324	c1c(c(=O)[nH]c(=O)[nH1])Cl	C01646314	-12.42	-5.04	-16.81	8.99	0.44
5325	c1cc(c(cc1F)F)C=O	C02004034	-12.42	-1.29	-15.14	7.24	-3.24
5326	C/C=C/BrO	C03070145	-12.42	-3.2	-13.12	2.49	1.41
5327	Cn1nnc1SCC#N	C05749026	-12.42	-0.33	-18.14	8.23	-2.18
5328	CC(=O)/C=C/Cc1ccc1	C12370861	-12.42	-1.42	-13.25	6.45	-4.21
5329	c1cc(c(c1)F)F)NC(=S)N	C16125756	-12.42	-2.19	-16.04	8.62	-2.81
5330	CC[C@H]1[C@H](O)CC	C17059632	-12.42	-0.44	-12.27	2.47	-2.19
5331	C1[C@H]1[C@@H](C@H)1F)C(=O)Cl	C21989319	-12.42	-1.05	-13.06	4.25	-2.55
5332	CC(=O)/C=C/C)Cl	C22000861	-12.42	0.77	-16.65	6.11	-2.64
5333	c1ccc(cc1)Nc2ncccc2	C00282566	-12.41	1.06	-16.91	6.31	-2.87
5334	C=COCCCI	C01586527	-12.41	0.02	-13.15	3.09	-2.36
5335	CC[C@H](N+)(=O)[O-]Cl	C01586658	-12.41	-0.41	-12.16	2.92	-2.76
5336	CCOCC	C02031623	-12.41	-0.07	-11.22	1.24	-2.36
5337	CCOC(=O)CCN=C=O	C02555344	-12.41	-2.88	-12.56	3.7	-0.67
5338	CC(=O)OCCC#N	C04804419	-12.41	-1.55	-14.37	5.65	-2.13
5339	C1COCC=C1Cl	C05104113	-12.41	-0.02	-14.46	1.81	0.26
5340	COc1ccc2c(c1)[nH]n2	C05115788	-12.41	-3.66	-13.76	5.79	-0.79
5341	C=CC[C@H]1[C@H](C(F)F)F)O	C08698314	-12.41	-1.56	-11.74	2.02	-1.14
5342	c1c(cc(cc1F)Br)O	C12957254	-12.41	-0.7	-12.25	2.32	-1.77
5343	c1cc(c(cc1N))O	C14628844	-12.41	-1.11	-13.74	3.04	-0.59
5344	c1cc(nc2c1cc[nH]2)F	C14984906	-12.41	-2.07	-13.6	6.05	-2.79
5345	c1ccc(c(c1)C/C(=N/O)N)F	C16082806	-12.41	-1.78	-16.55	7.34	-1.43
5346	C/C=C/C=C/N/O	C17147402	-12.41	-1.25	-14.08	4.28	-1.37
5347	CN1C(=O)C(=O)N(C1=O)CC#N	C20296437	-12.41	-0.67	-19.43	8.87	-1.18
5348	c1nc2ncccc1N	C00167784	-12.4	-2.8	-16.12	9.93	-3.42
5349	CC(=O)NCC(=O)OC	C00399511	-12.4	-0.99	-16.65	5.57	-0.33
5350	c1c(nc(nc1N)N)N	C01511136	-12.4	-4.72	-14.99	5.65	1.66
5351	Cc1nnc(s1)[N+](=O)[O-]	C01615110	-12.4	-2.8	-14.02	7.14	-2.73
5352	C1CCSC1	C01680812	-12.4	-0.14	-11.24	1.88	-2.9
5353	C1C[C@H](C=C1)C#N	C01765792	-12.4	-1.17	-13.29	3.94	-1.88
5354	c1ccc(c(c1)c2cccc2)N	C02525621	-12.4	-1.13	-14.63	3.67	-0.31
5355	c1cc(c(c1)F)[N+](=O)[O-]F	C02557001	-12.4	-3.29	-15.2	8.47	-2.38
5356	CC1=CSCCO1	C04887560	-12.4	-0.39	-14.42	2.69	-0.27
5357	Cc1ccc(c(=O)[nH]1)C#N	C08612407	-12.4	-1.61	-17.5	6.57	0.14
5358	c1c(nc[nH]c1=O)N	C08613061	-12.4	-3.23	-16.79	5.3	2.32
5359	c1cc2c(cc1O)nsn2	C12341371	-12.4	-2.81	-14.89	5	0.3
5360	CC(=O)N=C(N)SC	C15024454	-12.4	-4.01	-13.44	5.28	-0.23
5361	c1cc(sc1N=C=O)Br	C19432378	-12.4	-2.17	-9.72	1.23	-1.74
5362	c1csc2c1[C@@H](C2)Cl	C19727151	-12.4	-0.3	-10.09	2.43	-4.44
5363	Cc1cc(ccc1S)F	C20247138	-12.4	-0.19	-9.7	1.49	-4
5364	c1cc(c(c1)F)OC(F)(F)F	C22057469	-12.4	1.25	-15.05	4.87	-3.47
5365	CC(=O)Nc1cc(ccc1F)F	C00398779	-12.39	-1.42	-14.16	5.99	-2.8
5366	CCC(=O)OCCI	C01680716	-12.39	-0.83	-14.4	4.21	-1.38
5367	CC(=CC(=O)N)C	C01684064	-12.39	-2.54	-14.46	4.73	-0.12
5368	Cc1ccc(cc1)SC	C01693361	-12.39	0.52	-14.31	2.29	-0.9
5369	Cc1cc(cs1)Br	C02528624	-12.39	-0.94	-13	1.55	0
5370	C1(=C(C(=O)SC1=O)Cl)Cl	C05478084	-12.39	1.11	-12.38	1.02	-2.14
5371	CC(=O)CSc1cn[nH]n1	C07344306	-12.39	-2.46	-14.72	5.73	-0.95
5372	Cc1c(c(on1)N)I	C12481600	-12.39	-3.48	-11.88	3.31	-0.34
5373	c1cc(ccc1C=C)COCl	C13542609	-12.39	-1.57	-11.51	3.11	-2.42
5374	c1cc2ncccc1N	C18555973	-12.39	-3.31	-13.77	6.69	-2
5375	c1cc(c(cc1F)C)N)F	C19482514	-12.39	3.66	-17.2	2.56	-1.41
5376	CCNc1ccc(c1)F)F	C19918384	-12.39	-3.41	-9.52	3.81	-3.26
5377	Cc1cc(c([nH+]c1)Cl)[O-]	C21981922	-12.39	-2.63	-12.68	3.83	-0.9
5378	c1c(cnc(c1[N+](=O)[O-])F)Br	C21981951	-12.39	-2.15	-11.34	4.08	-2.98
5379	Cc1ccc(nc1)C(F)F)F	C21985793	-12.39	-1.76	-11.33	4.13	-3.43
5380	Cc1cc(on1)C(=O)C	C26506537	-12.39	1.44	-15.46	4.02	-2.4
5381	c1cc(sc1)C(=C)C(=O)[O-]	C26515478	-12.39	0.76	-16.13	5.58	-2.6
5382	CC(=O)Cc1cccs1	C00163136	-12.38	-1.55	-12.72	5.64	-3.75
5383	c1cc(n2cccnc2c1)N	C00337657	-12.38	-1.6	-15.03	6.93	-2.67
5384	C=CC1OCCO1	C00396113	-12.38	0.15	-14.35	3.01	-1.2
5385	CSC1=[NH+][C]CN1	C01634181	-12.38	-1.08	-13.93	2.79	-0.16
5386	c1cc(c(cc1N)C#N)F	C02565103	-12.38	1.44	-17.2	5.48	-2.1
5387	CC(=O)C1c(ccc1F)F	C02579282	-12.38	-0.18	-13.32	5.55	-4.43
5388	c1c(ncs1)CC#N	C02584053	-12.38	-1.49	-17.79	7.92	-1.01
5389	C1=Nc2c(non2)NN=C1	C03204866	-12.38	-4.53	-20.33	11.88	0.59
5390	CCOC(=O)[C@H]1[C@@H](C@H)1C=O	C04528550	-12.38	-0.81	-14.99	6.74	-3.31
5391	CN(C(=O)OCCC)N=O	C04804540	-12.38	-0.17	-15.67	4.5	-1.04
5392	c1cc(c(=O)[nH]c1)F	C08698105	-12.38	-3.16	-15.38	5.23	0.93
5393	c1c[nH]c(=O)c2c1ccc2	C16972974	-12.38	-2.15	-17.14	6.19	0.72
5394	c1cc(c(c1)F)Cn2c(ccn2)N)F	C19689160	-12.38	1.71	-17.09	6.91	-3.91
5395	COCC1nc(cs1)CCl	C26511167	-12.38	-2.25	-13.18	5.09	-2.04
5396	Cc1csc(n1)CF	C32500872	-12.38	-2.03	-12.27	4.34	-2.42

5397	c1cc(ncc1Br)Br	C00343301	-12.37	-1.58	-13.95	2.19	0.97
5398	CC(=O)COC(=O)C	C01640814	-12.37	-0.35	-15.76	6.59	-2.84
5399	COCc1ccco1	C01668230	-12.37	-1.16	-13.88	3.83	-1.16
5400	c1cnn(c1)CO	C01682023	-12.37	-4.98	-13.41	4.96	1.04
5401	C1=CC(=O)N(C1=O)CSC#N	C01868507	-12.37	0.48	-19.39	8.38	-1.86
5402	COC(=O)CN=C=O	C02547543	-12.37	-0.49	-12.04	2.14	-1.98
5403	COC(=O)CN=C=O	C03139118	-12.37	-2.15	-15.6	5.86	-0.48
5404	c1cc(ccc1N)[N+](=O)[O-]	C03860644	-12.37	-3.35	-13.61	6.72	-2.13
5405	c1cn(c(=O)[nH]c1=O)C/C=N/O	C04032019	-12.37	-2.64	-21.85	10.25	1.87
5406	c1cc(cc(c1)F)/C(=N/O)/N	C06863049	-12.37	-4.95	-13.98	5.76	0.79
5407	COC(=O)CN1C(=O)CSC1=O	C08092047	-12.37	1.88	-19.93	7.76	-2.08
5408	Cc1ccccc1N1CC#N	C13281490	-12.37	-6.07	-5.38	3.83	-4.74
5409	CS(=O)(=O)n1cc(cn1)Cl	C14218611	-12.37	-1.87	-18.95	8.61	-0.16
5410	C1=C[NH+]=C/C(=C/N=O)/N1	C17423937	-12.37	-3.67	-16.36	7.1	0.55
5411	c1cnc(nc1)NCC(F)(F)F	C19231842	-12.37	-2.26	-10.8	4.3	-3.61
5412	CC1=C(C(=O)CC1)O	C21300156	-12.37	-2.4	-14.73	5.53	-0.77
5413	CC(=O)OC	C01699947	-12.36	-0.86	-12.96	3.66	-2.21
5414	c1ccc(cc1)NCCCI	C01712525	-12.36	-1.15	-9.79	2.28	-3.69
5415	CC(=O)C[C@H]1CCC=C1	C02036659	-12.36	-0.89	-11.46	3.97	-3.98
5416	C=CCCO	C02038899	-12.36	-0.13	-13.75	3.99	-2.47
5417	c1c(ncs1)CO	C02527711	-12.36	-2.16	-14.93	4.04	0.68
5418	CC(=O)OCCCI	C04887626	-12.36	-1.1	-12.92	4.47	-2.81
5419	C=C/C=C/C#N	C05542734	-12.36	-1.27	-13.97	5.22	-2.34
5420	COC/C(=N/O)/N	C06453315	-12.36	-3.44	-14.97	4.06	1.99
5421	c1cnc(c1)C=O)Cl	C12958751	-12.36	-2.28	-11.31	3.36	-2.12
5422	CCOc1[nH]c(=O)c(cn1)F	C14982788	-12.36	-3.54	-15.84	6.88	0.15
5423	c1cc2c(nc1)NC(=O)C2	C14984260	-12.36	0.1	-16.96	6.31	-1.81
5424	CC/C=C/Cn1cnc1	C15776518	-12.36	-1.48	-11.42	5.59	-5.05
5425	C1[C@@H]2C=C[C@@H]2CC1=O	C17120047	-12.36	-0.83	-11.22	2.9	-3.21
5426	COC1ccc(c(c1)N)F	C21304447	-12.36	-2.09	-12.82	3.83	-1.28
5427	c1nnc(n1)CCO	C21983799	-12.36	-2.77	-16.38	5.84	0.95
5428	c1ccc2c(c1)[nH]c(n2)CO	C00158650	-12.35	-4.89	-13.7	6.74	-0.5
5429	C1C[C@H](C=C1)CO	C01767933	-12.35	-1.27	-12.15	2.14	-1.07
5430	Cn1cc(cn1)C#N	C02537518	-12.35	-0.17	-16.55	6.32	-1.95
5431	C(CBr)N=C=O	C02556964	-12.35	0.29	-14.45	1.86	-0.06
5432	Cn1ccnc1Br	C02577853	-12.35	-2.1	-12.2	4.75	-2.81
5433	[C@@H](C)[O]C[C@@H](F)(F)C(F)(F)F	C04266028	-12.35	-2.33	-10.9	4.1	-3.22
5434	C1(=S)NCC(=S)NN1	C05566462	-12.35	-2.9	-16.35	3.67	3.24
5435	c1nc(c(cn1)Cl)N[O-]	C08964409	-12.35	-4.53	-14.67	4.38	2.46
5436	CCNC1=NCCCS1	C15417787	-12.35	-0.89	-12.07	2.6	-2
5437	C1CNC(=NH2+)NC1=O	C16990869	-12.35	-3.85	-15.68	6.73	0.46
5438	c1cc(=O)[nH]c(c1[N+](=O)[O-])N	C21985741	-12.35	-4.84	-19.16	11.42	0.22
5439	Cc1c(nc(nH1)Cl)C	C22126106	-12.35	-1.6	-13.57	5.29	-2.48
5440	C(#N)Sc1c(nc(n1)N)N	C32106105	-12.35	-3.5	-17.96	9.33	-0.22
5441	c1ccc2c(c1)OC(O2)(F)F	C00157363	-12.34	0.82	-16.31	4.2	-1.05
5442	Cc1c(nc(nH1)O-)C	C00162747	-12.34	-4.4	-15.08	5.28	1.86
5443	Cc1ccc(c1)O)N	C01433370	-12.34	-3.64	-11.43	2.99	-0.26
5444	Cc1ccc(c1)N=C=O	C01845941	-12.34	-1.41	-10.43	1.91	-2.4
5445	C(CC(=O)Cl)CCI	C02242611	-12.34	-1.05	-12.57	4.32	-3.03
5446	Cc1cc(nc1)F)N	C02384018	-12.34	-1.79	-16.27	5.11	0.61
5447	c1c(c(cc1)F)F)C=O	C04290143	-12.34	-1.76	-13.84	6.04	-2.78
5448	c1cc(c(nc1)C=O)N	C04352694	-12.34	-5.65	-15.55	9.23	-0.38
5449	C[C@H]([N+](=O)[O-])Cl	C04409862	-12.34	-0.5	-12.94	3.35	-2.25
5450	C[C@H]1CN(C(=NH2+))S1C	C05125599	-12.34	0.01	-14.23	3.94	-2.07
5451	c1c(c(n1)C(=S)N)N)C#N	C06495096	-12.34	-1.84	-17.09	7.9	-1.32
5452	C=CC(=O)OC/C=C)Cl	C08580935	-12.34	-0.3	-13.14	4.73	-3.64
5453	CCOC(=S)S	C12358685	-12.34	-1.06	-13.57	4.17	-1.88
5454	c1csc2n1c(cn2)C#N	C13211756	-12.34	-0.25	-14.85	6.11	-3.35
5455	CCc1ccc(o1)C#N	C15783907	-12.34	-0.2	-12.54	3.92	-3.52
5456	CC(=O)OCc1ccc(nH1)c1=O	C16998256	-12.34	-0.67	-19.15	7.85	-0.38
5457	CN(C)c1nc(nH1)N=[N+]=[N-]	C17024977	-12.34	1.16	-15.95	5.28	-2.84
5458	CCNC(=S)N	C18191765	-12.34	-1.13	-12.03	1.81	-1
5459	c1ccc2c(c1)c(c(nH2)N)C=O	C19087881	-12.34	-3.52	-11.3	4.45	-1.97
5460	c1c(nH1)n1N	C21303334	-12.34	-5.68	-13.26	5.47	1.13
5461	Cc1c(ncn1)C	C00003183	-12.33	-0.65	-14.39	4.23	-1.52
5462	COc1cccc(c1)N	C00157531	-12.33	-2.01	-12.34	3.28	-1.25
5463	CCn1c(cc(=O)[nH]c1=O)N	C00399854	-12.33	-4.42	-17.6	9.81	-0.11
5464	c1cc(cc(c1)O)[N+](=O)[O-]	C01576887	-12.33	-3.04	-13.66	6.12	-1.75
5465	c1c(ncs1)CONC(=O)N	C01705603	-12.33	-4.62	-18.89	10.34	0.84
5466	C[C@H]1CCC(=O)C1	C02039266	-12.33	-0.63	-12.01	3.13	-2.82
5467	C(=NC)Cl)Cl)Cl)O	C04262410	-12.33	-0.18	-12.17	0.45	-0.42
5468	CC1=NCC[C@H]1[N+](=O)[O-]	C05306562	-12.33	-0.96	-17.4	4.54	1.48
5469	c1nc(nn1)CC(F)F[N+](=O)[O-]	C12397049	-12.33	-2.81	-16.14	12.32	-5.71
5470	c1c(nH1)c(=O)[nH]c1=S)[O-]	C17779396	-12.33	-3.47	-16.8	6.86	1.08
5471	CCc1ccn(n1)C	C26547541	-12.33	-0.32	-14.06	4.67	-2.62
5472	Cc1cc[nH+]c(c1)N[N+](=O)[O-]	C01605247	-12.32	-5.03	-17.13	13.02	-3.18
5473	Cc1ccc(cc1)NO	C01607220	-12.32	-3.52	-13.65	4.16	0.69
5474	C(#N)/C(=C/C#N)N)N	C02039806	-12.32	-2.62	-15.08	4.43	0.95
5475	COC(=O)OCC=C	C02504725	-12.32	-0.9	-12.21	3.43	-2.64
5476	c1csc(n1)C=O	C02512364	-12.32	-2.17	-16.71	7.62	-1.05
5477	c1cn(nc1)C(=O)NN(C)F)F	C02521253	-12.32	-1.53	-20.14	8.6	0.75
5478	c1(c(c(c(c1)F)Cl)F)F)O	C02530822	-12.32	0.21	-13.43	2.29	-1.4
5479	C=CCOCC(C(F)F)(F)F	C02576921	-12.32	-1.18	-10.95	2.88	-3.08
5480	CSC(=NH2+)N	C04676170	-12.32	-2.72	-11.89	2.12	0.17
5481	CC(=O)CCn1ccnc1	C05480858	-12.32	-2.21	-15.3	6.53	-1.34
5482	C/C(=N)OC(=O)C/C(=O)C	C05543789	-12.32	-1.63	-14.16	6.4	-2.93
5483	CC1=C[C@H]([OC1=O)O	C05665331	-12.32	-2.54	-15.46	6.8	-1.12
5484	C(#N)N=C(N)O	C06661263	-12.32	-7.48	-12.23	5.82	1.57
5485	c1cc(c(c1)F)C(F)F)O	C08100952	-12.32	-2.31	-11.4	3.39	-2
5486	CCn1ccc(c1)C=O	C08728204	-12.32	-1.47	-13.46	6.07	-3.47

5487	CC(C)CCN=C=O	C11802388	-12.32	0.25	-13.36	1.66	-0.87
5488	c1cc2c(c[nH]c2nc1)C#N	C14984912	-12.32	-4.86	-11.91	7.54	-3.09
5489	C(C(=NH2+)N)OCC(F)(F)F	C19427472	-12.32	-5.84	-13.85	7.11	0.24
5490	c1cc(c(=O)oc1)I	C21989735	-12.32	-0.36	-16.69	8.24	-3.51
5491	c1nncn1NC(=[NH2+])N	C26953640	-12.32	-2.53	-18.56	10.95	-2.19
5492	c1cnc1Cn2c(ccn2)N	C00819617	-12.31	0.15	-16.93	6.8	-2.33
5493	#C#CC1c1ccccc1O	C01639886	-12.31	-2.15	-15.01	5.53	-0.68
5494	c1ccc(cc1)C[n+] ₂ cc(on2)[O-]	C01682005	-12.31	-2.41	-14.45	9.52	-4.96
5495	CCC(=O)Br	C01846004	-12.31	-0.68	-12.08	2.5	-2.04
5496	Cc1c(oc(=O)o1)C	C02504803	-12.31	-2.34	-13.24	6.34	-3.06
5497	CC(=O)Cc1ccc(cc1F)F	C02579281	-12.31	-1.85	-12.33	6.34	-4.46
5498	CC(=O)n1c(nc(n1)N)N	C03163360	-12.31	-2.43	-12.6	4.98	-2.26
5499	Cc1ccnnc1C(=O)N	C03848319	-12.31	-3.45	-14.43	5.64	-0.07
5500	c1(nc(nH)n1)[S-])C(F)(F)F	C04716371	-12.31	-7.14	-14.47	11.45	-2.14
5501	c1ccc(cc1)NNC(F)(F)F	C05224748	-12.31	-0.31	-14.56	1.88	0.68
5502	c1cc(c(nc1)Cl)C(=N/O)/N	C06658112	-12.31	-4.16	-15.79	7.67	-0.03
5503	Cc1ccn(n1)CCl	C09547120	-12.31	-2.38	-10.6	3.98	-3.31
5504	C1C/C(=C(\C(F)(F)F)[O-])/C(=O)C1	C12394374	-12.31	-4.03	-8.93	3.42	-2.77
5505	c1(c(nH)nc1N)C(F)(F)Br	C12395922	-12.31	-2.2	-11.9	2.68	-0.9
5506	CCC(=[NH2+])NN	C16082678	-12.31	-2.88	-12.77	3.01	0.33
5507	c1ccc(cc1)N=C=S	C00164776	-12.3	-0.93	-11.96	4.62	-4.04
5508	COc1ccc(cc1)Cl	C00388374	-12.3	0.98	-14.74	2.26	-0.81
5509	C/C=C/[C@H]1C=CC(=O)O1	C01668307	-12.3	-0.78	-15.08	7.16	-3.6
5510	C=CCN1C(=O)C=CC1=O	C01720445	-12.3	-0.89	-14.91	5.81	-2.31
5511	C1CCC(C1)CO	C01845720	-12.3	-3.28	-9.29	1.81	-1.53
5512	c1cc2cnc1cc2	C01847613	-12.3	-1.28	-14.41	5.74	-2.35
5513	c1cnn(c1)CC#N	C02538878	-12.3	-2.06	-17.43	9.43	-2.25
5514	C=C=C/[P@@H]1(=O)[O-]	C05377186	-12.3	-5.79	-13.69	7.96	-0.78
5515	C(=C/C#N)C=C/C#N	C05409892	-12.3	-1.97	-15.53	8.58	-3.39
5516	CCOC(=O)O	C05856362	-12.3	-4.68	-11.25	4.23	-0.61
5517	Cc1nccn1C	C08294951	-12.3	-1.06	-14.07	5.46	-2.62
5518	Cc1c(c[nH]n1)/C=N/O	C12525130	-12.3	-3.06	-15	5.3	0.46
5519	Cc1[nH]c2cc(ccc2n1)F	C12672023	-12.3	-4.06	-11.79	6.73	-3.19
5520	CC1NNC(=S)NN1	C18204142	-12.3	-0.97	-15.43	3.8	0.31
5521	CCc1cccc1S	C19735106	-12.3	-1	-8.48	1.66	-4.49
5522	c1ccc(cc1F)NCCO)F	C20045173	-12.3	-2.35	-13.6	4.35	-0.69
5523	c1c(nsn1)N	C26479221	-12.3	-4.19	-14.2	5.35	0.74
5524	CCNc1cc(ccn1)Cl	C32914833	-12.3	0.75	-12.76	2.69	-2.98
5525	COc(=O)CSCC=C	C01626921	-12.29	-0.82	-13.03	5.17	-3.62
5526	C1CN=C(N1)Cl	C01670679	-12.29	-0.89	-14.29	2.76	0.14
5527	COC(=O)C[C@@H]1CSCC1=O	C05759397	-12.29	-0.36	-16.27	8.28	-3.94
5528	c1(c[nH]c(=O)[nH]c1=O)N/O	C05783668	-12.29	-5.85	-18.88	7.88	4.56
5529	C(c1c(non1)N)Oc2c(non2)N	C06691161	-12.29	-2.7	-21.26	9.18	2.5
5530	c1c(cnc(c1[N+](=O)[O-])Cl)F	C08698159	-12.29	-2.07	-12.82	3.68	-1.08
5531	c1cc([nH]c1)C(=O)CC#N	C14007813	-12.29	-2.04	-17.94	10.32	-2.63
5532	c1c(c(nH)1)N=[N+]=[N-])C(=O)N	C16952135	-12.29	-3.23	-19.09	7.46	2.57
5533	C=CCn1c(nnn1)N	C16954942	-12.29	-3.3	-16.07	8.88	-1.79
5534	CC(=O)OC/C=C/Cl	C17311824	-12.29	-1.28	-12.46	4.59	-3.13
5535	c1ccc(cc1)CNC(=S)NN)F	C20426753	-12.29	1.66	-21.89	10.74	-2.8
5536	#CCc1cc(ccc1F)N	C21984820	-12.29	0.45	-16.47	6.42	-2.7
5537	#CCCN1CCCC1=O	C21993361	-12.29	0.27	-16.95	7.24	-2.85
5538	c1cnn(c1)C[C@H]2CO2	C22215419	-12.29	-2.76	-14.27	6.03	-1.29
5539	COc1cncnc1N	C26440874	-12.29	-1.44	-15.68	5.85	-1.02
5540	CC(C)COC(=O)Cl	C00388452	-12.28	1.16	-11.84	1.65	-3.24
5541	c1ccc(cc1)CCC(=O)N)O	C01433352	-12.28	-2.33	-16.81	6.67	0.19
5542	CC(=O)OCCBr	C01566591	-12.28	0.36	-14	4.29	-2.93
5543	c1c[nH]c2c1ncnc2N	C01575342	-12.28	-3.02	-16.19	8.08	-1.15
5544	COCC(=O)Cl	C01631211	-12.28	-1.56	-13.51	4.36	-1.57
5545	Cc1nccnc1)Cl	C01644965	-12.28	-2.36	-11.33	3.72	-2.3
5546	C(CC=O)CCl	C01681994	-12.28	-0.98	-13.34	4.53	-2.49
5547	CC(=O)OCCl	C01845923	-12.28	-1.35	-13.99	4.38	-1.31
5548	CCCC#CC#N	C01873910	-12.28	-0.29	-12.8	3.52	-2.71
5549	COC(=O)CCC(F)(F)F	C02525281	-12.28	-0.18	-12.54	3.48	-3.04
5550	c1c(cc(c1F)F)F)CC#N	C02575057	-12.28	-2.41	-15.49	9.45	-3.83
5551	c1cc(n(c1)CCC#N)C=O	C02577970	-12.28	-2.19	-16.09	9.83	-3.83
5552	CNC(=S)Nc1ncco1	C05566430	-12.28	-1.47	-16.8	5.55	0.44
5553	CCc1csc(n1)[S-]	C05599578	-12.28	-1.55	-14.62	3.18	0.7
5554	C=C/C=C/CCC(=O)C=[N+]=[N-]	C05665619	-12.28	0.32	-16.32	6.04	-2.33
5555	Cc1c(=O)[nH]c(=O)[nH]n1	C11666592	-12.28	-1.14	-18.58	5.83	1.61
5556	C1CC1([NH+])=c ₂ /c(c(c2=O)[O-])[O-]	C15768417	-12.28	-1.41	-16.8	5.02	0.91
5557	c1cnc(nH)c1=O	C18081263	-12.28	-3.77	-15.81	8.27	-0.96
5558	C1CCC(C1)CCC=O	C19089807	-12.28	-1.75	-10.4	3.84	-3.97
5559	CCC(=O)c1cncn1C	C19091708	-12.28	0.05	-13.15	4.02	-3.18
5560	c1cnc(nc1)NO	C26441007	-12.28	-3.11	-17.23	8.75	-0.7
5561	c1cc(ccc1CCO)O	C00164581	-12.27	-1.83	-14.32	3.68	0.2
5562	Cc1ccc(o1)C=O	C00900814	-12.27	-1.85	-15.17	7.52	-2.76
5563	c1c(=O)[nH]c(nc1Cl)[O-]	C01494932	-12.27	-1.39	-16.95	5.34	0.73
5564	c1c2c(nc(n1)N)SCC2	C01703705	-12.27	1	-17.02	6.37	-2.62
5565	c1cc(c(c1)F)C#N)O	C02586041	-12.27	0.25	-18.09	7.06	-1.49
5566	c1csc2c1c(=O)[nH]cn2	C04023433	-12.27	-2.61	-17.21	9.65	-2.1
5567	c1csc(n1)NCCO	C13539253	-12.27	-3.61	-14.12	5.03	0.43
5568	Cn1c(c(sc1=S)C#N)N	C13547304	-12.27	-3.7	-14.05	7.93	-2.46
5569	CCC/C(=N/O)/N	C15020970	-12.27	-2.72	-13.8	4.04	0.21
5570	CCOC(=O)[C@H]1[C@H]1F	C15442312	-12.27	-1.49	-13.56	6.28	-3.51
5571	C=C(Cc1ccccc1)C=O	C21998734	-12.27	0.12	-13.7	5.93	-4.63
5572	C=Cn1cnc1C(=O)C(F)(F)F	C32620402	-12.27	1.23	-14.37	4.9	-4.04
5573	Cc1ccsc1C=O	C00157152	-12.26	0.73	-15.24	5.14	-2.9
5574	c1c(c(=O)[nH]c(=O)[nH]1)N	C01236370	-12.26	-3.72	-19.08	7.96	2.58
5575	C1CC=C[C@H](C1)c2nc(nc(n2)N)N	C01673374	-12.26	-0.11	-13.06	5.02	-4.11
5576	CCC(=O)Oc1ccccc1	C01694849	-12.26	-0.82	-11.76	5.26	-4.95

5577	CSCCC=O	C01733699	-12.26	-1.29	-13.41	4.8	-2.36
5578	COC(=O)CSCCCI	C01737053	-12.26	-0.58	-12.75	4.75	-3.68
5579	CCCSC	C02038334	-12.26	-0.37	-10.01	1.21	-3.08
5580	COCCNC(=O)C(F)F	C03165342	-12.26	-0.34	-15.78	4.01	-0.15
5581	C/C(=C/C(=O)OC)/OC(=O)C	C04583015	-12.26	-0.36	-14.92	5.92	-2.9
5582	C(#N)[C@H](F)	C08698381	-12.26	-0.15	-12.92	3.17	-2.36
5583	CC(=N/N=C([NH-])/N[N+](=O)[O-])C	C13136442	-12.26	-0.91	-15.23	6.87	-2.99
5584	C/C=C/C1OCCO1	C16970435	-12.26	0.24	-13.56	2.85	-1.79
5585	Cc1ccc(nn1)Br	C19872637	-12.26	-1.54	-13.9	5.42	-2.24
5586	Cn1nc(nn1)[N-][N+](=O)[O-]	C20428581	-12.26	0.02	-17.98	7.92	-2.22
5587	CC(=O)c1ccncc1	C01555299	-12.25	-2.53	-12.71	5.34	-2.36
5588	c1cc(sc1Br)Br	C01673411	-12.25	-0.84	-13.07	0.69	0.96
5589	c1cc2c(cc1F)[nH]c(=O)o2	C01728885	-12.25	-1.51	-15.76	5.33	-0.31
5590	COC(=N)C(F)F	C04897098	-12.25	-1.98	-13.1	2.11	0.71
5591	c1cc(c(cc1F)F)C/C(=N/O)/N	C06453297	-12.25	-1.61	-17.22	6.29	0.29
5592	c1c(c([nH]c(=S)n1)[O-])Cl	C06565555	-12.25	-4.61	-15.82	9.73	-1.55
5593	CCC(=O)Cc1c[nH]nc1	C12359063	-12.25	-1.73	-15.54	7.07	-2.05
5594	CS/C(=NIC#N)/S	C12405130	-12.25	-1.84	-12.23	5.38	-3.57
5595	CCc1[nH]c(nn1)[S-]	C14128798	-12.25	-2.96	-15.21	8.39	-2.47
5596	C1C(=NNC1=O)N	C18145753	-12.25	-6.06	-15.21	5.43	3.6
5597	c1c(c(nc1Br)F)N	C19800981	-12.25	-0.56	-14.63	3.94	-0.99
5598	c1cc(ncn1)S(=O)(=O)N=[N+]=[N-]	C32602802	-12.25	1.29	-20.74	5.55	1.65
5599	c1cc(c(c1)F)c2nccn2)N	C00159344	-12.24	-1.07	-17.69	7.88	-1.35
5600	c1cc(ncc1CC#N)Cl	C01387124	-12.24	-2.91	-14.77	8.73	-3.28
5601	CC(=C)CC#N	C01635623	-12.24	-1.19	-12.81	4.29	-2.53
5602	CC(=C)C(=O)OC	C01680392	-12.24	-1.95	-11.79	3.96	-2.46
5603	CCOCCI	C02031622	-12.24	-0.8	-11.61	2.31	-2.14
5604	c1nc(c(c(n1)N)NC=O)N	C02558610	-12.24	-2.97	-19.19	8.96	0.98
5605	COC(=O)C(C(F)F)F(F)F	C02565738	-12.24	1.52	-13.48	4.34	-4.61
5606	c1(=O)c(=S)[nH]nc([nH]1)[O-]	C03954265	-12.24	-5.36	-18.83	7.25	4.7
5607	Cc1cc(nn1)[O-]	C05296681	-12.24	-1.66	-14.66	6.24	-2.16
5608	C/C(=C1/CCCCC1=O)/[O-]	C18037976	-12.24	-4.11	-9.94	4.22	-2.41
5609	COc1ccc(cn1)N=C=S	C19840574	-12.24	-0.13	-13.66	3.07	-1.52
5610	c1cc(ccc1F)SCC(=NH2+)N	C19848161	-12.24	1.18	-19.41	8.36	-2.38
5611	c1c(c(cc1Cl)F)Br)N	C21300420	-12.24	-4.17	-8.46	3.03	-2.64
5612	C1CC=C(OC1)C#N	C26897037	-12.24	0.83	-14.84	4.15	-2.38
5613	CC(=O)Nc1ccc(cc1)F	C00145421	-12.23	-1.05	-15.21	6.75	-2.72
5614	c1cc(c2nccnn2c1)N	C01385374	-12.23	-2.63	-14.72	7.26	-2.14
5615	c1cc2nccnn2cc1N	C01597529	-12.23	-4.42	-18.47	10.86	-0.19
5616	C/C=C(C)C#N	C01676639	-12.23	-1.46	-11.85	3.96	-2.88
5617	c1c(cc1F)F)N+](=O)[O-]	C01706151	-12.23	-0.15	-12.4	2.69	-2.38
5618	CN(C)C(=O)Cl	C01712063	-12.23	-1.01	-14.29	4.14	-1.07
5619	CC(=C1C=CC=C1)C	C01719654	-12.23	-0.01	-10.34	2.52	-4.4
5620	CCC(=O)c1nccs1	C02020149	-12.23	0.83	-14.78	4.06	-2.34
5621	C/C=C/CC#N	C02037705	-12.23	-1.06	-12.76	4.6	-3.01
5622	c1cocc1C=O	C02040441	-12.23	-1.87	-15.67	6.98	-1.66
5623	Cc1cc(ccn1)Cl	C02391146	-12.23	-1.68	-9.95	2.35	-2.95
5624	c1c(sc1)CO	C02527712	-12.23	-1.64	-16.42	5.09	0.74
5625	Cn1c(cen1)C(=O)Cl	C02549378	-12.23	1.12	-15.27	3.57	-1.65
5626	CC(=O)OCC(F)F	C02557127	-12.23	-0.02	-13.33	3.82	-2.7
5627	c1c[nH]cc1C=O	C02581109	-12.23	-3.04	-15.64	8.09	-1.64
5628	C(CS)CS	C03860693	-12.23	-0.07	-11.36	1.68	-2.49
5629	C([C@H](C(F)F)F)O)Br	C04242156	-12.23	-1.01	-13	2.45	-0.66
5630	c1[nH]c(c(n1)C(=O)N)F	C04771527	-12.23	-4.52	-17.79	9.24	0.85
5631	CCS/C(=[NH+]/N)/N	C06411412	-12.23	-3.68	-14.71	2.82	3.34
5632	C[C@H](C(=O)OC)F	C06491528	-12.23	-0.6	-13.46	4.03	-2.21
5633	C/C=C/Cc1ccc(cc1)O	C08614342	-12.23	-0.47	-14.44	2.76	-0.08
5634	C1C[C@H](OC1)C(=O)Cl	C11731532	-12.23	1.9	-15.93	4.25	-2.44
5635	c1c(cnc1O)Cl	C12359952	-12.23	-1.12	-18.22	4.86	2.24
5636	c1cc(ccc1C(=O)C(=N/N)F	C16400651	-12.23	3.3	-20.95	7.4	-1.98
5637	CC([NH+]=C(N))SCC	C16911655	-12.23	-1.41	-11.21	2.47	-2.08
5638	c1cc(ccc1F)NCC(F)F	C20051071	-12.23	-3.06	-8.95	3.42	-3.64
5639	c1c[nH+]c(c1Br)O)N	C21981839	-12.23	-4.38	-12	3.87	0.29
5640	c1cccc(c1)n2cnnn2)O	C31772037	-12.23	-1.35	-17.08	8.03	-1.84
5641	Cc1cnc1C	C00003182	-12.22	-1.74	-12.62	3.9	-1.75
5642	COC1=CC(=O)CC1	C00395539	-12.22	-2.07	-14.47	6.29	-1.96
5643	Cc1ccc(cc1)OC(=S)Cl	C00395624	-12.22	0.77	-15.03	2.28	-0.23
5644	CCCC(=O)SC	C00409240	-12.22	-0.45	-13.38	2.41	-0.81
5645	CSccncc1n)N	C01675981	-12.22	-2.09	-15.65	3.86	1.66
5646	c1nc(c(n1)N)C(=O)N	C01699717	-12.22	-1.61	-18.17	4.72	2.83
5647	c1c(sc1)Br)Br	C01756180	-12.22	-0.94	-14.05	1.26	1.51
5648	C(#N)C(C(F)F)F	C01847433	-12.22	0.62	-11.67	1.2	-2.36
5649	c1(c(nc2c(n1)non2)NN)N	C02360407	-12.22	-9.59	-14.67	11.72	0.33
5650	C[C@H](C(=O)C)S	C04802667	-12.22	-1.22	-11.9	2.95	-2.04
5651	CC(=C)CNC(=S)N	C05601328	-12.22	-1.34	-16.13	2.48	2.77
5652	CO[C@H]1CN=C1	C06403193	-12.22	-2.38	-15.35	3.51	2.01
5653	CC(=O)[C@H]1C(=O)COC1=O	C06562806	-12.22	-3.26	-17.72	9.02	-0.26
5654	C=CCOC1cccc1	C08294968	-12.22	1.63	-15.19	3.67	-2.32
5655	c1c(c(n1)CCO)Br	C12357746	-12.22	-3.04	-12.64	3.85	-0.39
5656	c1cnn(c1N)CC(F)F	C12396453	-12.22	0.89	-15.48	4.15	-1.77
5657	COCc1ccncc1	C15858171	-12.22	0.24	-13.44	3.3	-2.31
5658	C/C=C/C(=O)OC(C)C	C16892842	-12.22	0.43	-12.3	3.53	-3.87
5659	c1c(cc1c1F)F)NC(=O)N	C19260055	-12.22	-4.8	-16.52	9.59	-0.5
5660	C1CCC(C1)OCC#N	C19486556	-12.22	-0.47	-14.11	5.45	-3.08
5661	c1ncc(n1)CC(C(=N/O)/N	C19503104	-12.22	-3.36	-16.75	8.61	-0.72
5662	C1CCc2c(c([nH]2)C=O)C1	C20270533	-12.22	0.37	-15.53	4.67	-1.74
5663	Cc1ccc(c1)F)NC(=O)N	C20372350	-12.22	-1.48	-18.15	8.25	-0.85
5664	[H]N=C/C1C(=CCS1)C(=O)NC	C26422384	-12.22	-2.99	-15.42	6.13	0.06
5665	COC(=O)C1cn[nH]n1	C26507098	-12.22	-0.48	-19.56	8.52	-0.71
5666	COC(=O)c1ccsc1N	C00115816	-12.21	-3.04	-11.91	4.42	-1.67

5667	c1c(c(co1)C=O)CO	C00332260	-12.21	-5.08	-13.01	5.58	0.3
5668	c1nncn1)CCO	C01557213	-12.21	-2.75	-18.2	6.83	1.91
5669	C[C@@H]1C[C@H]1C(=O)Cl	C01766063	-12.21	-1.05	-12.68	2.41	-0.89
5670	CCC(=O)OC(C)C	C02031573	-12.21	-1.51	-10.85	3.61	-3.46
5671	CC/[NH+]=C/c1ccccc1	C03083158	-12.21	-0.99	-14.06	2.71	0.13
5672	CCOC(=O)CSC(=[NH2+])N	C05315506	-12.21	-1.58	-15.35	3.62	1.09
5673	c1c(ncnc1)Cl	C06643288	-12.21	-0.34	-9.81	1.22	-3.29
5674	c1ncnc2c1C(=O)OC2=O	C08100888	-12.21	-3.01	-12.05	5.62	-2.77
5675	Cc1cc(c[nH]c1=O)Br	C08698070	-12.21	-3.96	-12.99	6.75	-2.02
5676	CC/C=C/C#N	C13525896	-12.21	-0.78	-13.33	4.79	-2.88
5677	C(C(OC(F)(F)F)(F)F)F	C14611416	-12.21	-1.79	-11.76	2.74	-1.41
5678	c1ccnc(c1)C(=O)C(F)F	C16159011	-12.21	-1.55	-12.87	5.11	-2.9
5679	C[C@H]1C=CCC1=O	C18208228	-12.21	-1.33	-13.42	5.28	-2.74
5680	Cc1cnc(s1)Br	C19046001	-12.21	-0.39	-12.42	3.02	-2.43
5681	C1CSC[C@H]1S	C20476695	-12.21	0.34	-11.6	2	-2.96
5682	c1c(ncn1)C(F)(F)F	C26440929	-12.21	-3.48	-16.4	8.32	-0.65
5683	c1c(nc(o1)Br)CO	C30678074	-12.21	-2.98	-16.07	4.78	2.06
5684	c1cc2c(cc1O)OCO2	C00164504	-12.2	-0.76	-15.84	4.62	-0.21
5685	CC(=O)CCCl	C01664673	-12.2	0.63	-13.82	3.59	-2.6
5686	COCCc1ccccn1	C01666110	-12.2	0.33	-13.53	3.53	-2.52
5687	C=C(COC(=S)S)Cl	C01681477	-12.2	-1.2	-12.76	4.5	-2.75
5688	Cn1c(=O)[nH]c(=O)cn1	C01684202	-12.2	-1.44	-17.6	5.8	1.03
5689	COC(=O)C(C(OC)(F)F)(F)F	C01845749	-12.2	1.88	-14.45	3.3	-2.94
5690	C(CN=C=S)CCl	C02390117	-12.2	-0.97	-14.55	2.37	0.96
5691	COc1ccc(c(c1)F)O	C02545252	-12.2	-2.02	-13.41	3.94	-0.71
5692	C=C(c1ccccc1)NNC=O	C03250356	-12.2	2	-19.51	6.59	-1.28
5693	c1cc(c(nc1)[N+]=[O])N	C04085943	-12.2	-2.36	-18.66	10.65	-1.84
5694	CNC(=O)Nc1ccncc1	C06378866	-12.2	0.29	-19.47	7.36	-0.38
5695	c1c(ncnc1N)C(F)F	C08764206	-12.2	-3.85	-10.81	4.18	-1.72
5696	c1(c(non1)/N=[N+]/(c2c(non2)N)[O-])N	C12428225	-12.2	-3.54	-16.14	7.62	-0.14
5697	c1c[nH]ccc1=O	C13515858	-12.2	-1.61	-15.59	6.5	-1.51
5698	c1c(c(sc1Br)C#N)N	C16696880	-12.2	-3.06	-10.62	3.34	-1.86
5699	CCn1ccncc1C=O	C16902428	-12.2	-1.87	-12.73	5.11	-2.71
5700	c1cc(c(cc1F)NC(=O)N)F	C19279583	-12.2	-4.22	-16.15	8.75	-0.59
5701	C#CCNCC(F)F	C20033242	-12.2	0.14	-14.28	3.38	-1.44
5702	c1cc(c(cc1F)NC(=O)N)F	C21302798	-12.2	-2.56	-13.93	3.43	0.85
5703	c1ccc(cc1)C(=O)CC#N	C01555580	-12.19	-2.1	-11.84	6.5	-4.75
5704	CC(=O)O[C@H]1CC(=O)C=C1	C01591482	-12.19	1.49	-17.88	5.78	-1.57
5705	Cc1c(c(no1)N)Br	C02510208	-12.19	-2.28	-11.82	3.58	-1.66
5706	[H]N=C(\C(C(C(F)(F)F)(F)F)(F)F)[O-]	C04348144	-12.19	-3.5	-12.17	3.71	-0.24
5707	CC1=C[C@H](CCC1)O	C04528633	-12.19	-0.9	-11.85	1.99	-1.43
5708	C1CC=CSC1	C05217520	-12.19	-0.5	-12.91	1.51	-0.29
5709	C1C[C@@H](OC1)Cl	C05600268	-12.19	1.39	-12.71	2.01	-2.87
5710	CC[C@H]1CCCCO1	C05719152	-12.19	0.29	-13.34	1.15	-0.29
5711	c1[nH]c(=O)c(c(n1)N)N	C09144851	-12.19	-6.86	-14.77	5.79	3.66
5712	Cc1cc(c(nc1)F)Cl	C16159754	-12.19	-1.66	-11.62	4.01	-2.91
5713	C=C(CC#N)Cl	C19479444	-12.19	-0.46	-14.47	5.56	-2.82
5714	C=CCNCC(F)F	C20033533	-12.19	-0.77	-11.57	1.84	-1.69
5715	C=CCNCC(=C)Br	C21953591	-12.19	-0.63	-10.32	1.02	-2.25
5716	C1CC(=C[C@H]1O)Br	C21994686	-12.19	-0.21	-14.04	2.96	-0.91
5717	c1ccc1/C=C/C=O	C25722042	-12.19	-3.31	-12.67	6.44	-2.66
5718	Cc1c(ncnc1)C(F)F	C26512550	-12.19	-2.63	-15.4	6.17	-0.34
5719	C=CCOC(=O)[C@H](C=C)O	C01598480	-12.18	-1.9	-12.24	3.86	-1.89
5720	Cc1ccc(cc1)N=C	C01628277	-12.18	-2.01	-12.95	3.88	-1.11
5721	CO/C=C/C#C	C01692444	-12.18	-1.88	-11.16	3.01	-2.15
5722	COC(=O)C(=O)N	C01707270	-12.18	-2.92	-14.67	4.96	0.46
5723	c1(c(nc[nH]1)Cl)Cl	C01756167	-12.18	-2.86	-12.85	2.66	0.87
5724	CCC(=O)ONO	C01763327	-12.18	-2.69	-14.37	5.62	-0.75
5725	c1(c(sc(n1)F)Cl)C(F)F	C02540189	-12.18	-1.81	-10.21	2.32	-2.48
5726	CCOC1=CCCCC1	C04428694	-12.18	-0.88	-11.96	1.53	-0.87
5727	Cn1cc(cn1)C(=O)Cl	C04519971	-12.18	0.7	-15.87	5.04	-2.05
5728	C/(C(=C)Cl)Cl)SC#N	C05941607	-12.18	-0.56	-12.57	2.84	-1.89
5729	C1C[C@@H](C[C@H]1)SC#N)O	C05975913	-12.18	-0.09	-14.73	4.06	-1.43
5730	C[C@H](c1nc(c1)C(=O)N)O	C06933237	-12.18	-4.81	-16.43	6.45	2.61
5731	CCc1nnc(s1)Br	C11920181	-12.18	-1.87	-12.24	4.17	-2.24
5732	C1C=C2[C@H](C1=O)C=C2=O	C15022466	-12.18	-1.92	-12.63	5.2	-2.82
5733	C=C[C@H](C=C)O	C18088144	-12.18	-1.24	-14.42	2.41	1.07
5734	c1cc(ccc1c2cc[nH]n2)F	C18217709	-12.18	-0.7	-13.09	4.93	-3.33
5735	c1ccc(c(c1)[C@H]2CO2)F	C19730664	-12.18	-0.94	-11.64	3.16	-2.76
5736	C/(C=C/C)Cl)O	C33359474	-12.18	-1.37	-13.97	3.71	-0.56
5737	c1cnc(cc1Cl)C#N	C00065282	-12.17	0.72	-14.61	4.39	-2.67
5738	c1cc2c(cc[nH]2)cc1N	C00153906	-12.17	-1.95	-13.02	4.49	-1.69
5739	c1c(c(ncn1)NN)Cl	C00967357	-12.17	-4.42	-9.73	3.46	-1.47
5740	c1cnc2nncn2c1	C01601189	-12.17	-4.39	-18.71	12.5	-1.57
5741	c1cc2c(cc1O)cc(=O)[nH]2	C01608403	-12.17	-4.39	-15.73	7.35	0.6
5742	c1c(c(cs1)Br)Br	C01653761	-12.17	-1.31	-9.44	1.95	-3.38
5743	C1CCN(C1)C#N	C01676633	-12.17	1.41	-13.14	4.03	-4.47
5744	C[C@H]1(CCC=C1)O	C01713309	-12.17	-1.2	-11.88	1.91	-1
5745	COC(=O)[C@H](C(F)F)F	C01847475	-12.17	-0.59	-13.3	4.33	-2.61
5746	c1ccc(cc1)C(c2n[nH]c(=O)n2)N	C01857157	-12.17	-1.99	-15.1	7.32	-2.4
5747	C1(=O)C(=O)NC(=O)C(=O)N1	C01870442	-12.17	1.07	-20.84	5.91	1.68
5748	c1c(csc1Br)Br	C02168779	-12.17	-0.55	-13.53	1.03	0.88
5749	C(CCl)N=C=S	C02390110	-12.17	0.25	-14.53	1.2	0.91
5750	Cn1ccc(n1)C#N	C02565746	-12.17	-0.29	-16.84	6.91	-1.95
5751	C1=CC(=NO)C=CC1=NO	C03875735	-12.17	-5.34	-15.34	7.09	1.42
5752	C(=NC(=O)Cl)=O	C04528639	-12.17	-0.01	-15.1	1.55	1.39
5753	c1c(c([nH]1)Br)Br	C04552403	-12.17	-0.58	-12.9	2.83	-1.52
5754	c1[nH]c(c(n1)C(=O)N)SC#N	C05605533	-12.17	-6.66	-13.69	7.98	0.21
5755	CC[C@@H](C)N(=O)O	C06001708	-12.17	-2.51	-12.09	2.99	-0.56
5756	c1c(c(c(n1)[O-])Cl)Cl	C08612671	-12.17	-0.57	-15.73	4.86	-0.73

5847	CC(=O)c1csc(n1)N	C03888881	-12.12	-2.28	-13.79	5	-1.05
5848	Cn1c(=O)[nH]c(=O)c(n1)[S-]	C05893136	-12.12	-0.86	-16.47	4.21	0.99
5849	c1cc(oc1)Cn2c(cc(=O)[nH]c2=O)[O-]	C06059073	-12.12	-2.76	-20.28	9.35	1.57
5850	c1cc2c(cc1F)sc(n2)N	C17744334	-12.12	-1.9	-12.35	4.57	-2.44
5851	Cc1cc([nH]c1=O)Cl	C20358050	-12.12	-3.99	-16.79	9.84	-1.18
5852	C1[C@@@H](OC1)N=C=S	C26475813	-12.12	1.09	-15.16	2.55	-0.6
5853	c1cc2c(cc1F)no[n+][2][O-]	C00236905	-12.11	-3.13	-13.89	8.44	-3.53
5854	Cc1c2cccoc2[nH]n1	C00337341	-12.11	-3.77	-12.7	7.19	-2.84
5855	CCOC(=O)CC=C	C00389875	-12.11	-1.11	-12.04	3.73	-2.69
5856	c1cc(ccc1NC(=O)N)Br	C00394369	-12.11	-2.16	-16.08	6.85	-0.72
5857	CCCC(=O)OC=C	C00404766	-12.11	2.42	-14.45	3.46	-3.54
5858	c1cc(ncc1C(=O)N)F	C01600208	-12.11	-2.9	-16.02	6.42	0.38
5859	c1c(cc(c(c1O)C=O)O)O	C01670802	-12.11	-4.13	-17.51	7.46	2.08
5860	CCOC(C)C	C02031650	-12.11	-0.36	-10.73	1.24	-2.25
5861	c1cc(sc1)C(=O)CC#N	C02170146	-12.11	-1.83	-14.72	6.13	-1.68
5862	c1cc(cc(c1C(F)F)F)F	C02382347	-12.11	-2.27	-11.21	2.85	-1.48
5863	c1(c(nc(s1)F)Cl)C(F)F	C02540173	-12.11	-2.19	-12.06	3.38	-1.23
5864	[C@](C(F)(F)Cl)(N=O)(F)Cl	C05049403	-12.11	-2.34	-11.8	2.4	-0.37
5865	Cn1c(nnc1[S-])C(F)F	C06072296	-12.11	-0.28	-14.02	5.08	-2.89
5866	Cn1c(=S)[nH]c(n1)N	C15022151	-12.11	-1.6	-13.95	5.3	-1.86
5867	c1cc(cc(c1OCC#N)F)F	C15442724	-12.11	-3.21	-14.5	9.1	-3.51
5868	C/C=C/C1C(=O)NC(=S)S1	C16892172	-12.11	-0.6	-15.26	5.85	-2.1
5869	c1[nH]c2c(n1)nnnc2[O-]	C17284041	-12.11	-5.3	-19.3	10.16	2.34
5870	c1[nH]c2c(n1)c(=O)[nH]cn2	C18153302	-12.11	-6.93	-16.56	10.59	0.79
5871	c1cnccc1CNC(=S)NN	C26516090	-12.11	-0.68	-21	10.94	-1.39
5872	c1c([nH]c1Cl)CO	C26898271	-12.11	-2.77	-15.43	5.24	0.85
5873	C[S@@]([O-])Cc1ccccc1	C00013561	-12.1	-4.15	-15.05	9.93	-2.83
5874	c1cc(c(c1)O)O)O	C00330141	-12.1	-3.24	-16.04	5.31	1.87
5875	Cc1ccc(cc1)NC(=O)OC	C00395484	-12.1	-0.54	-16.69	5.46	-0.32
5876	C/C=C/Cl)O	C01530491	-12.1	-2.75	-12.96	2.66	0.95
5877	CCOC=C	C01586657	-12.1	-0.48	-11.82	1.88	-1.68
5878	C[C@]([H])(C(=O)OC)Cl	C01696573	-12.1	0.27	-13.17	3.46	-2.65
5879	C=C(C(=O)OCC(F)F)C(F)F	C02529929	-12.1	-0.95	-12.13	4.97	-3.99
5880	COCC(C(F)F)F	C02560088	-12.1	-0.67	-11.72	2.33	-2.04
5881	c1cc(ccc1NC#N)Cl	C02577553	-12.1	-5.94	-5.16	4.24	-5.24
5882	Cc1cnc(s1)CC#N	C03348992	-12.1	-2.15	-14.11	7.07	-2.9
5883	c1cc(c(c2c1non2)N)[N+](=O)[O-]	C04143698	-12.1	-1.08	-12.68	3.28	-1.62
5884	CC(=C)CSC	C05158304	-12.1	0.4	-12.37	1.32	-1.45
5885	CCN1C(=O)CCC(=O)N1	C05312033	-12.1	-2.02	-15.44	6.15	-0.79
5886	CON1C(=O)C(=O)NC1=O	C05526524	-12.1	-0.67	-17.48	5.4	0.66
5887	c1c(c(c[nH]1)F)F	C08700552	-12.1	-2.94	-13.42	6.11	-1.86
5888	Cc1cc(no1)NC(=O)N	C12926585	-12.1	-1.63	-17.68	7.02	0.18
5889	c1ccnc(c1)C(=S)N	C15858193	-12.1	-2.43	-15.71	7.66	-1.63
5890	c1cc(ncc1CO)N	C19850883	-12.1	-2.6	-17.37	6.76	1.12
5891	[H]/N=C/[Nc1ccc(cc1)F]N/C(=N/[H])/NN	C20458482	-12.1	-1.36	-13.97	7.03	-3.8
5892	C1[C@@]([H])([C@H]1F)C(=O)Cl	C21989321	-12.1	-0.02	-12.45	3.01	-2.65
5893	c1nc2n(n1)CC[NH2+]C2	C26894602	-12.1	-0.67	-16.21	5.41	-0.63
5894	C1C(CC1=O)CCl	C32625283	-12.1	-0.23	-13.43	4.52	-2.95
5895	Cc1c(nc[nH]1)C(F)F	C00039458	-12.09	-3.53	-12.44	6.58	-2.69
5896	c1ccc(cc1)NNC(=O)N)Cl	C00156647	-12.09	-1.78	-15.17	5.49	-0.63
5897	C(CCC)CC(=O)Cl	C01736654	-12.09	-0.82	-13.74	3.36	-0.88
5898	Cc1c(ccc1[O-])O	C02173520	-12.09	-0.98	-14.78	4.94	-1.28
5899	CC(=O)Nc1c(cc(cc1F)F)F	C02576930	-12.09	0.25	-15.61	6.15	-2.88
5900	c1cc(ccc1CC=O)Cl	C02581072	-12.09	-3.37	-9.54	4.89	-4.07
5901	COCC(=O)c1ccccc1	C05353997	-12.09	0.62	-13.94	2.83	-1.6
5902	c1c(c(nc(n1)N)Cl)[N+](=O)[O-]	C05438590	-12.09	-1.19	-13.29	4.49	-2.11
5903	CCO[C@]([H])(C)C=O	C05576053	-12.09	-0.89	-12.79	3.14	-1.54
5904	CCOCC(=O)Cl	C05650726	-12.09	-0.93	-14.64	4.28	-0.8
5905	c1c(nc(c(n1)N)C#N)C#N	C08698500	-12.09	-1.65	-16.55	6.38	-0.28
5906	Cc1ccc(cc1)N)C(F)F	C12359276	-12.09	-1.97	-13.71	4.2	-0.61
5907	c1c(c[nH]c(=O)c1N)Br	C15022241	-12.09	-0.77	-17.34	3.94	2.09
5908	C/C=C/Cl)CO	C16970422	-12.09	-1.7	-12.11	2.14	-0.43
5909	C/C=C/[C@H]1C=CC(=O)O1	C17299313	-12.09	-0.43	-15.24	7.08	-3.5
5910	CC(=O)[C@@]([H])(C#N)Cl	C22011853	-12.09	0.54	-14.52	4.1	-2.22
5911	CC/C=C/CCOC=O	G2008A006	-12.09	-1.45	-13.1	6.29	-3.83
5912	C=CCN=C=O	C01627092	-12.08	-0.67	-13.54	1.98	0.15
5913	C=COCC(F)F	C02040641	-12.08	-0.33	-12.88	3.3	-2.18
5914	CCOC(=O)/C=C/Br	C02380553	-12.08	-0.31	-10.83	2.33	-3.27
5915	CC[C@H]1CCC(=O)C1	C02507849	-12.08	-0.56	-11.19	3.06	-3.39
5916	Cc1ccsc1C#N	C02510165	-12.08	-1.82	-10.66	3.81	-3.4
5917	C(C=O)C(C(F)F)F	C02537055	-12.08	-0.72	-12.79	3.78	-2.35
5918	c1cc(cc(c1C(F)F)N)C#N	C02541529	-12.08	-3.88	-9.68	4.19	-2.72
5919	C(CCS)CS	C03860245	-12.08	-1.12	-9.37	1.45	-3.05
5920	c1nc(c2c(n1)[nH]nc2Br)N	C05479148	-12.08	-1.53	-13.67	4.37	-1.25
5921	c1cc(ccc1)SC(F)F	C15442446	-12.08	-0.18	-12.8	3.73	-2.84
5922	c1c(c(nc1)N)N	C17325862	-12.08	-7.59	-12.86	7.32	1.05
5923	CSc1[nH]c(=O)ccn1	C17946259	-12.08	-0.33	-16.39	6.16	-1.53
5924	c1cc(c(nc1)N)CO	C19735472	-12.08	-2.03	-17.49	6.65	0.8
5925	C[C@H](c1ccccc1O)O	C20030879	-12.08	-1.58	-16.08	5.58	0
5926	C[C@@]([H])(C#N)NCC=C	C20177399	-12.08	-0.34	-14.01	3.58	-1.3
5927	c1cc(cc(c1)F)/C=C/C=O	C21304317	-12.08	-3.54	-10.46	6.06	-4.14
5928	CCO[C@]([H])(C(C(F)F)F)F)F)F)O	C01693056	-12.07	-4.78	-6.88	2.04	-2.45
5929	c1c(ncs1)C#N	C02039551	-12.07	-2.59	-14.22	6.28	-1.55
5930	CC(C)OC(=O)Cl	C02041092	-12.07	0.28	-12.84	2	-1.52
5931	c1cnc(nc1)C#N	C02531032	-12.07	-2.8	-14.26	6.84	-1.85
5932	CCc1cc(cn1)N	C02537955	-12.07	-2.85	-11.64	3.87	-1.45
5933	c1c(cn1)CO[N+](=O)[O-]	C02552464	-12.07	-2.54	-17.02	6.91	0.58
5934	CC/C=C/C=C/C=O	C02567938	-12.07	-1.99	-13.63	5.37	-1.82
5935	C/C(=N)O/c1cc[nH]1	C12481579	-12.07	-3.71	-15.6	6.75	0.49
5936	C1C(O)I	C16083106	-12.07	-0.14	-12.81	2.25	-1.37

5937	c1c(n(c(=S)nn1)N)[O-]	C16382956	-12.07	-4.17	-14.79	6.98	-0.09
5938	C#CCNCC#C	C19798465	-12.07	-1.11	-12.82	3.19	-1.33
5939	Cc1cc(c(nc1)N)[N+](=O)[O-]	C20357575	-12.07	-2.26	-12.82	5.14	-2.13
5940	c1cc(ccc1N)Oc2cnccn2	C20444289	-12.07	-1.9	-16.01	6.47	-0.64
5941	CC(=O)N(c1ccccc1)O	C00403543	-12.06	-5.01	-14.51	7.74	-0.28
5942	C(C#CCO)NC(c=O)C(F)(F)F	C01614435	-12.06	-1.45	-16.91	5.61	0.69
5943	CC(=O)C1CCC1	C02384765	-12.06	-0.77	-11.54	3.31	-3.06
5944	CCCCCSC#N	C02507892	-12.06	-0.07	-12.72	2.82	-2.09
5945	CC(=O)c1ccn(n1)C	C02536626	-12.06	-2.2	-14.06	6.52	-2.32
5946	c1cc(c(cc1F)O)C(F)(F)F	C02560196	-12.06	-2.76	-10.61	2.96	-1.65
5947	c1cc(ccc1F)F)c2cno2	C02578080	-12.06	-0.17	-14.43	5.35	-2.82
5948	CCCN(C=O)C(F)(F)F	C03100060	-12.06	-1.66	-12.32	3.35	-1.42
5949	Cc1nnc(s1)Br	C04290646	-12.06	-2.04	-13.02	4.65	-1.64
5950	c1c(cc(c2c1[nH]cn2)F)F	C04430748	-12.06	-4.42	-13.8	7.05	-0.89
5951	C/(C=N)NC(=O)N)Cl	C04758465	-12.06	-1.61	-17.47	6.13	0.89
5952	CCc1c(nc(nc1)N)N	C05115159	-12.06	-2.99	-13.38	5.11	-0.79
5953	CCOC(=O)C(=NO)N	C05672512	-12.06	-2.88	-14.3	4.54	0.59
5954	CNC(=S)Nc1ccc(c(c1)F)F	C07571424	-12.06	0.58	-18.04	8.96	-3.56
5955	c1ccc(c(c1)N)n2cncn2	C12397685	-12.06	-0.01	-12.87	5.12	-4.29
5956	C1=CN=C2[C@H]1C=C(C=N2)Cl][O-]	C14401174	-12.06	-0.79	-15.49	5.51	-1.29
5957	Cn1cncc1C(=O)N	C16123785	-12.06	-2.95	-15.9	7.24	-0.45
5958	CCc1c(c(=O)[nH]cn1)F	C16158677	-12.06	-1.25	-15.09	3.96	0.31
5959	c1nc(c2c(n1)no[n+][2O-])N	C17353724	-12.06	-0.57	-17.26	7.74	-1.98
5960	c1cc(oc1)COCC#N	C19476664	-12.06	-1.82	-16.41	8.56	-2.38
5961	c1cc(sc1)[C@@H](C#N)N	C19984872	-12.06	-0.47	-15.16	4.71	-1.14
5962	c1cc(ncc1)N	C21303107	-12.06	-3.09	-16.95	8.23	-0.25
5963	C1C[C@@@H]2[C@H]1CCC2=C1)O	C25695675	-12.06	-0.63	-12.34	2.99	-2.09
5964	c1ccc(cc1)C(=O)N	C00152996	-12.05	-3.54	-14.18	6.61	-0.94
5965	c1cnc(nc1)NC=O	C00393958	-12.05	-1.37	-17.98	9.5	-2.2
5966	CCC(=O)c1ccc[nH]1	C01574407	-12.05	-2.31	-11.76	4.84	-2.82
5967	C=CC1OCCCC1	C01590522	-12.05	0.22	-15.27	2.99	0.01
5968	c1(c([nH]c[=O][nH]c1=O)C(F)(F)F)F	C01665340	-12.05	-3.14	-13.78	5.04	-0.16
5969	C1CC=C(C1)C#N	C02584532	-12.05	1.36	-13.91	3.81	-3.31
5970	C(CCl)C(=N)O)N	C04202657	-12.05	-3.01	-13.18	3.72	0.43
5971	CCOC(=O)C(C)C(F)	C08700944	-12.05	-0.73	-11	3.16	-3.47
5972	C1COc2c([nH]c[n2])S)O1	C08701396	-12.05	-2.41	-17.75	6.8	1.32
5973	Cc1c(cn[nH]1)C(=O)C	C15442858	-12.05	-3.69	-15.69	8.86	-1.52
5974	c1cc(oc1)C(=O)Nn2cncn2	C00055247	-12.04	-0.71	-17.35	9.33	-3.31
5975	c1cncnc1C(=O)N	C00391130	-12.04	-2.99	-16.36	6.94	0.37
5976	[C@H]1(C(=O)NC(=O)S1)Br	C01399351	-12.04	-0.33	-15.33	3.45	0.16
5977	Cc1c(cnc(n1)N)N	C01562299	-12.04	-5.97	-13.88	5.03	2.78
5978	C[C@H]1C=C[C@@H](S1)C	C01619184	-12.04	-1.15	-12.5	2.18	-0.56
5979	C=CC(=O)OCC#C	C01766086	-12.04	-0.38	-13.52	4.76	-2.9
5980	CO[C@H]1CCCC=CO1	C03861323	-12.04	-0.64	-11.57	2.36	-2.19
5981	c1cc(ncc1Cl)NC(=S)N	C04298864	-12.04	-2.29	-18.62	11.87	-3
5982	CSC(=S)N	C05734507	-12.04	-4.15	-12.35	1.81	2.65
5983	c1c(nc(s1)N)CO	C08698497	-12.04	-4.26	-14.03	4.8	1.45
5984	C(CCl)NC(=O)N1c(nnn1)N	C16981573	-12.04	-4.36	-12.97	6.38	-1.08
5985	c1cc(ccc1)OCC#N)N=O	C19277149	-12.04	-2.56	-14.82	7.15	-1.81
5986	C(=O)c1c(mns1)C(F)(F)F	C20445091	-12.04	-0.37	-14.34	3.98	-1.32
5987	COCC(=O)COCC=C	C20519037	-12.04	-0.44	-14.96	5.96	-2.6
5988	c1cc(sc1)CC(=O)[S-]	C00334133	-12.03	-2.83	-12.11	5.04	-2.12
5989	COCC(=O)Nc1ccccc1O	C00334817	-12.03	-0.25	-17.2	5.48	-0.06
5990	CCNC(=O)c1ccccc1	C00394619	-12.03	0.01	-16.59	6.1	-1.54
5991	C=CCCCO	C01632700	-12.03	-1.73	-11.76	2.06	-0.6
5992	CCCOCC(=O)CBr	C02545346	-12.03	-1.24	-10.93	3.61	-3.47
5993	Cn1c(ccn1)C=O	C02559423	-12.03	-3.5	-13.66	6.67	-1.55
5994	c1cc(oc1)CNC(=O)C(F)(F)F	C03165337	-12.03	-3.55	-11	4.11	-1.58
5995	[C@H](C(O)C(F)F)F)F)Cl	C03812964	-12.03	-2.08	-12.4	4.32	-1.87
5996	C1C[C@@@H](C=C[C@H]1O)O	C03860565	-12.03	-3.5	-13.13	3.08	1.52
5997	C#N)C(Br)Br	C04254227	-12.03	-0.04	-12.23	2.64	-2.4
5998	C1=C[C@@@H](C[C@@@H](C=C1)Br)O)O	C04978561	-12.03	-1.97	-14.32	4.01	0.24
5999	C=CCCN=C(S)S	C05600963	-12.03	0.03	-15.61	1.71	1.84
6000	COCC(=O)N(CCC)N=O	C05647924	-12.03	1.31	-15.58	3.28	-1.04
6001	c1cc(c(c(c1)F)C/C(=N)O)/N)F	C06453052	-12.03	0.51	-18.45	5.59	0.33
6002	Cn1c(c=O)cc[nH]c1=O	C08765763	-12.03	-4.08	-16.33	7.04	1.34
6003	C(=C(C(F)F)F)C#N	C12360021	-12.03	1.24	-14.38	3.8	-2.69
6004	c1nc(c2c(n1)N=CC2)N	C13518237	-12.03	-4.18	-14.67	8.5	-1.69
6005	c1cnc(cc1Br)[N+](=O)[O-]	C14982291	-12.03	-3.22	-11.03	5.04	-2.83
6006	Cc1c(sc(n1)N)Cl	C15021512	-12.03	-2.29	-11.76	3.44	-1.43
6007	c1cc(oc1)C=C/CO	C15416451	-12.03	-2.15	-14.1	5.02	-0.8
6008	c1cnc(cc1O)C#N	C15767237	-12.03	1.03	-18.53	5.66	-0.19
6009	CCc1ccc(s1)CS	C19424913	-12.03	-0.9	-8.61	2.09	-4.61
6010	c1cc(c(cc1Br)N)[N+](=O)[O-]	C19801685	-12.03	-2.16	-11.1	4.1	-2.87
6011	c1c(cnc(c1Br)N)C#N	C20246651	-12.03	-1.15	-13.51	4.51	-1.88
6012	CC(=O)c1ccc(c(c1)F)N	C20310704	-12.03	-0.95	-14.8	5.8	-2.08
6013	COCC(=O)Cn1cccc1C=O	C20447607	-12.03	-1.17	-15.33	8.2	-3.74
6014	c1cncnc1CNC(=O)N	C22148192	-12.03	-0.79	-21.65	9.35	1.05
6015	c1cc(oc1)c2cc(no2)C#N	C32005924	-12.03	-0.39	-12.72	4.37	-3.29
6016	Cc1nc(cs1)CCl	C00157256	-12.02	-1.5	-11.55	3.79	-2.76
6017	CCC(=O)OCC	C00388078	-12.02	-0.44	-12.34	3.7	-2.93
6018	CNC(=O)Nc1ccccc1	C00395001	-12.02	0.37	-18.01	7.3	-1.67
6019	c1c(ccc1C=O)C=O	C01296257	-12.02	-1.75	-14.13	6.08	-2.22
6020	COCC(=O)CCl	C01641046	-12.02	-1.1	-13.37	4.55	-2.1
6021	c1ccc2c(c1)CC(=O)O2	C01757785	-12.02	-0.63	-12.94	5.61	-4.07
6022	CC[C@H](N+)(=O)[O-])Br	C01758984	-12.02	0.07	-14.29	2.57	-0.37
6023	Cc1cnc(s1)Cl	C02507113	-12.02	-1.46	-13.72	3	0.16
6024	C[C@H](c1ccccc1F)O	C02598066	-12.02	-1.4	-11.57	3.08	-2.14
6025	c12c(sc(=S)s1)SSS2	C03194293	-12.02	-0.42	-11.9	0.81	-0.51
6026	COCC(=O)CS	C03860880	-12.02	-1.33	-13.25	4.27	-1.72

6027	C1C[C@H]2C(=C1)CC(=O)O2	C05600430	-12.02	-0.45	-13.57	5.47	-3.47
6028	C1CO[C@@H]1CBr	C16083109	-12.02	0.68	-13.64	2.61	-1.67
6029	C1C=C(NC1=O)N	C32599192	-12.02	-4.02	-15.91	7.89	0.03
6030	c1cc(cc1C(=O)N)C(F)F	C00086933	-12.01	-5.43	-10.8	4.36	-0.15
6031	COC(=O)C=C(F)F	C00158099	-12.01	-0.16	-11.94	2.95	-2.87
6032	Cc1ccc(cc1)N=C=O	C00159655	-12.01	-1.64	-11.2	1.77	-0.94
6033	c1ccc(c1)N=C=O	C00164828	-12.01	0.31	-14.09	2.65	-0.89
6034	COC1c(cc(c1F)F)F	C00406983	-12.01	0.32	-11.61	2.54	-3.27
6035	Cn1cnc(c1[N+](=O)[O-])Cl	C01299831	-12.01	-3.18	-11.57	7.18	-4.44
6036	Cn1c(=NC#N)n(n1)C	C01564396	-12.01	-0.13	-12.74	4.48	-3.62
6037	CC/C=C(C)C=O	C02034338	-12.01	-0.89	-12.12	3.96	-2.95
6038	CCOC(=O)C@H(C)Cl	C02034883	-12.01	-0.55	-11.4	3.29	-3.35
6039	c1nc2c(s1)ncs2	C02519608	-12.01	-2.27	-18.06	7.18	1.13
6040	C=CCCC#N	C02539655	-12.01	-0.66	-12.53	4.82	-3.64
6041	c1cscc1C(=N/O)N	C02547398	-12.01	-1.61	-14.82	4.9	-0.48
6042	c1ccc2c(c1)[C@H](C2=O)Cl	C03848334	-12.01	2.15	-14.33	4.29	-4.12
6043	C=CCN1CCSC1=[NH2+]	C03865387	-12.01	-0.69	-12.5	4.02	-2.83
6044	Cn1c(cnc1CC)Cl	C04206489	-12.01	0.06	-12.95	4.29	-3.42
6045	CCOC(=O)c1c(c[nH]n1)C=O	C04453807	-12.01	0.56	-15.85	5.14	-1.86
6046	c1c(nc[nH]1)CCO	C04533393	-12.01	-5.42	-14.67	6.15	1.93
6047	C/C=C/C(=O)OC	C04777523	-12.01	-0.18	-11.88	3.75	-3.71
6048	Cc1cc(cs1)C=O	C04999814	-12.01	-0.75	-13.83	5.55	-2.98
6049	COCNc1ccccc1	C05329528	-12.01	-3.18	-12.91	2.85	1.22
6050	CCn1c(cc(=O)[nH]c1=O)[O-]	C05346557	-12.01	-3.4	-18.24	8.45	1.19
6051	CC(=O)Nc1cc[nH]1	C08733367	-12.01	-5.75	-13.55	7.99	-0.71
6052	COC(=O)C(=N)[O-]C#N	C12504657	-12.01	-1.94	-15.35	5.71	-0.43
6053	c1cc(nc1)CNC(=O)C(F)F	C13208169	-12.01	-3.94	-11.43	4.95	-1.59
6054	c1c(sc(n1)Cl)[N+](=O)[O-]Cl	C19841416	-12.01	-2.47	-9.53	2.69	-2.71
6055	c1cc(ncc1CO)C#N	C21987003	-12.01	-1.34	-17.79	7.38	-0.26
6056	CC1=NCCC1	C25695470	-12.01	-1.13	-12.28	2.58	-1.18
6057	c1c(cnc(n1)NO)Br	C26441014	-12.01	-3.36	-14.94	7.25	-0.97
6058	c1cc(cc(c1F)N)c2ncnc(n2)N	C00089558	-12	-0.41	-10.6	5.13	-6.12
6059	CCOC(=O)C@H(C)O	C00391792	-12	-3.81	-13.34	6.23	-1.08
6060	COC(=O)C1cnc(s1)N	C00574159	-12	-2.05	-15.52	7.48	-1.91
6061	COC([C@H](F)Cl)F	C02040627	-12	-1.32	-11.3	2.25	-1.64
6062	c1c(cc(c1C)C#N)F)F	C02575072	-12	-2.31	-13.11	7.21	-3.78
6063	C=CCOCC1	C04203523	-12	-0.22	-11.73	2.53	-2.57
6064	[C@H](C(F)F)(C(F)F)C1O	C04958291	-12	-0.48	-13.16	2.23	-0.59
6065	c1c[nH]c(=O)cc1N	C14982073	-12	-3.84	-16.25	5.31	2.77
6066	c1cc2c(cc1F)[nH]nc2O	C14983479	-12	-1.23	-15.74	4.07	0.9
6067	CCOc1cc([nH]n1)C	C17058893	-12	-0.1	-15.07	4.09	-0.92
6068	Cc1c(n2c(nc(n2)nn1)[O-]	C17128112	-12	-5.54	-9.92	6.36	-2.88
6069	C/C(=N/O)/c1ccsc1	C17142597	-12	-2.91	-12.22	4.42	-1.28
6070	C/C=C/OC(=O)CC#N	C21986548	-12	-2.61	-15.29	9.35	-3.44
6071	C/C(=N/O)/c1ccccc1	C00160850	-11.99	-1.61	-14.32	4.63	-0.69
6072	c1cnc(cn1)C(=S)N	C00165372	-11.99	-3.61	-16.22	8.1	-0.27
6073	c1cc(c(nc1)Cl)CO	C00168331	-11.99	-1.52	-14.08	4.15	-0.54
6074	c1c(c(=O)[nH]c(=O)[nH]1)I	C01092752	-11.99	-4.9	-15.19	8.12	-0.02
6075	CN1C(=O)C@H([SC1=S)Br	C01690538	-11.99	1.08	-13.69	3.44	-2.82
6076	c1nncn1NC(=O)N	C01881932	-11.99	-5.64	-19.36	11.03	1.98
6077	c1cc(c(cc1C#N)O)N	C02022082	-11.99	-0.92	-12.82	6.07	-1.31
6078	C1C(=CS(=O)(=O)O1)Br	C02025439	-11.99	-0.83	-18.02	3.57	0.3
6079	c1cc(c(cc1CC#N)F)Cl	C02527783	-11.99	-2.97	-12.24	7.89	-4.67
6080	c1cc(c(cc1NC#N)Cl)O	C06093070	-11.99	-5.04	-12.11	5.63	-0.46
6081	CCn1c(=O)[nH]c(=O)cn1	C16887532	-11.99	0.55	-18.32	5.64	0.15
6082	c1cc2c(cc1N)OCCO2	C00164370	-11.98	-0.63	-15.09	4.52	-0.79
6083	C=C[C@H]([C@H](C=C)O)O	C00389840	-11.98	-1.14	-14.09	2.57	0.67
6084	CCOC(=O)C(=O)OCC	C01648270	-11.98	0.58	-12.66	3.62	-3.53
6085	CCOC(=O)C[N+](=O)[O-]	C01675129	-11.98	-1.02	-15.31	7.28	-2.92
6086	c1cnc(cn1)C=O	C02391857	-11.98	-3.14	-17.36	8.52	0.01
6087	CCOCn1cc(cn1)N	C02537655	-11.98	-0.23	-15.73	4.04	-0.06
6088	CC(C)C(=O)CC(=O)C	C03848396	-11.98	-2.37	-10.43	3.68	-2.86
6089	C1(=O)C(=O)C(=O)C(=O)C(=O)C1=O	C03861007	-11.98	1.61	-17.34	5.44	-1.69
6090	C(CSC(=[NH2+])N)O	C03865389	-11.98	-3.63	-14.32	3.96	2.01
6091	c1ccnc(c1)/C=N/O	C04758521	-11.98	-3.55	-15.99	7.85	-0.28
6092	COP(=O)(C=[N+]=[N-])OC	C05493067	-11.98	-2.55	-12.61	5.79	-2.61
6093	CC(=O)CCc1cccs1	C11631233	-11.98	-1.59	-10.25	4.12	-4.26
6094	c1oc(c1C#N)Br	C12370773	-11.98	-2.4	-11.27	4.37	-2.68
6095	C(#N)/C(=C(\C#N)/Cl)F	C17174231	-11.98	-0.68	-11.8	3	-2.5
6096	Cc1c(ncnc1)N)N	C25491255	-11.98	-3.2	-14.46	6.45	-0.76
6097	c1cc(ccc1)[N+](=O)[O-]N	C00047987	-11.97	-2.98	-12.36	5.66	-2.3
6098	COC(=O)C@H(CSCC1=O	C00160859	-11.97	2.69	-16.11	4.35	-2.9
6099	Cn1c(=S)[nH]c(=S)cn1	C01689464	-11.97	-1.49	-14.03	6.24	-2.7
6100	CCCCN=C=S	C01733350	-11.97	-0.66	-13.11	1.19	0.61
6101	C/C(=C/c1ccoc1)/C=O	C01850921	-11.97	-0.03	-15.88	5.98	-2.04
6102	Cc1ccc(cc1)NCC#N	C01867042	-11.97	-4.39	-11.6	4.9	-0.88
6103	c1nc(no1)CC1	C02169235	-11.97	-2.1	-14.54	5.26	-0.6
6104	Cc1cscc1C	C02383464	-11.97	-0.39	-12.31	1.63	-0.9
6105	c1ccc(c(c1)NC(=[NH2+])N)F	C02526901	-11.97	0.35	-20.16	10.46	-2.63
6106	c1cc(ncc1C=O)Br	C02527534	-11.97	-1.59	-13.53	5.44	-2.29
6107	Cc1ccnnc1C(F)F	C02536622	-11.97	-1.47	-13.05	4.76	-2.21
6108	c1nc([n-]n1)NC=O	C03954260	-11.97	-2.6	-18.09	8.09	0.63
6109	c1ccc(cc1)N=C(C#N)C#N	C04265762	-11.97	-1.03	-10.98	3.24	-3.2
6110	CC(=O)c1cc(c(cc1F)F)F	C04290138	-11.97	0.72	-15.08	5.26	-2.88
6111	c1nncn1N	C04692512	-11.97	-3.81	-13.18	7.1	-2.08
6112	C[C@H](c1cc([nH]1)O)O	C05387056	-11.97	-5.12	-16.3	5.39	4.06
6113	C=C[C@H]([C#C]O	C12363479	-11.97	-1.45	-12.54	2.59	-0.56
6114	Cn1cc(nn1)N	C19089902	-11.97	-3.53	-15.39	6.98	-0.03
6115	COc1ccc(cc1)S	C197330599	-11.97	-0.42	-10.8	2.1	-2.84
6116	CC(=O)Nc1ccc(cc1F)F	C00079075	-11.96	-1.53	-12.96	5.3	-2.77

6117	COC(=O)c1ccoc1	C01567963	-11.96	-0.9	-14.4	5.79	-2.45
6118	COC(=O)C(=C)CC=C	C01573411	-11.96	-1.13	-12.14	4.01	-2.7
6119	c1c(c(c(c1F)F)F)CC#N	C02382107	-11.96	-2.15	-14.14	8.67	-4.34
6120	C(/C=C/C(C(C(F)F)F)F)F)O	C02530856	-11.96	-2.7	-10.05	3.13	-2.33
6121	c1cn(nc1[N+](=O)[O-])C(F)F	C02534798	-11.96	-5.9	-8.71	5.95	-3.3
6122	c1c(cc(c1F)C(=O)Cl)F	C02545260	-11.96	2.68	-15.04	2.91	-2.51
6123	Cn1c(nnn1)SC	C03108049	-11.96	-1.43	-15.59	6.22	-1.16
6124	Cc1cc(not)NC(=O)C(F)F	C03165372	-11.96	-1.84	-11.71	3.93	-2.34
6125	C1C(=CC(=O)CO)O	C04622256	-11.96	-5.59	-15.6	8.82	0.42
6126	COC1=NO[C@H]2[C@H](OC=C2	C06169744	-11.96	-1.94	-15.84	5.25	0.58
6127	CCC/C=C/CO	C15272642	-11.96	-0.74	-11.62	2.15	-1.75
6128	c1c(c(c(c1F)Cl)F)N[N+](=O)[O-]	C16158749	-11.96	-3	-8.29	2.16	-2.83
6129	CC[C@H](C)(NH2+)CC(F)F	C19504671	-11.96	-0.37	-10.75	1.55	-2.38
6130	c1c(cc(c1[N+](=O)[O-])F)F	C21982378	-11.96	-0.42	-11.85	4.27	-3.96
6131	Cc1cccc(c1N)N	C00153100	-11.95	-4.76	-8.92	2.64	-0.92
6132	c1cscc1C(=O)CBr	C00158757	-11.95	1.05	-15.42	5.98	-3.55
6133	C/C=C/[C@H](c1cccc1)O	C01591833	-11.95	-1.14	-13.17	2.3	0.06
6134	C=C/C=C/C=O	C01692349	-11.95	-1.33	-13.56	5.31	-2.37
6135	c1cnnnc1	C01847599	-11.95	-1.94	-14.88	5.4	-0.53
6136	c1c(cnc(n1)Cl)I	C02028368	-11.95	1.06	-16.22	2.25	0.96
6137	CC(=O)c1ccc(s1)C=O	C02566479	-11.95	-0.96	-14.78	6.69	-2.9
6138	c1cnc(cc1C(F)F)Cl	C02584286	-11.95	0.77	-13.79	2.82	-1.75
6139	Cn1cn[nH]c1=S	C04529133	-11.95	-2.45	-13.73	7.08	-2.86
6140	Cn1cnnn1	C06072454	-11.95	-1.89	-14.32	5.17	-0.91
6141	C=CCSC(=[NH2+])N	C06668743	-11.95	-2.73	-9.78	2.13	-1.57
6142	c1cc(=O)[nH]c(c1)F	C08698075	-11.95	-2.83	-16	5.89	0.99
6143	COC(=O)C=C(Cl)CCBr	C17062716	-11.95	-0.46	-12.75	4.94	-3.68
6144	c1ccc2c(c1)C[C@H](O2)N=C=O	C19428274	-11.95	-0.81	-15.16	4.42	-0.4
6145	CNc1c(cccc1F)F	C20359426	-11.95	-1.44	-11.19	3.22	-2.54
6146	c1cc(c(c1N)[N+](=O)[O-])O	C25723529	-11.95	-1.43	-15.76	6.08	-0.85
6147	CC(=O)Cc1ccc(cc1)F	C00156292	-11.94	-1.59	-11.97	6.03	-4.42
6148	Cc1ccc(o1)C(=O)C	C01596545	-11.94	-1.44	-12.02	4.51	-2.99
6149	c1cnnnc1	C01682358	-11.94	-1.91	-14.52	5.69	-1.2
6150	CCSCC1	C01712614	-11.94	0.27	-9.68	1.14	-3.66
6151	COc1nc(ns1)N	C02506770	-11.94	-2.05	-15.73	5.12	0.71
6152	c1nnc(n1)CC#N	C02569385	-11.94	-2.83	-17.25	11.28	-3.14
6153	CC(C=O)c1ccccc1	C02571387	-11.94	-2.2	-11.04	4.44	-3.14
6154	CCc1[nH]ccn1	C08283843	-11.94	-0.14	-14.68	4.96	-2.08
6155	c1c[nH]c2c1nc(on2)Br	C21303791	-11.94	-1.68	-15.99	7.74	-2.01
6156	c1c(c[nH+]c(c1Br)F)[O-]	C21981944	-11.94	0.23	-18.09	6.19	-0.27
6157	c1cc(ccc1CC#N)Cl	C00157142	-11.93	-2.41	-13.84	6.39	-2.06
6158	COc1ccc(cc1)O	C00394208	-11.93	-0.73	-14.12	3.84	-0.93
6159	c1ccc(c(c1)C(=O)C=O)O	C01562451	-11.93	0.02	-19.75	10.44	-2.64
6160	C1CCC(C1)CC#N	C01627371	-11.93	-0.9	-11.63	4.51	-3.91
6161	C=COCCO	C02031158	-11.93	-2.98	-13.62	4.12	0.55
6162	C1SCS(=[NH2+])N1CCCI	C02391995	-11.93	-0.08	-13.25	4.29	-2.88
6163	C1CCN/C(=[NH+]/C#N)/C1	C04106190	-11.93	0.21	-16.58	8.5	-4.06
6164	C[C@H](C(=O)C)S	C04802659	-11.93	-1.38	-12.71	4.3	-2.13
6165	CC(=O)C[P@@](O)(P@)(O)OC	C05188567	-11.93	-5.28	-12.6	6.03	-0.08
6166	c1cncnc1C=N/O	C05369331	-11.93	-1.62	-18.46	7.47	0.68
6167	c1cc(c(nc1)C#N)O	C13282563	-11.93	-0.66	-18.39	7.32	-0.21
6168	CCOC(=O)c1cccnc1N	C19818956	-11.93	-1.94	-12.03	4.48	-2.43
6169	c1cc(c(cc1C(F)F)F)C#N	C00155280	-11.92	1.36	-13.55	4.41	-4.14
6170	C1C[C@H](C(=O)C)Cl	C01690074	-11.92	-0.64	-12.26	3.79	-2.8
6171	CC[C@H](C(=[NH+](=O)[O-])Br	C02042099	-11.92	-0.92	-13.12	2.46	-0.35
6172	CCOC(=O)c1ccc(nc1)F	C02383121	-11.92	1.48	-13.46	3.43	-3.36
6173	C(CCl)N(C(=O)O)N=O	C04683405	-11.92	-0.57	-15.52	3.77	0.39
6174	CO/C=C/Cl/C	C04758251	-11.92	-2.24	-11.55	4.26	-2.39
6175	c1(c(non1)N)c2nc(on2)[O-]	C05753650	-11.92	-2.16	-17.63	6.18	1.68
6176	c1cc[nH]c(c1=O)c1	C08737707	-11.92	-2.84	-14.81	4.79	0.93
6177	Cc1[nH]c(=O)ccn1	C18038081	-11.92	-2.51	-16.67	8.23	-0.98
6178	COc1cnc(nc1)Cl	C21298676	-11.92	1.49	-16.14	4.04	-1.31
6179	c1c(noc1C2CC2)C#N	C32005417	-11.92	2.1	-14.86	4.32	-3.49
6180	c1cc(c(c1)N=C=O)F(C)F(F)F	C00152311	-11.91	-2.56	-10.71	4.3	-2.95
6181	c1cc(c(cc1O)O)O	C00388437	-11.91	-2.04	-18.17	5.75	2.55
6182	c1cc(ccc1O)I	C00391103	-11.91	-0.32	-15.14	2.29	1.26
6183	c1ccc2cnncc2c1	C00404458	-11.91	-2.3	-13.37	6.67	-2.91
6184	c1c2cn(c1)CCC2=O	C01706477	-11.91	-1.14	-14.76	7.09	-3.1
6185	CCOCc1ccc(cc1)F	C02381233	-11.91	-1.73	-11.29	3.28	-2.17
6186	COC(=O)CNC=O	C02384738	-11.91	-1.41	-16.27	6.15	-0.39
6187	Cc1ccn(n1)CC#N	C02537500	-11.91	-3.25	-15.97	10.03	-2.72
6188	C#CCOC1ccccc1N	C09239393	-11.91	-2.23	-11.69	4.43	-2.41
6189	c1(nnc(s1)NN)C(F)F	C12336338	-11.91	-5.84	-11.45	5.91	-0.53
6190	Cc1c[nH]c(=O)cn1	C16955422	-11.91	-3.36	-17.02	8.63	-0.16
6191	CC1=CN[C@H](C=C1)O	C22060898	-11.91	-2.94	-14.86	4.87	1.01
6192	c1cc(ccc1NC(=S)NN)F	C00164366	-11.9	-1.02	-17.41	9.14	-2.61
6193	CC(=CC=O)C	C00896834	-11.9	-1.28	-12.92	4.59	-2.29
6194	Cc1nnc(n1)N/C	C01049738	-11.9	-3.21	-14.58	7.76	-1.87
6195	COSc1ccccc1	C01557882	-11.9	-0.2	-15.23	3.3	0.24
6196	C/C=C/C(=O)OC	C01561844	-11.9	-0.6	-12.64	3.94	-2.61
6197	CC(=O)SC(=O)C	C01680715	-11.9	-0.15	-16.55	6.2	-1.39
6198	CCN(CC)C#N	C01688361	-11.9	1.18	-12.3	3.98	-4.77
6199	CC(=O)CCSC	C01850546	-11.9	1.11	-13.57	3.63	-3.06
6200	c1ccc(cc1)NC(=O)CF	C02040810	-11.9	-2.37	-17.42	10.63	-2.73
6201	COC(=O)C1=CCCC1	C02561362	-11.9	2.4	-14.59	3.92	-3.63
6202	Cc1ccc(o1)/C=C/[N+](=O)[O-]	C03119557	-11.9	-0.65	-12.29	5.31	-4.27
6203	COC(=O)NC=C(Cl)Cl	C03164822	-11.9	-0.34	-13.98	2.77	-0.34
6204	C1CC(=O)N(C1)CCO	C04521571	-11.9	-3.81	-14.44	6.18	0.18
6205	C/C(=N/OC)/C(=O)C	C05412611	-11.9	0.15	-13.35	2.99	-1.68
6206	CCOC(=O)C=C/N=[N+]=[N-]	C05828240	-11.9	0.19	-12.43	2.62	-2.27

6207	c1c[nH]c2c1cc(cn2)l	C06643321	-11.9	-0.93	-11.42	4.21	-3.76
6208	c1c(=S)[nH]c(n1)l[O-]	C08615435	-11.9	-3.14	-17.54	5.25	3.54
6209	c1c2c(c(nc1N)O)n[nH]n2	C08659459	-11.9	-5.4	-16.78	6.28	4
6210	CC/C=C/COC=O	C14438701	-11.9	-1.49	-12.99	6.42	-3.83
6211	Cc1ccc2cn[nH]c2c1	C14983527	-11.9	-0.63	-12.48	4.1	-2.89
6212	CNc1[nH]ncc(=O)n1	C17106102	-11.9	-1.96	-17.78	6.06	1.77
6213	[H]N=C(Nc1cc(=O)n1)C(=O)[NH+]=C(N)N	C20459083	-11.9	-4.06	-17.58	12.65	-2.91
6214	c1c(c(cnc1Cl)Cl)Cl	C21986485	-11.9	0.89	-11.17	1.47	-3.09
6215	C#C[C@H](c1cccc1Cl)O	C21998451	-11.9	-1.31	-13.26	5.42	-2.76
6216	c1c(c(n1)CC#N	C26547910	-11.9	-1.06	-17.08	8.47	-2.22
6217	Cn1c(=O)ccc(n1)Br	C29865944	-11.9	-2.93	-12.44	5.03	-1.56
6218	c1ccc2c(c1)cncc2	C00160344	-11.89	-0.82	-13.2	5.61	-3.48
6219	C[C@H](c1cccc(c1)N)O	C00404425	-11.89	-2.27	-12.82	3.63	-0.44
6220	CCCC=O	C01667603	-11.89	-1.3	-11.55	3.55	-2.59
6221	CCc1cccc(c1)N	C02034642	-11.89	-1.02	-9.91	1.92	-2.88
6222	CC(=C)CCCC#N	C02567414	-11.89	-0.08	-12.68	4.9	-4.03
6223	Cc1ccsc1C(=O)N	C02573585	-11.89	-0.01	-16.48	5.39	-0.79
6224	c1cc(c(cc1N)[N+](=O)[O-])N	C03860651	-11.89	-3.14	-14.24	6.32	-0.83
6225	C(CC)/C(=N)N	C04202658	-11.89	-0.99	-13.17	2.83	-0.55
6226	C(CN[N+](=O)[O-])N	C04530237	-11.89	-3.88	-15.93	8.41	-0.49
6227	[H]N=C[C@H](C(=O)OCC)[N+](=O)[O-]	C04876799	-11.89	-1.72	-14.51	3.6	0.74
6228	c1nnnc1N2C=CCC=C2	C05778327	-11.89	-1.15	-12.38	6.84	-5.19
6229	C/C=N/C(=O)N)Cl	C17002775	-11.89	-1.99	-17.06	6.24	0.91
6230	C1=C[C@@H](C(=C1)CCO)S	C21991846	-11.89	-2.94	-11.4	3.93	-1.47
6231	c1cc(nc(c1)F)N	C21999170	-11.89	-1.45	-13.97	5.35	-1.82
6232	c1cnc(c1NC2CC2)N	C32914848	-11.89	-3.25	-11.41	5.46	-2.69
6233	c1ccc(c(=O)cc1)O	C00392003	-11.88	-3.33	-16.53	9.96	-1.97
6234	c1csc(c1Br)Cl	C01023254	-11.88	-0.75	-9.62	1.88	-3.39
6235	C1C(=O)NC(=O)CS1	C01668590	-11.88	0.65	-18.05	5.54	-0.01
6236	CCOc1ccc(cc1)C	C01693363	-11.88	1.23	-14.44	2.5	-1.17
6237	C[C@H](C#N)O(C=O)C	C01697346	-11.88	0.34	-14.45	4.9	-2.68
6238	CC#CCO	C02015866	-11.88	-1.6	-12.51	3	-0.77
6239	c1cc(cc(c1)OC(F)F)F)O	C02390049	-11.88	-0.33	-13.75	2.89	-0.69
6240	Cc1ccccn1=N=O	C03860654	-11.88	-1.11	-11.62	3.68	-2.83
6241	c1ccc(c1Br)C=O	C04208980	-11.88	-2.55	-12.42	5.25	-2.17
6242	CCCC[C@H](C#C)O	C04283778	-11.88	-1.92	-10.37	2.21	-1.81
6243	Cc1cccc(n1)O	C12358764	-11.88	-2.66	-14.6	4.92	0.47
6244	Cn1c(ccn1)C#N	C12396642	-11.88	-2.37	-11.64	4.07	-1.95
6245	C1C/C(=[NH+])C#N)NC1	C13400701	-11.88	2.27	-16.78	6.44	-3.81
6246	c1c[nH]c2c1ncc(c2)C#N	C14401082	-11.88	-1.34	-14.97	6.85	-2.42
6247	C/C(=N/O)/C(F)F	C14628482	-11.88	-1.94	-13.63	3.87	-0.18
6248	C1CC1c2nc(no2)CCl	C19090180	-11.88	2.46	-15.99	4.08	-2.43
6249	CSc1ccc(s1)C#N	C00165400	-11.87	-0.47	-13.6	3.3	-1.1
6250	CC(=O)NCc1ccc(cc1)N	C00391625	-11.87	-0.38	-19.84	6.26	2.08
6251	CC(C)SC#N	C01690285	-11.87	0.47	-12.67	2.96	-2.64
6252	#CCOCC#N	C01732677	-11.87	-1.38	-13.63	5.61	-2.46
6253	C(=NO)(C(=O)N)C(=O)N	C01841944	-11.87	-5.67	-17.23	7.02	4.01
6254	c1cc(c(cc1Br)F)[N+](=O)[O-]	C02387727	-11.87	-1.08	-11.05	4.6	-4.34
6255	COC(=O)C(C(F)F)Cl(F)F	C02530825	-11.87	-0.19	-10.69	1.98	-2.97
6256	CCO[C@H](C)C=CO1	C03875718	-11.87	-0.18	-11.07	2.34	-2.96
6257	CC(=O)NCC(=S)N	C05423714	-11.87	-2.2	-16.54	4.43	2.44
6258	c1c(ocnc1C(=O)N)CO	C06658124	-11.87	-4.27	-17.8	7.24	2.96
6259	CCCc1cc(n[nH]1)N	C12359877	-11.87	-2.31	-12.1	4.15	-1.61
6260	CC(=N)[NH+]=C(N)SC)C	C12620338	-11.87	-0.05	-13.74	4.03	-2.1
6261	c1cnc2c(c1N=[N+]=[N-])n[nH]n2	C17061572	-11.87	-5.87	-13.47	6.52	0.95
6262	CSc1c(nc([nH]c1=O)N)N	C17106178	-11.87	-3.7	-14.94	5.12	1.65
6263	c1cnc(cc1N)Br	C19015174	-11.87	-0.35	-14.48	3.91	-0.95
6264	CN(C)c1ccncc1	C19075763	-11.87	-1.3	-11.56	3.47	-2.48
6265	C(=C/[O-])C(=O)C(F)F)F	C20230759	-11.87	-0.37	-15.33	5.55	-1.72
6266	C[C@H]1CC=NN1	C28224156	-11.87	-1.09	-12.82	2.82	-0.78
6267	Cc1ccc(s1)C=O	C00152265	-11.86	-2.36	-10.88	4.41	-3.04
6268	c1cc(c(nc1)Cl)[N+](=O)[O-]	C00164421	-11.86	-1.75	-14.14	6.84	-2.81
6269	C1=CC(=O)N(C1=O)C(=O)N	C00207571	-11.86	-3.24	-19.44	10.92	-0.1
6270	CSC(=C(C)Cl)Cl	C01603556	-11.86	-0.65	-11.64	0.96	-0.53
6271	c1c(=O)[nH]cnn1	C02506112	-11.86	-4.12	-15.61	7.87	-0.01
6272	c1cc(c(cc1F)F)C=N)O	C02507110	-11.86	-1.61	-15.03	6.51	-1.72
6273	C(CN=C=O)CCl	C02539356	-11.86	-0.95	-13.58	3.15	-0.48
6274	CCOC(=O)c1cnns1	C02571484	-11.86	0.08	-13.63	3.79	-2.11
6275	Cc1ccccc1CSC#N	C03848393	-11.86	-0.96	-12.17	3.45	-2.17
6276	C=CCN(C=O)C(=O)NN	C04550592	-11.86	-1.24	-20.38	4.78	4.98
6277	c1c2c(c(=O)[nH]n1)CCC2	C04625950	-11.86	0.67	-18.22	7.18	-1.49
6278	CCCN(C(=O)C)N=O	C05049226	-11.86	-0.27	-12.94	2.77	-1.42
6279	c1ccc2c(c1)c(=O)nn[nH]2	C08613136	-11.86	-2.8	-14.54	6	-0.52
6280	CCOC(=O)c1cc(=O)[O-]	C12398478	-11.86	0.04	-15.75	5.29	-1.44
6281	c1cnc1NC(=O)CCl	C12505051	-11.86	-3.17	-14.08	7.47	-2.09
6282	c1cnc(c1)C=[N+](O)/[O-]	C13213551	-11.86	0.02	-15.35	6.37	-2.89
6283	c1cc2c(cc1N)[nH]c(=O)[nH]2	C18276088	-11.86	-4.45	-14.42	6.57	0.45
6284	C[C@H]1C(C1)S	C20476539	-11.86	-0.68	-9.21	1.39	-3.36
6285	c1cc(cc(c1)F)C(=O)[H](C)Br)O	C32914675	-11.86	-1.29	-11.56	3.69	-2.7
6286	Cc1nc(cs1)C(=S)N	C00121471	-11.85	-2.84	-14.78	7.19	-1.42
6287	c1c(c(c(c1F)F)C#N)F)F	C00155260	-11.85	1.85	-13.63	3.97	-4.04
6288	c1cc2cncn2cc1N	C01705760	-11.85	-3.95	-14.22	8.29	-1.97
6289	CCC[C@H]1[N+](=O)[O-]Cl	C02042100	-11.85	-0.93	-12.81	2.78	-0.9
6290	c1cc(oc1)C(=O)[C@H]2C=CC=[NH+]+2	C02173476	-11.85	-0.2	-16.96	6.4	-1.09
6291	c1cc(ccc1C#CCO)F	C02525748	-11.85	-2.4	-12.09	4.95	-2.31
6292	CC(=O)OCCS	C04558439	-11.85	-0.91	-14.09	5.03	-0.87
6293	C(C#N)SC(=[NH2+])N	C05112697	-11.85	-3.35	-14.63	5.33	0.79
6294	CCOCc1cccc1O	C05334404	-11.85	-0.05	-15.68	3.3	0.58
6295	C/N=C(/n1cncn1)S	C05412972	-11.85	-1.79	-14.36	3.62	0.68
6296	COC[C@H]1C(=C(C(=O)O1)Cl)Cl	C05701326	-11.85	-1.5	-13.77	4.09	-0.67

6297	c1cnn2c1NCCC2	C12396623	-11.85	-3.13	-12.32	5.37	-1.77
6298	c1cn(nn1)CC#N	C12505475	-11.85	-1.42	-17.65	9.11	-1.9
6299	C1C=NC(=CC1=O)Br	C14982269	-11.85	0.02	-15.52	4.05	-0.4
6300	C=CCC(=O)c1cccc1	C17719794	-11.85	0.13	-12.05	4.36	-4.29
6301	C(=N/C(=C(C#N)N)/C#N)N	C22000648	-11.85	-4.09	-14.39	6.68	-0.05
6302	C#C[C@H](c1cccc1)N	C32501210	-11.85	-0.42	-12.01	3.19	-2.61
6303	c1cc(c(cc1C#N)Cl)N	C00157168	-11.84	-0.86	-12.96	4.39	-2.41
6304	c1cc(oc1)OC(=O)c2ccco2	C00240839	-11.84	0.24	-15.36	7.12	-3.84
6305	c1cccc1C1Br	C00331843	-11.84	-2.38	-12.11	2.28	0.37
6306	CC(C)OC(=O)CS	C00395104	-11.84	-1.91	-12.94	4.05	-1.03
6307	CCc1cnccc1C	C00967180	-11.84	-0.78	-10.43	2.86	-3.49
6308	c1cnc(nc1Cl)Cl	C01571020	-11.84	-2.68	-11.23	4.22	-2.15
6309	CC[C@H](C)OC(=O)C(F)(F)F	C01686418	-11.84	-0.73	-9.54	1.85	-3.42
6310	Cc1ccn2c(c1)n[nH]c2=O	C01696466	-11.84	-5.13	-11.57	7.35	-2.49
6311	Cn1ccc(c1)C=O	C02581754	-11.84	-2.35	-14.58	8.03	-2.94
6312	C(=O)C(C(F)(F)Cl)(F)F	C05287061	-11.84	-3.92	-11.73	3.76	0.05
6313	CC(=O)/C=C/c1cccc1	C12370860	-11.84	-2.14	-10.12	4.53	-4.11
6314	C1CSC(=[NH2+])N1	C18354955	-11.84	-2.35	-13.06	4.12	-0.54
6315	c1cc(nc(c1N=O)N)N	C19944846	-11.84	-2.6	-19.47	9.38	0.84
6316	c1cccc(c1)NCC(F)(F)F	C21794619	-11.84	-2.27	-10.55	3.96	-2.98
6317	c1cc(c(cc1Cl)Cl)N	C00157569	-11.83	-0.87	-10.45	1.97	-2.48
6318	c1cc(c(nc1)[N+](=O)[O-])[O-]	C00331852	-11.83	-3.38	-17.76	11.27	-1.95
6319	c1c(nc2c1[n+](on2)[O-])Br	C01252138	-11.83	-2.07	-13.58	7.25	-3.43
6320	COCCOC=C	C01577176	-11.83	-0.27	-14.04	3.48	-1
6321	c1[nH]c2c(n1)c(nc(n2)F)N	C01641355	-11.83	-4.56	-13.97	7.91	-1.21
6322	CC[C@H](C=C)O	C01692449	-11.83	-0.56	-11.88	1.48	-0.87
6323	c1cc([nH]c1)C(=O)OCC#N	C01721192	-11.83	0.67	-17.12	6.47	-1.85
6324	CC[C@H](C=C)O	C02032295	-11.83	-0.14	-13.33	1.51	0.13
6325	c1cncc(c1C=O)Br	C02559660	-11.83	-0.75	-12.14	3.27	-2.21
6326	C1C[C@H](C)C=C1/C=C/C=C=O	C04429376	-11.83	-1.78	-10.55	4.81	-4.31
6327	C(=O)C(C(F)(F)F)F	C05178393	-11.83	-0.16	-11.67	1.29	-1.29
6328	C/C=C/C=C/N=O	C08612527	-11.83	-1.41	-12.71	3.72	-1.42
6329	COC/C(=C)SC#N)/Br	C12432974	-11.83	-2.16	-12.19	3.69	-1.17
6330	CC(=O)CSC#N	C16138990	-11.83	0.33	-15.77	5.74	-2.13
6331	CSc1nc(on1)N	C16939852	-11.83	-2.74	-17.19	7.15	0.95
6332	Cc1cnccc1NN	C19089984	-11.83	-2.18	-12.72	3.97	-0.9
6333	c1cc(c(cc1OCCON)F)F	C19727807	-11.83	-2.51	-14.15	6.57	-1.75
6334	CC(=O)NCc1cccc1F	C21269818	-11.83	1.72	-18.51	7.64	-2.68
6335	C1CC(=CC(=O)C1)Br	C26895294	-11.83	-0.08	-12.66	4.18	-3.27
6336	Cn1ccc(=[NH2+])cc1	C00059393	-11.82	-3.07	-13.89	7.84	-2.69
6337	CNC(=O)Cc1cccc1	C00168784	-11.82	-4.91	-11.34	6.95	-2.52
6338	C=C1CC(=O)O1	C01609482	-11.82	-1.57	-13.13	5.2	-2.32
6339	C[C@H](C(=O)Cl)OC(=O)C	C02516988	-11.82	0.16	-13.26	4.54	-3.26
6340	Cn1cc(c(n1)C(F)(F)F)N	C02537831	-11.82	-3.35	-12.86	5.39	-1
6341	CC(=O)SCCCC#N	C02584630	-11.82	-2.5	-12.69	6.81	-3.43
6342	c1c(cnc1Br)Cl	C02599049	-11.82	-0.52	-13	1.33	0.37
6343	c1cc(oc1)CSC(F)F	C03284957	-11.82	0.8	-14.06	3.61	-2.17
6344	CC/C(=C(C)C(=O)C)/O	C03848380	-11.82	-1.9	-11.06	3.86	-2.72
6345	C[C@H](C(F)(F)F)OC(=O)C	C04290183	-11.82	0.63	-12.91	3.64	-3.18
6346	C(NN(C)=N[N+](=O)[O-])/N)O	C06021264	-11.82	-3.46	-19.51	6.25	4.91
6347	Cc1cc(n[H]c(=O)c1	C09638365	-11.82	-1.21	-16.08	4.75	0.73
6348	c1cc(nc(c1)Cl)O	C12358726	-11.82	-1.74	-16.04	5.29	0.67
6349	COC(=O)c1ccnnc1	C12359421	-11.82	1.14	-16.58	5.32	-1.71
6350	COC(=O)[C@H](C(F)(F)F)N	C15442471	-11.82	-1.67	-13.78	3.97	-0.34
6351	C(=O)[C@H](C(F)(F)F)Cl	C16159145	-11.82	0.33	-10.57	0.73	-2.31
6352	CC/C=C/C=C=O	C20231660	-11.82	-1.1	-12.41	5.18	-3.49
6353	CN1C(=O)C=C[C@H](C1=O)N	C29786782	-11.82	-4.55	-14.39	6.11	1
6354	c1ccc(cc1)CCC(=O)N	C00074758	-11.81	-1.33	-15.91	7.28	-1.85
6355	c1cc(oc1)c2nsc(=O)o2	C00076458	-11.81	0.01	-15.25	4.6	-1.18
6356	Cc1cc(ncc1)C	C00388629	-11.81	-1.62	-11.27	3.98	-2.9
6357	Cn1cnc1C(=O)N	C01401586	-11.81	-3.69	-15.75	6.08	1.55
6358	CC(C)OC=C	C01586530	-11.81	0.16	-10.55	1.5	-2.92
6359	CC/C=C/C#N	C02012972	-11.81	-1.14	-11.53	3.94	-3.08
6360	CC(=O)OCC(F)F	C02539797	-11.81	-1.72	-13.07	5.59	-2.61
6361	c1cc(ccc1OCC(=O)Cl)F	C02581492	-11.81	-3.52	-12.03	5.52	-1.78
6362	COC(=O)CNC(=O)Cl	C03270957	-11.81	-2.21	-14.76	6.34	-1.19
6363	CC1=NN[C@H](C1)c2ccco2	C04995369	-11.81	0.18	-14.3	4.58	-2.26
6364	C(C#N)c1c(n[H]n1)N	C05072563	-11.81	-2.91	-17.44	8.19	0.36
6365	CNC(=S)Nc1nccn1C=O	C05566432	-11.81	-0.48	-17.94	5.66	0.95
6366	CCc1cccn1	C11920572	-11.81	-0.17	-12.58	4.02	-3.08
6367	Cn1c(c(cn1)C=O)N	C12370882	-11.81	-4.95	-15.04	8.96	-0.77
6368	Cc1c(c([nH]n1)N)N	C12506145	-11.81	-3.25	-11.39	3.75	-0.92
6369	C=CC[C@H](c1cccc(c1)F)O	C15441108	-11.81	-1.02	-10.71	3.19	-3.27
6370	c1cnccc1CCC=O	C19682808	-11.81	-1.01	-14.89	7.05	-2.96
6371	COCC1ncc(c(n1)Cl)F	C32914840	-11.81	-1.6	-12.36	3.73	-1.58
6372	N(C(=O)C)c1cccc1	W2004A008	-11.81	-0.48	-15.2	6.57	-2.69
6373	O=N(=O)c1ccc(O)cc1	nphen1	-11.81	-1.43	-14.19	5.45	-1.64
6374	CC(=O)Nc1ccc(cc1F)N	C01574393	-11.8	-1.78	-14.75	5.84	-1.11
6375	C1OC2=CC(=O)C(=O)C=C2O1	C01592536	-11.8	-1.05	-15.44	6.61	-1.93
6376	c1cc(ccc1/C=C/C#N)F	C01624976	-11.8	-1.66	-12.76	5.51	-2.89
6377	CC[C@H](C)[C][N+](=O)[O-]	C01758976	-11.8	-0.73	-11.86	3.74	-2.96
6378	c1cc(oc1)CSSC(=[NH2+])N	C01764133	-11.8	-2.67	-14.05	4.01	0.9
6379	c1c(c(n1CC)[N+](=O)[O-])Cl	C02536478	-11.8	-4.13	-12.21	8.44	-3.9
6380	c1cc(cc(c1)O)/C=N/O	C02573571	-11.8	-3.16	-13.79	4.61	0.53
6381	c1cc(sc1C(=O)C(F)(F)Cl	C02579824	-11.8	-0.07	-11.74	1.84	-1.83
6382	c1c(c(c2c(c1F)n[nH]n2)N)F	C04714861	-11.8	-5.08	-13.87	4.73	2.42
6383	Cn1ccnnc1=[NH2+]	C04934539	-11.8	-2.77	-17.24	8.26	-0.05
6384	CC(=S)SC	C05167654	-11.8	-2.15	-12.1	5.26	-2.82
6385	CC(=O)C1=C(OCC1)O	C06293632	-11.8	-2.17	-17.14	7.75	-0.24
6386	C1C(=O)OC(=O)CS1	C08100926	-11.8	0.75	-16.96	7.17	-2.76

6387	c1cc(=O)[nH]c1C(F)(F)F	C08698270	-11.8	-2.27	-13.91	4.06	0.34
6388	c1cc(c(c1O)F)FBr	C12359201	-11.8	-1.3	-15.26	4.63	0.14
6389	CCCc1nc(on1)[C@@H](C)Cl	C12760971	-11.8	0.34	-12.55	3.37	-2.96
6390	c1cc(c(c1C(F)(F)N)F)F	C15443439	-11.8	-2.78	-8.71	2.44	-2.74
6391	c1nc([nH]n1)Scco	C18039855	-11.8	-4.15	-14.32	6.82	-0.14
6392	c1cc(ncn1)C=C/CO	C22066196	-11.8	-1.69	-15.39	6.07	-0.79
6393	[H]/N=C/1\C=C[C@H](S1)SCC	C31893621	-11.8	0.18	-13.37	4.03	-2.64
6394	c1csc(c1c(=O)N)N	C00078193	-11.79	-2.6	-15.71	5.46	1.06
6395	CNC(=O)c1cccc1N	C00294877	-11.79	-2.9	-13.55	5.4	-0.73
6396	Cc1cc(c(=O)[nH]n1)N	C00391334	-11.79	-2.17	-16.73	6.04	1.07
6397	C=Cn1ccc(=O)[nH]c1=O	C01086359	-11.79	-2.38	-16.7	8.25	-0.96
6398	c1c(nc(n1)N)N	C01511101	-11.79	-2.62	-14.94	5.29	0.48
6399	C[C@]12[C@H](O1)C(=O)C=CC2=O	C01559087	-11.79	-1.91	-14.63	4.34	0.41
6400	c1cnn2c(c1N)nnn2	C01703197	-11.79	-3.62	-19.02	10.71	0.14
6401	CC(=O)C(=O)Sc1cccc1	C01760963	-11.79	-1.61	-13.41	4.2	-0.97
6402	CCSC(=O)C	C01850956	-11.79	-0.64	-13.16	2.71	-0.71
6403	CO[C@]@H](C(F)F)O	C02040620	-11.79	-2.91	-11.68	2.47	0.32
6404	c1cc(c(c1)Cl)F	C02382265	-11.79	-0.58	-15.79	4.4	0.17
6405	Cc1c1ccc(n1)C(=O)Cl	C02521282	-11.79	-2.74	-12.03	5.83	-2.85
6406	c1cc(ccc1N)OCC(F)F	C02555218	-11.79	-3.79	-9.53	3.91	-2.37
6407	c1c([nH]cn1)C(=S)[S-]	C02557033	-11.79	-3.31	-12.65	6.66	-2.48
6408	c1ccc(c1)CC=OCl	C02581070	-11.79	-2.33	-8.88	3.48	-4.06
6409	C/C(=C/C(=O)c1cccc1O)/[O-]	C05114151	-11.79	-3.81	-12.95	7.52	-2.55
6410	CC(=O)C1=NCCS1	C05159440	-11.79	1.09	-17.03	5.12	-0.98
6411	c1c(nc([nH]1)C(=O)N)C(=O)N	C05595900	-11.79	-9.87	-16.77	10.72	4.14
6412	CCc1cc([nH]1)C(F)F	C12395948	-11.79	-2.76	-12.04	4.07	-1.06
6413	CCNc1nccc(n1)Cl	C21303232	-11.79	0.24	-13	4.3	-3.32
6414	c1ccc(cc1)Cn2c(ccn2)C=O	C22005383	-11.79	-1.29	-12.28	6.29	-4.5
6415	C1CCc2c(c([nH][nH+]2)N)C1	C25949884	-11.79	-3.18	-13.47	6.36	-1.5
6416	CC(=O)[C@]@H](C@]@H](C@H]1c2cccc2	C32005632	-11.79	1.11	-13.78	4.96	-4.09
6417	CCOc1ccc(cn1)C#N	C00166500	-11.78	-1.94	-13.01	4.28	-1.11
6418	Cc1c(c(s1)N)C#N	C01414956	-11.78	-4.19	-11.53	4.63	-0.68
6419	CC(=O)N(C)CC#C	C01669329	-11.78	-0.17	-16.1	6.92	-2.43
6420	c1c(c(ncn1)N)CO	C03650210	-11.78	-2.69	-17.95	7.93	0.94
6421	c1cc2c(cc1C#N)nc[nH]2	C04353499	-11.78	-2.2	-14.18	7.99	-3.39
6422	c1csc2c1[nH]c(c2)CO	C04967342	-11.78	-2.71	-14.71	6.25	-0.62
6423	c1c(nc(n1)CC(F)F)[N+]=[O-]	C12395040	-11.78	-3.12	-13.75	8.39	-3.29
6424	c1cc(c(=O)[nH]c1)C#N	C12471465	-11.78	-0.33	-18.97	6.85	0.67
6425	CCc1nc(on1)CCl	C12505491	-11.78	-0.98	-13.44	4.41	-1.76
6426	CC(=O)c1c2ccccc2[nH]n1	C16696733	-11.78	-2.74	-14.11	7.87	-2.81
6427	CC(=O)O/N=C1/CCOC1=O	C17164764	-11.78	-0.21	-18.27	10.2	-3.5
6428	c1[n-jc2c(n1)nnnc2N(=N+)=N-]	C17376063	-11.78	0.33	-20.96	9.08	-0.23
6429	c1cc(oc1)c2nc(cc2)C=O	C19723038	-11.78	0.91	-18.78	6.8	-0.72
6430	c1(nc2n1)[C@H](N=N2)N)N	C19798285	-11.78	-0.61	-19.19	7.61	0.41
6431	CCSCC#N	C19870197	-11.78	-1.35	-12.9	5.43	-2.96
6432	CNc1cc(cc1)F	C20054574	-11.78	-2.01	-9.96	2.88	-2.7
6433	C1[C@H]([C@@H]1C(=O)C=[N+]=[N-])C(=O)C=[N+]=[N-]	C32105329	-11.78	-0.79	-18.81	8.51	-0.7
6434	c1cc(c(cc1/C=N/O)Cl)F	C00106511	-11.77	-3.42	-11.59	5.36	-2.12
6435	CCOCCOCC(=O)Cl	C01845903	-11.77	-1.38	-12.57	3.17	-0.99
6436	c1(c(c(nc1)Cl)F)F)Cl)F	C01850900	-11.77	0.35	-9.78	0.43	-2.77
6437	Cc1cc(nc1)[O-]	C02030961	-11.77	-2.82	-15.9	7.51	-0.55
6438	CC/C=C/1/CCOC1=O	C02034940	-11.77	-0.83	-13.61	6.22	-3.56
6439	c1ccc(cc1)COCCl	C02242621	-11.77	-1.36	-13.18	3.13	-0.36
6440	CCOC(=O)C(C(F)F)Cl)F	C02525771	-11.77	0.28	-10	1.7	-3.75
6441	Cc1cc([nH]n1)CO	C03851840	-11.77	-4.42	-13.52	5.38	0.78
6442	[C@@](C(F)F)C1(OC(F)F)F)Cl	C04329297	-11.77	0.28	-9.56	0.16	-2.64
6443	C#CCOc1cccc1)C=O	C04487618	-11.77	-3.01	-13.6	8.64	-3.8
6444	[H]/N=C/1/CCCS1	C04521976	-11.77	-0.75	-12.59	3.1	-1.53
6445	c1(c(nsn1)Cl)Cl	C04529131	-11.77	-1.64	-13.6	1.7	1.77
6446	CCOC(=S)C	C05224467	-11.77	-0.87	-11.88	3.32	-2.34
6447	c1c([nH]c2c1c(ccn2)N	C14401132	-11.77	-3.32	-14.77	7.53	-1.23
6448	Cc1cccc(c1)OC(F)F	C14592876	-11.77	-0.26	-9.72	1.94	-3.73
6449	[H]/N=C(N)/NSC#N	C14989407	-11.77	-4.96	-14.91	8.7	-0.61
6450	C[C@]@H]1CNC(=NC1=O)N	C17313113	-11.77	-5	-13.64	6.67	0.21
6451	c1nc2c(ncn2[O-])nn1	C17380717	-11.77	-2.05	-17.82	6.92	1.17
6452	c1cc(ccc1O)[C@]@H]1C(=O)C(=O)N)F	C19480106	-11.77	0.92	-20.03	8.71	-1.37
6453	CC(=O)c1ccnc1N	C20357579	-11.77	1.12	-16.95	5.11	-1.05
6454	c1cc(ccc1)Cl)N	C00085247	-11.76	-1.59	-11.24	2.92	-1.86
6455	Cc1c(nc(=O)[nH]c1)F	C00333479	-11.76	-4.68	-16.75	8.54	1.13
6456	Cc1cccc1C(=O)C	C01081110	-11.76	1.08	-13.57	4.3	-3.57
6457	CC(O)C(=O)C(F)F	C01675528	-11.76	0.34	-11.43	2.16	-2.83
6458	C/C(=C/Br)/CO	C01683065	-11.76	-1.57	-13.44	2.02	1.22
6459	C[C@H](C(=O)OC)Cl	C02017921	-11.76	-0.59	-12	3.48	-2.64
6460	CCC(=O)CBr	C02030997	-11.76	-1.2	-12.45	4.56	-2.67
6461	c1cnc(c1)C(=O)CBr	C02546217	-11.76	0.65	-16.2	5.48	-1.69
6462	Cc1ccc(c(c1N)OC)F	C02558532	-11.76	-1.28	-14.4	4.43	-0.51
6463	c1cc(c(nc1)[N+]=[O-])Cl	C02566375	-11.76	-3.35	-13.77	9.03	-3.66
6464	C(COC1c(non1)N)O	C02566452	-11.76	-3.89	-17.89	6.74	3.29
6465	c1ccc(cc1)[C@]@H](CC#N)O	C02566594	-11.76	-3.33	-14.95	6.83	-0.31
6466	CO[C@H]1C=C[C@]@H](O1)OC	C03860392	-11.76	-2.4	-11.59	3.29	-1.07
6467	C1COC(=O)N1C(=O)CCl	C04207427	-11.76	0.67	-17.24	6.21	-1.41
6468	CCc1cc([nH]1)O	C04494836	-11.76	-2.91	-15.16	4.65	1.66
6469	c1ccc2c(c1)CNC(=NH+)2	C05517570	-11.76	-0.49	-13.94	5.76	-3.09
6470	CC[C@]@H](CC#C)O	C08737734	-11.76	0.6	-13.84	3.61	-2.13
6471	CN(/C(=N)/[N+]=[O-])O]/[NH-])N=O	C13527713	-11.76	-6.14	-16.94	12.92	-1.59
6472	C/C=C/C)C=N/O	C14590619	-11.76	-0.86	-13.72	2.09	-1.28
6473	c1cc(c(cc1C(F)F)F)O)Br	C14989337	-11.76	-3.08	-8.77	4.59	-2.5
6474	CCc1c([nH]c(=S)nn1)[O-]	C16887340	-11.76	-5.11	-12.9	5.02	1.22
6475	CCSc1nccc(n1)N	C19093154	-11.76	-0.22	-12.76	4.82	-3.6
6476	C[C@H](C(=O)C(F)F)N	C20285513	-11.76	-1.2	-13.8	3.44	-0.19

6477	Cc1cc(c([nH+]c1)Br)[O-]	C21981894	-11.76	-2.85	-11.61	3.68	-0.98
6478	c1c(c(ncn1)NCC(F)(F)F)N	C26475074	-11.76	-2.25	-13.44	5.65	-1.73
6479	c1cc(cnc1)C(=O)CBr	C00158589	-11.75	0.3	-14.59	5.54	-2.99
6480	COC(=O)c1ccc[nH]1	C00165735	-11.75	-0.69	-14.22	5.51	-2.35
6481	CC(=CCO)C	C00897129	-11.75	-1.47	-12.15	2.41	-0.54
6482	Cc1c(cccn1)Br	C00966625	-11.75	-0.33	-11.14	2.64	-2.92
6483	c1enn(c1N)CCO	C01559503	-11.75	-1.42	-16.3	5.11	0.86
6484	CCO[C@H](C(F)(F)F)O	C01692441	-11.75	-1.36	-12.19	2.37	-0.57
6485	Cc1ccc(cc1)[N+](=O)[O-]	C01700067	-11.75	-1.97	-10.48	5.06	-4.36
6486	c1c(cnn2c1nnc2)N	C01730470	-11.75	-5.01	-20.82	13.2	0.88
6487	Cc1cc[nH]c1C	C01845997	-11.75	-1.09	-12.81	2.72	-0.57
6488	Cc1c(noc1C)C	C02023198	-11.75	-1.45	-11.46	4.25	-3.09
6489	CC(C)Nc1ccccc1	C02031136	-11.75	-1.42	-8.22	1.64	-3.75
6490	COCCN=C=S	C02168500	-11.75	0.77	-14.8	2.99	-0.72
6491	c1c(ocn1Br)CO	C02523038	-11.75	-2.27	-14.96	5.29	0.19
6492	CNC(=O)C@H](F)I	C02525279	-11.75	-1.21	-13.76	4.23	-1.02
6493	Cc1cc(ncc1Cl)F	C02539940	-11.75	-0.76	-11.01	2.78	-2.76
6494	c1cc(ccc1[N+](=O)[O-])OC(F)F	C04255174	-11.75	-4.21	-11.29	5.87	-2.13
6495	C1CC=C(C1)C=O	C05133539	-11.75	-0.04	-15.57	4.86	-1.01
6496	C=C(c1ccccc1)Br	C08700557	-11.75	-1.27	-9.9	2.95	-3.54
6497	c1c(sc(n1)N)C(=O)N	C10037209	-11.75	-3.05	-18.15	7.6	1.85
6498	C(C(=O)Cl)C(F)F	C12953050	-11.75	0.47	-14.38	4.39	-2.24
6499	CN1C[C@H](CC1=O)N=C=O	C19732303	-11.75	-0.59	-18.04	6.28	0.6
6500	c1cc(c(nc1)N)C(=O)N	C19770044	-11.75	-3.14	-17.89	7.94	1.35
6501	c1nc(on1)C=O	C20443635	-11.75	-1.48	-15.93	5.85	-0.2
6502	c1cc(c(c1N)CC(=O)F)F	C21985443	-11.75	-1.22	-13.69	5.43	-2.27
6503	CCc1ccc(cc1N)C(F)F	C21987767	-11.75	-3.42	-9.19	4.25	-3.39
6504	c1cc2c(cc1N)scn2	C00332484	-11.74	-3.07	-13.09	5.72	-1.3
6505	c1cc(ccc1[N+](=O)[O-])OC=O	C01564798	-11.74	-2.18	-14.46	8.9	-4
6506	c1ccc(cc1)CNC(=O)CO	C01633995	-11.74	-0.08	-19.81	9.12	-0.97
6507	CNC(=O)C1CSn1	C01709779	-11.74	-1.09	-16.24	5.21	0.37
6508	C(C=C(C#N)C)C#N	C01718503	-11.74	-2.01	-16.59	10.32	-3.46
6509	C/C=C(\C)/CCO	C01995217	-11.74	-1.99	-11.61	2.97	-1.11
6510	CC(=O)OCC(C(C(F)(F)F)F)F(F)F	C02572311	-11.74	-1.56	-8.79	3.68	-5.07
6511	C1SCS1	C03860808	-11.74	-0.04	-10.77	2.08	-3.01
6512	C(C(=O)Cl)Cl	C03860850	-11.74	0.13	-13.59	3.53	-1.82
6513	c1cc(oc1)C(=O)NO	C04522246	-11.74	-4.69	-16.03	8.77	0.21
6514	c1[n-]c(c(n1)[N+](=O)[O-])I	C13207567	-11.74	-3.36	-11.98	7.1	-3.49
6515	CNC(=O)c1ccc(c(c1)F)F	C16649315	-11.74	-2.58	-15.07	8.04	-2.14
6516	CCCOC(=O)CS	C16678202	-11.74	-1.76	-10.88	4	-3.1
6517	c1cc(cnc1)CNn2cnnc2	C20879680	-11.74	-2.49	-14.25	8.91	-3.91
6518	CCN(C)C(=O)Cl	C21992762	-11.74	-0.73	-13.35	4.12	-1.79
6519	CC(=CC(=O)OC)C	C00388580	-11.73	2.11	-14.15	3.42	-3.1
6520	c1cc(ccc1[N+](=O)[O-])SC#N	C01095295	-11.73	-3.06	-13.25	6.62	-2.04
6521	CCCC(=O)OCC=C	C01561518	-11.73	-0.17	-10.89	3.27	-3.94
6522	COc1cc(ccn1)F	C01584800	-11.73	-0.82	-12.67	2.91	-1.15
6523	CCSC(=S)S	C01627213	-11.73	-1.81	-10.38	3.45	-2.99
6524	Cc1nnc(o1)Nc2ccccc2	C01639044	-11.73	1.18	-19	6.83	-0.74
6525	Cc1cccc(c1)OC	C01693360	-11.73	-1.23	-9.73	2.65	-3.42
6526	c1ccnc(c1)C(F)F	C01695077	-11.73	1.29	-16.03	4.28	-1.26
6527	c1ccc(cc1)CCCO	C01747839	-11.73	-1.49	-12.29	4.32	-2.26
6528	Cc1ccc(c(n1)F)N	C02384073	-11.73	-2.56	-14.95	5.16	0.62
6529	c1cc2c(nc1)onc2Cl	C03852480	-11.73	0.98	-18.35	6.6	-0.96
6530	Cc1c(ncnc1Cl)N	C03881110	-11.73	-3.52	-10.15	3.21	-1.26
6531	c1csc(n1)CO	C04277257	-11.73	-3.58	-13.99	5.21	0.62
6532	C(#N)C(=N[O-])C(=[NH2+])N[O-]	C04557733	-11.73	-5.15	-15.44	6.75	2.1
6533	C/C=C[C@H](CC=C)O	C04582346	-11.73	-0.3	-13.16	1.68	0.05
6534	CO/C=C\OC	C04712486	-11.73	-0.92	-13.63	3.97	-1.15
6535	c1cc(c(cc1)C(=N(O))N)F)F	C06862846	-11.73	-3.13	-13.33	4.44	0.29
6536	C(#N)[C@H](F)I	C08698380	-11.73	-0.21	-12.38	3.22	-2.37
6537	c1cc(oc1)C=C(C(=O)N	C16892204	-11.73	0.05	-18.13	7.75	-1.4
6538	C=CCSc1nnc(s1)N	C17173788	-11.73	-1.36	-10.63	2.34	-2.08
6539	c1cc(sc1)[C@H]2CO2	C19257652	-11.73	-1.78	-12.69	4.66	-1.92
6540	c1c(cc(c1F)F)GNN	C19264805	-11.73	0.76	-13.17	2.13	-1.44
6541	c1c(cn1)CC#N)N	C19810571	-11.73	-2.24	-18.68	9.81	-0.62
6542	c1[nH]nc(n1)C(=N(O))N	C22146424	-11.73	-5.82	-19.67	12.71	1.05
6543	c1cc(ccc1CO)SC(F)F	C32627931	-11.73	-2.02	-13.08	5.69	-2.32
6544	Cc1cc(not1)C(=S)N	C00166485	-11.72	-1.27	-15.54	6.66	-1.58
6545	COc1OCCCO1	C01590518	-11.72	-1.2	-12.99	3.47	-1
6546	CN(C)C(=O)OCC=C	C01615454	-11.72	-2.06	-11.89	4.54	-2.32
6547	c1ccc(cc1)Cc2[nH]cnc2	C01678932	-11.72	0.15	-17.82	5.97	-0.02
6548	COC(=O)NCC=C	C01716624	-11.72	-0.61	-14.89	4.34	-0.55
6549	COC(=O)C[N+](=O)[O-]	C01733869	-11.72	-1.66	-15.42	7.58	-2.22
6550	CCCCC(=O)Cl	C01847704	-11.72	-0.24	-12.87	2.62	-1.23
6551	CC(=CCCCO)C	C02539466	-11.72	-1.84	-12.55	1.99	0.68
6552	CCc1c[nH]nc1C	C03848357	-11.72	-2.64	-10.82	3.93	-2.19
6553	CO[C@H]1CCC=CO1	C03861322	-11.72	-0.58	-11.31	2.37	-2.2
6554	CC/C=N/C(C)	C05663759	-11.72	-1.55	-11.49	2.79	-1.47
6555	CO[C@H](C(F)(F)F)F	C08698306	-11.72	-1.28	-11.78	2.64	-1.29
6556	CS/C(=N/C#N)/NCC=C	C13142991	-11.72	0.17	-11.79	3.1	-3.2
6557	c1c(c(cnc1Cl)[N+](=O)[O-])Cl	C15021894	-11.72	-0.18	-11.14	2.78	-3.18
6558	c1ccc(c(c1)CNCC(F)F)F)F	C19517343	-11.72	0.3	-11.87	3.26	-3.42
6559	c1c(c(c(c(n1)N)F)C(F)F)N	C19735234	-11.72	-0.01	-16.76	5.3	-0.24
6560	C=C1CCCC1=O	C21982784	-11.72	1.78	-13.97	3.72	-3.25
6561	c1c(nc[nH]1)C#N	C26898378	-11.72	-6.28	-13.75	10.21	-1.9
6562	c1ccc(c1CS)Cl	C00404320	-11.71	-1.64	-11.79	1.94	-0.21
6563	Cc1ccc([nH]1)C=O	C01574403	-11.71	-1.65	-15.57	5.95	-0.44
6564	CCCCSC#N	C01576854	-11.71	0.11	-12.56	2.8	-2.05
6565	COc1c2c(ncn1)scn2	C01699131	-11.71	-1.01	-17.04	4.8	1.54
6566	c1cc(c(c1)Br)OO	C02019194	-11.71	-1.37	-14.52	4.46	-0.27

6567	C1COC(O1)CCBr	C02242714	-11.71	-0.66	-11.77	2.68	-1.96
6568	c1cc(c(cc1F)F)C(=O)C=O	C02524869	-11.71	-0.78	-18.99	11.99	-3.93
6569	C(CCBr)CC#N	C03860244	-11.71	-2.31	-11.26	5.55	-3.69
6570	c1nc(c(c(n1)C)[N+](=O)[O-])N	C03866077	-11.71	-1.88	-12.02	4.13	-1.93
6571	C1COC(=O)C=C1	C04521393	-11.71	-1.43	-15.19	7.24	-2.33
6572	Cc1cc(on1)COC	C05793354	-11.71	-2.52	-12.73	4.82	-1.28
6573	C(=C)[N+](=O)[O-]C(F)F	C08579998	-11.71	-1.05	-15.42	7.55	-2.8
6574	COC(=O)Cn1ccn1	C12395003	-11.71	-1.52	-16.82	9.23	-2.6
6575	Cc1cnc(s1)[N+](=O)[O-]	C15783909	-11.71	-2.62	-13.22	7.62	-3.48
6576	c1ccc2c(c1)ncn2N	C15882019	-11.71	-2.31	-12.83	6.39	-2.96
6577	Cc1c(ccc(c1F)[N+](=O)[O-])F	C32914723	-11.71	-1.3	-10.98	4.95	-4.37
6578	C1C[C@]@H](OC1)CCl	C01641196	-11.7	1.37	-13.24	2.52	-2.35
6579	c1ccc(cc1)C(=O)CCl	C01673519	-11.7	1.15	-14.38	5.76	-4.23
6580	C=CC(=C)[O-]	C01680420	-11.7	-1.49	-13.03	3.2	-0.38
6581	Cc1cc(c(nc1)Cl)N	C02585529	-11.7	-3.37	-10.85	3.93	-1.42
6582	c1cn(cn1)c2nc[nH]n2	C05819380	-11.7	-1.05	-11.63	5.81	-4.82
6583	c1c(cc(c2c1[nH]nc2)F)Cl	C14984002	-11.7	0.96	-12.7	2.8	-2.77
6584	C[C@]@H](c1cnnc1)[NH3+]	C20441652	-11.7	-1.62	-12.7	3.34	-0.72
6585	c1cc[n+](cc1)c2c(c(=O)c2=O)[O-]	C26329912	-11.7	-0.56	-17.27	9.71	-3.58
6586	CCc1c(c(no1)C)N	C26441268	-11.7	-2.3	-12.98	5.25	-1.67
6587	c1cc(c(c1)O)F	C26892777	-11.7	0.2	-13.15	3.6	-2.35
6588	COC(=O)c1ccc1	C00388192	-11.69	0.24	-14.53	5.13	-2.53
6589	C(CBr)NC(=O)C(F)F	C01601783	-11.69	-1.4	-14.41	4.32	-0.21
6590	Cc1ccn2cncn2c1	C01696467	-11.69	-2.56	-13.92	9.71	-4.92
6591	CC[C@]@H](C@]@H)(C(O)[N+](=O)[O-])	C01759010	-11.69	-0.69	-13.73	3.9	-1.16
6592	COCC=C	C01845913	-11.69	-0.52	-11.34	1.47	-1.31
6593	c1ccc(cc1)CSC(=S)N	C02003005	-11.69	-2.22	-12.86	7.01	-3.61
6594	c1cnc([nH]1)CO	C02509361	-11.69	-3.08	-14.69	5.31	0.77
6595	Cc1c(cco1)C(=O)Cl	C02521278	-11.69	-2.49	-9.89	3.42	-2.74
6596	c1ccc(c(c1)O)OC(F)F	C02560218	-11.69	-1.57	-12.82	3.63	-0.93
6597	c1cc(c(cc1)O)C#N	C02581327	-11.69	1.07	-19.99	6.27	0.97
6598	c1cnc(cn1)C(=O)N=C(N)N	C06119119	-11.69	1.97	-24.8	10.77	0.38
6599	c1cc(=O)[nH]cc1C=O	C08698108	-11.69	-3.09	-16.68	6.73	1.35
6600	C1=NC2=NC(=O)NC(=O)C2=N1	C12493517	-11.69	-3.49	-16.37	7.17	1.01
6601	C[C@H]1CC(=NO1)[N+](=O)[O-]	C15783915	-11.69	-1.79	-11.75	4.79	-2.95
6602	Cc1ccc(cc1)C(=N/O)N/F	C15922637	-11.69	-4.11	-9.91	3.92	-1.59
6603	Cc1cnc(c1)C=O	C20443799	-11.69	-3.18	-12.62	5.05	-0.93
6604	CC(=O)C[NH2+]c1ccccc1	C26439299	-11.69	-2.16	-10.9	4.62	-3.24
6605	Cc1c(c([nH]n1)N)[N+](=O)[O-]	C32107407	-11.69	-4.35	-14.73	8.19	-0.8
6606	CCN1ccc(=N)cc1	C00059392	-11.68	-2.8	-13.13	7.55	-3.3
6607	c1cc(c2cc[nH]c2)N1	C00153904	-11.68	-0.89	-13.24	4.25	-1.8
6608	c1cc(cc1)C@]@H](C#CBr)O	C01304685	-11.68	-0.07	-15.03	2.88	0.53
6609	c1c(c([nH]1)C(F)F)C#N	C01396895	-11.68	-0.18	-14.86	4.88	-1.52
6610	c1ccc2c(c1)occc2	C01684620	-11.68	-2.24	-16.17	8.84	-2.11
6611	CCC(=O)Cl	C01730995	-11.68	-0.66	-11.86	2.78	-1.94
6612	C(NC(=O)N)OC(=S)S	C01733729	-11.68	-2	-18.81	6.66	2.46
6613	C#CCSP(=O)(O)O	C01755932	-11.68	-6.96	-11.45	10.93	-4.2
6614	Cc1ccsc1C(=O)Cl	C02504559	-11.68	1.82	-16.55	3.61	-0.55
6615	c1c(ocn1)C=O	C02577850	-11.68	-2.48	-15.67	5.82	0.65
6616	Cc1ccn(c1)N	C02581942	-11.68	-3.39	-14.56	4.69	1.58
6617	c1cc(sc1)C(=O)C(O)O	C03051942	-11.68	-1.92	-16.4	6.31	0.33
6618	C/(C(=NH+)/N)/N)Cl	C04203873	-11.68	-3.56	-12.58	4.26	0.2
6619	CSC1=NCCS1	C04276728	-11.68	-0.45	-12.92	2.94	-1.25
6620	CNC(=S)NC(=S)N	C05187302	-11.68	-2.86	-15.36	3.56	2.98
6621	c1c2c(=O)[nH]c(nc2n[nH]1)N	C08579359	-11.68	-4.08	-16.04	6.47	1.98
6622	CCc1cc(ccn1)Cl	C08698219	-11.68	-0.55	-12.39	2.73	-1.47
6623	CO[C@]@H](C(F)F)F	C08698307	-11.68	-1.47	-11.47	2.59	-1.33
6624	CSc1ncc(c(n1)[O-])F	C08952557	-11.68	-0.76	-16.77	7.36	-1.51
6625	c1c[nH]c(=O)cc1C#N	C12471987	-11.68	-1.4	-16.75	5.51	0.95
6626	c1c(cc(c1O)C=O)F)F	C16159087	-11.68	-2.95	-14.06	6.5	-1.16
6627	C#CC[C@]@H](CC)O	C21989128	-11.68	-1.17	-13.29	4.01	-1.24
6628	c1ccc(cc1)OCC(=O)N	C00123519	-11.67	-1.45	-18.11	9.26	-1.37
6629	Cn1ccn1CCl	C00158948	-11.67	-0.2	-13.68	5.34	-3.14
6630	c1ccc(c(c1)N)n2ccn2	C00161845	-11.67	-1.17	-11.75	4.46	-3.2
6631	CCOC1=CC(=O)CC1	C00395538	-11.67	-1.43	-13.58	6.03	-2.69
6632	CCNC(=O)CBr	C01673002	-11.67	-0.92	-15.51	5.9	-1.14
6633	c1csccc1=O	C01716966	-11.67	-1.65	-16.24	8.53	-2.31
6634	CC(=O)c1ccc(c(n1)F)	C01732272	-11.67	-3.54	-10.04	4.44	-2.52
6635	CCOCCOCC	C01866961	-11.67	-0.13	-11.72	1.95	-1.78
6636	C(C(F)F)OC(F)F	C01995123	-11.67	-0.5	-12.6	2.97	-1.54
6637	CCNC(=S)OCC	C05459724	-11.67	-2.11	-12.9	1.66	1.68
6638	COP(=S)OC	C05701293	-11.67	-3.46	-11.59	12.02	-8.64
6639	C/C=C(\C)/C=NCC	C16137303	-11.67	2.24	-14.04	2.69	-2.56
6640	c1cc(c(cc1Nc2nccs2)Cl)F	C20430005	-11.67	-0.11	-12.5	5.47	-4.52
6641	C1CNC(=NC#N)N1	C20466852	-11.67	-1.38	-16.36	9.02	-2.94
6642	Cc1cc(c(cn1)F)Cl	C21982020	-11.67	0.63	-11.8	2.47	-2.97
6643	C[C@]@H]1N=CCS1	C21999663	-11.67	-2.38	-11.98	3.9	-1.22
6644	Cc1cc(ncn1)NN	C25491323	-11.67	-1.48	-15.06	6.21	-1.35
6645	c1cnc2c1NC(=O)C2	C26894783	-11.67	-3.05	-13.93	6.13	-0.82
6646	CCn1ccn1	C00403991	-11.66	-0.69	-14.12	4.46	-1.31
6647	c1cc(cc(c1))O	C00404435	-11.66	-1.27	-14.18	2.56	1.23
6648	C=CCOC1ccnc(n1)N	C01644915	-11.66	-0.42	-17.19	4.14	1.82
6649	CCCN=C=O	C02041061	-11.66	-0.66	-12.17	1.76	-0.59
6650	c1cnc(c(c1C(F)F)F)F)Cl	C02525284	-11.66	0.29	-13.73	3.99	-2.22
6651	C(CO)NC(=O)c1c(no[n+]1[O-])N	C03033217	-11.66	-7.98	-14.14	7.19	3.26
6652	c1cc(cc(c1)N)CO	C03861383	-11.66	-2.49	-13.36	3.88	0.3
6653	c1cnc(cc1C(F)F)F)O	C12359082	-11.66	0.07	-16.19	4.13	0.33
6654	c1c(c(nnc1[O-])Cl)Cl	C17062759	-11.66	-6.54	-10.74	4.42	1.2
6655	CCc1ccn(n1)CC	C26547544	-11.66	-2.02	-10.58	4.46	-3.52
6656	COC(=O)c1c(ccs1)N	C00105231	-11.65	-3.01	-12.26	5.26	-1.65

6657	CNC(=O)Nc1ccc(cc1)Cl	C00392864	-11.65	-0.51	-16	6.81	-1.95
6658	Cn1cccc1[N+](=O)[O-]	C01573937	-11.65	-2.02	-14.07	6.3	-1.85
6659	c1onc(cc1C(=O)N)F	C01595323	-11.65	-3.77	-15.49	6.37	1.24
6660	CCOC(=O)CNC=O	C01653017	-11.65	-1.64	-15.17	5.71	-0.55
6661	CCOC(=O)CNO	C01702711	-11.65	-3.98	-13.36	4.23	1.47
6662	C/C=C(C)/C@H](C)O	C01730155	-11.65	-0.67	-11.26	1.55	-1.26
6663	C=CCSCC(=O)Cl	C01743786	-11.65	-0.42	-14.16	3.95	-1.02
6664	CCOC(=O)[C@H](C(=O)C(F)F)Cl	C02390290	-11.65	2.1	-13.17	2.87	-3.45
6665	Cc1cc(no1)N=C=S	C02582838	-11.65	-0.4	-14.73	4.73	-1.24
6666	CC(C)C#CO	C05358665	-11.65	-3.52	-10.64	3.13	-0.61
6667	CS/C(=N/c1cccc1)/N	C06485236	-11.65	0.06	-11.48	3.1	-3.34
6668	COc1ncc(s1)Br	C08614804	-11.65	-0.61	-12.49	1.99	-0.54
6669	c1cc(c(cc1O)F)OC(F)F	C12359205	-11.65	0.9	-14.81	3.43	-1.17
6670	C/C(=N/O)/N)Cl	C12504756	-11.65	-4.14	-13.06	4.59	0.96
6671	[H]/N=C(N)/N/C(=N/[H])/N(C)C	C12859773	-11.65	-0.95	-16.45	7.59	-1.84
6672	c1c[nH]c(=O)c2c1nc[nH]2	C17300860	-11.65	-3.6	-17.84	10.68	-0.89
6673	CCNc1cncn1	C21985100	-11.65	1.05	-14.09	5.33	-3.94
6674	C[C@H](C#N)OC(=O)n1ccnc1	C21991411	-11.65	-1.84	-12.22	5.99	-3.58
6675	CCOC(=O)n1cnnn1	C21999832	-11.65	-0.33	-14.97	5	-1.36
6676	c1cc2c(cc1CBr)non2	C00158673	-11.65	-3.14	-12.53	4.83	-0.83
6677	c1cc(cc(c1)O)C(F)F	C00164582	-11.64	-4.63	-9.18	3.24	-1.07
6678	COc1ccc(cc1)OC(=O)Cl	C00409390	-11.64	-1.66	-11.85	3.67	-1.8
6679	c1c2n(cn1)C(=O)NCC2	C01401979	-11.64	-0.89	-16.55	7.74	-1.94
6680	CCCCNC(=O)S	C01661308	-11.64	1.05	-15.09	3.59	-1.19
6681	c1ccc2c(c1)[nH]c(n2)NN	C01668389	-11.64	-5.37	-10.9	7.18	-2.56
6682	C1C=C[C@@H]2[C@H]1C(=O)C2	C01669120	-11.64	-0.62	-11.29	3.48	-3.22
6683	c1c(c(=O)[nH]c(=O)[nH]1)[S-]	C01680613	-11.64	-4.37	-16.61	8.58	0.75
6684	CC(C)C(=O)Cl	C01850092	-11.64	1.6	-13.22	2.39	-2.4
6685	CC/C=C(C)C#N	C02032406	-11.64	-1.48	-11.97	4.24	-2.43
6686	C(C(=N/O)/N)CBr	C02547089	-11.64	-2.21	-13.99	4.8	-0.25
6687	c1cc2c(cc1C(=O)Cl)non2	C02565039	-11.64	-3.05	-10.86	3.68	-1.41
6688	C[C@H]1C(=O)CCO1	C03880801	-11.64	-0.53	-12.92	2.95	-1.13
6689	C1C(=O)O[C@@H](S1)C(F)F	C04204970	-11.64	0.03	-14.08	5.27	-2.86
6690	CNc1ncc(cn1)Br	C04208971	-11.64	-1.46	-10.06	3.05	-3.17
6691	C1COC=CO1	C05134270	-11.64	-1.03	-12.68	2.98	-0.91
6692	C(CO)n1c(c(c(n1)N)[N+](=O)[O-])N	C07036852	-11.64	-6.83	-15.12	6.54	3.77
6693	c1c(ccc2c1[nH]nc2)F	C14983251	-11.64	-2.79	-12.71	4.58	-0.72
6694	c1c2c(cn1)nc([n-]2)C(F)F	C17164797	-11.64	-0.41	-12.47	4.05	-2.81
6695	c1cc(cc(c1)F)CC(=O)NN	C19262827	-11.64	-6.16	-14.34	10.3	-1.44
6696	c1cnc(c(c1N)N)Cl	C20028387	-11.64	-4.95	-13.71	6.43	0.59
6697	Cc1c(csn1)C=O	C20441798	-11.64	1.1	-16.04	4.99	-1.7
6698	Cc1nc(ns1)C=O	C20443860	-11.64	-2.36	-15.53	7.14	-0.89
6699	c1cnc(c1)Cn2cccc2	C00156227	-11.63	1.05	-13.18	5.26	-4.76
6700	C/C(=N/N)C(=O)	C00897463	-11.63	-1.65	-14.17	5.49	-1.29
6701	C=CCOCCO	C01664999	-11.63	-3.12	-12.69	3.8	0.37
6702	COC(=O)[C@H](C#N)Br	C01702492	-11.63	-1.48	-13.64	5.41	-1.92
6703	c1cn(nn1)CCO	C02513900	-11.63	-3.22	-16.59	6.91	1.26
6704	C(=C/C(F)F)C(=O)N	C02556478	-11.63	-0.93	-15.94	5.14	0.1
6705	c1ccc(cc1)S/C=C/C=O	C05485505	-11.63	-1.86	-13.98	5.33	-1.12
6706	COC(=O)c1c[nH]cn1	C08101003	-11.63	-0.1	-15.96	6.6	-2.16
6707	C[C@H]1[C@H]([O]1)C(F)F	C08101014	-11.63	-0.94	-12.07	2.89	-1.51
6708	c1cc(ncc1Cl)C(=O)N	C14982479	-11.63	-2.77	-13	4.24	-0.1
6709	C1C=C2[C@@H](C1=O)C=CC2=O	C18722504	-11.63	-2.31	-12.6	6.24	-2.96
6710	c1c(cncc1N)C(F)F	C26459981	-11.63	-3.33	-11.85	4.6	-1.05
6711	c1c(csn1)N	C26510219	-11.63	-2.05	-14.14	4.51	0.05
6712	c1ccc2c(c1)cn(n2)Cl	C00331522	-11.62	-2.43	-13.51	5.06	-0.74
6713	COc1c(non1)N	C00967422	-11.62	-2.36	-16.05	5.23	1.57
6714	c1cc(c(cc1NC=O)F)F	C01595327	-11.62	-2.79	-16.34	9.58	-2.08
6715	c1[n+](cc(c1[N+](=O)[O-])F)[O-]	C02559899	-11.62	0.44	-19.43	10.17	-2.79
6716	c1cc(sc1)/C=C/C(=O)NC(=O)N2	C03120775	-11.62	0.96	-17.94	5.99	-0.63
6717	COCC/C(=[NH+]/N)/N	C04203882	-11.62	-2.51	-13.43	3.39	0.93
6718	C(#N)c1c(non1)C(=[NH+]/N)/N	C04771246	-11.62	0.52	-15.29	2.14	1.01
6719	C/(C=C/CO)O	C05112523	-11.62	-5.14	-12.59	3.84	2.26
6720	CC(=O)NCC(N)C(=O)N	C05196943	-11.62	-0.54	-18.06	5.91	1.07
6721	COc1CCCC1	C05997769	-11.62	-0.54	-9.8	1.23	-2.52
6722	[H]/N=C1/C(=N/O)/SC(=N1)[O-]	C06083804	-11.62	-6.27	-14.18	6.17	2.66
6723	Cc1cccnc1NN=O	C13213090	-11.62	-0.92	-15.22	6.48	-1.95
6724	c1ccc(cc1)CN2NC(=O)ON2	C17024860	-11.62	-1.07	-14.36	5.76	-1.95
6725	c1c(c(c(nc1F)F)F)NN	C21990772	-11.62	-2.22	-14.39	5.22	-0.23
6726	Cc1cc(c(nc1)N)Cl	C26466278	-11.62	-1.05	-11.7	3.15	-2.02
6727	C1C[C@H]2C(=CC=CC2=O)C1	C01847232	-11.61	-2.37	-9.79	3.14	-2.58
6728	C[C@H](C(=O)C)Cl	C02038107	-11.61	-1.41	-12.49	4.75	-2.46
6729	C(C(=O)N=C=O)Cl	C02242678	-11.61	-0.05	-16.5	4.22	0.72
6730	COC(=O)c1nc([nH]n1)N	C02584075	-11.61	-2.85	-13.88	6.51	-1.4
6731	c1c(c([nH]n1)C(=N/O)/N)Cl	C04335930	-11.61	-5.17	-12.83	5.1	1.28
6732	Cc1c(c(on1)N)SC#N	C12372272	-11.61	-2.45	-15.39	6.39	-0.16
6733	C[C@H](C)C(=O)C	C14592827	-11.61	1.41	-13.64	3.45	-2.82
6734	c1cc(c(c(c1C#N)F)Cl)F	C16158182	-11.61	-2.28	-10.57	5.27	-4.03
6735	CCc1c[nH]nc1N	C21985136	-11.61	-2.31	-14.72	6.37	-0.94
6736	CCOC(=O)C1CC(=O)C1	C32915207	-11.61	-0.19	-13.02	4.88	-3.27
6737	CC(=O)Nc1cccnc1	C00152540	-11.6	-0.71	-16.42	6.89	-1.37
6738	Cc1ccc(cc1)CON	C00167561	-11.6	-0.9	-11.52	3.08	-2.26
6739	C=CC[C@H](c1ccc1)O	C00403958	-11.6	0.5	-13.28	2.93	-1.75
6740	C[C@H](c1cccc1)O	C00896625	-11.6	-1.19	-11.35	3	-2.06
6741	c1cc2nncn2nc1N	C01560835	-11.6	-5.15	-18.99	12.25	0.29
6742	C1(C(=O)NC(=O)NC1=O)Cl	C01668485	-11.6	1.17	-19.55	5.06	1.72
6743	C1CCN(CC1)Br	C01716333	-11.6	0.44	-10.44	0.87	-2.48
6744	Cc1ccc(c(n1)F)C#N	C02384011	-11.6	-1.09	-15.28	6.61	-1.83
6745	Cc1c(snn1)C#N	C02510173	-11.6	-1.74	-11.35	3.14	-1.65
6746	COc1c(ccc(c1F)O)F	C02527861	-11.6	-0.23	-15.82	5.29	-0.84

6747	c1csc(c1Cl)Cl	C02584557	-11.6	-2.11	-11.35	2.02	-0.16
6748	Cn1cncc1C#N	C04262654	-11.6	-2.68	-11.41	5.54	-3.05
6749	C/C(=C/C(=O)C)Br/[O-]	C04714958	-11.6	0.79	-12.72	2.44	-2.1
6750	C/C=C/C=C=O	C04759170	-11.6	-0.72	-14.33	5.02	-1.58
6751	c1c[nH]c(=O)cc1	C12370900	-11.6	-4.34	-13.1	7.73	-1.88
6752	c1(c(non1)N)c2nc([nH]n2)N	C16948454	-11.6	-4.32	-15.67	8.72	-0.33
6753	c1c[nH]c(=O)c1[O-]Cl	C171111113	-11.6	-2.88	-16.86	5.36	2.78
6754	Cc1ccc(o1)[C@@H](C)Cl	C19413953	-11.6	0.67	-11.35	3.22	-4.14
6755	CCc1cnc(o1)C=O	C20445052	-11.6	-1.5	-15.77	6.35	-0.68
6756	CCOC(=O)[C@@H]1C[C@H]1CO	C21984006	-11.6	-4.62	-12.17	6.62	-1.44
6757	C1CC(=O)C(=C1)Br	C30677948	-11.6	-2.23	-13.02	6.49	-2.85
6758	CN(C)CCl	C31667387	-11.6	-1.11	-11.27	1.51	-0.73
6759	c1cc(ccc1Cc2ncc2)N	C32006826	-11.6	-3.11	-17.7	8.04	1.16
6760	c1ccc(cc1)c2cc([nH]n2)[O-]	C00133300	-11.59	-3.05	-13.9	5.01	0.36
6761	[C@H](c1ccc(o1)O	C00164796	-11.59	-1.47	-14	4.63	-0.75
6762	CCc1ccccc1F	C00388676	-11.59	2.03	-14.98	4.28	-2.92
6763	COc1=O)CCOCc=C	C01599222	-11.59	0.23	-13.86	3.74	-1.7
6764	c1ccc(cc1)C2=NC2	C01712323	-11.59	-1.84	-12.07	4.15	-1.84
6765	CCCN=C=S	C01845905	-11.59	-0.03	-13.38	1.19	0.62
6766	c1cc(c(cc1Cl)O)CO	C01872360	-11.59	-1.25	-14.32	3.73	0.25
6767	COc1=O)CN1CCSC1=[NH2+]	C02454574	-11.59	0.93	-17.28	7.48	-2.71
6768	c1cc(c(c1)F)F)N=C=S	C02506747	-11.59	0.6	-15.12	4.21	-1.27
6769	c1cc(c(c1)N)O	C02512960	-11.59	-3.2	-10.34	2.56	-0.62
6770	Cc1cnn(c1)CC=O	C02537469	-11.59	-2.58	-14.04	7.3	-2.27
6771	C=Cc1cnc1	C05976084	-11.59	-1.21	-11.1	4.17	-3.44
6772	CCc1cnc1	C06755998	-11.59	-3.02	-13.82	3.96	1.29
6773	CNOC(=O)c1ccc(o1	C15780035	-11.59	0.03	-14.95	5.62	-2.3
6774	c1c(cnc(=O)[nH]1)F	C16697945	-11.59	-2.12	-16.04	4.23	2.34
6775	[C@H]1C=C[C@H](S1)C	C16981767	-11.59	-0.76	-9.16	2.18	-3.84
6776	C(SC(=[NH2+])N)SC(=[NH2+])N	C17289287	-11.59	-2.53	-13.17	2.96	1.14
6777	c1cc(c([nH]c1)C[NH3+])O	C20443406	-11.59	-1.21	-17.93	5.67	1.88
6778	CCc1nc(cs1)CS	C31890184	-11.59	-0.87	-11.17	3.6	-3.15
6779	Cc1ccc(cc1)NC(=O)C	C00080878	-11.58	-0.24	-15.09	6.81	-3.07
6780	Cc1ccc(cc1)N)Cl	C00407045	-11.58	-2.82	-11.19	1.97	0.46
6781	CCOC(=O)Cc1ccc(s1	C00409165	-11.58	1.14	-12.95	4.71	-4.47
6782	COc1=O)Cn1cnc1	C01390106	-11.58	-1.11	-17.54	10.69	-3.62
6783	c1c(c(cc1O)O)O	C01727808	-11.58	-4.36	-17.52	6.17	4.12
6784	C1CSC(=N)S1	C01736448	-11.58	0.5	-14.91	4.27	-1.43
6785	Cn1cc(c(n1)C(=O)N)N	C02558393	-11.58	-4.95	-16.26	7.02	2.61
6786	c1cc(cc1)OC(F)F)O	C02560136	-11.58	0.73	-16.93	4.9	-0.27
6787	[C@H](c1ccc(cc1)O	C04262371	-11.58	-0.39	-12.27	2.41	-1.33
6788	Cc1cc(sc1)CO	C04277326	-11.58	-1.29	-12.9	3.68	-1.08
6789	C1[C@H](C=C[C@H]1O)O	C04761434	-11.58	-2.68	-13.96	3.2	1.85
6790	c1([nH]c1c([nH]1[O-])N)[O-]N	C05123717	-11.58	-4.52	-18.7	9.35	2.29
6791	c1c(cc(c1C#N)O)F)F	C16158096	-11.58	1.26	-15.58	4.32	-1.58
6792	CCSc1cnc(s1)N	C19440122	-11.58	-0.06	-14.61	5.39	-2.31
6793	Cc1nc(cnn1)N	C19801101	-11.58	-4.6	-14.67	7.88	-0.19
6794	c1[nH]nc(n1)c2c(non2)N	C01052727	-11.57	-6.38	-14.43	10	-0.77
6795	COCCOC(=O)CBr	C01598909	-11.57	0.35	-16.34	4.93	-0.5
6796	C#CCOCCBr	C01639893	-11.57	0.18	-14.83	3.82	-0.74
6797	C1C[C@H](C[C@H](C1)SC#N)O	C01665881	-11.57	-0.57	-13.97	4.09	-1.12
6798	Cn1nc(nn1)CCO	C01726461	-11.57	-3.11	-15.82	6.16	1.2
6799	C(C(F)F)OC(C(F)F)F)F	C02560091	-11.57	-0.45	-10.77	3.32	-3.67
6800	CCc1cnc1	C02584490	-11.57	-1.78	-14.58	8.62	-3.83
6801	CN1CCCC1=O	C03860621	-11.57	-1.12	-14.66	5.87	-1.66
6802	C1CSCSC1	C03861206	-11.57	0.24	-10.63	2.01	-3.19
6803	C/C=C/C(C)C	C04533109	-11.57	-2.22	-12.28	2.11	0.82
6804	C1CC1C#CCO	C06665111	-11.57	-1.75	-12.92	4.44	-1.33
6805	c1cc(cnc1)NC=C(C#N)C#N	C12484090	-11.57	-1.15	-16.18	8.82	-3.07
6806	CCSc1nnc(s1)N	C17744349	-11.57	-1.34	-14.36	5.62	-1.49
6807	c1csc2c1[C@H](CC2)O	C19727104	-11.57	-0.49	-14.52	4.96	-1.53
6808	Cc1cc(ncn1)OC	C19872635	-11.57	0.08	-13.89	3.63	-1.4
6809	C1=C2[C@H](N=CN=C2N=N1)N	C20230335	-11.57	-2.11	-16.59	6.01	1.12
6810	Cc1cc(ncn1)C=O	C20443755	-11.57	-2.2	-11.48	4.3	-2.19
6811	Cc1c(ccnc1)F)Br	C21981953	-11.57	-2.36	-9.35	3.01	-2.88
6812	c1cc2c(cc1F)nc([nH]2)CC#N	C26471035	-11.57	-6.2	-12.24	10.38	-3.52
6813	c1c(nns1)CO	C32627325	-11.57	-3.37	-15.03	5.61	1.22
6814	CC(=O)Nc1ccccc1	C00142824	-11.56	-0.73	-14.85	6.68	-2.65
6815	C=Cc1c[nH]c(=O)[nH]c1=O	C01574276	-11.56	-2.43	-20.51	10.16	1.22
6816	c1csc(c1)C(=O)C=O	C01695362	-11.56	1	-21.01	9.75	-1.32
6817	COc1=O)Cc1csc(n1)N	C02028787	-11.56	-2.88	-13.63	7.02	-2.07
6818	c1csc2c1c(ncn2)N	C02243965	-11.56	-0.79	-14.66	5.91	-2.01
6819	CCc1ccc(cc1)C#N	C02565985	-11.56	-0.94	-11.77	3.49	-2.34
6820	[C@H](C(F)F)OC(F)F)F	C03776875	-11.56	-0.64	-12.65	3.33	-1.6
6821	C(CS)OC(=S)S	C04429747	-11.56	-1.76	-12.06	4.22	-1.96
6822	[C@H](C=C[C@H](C)O)O	C04743006	-11.56	-2.8	-13.3	3.44	1.11
6823	COP(O)OC	C05020018	-11.56	-1.62	-13.76	5.6	-1.78
6824	c1nc([nH]n1)CO	C06585091	-11.56	-4.89	-14.87	5.49	2.71
6825	c1c(c(nc1)SC(=[NH2+])N)N)F	C09189663	-11.56	-1.2	-15.05	4.69	0
6826	c1cc(cc1)F)OCCNO	C19727909	-11.56	-2.49	-14.45	5.65	-0.26
6827	c1cnc(nc1)/C=N/O	C22016729	-11.56	-3.1	-16.88	8.12	0.3
6828	Cc1ccc(cn1)C(F)F)F	C30714873	-11.56	0.15	-11.38	2.97	-3.3
6829	c1cc(cc1)F)C(=O)C(F)F)F	C01601803	-11.55	1.65	-13.02	2.98	-3.17
6830	CCCN[+](=O)[O-]	C01668639	-11.55	-1.11	-13.13	4.22	-1.54
6831	CC(=O)C(F)F)F	C01693867	-11.55	-1.06	-11.75	2.99	-1.74
6832	CC(=CCOC)C	C01765828	-11.55	-0.71	-11.44	1.67	-1.06
6833	CC1(C=CC(=O)C=C1)O	C01851971	-11.55	-2.29	-14.27	5.72	-0.71
6834	C1CCC(C1)CC(=O)Cl	C02560067	-11.55	-0.69	-12.58	2.59	-0.88
6835	Cc1ccc(cc1)CN=C=O	C02568122	-11.55	-1.82	-10.56	2.9	-2.06
6836	[C@H]1(C=C(C(=O)O1)Cl)Cl)[O-]	C03882174	-11.55	-1.96	-14.26	5.4	-0.72

6837	c1cc(ccc1CC(=O)NN)F	C03888145	-11.55	-5.68	-13.27	8.82	-1.41
6838	Cc1c(oc1Br)C	C04198776	-11.55	-0.47	-11.87	3.78	-2.99
6839	CCOC(=O)c1cnoc1	C04208879	-11.55	-0.73	-13.28	5.21	-2.76
6840	CN(C)C(=NH2+)SC	C04620596	-11.55	-1.09	-13.04	2.54	0.04
6841	C(C(=O)N)NC(=O)C=[N+]=[N-]	C04727053	-11.55	-1.94	-20.11	7.94	2.56
6842	c1(=O)[nH][nH]c(=O)n1N	C04761831	-11.55	-4.39	-16.58	6.97	2.44
6843	c1cc(ncc1[N+](=O)[O-])NN=O	C05933595	-11.55	-3.32	-12.8	6.37	-1.8
6844	C[C@@H](c1cccs1)S	C06661650	-11.55	-0.44	-9.38	2.07	-3.8
6845	Cn1cnc(c1N)/C(=N/O)/N	C17041968	-11.55	-4.55	-16.71	9.4	0.32
6846	Cc1ccsc1CNN	C19271386	-11.55	1.01	-13.6	2.25	-1.21
6847	c1c(cnc1C#N)CO	C21984979	-11.55	-2.04	-15.35	6.2	-0.35
6848	COC(=O)C1CC1	C00164516	-11.54	-0.63	-11.75	3.69	-2.85
6849	Cc1cc(ccn1)[N+](=O)[O-]	C00332953	-11.54	0.26	-12.96	4.26	-3.1
6850	C[C@H](C(=O)OC)Br	C02046232	-11.54	-0.81	-11.29	3.31	-2.74
6851	CCNc1ccccc1F	C02557563	-11.54	-1	-12.55	2.41	-0.4
6852	CC(=O)O[C@@H]1CS(=O)(=O)C=C1	C04304352	-11.54	-1.03	-19.42	9.63	-0.72
6853	Cc1ccc(cc1)NC(=O)NO	C04809417	-11.54	-1.69	-22.45	10.76	1.84
6854	C1C(=O)COC1=O	C05187742	-11.54	-4.37	-14.31	6.73	0.41
6855	Cc1c[nH]nc1c2ccco2	C05212214	-11.54	0.26	-14.11	4.86	-2.56
6856	C=CC(=O)Nn1ccccc1	C05283019	-11.54	0.41	-18.71	7.2	-0.44
6857	CC(=C)C/N=C/C)S	C05423668	-11.54	-0.57	-13.77	1.77	1.04
6858	CCOC(=O)[C@H](C)OC(=O)C	C05575470	-11.54	-0.07	-13.22	5.68	-3.93
6859	CCn1c(non1)N	C05956921	-11.54	-3.11	-14.65	5.87	0.35
6860	C1C(=O)N(C(=O)S1)CCBr	C08804400	-11.54	0.92	-14.83	4.69	-2.32
6861	c1cc(c(c1)Br)O)N	C12471080	-11.54	-1.24	-13.04	3.13	-0.39
6862	c1c(c(nc1F)[O-])[O-]C#N	C12958601	-11.54	-1.76	-19.59	6.04	3.76
6863	c1c(cc(cc1F)Br)N	C15442259	-11.54	-0.6	-10.73	2.13	-2.33
6864	c1c(cnc(c1[N+](=O)[O-])N)Br	C19202471	-11.54	-1.88	-11.32	3.72	-2.07
6865	c1ccc(c(c1)CNC(=S)N)F	C20586255	-11.54	-0.21	-20.91	12.47	-2.89
6866	C1[C@H]2C(=O)C=C[C@@H](O1)O2	C22061526	-11.54	-2.01	-13.66	4.92	-0.79
6867	CC(=O)N1C(cc(=O)[nH]c1=O)N	C26506240	-11.54	-2.1	-16.49	6.04	1
6868	CCC(=O)c1cccnc1	C01995302	-11.53	-1.24	-12.12	4.87	-3.04
6869	C(c1nc(nc(n1)N)N)Cl	C02023116	-11.53	-1.82	-12.39	5.11	-2.43
6870	Cn1c(=O)ccc(n1)Cl	C02391439	-11.53	-2.81	-12.48	5.19	-1.44
6871	CCn1cc(cn1)C(=O)Cl	C02521290	-11.53	-2.13	-11.46	4.86	-2.8
6872	c1cc2c(c(c1)O)[nH]n2	C02571481	-11.53	-6.41	-15.9	9.87	0.91
6873	c1c(cc(c(c1F)F)CO	C02575053	-11.53	-1.8	-13.23	4.86	-1.35
6874	c1ccc2c(c1)[C@@H](C2=O)Cl	C03848331	-11.53	-1.75	-9.93	4.2	-4.06
6875	c1(c(nc1nc1)N)N)N=O	C03861400	-11.53	-1.4	-16.69	5.48	1.08
6876	CCCCON(O)O	C04235229	-11.53	-3.36	-13.39	4.7	0.52
6877	c1ccn2cc(nc2c1)C=O	C04262674	-11.53	-4.39	-10.85	7.27	-3.56
6878	CCOCCSC(=NH2+)N	C04650241	-11.53	-2.59	-14.08	3.07	2.08
6879	C/C=C\CCCO	C05225098	-11.53	-0.99	-11.37	2.04	-1.22
6880	Cn1c(=O)[nH]c(=O)n(c1=O)C	C05296475	-11.53	-0.82	-14.85	4.62	-0.47
6881	c1cn(c(n1)[N+](=O)[O-])CCCl	C13207468	-11.53	-2.62	-11.95	8.88	-5.84
6882	c1d[nH]c2c1cnc(c2)Cl	C14985682	-11.53	1.77	-15.91	5.14	-2.52
6883	c1cc(ncc1N)CO	C21985574	-11.53	-2.54	-17.33	6.75	1.59
6884	CCOC(=O)C(C)C	C00391109	-11.52	-0.49	-10.87	3.3	-3.46
6885	c1ccc(c(cc1)F)N	C00409350	-11.52	-0.64	-13.81	2.17	0.77
6886	C/C=C/C)C(=O)N	C01763171	-11.52	-1.09	-14.83	4.72	-0.32
6887	CSc1ccc(cc1)C=O	C02166804	-11.52	0.44	-13.12	5.07	-3.91
6888	CNC(=O)c1c(nc1)[O-]N	C03165662	-11.52	-6.71	-10.43	5.51	0.11
6889	C/C(=C=C)CO	C04701646	-11.52	-0.75	-12.42	2.76	-1.1
6890	c1c(snn1)N	C05439122	-11.52	-3.54	-14.67	5.89	0.8
6891	C1C(=O)N/C(=N/C(=NH2+))N)/S1	C12844147	-11.52	1.34	-17.07	4.9	-0.7
6892	c1cc(cc(c1)Cl)CN=C=O	C19730707	-11.52	-1.82	-10.85	3.19	-2.03
6893	c1cc(sc1)[C@@H](C(F)F)N	C20475297	-11.52	-1.29	-11.25	2.75	-1.73
6894	c1cncc(c1C(=O)N)N	C30678199	-11.52	-3.94	-17.16	7.56	2.01
6895	CCCNc1nnns1	C32603393	-11.52	-1.9	-14.1	5.87	-1.39
6896	c1ccc(c2c(c1)nsn2)N	C00161237	-11.51	-1.7	-13.91	4.38	-0.28
6897	c1cnc2nc(nc2c1)CCl	C01301235	-11.51	-3.32	-14.08	11.1	-5.21
6898	Cc1ccncc1CO	C01656171	-11.51	-2.63	-13.32	5.06	-0.61
6899	CCOC(=O)NC(=O)O	C01757823	-11.51	-6.49	-15.15	8.61	1.51
6900	C1C[C@H](OC1)CCl	C02033089	-11.51	-0.31	-11.44	2.56	-2.31
6901	c1cc(c(c(c1)F)F)C(=O)Cl	C02584346	-11.51	-1.34	-14.96	6.78	-1.99
6902	c1cc(cc(c1)F)NC(=O)C(F)F	C03196213	-11.51	-2.4	-10.53	3.63	-2.21
6903	Cc1cc(cc1)C=O	C04208884	-11.51	-2.84	-13.39	7.04	-2.33
6904	CCOC(=O)[C@H](C)S	C04802725	-11.51	-0.93	-11.22	3.61	-2.98
6905	c1csc(c1[N+](=O)[O-])N	C05522052	-11.51	-4.09	-14.6	6.48	0.7
6906	c1cn2c(n1)c(c[nH]2)C#N	C05647555	-11.51	-4.05	-18.08	13.25	-2.63
6907	c1cnccc1C(=O)CCl	C11919359	-11.51	1.19	-16.41	6.56	-2.86
6908	c1cncc2c1[nH]nc2C(F)F	C11919527	-11.51	-1.72	-12.44	4.44	-1.79
6909	Cc1c(ncn1)C(=O)Cl	C16124695	-11.51	-2.26	-13.74	4.78	-0.3
6910	CCn1ccncc1Cl	C30677689	-11.51	-1.27	-11.52	4.63	-3.35
6911	c1ccc2c(c1)[nH+]nn2N	C00230381	-11.5	-3.92	-14.18	7.32	-0.73
6912	CC(=C)C(=O)OCCCl	C01561514	-11.5	-0.9	-11.24	4.42	-3.78
6913	CCn1cc(c(=O)[nH]c1=O)F	C01600523	-11.5	-2.22	-18.39	9.11	-0.01
6914	c1cc(cc2c1ccs2)N	C01666822	-11.5	-1.95	-10.6	3.76	-2.72
6915	C[C@H](CC=C)O	C02031653	-11.5	-1.68	-10.78	1.62	-0.66
6916	C1Sc2c(sc(=O)s2)S1	C02508341	-11.5	0.77	-14.72	3.49	-1.04
6917	c1c(n[n-]n1)C=O	C04353756	-11.5	-4.49	-15.61	8.06	0.54
6918	c1cc2cn[nH]c2cc1O	C06093719	-11.5	-0.73	-17.55	6.93	-0.16
6919	COc1ccncc1	C06424941	-11.5	-0.46	-16.45	5.6	-0.18
6920	c1cc(c(cc1)F)C(=N/O)/N)F	C06862924	-11.5	-0.41	-16.81	5.46	0.26
6921	CCOC(=O)[C@H](C(F)F)F	C08698297	-11.5	-0.31	-11.87	4.03	-3.35
6922	C1(=O)C(=NC(=S)N1)[O-]	C17744176	-11.5	-5.04	-17.81	9.36	1.99
6923	c1c(noc1C2CC2)CCl	C19093263	-11.5	2.71	-13.81	3.85	-4.24
6924	c1nc([nH]n1)SC[C@@H]2CO2	C19863792	-11.5	-6.27	-13.06	9.46	-1.62
6925	COc1cc(sc1)C(=O)Cl	C21982418	-11.5	-1.44	-11.44	3.66	-2.29
6926	C1C[C@H](C(=O)C1)C(F)F	C22014869	-11.5	-0.8	-11.92	4.36	-3.14

6927	C[C@H](c1cccs1)Cl	C32005547	-11.5	-0.38	-9.2	2.18	-4.1
6928	C1COC(=O)C#N	C32628066	-11.5	0.88	-16.12	5	-1.27
6929	Cc1c[nH]cc1C(=O)C	C00076525	-11.49	-4.14	-12.42	7.75	-2.68
6930	c1cc(cc(c1)O)C=O	C00901630	-11.49	-2.99	-14.27	6.81	-1.04
6931	CCC(=S)N(C)O	C01629969	-11.49	-2.81	-12.91	5.42	-1.19
6932	CNc1cncnc1N	C01654212	-11.49	-2.02	-13.67	4.62	-0.43
6933	CCOC[N+](=O)[O-]	C01666927	-11.49	-0.63	-11.24	3.41	-3.02
6934	c1cnc(nc1C#N)Cl	C01689926	-11.49	-2.86	-12.62	6.04	-2.06
6935	C(=C(C)Cl)(C(=O)N)Cl	C01733712	-11.49	-1.46	-12.59	2.87	-0.31
6936	c1ccc(cc1)C[C@H](CF)O	C02045792	-11.49	-4.22	-9.41	4.71	-2.57
6937	C(C/C(=N/O)/N)CCl	C02547116	-11.49	-2.11	-14.21	4.95	-0.12
6938	CC/C=C/C/C=O	C02560463	-11.49	-2.13	-9.91	2.41	-1.87
6939	CC(=O)O[C@H]1Cc2c1cccc2	C03847740	-11.49	-0.06	-12.15	5.86	-5.14
6940	c1cnc(nc1)F	C06119128	-11.49	-2.07	-15.18	5.98	-0.23
6941	C=C[C@H](CCBr)O	C06129902	-11.49	-0.83	-10.75	1.64	-1.55
6942	COC(=O)C=CNc1cccc1	C06664522	-11.49	-1.42	-13.66	4.82	-1.23
6943	COCCS	C12481545	-11.49	-0.45	-11.16	1.18	-1.07
6944	c1cc(c(nc1)C(=O)N)N	C26897415	-11.49	-6.41	-12.79	5.95	1.76
6945	CC(=O)Nc1ccsc1	C00402245	-11.48	-0.56	-17.74	6.46	0.37
6946	COC=C=C	C01585463	-11.48	-0.68	-12.17	3.03	-1.66
6947	CSC(=O)SC	C01757801	-11.48	-0.78	-12.6	2.19	-0.3
6948	c1c(cc(c1F)N=C=O)F)Br	C02389297	-11.48	0.05	-12	1.7	-1.23
6949	c1[nH]c(=O)c2c(n1)CCC2	C16855224	-11.48	-2.58	-15.66	9.19	-2.43
6950	c1cnn(c1)CCC=O	C19089272	-11.48	-1.32	-15.31	7.4	-2.26
6951	CSc1cncn1N	C19093284	-11.48	1.22	-14.38	4.61	-2.92
6952	c1ccc(cc1)CCN[NH3+]	C19166991	-11.48	0.82	-13.45	3.07	-1.92
6953	c1(nnc(s1)N)C(F)F	C20475421	-11.48	-5.19	-14	8.4	-0.69
6954	c1cc2c(cc[nH]2)cc1O	C00395637	-11.47	-1.62	-13.88	5.19	-1.16
6955	C/C=C/C#N	C01645020	-11.47	-1.47	-11.63	4.14	-2.52
6956	C[C@H]1C(=O)CCO1	C03880802	-11.47	-0.3	-13.13	3.05	-1.08
6957	CNSc1nncs1	C04454362	-11.47	-2.09	-13.99	4.87	-0.26
6958	c1cc(ccc1/C=N/O)[N+](=O)[O-]	C04759249	-11.47	-4.63	-13.19	7.22	-0.87
6959	C/C=C/C=C(=O)N	C04976360	-11.47	-0.92	-15.34	5.47	-0.68
6960	C#C/C=N=C1cccc1	C18061018	-11.47	-0.62	-11.26	4.25	-3.85
6961	c1cc(oc1)[C@H]2CO2	C19730638	-11.47	-1.84	-13.83	5.49	-1.29
6962	CNc1nc([nH]n1)N	C19802099	-11.47	-3.96	-14.89	9.44	-2.06
6963	c1cncn1CO	C26547719	-11.47	-2.89	-14.96	5.8	0.58
6964	COC(=O)c1cncn1	C00157407	-11.46	0.5	-16.67	5.86	-1.15
6965	CCOc1cccc1N	C00157538	-11.46	-1.48	-10.47	2.61	-2.12
6966	c1ccnc(c1)C=O	C00158582	-11.46	-2.12	-16.07	8.6	-1.87
6967	Cc1cc(=O)n(c(n1)N)C	C00405742	-11.46	-6.22	-11.48	8.55	-2.31
6968	CC[C@H](C=C)C)O	C01592387	-11.46	-0.41	-11.22	1.47	-1.31
6969	c1c(c(c1/c(=[NH+])/N)/[nH]1)F)N)F	C02386480	-11.46	-2.87	-12.63	3.5	0.54
6970	Cc1nc2nncn2c(n1)[O-]	C02508182	-11.46	-2.24	-15.97	11	-4.25
6971	c1cc2c(cc1Cl)OC(O2)(F)F	C02540166	-11.46	0.24	-11.18	2.59	-3.12
6972	Cc1nncn1N	C04202754	-11.46	-4.22	-14.82	6.53	1.05
6973	C(CS)OCCS	C04362791	-11.46	-1.28	-12.42	1.1	1.14
6974	C[S+](C)CCC#C	C04773266	-11.46	0.48	-10.75	1.65	-2.84
6975	c1ccc(c1)c2ccn[nH]2)N	C04822927	-11.46	-1.11	-12.94	4.66	-2.06
6976	c1c(c2c(nc[nH]2)nn1)Cl	C04877273	-11.46	-5.05	-12.56	8.4	-2.25
6977	Cc1cc([nH]c1)CO	C15020415	-11.46	-2.62	-13.81	5.17	-0.21
6978	C1C=C(COCO1)Br	C15042936	-11.46	-0.05	-12.57	2.89	-1.73
6979	c1cc(c(cc1F)C(=C)C=O)/[O-]O	C15442682	-11.46	-1.67	-15.19	7.96	-2.56
6980	CCc1cc(cnc1)C	C15781891	-11.46	-1.08	-9.43	2.72	-3.68
6981	CCOC(=O)C=CCl	C17063870	-11.46	0.38	-10.45	2.81	-4.2
6982	CCOc1ccnnc1N	C19092421	-11.46	-1.57	-12.11	3.64	-1.41
6983	CC(=CC(=O)C)BrC	C26506285	-11.46	-0.75	-11.04	4.13	-3.8
6984	c1cnc(cc1[N+](=O)[O-])Cl	C00151260	-11.45	0	-12.58	4.11	-2.98
6985	CCC(=O)CC(=O)CC	C00388711	-11.45	-1.99	-11.97	4.15	-1.64
6986	Cc1c([nH]nc1C(=O)OC	C00402175	-11.45	-1.17	-14.44	4.37	-0.22
6987	CC[C@H](c1ccco1)O	C00403956	-11.45	-1.65	-11.34	2.87	-1.33
6988	c1cc(ccc1C(F)F)NC=O	C01595333	-11.45	-2.48	-14.64	7.5	-1.83
6989	c1cnc(c1)/C=N/N	C01606671	-11.45	-2.39	-17.18	5.68	2.44
6990	CC(=O)CSC(=O)C	C01626914	-11.45	-0.29	-15.53	5.34	-0.96
6991	Cc1c(non1)CCl	C02387467	-11.45	-1.36	-14.84	6.51	-1.76
6992	CC(=O)C(C(F)F)F	C02530897	-11.45	-1.47	-12.36	4.69	-2.3
6993	C1CC(=O)N(C1)CCl	C03865397	-11.45	-0.76	-14.67	6.29	-2.3
6994	c1ccc(c1)c2cnc2)N	C04271694	-11.45	-1.17	-14.55	4.92	-0.64
6995	C1=C(C(=C(C1=O)Cl)Cl)[O-]	C04390919	-11.45	-4.9	-8.87	3.39	-1.06
6996	C1CSCC1=O	C04521395	-11.45	-0.5	-12.39	3.6	-2.16
6997	C(CSC(=[NH2+])N)C#N	C04721608	-11.45	-1.72	-15.19	6.42	-0.97
6998	COc1ccc(c(=O)[nH]1)[N+](=O)[O-]	C05285616	-11.45	-1.22	-15.05	3.66	1.16
6999	c1cc([nH]c1)c2ccc2	C05749268	-11.45	1.19	-16.47	4.8	-0.96
7000	c1c(nsn1)OC[C@H]2CO2	C12505812	-11.45	-1.54	-16.02	4.43	1.68
7001	Cn1c(nnn1)S#CCO	C17087008	-11.45	-1.9	-19.78	9.83	0.4
7002	CN1C(=O)C(=O)N(C1=O)CC(=O)OC	C20297290	-11.45	-0.55	-17.51	8.26	-1.65
7003	c1cc(cc(c1)F)CNC(=O)N	C20473623	-11.45	-0.02	-20.02	8.95	-0.36
7004	CCCNc1c(ccc1)F	C20476107	-11.45	0.41	-11.07	2.96	-3.75
7005	c1c(ncn1)Cl)C=O	C26461796	-11.45	-1.39	-12.18	4.09	-1.97
7006	Cc1nc(cs1)C#N	C00166074	-11.44	-0.58	-14.8	5.92	-1.99
7007	CCOc1c[nH]nc1C	C00401174	-11.44	-2.8	-13.87	4.62	0.61
7008	CN1C(=O)CC(=O)NC1=O	C01574468	-11.44	0.49	-18.21	5.86	0.42
7009	CN(C)N=C	C01604464	-11.44	-1.21	-12.29	2.96	-0.91
7010	COC(=O)Nc1cc2csc2n1	C01610328	-11.44	-0.98	-18.67	7.79	0.42
7011	COCC/C=C/CCl	C01640003	-11.44	-0.75	-9.91	2.16	-2.95
7012	CC(C)OC(=O)N(C)[N+](=O)[O-]	C01646516	-11.44	-2.07	-11.52	3.69	-1.54
7013	COc1cccc(=O)cc1	C01686793	-11.44	-3.53	-12.49	7.23	-2.65
7014	CC(C)OC(=S)S	C01706841	-11.44	-1.62	-11.4	3.96	-2.39
7015	c1ccc(cc1)C(=O)OCC#N	C01715383	-11.44	1.43	-13.96	5.58	-4.5
7016	C=C1CCOC1=O	C01740871	-11.44	-1.47	-14.47	6.83	-2.33

7017	c1ccc(c(c1)C(=O)Cl)O	C01997104	-11.44	0.34	-16.54	4.84	-0.08
7018	COC(=O)Nc1cccc(c1)O	C02019518	-11.44	-0.38	-19.98	7.56	1.35
7019	CCOC(=O)N[N+](=O)[O-]	C02032486	-11.44	-4.46	-16.95	8.89	1.09
7020	C(C(C(F)F)(F)OC(F)F	C02560092	-11.44	-1.59	-10.99	4.67	-3.53
7021	C1C(=O)NC(=S)S1	C03875936	-11.44	-2.08	-16	6.49	0.14
7022	CCc1ccc(cc1)N=O	C04962854	-11.44	-2.14	-11.74	3.24	-0.8
7023	[C@H]1CCCO1	C05226872	-11.44	-0.01	-11.22	1.59	-1.8
7024	Cc1[nH]c(cn1)[C@H](C(F)F)F)O	C05285761	-11.44	-4.03	-13.9	6.98	-0.49
7025	c1c(c[nH]1)[N+](=O)[O-]C#N	C05491120	-11.44	0.42	-17.22	6.06	-0.7
7026	[C@H](CO)N(N=O)O	C05758863	-11.44	-3.4	-14.25	4.81	1.41
7027	c1ccc(c(c1)C(=O)S)O	C05846849	-11.44	-0.25	-16.5	4.89	0.43
7028	CC(=O)Oc1cnc(s1)Br	C12359407	-11.44	-0.82	-15.11	4.96	-0.46
7029	c1cnc(c1)CC/C(=N/O)/N	C12395541	-11.44	-3.49	-14.78	6.48	0.36
7030	c1ccc2c(c1)c(n[nH]2)C=O	C14909878	-11.44	-3.88	-14.04	8.61	-2.14
7031	C(C(=O)C(F)F)C(F)F	C16082660	-11.44	0.47	-13.63	4.39	-2.39
7032	C1C2c2c(sc(n2)C=O)C1	C20441872	-11.44	-3.45	-10.72	5.35	-2.62
7033	[C@H](C(=O)c1ccco1)Cl	C32005842	-11.44	1.12	-13.35	4.19	-3.39
7034	c1c(cc(cc1N)N)N	C00133679	-11.43	-2.3	-13.85	3.26	1.47
7035	CCOCCBr	C01586364	-11.43	-0.25	-10.98	2.13	-2.34
7036	C1C(CS1)Cl	C01674496	-11.43	-0.09	-12.06	3.53	-2.81
7037	c1(c(c(=O)c(=O)c1=O)O)O	C02556258	-11.43	-4.69	-17.7	7.79	3.18
7038	c1cc(c(cc1O)F)C(F)F	C02560195	-11.43	-0.72	-13.24	4.02	-1.5
7039	CC(=O)CSC	C02560605	-11.43	-1.06	-13.53	5.52	-2.35
7040	Cc1ccc(o1)C(=O)N	C02750187	-11.43	-3.66	-13.37	5.71	-0.11
7041	c1c(csc1C(F)F)Br	C04290564	-11.43	0.06	-13.37	2.88	-1
7042	c1c(cnc1Cl)C=O	C06643293	-11.43	-0.02	-14.55	5.4	-2.26
7043	C/C=C/CO	C12358664	-11.43	-2.08	-11.65	2.3	0
7044	Cc1c(cn(n1)C)Cl	C16697473	-11.43	-2.3	-10.59	4.16	-2.69
7045	c1cc(c(cc1F)F)O[C@H]C(=NH2+)N	C19519793	-11.43	2.34	-20.81	8.45	-1.42
7046	c1ccc(cc1)Cc2cncn2N	C19785799	-11.43	0.17	-14.32	6.53	-3.81
7047	CC(=O)c1cccnc1N	C19851162	-11.43	-2.28	-13.19	5.56	-1.52
7048	c1c(c(cc(c1)O)O)N	C21303657	-11.43	-2.39	-16.85	5.82	1.99
7049	c1cc(ncc1C(=O)N)Cl	C00163243	-11.42	-2.95	-14.52	6.03	0.02
7050	c1cc(ccc1C(=S)N)F	C00165748	-11.42	-1.19	-16.17	8.8	-2.87
7051	C/C=C/[C@H]1C=CC(=O)O1	C01668309	-11.42	-0.34	-15.2	7.77	-3.65
7052	Cc1ccc(cc1)OCC#C	C01869848	-11.42	-2.67	-10.44	3.79	-2.11
7053	C=CCCC#N	C02034589	-11.42	0.02	-12.79	4.32	-2.97
7054	COP1OCCO1	C02038442	-11.42	-0.49	-13.97	3.81	-0.78
7055	c1cc(c(c(c1)F)C(=NH2+)NO)F	C02547181	-11.42	-2.11	-17.4	8.68	-0.58
7056	c1cc(ccc1NN)[N+](=O)[O-]	C03860923	-11.42	-2.27	-14.09	6.91	-1.98
7057	C1=C[C@H]([C@H]1C(=C1)F)O)O	C04262267	-11.42	-1.45	-15.52	4.8	0.74
7058	Cn1cc(nc1)C#N	C04262658	-11.42	-2.48	-14.06	8.35	-3.23
7059	Cc1ccc(c(c1)F)NC(=S)N	C12505971	-11.42	-0.47	-15.93	8.17	-3.19
7060	c1c[nH]c(=O)c(c1N)Cl	C14982027	-11.42	-1.92	-16.65	4.94	2.21
7061	c1cnc(cn1)NC2CC2	C18857979	-11.42	-0.74	-12.69	3.83	-1.82
7062	CCc1cc(cs1)CO	C19754888	-11.42	-1.49	-12.46	4.29	-1.76
7063	COC(=O)Nc1ccc(cc1)N)F	C19815646	-11.42	-3.9	-15.03	8.14	-0.63
7064	c1cc(sc1)SCC(=NH2+)N	C20078234	-11.42	0.62	-19.92	9.57	-1.68
7065	C1[C@H]([C@H]1F)C(=O)Cl	C21989325	-11.42	-0.03	-13.1	4.33	-2.63
7066	CC(=O)OCCOCCl	C26896288	-11.42	-0.52	-14.44	5.87	-2.34
7067	c1cc2n(c1)CCN=C2	C00185897	-11.41	0.56	-16.78	3.73	1.09
7068	C1SCCS1	C00901172	-11.41	0.54	-10.43	1.65	-3.18
7069	c1cncn(n1)NCCCl	C01557212	-11.41	-1.53	-13.8	6.59	-2.67
7070	C=C(CO)Cl	C01562139	-11.41	-2.53	-11.96	3.08	0
7071	CC(=O)Cl	C01613258	-11.41	-1.18	-12.26	4.43	-2.4
7072	C1CS[C@H]1O	C01763631	-11.41	-1.3	-12.27	2.68	-0.52
7073	CCOC(=O)[C@H]([C@H]1C)C#N)F	C02035879	-11.41	-0.9	-12.3	5	-3.21
7074	C=C(c1cccs1)NN	C02519476	-11.41	-3.92	-8.29	2.66	-1.87
7075	c1c(cc(c(c1)F)O)Br)F	C02545225	-11.41	0.33	-13.98	2.24	0
7076	C1COCC(=C1)CO	C05190737	-11.41	-1.01	-15.74	3.45	1.89
7077	CCNC(=O)C(F)F	C05471984	-11.41	-0.87	-13.13	3.44	-0.85
7078	Cc1ccc(cc1)NC(=O)NN	C06300383	-11.41	-0.45	-22.49	6.93	4.6
7079	C1C(=O)NC(=S)NC1=O	C08727446	-11.41	-3.42	-16.64	7.67	0.98
7080	C/C(=N/O)/C1CC1	C13509755	-11.41	-1.48	-11.86	3.2	-1.27
7081	c1cc2c[nH]nc2cc1NC(=S)N	C13598839	-11.41	-1.92	-14	5.64	-1.13
7082	C(CO)n1nc(n1)N	C16954938	-11.41	-3.54	-15	6.19	0.95
7083	CNC(=O)Oc1ccc[nH]c1=O	C17064144	-11.41	-0.32	-23.16	10.19	1.87
7084	c1ccc2c(c1)CN(C2)N	C19171334	-11.41	-1.23	-11.75	2.99	-1.43
7085	C1CNCC1(F)F	C19735230	-11.41	-1.02	-11.76	1.84	-0.46
7086	CCSCC(=NH2+)N	C19870377	-11.41	-4.49	-13.65	7.43	-0.71
7087	C=C/C=C/CCO	C31776272	-11.41	0.53	-13.27	3.16	-1.84
7088	c1cc(cc(c1)O)CO	C00388761	-11.4	-1.99	-15.02	4.73	0.88
7089	CNC(=O)Nc1ccc(cc1)O	C01601880	-11.4	-0.07	-22.93	8.51	3.08
7090	CC[C@H]([C(F)F)Cl)O	C01675523	-11.4	-2.06	-11	1.61	0.05
7091	C1CCC(C1)OC(=O)Cl	C02516857	-11.4	1.84	-13.86	1.76	-1.14
7092	C=CCCCC#N	C02517086	-11.4	-0.95	-12.56	4.78	-2.68
7093	c1cc(c(c(c1)F)F)[N+](=O)[O-]	C02565580	-11.4	-2.73	-14.46	8.1	-2.31
7094	COC(=O)[C@H](C(F)F)F)O	C02576920	-11.4	-1.66	-12.87	3.87	-0.73
7095	c1[nH]c(c(n1)C(=O)N)N	C03861263	-11.4	-3.15	-18.71	8.92	1.53
7096	C(C/C(=N/N)/N)CCl	C04203891	-11.4	-1.67	-13.38	4.51	-0.87
7097	C1C(=O)OCC(=O)O1	C04284649	-11.4	-0.74	-15.48	6.36	-1.54
7098	CC1=C[C@H]([C@H]1)O	C04528632	-11.4	-0.86	-10.99	1.87	-1.42
7099	C1=CNC(=N[C@H]1)S	C05496923	-11.4	-4.85	-13.86	4.37	2.94
7100	C=C[C@H](C#C)O	C12363481	-11.4	-0.05	-12.95	2.33	-0.72
7101	c1[nH]c(nc(=O)[nH+])1N	C18180628	-11.4	-4.94	-17.25	10.8	0
7102	c1cc(ncc1C#N)NN	C20285773	-11.4	-1.81	-15.49	7.19	-1.29
7103	c1cc(c(cc1F)F)Nc2nccn2)N	C00088763	-11.39	-1.04	-8.72	4.69	-6.33
7104	c1csc(n1)NC=C(C#N)C#N	C00093624	-11.39	-1.97	-13.02	6.94	-3.33
7105	Cc1cc[nH]1)O	C01471020	-11.39	-4.12	-14.46	4.99	2.2
7106	C1COCC1	C01692451	-11.39	0.39	-11.1	1.21	-1.88

7107	C1C2COP(O)O2	C01765038	-11.39	-1.45	-13.56	3.38	0.23
7108	CNC(=O)c1c(cn(n1)C)N	C02537279	-11.39	-4.33	-15.57	7.41	1.1
7109	c1cn(nc1C(F)F)F)CC#N	C02537523	-11.39	-4.49	-15.98	12.14	-3.05
7110	CCOC(C(F)F)F)F	C02539799	-11.39	-1.09	-11.01	2.67	-1.96
7111	C(C#N)C(=S)N	C05112695	-11.39	-2.92	-13.71	5.53	-0.29
7112	c1c2c([nH]n1)ncn(c2=O)N	C05479371	-11.39	-4.33	-20.52	9.69	3.76
7113	c1c(c[nH]1)F	C06091386	-11.39	-2.17	-13.35	4.04	0.1
7114	CC[C@H](C)ON=O	C06129975	-11.39	-1.04	-10.1	2.48	-2.73
7115	C1[C@H](CSC(=[NH+1])N)Br	C08614816	-11.39	-0.92	-11.28	2.08	-1.27
7116	c1c(c(=O)c(c[nH]1)Cl)Cl	C11757584	-11.39	-0.48	-14.64	2.52	1.21
7117	C#CC[C@H](c1cccc1)O	C12361905	-11.39	-0.26	-11.52	3.59	-3.2
7118	c1c(c(c(n1)N)[O-])F)Cl	C21981847	-11.39	-4.46	-15.24	7.98	0.33
7119	CCc1cc(no1)CO	C26547721	-11.39	-1.86	-14.51	5.62	-0.64
7120	C1C=C(C(=O)O1)Br	C30677954	-11.39	-3.09	-14.45	8.56	-2.41
7121	Cc1ccc(s1)/C=N/O	C00334142	-11.38	-2.91	-12.79	5.84	-1.53
7122	COCCBr	C01627348	-11.38	-0.18	-11.82	2.17	-1.55
7123	CCOC(C=O)C	C01697403	-11.38	0.71	-12.94	3.86	-3.02
7124	Cc1c(=O)n(c(n1)N)N	C02022931	-11.38	-5.87	-15.93	7.84	2.58
7125	CCCC(=O)C=C	C02039390	-11.38	-0.38	-11.59	3.67	-3.08
7126	c1c(cn(n1)CC(F)F)F)N+](=O)[O-]	C02534799	-11.38	-3.65	-13.02	8.73	-3.45
7127	COC1=NC=CC1	C04268437	-11.38	-2	-12.68	2.76	0.55
7128	c1cn[nH]c1CO	C04343992	-11.38	-4.06	-14.44	5.93	1.19
7129	CCCCOC(=O)CS	C04501341	-11.38	2.78	-14.42	3.93	-3.68
7130	c1cn(c(=O)[nH]c1=O)CCBr	C04785827	-11.38	-2.44	-16.85	9.48	-1.59
7131	CCNc1cccc1N	C05139781	-11.38	-4.36	-10.88	2.36	1.5
7132	c1cc(cc(c1)F)C(=O)C=O	C05240957	-11.38	-0.66	-14.38	7.56	-3.9
7133	c1cc(c(cc1)C=N)O)O	C05723016	-11.38	-3.44	-16.64	6.68	2.02
7134	Cc1nc(no1)CC#N	C09596237	-11.38	-1.8	-16.57	7.77	-0.78
7135	COC(=O)c1c([nH]cn1)N	C17419483	-11.38	-0.42	-16.73	7.22	-1.45
7136	c1cc(cc(c1)F)C@H]2CO2	C18899433	-11.38	-2.4	-11.33	5.08	-2.73
7137	CCOC(=O)c1cn(c([nH]1)N	C19091522	-11.38	-1.08	-13.89	6.14	-2.55
7138	C1CC(C1)N=C=O	C19477720	-11.38	0.68	-13.13	1.71	-0.64
7139	c1c(cnc1Cl)CO	C21303204	-11.38	-1.86	-13.68	4.59	-0.43
7140	Cc1ccc(n1C)C#N	C00160266	-11.37	0.44	-12.54	4.26	-3.53
7141	c1c(=O)[nH]c(=O)[nH]c11	C01682350	-11.37	-1.25	-15.46	5.06	0.28
7142	CCSCCBr	C01687819	-11.37	-0.69	-8.01	1.08	-3.75
7143	c1ccc2c(c1)OS(=O)O2	C01710890	-11.37	-2.61	-18.29	11.26	-1.74
7144	C[C@H](C=C)O	C01758745	-11.37	-1.9	-11.37	2.01	-0.11
7145	CC[C@H](CC#C)O	C01765496	-11.37	-0.31	-12.73	3.07	-1.39
7146	Cc1cccn1	C01845812	-11.37	-1.77	-14.01	4.32	0.09
7147	c1c(cc(c1F)O)F)Br	C02560118	-11.37	-0.21	-13.72	2.45	0.1
7148	c1(c(c(c1F)F)F)F)O)O	C02572594	-11.37	-3.4	-13.03	4.86	0.2
7149	C(=O)C(=O)C(F)F)F	C02598062	-11.37	-0.91	-14.03	5.57	-2
7150	c1c(c(n[nH]1)O)N+](=O)[O-]	C04149782	-11.37	-5.93	-16.87	9.72	1.7
7151	CCOCCO	C04283944	-11.37	-2.49	-12.57	3.51	0.19
7152	C(C(=O)Cl)F)F	C04329299	-11.37	-1.2	-11.51	2.88	-1.54
7153	C1[C@H](CC=C1)C#N	C04787443	-11.37	0.36	-11.36	3.36	-3.73
7154	c1csc(n1)NC2=NC(=O)CS2	C05778643	-11.37	-0.87	-18.18	9.97	-2.29
7155	c1cc(c(c1O)F)C(=O)F	C12956563	-11.37	-3.13	-14.59	7.35	-1
7156	c1cnccc1NC(=O)C(F)F)F	C13208290	-11.37	-3.67	-11.21	5.07	-1.56
7157	CC(=O)N1CCCC1=O	C14684424	-11.37	-1.78	-15.28	6.02	-0.33
7158	c1nc(c(s1)C=O)Cl	C14982499	-11.37	-1.66	-13.36	5.18	-1.54
7159	c1cc(c(=O)[nH]c1)CO	C19091101	-11.37	-4	-16.63	8.5	0.76
7160	CC(=O)Cc1cccc1N	C19801521	-11.37	-2.07	-13.3	6.87	-2.87
7161	C[C@H](C(=[NH2+])N)N+](=O)[O-]	C26898079	-11.37	-6.68	-14.95	10.94	-0.67
7162	COC(=O)c1c(ccc1F)N	C00164468	-11.36	-3.14	-12.43	6.61	-2.41
7163	c1cc(ccc1CON)Cl	C00169388	-11.36	-1.27	-10.82	2.88	-2.15
7164	CNc1nccc(n1)N	C00331866	-11.36	0	-18.75	4.97	2.41
7165	c1cc(c(cc1Cl)Cl)O	C00388057	-11.36	-1.26	-10.72	2.55	-1.93
7166	C1CN(C(=O)N1)C(=O)CC1	C00806258	-11.36	-2.34	-15.3	6.55	-0.28
7167	CC(=O)C(=O)N	C01581119	-11.36	-2.7	-13.65	3.83	1.16
7168	c1c(cc(c(c1F)N+](=O)[O-])F)F	C01706148	-11.36	-1.25	-11.06	4.52	-2.95
7169	C[C@H](CC1)N+](=O)[O-]	C01758981	-11.36	0.49	-14.13	5.11	-2.83
7170	C1CCC(C1)C(=O)Cl	C02242641	-11.36	0.41	-10.44	2.08	-3.41
7171	C1C[C@H](OC1)CC#N	C04207146	-11.36	-0.54	-15.18	6.56	-2.2
7172	Cc1ncc(n1C)Br	C04352760	-11.36	-0.9	-11.86	4.43	-3.03
7173	[H]N=c/1\onc(s1)c2c(non2)N	C04481985	-11.36	-1.86	-13.91	2.38	2.02
7174	C(C(F)F)FS	C04501362	-11.36	-0.67	-10.94	2	-1.75
7175	Cn1cnn(c1=O)C	C05425304	-11.36	-3.46	-14.58	9.13	-2.45
7176	C(=O)(C(O)(O)O)C(F)F)F	C08698296	-11.36	-4.66	-13.43	4.29	2.45
7177	c1ccc(c(c1)C(=O)C)Cl)N	C15021946	-11.36	-1.99	-11.32	4.88	-2.93
7178	[C@H](C(=O)F)F)Cl	C16159210	-11.36	-0.02	-12.76	2.92	-1.5
7179	c1cc(ccc1CCC=O)F	C19682816	-11.36	-3.79	-9.44	6.22	-4.35
7180	COC(=O)Nc1cc(ccc1F)N	C19815589	-11.36	0.02	-17.4	6.59	-0.58
7181	COCCNc1ccc(cc1F)F	C20053295	-11.36	0.85	-13.05	3.36	-2.52
7182	COCCNc1ncccn1	C21511690	-11.36	0.13	-14.32	5.26	-2.42
7183	Cc1c(non1)CS	C23993717	-11.36	-1.14	-14.79	5.97	-1.4
7184	c1nc(c(c(n1)NN)F)CF	C26466574	-11.36	-1.29	-14.08	5.43	-1.43
7185	CSc1ncc(n1)O	C00392495	-11.35	0.35	-18.34	4.82	1.82
7186	c1c(c(nc(=O)[nH]1)N)Br	C00967468	-11.35	-3.19	-19.43	10.2	1.07
7187	C=C1C=CC1=O	C01558090	-11.35	-1.5	-14.28	5.47	-1.04
7188	CC(=O)Nc1c(cc(cc1F)N)F	C01592344	-11.35	0.07	-19.88	8.21	0.25
7189	CCOC(=O)C=O	C01681280	-11.35	-0.81	-15.32	6.95	-2.17
7190	C(CCC)CC#N	C01693305	-11.35	-2.05	-11.27	5.58	-3.61
7191	C[C@H](C(=O)OC)NC(=O)C(F)F)F	C02145546	-11.35	1.29	-14.34	3.77	-2.07
7192	C#CCCC#N	C02390304	-11.35	-1.04	-12.01	4.62	-2.92
7193	c1cc(c(cc1F)F)NC(=S)S	C02565033	-11.35	-2.24	-14.36	4.92	0.34
7194	Cc1c(c(n[nH]1)N)Br	C04244008	-11.35	-4.88	-11.95	6.01	-0.53
7195	Cc1c(ccn1)C(=O)Cl	C04277260	-11.35	-1.33	-14.23	4.5	-0.29
7196	[H]N=C(N)/S[C@H]1CCC[C@H]1O	C04429056	-11.35	0.06	-15	3.3	0.29

7197	C1CCC(=CC1)C#N	C04521340	-11.35	1.48	-14.61	3.5	-1.73
7198	CC(C)CCN=O	C05359504	-11.35	-1.72	-12.46	2.96	-0.13
7199	CC/C=N/N(C)C	C05734086	-11.35	-0.27	-12.93	2.7	-0.85
7200	C1CC(=O)OC1=O	C08681668	-11.35	-4.48	-14.62	6.81	0.94
7201	COCCCN=C=O	C11802362	-11.35	-1.88	-13.6	3.27	0.85
7202	C1C[C@H](OC1)CN=C=O	C11802363	-11.35	-0.91	-14.54	3.71	0.38
7203	Cn1ccc(n1)	C12370361	-11.35	-0.77	-12.8	4.58	-2.36
7204	C1CC(=O)CCC1C(=O)Cl	C16124708	-11.35	-0.28	-13.42	5.43	-3.08
7205	[C@H]1(C(=O)C(=O)NC(=N1)N)[NH3+]	C16891331	-11.35	-5.07	-17.79	8.91	2.61
7206	CCOC(=O)C1c(c[nH]1)N	C17946019	-11.35	0.77	-15.74	4.22	-0.61
7207	C1CC1c2nc([nH]n2)N	C18194322	-11.35	-3.11	-12.54	7.36	-3.06
7208	c1cc2c(cc1Cl)C(F)F	C21985250	-11.35	-2.86	-8.42	3.15	-3.22
7209	Cc1cc[nH]c1C=O	C26898381	-11.35	-2.16	-12.77	5.49	-1.9
7210	CNC(=S)Nc1ccc(cc1)F	C00072259	-11.34	0.45	-17.61	9.33	-3.5
7211	CCOC(=O)c1ccc1	C00164474	-11.34	2.19	-15.37	5.11	-3.26
7212	c1cc(ccc1[N+](=O)[O-])SN	C01583414	-11.34	-0.47	-12.97	4.84	-2.74
7213	c1c(c(cc(c1Cl)F)Cl)N	C01706155	-11.34	-3.85	-9.95	2.17	0.28
7214	CCC(=C)C=O	C01845569	-11.34	-1.45	-12.04	4.5	-2.35
7215	C1COC(O1)C(F)F	C02525293	-11.34	-2.25	-11.69	3.72	-1.12
7216	CC(=O)C1ccc(c1)F	C02600072	-11.34	-1.38	-11.67	6.14	-4.43
7217	Cc1cc(nn1)N[N+](=O)[O-]	C05003197	-11.34	-5.17	-12.67	8.63	-2.13
7218	c1cc2c(c1)Onc[nH]2	C05286233	-11.34	-3.64	-14.74	8.13	-1.09
7219	c1c(nc(c1Cl)Cl)N	C08698162	-11.34	-1.68	-12.77	4.19	-1.08
7220	CCSc1nc(sn1)N	C17173608	-11.34	-4.91	-8.36	3.88	-1.94
7221	C1CC(=O)N(C1)CC#N	C19508742	-11.34	-1.9	-16.63	9.43	-2.23
7222	CC(=O)C1=CNCCC1	C20280751	-11.34	-3.73	-11.49	5.91	-2.03
7223	COCC(=O)COCCC=C	C20519084	-11.34	-0.8	-13.02	5.73	-3.24
7224	COCC1ccc(cc1)N	C22204322	-11.34	-1.23	-12.66	4.02	-1.47
7225	c1c(cc(n1)Br)C=O	C30678087	-11.34	-3.85	-15.32	8.14	-0.31
7226	Cc1cn2ccccc2n1	C00151684	-11.33	-1.59	-12.36	6.92	-4.3
7227	c1cc(cnc1)C(=O)NN	C00152498	-11.33	2.44	-21.24	7.12	0.35
7228	Cc1[n-]c([nH]1)NC(=O)N	C01667220	-11.33	-2.3	-20.08	7.52	3.53
7229	CC[C@H](C(=C)C)O	C02038914	-11.33	-1.13	-10.49	1.46	-1.17
7230	C=CCOC(=O)C[C@H](C=C)O	C02159825	-11.33	-0.68	-12.13	3.55	-2.07
7231	c1cc(c(c1)Br)O	C02510737	-11.33	-0.46	-14.89	3.56	0.45
7232	c1cc(c(c1)F)C(=O)N=C=O	C02568127	-11.33	2.87	-19.24	5.93	-0.89
7233	C/(C=C/Br)Br	C02584386	-11.33	-3.11	-11.14	3.3	-0.38
7234	c1ccc(cc1)C[P@H](=O)[O-]	C03958319	-11.33	-1.8	-15.34	7.68	-1.86
7235	c1c(nnn1c2c(non2)N)[N+](=O)[O-]	C04171179	-11.33	-0.7	-14.23	5.42	-1.82
7236	c1[nH]c(c(n1)[N+](=O)[O-])Br	C04714979	-11.33	-3.61	-11.45	6.94	-3.2
7237	c1ccc(cc1)NC(=O)C=N/O	C05933783	-11.33	-4.31	-17.4	8.9	1.49
7238	CCOCCI	C06661811	-11.33	-0.93	-10.76	1.91	-1.56
7239	c12c([nH]c(=O)[nH]1)nc([nH]c2=O)N	C13527382	-11.33	-4.88	-14.95	6.86	1.64
7240	CC(C)OC(=O)OCCI	C21299034	-11.33	-1.52	-10.79	4.19	-3.22
7241	CC(C)(C#N)Nn1cncn1	C00256496	-11.32	-2.6	-14.94	9.01	-2.79
7242	Cc1csc1C=O	C00334132	-11.32	1.28	-13.77	3.98	-2.8
7243	Cc1nc2ccnnc2n1	C01571375	-11.32	-1.04	-15.74	6.09	-0.63
7244	C1CCC(C1)CO	C01674839	-11.32	-0.88	-11.29	1.84	-0.98
7245	CCOC(=O)CC=C	C01676796	-11.32	-0.64	-12.19	3.62	-2.11
7246	Cc1ccccc1[N+](=O)[O-]	C01700065	-11.32	-2.61	-9.9	5.42	-4.22
7247	C(=N/NC(=O)N)C(=O)N	C04266474	-11.32	-3.68	-17.49	8.71	1.14
7248	CCOC(=O)c1c([nH]n1)C	C05285437	-11.32	-0.21	-14.26	4.6	-1.45
7249	C/C=NN(C)C=O	C05353490	-11.32	-2.17	-13.62	5.96	-1.49
7250	c1c([nH]n1)O	C06452783	-11.32	-3.1	-13.97	4.78	0.96
7251	c1c(c(nc(n1)N)N)CO	C13281672	-11.32	-2.84	-16.02	6.2	1.33
7252	c1cnccc1CC[NH2+]	C19168812	-11.32	0.17	-15.38	4.46	-0.55
7253	c1ccc2c(c1)C[C@H](O2)CN[NH3+]	C19272957	-11.32	-2.01	-11.55	3.6	-1.36
7254	c1cc(c(cc1Cl)N=C=O)F	C19511315	-11.32	-0.49	-10.89	2.33	-2.27
7255	c1c(cc(cc1F)NCC(F)F)F	C20054573	-11.32	-3.28	-7.51	3.17	-3.69
7256	c1cc2c(cc1OC=O)OCO2	C21300262	-11.32	-1.4	-14.48	7.04	-2.48
7257	c1cnc(c(n1)C#N)Cl	C00161160	-11.31	-2.44	-13.9	6.29	-1.25
7258	c1nc(nc1)c2c(non2)N	C01052718	-11.31	-2.39	-16.71	7.13	0.66
7259	CCCc1ccc(cc1)N	C01683314	-11.31	-1.85	-11.39	1.77	0.16
7260	CC[C@H](C)[N+](=O)[O-]	C01758996	-11.31	-1.29	-14.36	5.59	-1.23
7261	C=CC(=O)OCCO	C01850233	-11.31	-1.82	-15.23	6.04	-0.3
7262	C[C@H](C(=O)N)OC(=O)C	C01871132	-11.31	-1.91	-16.83	7.97	-0.53
7263	COCCCI	C02031633	-11.31	-0.97	-11.32	2.39	-1.41
7264	c1[nH]c2c(n1)c(ncn2)NO	C02558668	-11.31	-4.21	-15.98	9.8	-0.91
7265	C=CCOC([C@H](F)Cl)F	C04240027	-11.31	-0.24	-11.14	2.17	-2.1
7266	c1cc(ccc1N=C=O)[N+](=O)[O-]	C04262255	-11.31	-3.28	-12.77	6.72	-1.98
7267	c1cc2c(cc1Cl)nc[nH]2	C05425423	-11.31	-6.21	-8.96	7.55	-3.68
7268	c1(c(non1)N)C(=NH+)(N)N	C05510648	-11.31	-3.16	-17.74	5.48	4.12
7269	c1cc2c(cc1F)sc(=O)[nH]2	C14984961	-11.31	-2.99	-12.81	4.51	-0.01
7270	CC1=CC=C(N1)N)C	C30678136	-11.31	-3.43	-10.12	4.09	-1.85
7271	c1ccc(cc1)c2cn[nH]n2	C00027320	-11.3	0.65	-15.14	5.59	-2.39
7272	c1cc2c(cc[nH]2)cc1C#N	C00157017	-11.3	-1.69	-11.53	5.55	-3.63
7273	c1ccc(c1)C#N)Cl	C00157274	-11.3	-2.11	-10.13	4.84	-3.89
7274	C(CCCCC)CCO	C01666983	-11.3	-1.63	-10.7	2.66	-1.62
7275	Cn1c(=O)ccs1	C01849933	-11.3	-2.31	-15.92	8.34	-1.4
7276	CCOC(=O)[C@H](C)Br	C01866959	-11.3	-0.19	-10.74	3.1	-3.48
7277	CC/C=C/COCC=O	C02010172	-11.3	-0.96	-14.3	6.32	-2.36
7278	COCC(F)F	C02560087	-11.3	-1.51	-11.27	2.71	-1.23
7279	CC(=O)OCCP	C02577210	-11.3	-2.04	-10.89	3.88	-2.25
7280	C=CCOCCBr	C04203464	-11.3	-0.43	-10.43	2.29	-2.73
7281	CCn1cn[nH]c1=S	C04218214	-11.3	-2.14	-12.62	6.89	-3.44
7282	C1C/C(=N/O)NC1	C04579230	-11.3	-0.91	-14.93	4.48	0.06
7283	CSC(=O)c1cscn1	C12471791	-11.3	-1.38	-13.18	5.18	-1.93
7284	c1cc(cnc1)[P@H](=O)O	C13222833	-11.3	-2.95	-16.94	8.54	0.05
7285	c1cc(nc(c1)F)OC(F)F	C16158729	-11.3	-0.13	-17.16	7.51	-1.52
7286	CCc1c([nH]c(nc1=O)N)N	C17040265	-11.3	-3.78	-14.6	5.68	1.39

7287	COC(=O)c1c[nH]nc1N	C18217582	-11.3	-0.95	-15.26	5.45	-0.54
7288	Cn1c(=O)cc(nc1[O-])Cl	C18272301	-11.3	-0.83	-14.51	4.95	-0.92
7289	Cc1ccccc1CNN	C19171889	-11.3	1.06	-12.86	2.39	-1.89
7290	c1ccc(cc1)[C@H]2CO2	C00901249	-11.29	2.13	-14.17	3.52	-2.76
7291	CCCCSCC	C01555231	-11.29	-0.59	-10.85	1.09	-0.94
7292	CSCCO	C01577077	-11.29	-2.74	-10.94	2.34	0.05
7293	C=CCSc1ccsc1	C01663925	-11.29	0.18	-13	2.23	-0.69
7294	CC(=O)c1ocnn1C	C02536627	-11.29	0.99	-15.87	5.64	-2.05
7295	C1CC(=O)C=C1O	C03861294	-11.29	-3.1	-14.8	6.94	-0.34
7296	CCOC(=O)c1c(non1)C	C04343169	-11.29	2.31	-13.69	2.74	-2.64
7297	CC(=O)C=C\OC	C04758442	-11.29	-2.29	-13.79	6.91	-2.12
7298	C/C=NNC(=O)N	C05004577	-11.29	-4.33	-14.76	6.46	1.33
7299	Cc1c[nH]c(=O)nc1	C14982937	-11.29	-3.63	-15.79	5.96	2.16
7300	c1cc2ncc(n2nc1)N	C15020289	-11.29	-3.6	-13.92	7.84	-1.6
7301	c1ccc(cc1)C=NNC=O	C17111335	-11.29	-0.89	-14.31	6.4	-2.49
7302	C=C(C#N)/C(=O)N\N	C17286555	-11.29	-4.48	-15.36	5.97	2.57
7303	c1cc(oc1)/C=C\#N	C17376753	-11.29	-1.02	-14.67	7.6	-3.2
7304	Cc1ccc(s1)CNN	C19413030	-11.29	-1.25	-11.06	2.36	-1.33
7305	c1cc(oc1)c2cc([nH]n2)C=O	C20270497	-11.29	1.03	-18.21	7.87	-1.98
7306	COC(=O)Cn1ccccc1=O	C20302817	-11.29	-1.64	-18.05	11.92	-3.52
7307	c1cc(sc1)[C@H](C(F)F)N	C20475296	-11.29	-1.83	-10.3	2.52	-1.69
7308	Cc1c(cccc1Cl)N	C00157621	-11.28	-2.37	-8.43	2.26	-2.74
7309	Cc1c(c(on1)C)C=O	C00158502	-11.28	-1.95	-12.06	5.2	-2.47
7310	C[C@@H]1C(=O)C=C(C1=O)[O-]	C01761600	-11.28	-4.25	-15.28	8.36	-0.12
7311	CCOCc1ccc(cc1)N	C02584494	-11.28	-1.45	-10.03	2.81	-2.6
7312	CC1=CC[C@H]1O	C05757640	-11.28	-0.87	-10.45	1.73	-1.69
7313	c1cc(oc1C=O)c2ccn[nH]2	C06666971	-11.28	-0.91	-19.49	11.58	-2.47
7314	C1CC1/C(=N/O)/N	C08146674	-11.28	-3.06	-12.54	4.11	0.21
7315	CCC/C=C\OC(=O)C	C20230653	-11.28	0.96	-11.88	4.2	-4.57
7316	c1cc(c(cc1F)[C@H]2CO2)F	C22215708	-11.28	-1.07	-10.88	3.48	-2.81
7317	C1CC(=C(C=C1)Br)O	C30677946	-11.28	0.07	-14.02	5.99	-3.33
7318	CNc1cc(nh+)c(n1)N	C32914851	-11.28	-2.91	-12.8	5.85	-1.43
7319	c1cnc2nc(cn2c1)CBr	C00078830	-11.27	-3.11	-13.59	10.7	-5.27
7320	c1cc2c(cc1C#N)OCO2	C00388101	-11.27	-2.56	-11.09	4.95	-2.56
7321	C1CNc2(non2)N1	C01052690	-11.27	-3.66	-16.54	9.25	-0.33
7322	CCSCCO	C01687820	-11.27	-2.88	-10.17	2.27	-0.48
7323	CCOC(=O)CN(C)C#N	C01690411	-11.27	-2.56	-11.74	8.23	-5.21
7324	C[C@@H](COC)C(F)F	C01709839	-11.27	-2.62	-11.46	3.3	-0.5
7325	COC(=O)C(C(=O)OC)C(F)F	C02003934	-11.27	-0.03	-12.81	4.25	-2.68
7326	C[C@H](C(=O)OC)O	C02034809	-11.27	-1.16	-13.85	4.11	-0.37
7327	CC(=C)CNC(=S)NN	C03269650	-11.27	0.21	-17.78	7.9	-1.6
7328	Cc1c[nH]nc1O	C03861216	-11.27	-3.74	-15.27	5.47	2.27
7329	C1CSCC(=O)N1	C04137257	-11.27	-2.94	-13.2	5.48	-0.61
7330	C1COC(=O)[C@H]1N=C=S	C04266335	-11.27	-0.28	-15.9	6.88	-1.97
7331	CC#C[C@H](C)O	C05158110	-11.27	-1.11	-12.15	2.81	-0.83
7332	CSC/C(=N/O)/N	C06794381	-11.27	-3.17	-15.39	5.47	1.82
7333	c1n([nH]c1N+)(=O)[O-]C2CC2	C12396626	-11.27	0.46	-11.26	3.13	-3.61
7334	Cc1cccc(c1F)C#N	C16158454	-11.27	-1.34	-11.33	5.52	-4.12
7335	CCNc1ccnc(n1)Cl	C19091606	-11.27	-4.52	-9.28	4.68	-2.15
7336	CC(=O)N(C)CC=O	C19679292	-11.27	-3.45	-12.84	6.28	-1.28
7337	c1c(con1)C=O	C20417325	-11.27	-2.61	-15.28	7.95	-1.33
7338	C1COC(OC1)CCBr	C00155380	-11.26	-0.74	-10.46	2.61	-2.66
7339	C(C(=O)C(F)F)F	C01655707	-11.26	-1.09	-12.19	4.85	-2.82
7340	c1c(c(sc1Cl)Cl)Cl	C02244224	-11.26	-0.69	-11.09	0.41	0.12
7341	Cc1c(ccc(n1)Cl)F	C02539926	-11.26	-1.78	-11.32	2.64	-0.8
7342	CC(=O)CSC(=[NH2+])N	C04768945	-11.26	-0.3	-16.88	4.34	-2.58
7343	CNc1c(c(c(c1F)F)F)F	C05996550	-11.26	-0.68	-10.01	1.59	1.16
7344	COc1cnc(c1)Cl	C08614795	-11.26	-1.53	-12.55	2.68	0.14
7345	c1cnn(c1)c2ccc(cc2N)F	C12398078	-11.26	-1.4	-11.04	4.5	-3.32
7346	c1c(cc(c2c1[nH]nc2)O)F	C14983372	-11.26	0.54	-15.95	4.42	-0.27
7347	C=N/N=C/C1cncn1)N	C15229050	-11.26	-1.96	-15.72	6.57	-0.15
7348	CCOC(=O)c1ccc(n1)N	C17061541	-11.26	-2.33	-13.49	3.92	0.64
7349	C(=N/O)C=N/O	C18120428	-11.26	-6.02	-11.96	3.96	2.76
7350	c1c(cnc(c1Br)N)Cl	C19721329	-11.26	-0.55	-11.26	2.49	-1.94
7351	Cn1c(c(cn1)Br)C(F)F	C26513441	-11.26	-0.77	-10.42	2.62	-2.69
7352	c1cc(c(nc1)C(F)F)Cl	C30714862	-11.26	-3.12	-9.79	4.9	-3.24
7353	COc1ccccc1O	C00389516	-11.25	-2.16	-12.39	4	-0.71
7354	CCCc1[nH]ccn1	C00389830	-11.25	-1.77	-11.73	4.86	-2.61
7355	CCOC(=O)[C@H]1[C@H](O1)C	C02016528	-11.25	-0.73	-14.83	6.21	-1.9
7356	CCO[C@H]1C=CC(=O)O1	C05316521	-11.25	-2.43	-13.56	7.19	-2.45
7357	c1nc2n(n1)C(=O)CS2	C05778321	-11.25	-2.68	-16.07	9.63	-2.13
7358	c1cnc2c1cnc2	C06119163	-11.25	-3.08	-13	4.63	0.2
7359	COC(=O)c1[n-]cnn1	C12398239	-11.25	-0.78	-15.98	7.72	-2.21
7360	c1c(cn1)CO	C12957939	-11.25	-4.44	-13.77	6.98	-0.02
7361	c1csc(c1)[C@H](C#N)N	C21950032	-11.25	-1.32	-13.82	5.05	-1.16
7362	c1c(c(c(c1N)[O-])F)F	C21981831	-11.25	-3.62	-16.94	8.63	0.69
7363	Cc1cc(n1)NC=O	C23993713	-11.25	-2.17	-16.27	8.6	-1.4
7364	CC[C@H](c1cccs1)O	C32005453	-11.25	-1.59	-10.78	3.07	-1.95
7365	c1c(c(cs1)Br)CO	C00334083	-11.24	-1.83	-10.65	2.35	-1.11
7366	c1cc2c(cc1C#N)no[n+]2[O-]	C00509558	-11.24	-3.11	-14.86	10.48	-3.75
7367	CC(=O)CCOC	C01571067	-11.24	-0.74	-13.06	3.96	-1.4
7368	CC1=NCC(=O)O1	C01578443	-11.24	-1.9	-15.3	4.52	1.44
7369	CN(CC=C)C=O	C01695273	-11.24	-0.99	-13.78	5.23	-1.7
7370	CNC(=O)C(F)F	C01845674	-11.24	-2	-13.1	4.01	-0.15
7371	c1c(nc(s1)Br)CO	C04198769	-11.24	-2.25	-12.25	3.13	0.13
7372	c1cnc(c1)OCCO	C05286613	-11.24	-3.16	-13.82	5.5	0.23
7373	c1cc(sc1(=O)Cl)Br	C06335011	-11.24	-0.99	-12.99	2.37	0.37
7374	C(C(F)F)OC(=O)N	C08390489	-11.24	-2.96	-13.65	4.4	0.96
7375	C\1COC(=O)/C1=C/[C@H]2CO2	C16037740	-11.24	-1.23	-15.08	6.97	-1.9
7376	[H]/N=C(C(CCC))OCC	C17002002	-11.24	-1.43	-11.19	2.22	-0.83

7377	Cc1cnn(c1)CCO	C19092565	-11.24	-2.49	-12.63	4.36	-0.47
7378	c1cc(c(cc1F)Cl)CS	C19414866	-11.24	0.38	-9.57	2.41	-4.47
7379	c1csnc1C=O	C20443576	-11.24	-1.41	-17	8.39	-1.21
7380	c1cn2c(n1)nc(cn2)C(F)(F)F	C21994021	-11.24	-3.84	-11.22	7.95	-4.13
7381	CCOC(=O)C	C00895412	-11.23	-0.42	-12.47	4	-2.34
7382	c1cnc(n2c1nnc2)[O-]	C01613013	-11.23	-3.67	-19.81	10.63	1.61
7383	C#C/C=N/NC(=O)N	C01686584	-11.23	-2.23	-17.25	6.45	1.81
7384	CC(=O)OCc1ccc(o1)[N+](=O)[O-]	C01693515	-11.23	-0.92	-14.71	8.16	-3.76
7385	C/C=C/CO	C01758744	-11.23	-1.22	-12.25	2.31	-0.05
7386	CC[C@H]1C(=CC(=O)O1)[O-]	C02044283	-11.23	-0.26	-14.32	4.67	-1.33
7387	CC[C@H]1CCCC1=O	C02162286	-11.23	0.82	-11.62	3.01	-3.43
7388	C1C[C@H](OC1)CN=C=S	C02164322	-11.23	-0.55	-12.35	3.37	-1.7
7389	c1cc2cc[nH]c2c(c1)N	C02389399	-11.23	-2.29	-11.5	4.51	-1.95
7390	C/C(=C/Br)/C#N	C02539354	-11.23	-2.14	-12.12	4.5	-1.47
7391	C(CC#N)CSC(=NH2+)N	C04642990	-11.23	-2.36	-13.61	6.27	-1.53
7392	c1ccc2c(c1)C(=[N+]=[N-])N=N2	C05464544	-11.23	1.5	-16.41	5.32	-1.64
7393	CCON=O	C05650763	-11.23	-0.89	-11.1	2.4	-1.64
7394	[H]/N=C/[N-][N+](=O)[O-]SC	C05721282	-11.23	-3.64	-17.04	9.22	0.23
7395	CNc1c(cnc(n1)NN)F	C06639728	-11.23	0.7	-15.05	4.37	-1.26
7396	Cc1ccc(nn1)NN	C11567889	-11.23	-4.55	-13.34	7.27	-0.6
7397	c1ccc(cc1)Sc2nccs2	C15781452	-11.23	-0.01	-11.3	4.58	-4.51
7398	c1cc(c(c1C#N)F)FBr	C16159965	-11.23	-2.73	-9.9	5.21	-4.12
7399	CC/C=C/C=C/C=O	C20231657	-11.23	-0.59	-11.98	4.85	-3.51
7400	C=C[C@@H]1C(=C)CCCCO1	C21990744	-11.23	-0.72	-8.98	1.71	-3.24
7401	c1cc(oc1)[C@H](C)[N+](=O)[O-]O	C00055278	-11.22	-0.06	-15.77	5.66	-1.06
7402	CNC(=O)c1cccc1	C00336927	-11.22	-1.67	-14.15	6.67	-2.06
7403	c1ccc2c(c1)C[C@H]3[C@H]2O3	C01433171	-11.22	-0.63	-11.75	4.21	-3.05
7404	c1c(cnc1F)C(=O)N	C01596084	-11.22	-0.91	-17.05	6.36	0.37
7405	c1c(c(nc(n1)Cl)Cl)F	C01696262	-11.22	0.23	-13.77	2.42	-0.09
7406	C1=CC(=O)N(C1=O)CO	C01868506	-11.22	-3.89	-17.4	8.21	1.86
7407	CC/C=C(C)/CO	C02039394	-11.22	-0.74	-13.34	2.38	0.47
7408	COCC(C(F)F)F	C02572596	-11.22	-0.81	-11.3	2.85	-1.96
7409	c1c(c(nc(c1)F)F)Cl	C02585564	-11.22	0.67	-11.18	2.03	-2.73
7410	C#CCNC(=O)CCCl	C03091475	-11.22	0.14	-15.44	4.4	-0.32
7411	Cc1ccnnc1N	C03123182	-11.22	-2.87	-13.93	4.29	1.29
7412	c1nc(c(c(n1)[O-])F)CF	C03130171	-11.22	-2.43	-14.73	4.77	1.16
7413	c1c(nc(s1)C=S)Br	C04198787	-11.22	-1	-11.47	3.88	-2.63
7414	CS(=O)(=O)c1[n-jnc(n1)[N+](=O)[O-]	C04537580	-11.22	-7.01	-15.22	12.21	-1.2
7415	COC(=O)Cn1ccc(=O)[nH]c1=O	C05175369	-11.22	-2.99	-19.45	11.37	-0.15
7416	Cc1cc(c(nc1)Br)N	C08698240	-11.22	-3.52	-10.14	3.92	-1.48
7417	Cc1c(c[nH]1)C(=O)OC	C08699843	-11.22	1.42	-16.24	5.23	-1.63
7418	c1cc2c(c1)C(=O)nsn2	C12375028	-11.22	-1.97	-15.4	5.88	0.27
7419	COc1nc(c(nn1)F)[O-]	C12958963	-11.22	-1.42	-16.45	4.82	1.83
7420	CNc1ccc(nc1)Cl	C19230648	-11.22	-0.67	-11.27	3.02	-2.3
7421	Cc1nccc(n1)C=O	C20442771	-11.22	-0.8	-13.22	4.49	-1.69
7422	Cc1c(cc(cn1)Br)N	C21993122	-11.22	-0.07	-13.94	4.32	-1.53
7423	c1nccc2c1cc(s2)C=O	C30677829	-11.22	-3.57	-10.25	5.39	-2.79
7424	c1ccc(cc1)NNC(=O)N	C00001924	-11.21	0.98	-18.31	6.42	-0.29
7425	c1ccc(c(c1)C(=O)NN)O	C00110435	-11.21	-2.37	-17.97	8.96	0.17
7426	c1csc2n1cc(nc2)Br	C01571473	-11.21	-1.31	-16.89	6.73	0.26
7427	CCOC1CCCC1	C02034347	-11.21	-1.42	-11.05	2.3	-1.05
7428	CCOP(O)O	C02037673	-11.21	-4.8	-12.8	6.69	-0.31
7429	Cn1cnc(c1C=O)Br	C02382641	-11.21	-2.6	-11.16	5.52	-2.97
7430	c1cc(c(nc1)F)C=O	C02384094	-11.21	-2.99	-16.81	10.41	-1.82
7431	CC[C@H](C)N=C=O	C02387312	-11.21	0.75	-12.87	1.81	-0.9
7432	Cn1ccc(n1)N=C=S	C02522255	-11.21	-1.76	-12.58	6.17	-3.04
7433	C1C[C@H](C)CC(=O)C=O	C03875685	-11.21	-0.61	-11.16	3.77	-3.21
7434	C(=N/O)c1c(c(c(c1F)F)F)F	C04801780	-11.21	-0.61	-13.16	4.4	-1.84
7435	C1CO[C@H](CO1)CCl	C05191059	-11.21	-0.15	-15.06	3.19	0.81
7436	C/C(=N/O)/C(=N/O)/C	C12358611	-11.21	-6.64	-13.92	8.74	0.61
7437	CCOC(=O)C(=[N+](=O)[O-])[C](=O)C	C12413614	-11.21	-1.42	-14.12	6.91	-2.58
7438	c1ccc(c1)C=C/NC=O	C12495746	-11.21	-1.13	-15.79	7.21	-1.5
7439	c1cc(c(c1)Cl)N=C=O	C12505369	-11.21	-2.44	-9.88	3.43	-2.32
7440	CC(=O)Oc1ccc(nc1)C#N	C16678104	-11.21	-1.08	-13.89	7.13	-3.37
7441	C/C=C/C1OCC=CCO1	C16892844	-11.21	-0.52	-10.77	3.04	-2.96
7442	Cn1cccc1/C=N/O	C17021793	-11.21	-3.79	-11.65	5.28	-1.05
7443	CCOC(=O)C=C(C(F)F)F	C17142398	-11.21	-0.3	-13.42	6.1	-3.59
7444	CCCN=C/C/1C=CC=[NH+]1	C17378193	-11.21	-1.05	-10.71	3.1	-2.56
7445	CN/C(=N/C#N)/SC	C18043329	-11.21	-0.7	-11.58	3.06	-1.99
7446	C1CCN(C(=O)C1)CCC#N	C20296503	-11.21	1.84	-18.03	8.26	-3.28
7447	c1nnc2n1NC(=O)CS2	C26894428	-11.21	-1.72	-16.52	8.67	-1.64
7448	COc1cnc(cn1)N	C33358876	-11.21	-1.09	-16.88	5.42	1.34
7449	c1cscc1CC(=O)NN	C00120974	-11.2	-4.74	-13.46	7.63	-0.62
7450	Cc1cnc(s1)NC	C00330650	-11.2	-3.68	-9.53	4.01	-2
7451	COCC1c[nH]c(=O)[nH]c1=O	C00334157	-11.2	-4.83	-14.87	7.3	1.2
7452	CC(=C)C#N	C01571157	-11.2	-1.97	-11.3	4.32	-2.25
7453	c1c(c(=O)[nH]c(=O)n1O)C#N	C01604744	-11.2	1.09	-22.05	9.41	0.36
7454	CC(=C)C(=O)Oc1cccc1	C01725147	-11.2	-0.56	-10.73	5.33	-5.24
7455	COc(C(F)F)F	C01847428	-11.2	-0.62	-12.11	2.83	-1.31
7456	CC[C@H](C#CC)O	C02390326	-11.2	0.4	-12.68	2.58	-1.5
7457	C/C(=[NH+]/C#N)/N	C02575364	-11.2	-3.98	-12.69	7.08	-1.61
7458	c1ccc(c1)N)NC(=O)N	C03163091	-11.2	-0.58	-22.08	7.76	3.7
7459	c1c(nc(n1)Br)CCO	C04203470	-11.2	-3.18	-12.17	3.9	0.25
7460	C(#N)c1c(n[nH]n1)Br	C04531248	-11.2	-5.3	-11.05	3.57	1.59
7461	Cn1cnc2c(c1=O)n[nH]n2	C04622295	-11.2	-6.99	-18.29	11.99	2.1
7462	c1cc(c(c1)O)ClO	C05784422	-11.2	-0.8	-16.79	4.35	2.05
7463	C1C=CC(=O)CO1	C06760908	-11.2	-1.7	-14.97	5.4	0.06
7464	CC(=O)Oc1cc(sc1)C=O	C12359442	-11.2	-0.53	-15.54	8.24	-3.38
7465	c1c2c(ncn1)ncnc2[O-]	C17157982	-11.2	-5.28	-15.2	11.08	-1.81
7466	CCc1ncc(cn1)C#N	C19093025	-11.2	-0.84	-11.4	3.89	-2.85

7467	c1ccc(cc1)O[C@@H]C(=[NH2+])N	C19510023	-11.2	1.25	-20.4	9.28	-1.33
7468	Cc1cc(oc1N)C#N	C21981876	-11.2	0.2	-15.36	5.87	-1.92
7469	CCOc1ccc(nc1)Cl	C21981935	-11.2	0.07	-12	3.3	-2.58
7470	c1cn(cn1)C[C@H]2CO2	C22178514	-11.2	-3.06	-13.34	7.49	-2.29
7471	c1ccc(cc1)Nc2[n-]c(nn2)O	C25490371	-11.2	-1.7	-18.43	9.2	-0.27
7472	c1cscc1C(=O)CC#N	C00108546	-11.19	1.12	-20.54	11.6	-3.37
7473	c1ccc2c(c1)nn(n2)N	C00333062	-11.19	-0.7	-16.26	6.46	-0.68
7474	COc1ccc(cc1)OC#N	C00369358	-11.19	-1.01	-12.6	2.79	-0.38
7475	Cn1ccnc1I	C00967464	-11.19	-1.68	-10.87	4.54	-3.18
7476	C=C([C@H](CO)O)Cl	C01661160	-11.19	-2.65	-13.75	3.35	1.86
7477	C=COC(=O)N	C01720047	-11.19	-3.1	-13.94	4.6	1.25
7478	c1(c(ss1)C(F)(F)C(F)(F)F)	C01765084	-11.19	-1.23	-7.35	0.62	-3.23
7479	CC[C@H](C)[N+](=O)[O-]	C02034490	-11.19	-0.86	-11.17	3.8	-2.96
7480	CCCC(=O)CC	C02034635	-11.19	-0.4	-10.96	3.45	-3.27
7481	CC(=O)Cn1cc(cn1)Cl	C02537946	-11.19	-2.97	-14.21	8.9	-2.91
7482	c1cnc(cn1)NC(=S)N	C02538964	-11.19	-2.14	-19.01	11.45	-1.49
7483	C(=O)C(F)BrN	C04566219	-11.19	-3.01	-12.03	3.29	0.56
7484	[H]/N=c1/n(c(cs1)C)N	C04619757	-11.19	-2.92	-15.3	4.67	2.36
7485	c1cnn(n1)C(=O)O	C05605229	-11.19	-5.89	-17.09	11.25	0.54
7486	CCSC#N	C05648398	-11.19	0.73	-12.8	2.84	-1.96
7487	[H]/N=C/C(C)C)OC	C05715333	-11.19	-1.04	-12.27	2.2	-0.08
7488	c1c(c(=O)[nH]cn1)C(=O)N	C08672865	-11.19	-3.89	-18.1	8.35	2.45
7489	c1ccc2c(c1)ncn2N[N+](=O)[O-]	C13230357	-11.19	-1.66	-10.89	5.31	-3.95
7490	CS/C(=NH+)]N)/N	C16248586	-11.19	-2.92	-12.71	3.89	0.55
7491	C(=N/C(=O)N)NC(=O)N	C17145934	-11.19	-3.23	-17.99	6.25	3.78
7492	c1[nH]c2c(n1)ncnc2N(N=O)O	C17174526	-11.19	-2.55	-17.23	11.1	-2.51
7493	c1nc(c2c(n1)nsn2)N	C17298966	-11.19	-2.22	-16.45	7.66	-0.19
7494	C(C(F)(F)F)NN	C19166968	-11.19	-2.96	-10.57	2.02	0.32
7495	c1ccc(c(c1)NC(=O)CC#N)F	C00091998	-11.18	-4.24	-15.23	11.48	-3.19
7496	CC(=O)Nc1cc(c(c1F)F)F	C00398900	-11.18	-1.92	-12.04	5.14	-2.36
7497	CC1=[NH+]]C(=O)CN1	C01600181	-11.18	-2.67	-15.56	6.27	0.78
7498	CSc1cc(ncn1)N	C01675805	-11.18	0.01	-16.5	3.68	1.63
7499	CCCCOC(=O)C	C01699905	-11.18	1.48	-12.89	3.82	-3.59
7500	CC1=CC(=O)N(C1=O)N	C01731977	-11.18	-3.46	-15.99	6.07	2.19
7501	C=CCCCOCCI	C02244264	-11.18	-1.83	-10.56	2.05	-0.84
7502	C1C=C(CS1(=O)=O)N=C=S	C02454917	-11.18	0.22	-18.84	8.05	-0.61
7503	COc1c(cc(c1O)O)O	C02566737	-11.18	-1.85	-18.1	6.3	2.47
7504	C1CCO[C@H](C1)O	C03606317	-11.18	-1.04	-12.6	2.73	-0.26
7505	C(=O)(C(=O)NO)NO	C04775726	-11.18	-8.08	-15.01	8.89	3.02
7506	CNC(=O)NCC(F)(F)F	C04804438	-11.18	-3.04	-13.97	5.18	0.66
7507	C[C@H](CCS)CS	C05420301	-11.18	-0.44	-8.72	1.26	-3.29
7508	Cc1cc(c(nc1)Cl)F	C08698182	-11.18	0.92	-14.91	3.77	-0.95
7509	CCCCN/C(=N/O)N	C13536006	-11.18	-0.98	-13.31	4.15	-1.04
7510	c1cc(oc1)CNCC#N	C20056646	-11.18	-1.44	-15.71	7.33	-1.36
7511	C1=C(C(=NC(=O)[C@@H]1Cl)Br	C22000015	-11.18	-1.76	-14.4	6.31	-1.33
7512	Cc1nc(co1)Cl(=O)N	C22606247	-11.18	-2.56	-17.75	6.82	2.3
7513	c1cn(cn1)C(=O)NCC(=O)N	C32628556	-11.18	-5.18	-16.75	10.05	0.7
7514	c1cc(ccc1CO)OC(F)F	C00160555	-11.17	-3.73	-12.13	5.66	-0.97
7515	c1(c(non1)C(=O)N)C(=O)N	C01083685	-11.17	-3.65	-17.47	7.4	2.55
7516	c1cnn2c(n1)nnn2	C01504564	-11.17	-4.46	-19.78	14.61	-1.54
7517	C1CSCC(=O)O1	C01604633	-11.17	-1.01	-12.73	4.94	-2.38
7518	C[C@H]1CCCS1	C02039245	-11.17	0.47	-10.13	1.89	-3.4
7519	C[C@H](C(=O)C)F	C02386513	-11.17	-0.8	-11.26	2.97	-2.09
7520	CCn1ccc(n1)N=C=S	C02537537	-11.17	0.39	-14.06	6.16	-3.66
7521	CCOc1ccc(c(c1)F)Cl	C02567847	-11.17	0.19	-12.92	2.9	-1.33
7522	c1c(sc(n1)Cl)CCI	C02572329	-11.17	-1.36	-13.47	3.18	0.48
7523	CCn1cc(cn1)CO	C02578416	-11.17	-2.39	-14.14	5.87	-0.5
7524	C[C@H](CCl)/C(=[NH+])N)/N	C04203877	-11.17	-1.55	-11.89	2.87	-0.59
7525	c1cc(c(c(c1)F)C(=O)C=O)F	C05240975	-11.17	-3.22	-12.58	8.64	-4
7526	c1c2c(c(nn1)NN)n[n-]n2	C05543320	-11.17	-1.73	-17.86	6.7	1.72
7527	c1[nH]c(c(n1)Br)Br	C08294931	-11.17	-3.77	-10	4.98	-2.39
7528	CS(=O)(=O)n1cccn1	C13948093	-11.17	-2.31	-18.83	9.73	0.24
7529	c1cscc1CNCC(F)(F)F	C19435440	-11.17	-1.08	-10.62	3.1	-2.58
7530	CC/C=C/C=C)CO	C20231651	-11.17	-0.44	-12.08	3.15	-1.8
7531	CCc1nc(noc1)CCI	C20368531	-11.17	2.99	-15.65	3.86	-2.36
7532	c1cc(oc1)C(=O)c2[nH]cc[nH+]2	C00167322	-11.16	-0.91	-15.57	7.79	-2.46
7533	c1cc(ccc1NC=O)Br	C00396370	-11.16	-1.68	-14.12	7.02	-2.39
7534	C1C(=C(C(=O)O1)Cl)Cl	C01669133	-11.16	-0.99	-13.05	5.54	-2.67
7535	C=CCON	C01716621	-11.16	-1.49	-11.63	2.08	-0.14
7536	c1(c(=O)ssc1Cl)Cl	C01722340	-11.16	1.63	-14.82	1.99	0.04
7537	COC(=O)CC(=O)Cl	C02170332	-11.16	-2.04	-13.6	7.16	-2.67
7538	c1c(cn(n1)CC(F)(F)F)N	C02521254	-11.16	-1.4	-14.62	5.85	-1
7539	c1cc(nc(c1)F)C(=O)Cl	C02525419	-11.16	-2.73	-11.03	5.03	-2.44
7540	C(CBr)CC(=O)Cl	C02560396	-11.16	-0.69	-13.37	3.28	-0.38
7541	c1ccc(cc1)COCC#N	C03130524	-11.16	0.55	-17.09	6.99	-1.61
7542	Cn1cccc1C(=O)N	C03262883	-11.16	-0.34	-16.31	6.09	-0.59
7543	c1ccc(cc1)N=S=O	C04521868	-11.16	-1.34	-20.22	11.59	-1.2
7544	CN(CCO)N=O	C05066705	-11.16	-4.04	-13.5	4.66	1.72
7545	C/C=C/C=C)COC(=O)C	C05282693	-11.16	-0.6	-12.48	4.2	-2.28
7546	CC/C=C)CCC=O	C06661796	-11.16	-0.58	-12.85	3.96	-1.7
7547	[C@H](C(=O)N)(F)I	C08698285	-11.16	-3.17	-12.55	4.29	0.26
7548	Cc1ccnc(c1)NN	C11567887	-11.16	-1.92	-11.88	4.15	-1.51
7549	c1cnn2c1ncc(c2)N	C12396940	-11.16	-3.3	-14.37	7.51	-1
7550	COc1cc(coc1)C=O	C16943643	-11.16	-2.76	-12.36	5.11	-1.15
7551	C1[C@@H](C=C)C[C@H]2[C@H]1O2)O	C17000696	-11.16	-2.19	-13.55	3.88	0.69
7552	CCn1c(nnn1)N	C17024933	-11.16	-1.21	-15.95	7.56	-1.56
7553	C1CC(=NC1)C[N+](=O)[O-]	C20445714	-11.16	2.5	-15.8	3.18	-1.05
7554	c1cnc(cc1Br)C#N	C00065167	-11.15	0.54	-13.3	4.35	-2.75
7555	C1C=C[C@H]2[C@H]1C(=O)C2(Cl)Cl	C00159161	-11.15	0.83	-11.09	2.99	-3.88
7556	CCC(=NO)CC	C00160693	-11.15	-1.42	-11.82	3.27	-1.18

7557	c1nc2c(c(n1)N)CCC2	C00248748	-11.15	-0.24	-13.22	4.7	-2.39
7558	Cc1c([nH]c(nc1=O)N)N	C00330433	-11.15	-4.24	-15.8	9.12	-0.23
7559	c1ccnc(c1)Nc2ncccn2	C01267756	-11.15	2.09	-14.92	7.13	-5.45
7560	CCN1C(=O)CSC1=O	C01319370	-11.15	1.22	-15.25	4.67	-1.79
7561	CCCC(=O)C#C	C01613266	-11.15	-0.32	-12.41	4.66	-3.08
7562	C[C@H](C(=O)C(=C)C)O	C01663924	-11.15	-0.58	-11.28	2.24	-1.52
7563	c1c(sc(n1)[S-])N	C01699988	-11.15	-4.52	-15.72	9.56	-0.47
7564	C[C@@H](CCC=C)O	C02003061	-11.15	-0.48	-12.48	1.49	0.33
7565	c1c(cnc(c1C=O)Cl)F	C02384081	-11.15	-0.51	-14.76	6.38	-2.26
7566	C1C=CC(=O)S1	C02545307	-11.15	-1.96	-14.07	6.93	-2.04
7567	c1(nc(sn1)[S-])S	C04170603	-11.15	-2.21	-13.78	6.99	-2.15
7568	C=CCOc1ccc(cc1)N	C05000140	-11.15	-2.19	-9.63	3.05	-2.39
7569	C[C@@H](c1cccn1)O	C05319867	-11.15	-1.76	-11.97	3.4	-0.83
7570	c1cnc([nH]1)CC#N	C12520175	-11.15	-2.1	-17.45	10.3	-1.9
7571	C/C(=N/O)/C(F)F	C16082659	-11.15	-2.66	-12.19	3.97	-0.27
7572	c1nnc(n1)CCC(=S)N	C19476287	-11.15	-2.92	-15.39	9.78	-2.62
7573	C[C@H]1C=NN([C@@H]1C)C	C22205956	-11.15	-1.02	-11.24	3.33	-2.21
7574	CCc1ccc(c(c1)O)O	C00002501	-11.14	-1.4	-13.49	4.46	-0.72
7575	COc1ncccn1	C00330839	-11.14	-1.67	-15.73	5.85	0.4
7576	c1cc(cc1C(=O)NN)[N+](=O)[O-]	C01041279	-11.14	-5.1	-12.57	6.39	0.13
7577	C(CO)NC(=O)C(F)F	C01602826	-11.14	-3.21	-14.64	4.96	1.75
7578	CC=C/C=O	C02031161	-11.14	-1.07	-12.12	4.57	-2.52
7579	CCOC(=O)c1c(snn1)N	C02196992	-11.14	-2.43	-13.51	5.29	-0.49
7580	Cc1c(c(c(c1F)OC)F)F	C02526254	-11.14	0.99	-10.73	2.18	-3.58
7581	C(CCB)CO	C02560614	-11.14	-1.39	-11.41	2.36	-0.7
7582	C[C@@H](C(F)F)OC(=O)C	C02579126	-11.14	0.04	-11.6	3.54	-3.11
7583	CCN(CC)N=O	C03875370	-11.14	-1.17	-12.25	3.77	-1.48
7584	CC(=O)OCCCS	C04763523	-11.14	-0.79	-13.66	4.25	-0.94
7585	C/C=N/N(C)C	C05187253	-11.14	-0.45	-12.79	2.96	-0.85
7586	C[C@H](C#CC(F)F)O	C05531338	-11.14	-2.64	-10.16	2.64	-0.99
7587	C1CC=C([C@H](C1)O)[N+](=O)[O-]	C05566682	-11.14	-2.94	-11.13	5.23	-2.29
7588	c1nc2n(n1)[C@H]1[C@@H](C=NN2)[N+](=O)[O-][O-]	C05670174	-11.14	-1.75	-18.01	5.76	2.86
7589	CC(=C1C(=NC(=S)S1)[O-])C	C08971986	-11.14	-2.39	-12.04	5.81	-2.52
7590	Cc1ccnc1NC(=NH2+)[S-]	C13571573	-11.14	-0.32	-12.07	4.36	-3.11
7591	C[C@@H]([C@H]1[C@H](O1)[C@@H](C)O)O	C17020278	-11.14	-1.67	-13.87	3.19	1.21
7592	c1cc(ccc1C=O)OC(=O)C(F)F	C31976025	-11.14	-1.52	-11.01	5.84	-4.45
7593	C[C@H](Cc1ccc(cc1)F)O	C32005747	-11.14	-2.85	-8.88	3.13	-2.54
7594	CCc1nc(cs1)C	C00396075	-11.13	-1.27	-10.25	3.28	-2.9
7595	CNC(=O)c1cccc1O	C00406312	-11.13	-1.93	-16.24	8.07	-1.02
7596	CCO[C@@H]1CCCO1	C00407008	-11.13	0.23	-14.07	2.56	0.14
7597	CC(=C)C=O	C01586526	-11.13	-1.38	-12.6	4.64	-1.8
7598	C(COC(=O)CBr)C#N	C01672183	-11.13	-1.09	-16.58	8.43	-1.89
7599	C(CCC)CO	C01712476	-11.13	-1.34	-11.64	2.47	-0.63
7600	C=C(CCC#N)C#N	C01995300	-11.13	-3.06	-13.77	9.11	-3.41
7601	CCc1nc(sn1)N	C02506771	-11.13	-0.68	-14.15	4.73	-1.04
7602	COc1ccc(cc1O)F	C02516795	-11.13	-2.4	-11.46	4.02	-1.29
7603	c1ccc(c(c1)N)CC#N	C03263977	-11.13	-1.78	-11.7	6.08	-3.74
7604	COC(=O)c1c(c[nH]n1)[N+](=O)[O-]	C04343026	-11.13	-1.73	-14.71	7.36	-2.06
7605	CNC(=S)Nc1cccn1	C05569913	-11.13	0.34	-18.65	9.37	-2.2
7606	c1(c(snn1)[O-])C(=O)N	C06057080	-11.13	-4.52	-19.71	9.52	3.58
7607	c1cnc([n+](c1N)[O-])N	C21984663	-11.13	-5.36	-16.65	11.89	-1.01
7608	c1c(csc1C=O)Br	C00120279	-11.12	-1.14	-14.9	4.9	0.02
7609	c1cc(c(cc1N)Cl)Cl	C00157572	-11.12	-2.14	-9.32	2.74	-2.39
7610	c1nnc2n1nc(s2)[S-]	C01596618	-11.12	-0.55	-18.58	6.28	1.73
7611	C[C@H]1[C@@H]1[C@H]1C(=O)Cl	C01766064	-11.12	-0.93	-11.65	2.35	-0.89
7612	Cc1cc(ccc1F)C#N	C02510727	-11.12	-1.38	-10.4	3.39	-2.72
7613	C1[C@H](C=CC1=O)O	C04202495	-11.12	-3.25	-14.18	6.13	0.17
7614	C1C(=O)O[C@H](S1)C(F)F	C04204971	-11.12	-1.4	-11.08	4.15	-2.79
7615	c1cc(c(cc1C(F)F)O)F	C04265115	-11.12	-3.16	-9.47	3.13	-1.63
7616	C1CCONC1	C04992731	-11.12	-1.02	-11.6	2.07	-0.56
7617	C(=C(C=O))C=O	C05178379	-11.12	-3.08	-13.01	6.35	-1.38
7618	c1ccc(cc1)Nc2ncccn2	C06665762	-11.12	2.56	-14.91	4.31	-3.09
7619	c1cnc2ncc(n2c1)N	C12357305	-11.12	-4.07	-14.41	10.55	-3.2
7620	c1ccc(cc1)/C=C/C#N	C13532158	-11.12	-2.31	-10.77	6.4	-4.45
7621	c1cc2c(cc1F)[nH]nc2Br	C14983474	-11.12	-0.36	-10.93	3	-2.83
7622	C=CCC[C@H](CO)O	C16123974	-11.12	-4.62	-11.36	3.75	1.1
7623	c1cc(c(c1Cl)[N+](=O)[O-])F	C16158176	-11.12	-3.51	-10.78	7.51	-4.35
7624	C1=C/C(=C/NNC(=O)N)/[NH+]=C1	C17380264	-11.12	0.34	-18.75	6.93	0.36
7625	c1cc(=O)[nH]cc1CO	C21297324	-11.12	-3.74	-17.56	9.24	0.93
7626	Cn1c(nc(n1)[N+](=O)[O-])N=[N+]=[N-]	C32602714	-11.12	1.09	-15.29	6.67	-3.59
7627	CC(=O)Nc1cccc1N	C00039703	-11.11	-1.59	-15.43	7.2	-1.29
7628	C1CS[C@H](CS1)C#N	C00159877	-11.11	1.86	-13.42	3.89	-3.44
7629	CCC[C@@H](C#C)O	C01765495	-11.11	0.37	-12.24	2.18	-1.41
7630	c1c([nH]c(=O)[nH]c1=O)CCl	C02008825	-11.11	-2.96	-16.63	8.34	0.15
7631	c1cc(ccc1NC(=O)NN)Cl	C02528216	-11.11	-1.94	-14.83	6.55	-0.9
7632	C1CCSCC1	C04416382	-11.11	0.78	-9.74	1.22	-3.36
7633	Cc1c(cccn1)C#N	C07277618	-11.11	-0.81	-11.94	4.34	-2.7
7634	C=CCn1cc(cn1)CO	C27832618	-11.11	-2.36	-14.44	6.59	-0.9
7635	c1c(cc(c1F)C(F)F)F	C00116711	-11.1	-2.42	-11.52	4.67	-1.83
7636	COC(=O)c1cc(no1)[O-]	C00389603	-11.1	-0.39	-16.02	5.96	-0.66
7637	CC(C)C(=O)C	C01699949	-11.1	-0.89	-11.04	3.35	-2.53
7638	C1C(=O)OCC(=O)N1	C02028750	-11.1	-2.3	-15.92	6.74	0.38
7639	CC(=O)Oc1cccc(c1)C=O	C02146872	-11.1	-2.24	-15.49	10.71	-4.09
7640	CC(=O)C=C/c1ccc[nH]1	C02518984	-11.1	0.84	-15.45	6.8	-3.29
7641	Cc1cnc(nc1N)Cl	C02583509	-11.1	-4.73	-12.91	5.02	1.52
7642	c1cnc1CCCO	C08294976	-11.1	-2.22	-12.85	4.85	-0.88
7643	c1cnc(c(c1C)[N+](=O)[O-])N	C22048227	-11.1	-2.88	-11.71	5.59	-2.1
7644	c1cc2c(c3c1non3)non2	C00328553	-11.09	-0.02	-14.2	4.81	-1.68
7645	c1ccc2c(c1)[nH]c(=O)s2	C00395576	-11.09	-3.67	-13.33	5.94	-0.03
7646	c1ccc(c(c1)CC#N)Cl	C00406929	-11.09	-1.01	-13.52	5.44	-2

7647	c1cnc(n(c1=O)[N+](=O)[O-])[O-]	C01309107	-11.09	-6.08	-19.01	14.44	-0.44
7648	CNC(=O)c1c(n(n1)C)N	C01417947	-11.09	-5.72	-14.21	7	1.84
7649	CCCCOC(=O)C=C	C01532055	-11.09	1.68	-12.66	3.88	-3.99
7650	CO[C@H](CBr)C=C	C01667154	-11.09	-0.03	-12.12	1.51	-0.46
7651	c1cc(c2nnnn2c1)N	C01683864	-11.09	-2.98	-17.81	9.79	-0.09
7652	Cc1ccnn1CC#N	C02537502	-11.09	-1.01	-15.09	7.66	-2.65
7653	Cc1c2ccc(cc2[nH]n1)F	C03913595	-11.09	-0.48	-11.84	4.13	-2.91
7654	CC(C)CC(=O)/C(=N/N)/N	C04203888	-11.09	2.11	-15.53	3.02	-0.68
7655	Cn1c(=O)[nH][nH]c1=O	C06072207	-11.09	-5.31	-15.87	9	1.09
7656	C1C[C@H](OC1)C(=O)Cl	C11731531	-11.09	-1.37	-11.51	4.25	-1.49
7657	c1cc(cc(c1)Cl)CS	C19421408	-11.09	-1.11	-7.83	2.29	-4.44
7658	CCCNc1cccc[nH]1	C20015472	-11.09	-1	-9.89	3.03	-3.23
7659	COc1c(cn(n1)CC(F)F)N	C20348918	-11.09	-4.33	-13.51	6.14	0.61
7660	C1=C(C=NC(=O)[C@H]1Cl)Br	C22000018	-11.09	-1.65	-14.44	6.35	-1.34
7661	c1cn(c(=O)[nH]c1=O)CC#N	C26515441	-11.09	-3.15	-21.53	14.42	-0.84
7662	c1cc(oc1)CNC(=O)CCl	C00122762	-11.08	-0.54	-15.39	6.79	-1.94
7663	c1cc(oc1)C(=O)/C(=N/O)/C#N	C00138927	-11.08	-0.44	-17.4	7.22	-0.46
7664	c1cc(ncc1C(F)F)Br	C00166552	-11.08	-1.98	-10.43	2.56	-1.24
7665	Cc1c(cno1)C(=O)C	C00169509	-11.08	-1.66	-11.7	4.82	-2.53
7666	Cc1ccc(nc1)[N+](=O)[O-]	C00330898	-11.08	-2.79	-12.42	8.04	-3.92
7667	CCOC(=O)C(=O)N(C)C	C01603528	-11.08	-0.06	-13.39	4.41	-2.03
7668	C#C/C=C/CO	C01667503	-11.08	-1.97	-12.34	3.81	-0.57
7669	C(CO)Cl	C01845916	-11.08	-3.17	-9.96	2.56	-0.5
7670	c1c(cc(c1O)F)FBr	C02574963	-11.08	-1.21	-12.93	3	0.05
7671	CC/C=C/C[C@H](C)O	C04283838	-11.08	-1.65	-9.41	1.71	-1.73
7672	CO[P@H](=O)CCl	C04974704	-11.08	-0.75	-14.24	5.39	-1.47
7673	C1C@HC=C1)O	C05426112	-11.08	-1.61	-12.61	1.96	1.17
7674	c1cnc(nc1)NNC=O	C06599348	-11.08	-4.42	-16.79	7.83	2.3
7675	Cc1cncnc1	C14983067	-11.08	-0.52	-9.52	2.19	-3.24
7676	c1c2c(nc[nH]2)nc(n1)C(F)F	C26506868	-11.08	0.11	-15.77	7.57	-2.99
7677	c1cn(cn1)C(=O)N2ccnc2	C00155422	-11.07	-1.26	-11.63	6.2	-4.38
7678	Cc1ccc(o1)/C=N/O	C00169291	-11.07	-0.66	-16.3	7.48	-1.59
7679	Cn1ccc(=O)[nH]c1=O	C00409298	-11.07	-3.11	-17.41	9.75	-0.3
7680	c1nc(c2c(n1)[nH]c(n2)Br)N	C00967449	-11.07	-3.44	-10.98	4.79	-1.43
7681	CN1C(=O)CSC1=O	C01101310	-11.07	0.49	-15.54	4.87	-0.88
7682	CC(=C)CO	C01661231	-11.07	-2.08	-10.99	2.26	-0.26
7683	CCOC/C(=C/Cl)/C	C01683072	-11.07	-0.53	-11	1.56	-1.1
7684	c1cc(c(c1N)F)Cl)F	C01706154	-11.07	0.5	-15.22	3.97	-0.32
7685	C1ccc(c(n1)F)O	C02384075	-11.07	-2.5	-15.11	5.93	0.6
7686	c1ccc2c(c1)c(no2)CBr	C02509747	-11.07	1.45	-14.45	5.95	-4.02
7687	Cc1c2c([nH]n1)CCCC2	C04317853	-11.07	-2.86	-9.75	4.49	-2.95
7688	c1c[nH]c2c1CCCC2	C04521854	-11.07	-1.9	-11.87	2.69	0.01
7689	C[C@@H]1(CCC=C1)O	C05049663	-11.07	-0.68	-11.17	1.84	-1.07
7690	C[C@H]1CCCCO1	C05226869	-11.07	0.03	-10.78	1.52	-1.84
7691	c1csc(c1O)C(=O)N	C11848541	-11.07	-3.99	-16.47	8.07	1.32
7692	c1c([nH]c2c1c(=O)[nH]cc2	C14985678	-11.07	-1.84	-17.23	7.03	0.97
7693	C/C(=C/C(=O)OC)/OC	C17328156	-11.07	-1.86	-10.86	3.66	-2.01
7694	C=CCOc1c(non1)N	C26442172	-11.07	-0.61	-17.56	6.56	0.54
7695	C(C(=O)NN)NC(=O)C(F)F	C32501070	-11.07	-6.14	-15.53	8.48	2.13
7696	c1ccc2c(c1N)Nnon2	C00160421	-11.06	-3.86	-12.89	5.28	0.41
7697	Cc1ccc(s1)Br	C00403354	-11.06	-0.24	-12.56	1.6	0.13
7698	C[C@H]1CC[C@H](C1=O)C	C01575590	-11.06	1.17	-11.95	3.11	-3.39
7699	C1C[C@H](C=C1)C(=O)N	C01732795	-11.06	-3.5	-12.17	5.18	-0.57
7700	C/C=C/C)C#N	C02035672	-11.06	-1.26	-11.13	4.12	-2.8
7701	c1ccc2c(c1)F)C(=O)C2	C03847841	-11.06	-1.1	-13.24	6.97	-3.69
7702	c1c(c([nH]n1)C#N)Br	C04216077	-11.06	1.11	-14.19	3.28	-1.27
7703	CCCS	C04706588	-11.06	-0.52	-10.89	0.72	-0.38
7704	C/C=C/CSC	C05132858	-11.06	-0.79	-10.7	1.47	-1.04
7705	C1COCC(=C1)C=O	C05190728	-11.06	-1.11	-15.62	5.82	-0.16
7706	CC(=O)N[N-]C(=N[N+](=O)[O-])[O-]	C06073646	-11.06	-3.05	-18.37	8.77	1.59
7707	CC(=O)c1c(cccn1)F	C08698164	-11.06	-2.09	-14.41	6.71	-1.28
7708	C/C=C/C=C)CO	C13546465	-11.06	-2.07	-10.37	2.42	-1.04
7709	CCC(=O)OCCCl	C16609984	-11.06	-0.7	-11.19	4.31	-3.48
7710	CCc1c(=O)[nH]c(=O)[nH]n1	C16887345	-11.06	0.61	-18.12	5.53	0.92
7711	C/[NH+]=C/c1ccc(cc1)[N+](=O)[O-]	C16978838	-11.06	-1.51	-12.27	5.34	-2.62
7712	C[C@H](CS)S	C17327670	-11.06	0.22	-10.56	1.63	-2.35
7713	COCC(=O)CNCC#C	C20033525	-11.06	-1.45	-14.11	5.78	-1.28
7714	c1cnncc1/C=N/O	C00332246	-11.05	0.09	-19.16	7.79	0.24
7715	CC(=C)COCC(=O)N	C00393731	-11.05	-2.85	-13.15	4.48	0.47
7716	CCCC(=O)C	C00901192	-11.05	-0.39	-11.68	3.67	-2.65
7717	CCCCSCCO	C01640796	-11.05	-1.19	-10.16	2.08	-1.79
7718	c1c(nc(s1)Br)Br	C02245232	-11.05	-1.57	-13.87	2.83	1.56
7719	Cn1cc(nc1)CO	C03880803	-11.05	-2.86	-13.38	6.08	-0.89
7720	C/C(=C/C(=O)C)N/[O-]	C04714960	-11.05	-0.94	-10.62	2.04	-1.53
7721	Cc1c(nnn1)[O-]	C05285766	-11.05	-2.99	-17.25	8.2	0.99
7722	C=Cn1cccc1O	C05377636	-11.05	-2.42	-13.37	4.92	-0.18
7723	CC[C@H](C)S	C06661091	-11.05	-0.41	-8.71	0.77	-2.71
7724	CCn1c(nnn1)[S-]	C06880576	-11.05	-1.63	-12.7	4.72	-1.43
7725	c1cc(ccc1NC(=O)/C=N/O)F	C07991482	-11.05	-2.49	-18.88	10.22	0.1
7726	c1cnc(c1Br)CO	C13213192	-11.05	-2.51	-11.48	3.53	-0.59
7727	[C@H](C(=O)F)F)Cl	C16159208	-11.05	0.02	-12.49	2.88	-1.45
7728	c1c(c(n[nH]c1=O)Cl)[O-]	C17063299	-11.05	-2.35	-18.52	6.14	3.68
7729	COCC1cccc(c1)N	C19398609	-11.05	-0.21	-13.38	4	-1.46
7730	C=CCOCC#N	C26515255	-11.05	-1.33	-12.63	5.4	-2.49
7731	C1COCC=C1C(=O)C(F)F)Br	C32628529	-11.05	1.38	-12.86	3.09	-2.66
7732	c1cc(sc1)C(=O)NN	C00153618	-11.04	-3.1	-14.18	6.47	-0.23
7733	C[C@H](C)C)O	C01692450	-11.04	-0.66	-11.15	1.67	-0.9
7734	c1cnn(c1)c2nncn2N	C02454447	-11.04	-1.87	-13.11	8.63	-4.69
7735	Cc1ccccc1/C=N/O	C02573583	-11.04	-0.67	-13.32	5.16	-2.2
7736	c1(nnc(s1)Br)Br	C05003393	-11.04	-1.26	-13.42	2.49	1.14

7737	CN(C=S)N	C05688656	-11.04	-3.67	-13.38	2.88	3.13
7738	Cc1ncc(c(n1)N)C=O	C11919726	-11.04	-6.39	-9.64	5.92	-0.93
7739	c1[nH]c2c(n1)C(=N+)([N2])[O-]N	C17173461	-11.04	-8.86	-17.09	15.05	-0.13
7740	CC[C@H](c1cccc1)Cl	C32005476	-11.04	1.76	-11.65	2.84	-4
7741	Cc1ccc(c(c1)O)NC(=O)C	C00409297	-11.03	-1.26	-15.35	6.61	-1.03
7742	CCOC(=O)C=C(\C)/C#N	C01679009	-11.03	0.3	-11.33	3.51	-3.51
7743	CNNC(=O)OC	C01766230	-11.03	-2.17	-14.3	4.59	0.86
7744	Cn1c(=O)[nH][nH]c1=S	C04204671	-11.03	-6.6	-15.37	11.94	-1.01
7745	C#C/C=NNC(=O)N	C04962248	-11.03	-3.05	-16.51	7.1	1.42
7746	C[C@H]1CCOC1	C06037606	-11.03	-0.24	-10.61	1.48	-1.66
7747	Cc1c(scn1)C(=O)C	C06069129	-11.03	1.23	-17.33	5.38	-0.31
7748	c1c(cn(n1)CC(F)F)C=O	C12357569	-11.03	-3.45	-12.94	8.08	-2.72
7749	CC(C)/C(=N)O/C	C14590616	-11.03	-1.44	-12.65	4.13	-1.07
7750	c1cncc(=O)[nH]1	C14684052	-11.03	-2.22	-16.04	4.97	2.26
7751	CCc1ccc(nc1)C=O	C19090982	-11.03	-0.56	-11.47	3.97	-2.97
7752	c1c(nc(cn1)Cl)NN	C20282017	-11.03	-3.98	-13.23	6.1	0.09
7753	Cc1cncc(cc1)Cl	C21981799	-11.03	1.39	-11.6	2.44	-3.26
7754	C1C[C@H](OC1)N=C=S	C26475807	-11.03	0.71	-14.47	3.23	-0.51
7755	COCC(=O)CNC(=S)NN	C26515630	-11.03	-3.09	-16.12	9.05	-0.87
7756	C[C@H]1CC=NN1	C28224152	-11.03	0.09	-13.19	2.84	-0.77
7757	c1c(ncn1)C(=O)NN	C30677889	-11.03	-3.87	-18.05	7.85	3.04
7758	C1C[C@H](OC1)CBr	C00158845	-11.02	-0.24	-10.78	2.38	-2.38
7759	c1cc(ccc1)NN=C(C#N)C#N)F	C00358054	-11.02	-1.8	-10.95	4.34	-2.61
7760	C=C[C@H]1COCC(=O)O1	C00403302	-11.02	-0.63	-14.91	6.93	-2.4
7761	c1c[n+](ccc1Cl)[O-]	C00407058	-11.02	-1.64	-17.78	11.02	-2.63
7762	c1ccc(cc1)[C@H](C#C)BrO	C01304686	-11.02	-0.39	-13.97	2.86	0.48
7763	c1cc(nc(c1)F)NNC(=O)N	C01391062	-11.02	-2.4	-19.28	10.27	0.39
7764	CC(=O)N(CN(C)[N+](=O)[O-])	C01610828	-11.02	0.96	-17.78	6.44	-0.63
7765	C[C@H](C1CCCC1)O	C01700002	-11.02	-1.31	-9.33	1.32	-1.69
7766	COc1c(=O)c(=O)c1OC	C02145277	-11.02	-2.87	-11.46	3.82	-0.51
7767	CCn1ccc(n1)C(=O)C	C02536625	-11.02	-2.21	-12.05	6.25	-3
7768	Cc1ccc(cc1)P(=O)([O-])[O-]	C03097907	-11.02	-3.41	-14.1	8.15	-1.66
7769	CCC1=CCCC1=O	C04273483	-11.02	-1.02	-11.76	5.24	-3.48
7770	C(#N)c1c(c2c(nc1n)non2)N	C04343049	-11.02	-2.76	-13.49	5.07	0.16
7771	C1C[C@H](C=C1)C(=O)N	C05217616	-11.02	-2.16	-13.29	5.07	-0.64
7772	CC[C@H](C)S	C05298826	-11.02	-0.55	-10.4	0.66	-0.72
7773	C[C@H](CO)N(N=O)O	C06020795	-11.02	-4.52	-12.7	4.8	1.4
7774	c1cncc(cc1C=O)F	C08698252	-11.02	-1.79	-16.25	8.08	-1.05
7775	[C@H](C(=O)N)(F)I	C08698286	-11.02	-2.42	-13.23	4.4	0.23
7776	Cc1nc2c(ccn2)c(=O)c1O	C11919574	-11.02	0.86	-17.82	8.12	-2.18
7777	CO/N=C(C(=N)O)N)/N	C13477947	-11.02	-2.41	-13.03	3.55	0.87
7778	C[C@H](O)OC(F)F	C16159293	-11.02	-1.55	-11.69	2.05	0.17
7779	Cc1c(c(=O)[nH]cn1)N	C17062002	-11.02	-3.01	-15.63	5.39	2.23
7780	CSc1nc(cnn1)[O-]	C18181842	-11.02	-3.4	-15.31	7.49	0.2
7781	COCC(=O)CNCC=C	C20033808	-11.02	0.04	-13.7	3.96	-1.32
7782	C1COCC[C@H]1C=N/O	C20283003	-11.02	-3.27	-13.15	4.81	0.59
7783	c1cc(ccc1OC(F)F)Br	C00056737	-11.01	0.11	-10.83	1.26	-1.55
7784	c1cc(ccc1CO)OC(F)F	C00167206	-11.01	-0.9	-13.38	3.47	-0.2
7785	Cc1nc(c(o1)N)C#N	C00335545	-11.01	-4.32	-15.15	6.51	1.96
7786	CNc1nnnn1C	C01577919	-11.01	-2.17	-14.9	7.69	-1.63
7787	CC[C@H](C[C@H]1CCCO1)O	C01597025	-11.01	0.55	-14.34	1.42	1.36
7788	CCSC#N	C01648252	-11.01	-0.98	-10.74	2.99	-2.27
7789	c1cc(c(cc1OC(F)F)N)O	C02386507	-11.01	0.18	-15.06	3.03	0.83
7790	c1cc(cc(c1)OC(F)F)C=O	C02560126	-11.01	-4.35	-12.17	7.57	-2.06
7791	c1cc(c2nccn2c1)O	C03880832	-11.01	-2.54	-15.33	8.54	-1.68
7792	CCOC(=O)[C@H](C)O	C04291190	-11.01	-3.11	-12.2	5.98	-1.68
7793	C(=O)[C@H](C(F)F)C(F)Cl	C16159144	-11.01	-0.15	-8.77	0.58	-2.67
7794	CCCC[C@H](C=C)C	C17377825	-11.01	-1.81	-7.99	1.41	-2.63
7795	C1C=C[C@H]2[C@H]1CC2=O	C19230141	-11.01	-0.65	-11.06	3.95	-3.25
7796	Cc1cc(c[nH]c1)F	C21981955	-11.01	-3.43	-14.34	6.98	-0.22
7797	c1cc2c(cc1S)OCO2	C31829378	-11.01	0.21	-12.37	3.66	-2.51
7798	c1cc2c(nsc2nc1)[O-]	C00080837	-11	-3.03	-14.22	6.84	-0.6
7799	Cn1cncc1CC#N	C00330926	-11	-1.41	-15.26	9.25	-3.58
7800	c1cc(ccc1C=C/C)O	C01530240	-11	-1.92	-16.55	7.51	-0.03
7801	CC(=O)C(=O)C=C(C(F)F)C(F)F	C01673726	-11	-1.87	-8.1	3.25	-4.28
7802	c1ccc(cc1)/C=C/C=N/O	C01679302	-11	-1.31	-13.88	4.36	-0.17
7803	CCOC(=O)CC=O	C01764589	-11	-3.59	-14.32	7	-0.08
7804	c1ccc(c(c1)NN=C(C#N)C#N)F	C02168607	-11	-0.23	-12.2	4.23	-2.8
7805	CCc1ccc(cc1)O	C02566153	-11	-1.26	-13.49	3.88	-0.12
7806	C[C@H](CBr)O	C03861677	-11	-1.56	-11.54	2.48	-0.38
7807	c1[nH]c(c(n1)C(=O)N)[N+](=O)[O-]	C03944779	-11	-5.23	-15.88	11.19	-1.08
7808	C1C[C@H](OC=C1)C=O	C04529095	-11	-0.76	-12.96	3.6	-0.88
7809	c1(c(=S)ssn1)Cl	C05510634	-11	-1.34	-13.51	2.15	1.69
7810	C1C[C@H](C[C@H](C1)SC#N)O	C05975924	-11	-1.66	-12.15	4.13	-1.32
7811	CS/C=C/c1cccc1	C06019647	-11	0.08	-12.22	2.28	-1.14
7812	CC1=CC[C@H](CC1)C#N	C06130090	-11	-0.28	-11.91	3.33	-2.14
7813	c1cc([nH]c1)c2[nH]c(=O)on2	C12367568	-11	-0.46	-16.11	6.87	-1.3
7814	C/C(=N)C1CCCC1)/N	C15782363	-11	0.57	-14.03	4.84	-2.38
7815	CC(=O)c1ncccn1	C16696745	-11	-2.13	-14.1	7.44	-2.21
7816	c1cc(ccc1C(=O)N=[N+]=[N-])[O-]	C17724808	-11	1.05	-17.93	4.27	1.62
7817	c1cncc(cc1CO)N	C19092522	-11	-3.22	-13.96	5.12	1.05
7818	Cc1nsc1C=O	C20443693	-11	0.34	-15.79	6.21	-1.76
7819	c1cc(oc1)c2ccc(o2)C=O	C22201052	-11	0.75	-17.73	9.7	-3.72
7820	C[C@H](CCS)S	C25695480	-11	0.76	-10.93	2.2	-3.04
7821	C[C@H](C(=NH2+))N)[N+](=O)[O-]	C26898076	-11	-5.69	-16.24	11.6	-0.67
7822	CC(=O)C1CCCC1	C01681283	-10.99	1.85	-12.67	3.36	-3.53
7823	CCCOCCC	C02041060	-10.99	-0.19	-11.17	1.1	-0.72
7824	CCO/C=C/C(=O)C(F)F	C02557016	-10.99	0.18	-11.9	3.46	-2.73
7825	c1c(nc(s1)CC#N)CBr	C03167461	-10.99	-2.11	-13.6	8.04	-3.31
7826	c1c(c[nH]c(=O)c1N)C(F)F	C03181875	-10.99	-3.8	-12.34	5.44	-0.29

7827	C[C@@H](c1cccc1)S	C04706573	-10.99	-0.8	-7.48	1.71	-4.42
7828	CC(C)C@H](C#C)O	C05226739	-10.99	-0.9	-10.75	1.97	-1.3
7829	C(=C(Cl)C(=O)N	C05282285	-10.99	-2.67	-13.23	4.49	0.43
7830	c1cc(cc(c1)N)C(F)F	C12358779	-10.99	0.81	-12	2.67	-2.47
7831	COCC(=O)C=N/O	C14455583	-10.99	-1.89	-15.41	6.34	-0.03
7832	c1[nH]c(=O)(c1N)[N+](=O)[O-]	C15021887	-10.99	-2.6	-17.78	7.42	1.97
7833	c1[nH]c(c(n1)C(=O)NO)N	C16954267	-10.99	-7.27	-15.86	10.66	1.48
7834	c1cc(c(c1NCCO)F)F	C20044958	-10.99	-2.96	-13.82	6.53	-0.73
7835	C1COC[C@H]1CCl	C20078000	-10.99	0.43	-11.17	1.86	-2.11
7836	c1cc(ccc1c2cc(no2)CC(=O)[O-])Cl	C20270420	-10.99	-0.47	-13.45	7.15	-4.22
7837	CC(=O)n1cc(cn1)I	C21301159	-10.99	-0.99	-11.1	3.64	-2.54
7838	c1cccc1CCC=O	C22003337	-10.99	-3.94	-10.6	6.35	-2.79
7839	CSc1c(c(=O)c1=O)N	C26329862	-10.99	-4.63	-13.38	7.5	-0.49
7840	c1cn2c(cc1)ncn2	C26894585	-10.99	-3.9	-7.67	5.23	-4.65
7841	c1cncc(c1CO)Cl	C26898627	-10.99	-0.06	-14.49	4.13	-0.56
7842	COc1ccc(c(c1)N)N	C00152529	-10.98	-2	-12.84	3.7	0.17
7843	COc1ccc(cc1F)N	C00389573	-10.98	-2.46	-11.94	4.7	-1.27
7844	COC(=O)C(=O)OC	C01532047	-10.98	0.37	-13.39	4.07	-2.04
7845	C[C@@H](C(C)C(=O)N	C01594371	-10.98	-3.69	-11.68	4.53	-0.14
7846	CC[C@H](/C=C/C)O	C01609494	-10.98	-0.7	-10.21	1.45	-1.52
7847	C=C/C=C/C1/CCOC1=O	C02034937	-10.98	1.24	-15.94	7.05	-3.33
7848	C=CCCCC[N+](=O)[O-]	C02557923	-10.98	-0.01	-13.02	3.56	-1.52
7849	Cc1cncc(c1)C#N	C02582041	-10.98	1.19	-14.64	5.28	-2.81
7850	c1cnc(nc1)NC(=S)N	C02582351	-10.98	-0.11	-18.62	10.71	-2.94
7851	CC(=O)OCC=O	C02584547	-10.98	-1.68	-14.27	6.6	-1.63
7852	C(Cl(=O)NCC(F)F)Cl	C03252688	-10.98	-1.92	-13.33	5.7	-1.43
7853	c1cc2c(cc1C#N)CCO2	C04253977	-10.98	-1.77	-10.08	4.36	-3.49
7854	CC(C)c1ccncc1	C08294971	-10.98	-1.52	-8.64	2.58	-3.4
7855	CCc1nnc(o1)[S-]	C08731367	-10.98	-2.19	-14.7	4.73	1.19
7856	Cc1ccc(c(c1F)C#N	C12359232	-10.98	2.22	-16.06	6.13	-3.25
7857	C1CC1c2[nH]c(nn2)[S-]	C12505190	-10.98	1.23	-14.97	5.6	-2.85
7858	c1[nH]c(c(n1)[O-])C(=O)N	C13283660	-10.98	-6.94	-16.36	9.29	3.03
7859	CC(=O)OCC(=O)OC	C14442398	-10.98	0.46	-14.77	5.97	-2.64
7860	C1CO[C@H](CO)Cl	C14983036	-10.98	-1.2	-10.51	2.67	-1.94
7861	c1ccc(cc1)N/N=C(C#N)/C(=O)N	C14983473	-10.98	-1.86	-17.54	9.09	-0.67
7862	C/C=N/N(C)C	C20230282	-10.98	-0.85	-11.73	3.24	-1.64
7863	Cc1cc(cnc1Br)F	C21299171	-10.98	0.74	-11.26	2.55	-3.01
7864	c1ccc(c1Br)C(=O)Cl	C26340353	-10.98	0.95	-13.94	5	-2.99
7865	CCC(=O)CC	C01648158	-10.97	0.66	-12.37	3.49	-2.74
7866	CCN1CC1=C	C01684539	-10.97	-0.34	-12.96	2.05	0.28
7867	c1c(ncs1)C(=O)NN	C02353142	-10.97	-3.88	-15.18	6.84	1.25
7868	Cc1ccc(cc1F)OC	C02512464	-10.97	0.96	-13.48	3.24	-1.69
7869	c1cc(c(cc1C#N)C(F)F)F	C03880152	-10.97	-2.87	-8.71	4.71	-4.1
7870	Cc1cc([nH]n1)C=O	C04244055	-10.97	-0.25	-15.56	5.93	-1.09
7871	C(#N)C(Cl)Cl	C04283780	-10.97	-0.26	-11.65	3.15	-2.21
7872	C1[C@@H](C(C=C1)CC#N	C04994803	-10.97	-1.68	-10.02	5	-4.27
7873	CCO/C=C/C(=O)C(F)F	C05952650	-10.97	-2.76	-10.2	6	-4
7874	c1nc([nH]n1)NC2=NCCO2	C06585097	-10.97	-0.08	-19.26	4.99	3.37
7875	C=CCNc1ncco1	C08699322	-10.97	-1.29	-13.33	4.13	-0.49
7876	Cc1nnc(s1)NN	C09584705	-10.97	-4.4	-13	6.64	-0.2
7877	c1c(=O)[nH]cnc1NN	C13303321	-10.97	-1.8	-17.28	5.84	2.27
7878	C/C=C/C=C/C=O	C13540493	-10.97	-0.31	-12.43	4.73	-2.96
7879	CCOC1CCCC1O	G2008A004	-10.97	-1.72	-11.32	4.09	-2.02
7880	Oc1c(cccc1)CC=C	W2004A002	-10.97	-0.58	-10.25	2.71	-2.86
7881	c1cc(c(cc1C(F)F)F)N	C00092915	-10.96	-5.63	-7.59	3.24	-0.98
7882	CCOC(=O)c1cncc1C	C00156448	-10.96	-0.1	-12.88	5.19	-3.17
7883	c1c(ccnc1C#N)C#N	C00332342	-10.96	-1.33	-12.71	5.74	-2.67
7884	CCOc1cccc(c1)Cl	C00403340	-10.96	-2.64	-9.58	2.12	-0.87
7885	c1c([n+](c(n1)Cl)[O-]	C01581402	-10.96	-3.81	-17.24	11.37	-1.28
7886	CC(C)SCCO	C01596246	-10.96	-3.24	-9.06	2.25	-0.91
7887	CCCc1ccc(cc1)O	C01692500	-10.96	-1	-12.58	2.52	0.11
7888	CC(C)SCC#C	C01732652	-10.96	-0.52	-11.18	2.55	-1.82
7889	C1CN(C(=O)N1)C(=O)Cl	C02083216	-10.96	-2.14	-16.13	7.05	0.26
7890	CC/C=C/C(=O)OC	C02508321	-10.96	-0.96	-10.53	3.74	-3.21
7891	CCOCCC(=O)C	C02522795	-10.96	-1	-11.94	4.17	-2.2
7892	CCO[C@H]1CCC=CO1	C03875719	-10.96	0.2	-10.54	2.33	-2.96
7893	c1c(c2c(c1F)F)nc([nH]2)F	C04430556	-10.96	-4.68	-9.55	6.64	-3.36
7894	CN(C(=O)c1cccc1)O	C05497333	-10.96	-3.28	-12.77	6.67	-1.59
7895	COCCSC(=NH2+)N	C05607027	-10.96	-2.73	-13.5	3.09	2.17
7896	c1c(on[n+1]CCC#N)[O-]	C06224219	-10.96	-3.24	-17.59	12.93	-3.06
7897	Cc1cncc(c1)N=C=S	C11535835	-10.96	0.54	-15.53	4.2	-0.17
7898	CCC/C=N/O	C13514543	-10.96	-3.19	-11.45	4.18	-0.49
7899	C(=O)([C@](C(F)F)F)Cl	C16159142	-10.96	-0.32	-8.71	0.73	-2.65
7900	CC[C@H](/C=C/C)O	C17377821	-10.96	-0.59	-10.11	1.25	-1.51
7901	c1ccc2c(c1)nc(s2)F	C00152323	-10.95	-0.68	-14.17	4.16	-0.26
7902	c1ccc(cc1)OC(=O)Cl	C00161080	-10.95	-1.87	-10.26	5.96	-4.79
7903	Cc1c(no[n+1][O-])C(=O)N	C01504370	-10.95	-3.86	-15.09	7.87	0.13
7904	CC(C)Sc1[nH]ncn1	C01573438	-10.95	1.56	-12.84	3.74	-3.41
7905	CCC(CC)O	C01648159	-10.95	-1.2	-9.96	1.28	-1.06
7906	CC(C)CN=C=S	C01846032	-10.95	-0.19	-12.29	1.17	0.37
7907	CSc1cn[nH]c(=O)n1	C02568446	-10.95	-3.53	-15.98	7.99	0.57
7908	C[C@H](C)COC1	C04918919	-10.95	-0.39	-10.46	1.51	-1.6
7909	c1c(nnn1CO)[N+](=O)[O-]	C05567174	-10.95	-2.78	-17.82	9.05	0.61
7910	[H]N=C(c1cc2c(cc1n)non2)O	C05670199	-10.95	-10.51	-8.09	4.63	3.02
7911	CN(C)C(=S)N	C05688714	-10.95	-1.14	-13.69	2.77	1.12
7912	Cc1cnc(nc1)[O-]SC	C08616644	-10.95	-2.09	-13.07	6.21	-2
7913	CC[C@H](C(=O)C(F)F)Br	C08700959	-10.95	-0.42	-9.02	1.69	-3.2
7914	c1ccc2c(c1)[nH]c(=S)[nH]2	C12341568	-10.95	-1.97	-15.06	9.4	-3.32
7915	C=CCSc1ccccn1	C13284240	-10.95	0.08	-10.28	3.35	-4.11
7916	CCc1[nH]c2cccnc2n1	C26439558	-10.95	-3.1	-11.99	7.22	-3.08

7917	C(COC(F)(F)F)O	C32629454	-10.95	-3.26	-12.96	4.21	1.05
7918	c1ccc2c(c1)cc(o2)Br	C00158632	-10.94	-1.36	-12.24	3.26	-0.59
7919	C(CCl)OCCCl	C01599332	-10.94	-0.31	-11.21	3.23	-2.66
7920	CCCCCN=C=O	C01841178	-10.94	-1.78	-10.68	1.75	-0.22
7921	CCCCOCC	C02031618	-10.94	-0.47	-10.84	1.18	-0.81
7922	C1CSC[C@H]1O	C02033249	-10.94	-1.71	-11.63	2.81	-0.4
7923	c1c(nn(c1C(F)F)N+)(=O)[O-])C(F)F	C02537490	-10.94	-4.36	-10.31	7.2	-3.47
7924	C=CCOC(C(F)F)F(C(F)F)F	C02584266	-10.94	0.01	-7.75	0.89	-4.08
7925	CO[C@H]1C=C[C@H](O1)OC	C03860391	-10.94	-2.07	-11.66	3.9	-1.12
7926	C(N=C=S)Cl	C03860854	-10.94	-0.44	-13.49	2.07	0.92
7927	CCCC[C@H](C=C)O	C04521547	-10.94	-0.38	-12.16	1.44	0.16
7928	CC(=NNC)C	C04744395	-10.94	-0.61	-11.7	2.76	-1.17
7929	CCOC(=O)c1nc[n-]n1	C05575597	-10.94	-2.24	-13.06	4.16	0.19
7930	Cc1cccn1C=C	C06303114	-10.94	-1.89	-9.68	2.82	-2.19
7931	COc1cc(ccn1)Br	C08698203	-10.94	-0.19	-11.91	2.71	-1.55
7932	Cc1cc(on1)CO	C12370187	-10.94	-1.81	-14.94	5.85	-0.03
7933	Cc1cc(cnc1N)Cl	C19735877	-10.94	0.28	-13.06	3.85	-2
7934	CCc1cncnc1Cl	C21299588	-10.94	-1.32	-9.85	3.42	-3.19
7935	c1cc(c(cc1C(=O)NN)F)F	C00127687	-10.93	-3.1	-15.82	8.91	-0.92
7936	CC1=NNC(=O)CC1	C00152911	-10.93	-1.32	-15.56	6.57	-0.62
7937	C(c1[nH]nc(n1)CO)O	C01509969	-10.93	-7.03	-16.92	7.93	5.09
7938	c1(=O)(c(nsc1Cl)Cl	C01608420	-10.93	-0.39	-11.62	2.51	-1.43
7939	C[C@H](COC(=O)C)O	C01668304	-10.93	-1.65	-14.07	5.45	-0.67
7940	Cc1ccn2c(c1)nnn2	C01683868	-10.93	-3.83	-14.29	9.65	-2.47
7941	Cn1c(=S)[nH]c(=O)cn1	C01689467	-10.93	-1.54	-15.09	6.8	-1.11
7942	C=C(COCCO)Cl	C01708309	-10.93	-2.44	-13.33	4.86	-0.02
7943	C/C=C(C)/[C@H](C)O	C01730156	-10.93	-0.98	-10.33	1.6	-1.23
7944	COCCCB	C02392168	-10.93	1.03	-11.8	1.94	-2.1
7945	C(=O)(OC(C)Cl)Cl	C04261978	-10.93	1.05	-12.25	0.77	-0.5
7946	c1(c([nH]nc1O)N)N=O	C04552327	-10.93	-5.99	-18.39	9.42	4.03
7947	C(=O)(C(C(F)F)F)F)NN	C04742735	-10.93	-3.97	-11.37	4.28	0.13
7948	CCC1=CC(=O)CCC1	C04802706	-10.93	-0.57	-14.29	5.02	-1.09
7949	CCOc1cnc(o1)C	C05336805	-10.93	-1.51	-13.01	3.88	-0.29
7950	c1cc(ccc1N)OCC(F)F	C05933315	-10.93	-1.26	-13.48	6.01	-2.2
7951	CCn1c(cc(n1)C(F)F)N	C12357880	-10.93	-4.77	-9.31	5.37	-2.23
7952	c1cnc(nc1/C=N/O)N	C12505529	-10.93	-4.71	-13.69	7.19	0.29
7953	c1cc(sc1)SCCBr	C20078018	-10.93	-1.01	-7.19	2.02	-4.75
7954	c1cc(c(c(c1)Cl)CO)F	C00154651	-10.92	-2.71	-12.7	3.87	0.62
7955	c1c(cc(cc1O)O)N	C00157870	-10.92	-3.55	-14.4	4.53	2.5
7956	Cc1ccc(cc1)CO	C00896402	-10.92	-1.72	-10.86	3.33	-1.67
7957	C(COCCCl)O	C01641057	-10.92	-2.43	-13.07	4.33	0.25
7958	C/C=C(C=O)Cl	C01670683	-10.92	-2.19	-13.78	6.25	-1.2
7959	CCOC(=O)[C@H]1C[C@H]1C#N	C01728350	-10.92	-1.92	-10.71	5.48	-3.77
7960	C1CSCCO1	C03861039	-10.92	0.05	-11.42	2.13	-1.68
7961	c1ccc(c(c1)NNC(=S)N)F	C03883266	-10.92	0.92	-16.95	8.01	-2.89
7962	c1cc(c(c1)[N+](=O)[O-])N)N	C04087238	-10.92	-2.91	-13.02	5.96	-0.96
7963	COc1ccc(cn1)O	C04204273	-10.92	-1.23	-14.88	4.03	1.17
7964	C1CCC(C1)N=[N+]=[N-]	C04748490	-10.92	0.76	-12.63	1.17	-0.22
7965	C1[C@H](C=C[C@H]1O)O	C04761430	-10.92	-2.58	-13.42	3.2	1.88
7966	CC(C)C[C@H](C#C)O	C05227368	-10.92	-0.06	-11.3	2.17	-1.72
7967	C(CO)NC(=S)C(=S)N	C05501770	-10.92	-4.83	-14.5	3.4	5.01
7968	C1[C@H]2[C@H]1C(=O)OC2=O	C08100975	-10.92	-1.85	-13.28	7.32	-3.12
7969	CSsc1nc(c(nn1)CF)[O-]	C08619367	-10.92	-4.52	-15.01	9.45	-0.84
7970	COc1cc(c(cc1F)F)N	C08729943	-10.92	-2.32	-11.41	4.17	-1.37
7971	Cc1ccc(s1)N=C=O	C12370780	-10.92	0.62	-11.7	2.07	-1.91
7972	COc1cccnc1N	C14982093	-10.92	-1.69	-12.78	4.28	-0.72
7973	c1cc2c(c1)F)CCN2	C16083046	-10.92	-1.67	-9.5	3.01	-2.76
7974	CSsc1nsc2n1c(nn2)N	C16928843	-10.92	-4.14	-10.9	7.78	-3.66
7975	c1(nc(on1)N)N	C16951984	-10.92	-5.84	-14.98	8.24	1.65
7976	C(CON)CSC(=NH2+)N	C17004063	-10.92	-0.89	-14.43	3.48	0.93
7977	c1c(=O)c(c([nH]n1)[O-])Cl	C17062760	-10.92	-3.59	-16.48	5.62	3.53
7978	C(=C(N)N)C(=O)N	C20405516	-10.92	-5.37	-15.4	6.81	3.04
7979	[H]/N=C(\Nc1cccc1F)/N/C(=N/[H])/NN	C20458476	-10.92	-1.72	-11.99	6.71	-3.92
7980	c1cc(c(nc1)Cl)C#N	C00091827	-10.91	-1.7	-12.65	6.03	-2.59
7981	c1cc(ccc1C(=O)NN)F	C00153714	-10.91	-3.01	-14.05	7.05	-0.9
7982	C1CCC(C1)O	C00901228	-10.91	-0.97	-10.87	1.67	-0.74
7983	CCOC(=O)[C@H](C)CCl	C01690412	-10.91	1.29	-10.84	2.49	-3.86
7984	CC(=O)OC[C@H](CC)O	C02041688	-10.91	-0.94	-16.16	5.85	0.35
7985	CC(=O)OCCSC	C02165902	-10.91	1.57	-13.87	4.69	-3.31
7986	CCCSsc1[nH]ncn1	C02243770	-10.91	-2.07	-11.45	6.33	-3.72
7987	C=CCN1C(=O)CSC1=O	C02798866	-10.91	1.25	-14.81	4.76	-2.1
7988	C#CCOC(=O)C(C(F)F)C(F)F	C03100049	-10.91	-0.23	-9.68	4.47	-5.46
7989	Cc1ccc(c1)OC(=O)C	C04284473	-10.91	-1.62	-10.25	5.78	-4.83
7990	CCCC/C=C/C(=O)C(F)F/[O-]	C04552333	-10.91	-2.86	-7.16	2.42	-3.32
7991	C[C@H]1C(=O)NC(=S)N1	C05735524	-10.91	-1.23	-16.18	3.58	2.92
7992	c1nc(c(c(n1)NN)N)N	C05940982	-10.91	-4.12	-13.67	5.73	1.15
7993	c1cc(cnc1)c2nsc(=O)o2	C06536527	-10.91	-0.69	-15.28	4.12	0.93
7994	CCn1ccc(n1)CO	C12398019	-10.91	-4.45	-11.79	5.83	-0.51
7995	CCc1cc(on1)CO	C12398318	-10.91	-1.82	-13.64	5.63	-1.08
7996	c1cc(=O)[nH]cc1C(=O)N	C12505139	-10.91	-6.98	-15.03	7.6	3.5
7997	CCc1nc(on1)[C@H](C)Cl	C12760976	-10.91	0.07	-11.44	3.38	-2.91
7998	C[C@H](/C=N/O)c1cccc1	C13537506	-10.91	-2.73	-10.96	5.28	-2.5
7999	COc1ccc(nc1)C#N	C14628952	-10.91	1.47	-15.99	5.31	-1.7
8000	C=CC[C@H]1CC(C)/C1=N/O	C17175976	-10.91	0.02	-12.87	4.25	-2.31
8001	c1cc(ccc1NN)S(C)F)F	C21298186	-10.91	-0.37	-11.82	4.02	-2.74
8002	c1cc(cc(c1)F)/C=C/C(=O)N	C25723331	-10.91	-1.21	-15.96	7.86	-1.6
8003	c1cc(sc1CB)C#N	C26422793	-10.91	-1.71	-8.97	3.97	-4.21
8004	CCOc1ccc(c(c1)N)Cl	C32006644	-10.91	-1.03	-10.72	3.2	-2.36
8005	CCOC(=O)c1cncnc1	C00404120	-10.9	0.46	-12.03	3.97	-3.29
8006	c1cnc2c(n1)cncn2	C00897037	-10.9	-4	-13.72	8.31	-1.49

8007	CC(C)CC(=O)C	C01482107	-10.9	-0.43	-10.76	3.35	-3.06
8008	C=C1CC(C1)C#N	C02018664	-10.9	0.36	-12.87	4.9	-3.29
8009	C[C@@H](C=C)O	C02034518	-10.9	-1.45	-11.38	2.01	-0.08
8010	C[C@H](C1CCCC1)O	C02042927	-10.9	-0.22	-9.97	1.16	-1.87
8011	C/C=C/[C@@H](CC(=C)C)O	C02166487	-10.9	-0.75	-11.58	1.66	-0.24
8012	CC(=O)c1ccn(c1)C	C02539414	-10.9	-1.54	-11.87	6.01	-3.5
8013	c1ccc(cc1)C2OCCO2	C02571426	-10.9	-0.97	-10.11	3.33	-3.14
8014	Cc1ccc(cc1)OBr	C12359324	-10.9	-2.5	-11.93	2.65	0.88
8015	c1c[nH]c(=O)c1[O-]Br	C14982237	-10.9	-1.91	-16.78	5.19	2.6
8016	CCc1nc(no1)CCl	C20363164	-10.9	-0.87	-12.54	4.28	-1.77
8017	c1([nH]c(=S)nc(n1)N)N	C01586434	-10.89	-1.49	-12.52	4.62	-1.5
8018	C[C@@H](C(=O)OC)Br	C01589664	-10.89	0.36	-11.77	3.27	-2.74
8019	Cc1ccc(c(c1)O)CCl	C01595511	-10.89	-2.44	-12.27	3.61	0.2
8020	C[C@@H]1CCC(=O)C1	C01621822	-10.89	-0.62	-10.66	3.22	-2.83
8021	CCn1cnc(=O)[nH]c1=O	C01708261	-10.89	-3.98	-18.21	11.84	-0.54
8022	C[C@@H]1[C@H](O1)C(F)(F)F	C02560333	-10.89	-1.06	-11.33	2.94	-1.44
8023	COC(=O)C(F)F	C02579127	-10.89	-0.92	-12.81	4.67	-1.84
8024	c1cc(nc(c1)F)C(F)(F)F	C02598026	-10.89	0.88	-14.91	5.54	-2.4
8025	CCCCc1cc[nH]n1	C03628192	-10.89	-1.48	-9.64	3.25	-3.02
8026	CCC(=O)C(=O)OCC	C04528565	-10.89	-0.37	-11.86	3.38	-2.03
8027	CN(C)/C(=N)C#N/N	C05446329	-10.89	2.22	-15.98	7.2	-4.34
8028	c1ccc(c(c1)N)C(S)N/F	C06095140	-10.89	-1.41	-17.88	11.11	-2.71
8029	C([C@@](OC(F)(F)F)Br)(F)F	C08698308	-10.89	0.32	-11.19	2.02	-2.03
8030	CCn1ccc(n1)CC#N	C12397777	-10.89	-2	-14.73	9	-3.16
8031	C[C@H](CC=C)C=O	C14592828	-10.89	-0.18	-11.86	3.89	-2.75
8032	c1nc([nH]n1)SSc2[nH]ncn2	C17957808	-10.89	-2.96	-13.27	8.66	-3.33
8033	C1C(=O)N[C@H](S1)N	C25952641	-10.89	-3	-14.86	5.03	1.93
8034	COCc1csc(n1)N	C31772050	-10.89	-2.17	-13.45	5.28	-0.55
8035	Cc1ccc(o1)/C=C/C(=O)C	C00259259	-10.88	-1	-13.2	5.29	-1.97
8036	c1cc(ccc1NC(=O)NO)Cl	C00395135	-10.88	-3.41	-16.85	10.26	-0.88
8037	COC(=O)Cn1cncn1	C01107120	-10.88	-0.26	-17.74	8.91	-1.8
8038	c1c(csc1C=O)CCl	C01296251	-10.88	-1.71	-14.11	5.56	-0.62
8039	C/C=C/C=O	C01686876	-10.88	-1.25	-12.43	4.75	-1.95
8040	c1([nH]c(=O)O)c2n[nH]c(=O)O2	C01708978	-10.88	-0.73	-21.76	5.87	5.75
8041	C[C@@H](C#C)OC	C02025155	-10.88	-1.03	-11.16	2.82	-1.51
8042	COC[C@@H](C=C)O	C02036145	-10.88	-0.77	-13.21	2.84	0.26
8043	CC[C@H](C=C)C(O)	C02164152	-10.88	-0.11	-9.71	1.18	-2.23
8044	C[C@@H](C(=O)C)OC(=O)C	C02169175	-10.88	0.26	-14.25	6.48	-3.38
8045	C[C@H](c1ccccc1)O	C02561250	-10.88	-1.6	-13.31	3.93	0.1
8046	C[C@H]1CCCC(=O)O1	C03860819	-10.88	-1.04	-13.4	6.17	-2.61
8047	C1CCC(=CC1)C=O	C04977523	-10.88	-1.15	-13.36	4.62	-0.99
8048	C/C=C(\C)/C=N/NC	C05371598	-10.88	-1.28	-12.66	2.76	0.29
8049	CCC(=S)N	C05501503	-10.88	-1.91	-11.2	1.66	0.58
8050	c1cc(ccc1C/C(=N/O)/N)N	C06535467	-10.88	-2.12	-17.19	5.5	2.93
8051	c1cc(cc(c1)N)/C(=N/O)/N	C12647933	-10.88	-0.53	-16.28	5.25	0.68
8052	c1cc2c(cc1F)n[nH]c2C=O	C14983482	-10.88	0.06	-13.91	5.2	-2.22
8053	C[C@H](COC(F)F)O	C16159289	-10.88	-2.17	-11.96	2.84	0.41
8054	c1c(sc(=S)[nH]1)O	C17061538	-10.88	-5.34	-15.37	9.64	0.18
8055	C=C[C@H]1C(=C)CCC(=O)O1	C21990748	-10.88	0.05	-12.44	5.34	-3.83
8056	Cc1nc(on1)CCCl	C26515414	-10.88	1.93	-14.68	3.79	-1.91
8057	c1c(c(c(n1)Br)N)Cl	C26894759	-10.88	0.19	-11.86	2.26	-1.47
8058	CS(=O)(=O)n1cncn1	C32603711	-10.88	-0.38	-20.09	10.36	-0.76
8059	CCc1ccc(c(c1)N)O	C00125075	-10.87	-1.39	-14.1	2.91	1.71
8060	c1cncn(c1)C(=O)CBr	C00158584	-10.87	1.68	-14.09	4.68	-3.15
8061	c1cc(c(cc1F)F)NC(=O)CC#N	C00167765	-10.87	-4.66	-14.29	11.32	-3.24
8062	COCOC(=O)C=C	C01608907	-10.87	0.77	-14.59	5.1	-2.14
8063	CCOC(=O)/C=C/CF	C01614532	-10.87	-1.25	-10.84	4.71	-3.5
8064	CC(C)C[N+](=O)[O-]	C01666939	-10.87	-0.87	-10.53	3.45	-2.92
8065	CC(=O)/C=C/C(=O)C	C01718551	-10.87	1.4	-15.35	4.66	-1.57
8066	c1ccc(cc1)C=C([O-])[O-]O	C01767981	-10.87	-2.85	-13.83	6.11	-0.3
8067	COnc2ccccc2nn1	C01865819	-10.87	2.46	-17.49	6.24	-2.07
8068	CNc1nnc(s1)[S-]	C02171944	-10.87	-1.38	-13.76	5.12	-0.85
8069	COc1ccc(c(c1)O)N	C02510157	-10.87	-2.97	-12.93	4.19	0.84
8070	Cc1cnc(n1)C(F)F	C02536621	-10.87	-4	-9.79	5.21	-2.29
8071	C[C@@H]1C(=O)CCS1	C05227198	-10.87	-0.85	-10.42	3.1	-2.7
8072	CCNNC(=S)N	C05784958	-10.87	-0.04	-16.03	2.76	2.45
8073	C/(C=C)CC#N)C#N	C08580903	-10.87	-1.08	-16.06	9.56	-3.28
8074	Cc1[nH]c2c(n1)c(nnn2)N	C08581302	-10.87	-5.05	-13.84	8.08	-0.07
8075	Cc1c([nH]cn1)CCl	C08614793	-10.87	-0.95	-12.55	5.53	-2.89
8076	C[C@H](C(=O)Cl)NC(=O)C	C11892560	-10.87	0.68	-15.2	4.63	-0.99
8077	CN/C(=N/O)/c1c(non1)N	C13477019	-10.87	-0.09	-19.05	7.36	0.92
8078	Cc1c(c(n1)N)I	C15021713	-10.87	-1.99	-10.41	3.4	-1.88
8079	CCc1nc(cs1)CO	C19092941	-10.87	-1.29	-13.09	3.99	-0.48
8080	CC1(C[C@H]1C(=O)Cl)C	C20357971	-10.87	1.08	-10.72	2.25	-3.49
8081	CCC(=O)[C@H](C#N)Cl	C21982971	-10.87	-0.32	-14.54	6.88	-2.88
8082	CCOC(=O)c1c(ccs1)N	C26506189	-10.87	-1.07	-13.08	5.7	-2.43
8083	c1c(nc2n1CCS2)C=O	C29753875	-10.87	-3.52	-12.92	8.22	-2.65
8084	Cc1ccccc1	M1995A019	-10.87	0.18	-7.96	1.51	-4.6
8085	c1cc(ccc1CO)C(F)(F)F	C00166036	-10.86	-2.56	-11.47	3.64	-0.48
8086	CCn1c(cc(n1)C)N	C00167530	-10.86	-3.62	-10.38	5.08	-1.94
8087	c1c(ncnc1Br)C(=O)ON	C00481335	-10.86	-2.45	-10.54	4.15	-2.01
8088	Cc1c(non1)COC(=O)C	C00529501	-10.86	0.85	-17.13	7.55	-2.14
8089	C=CCCO	C01530356	-10.86	-3.03	-9.83	1.96	0.04
8090	CC(=O)Cc1ccc1	C01583724	-10.86	-1.15	-13.94	7.14	-2.92
8091	C(C(CCl)Cl)Cl	C01667602	-10.86	1.17	-11.91	3.35	-3.48
8092	c1cc(ccc1C#N)N2N=N2	C03845422	-10.86	-1.19	-11.32	3.63	-1.98
8093	c1cc(c(c(c1)F)N)C(F)(F)F	C04240283	-10.86	-1.93	-9.62	2.37	-1.68
8094	C1C(C=NC=C1C#N)C#N	C04390916	-10.86	-1.7	-15.24	7.78	-1.71
8095	C[C@@H](CC#C)O	C05226622	-10.86	-1.34	-12.07	3.16	-0.61
8096	C[C@@H]1CC(=O)NN1	C05758013	-10.86	-4.28	-12.17	5.03	0.56

8097	c1cc(cnc1)CC(=O)N	C12359076	-10.86	-1.57	-17.81	8.66	-0.14
8098	C(=NNC(=O)N)C=[N+](O)[O-]	C13404426	-10.86	-2.9	-17.55	8.44	1.15
8099	C1C[C@H]([C@H](C1)Cl)O	C16137618	-10.86	-1.49	-10.36	2.08	-1.1
8100	CSc1c(c[nH]c(=O)n1)F	C16952036	-10.86	-5.83	-14.77	10.37	-0.62
8101	c1c(ccnc1N)CO	C21985268	-10.86	-2.13	-17.64	7.21	1.7
8102	CC(=O)C1=CC=C(C1)Br	C27840696	-10.86	-0.78	-10.23	3.97	-3.83
8103	c1cc2c(cc1Cl)[nH]nc2N	C00154498	-10.85	-4.35	-8.8	4.25	-1.95
8104	Cc1[nH]nc(n1)C	C01435792	-10.85	-2.1	-14.26	7.63	-2.12
8105	CCCN=C=O	C01575578	-10.85	-0.79	-11.94	1.73	0.14
8106	C[C@H](CC)OC(=O)C	C01627215	-10.85	-0.52	-11.62	4.67	-3.38
8107	c1c2c([nH]c(=O)[nH]2)nc(n1)Cl	C01691607	-10.85	-7.01	-9.75	6.16	-0.25
8108	C[C@H]1C(=O)C=C(C1=O)[O-]	C02037771	-10.85	-6.16	-15.24	10.47	0.09
8109	c1cc(c(c1)F)FCCO	C02386435	-10.85	-0.2	-13.5	4.95	-2.11
8110	c1cc(cnc1)C(=O)c2ccco2	C02392765	-10.85	0.35	-13.88	6.09	-3.4
8111	CS/C(=NN)/NN	C04280916	-10.85	-4.73	-11.21	4.53	0.56
8112	c1ccc2c(c1)cc(s2)C#N	C06118051	-10.85	-0.6	-12.89	4	-1.36
8113	C1COC(=CO)C=O	C06855242	-10.85	-1.94	-16.13	8.67	-1.46
8114	COc1ccc(cn1)Cl	C08494087	-10.85	-1.61	-10.53	2.51	-1.22
8115	c1cnnc2c1c(ncn2)[O-]	C09307071	-10.85	-3.69	-18.09	12.21	-1.29
8116	c1cn(nc1N)CC(F)F	C12357564	-10.85	-1.09	-14.96	6.94	-1.73
8117	CN(C)C(=O)c1cn[nH]c1N	C14608622	-10.85	-2.24	-15.35	6.74	0
8118	c1cc(ncn1N)[N+](=O)[O-]	C14982121	-10.85	-4.22	-14.9	9.99	-1.71
8119	C=CCOCC=C	C15217376	-10.85	-0.56	-9.75	2.1	-2.64
8120	CCn1cc(cn1)Br	C16124257	-10.85	0.04	-11.54	3.65	-3
8121	c1ccnc(c1)NC=C(C#N)C#N	C00136835	-10.84	-1.44	-15.43	9.81	-3.78
8122	Cc1[nH]cc(n1)C(=S)N	C00164983	-10.84	-4.75	-13.92	8.93	-1.11
8123	CCOC(=O)CC	C01697400	-10.84	-1.42	-9.34	3.44	-3.52
8124	CC[C@H]([C@H]([C@H](C)[N+](=O)[O-])O-])O	C01759007	-10.84	-2.12	-10.13	3.4	-1.99
8125	CN1C(=O)CNC1=S	C02537633	-10.84	-1.66	-13.45	4.31	-0.04
8126	c1cc(c(cc1F)N)n2cnnc2	C02538780	-10.84	-2.19	-9.3	4.9	-4.25
8127	c1c(cc(c1N)F)C#N	C02559543	-10.84	0.05	-12.66	3.86	-2.1
8128	C[C@H](C(=O)C(F)F)Br	C02560294	-10.84	1.2	-11.33	2.02	-2.72
8129	CC(=O)SCCC#N	C02584629	-10.84	-1.1	-14.94	6.89	-1.69
8130	c1cc(=O)nc1[O-]CCO	C04353786	-10.84	-4.64	-17.84	8.67	2.97
8131	C/C=C/C#N	C05023934	-10.84	-1.51	-11.91	4.6	-2.02
8132	C1COC(=O)[C@@H]1Cl	C05134260	-10.84	-0.54	-13.43	5.58	-2.45
8133	CC(=O)CC(=O)OC	C05159232	-10.84	-5.34	-12.31	7.82	-1.02
8134	c1c(c(n[nH]c1=O)[O-])Cl	C08614601	-10.84	-2.88	-18.6	5.82	4.81
8135	c1c(c[nH]c(=O)c1[N+](=O)[O-])O	C08649837	-10.84	-1.28	-18.44	6.92	1.96
8136	C1CO[C@H]1CBr	C16083110	-10.84	1.35	-13.13	2.64	-1.69
8137	c1(nnc(c1)N)C(=O)NN	C16952808	-10.84	-5.17	-17.92	6.26	6
8138	C1(=O)C(=O)[C@@]2([C@]1(C2=O)O)O	C16955511	-10.84	-2.31	-17.63	5.16	3.95
8139	c1c2c(ncn1)CNC2=O	C25923627	-10.84	-1.54	-17.37	8.09	-0.01
8140	c1cc2nc(cn2cc1)FBr	C32911311	-10.84	-1.59	-9.66	4.68	-4.27
8141	C[C@H](C(=O)C)O	C00895240	-10.83	-1.9	-12.87	4.47	-0.54
8142	Cc1c[nH]c(=O)[nH]1	C00967419	-10.83	-2.67	-15.6	7.35	0.1
8143	CCOC(=O)NN	C01640794	-10.83	-3.05	-13.71	4.89	1.04
8144	CCCSCC=C	C01644622	-10.83	0.31	-11.03	1.17	-1.28
8145	Cc1[nH]c2c(n1)ncn2	C01761937	-10.83	-3.08	-15.72	9.95	-1.98
8146	CC[C@H](CC#C)O	C02032398	-10.83	-0.42	-12.13	3.06	-1.34
8147	c1(c(c(c(c1)F)Br)F)F)N	C02167091	-10.83	0.73	-12.44	1.78	-0.91
8148	c1cc(nc(c1)F)C(=O)N	C02525420	-10.83	-3.13	-13.51	5.51	0.31
8149	C1CN(C(=O)N1N=O)N=O	C04887030	-10.83	0.18	-18.55	8.3	-0.76
8150	Cc1cc(c(s1)CO	C06857783	-10.83	-1.83	-11.31	3.46	-1.16
8151	c1c(nc[nH]1)CC#N	C08100958	-10.83	-1.14	-17.21	9.96	-2.45
8152	C/C(=C(C(=O)OC)NC	C15839430	-10.83	2.37	-14.74	3.91	-2.37
8153	Cn1nc(c1C(=N/O)N)N	C17044453	-10.83	-4	-16.45	8.81	0.81
8154	c1nc(nc1)NC2CC2	C18857994	-10.83	-1.12	-10.16	4.18	-3.73
8155	c1cc2c(c[nH]c2nc1)CC#N	C21304030	-10.83	-4.75	-13.1	10.69	-3.66
8156	CC[C@H](C(=O)OC)O	C00393219	-10.82	-0.59	-13.87	3.87	-0.23
8157	c1(c(non1)N)c2nc(on2)N	C01066115	-10.82	-1.82	-17.42	6.24	2.19
8158	C1COC(O)CCO	C01651845	-10.82	-2.81	-14.81	4.1	2.7
8159	c1cc(ccc1N)NC(=O)N	C01683199	-10.82	-0.31	-22.03	7.63	3.88
8160	C1[C@H](OCO1)CCl	C02045101	-10.82	-0.6	-12.27	3.21	-1.16
8161	CCCN1ccc(n1)C=O	C02538042	-10.82	-2.77	-11.06	5.87	-2.86
8162	c1ccc(cc1)C(=C)C(=O)C(F)F/[O-]	C04243029	-10.82	-3.54	-9.07	4.51	-2.72
8163	COC1=CCOCC1	C04521391	-10.82	-0.7	-12.74	2.61	0.01
8164	c1c(c(cc1F)[N+](=O)[O-])F)N	C04783291	-10.82	1.56	-18.11	6.49	-0.76
8165	C(CCl)ON	C04887608	-10.82	-2.38	-11.81	2.68	0.69
8166	c1ccn(c(=O)c1)N	C05521768	-10.82	-1.79	-17.27	9.33	-1.09
8167	c1ccnc(c1)C(=O)CC#N	C08729875	-10.82	-4	-12.13	8.28	-2.96
8168	Cn1c(ccn1)C(F)F)N	C12357879	-10.82	-4.96	-9.87	5.57	-1.55
8169	C=CCNc1ccc([nH+]1)N	C19961570	-10.82	-3.4	-10.5	4.42	-1.35
8170	c1ccc(c1)[C@@H](C(F)(NH3+))F	C20285900	-10.82	-2.43	-9.24	3.23	-2.38
8171	CN(c1ccc(nn1)Cl)N	C00152907	-10.81	-2.24	-12.3	5.38	-1.64
8172	CC(=O)Oc1ccc(cc1)Br	C01596299	-10.81	-0.63	-13.45	4.81	-1.53
8173	C=CCOC(=O)N	C01664995	-10.81	-0.61	-16.01	4.72	1.08
8174	Cc1ccc(cc1)CCO	C01680826	-10.81	-1.56	-10.28	3.47	-2.44
8175	CCOC(=O)c1ccnc(c1)F	C01682853	-10.81	1.89	-13.61	4.19	-3.28
8176	CCOC(=O)C#C	C01690295	-10.81	-1.13	-12.75	5.77	-2.7
8177	CC(=O)c1cccc1O	C01699884	-10.81	-0.14	-14.48	6.4	-2.6
8178	c1cc(sc1)C=C/CO	C01743779	-10.81	-1.84	-14.48	4.04	1.47
8179	COC(=O)c1ccc([nH]1)C=O	C01765334	-10.81	-0.1	-16.06	7.38	-2.04
8180	CCCCC#CC=O	C01995132	-10.81	-0.71	-12.86	4.88	-2.11
8181	c1cncc(c1Cl)C(F)F)F	C02578099	-10.81	-2.85	-9.14	2.91	-1.73
8182	C=CN1CCCC1=O	C03590964	-10.81	-0.55	-13.76	5.86	-2.37
8183	CNC(=S)N(C)N	C05187279	-10.81	-3.15	-14.06	2.64	3.77
8184	CNc1nc(nc1N)N	C13284856	-10.81	-5.46	-10.55	5.13	0.06
8185	c1cc2c(cc1F)[nH]c(n2)CO	C14987601	-10.81	-5.27	-10.75	5.73	-0.53
8186	CCOC(=O)/C=C/C=C/C	C16893048	-10.81	-0.28	-10.22	4.04	-4.36

8187	C#CCN[C@H]1CCSC1	C19875381	-10.81	0.06	-11.39	3.18	-2.65
8188	C[C@@H]([C@@](C(F)(F)F)(O-))F	C20232458	-10.81	-2.5	-11.17	3.6	-0.75
8189	c1cnccc1C(=O)NN	C00001590	-10.8	-3.67	-15.27	7.68	0.47
8190	CCn1c(nnn1)N	C01462461	-10.8	-4.73	-12.88	7.22	-0.42
8191	Cc1nc(nc(n1)N)N	C01555389	-10.8	-1.47	-12.41	5.12	-2.04
8192	CC1=C[P@@](=O)(CC1)O	C01560250	-10.8	-2.5	-14.91	6.77	-0.15
8193	CCCOCC(=O)C(F)F	C01713566	-10.8	-0.78	-8.36	1.6	-3.26
8194	CCOC(=O)CF	C01720173	-10.8	-1	-12.88	5.48	-2.4
8195	c1cc(c(c1)F)O)C=O	C02242717	-10.8	-1.18	-13.64	5.1	-1.08
8196	C(=O)(C(F)F)Cl)N	C03880139	-10.8	-2.31	-12.67	3.52	0.66
8197	c1c[nH]c2c1cc(cn2)Br	C04352690	-10.8	-0.79	-15.39	4.43	0.95
8198	C(C(=O)CS)S	C05496914	-10.8	-1.77	-12.56	4.07	-0.54
8199	CC(=O)c1ccnc1F	C08698255	-10.8	0.64	-19.16	10.09	-2.36
8200	CCC#COCC	C12418183	-10.8	0.26	-10.93	2.91	-3.03
8201	COCC(=O)c1ccsc1	C12959134	-10.8	1.69	-14.21	4.82	-3.1
8202	CCC[C@H]([C@H](C)C)O	C20231670	-10.8	-1.52	-9.56	2.31	-2.02
8203	c1cc(c(cc1O)C#N)F	C32914668	-10.8	1.27	-17.54	6.96	-1.49
8204	c1cnc(nc1)NC=C(C#N)C#N	C00093631	-10.79	-1.62	-13.39	8.47	-4.25
8205	Cn1cccc1CC(=O)OC	C00156541	-10.79	0.26	-13.6	6.48	-3.93
8206	c1cc(c(cc1)F)CBr	C00161640	-10.79	-0.29	-11.89	2.24	-0.85
8207	CCOC1CCCCC1O	C00404747	-10.79	-1.77	-11.07	4.07	-2.02
8208	COCC(C(=O)OCC=C	C01599221	-10.79	1.34	-13.83	3.22	-1.52
8209	c1cn(ccc1=O)[O-]	C01731907	-10.79	-4.71	-17.26	11.35	-0.17
8210	C1CCN(CC1)Cl	C02038843	-10.79	0.81	-10.48	1.27	-2.39
8211	c1cc(c(c1N)N)C(F)F	C02243181	-10.79	-2.99	-9.76	2.97	-1.02
8212	COC(=O)c1c(c[nH]1)Br	C03832441	-10.79	0.42	-13.76	4.24	-1.68
8213	C1CC(=O)SC1	C04501380	-10.79	-0.6	-13.26	5.16	-2.09
8214	CCOC(=O)O[C@H](C)Cl	C04521313	-10.79	-0.69	-10.62	3.88	-3.36
8215	C[C@H]1CCCC(=O)O1	C04521558	-10.79	-0.5	-12.65	5.43	-3.07
8216	C(CSC(=NH2+)N)ON	C04887234	-10.79	-0.41	-15.69	3.75	1.57
8217	C1C(=O)N(CS1)CCO	C05621429	-10.79	-1.67	-16.65	4.91	2.62
8218	c1ccc2c(c1)c(n[nH]2)I	C14909873	-10.79	-3.72	-8.16	4.22	-3.14
8219	c1cc2c(c1)F[nH]c2[O-]	C14985619	-10.79	-3.36	-13.2	4.72	1.05
8220	C/C(=C)1/C(=O)C(=O)NC1=O/[O-]	C18192858	-10.79	-4.06	-13.47	5.05	1.68
8221	C[C@@H]([C@H](C(=O)NCC(F)F)F)F[NH3+]	C19426015	-10.79	-2.51	-13.19	4.21	0.7
8222	c1cc(ccc1)OCC=O	C19729374	-10.79	0.3	-16.47	6.86	-1.48
8223	c1cc(nc1C)OCC#N	C19872670	-10.79	0.79	-14.23	4.63	-0.98
8224	CCOC(=O)[C@@H]1C[C@@H]1CO	C21984003	-10.79	-2.22	-12.43	5.13	-1.27
8225	Cc1c(ncn1)C)Br	C22001029	-10.79	-2.44	-10.66	6	-3.68
8226	c1c(cnc(n1)Cl)C=O	C22113854	-10.79	0.82	-17.1	7.15	-1.67
8227	Cn1c(ccn1)I	C26340339	-10.79	-1.85	-9.33	2.84	-2.45
8228	COC(=O)CNC(=O)c1cc[nH]n1	C00045729	-10.78	-4.59	-12.13	6.39	-0.46
8229	c1c(c(c(n1)Cl)N)Cl	C00967450	-10.78	-4.02	-11.05	3.4	0.89
8230	c1nc(c2c(n1)sn2)[O-]	C01416783	-10.78	-6.11	-17	12.56	-0.24
8231	C=COCC=O	C01653065	-10.78	-0.56	-13.06	4.94	-2.1
8232	C=C[C@H]([C1CCCC1)O	C01664511	-10.78	-1.46	-9.39	2.64	-2.57
8233	c1c(oc1C)CCC(=O)Cl	C01769379	-10.78	-1.86	-12.38	4.91	-1.45
8234	CCCCCOC=C	C02037287	-10.78	-0.2	-10.41	1.56	-1.72
8235	c1csc(n1)NC(=O)C(=O)N	C02361933	-10.78	2.3	-23.49	7.32	3.09
8236	C[C@@H]([C@H](C(F)F)F)F)O	C04269612	-10.78	-0.83	-10.86	1.88	-0.96
8237	C[C@@H]1C[C@H]([C@H]1)O1	C04501394	-10.78	2.92	-15.79	5.21	-3.12
8238	CC(S+)(C)C	C05339219	-10.78	0.08	-9.17	0.15	-1.84
8239	C(=O)NNC(=S)N	C05410159	-10.78	-5.39	-15.78	7.15	3.24
8240	CCO[C@@H]1CCC(=O)O1	C05765982	-10.78	-0.11	-15.51	5.69	-0.85
8241	C[C@H]([C@H](CO)C=C	C06020791	-10.78	-1.2	-11.92	1.83	0.5
8242	c1ccc2c(cc1F)c(n[nH]2)N	C06188243	-10.78	-1.71	-12.02	4.64	-1.69
8243	C[C@H]([C@H](c1ccnc1)NO	C06733579	-10.78	-2.3	-12.32	3.77	0.07
8244	C1CC(C1)/C(=N)O)N	C15937658	-10.78	-3.65	-10.76	3.8	-0.17
8245	C1C(CO1)Br	C16083105	-10.78	-0.09	-12.22	2.57	-1.04
8246	[C@@](C(F)F)Cl)(N=O)(F)Cl	C16924550	-10.78	-1.18	-11.12	2.37	-0.85
8247	CNC(=S)Nc1cccc1F	C17083483	-10.78	0.36	-15.48	7.91	-3.57
8248	C[C@H]1C(=O)NCCS1	C00405461	-10.77	-3.03	-11.66	5.05	-1.13
8249	CC(=O)OC1CSC1	C01639980	-10.77	-0.97	-13.79	4.8	-0.8
8250	c1ccc(c(c1)N)NC(=O)C(F)F	C01680578	-10.77	-4.12	-9.79	4.66	-1.53
8251	c1ccc(cc1)[P@@H]([O-])O	C01996013	-10.77	-3.68	-13.81	7.91	-1.18
8252	CNc1ccc(cc1)C#N	C02565984	-10.77	-0.91	-11.67	4.45	-2.63
8253	c1cc(oc1C(F)F)C(F)F	C02566563	-10.77	-0.46	-9.07	2.56	-3.8
8254	COC(=O)[C@H](C)Br	C03164544	-10.77	1.15	-12.68	3.61	-2.85
8255	[H]/N=C\1/CC(=NN2C1=NN2)N=[N+]=[N-]	C04878745	-10.77	-4.33	-12.68	4.56	1.68
8256	CN(C)N=C/COC	C05081178	-10.77	-0.85	-11.7	3.07	-1.28
8257	CC(C)[N+](=O)[O-]	C05167659	-10.77	-0.82	-11.24	3.64	-2.35
8258	c1nc([nH]n1)NN	C05522092	-10.77	-5.21	-16.26	5.78	4.92
8259	c1c(c(n2c(n1)ncn2)[O-])C#N	C06658038	-10.77	-5.86	-19.4	18.13	-3.64
8260	c1cc(oc1)CNC(=O)CBr	C09877392	-10.77	-0.25	-14.82	6.34	-2.04
8261	CCC(=O)/C(=N)O/C	C14649264	-10.77	-1.42	-12.09	3.25	-0.51
8262	CO/C=C/COCO	C17196620	-10.77	-0.94	-12.77	3.28	-0.35
8263	Cc1cc(=O)[nH]cn1	C18211990	-10.77	-5.42	-13.08	9.21	-1.49
8264	CCn1ncc(n1)N	C19089911	-10.77	-2.1	-12.33	4.68	-1.01
8265	c1ccc(c(c1)CC[NH2+])N)F	C19168010	-10.77	0.67	-12.92	3.41	-1.94
8266	c1ccc(cc1)Cc2c[nH]nc2N	C19730117	-10.77	-0.36	-14.56	7.15	-3
8267	c1cc(c(cc1OCCO)F)F	C19786125	-10.77	-2.51	-13.21	6.26	-1.31
8268	c1(c(c(c(c1F)N)F)F)N+=[O-][O-]N	C19910277	-10.77	-2.83	-12.82	5.87	-0.98
8269	C1COC[C@H]1/C=N/O	C20283008	-10.77	-3.59	-12.82	4.92	0.72
8270	c1nc(c(s1)C=O)C=O	C20357651	-10.77	-2.41	-16.99	9.6	-0.96
8271	Cc1cc(c(nc1)N)O	C21981859	-10.77	-4.14	-13.47	6.6	0.23
8272	c1ccc(c(c1)CO)Cl	C00157459	-10.76	-1.67	-10.07	2.74	-1.76
8273	c1c(csc1[N+](=O)[O-])C=O	C00159715	-10.76	-4.64	-9.18	6.04	-3
8274	CCOC(C)OCC	C00404268	-10.76	-0.32	-10.58	2.43	-2.3
8275	Cn1c(cc(n1)O)C(F)F	C01046981	-10.76	-3.14	-12.71	4.11	0.98
8276	c1csc(n1)N[C@@H](C(F)F)F)O	C01558268	-10.76	-3.11	-12.11	4.02	0.44

8277	COCc1ccccc1	C01574322	-10.76	-0.26	-11.69	2.03	-0.83
8278	CCOC(=O)/C=C/C	C01680395	-10.76	-0.48	-10.56	3.68	-3.39
8279	CCCCOC(=O)CF	C01847502	-10.76	0.59	-13.09	5.44	-3.71
8280	CC(=C)C(=O)OCC(C(F)F)(F)F	C02579124	-10.76	0.34	-9.72	3.32	-4.69
8281	C1COC(OC1)CCCI	C05190715	-10.76	-0.01	-14.01	2.75	0.5
8282	CC[C@H](C#CC(F)F)F	C05467588	-10.76	0.03	-11.62	2.3	-1.46
8283	c12=c(nn1)ssnc2S	C06862762	-10.76	-0.42	-13.24	3.9	-1
8284	C1CC1N=C=O	C11802355	-10.76	-0.82	-11.77	1.96	-0.12
8285	COC(=O)C1Oc2ccccc2O1	C14608629	-10.76	-0.87	-12.79	6.5	-3.59
8286	c1cc2cc[nH]c2cc1I	C14983495	-10.76	-0.02	-10.9	3.41	-3.25
8287	C1C=CCC1C(=O)N	C15021095	-10.76	-2.26	-13.05	5.2	-0.65
8288	C1=C([C@H](C(=O)N=C1)N)[NH3+]	C15021943	-10.76	-3.6	-18.09	9.12	1.81
8289	C/C(=C/C(=O)OC)/N	C15975165	-10.76	0.77	-15.36	4.93	-1.09
8290	C[C@H](Cc1ccccc1)O	C20412681	-10.76	-4.19	-9.18	3.8	-1.19
8291	CC(=O)c1ccc(c(c1)N)F	C21985959	-10.76	-1.06	-13.29	5.73	-2.14
8292	c1c(c(n1)CCC#N)Br	C26547491	-10.76	-3.44	-10.2	6.31	-3.42
8293	c1c(c(n[nH]1)N)C2CC2	C26897708	-10.76	-5.27	-10.56	6.4	-1.33
8294	Cn1ccnc1CC#N	C00331886	-10.75	-0.94	-15.35	8.55	-3
8295	c1ccc(cc1)F)NNC(=S)N	C01396307	-10.75	0.23	-17.04	8.94	-2.87
8296	c1ccc(cc1)C(=O)C=O	C01634211	-10.75	-2.16	-13.49	8.72	-3.82
8297	CC1OCCO1	C01680769	-10.75	-0.31	-11.99	2.27	-0.72
8298	Cc1cccc(c1)NC	C01699966	-10.75	-0.13	-9.82	2.16	-2.96
8299	CC#CC(=O)C	C01723675	-10.75	-1.38	-12.72	5.11	-1.76
8300	C(C(C(=O)N)(F)F)(F)F	C02149987	-10.75	-2.2	-13.62	4.74	0.34
8301	C/N=C/c1ccccc1F	C05829901	-10.75	-0.82	-12.06	5.12	-2.99
8302	Cc1ccc(nc1)CCO	C08701027	-10.75	-2.25	-11.26	3.9	-1.14
8303	c1cc(cnc1)[C@H]2[C@H](O2)C#N	C13213076	-10.75	-1.57	-13.79	6.57	-1.97
8304	C/C(=N/O)/c1ccccc1N	C14417908	-10.75	-3.72	-10.14	3.96	-0.85
8305	c1[nH]nc(n1)/N=C(N)/[NH+]=C(N)N	C16926091	-10.75	-5.95	-20.54	19.1	-3.37
8306	CCc1nnc(o1)N	C16942992	-10.75	-2.11	-14.85	3.47	2.74
8307	c1cc(sc1)CNCC(F)F	C19502962	-10.75	-1.2	-10.31	3.48	-2.73
8308	CO[C@H]1CC=COC1	C20232049	-10.75	-0.82	-10.55	2.02	-1.4
8309	c1cnc(cn1)NCC(F)F	C21054921	-10.75	-2.53	-11.38	4.76	-1.6
8310	Cc1ccc(s1)[C@@H](C)S	C26515584	-10.75	-0.1	-8.18	2.09	-4.55
8311	Cn1c(cnc1SC)C=O	C30678014	-10.75	-2.97	-10.92	6.08	-2.93
8312	CCOc1ccc2nncn2n1	C00108362	-10.74	-5.1	-13.93	8.42	-0.14
8313	CC(=O)Nc1cccc(c1)F	C00389744	-10.74	-1.96	-14.48	8.41	-2.72
8314	C=CCN(CC=C)C#N	C00393616	-10.74	1.29	-10.21	3.79	-5.62
8315	CC[C@H]1CCC(=O)O1	C00394775	-10.74	0	-13.23	5.65	-3.16
8316	c1cc(c(nc1)C=O)O	C01494953	-10.74	-3	-16.42	8.52	0.16
8317	CCSCC(=O)C	C01657459	-10.74	-1.05	-12.45	5.74	-2.98
8318	C(CC)SC(=NH2+)N	C01665216	-10.74	-2.05	-13.45	2.65	2.1
8319	C([C@H](C#N)Cl)Cl	C01670676	-10.74	-1.07	-10.62	3.72	-2.78
8320	CCOc1cccc(c1)O	C01680430	-10.74	-1.64	-11.55	3.89	-1.45
8321	c1ccc(c(c1)NC(=O)N)O	C01720564	-10.74	0.17	-21.75	7.07	3.77
8322	c1cn[nH]c1C(=O)NN	C04243758	-10.74	-4.94	-18.21	7.26	5.15
8323	CCO[P@@H](=O)[O-]	C04529330	-10.74	-4.73	-12.35	6.63	-0.28
8324	[H]/N=C/Cc1ccccc1)OCC	C04776794	-10.74	-1.52	-13.13	3.33	0.58
8325	CC(C)Nn1cnc1	C05284733	-10.74	-1.39	-14.88	6.04	-0.52
8326	C(CO)/C(=N)O/N	C06373467	-10.74	-5.51	-13.39	4.45	3.7
8327	c1cnc(c1)NNC(=S)N	C13281580	-10.74	0.71	-19.72	10.64	-2.37
8328	c1cc2c(cc1F)C(=O)CO2	C16083115	-10.74	-0.54	-12.22	4.72	-2.7
8329	[H]/N=C(\CCC)/OCC	C17014696	-10.74	-1.22	-10.54	1.95	-0.93
8330	CCc1ccc(s1)C=O	C00152280	-10.73	-1.7	-12.36	4.14	-0.82
8331	C1CCC(=O)C1	C00895304	-10.73	-0.57	-11.07	3.27	-2.37
8332	CC(=C)C(=O)OCCOC	C01608910	-10.73	1.02	-14.04	4.93	-2.64
8333	CCOCCC#N	C01688360	-10.73	-1.8	-11.15	4.17	-1.95
8334	Cc1nnc(n1)C	C01742597	-10.73	-2.62	-13.46	6.36	-1.01
8335	c1cc(c(cc1Cl)F)[N+](=O)[O-]	C01845796	-10.73	-1.1	-12.75	4.76	-1.64
8336	CC(=O)OCCCCI	C02031626	-10.73	-0.17	-11.34	4.15	-3.37
8337	CCO[C@H](C(=O)OCC)O	C02045745	-10.73	-3.48	-10.4	4.54	-1.4
8338	c1c(c(n1CO)[N+](=O)[O-])Cl	C04290898	-10.73	-5.16	-12.57	7.41	-0.42
8339	CSC(=[N-])C(C(F)F)(F)F	C04803484	-10.73	-2.07	-8.37	2.24	-2.53
8340	C=CCOCO	C04976091	-10.73	-2.74	-12.32	3.41	0.92
8341	C1C[C@@H](OC=C1)C#N	C05191294	-10.73	1.59	-15.17	4.4	-1.55
8342	CC(=O)NCC(=O)C=[N+]=[N-]	C05278618	-10.73	-1.46	-16.8	7.21	0.32
8343	c1c(c(n[n-]1)C#N)[N+](=O)[O-]	C05605780	-10.73	-2.9	-13.55	6.16	-0.44
8344	c1c2c(sc1CO)CCC2	C12336482	-10.73	-1.83	-11.29	4.37	-1.98
8345	c1cncnc1NC=C(C#N)C#N	C12495537	-10.73	-0.06	-16.81	9.21	-3.08
8346	c1cc(oc1)[C@@H](C#N)N	C19984404	-10.73	-1.01	-14.66	5.5	-0.55
8347	CC(=O)c1c(ccc1)[O-]	C32914750	-10.73	1.77	-19.72	8.9	-1.68
8348	Cc1cc(nnc1Cl)[O-]	C00337144	-10.72	-2.83	-13.91	4.71	1.31
8349	CC(=O)Nc1ccccc1O	C00404269	-10.72	-1.12	-15.42	6.49	-0.67
8350	C1C=C(C[C@H]2[C@H]1O2)Cl	C01678543	-10.72	0.59	-14.72	2.52	0.9
8351	Cc1c([nH]nc1C)C	C02168425	-10.72	-1.65	-11.17	4.24	-2.14
8352	c1ccc(cc1)C[C@@H]2CO2	C02545314	-10.72	0.88	-12.12	3.74	-3.23
8353	c1ccc(c(c1)/C=C/C(=O)N)F	C02783413	-10.72	0.32	-20.68	9.06	0.59
8354	C1CN(C(=O)NC1=O)N=O	C04917965	-10.72	-0.65	-17.38	7.38	-0.07
8355	CCC(CC)S	C05298733	-10.72	-0.58	-9.98	0.57	-0.73
8356	C[C@H]1C(=O)NC(=S)N1	C05751800	-10.72	-3.74	-13.67	3.67	3.02
8357	c1cc(=O)[nH]cc1[O-]	C13527001	-10.72	-2.57	-16.37	5.11	3.11
8358	C1C(=O)N=C(N)N	C13536079	-10.72	-1.62	-15.72	6.34	0.28
8359	Cc1ccccc1/C=C/O	C13541520	-10.72	-2.91	-9.1	5.81	-4.52
8360	Cc1c(onc1[O-])C	C16974812	-10.72	-2.35	-15.04	7.74	-1.07
8361	CCN(CC)/C(=N)O/N	C17064135	-10.72	-4.42	-10.81	6.08	-1.57
8362	Cc1c(sc(n1)Br)C	C19702750	-10.72	-0.36	-10.86	3.38	-2.88
8363	CCNc1ccc(cn1)Br	C20552434	-10.72	-4.34	-6.16	2.65	-2.88
8364	c1ccc(c(c1)N)n2ccn2	C22141362	-10.72	-2.2	-12.67	6.18	-2.03
8365	c1cc(c(cc1NC(=O)N)N)F	C22144609	-10.72	-4.42	-17.77	10.34	1.13
8366	c1cnc(n2c1nnc2)NN	C26894645	-10.72	-2.09	-12.81	7.23	-3.06

8367	Cc1nncn1C	C32628130	-10.72	-1.96	-14.08	8.49	-3.17
8368	CNC(=S)Nc1ccccc1	C00075391	-10.71	0.8	-17.2	9.18	-3.49
8369	Cc1cc(=O)[nH]c(=O)[nH]1	C00162484	-10.71	-2.98	-16.87	8.54	0.6
8370	c1ccc2c(c1)nc(o2)Cl	C00404788	-10.71	-0.13	-15.82	4.49	0.75
8371	CC(=O)SCCCCl	C01635551	-10.71	-0.52	-9.75	3.1	-3.53
8372	c1ccoc(c1)Br	C02572476	-10.71	-1.98	-11.09	2.53	-0.17
8373	CCCCCS	C03861659	-10.71	-0.47	-10.4	0.72	-0.57
8374	Cn1cc(c(n1)[N+](=O)[O-])N	C04014784	-10.71	-2.79	-17.34	9.39	0.03
8375	CSC1=NCCCC1	C04963521	-10.71	0.72	-10.5	1.46	-2.39
8376	c1cc(=O)[nH]nc1	C08672864	-10.71	-2.38	-15.84	7.59	-0.07
8377	c1c(csc1)CnN]Br	C20475276	-10.71	-0.26	-11.18	1.9	-1.17
8378	c1c(con1)CO	C26547904	-10.71	-2.04	-15.28	6.08	0.52
8379	C=CS(=O)(=O)c1ccccc1	C00391881	-10.7	1.25	-16.45	6.67	-2.17
8380	CNC(=O)c1ccc(cc1)F	C00398480	-10.7	-2.11	-14.7	6.2	-0.1
8381	CC(=O)c1ccc([nH]1)[N+](=O)[O-]	C01561732	-10.7	-3.21	-11.86	7.74	-3.37
8382	CCCC(=O)C(C(F)(F)F)(F)F	C01675533	-10.7	-0.73	-8.53	2.28	-3.72
8383	COCCCC=O	C01678736	-10.7	-2.04	-11.65	4.49	-1.5
8384	C1=CC(=O)N(C1=O)O	C02141013	-10.7	-3.41	-16.55	8.58	0.67
8385	CC(=O)CNC(=O)C	C02528183	-10.7	-1.49	-15.63	6	0.43
8386	CCOC(=O)C(=N+)[N-](C(F)(F)F)	C04255747	-10.7	0.21	-11.47	2.53	-1.96
8387	CC[C@H](CS)S	C05298876	-10.7	-0.7	-11.55	1.46	0.09
8388	C[C@H]1CC[C@H](C1)O	C05752028	-10.7	-0.48	-10.91	1.73	-1.04
8389	Cc1ccc(n1)N	C06071275	-10.7	-2.63	-12.29	3.04	1.19
8390	c1cc2c(c(c1)F)c([nH]2)Cl	C14985898	-10.7	-0.37	-12.69	5.13	-2.77
8391	c1cc(cc(c1)O)C(F)F	C15441916	-10.7	-0.99	-12.7	4.93	-1.94
8392	CO/C=N/c1cn2c(n1)CN=C2	C17142940	-10.7	-0.05	-18.08	8.9	-1.47
8393	CC(=O)Cn1ccnc1	C19092247	-10.7	-2.28	-14.64	9.8	-3.57
8394	c1[nH]nc(n1)n2nncn2	C19770068	-10.7	-5.5	-15.57	13.56	-3.2
8395	c1cc(c(cc1F)F)N=C=S	C00164717	-10.69	-0.26	-11.48	2.32	-1.27
8396	CSc1ccccc1N	C00388267	-10.69	-0.14	-10.94	2.95	-2.56
8397	Cc1c([nH]1)[O-]C(=O)NN	C01082446	-10.69	-3.14	-15.87	8.26	0.05
8398	#CC1OCCCCO1	C01590523	-10.69	0.63	-14.01	4.56	-1.87
8399	C[C@H](CSC)O	C01682807	-10.69	-1.27	-11.54	2.87	-0.75
8400	c1ccc2c(c1)CCOC2	C01691582	-10.69	-0.89	-9.01	2.59	-3.38
8401	CC(C)SC=O	C01743177	-10.69	-0.18	-12.58	4.24	-2.17
8402	CC[C@H](N+)(=O)[O-]Cl	C01758983	-10.69	-0.68	-11.81	2.72	-0.93
8403	c1ccc(cc1)[C@H](CBr)O	C01995624	-10.69	-0.76	-10.03	2.87	-2.78
8404	CC[C@H](C)CCO	C02034637	-10.69	-2.73	-8.77	1.79	-0.98
8405	CC(=O)OCCC#C	C02382826	-10.69	-0.02	-12.22	4.91	-3.36
8406	COCCOCC	C02563430	-10.69	-0.7	-11.86	2.92	-1.05
8407	C1CS(=O)(=O)C=C1SC(=NH2+)N	C05034100	-10.69	-1.08	-20.36	9.5	1.25
8408	CCCCN(C(=O)C)N=O	C05049224	-10.69	-1.13	-10.41	2.81	-1.97
8409	Cc1[nH]c(cn1)[C@H](C(F)(F)F)O	C05285760	-10.69	-4.29	-12.78	6.93	-0.55
8410	C/C=N/NCCC#N	C05496996	-10.69	-2.96	-12.44	6.35	-1.65
8411	COC(=O)CSc1cccs1	C05510951	-10.69	-1.18	-13.08	4.53	-0.96
8412	Cn1c(cnc1)[N+](=O)[O-]CO	C13207527	-10.69	-3.81	-13.72	9.2	-2.36
8413	CCOC(=O)n1ccnc1	C13284754	-10.69	-0.31	-11.62	4.56	-3.32
8414	c1cc(ncc1[O-])[N+](=O)[O-]	C14982964	-10.69	-2.26	-15.41	8.16	-1.19
8415	CN(C(=O)c1ccco1)O	C15780037	-10.69	-3.63	-13.47	7.33	-0.92
8416	C(=O)([C@](C(F)(F)F)(F)Cl)F	C16159147	-10.69	-0.31	-9.1	0.96	-2.24
8417	C1[C@H](C=C[C@H]2[C@H]1O2)O	C17000693	-10.69	-2.11	-13.58	4.26	0.74
8418	c1c(c(nc1)N)[O-]N=O	C17021588	-10.69	-5.45	-13.64	5.69	2.71
8419	c1c(c[nH]c1=O)N	C17426312	-10.69	-4.33	-17.25	7.28	3.62
8420	C1CC(=CC(=O)C1)N	C18200963	-10.69	-4.76	-15.7	10.96	-1.18
8421	CC[NH2+]NCC	C19168139	-10.69	-0.3	-11.27	1.51	-0.63
8422	c1nncn1NC(=NH2+)N=C(N)N	C20458929	-10.69	-5.93	-13.69	12.89	-3.96
8423	c1cnc(nc1C=O)N	C26895888	-10.69	-4.91	-14.51	10.07	-1.34
8424	C1[C@H](COC1)Br	C29865995	-10.69	0.14	-9.78	1.14	-2.2
8425	CSc1nc(c(s1)C#N)N	C00039461	-10.68	-2.55	-11.94	5.18	-1.36
8426	C1Cn2c(nnn2)NC1=O	C01427446	-10.68	0.26	-18.4	7.46	0
8427	Cc1ccc(n1)C	C01574315	-10.68	-0.73	-9.43	3.25	-3.77
8428	CC(=CCc1ccc(cc1)O)C	C01600126	-10.68	-0.28	-12.88	2.8	-0.32
8429	C(CSC(=O)N)CCl	C01755559	-10.68	-1.18	-13.26	4.36	-0.6
8430	c1ccc2c(c1)CC(C2)O	C01758758	-10.68	-1.1	-10.31	2.95	-2.22
8431	CC(=O)[C@H](OC)F	C01765112	-10.68	-0.8	-12.9	4.46	-1.44
8432	c1csc1C(=O)NN	C02574348	-10.68	-3.04	-15.1	7.65	-0.2
8433	C[C@H]1[C@H](CCO1)S	C04262497	-10.68	0.36	-11.21	1.97	-1.8
8434	CNC=C/1CCOC1=O	C04771842	-10.68	-1.93	-13.8	7.02	-1.97
8435	CC(=O)Cc1ccccc1	C08294932	-10.68	-1.38	-13.61	7.51	-3.19
8436	c1ccc(n1)N	C12336599	-10.68	-3.58	-13.57	4.5	1.97
8437	c1c([nH]c(=O)c(c1)N)Br	C14982016	-10.68	-2.93	-14.87	4.93	2.19
8438	C[C@H]1C@H1N=C=O	C19518769	-10.68	-1.4	-10.76	2.18	-0.7
8439	CSc1ccc(cc1)Br	C00167168	-10.67	-0.05	-12.47	1.88	-0.03
8440	c1cc(nc(c1)Cl)Cl	C00331613	-10.67	-1.75	-10.26	4.11	-2.77
8441	c1c(nc2[nH]ncn2c1=O)N	C01613014	-10.67	-3.75	-16.01	7.3	1.78
8442	CC(=O)CCO	C01672523	-10.67	-2.71	-12.42	4.14	0.31
8443	C=CCOC=O	C01680373	-10.67	-0.76	-14.22	6.44	-2.14
8444	CC(=O)CCC(=O)C	C01683671	-10.67	-1.11	-11.72	4.69	-2.54
8445	c1c([nH](ccc1S)[O-])	C01714990	-10.67	-1.78	-17.68	11.1	-2.31
8446	C(C#N)N(CC#N)[N+](=O)[O-]	C01724608	-10.67	-4.3	-16.51	12.49	-2.35
8447	CCCC/C=C/C=O	C02017189	-10.67	-0.71	-12.87	4.62	-1.71
8448	c1ccc(c(c1)C)F)N=C=O	C02509912	-10.67	-3.66	-9.74	3.98	-1.25
8449	c1ccnc(c1)Cn2c(ccn2)N	C03445805	-10.67	0.3	-17.04	8.55	-2.47
8450	Cc1cc(no1)NC(=O)C(=O)N	C04323353	-10.67	-1.74	-16.78	6.24	1.61
8451	CCC(=S)[O-]	C04775268	-10.67	-0.68	-12.28	2.66	-0.38
8452	CCNc1nnc(s1)[S-]	C05303815	-10.67	-4.21	-10.88	6.14	-1.72
8453	C=C[P@@H](=O)[O-]	C06665106	-10.67	-4.32	-12.05	6.29	-0.59
8454	c1cc(c(cc1CCO)F)Cl	C15441145	-10.67	-2.58	-9.17	3.45	-2.37
8455	CSc1nnc(=O)n1N	C16248851	-10.67	-3.83	-11.44	5.12	-0.52
8456	Cc1nc([nH]n1)CC#N	C16249007	-10.67	-1.12	-17.17	9.72	-2.09

8457	c1cc(sc1)CC[NH2+]	C19265147	-10.67	-0.95	-12.03	3.47	-1.16
8458	C[C@@H]1C[C@H]1N=C=O	C19518771	-10.67	0.72	-12.49	1.87	-0.77
8459	CN/C=C/[N+](=O)[O-]/SC	C19594774	-10.67	-0.85	-12.21	5.24	-2.86
8460	CCOC(=O)[C@H](C#N)N	C20064543	-10.67	-0.34	-15.49	5.66	-0.5
8461	Cc1c(c(n1)C)N)Cl	C20313735	-10.67	-5.51	-9.08	5.64	-1.72
8462	CCOCc1cc(on1)N	C26512604	-10.67	-1.07	-16.61	5.99	1.01
8463	CC(=O)c1ccc(cc1F)F	C00157303	-10.66	1.25	-16.87	7.21	-2.26
8464	C1CCO[C@H](C1)ON	C00403241	-10.66	-1.84	-11.86	3.75	-0.7
8465	Cc1c(ccn1)C=O	C02384488	-10.66	-2.85	-11.86	6.22	-2.18
8466	CC(=C)C#CCO	C02390306	-10.66	-2.75	-11.74	4.79	-0.96
8467	c1cc(ccc1CN=C=O)Cl	C02526521	-10.66	-2.25	-11.86	3.22	0.23
8468	CCSc1nnc(n1N)C(F)F	C02536951	-10.66	-2.03	-9.95	4.55	-3.22
8469	C(CC(F)F)Br)CO	C02555156	-10.66	-1.72	-11.4	3.29	-0.83
8470	C[C@H](c1ccc(cc1)O)O	C02566074	-10.66	-2.01	-12.5	3.74	0.11
8471	c1cc(ccc1C#N)SC(F)F	C02579163	-10.66	-1.34	-7.95	3.48	-4.85
8472	C1=CC(=O)C[C@H]1O	C04521580	-10.66	-4.17	-14.16	7.67	0
8473	c1(c(c(c1F)Br)F)F)O	C04644817	-10.66	0.77	-12.76	2.29	-0.96
8474	C/C(=C/C(=O)C(F)F)/OC	C04801703	-10.66	-2.3	-8.92	2.93	-2.37
8475	CC(C)CS	C05008005	-10.66	-0.49	-8.13	0.68	-2.71
8476	CCc1nc(no1)C(=N)O/N	C05019001	-10.66	-2.03	-17.06	6.42	2.02
8477	CN(C)C(=S)NN	C06371802	-10.66	-2.04	-13.24	2.46	2.17
8478	C/C=C/O)N	C08603167	-10.66	-2.14	-13.76	4.85	0.39
8479	Cc1cc(nnc1)Cl	C15444618	-10.66	-2.1	-11.58	5.12	-2.1
8480	CCSc1ccccc1N	C16576888	-10.66	-0.22	-9.55	2.47	-3.36
8481	C[C@H]1C=CC[C@H]2[C@@H]1COC2	C17355228	-10.66	-0.38	-8.37	1.43	-3.34
8482	Cc1ccnc1C(F)F	C21985789	-10.66	-2.68	-9.17	4.52	-3.33
8483	c1cnnc1c2cccn2	C22002470	-10.66	-0.83	-14.36	6.77	-2.23
8484	C1CCc2c(c(no2)C#N)C1	C24774066	-10.66	2.16	-13.44	4.28	-3.66
8485	c1cc(sc1)CC(=O)N	C00347395	-10.65	-3.74	-13.73	7.48	-0.67
8486	CCOCC	C01657408	-10.65	-0.1	-10.46	1.46	-1.54
8487	CC(=O)COC	C01688094	-10.65	-1.4	-13.07	5.38	-1.57
8488	CC(=C)CNC(=O)C	C01697869	-10.65	1.06	-15.53	5.31	-1.49
8489	CCOC(=O)C(C=O)C(F)F	C02556469	-10.65	0.73	-12.52	4.12	-2.98
8490	C[C@@H](c1ccccc1)NC=O	C04018178	-10.65	-1.35	-15.14	6.09	-2.25
8491	COc1ccc(=O)[nH]n1	C05115746	-10.65	-3.65	-14.94	5.64	2.3
8492	Cc1c[nH]c(=S)[nH]c1=O	C08602963	-10.65	-4.01	-13.09	5.4	1.05
8493	CN(C)C=C[N+](=O)[O-]	C12370856	-10.65	-2.4	-15.04	9.48	-2.7
8494	Cc1c(cn1)CC(F)F)C=O	C12395188	-10.65	-5.64	-9	6.96	-2.96
8495	Cc1cccc(n1)CCl	C15884435	-10.65	-0.28	-10.62	3.77	-3.51
8496	COC(=O)[C@@H](CS)N	C19230197	-10.65	-0.92	-12.7	3.23	-0.27
8497	C1Cc2c(sc2)CC#N)C1	C19422427	-10.65	-1.79	-13.02	8.03	-3.88
8498	COC(=O)Nc1ccc(cc1)Cl	C00270902	-10.64	-0.34	-15.25	4.91	0.04
8499	c1cc(c(c1)Cl)Cl)O	C00388511	-10.64	-2.14	-10.12	3.58	-1.96
8500	c1cc(ccc1)O)Cl	C00388513	-10.64	-1.75	-9.92	2.89	-1.86
8501	C=CCNc1ccnc(n1)N	C01644920	-10.64	-4.11	-13.06	4.41	2.12
8502	CCOC(=O)CON	C01683162	-10.64	-1.63	-13.7	5.52	-0.84
8503	CC[C@H]1C[C@H](C#C)O	C02044152	-10.64	-0.49	-11.62	2.21	-0.74
8504	c1c(c(cc1)Br)Br	C02245234	-10.64	-0.08	-12.77	2.59	-0.37
8505	CC(=O)N(C)OC	C02528020	-10.64	-1.04	-12.97	4.55	-1.18
8506	Cc1c(cnn1)C#N	C02537522	-10.64	0.37	-14.66	6	-2.35
8507	c1c(cnc(=O)[nH]1)Br	C04002614	-10.64	-2.42	-17.98	9.5	0.25
8508	CNC(=O)c1ccc1	C04099604	-10.64	-1.13	-14.64	5.97	-0.85
8509	COc1ncc(n1)Cl	C04228197	-10.64	-1.53	-12.8	3.69	0
8510	COCCn1cc(cn1)N	C11920295	-10.64	-1.61	-13.03	4.11	-0.12
8511	c1cc(cnc1)CCCO	C15884434	-10.64	-1.81	-12.69	4.8	-0.94
8512	C1=C(C(=[N+]=[N-])N=N)1)C(=O)N	C17419165	-10.64	-2.89	-16.9	7.15	2
8513	C1CCC(C1)CCN=C=S	C19090030	-10.64	0.9	-8.66	1.09	-3.97
8514	Cc1ccc(c(n1)N)C(=O)N	C20272877	-10.64	-3.15	-16.5	8.09	0.93
8515	c1ccc(c(c1)CC(=O)NN)F	C22166985	-10.64	-5.98	-13.05	9.83	-1.43
8516	c1ccc2c(c1)[nH]c(n2)Br	C00158652	-10.63	-2.62	-14.23	4.91	1.3
8517	c1nc2c(c(n1)scn2)N	C00337087	-10.63	-1.28	-15.14	6.39	-0.59
8518	COc1cccc(n1)N	C00404286	-10.63	-0.02	-15.31	4.15	0.56
8519	Cc1cc(=O)oc(=O)[nH]1	C00532355	-10.63	-2.93	-16.39	9.98	-1.29
8520	c1cnc(nc1N)C(F)F	C01685214	-10.63	-5.07	-10.03	5.71	-1.24
8521	c1ccc(cc1)Cn2ccnn2	C01756184	-10.63	0.69	-17.58	7.74	-1.48
8522	C[C@@H]1C[C@H]1C(=O)Cl	C01766066	-10.63	-0.9	-11.34	2.35	-0.75
8523	Cc1ncc(s1)OC	C01850481	-10.63	0.99	-14.05	3.87	-1.45
8524	CCOC(=O)C(=C)C#N	C02507893	-10.63	0.3	-14.14	6.28	-3.07
8525	c1cc(c(nc1)Cl)C(F)F	C02584285	-10.63	-2.55	-10.99	4.56	-1.65
8526	CC(=O)NBr	C03874381	-10.63	-2.11	-13.25	5.04	-0.31
8527	c1c(cc(c2c1CCO2)F)F	C04255033	-10.63	-2.25	-8.78	3.77	-3.37
8528	C(C(O)F)F(C(F)F)F	C04266097	-10.63	-4.94	-7.34	1.96	-0.31
8529	C1COC(=O)[C@H]1N=C=S	C04266338	-10.63	-0.21	-14.72	6.34	-2.04
8530	Cc1nnc(s1)N[N+](=O)[O-]	C04476324	-10.63	-5.06	-11.34	7.85	-2.08
8531	C(CS)CO	C04501370	-10.63	-3.56	-11.06	2.26	1.74
8532	C1C[C@@H](OC=C1)C=O	C04529089	-10.63	0.31	-15.81	6.21	-1.35
8533	CC1=CC[C@H](CC1)C=O	C04811480	-10.63	-0.77	-12.34	3.82	-1.34
8534	c1cc2c(nc1)sc(=O)o2	C05331463	-10.63	0.53	-14.86	6.11	-2.41
8535	c1nc2nnc(c(n2n1)[O-])N	C06057109	-10.63	-6.57	-18.24	12.07	2.11
8536	C/1(=N)O)C(=N)O)N=C(C(=O)N1)[O-]	C06382801	-10.63	-5.15	-16.44	8.59	2.36
8537	c1cc(c(c1N)F)C#N)F	C06658048	-10.63	1.03	-16.13	6.6	-2.12
8538	Cc1c(non1)c2ccn[nH]2	C06667833	-10.63	-0.25	-15.29	5.92	-1.01
8539	CNC(=S)n1c(ncn1)N	C08642390	-10.63	-7.18	-7.41	7.34	-3.39
8540	CC(=O)NCC(=O)Cl	C11892187	-10.63	-0.83	-14.21	4.74	-0.33
8541	c1cncc2c1[nH]cc2Cl	C14985673	-10.63	-3.64	-9.5	5.04	-2.52
8542	CCC(=O)[C@H](C)Br	C19843048	-10.63	-1.28	-11.03	4.88	-3.2
8543	c1ccc(cc1)CNCC#N	C19943362	-10.63	-1.83	-12.02	5.95	-2.73
8544	c1cc2c(cc1S)CCO2	C20431100	-10.63	-1.77	-8.21	2.65	-3.3
8545	CC(=O)c1cc(ccc1O)F	C00152766	-10.62	-0.44	-12.76	5.22	-2.63
8546	C[C@@H](C(=O)C)O	C00895238	-10.62	-2.11	-12.37	4.28	-0.41

8547	CCC(=O)C	C00901514	-10.62	-0.99	-11.37	3.85	-2.11
8548	c1c(non1)N)c2c(non2)N	C01063399	-10.62	-0.42	-15.09	4.05	0.84
8549	CC1=CC(=O)N(C1=O)CO	C01740833	-10.62	-4.27	-15.77	7.58	1.84
8550	C=C1CCC[C@@H]1O	C02032076	-10.62	-1.23	-9.51	1.69	-1.58
8551	C[C@@H]1C(=O)NC(O1)(C)C	C02048374	-10.62	-1.02	-14.42	4.23	0.6
8552	CC(C)C(=O)NN/C=C/Cl	C03282531	-10.62	0.14	-13.86	5.29	-2.19
8553	C1C[C@H]([C@H]2[C@H]1C2)O	C05049665	-10.62	-0.85	-10.83	2.15	-1.08
8554	CCOC1ccc(=S)[nH]1	C05576352	-10.62	-0.23	-15.77	4.43	0.95
8555	C(#N)[C@H](F)Br	C08698383	-10.62	-0.01	-12.28	3.7	-2.03
8556	c1cc(ccc1CC(=O)N)F	C09425746	-10.62	-0.95	-15.99	7.84	-1.52
8557	c1c2c(ncn1)N=CNC2	C17158014	-10.62	0.48	-18.58	9.82	-2.34
8558	C/C=C/[C@H]1C=CC(=O)O1	C17299316	-10.62	-1.1	-13.03	7.03	-3.52
8559	C[NH+]1CCN(CC1)C#N	C22002350	-10.62	0.03	-11.21	3.59	-3.03
8560	c1c(n[nH]1)CC#N	C26507092	-10.62	-2.28	-17.35	9.4	-0.4
8561	C(c1c(c(c(c1F)F)F)F)ON	C01564467	-10.61	1.42	-12.56	2.5	-1.97
8562	c1c(cc(c(c1F)NC(=S)NN)F)F	C02528165	-10.61	2.26	-18.66	8.7	-2.9
8563	c1csc(n1)NN	C02555415	-10.61	-3.33	-16.1	4.5	4.31
8564	Cc1[nH]c(nn1)[S-]	C02556115	-10.61	-2.9	-14.77	9.07	-2.01
8565	C1C[C@@H]2CC(=O)C=C2C1	C03122099	-10.61	0.89	-15.14	4.27	-0.62
8566	c1c(nc([nH]c1=O)N)N	C08602956	-10.61	-3.3	-15.94	5.95	2.68
8567	Cc1ccc1CO	C12370518	-10.61	-1.26	-13.94	4.98	-0.39
8568	CCn1cc[nH]c1=S	C12505185	-10.61	-1.18	-11.28	4.76	-2.92
8569	Cc1c(cnn1C)Br	C14988517	-10.61	-0.13	-12.04	4.04	-2.49
8570	c1csc(c1C(F)F)FBr	C15442246	-10.61	-2.43	-6.86	2.48	-3.8
8571	C[C@H](CC(F)F)F)O	C16082633	-10.61	-0.99	-12.2	3.34	-0.76
8572	c1cc2c(c(c1F)O)CC2=O	C16083119	-10.61	0.17	-13.15	5	-2.62
8573	c1[nH]c2c(=O)[nH]c(nc2n1)F	C17174075	-10.61	-3.46	-16.86	10.96	-1.25
8574	c1nc2c(c(n1)NN)nsn2	C17352449	-10.61	-1.56	-15.8	6.79	-0.05
8575	c1c(nc2n1CCS2)CCl	C20272874	-10.61	-1.8	-13.05	8.17	-3.93
8576	Cc1ccsc1Br	C00166959	-10.6	0.16	-12.49	1.8	-0.07
8577	c1cc2c(cc1C(=O)NN)non2	C00171002	-10.6	-4.26	-15.73	9.36	0.02
8578	c1c(ncn1NN)NN	C00967279	-10.6	-3.32	-13.31	5.92	0.11
8579	CNC(=O)c1ccccc1	C01561776	-10.6	-2.5	-14.5	7.04	-0.64
8580	C1C(=O)OC2(O)C=CC(=O)C=C2	C01585857	-10.6	-2.39	-13.05	7.18	-2.35
8581	CCOC(=O)[C@H](C)Cl	C01605305	-10.6	-0.3	-10.21	3.33	-3.42
8582	c1cc(ccc1N)CO)F	C02243178	-10.6	-1	-13.49	3.77	0.12
8583	CCOC(=O)c1cncc1N	C05175382	-10.6	-1.91	-12.46	4.36	-0.59
8584	CCCCN[N+](=O)[O-]	C05309281	-10.6	1.35	-16.59	4.14	0.5
8585	CC[C@H]1CC(=C)C)O	C05922828	-10.6	-2.64	-9.3	1.51	-0.17
8586	C([N-]/C(=N/[N+](=O)[O-])/N)O	C06013662	-10.6	-4.83	-16.13	4.86	5.5
8587	Cn1ccc(n1)C(=O)Cl	C06319681	-10.6	-2.71	-11.74	6.02	-2.17
8588	Cc1ncc(s1)C=O	C13483707	-10.6	-2.74	-12.58	6.5	-1.78
8589	COc1ccccc1O	C13512224	-10.6	0.47	-17.09	8.73	-2.71
8590	c1c(c(cc2c1OC(O2)(F)F)F)N	C15443437	-10.6	-0.33	-12.06	2.97	-1.17
8591	C/C=C(C(=N)N)C)C	C17002836	-10.6	-0.19	-10.94	3.07	-2.54
8592	CCn1cc(nn1)N	C19089904	-10.6	-1.05	-15.53	6.75	-0.77
8593	c1cc(c(nc1)n2ccnc2)N	C20285771	-10.6	-3.74	-11.05	7.31	-3.12
8594	CNC(=O)c1c([nH]cn1)N	C22130313	-10.6	-4.97	-15.6	9.61	0.36
8595	c1ccn(c1)Cc2cccnc2	C00074128	-10.59	-0.57	-10.49	5.14	-4.67
8596	c1cc(nc1CO)Cl	C00169496	-10.59	-2.52	-12.71	4.88	-0.24
8597	C(CC(=O)N)C(=O)N	C01235985	-10.59	-5.61	-15.63	7.03	3.62
8598	CC(=O)NCC#N	C01610226	-10.59	-1.54	-14.92	6.3	-0.43
8599	CC(=O)NCC#C	C01679299	-10.59	-0.37	-14.77	5.44	-0.89
8600	CCCC(=O)OCCO	C01729706	-10.59	-1.53	-13.35	5.31	-1.02
8601	C/C=C(\C)C(=O)N	C01763170	-10.59	-1.35	-14.79	5.64	-0.1
8602	CC(=O)OCCOC	C02041072	-10.59	1.66	-15.58	5.08	-1.75
8603	CSc1nnc(s1)[S-]	C02269606	-10.59	-1.93	-11.87	5.07	-1.87
8604	C=CCSc1nc([nH]n1)N	C02341236	-10.59	-3.78	-15.23	6.01	2.41
8605	CNC(=O)[C@H](F)Br	C02525276	-10.59	-1.15	-13.65	4.86	-0.66
8606	CC(C)Nc1ccc(c1)F	C02540332	-10.59	-1.91	-7.35	2.48	-3.81
8607	CNc1cc(nc(n1)N)F	C02565663	-10.59	-0.28	-17.29	4.65	2.33
8608	C1COC(OC1)CCO	C04748100	-10.59	-2.22	-15.03	4.07	2.59
8609	CCCC/C=C/C#N	C05103575	-10.59	-0.2	-12.94	4.89	-2.34
8610	CCCCNC(=S)[S-]	C05513833	-10.59	-0.05	-14.31	1.66	2.11
8611	c1cnc(nc1)Nc2ccc(cc2)F	C06665763	-10.59	0.86	-10.97	5.11	-5.59
8612	Cc1cc(n/c(=N/C#N)/[nH]1)[O-]	C08732302	-10.59	-0.43	-15.62	9.89	-4.43
8613	c1[nH]c2c([n+](cnc2n1)[O-])N	C12428237	-10.59	-5.12	-16.57	13.07	-1.97
8614	CC(=O)NNC(=O)N	C13404423	-10.59	-4.37	-16.53	6.33	3.98
8615	CS(=O)(=O)n1cc(cn1)Br	C14218543	-10.59	-1.79	-17.1	8.54	-0.25
8616	CC(=O)OCC=C(F)F	C14628854	-10.59	-0.83	-10.59	4.37	-3.54
8617	C1CSCCC1=O	C16046250	-10.59	0.27	-11.57	3.4	-2.7
8618	c1cc2c(=O)[nH]cnc2nc1	C18009656	-10.59	-3.49	-15.13	10.09	-2.06
8619	C#CCSc1cnc(s1)N	C19516851	-10.59	-1.75	-12.88	6.71	-2.66
8620	c1ccc(c(c1F)SCC(=[NH2+]))N	C19848079	-10.59	2.43	-20.68	10.02	-2.36
8621	CCCNc1ncccc1	C20548294	-10.59	-1.28	-10.04	4.43	-3.7
8622	C[C@H](CCS)S	C25695484	-10.59	0.4	-10.14	2.15	-3
8623	C1C=C[C@H]2[C@H]1OC(=O)[C@H]2C=O	C00336459	-10.58	-1.5	-13.14	7.06	-3
8624	CC(=C)C(=O)N	C01608589	-10.58	-2.16	-14.28	5.42	0.44
8625	Cn1c(=O)c(c[nH]c1=O)Br	C01713470	-10.58	-4.55	-13.38	8.36	-1.01
8626	Cc1cnn(c1)CC(=O)Cl	C02521306	-10.58	-3.26	-12.25	7.89	-2.95
8627	C#CCNC(=O)CCl	C02565077	-10.58	-1.15	-14.19	6.23	-1.48
8628	c1cc(c(cc1F)F)NC(=O)C(=O)N	C04858496	-10.58	-7.46	-8.07	4.5	0.46
8629	C1=NNC=NN1	C05133229	-10.58	-2.42	-14.78	5.66	0.96
8630	c1([nH]c(=O)sn1)[S-]	C06523894	-10.58	-4.45	-16.07	6.6	3.34
8631	CCc1cc(om1)CO	C13483628	-10.58	-1.38	-14.28	5.68	-0.6
8632	CC/C(=N)O/C(=O)OCC	C16889901	-10.58	0.26	-13.25	3.69	-1.27
8633	CCOC(=O)c1[nH]cnc(n1)N	C18168376	-10.58	-3.17	-13.32	8.24	-2.32
8634	c1c(cn(n1)CCBr)Cl	C19089276	-10.58	-3.41	-6.82	3.09	-3.45
8635	Cc1c(cn(n1)C)C=O	C20443711	-10.58	-2.17	-11.99	6.59	-3.02
8636	Cc1c(non1)C=O	C20446269	-10.58	-2.44	-15.34	8.39	-1.19

8637	C(=NC(C(F)(F)F)(Cl)Cl)=O	C26438340	-10.58	-0.55	-9.78	0.52	-0.77
8638	c1ccc(cc1O)O=C=O	C00154704	-10.57	-2.96	-15.02	7.32	0.09
8639	c1cn(c(=O)[nH]c1=O)CCC#N	C02325345	-10.57	-3.07	-20.85	13.73	-0.38
8640	c1cc2c(c(c1)F)[C@H](C2)O	C03847715	-10.57	-2.13	-10.67	4.04	-1.81
8641	CSc1ccc(c(c1)O)N	C04773741	-10.57	0.05	-16.89	3.97	2.3
8642	CC[C@H](C(=O)C)S	C04802634	-10.57	-1.25	-9.25	2.55	-2.61
8643	Cc1cc[nH]1CCO	C05386774	-10.57	-3.85	-11.91	4.88	0.3
8644	c1cc(=O)n(cc1C(F)(F)F)O	C05567248	-10.57	-2.66	-10.99	4.89	-1.8
8645	CC[C@H](C#N)Cl	C05924267	-10.57	0.25	-11.45	3.47	-2.83
8646	c1c(ncc(n1)Cl)C(=O)N	C06091417	-10.57	-2.52	-15.19	4.53	2.6
8647	CCOc1cc(cnc1)C=O	C06643312	-10.57	-3.42	-11.78	5.99	-1.36
8648	C(c1nc(nc1)c2c(non2)N)O	C06658068	-10.57	-0.33	-20.44	7.61	2.59
8649	c1ccc(c(c1)C=C[N+](=O)[O-])F	C17001716	-10.57	-1.83	-9.49	5.61	-4.86
8650	CCOC(=O)c1cnoc1O	C18217813	-10.57	-2.12	-11.88	5.03	-1.6
8651	CCNc1cccc(c1)F	C19920945	-10.57	-1.7	-7.45	2.45	-3.87
8652	COC(=O)CNC1cccc1F	C20052505	-10.57	-3.41	-9.11	5.35	-3.38
8653	c1c(ncn1)C(=S)N	C30677885	-10.57	-3.4	-17.32	9	1.15
8654	c1cc(ccc1C#N)OC(F)F	C00167211	-10.56	0.25	-13.35	5.39	-2.84
8655	C1C[C@H]2[C@@H]1C=C2	C01590021	-10.56	-0.32	-6.95	0.48	-3.78
8656	CC(C)CCC#N	C01693282	-10.56	0.15	-11.49	4.29	-3.5
8657	C=CC(=O)c1cccc1	C01702416	-10.56	1.69	-15.87	5.24	-1.61
8658	c1c(c(c(c1F)C=O)F)F	C02534395	-10.56	0.46	-12.09	4.37	-3.3
8659	C[C@H](CC=C=C(C)C)O	C03163363	-10.56	-0.3	-10.43	2.66	-2.49
8660	Cc1c(c[nH]n1)C#N[N+](=O)[O-]	C04878133	-10.56	-3.17	-10.34	4.88	-1.92
8661	C1C=C[C@H]2[C@@H]1[C@@H]2C=O	C05104757	-10.56	0.03	-13.85	4.2	-0.94
8662	C[C@@H]1C(=C(C(=O)O1)[O-])C(=O)C	C05120728	-10.56	-4.76	-13.85	9.82	-1.77
8663	CC[C@H](C(F)F)O	C08698396	-10.56	-1.26	-10.44	1.89	-0.76
8664	c1c(c(c[nH]c1=O)F)C=O	C15444615	-10.56	-3.35	-13.41	5.08	1.13
8665	C[C@@H]1CC[C@@H](O1)C	C17146431	-10.56	0.2	-10.1	1.71	-2.37
8666	C/C(=N/O)/Nc1cccc1	C17991431	-10.56	-1.11	-11.74	4.07	-1.77
8667	c1cc(ccc1F)NCC#N)F	C20045038	-10.56	-3.71	-9.19	5.4	-3.06
8668	C(C=C)Nc1cccc1	W2004A012	-10.56	-0.22	-8.36	1.74	-3.72
8669	c1ccc(cc1)C(=O)NC#N	C00392325	-10.55	-2.32	-11.39	7.87	-4.71
8670	CNC(=O)c1cccnc1	C00404444	-10.55	-1.91	-14.57	6.56	-0.62
8671	CCOCc1cnc(nc1)N	C01670184	-10.55	-1.99	-13.76	3.8	1.4
8672	CCO[C@H](C)C=O	C01680393	-10.55	-0.67	-11.73	3.39	-1.54
8673	CC1=C[F@@]1(=O)CC1OC	C01701241	-10.55	0.97	-14.67	4.95	-1.79
8674	C/C=C/1CCOC1=O	C01752912	-10.55	-1.47	-14.65	6.91	-1.34
8675	CC(=O)c1cnn(c1)C	C02531017	-10.55	1.4	-16.15	6.42	-2.21
8676	c1cc(ccc1F)c2ccno2)F	C02578081	-10.55	0.08	-12.75	4.94	-2.81
8677	C(C(F)(F)F)(C(F)F)F)O-	C03860857	-10.55	-1.58	-11.06	2.43	-0.34
8678	c1c(nc[nH]1)C=O	C04085738	-10.55	-3.12	-15.5	9.34	-1.27
8679	COC(=S)S	C04404464	-10.55	-2.47	-11.33	4.35	-1.09
8680	Cc1nc(c(n1N)N)C(=O)N	C04879118	-10.55	-8.86	-10.33	6.91	1.74
8681	c1nc([nH]n1)CC#N	C05650337	-10.55	-5.53	-12.92	10.19	-2.29
8682	COCCc1nnc(s1)Br	C11920186	-10.55	-2.83	-11.78	4.89	-0.84
8683	CCn1cc(c(n1)[N+](=O)[O-])Cl	C12395851	-10.55	-3.81	-10.95	8.3	-4.09
8684	CCCCON	C14986309	-10.55	-2.56	-9.22	1.93	-0.69
8685	c1(c(c(c(nc1N)F)Br)F	C16159829	-10.55	-3.29	-7.74	2.1	-1.61
8686	C[C@H]1[C@@H]1N=C=O	C19518770	-10.55	-1.05	-10.95	1.89	-0.44
8687	CCOC(=O)c1ccc(cc1)F	C21299997	-10.55	1.53	-12.44	5.05	-4.69
8688	Cn1c(nnn1)CCl	C26466853	-10.55	-1.7	-15.72	8.15	-1.28
8689	c1cc(sc1C=O)[N+](=O)[O-]	C00154896	-10.54	-4.49	-11.68	8.68	-3.04
8690	Cc1cc(n1)CO	C00158682	-10.54	-2.75	-12.59	4.83	-0.03
8691	C[C@H]1CCOCO1	C00388133	-10.54	-0.15	-11.64	2.49	-1.25
8692	CCOC(=O)CSC	C00407006	-10.54	-0.38	-11.81	4.84	-3.2
8693	CCCCO	C01530354	-10.54	-1.83	-10.41	1.87	-0.17
8694	CCCCCO	C01699882	-10.54	-2.6	-8.57	1.88	-1.25
8695	Cc1c(cccc1F)[N+](=O)[O-]	C01706175	-10.54	-0.92	-12.25	4.58	-1.94
8696	Cc1nnc(n1N)SC	C02536944	-10.54	-4.94	-9.3	5.99	-2.29
8697	CCNc1[nH]ncc(=O)n1	C05009506	-10.54	-3.78	-10.86	6.06	-1.95
8698	C(#N)(C(F)F)F	C05019026	-10.54	0.1	-10.31	1.41	-1.74
8699	C/C(=N/O)/CS	C05184170	-10.54	-2.47	-13.09	4.26	0.76
8700	CCC/C=N/NC(=S)N	C05460935	-10.54	1.41	-17.55	4.98	0.61
8701	c1c(c(n[nH]c1=S)S)[S-]	C08649840	-10.54	-2.29	-9.99	3.06	-1.32
8702	Cn1c(cnc1[N+](=O)[O-])C(=O)NN	C13207565	-10.54	-3.31	-14.36	8.95	-1.82
8703	C(=N/O)(C(=S)N)N	C13548708	-10.54	-4.22	-14.56	5.93	2.31
8704	CC(=O)O/N=C(/c1ncon1)N	C13633639	-10.54	-3.89	-20.36	14.18	-0.47
8705	c1c[nH]c(cc1=O)[N+](=O)[O-]	C14982962	-10.54	-4.05	-13.44	8.16	-1.21
8706	C/C(=N/O)C/C(=O)C	C16892202	-10.54	0.98	-12.92	3.07	-1.67
8707	c1cc(cc1)COCCC#N	C19474580	-10.54	-2.03	-12.09	6.63	-3.05
8708	COC(=O)COCCCl	C21990560	-10.54	-0.82	-14.36	7.36	-2.71
8709	c1ccc(cc1)[S@](=O)C=C(Cl)Cl	C26442914	-10.54	2.89	-16.78	7.21	-3.85
8710	c1cc(cnc1)/C(=C/C=O)/[O-]	C26515429	-10.54	0.32	-15.9	7.06	-2.03
8711	CSCc1cccc(c1)N	C32500881	-10.54	-1.09	-9.9	3.69	-3.24
8712	CC(=C)CCC=C)C	G2008A007	-10.54	0.28	-6.56	0.49	-4.74
8713	CCC(=O)c1cccs1	C00159604	-10.53	1.84	-16.08	4.43	-0.73
8714	Cc1cncnc1Br	C00331645	-10.53	-1.86	-11.32	2.6	0.05
8715	CC(=C1C(=O)NC(=O)N1)C	C01581674	-10.53	-2.96	-13.27	5.68	0.01
8716	CCOCc1ccc(c(c1)O)N	C01705932	-10.53	-3.69	-11.01	4.1	0.08
8717	C=NOCCc1c(c(c(c1F)F)F)F	C02556849	-10.53	1.61	-12.32	3.88	-3.7
8718	CC(=O)C1=CNC(=O)CC1	C04267740	-10.53	1.33	-17.22	6.78	-1.42
8719	CCOC(=O)O[C@@H](C)Cl	C04521312	-10.53	-0.21	-10.89	3.88	-3.3
8720	C1COC(=O)[C@H]1Cl	C05134263	-10.53	-0.55	-13.04	5.41	-2.36
8721	C[C@H](c1cccc1)S	C05138833	-10.53	-1.5	-6.22	1.59	-4.4
8722	Cc1nc(cs1)COC	C05943281	-10.53	-2.2	-10.1	3.45	-1.68
8723	Cc1c(c(=O)[nH]cn1)Cl	C08672847	-10.53	-1.11	-13.57	3.81	0.34
8724	c1cn(nc1C(F)F)CCO	C12357744	-10.53	-3.88	-11.6	5.61	-0.66
8725	c1cnc(c1)[N+](=O)[O-]Br	C12969571	-10.53	0.03	-12.1	4.42	-2.88
8726	COCc1ccc(nc1)NN=O	C13213271	-10.53	-3.16	-13.49	6.84	-0.72

8727	c1[nH]c2c(n1)[nH]c(=O)[nH]c2=O	C13517187	-10.53	-2.55	-16.92	8.7	0.24
8728	COc1c(O)ccc1	C16158968	-10.53	-0.94	-12.96	4.37	-1
8729	c1c(O)ccc2c(O)c1	C21813546	-10.53	-1.16	-11.26	4.96	-3.07
8730	CC(C)C(=O)OCCl	C22114223	-10.53	0.44	-11.67	3.95	-3.25
8731	Cc1cc(O)ccc1	M1995A020	-10.53	-0.64	-6.49	1.36	-4.76
8732	C1CCC(=O)CC(=O)C1	C00403358	-10.52	-5.36	-13.63	8.82	-0.36
8733	c1cc(O)c1C(=O)C(=O)NC(=O)N2	C01688442	-10.52	0.33	-17.4	6.68	-0.13
8734	CCOC#C	C01850917	-10.52	-0.76	-11.03	2.9	-1.63
8735	C[C@H](CO)Cl	C02041254	-10.52	-1.55	-10.59	1.77	-0.15
8736	COC1=CC(=O)OC1	C02149451	-10.52	-3.45	-13.03	7.52	-1.56
8737	CC(=O)c1ccc(O)cc1	C02173163	-10.52	-2.55	-10.35	5.28	-2.9
8738	C1COC(O)CBr	C02242713	-10.52	1.2	-13.47	3.11	-1.36
8739	C1=NC(=O)NC(=O)C1=[N+]=[N-]	C04215596	-10.52	-3.67	-19.24	9.32	3.07
8740	CNc1c2cn[nH]c2ncn1	C04353394	-10.52	-1.72	-13.09	6.18	-1.9
8741	C(=S)(C(=S)N)N	C04695122	-10.52	-8.45	-12.81	6.25	4.49
8742	CS1ccc(O)cc1	C15021754	-10.52	-1.07	-13.77	5.56	-1.23
8743	c1ccc(O)c1C#CO	C16053620	-10.52	-0.73	-14.35	6.82	-2.25
8744	CCc1c(O)n(C(=O)[nH]n1)N	C16161121	-10.52	0.85	-16.7	4.7	0.62
8745	c1ccc2=C(C(=O)c2)O	C16929807	-10.52	-3.71	-13.9	7.05	0.04
8746	c1cc(O)c(F)c1C(=O)C	C18899435	-10.52	0.97	-11.94	3.21	-2.76
8747	C[C@H]1[C@H]2NC(=O)C	C19518772	-10.52	-0.57	-11.16	2.15	-0.93
8748	Cc1cc(O)ccc1	C19721279	-10.52	-1.87	-9.94	4.22	-2.93
8749	[C@@H]1(C(=O)C(=O)O)C(Cl)C1	C19864827	-10.52	-0.19	-11.7	4.29	-2.92
8750	C#Cc1c[nH]c(=O)[nH]c1=O	C00005467	-10.51	-2.64	-19.12	10.41	0.84
8751	Cc1ccc(O)c1N(N)C(=O)C	C00152518	-10.51	-1.86	-14.37	7.39	-1.67
8752	c1(cc(O)c1)C1=O	C00896288	-10.51	-0.29	-12.66	4.38	-1.94
8753	C=CCN1C(=O)CNC1=O	C01408334	-10.51	-0.83	-16.13	6.93	-0.48
8754	c1cc2c(O)c1nsn2	C01557822	-10.51	-2.44	-17.52	7.36	2.09
8755	C=C[C@H](C)O	C01572827	-10.51	-1.27	-14.98	6.43	-0.69
8756	c1ccc(O)c1C(=O)N	C04770645	-10.51	-1.17	-14.63	6.93	-1.64
8757	CN(C(=O)N)C(=O)C	C05351574	-10.51	0.25	-16.01	4.18	1.08
8758	c1(=O)[nH]c(O)c1	C05706506	-10.51	-2.42	-14.92	5.01	1.82
8759	c1ccc(O)c1CNC(=O)CS	C08701494	-10.51	-0.22	-15.25	6.56	-1.6
8760	CN1C(=O)[C@H](C(=O)NC1=O)Cl	C15417086	-10.51	-0.29	-14.79	4.58	-0.01
8761	Cc1ccc(O)c1	C16697993	-10.51	-2.17	-16.51	6.78	1.4
8762	COCC1ccc(O)cc1	C19255060	-10.51	-0.31	-11.5	3.38	-2.09
8763	C[C@H](C#N)NCC=C	C20177396	-10.51	0.31	-13.68	4.44	-1.58
8764	Cc1ccc(O)c1	C20443741	-10.51	-1.79	-14.6	5.71	0.18
8765	c1ccc(O)c1N	C20548919	-10.51	-2.98	-14.19	7.08	-0.42
8766	Cc1ccc(O)c1	C28531853	-10.51	-3.87	-13.54	9.85	-2.94
8767	Cc1ccc(O)c1	C00058199	-10.5	-2.08	-11.09	4.67	-2
8768	C=C1[C@H](C)C(=O)C#N	C01571997	-10.5	-1.14	-13.88	6.66	-2.13
8769	COCC(C)C	C01845918	-10.5	-0.2	-8.56	1.1	-2.84
8770	C[C@H](C(=O)C)O	C02048535	-10.5	-0.52	-12.55	2.2	0.36
8771	CCCN1ccc(O)cc1	C02537951	-10.5	0.11	-13.35	4.99	-2.24
8772	CCN1ccc(O)cc1	C02559424	-10.5	-2.82	-14.69	9.3	-2.29
8773	c1(cc(O)c1)N	C04018140	-10.5	-2.92	-17.38	6.47	3.34
8774	C(CSCCS)S	C04362785	-10.5	-1.68	-6.41	1.08	-3.49
8775	C[C@H]1C(=O)NN=CN1	C05369229	-10.5	-3.15	-16.21	6.88	1.99
8776	c1cc(O)c1S(=O)(=O)O	C06467618	-10.5	-3.98	-19.27	8.6	4.15
8777	C[C@H](c1ccc(O)cc1)O	C06733580	-10.5	-3.02	-11.08	3.67	-0.07
8778	Cc1ccc(O)cc1	C12360060	-10.5	0.82	-11.49	3.42	-3.25
8779	c1[nH]c(O)c(c1)[O-]	C16886470	-10.5	-2.02	-17.44	5.15	3.81
8780	c1ccc(O)c1N	C17130304	-10.5	0.22	-13.35	5.42	-2.79
8781	CC(=O)C(=O)C	C18011157	-10.5	0.4	-11.17	3.87	-3.6
8782	c1ccc(O)c1O	C18887898	-10.5	-2.76	-11.54	4.35	-0.55
8783	c1cc(O)c1C	C19730642	-10.5	-1.97	-12.96	5.88	-1.46
8784	C1CCC2c(O)c1	C22126212	-10.5	-2.19	-10.32	5.33	-3.32
8785	c1ccc2c(O)c1	C26515438	-10.5	-1.25	-6.34	1.95	-4.86
8786	C1CN[C@H](CN1)C#N	C26898490	-10.5	-1.85	-14.76	5.01	1.1
8787	Cc1ccc(O)c1	C00401676	-10.49	-3.79	-11.84	5.55	-0.41
8788	CC(=O)Cn1c(O)[nH]c1=O	C01084291	-10.49	0.58	-18.76	10.94	-3.25
8789	C(CCO)CO	C01599375	-10.49	-3.68	-12.19	3.22	2.16
8790	Cc1ccc2ncnc2c1	C01683867	-10.49	-3.75	-14.02	9.64	-2.35
8791	c1ccc2c(O)[nH]c(O)c2	C01703681	-10.49	-2.46	-14.37	6.5	-0.16
8792	C[C@H]1C=CC(=O)C1=O	C01706889	-10.49	-2.04	-13.96	7.59	-2.08
8793	CC(=O)CCOC(=O)C	C01719223	-10.49	-1.3	-14.65	8.27	-2.82
8794	CC(=O)CCOC(=O)N	C01731398	-10.49	-0.83	-15.96	4.91	1.39
8795	CCCN1c(O)[nH]c(O)c1	C01757772	-10.49	0.65	-16.16	5.49	-0.47
8796	CC[C@H](C)CO	C02041128	-10.49	-1.45	-9.42	1.64	-1.27
8797	c1ccc(O)c1C(=O)C	C02559042	-10.49	-3.06	-15.44	9.23	-1.22
8798	CCOC(=O)OCCl	C02559058	-10.49	0.86	-12.04	4.03	-3.34
8799	COc1ccc(O)c1	C04344107	-10.49	-0.31	-13.85	3.77	-0.11
8800	CC[C@H](C(=O)C)Cl	C05227373	-10.49	-0.93	-10.66	1.92	-0.82
8801	c1ccc(O)c1CNC(=O)C(F)F	C06334837	-10.49	-4.02	-7.63	3.44	-2.27
8802	CC(=O)CSc1[nH]c1	C08334467	-10.49	-2.54	-13.25	8.35	-3.05
8803	c1[nH]c(O)c(O)c1	C08615382	-10.49	-2.53	-18.71	7.13	3.62
8804	c1[nH]c(O)c2c(O)c1	C13543038	-10.49	-6.35	-17.08	8.2	4.74
8805	Cc1ccc(O)c1	C14985731	-10.49	-4.83	-8.19	3.47	-0.94
8806	c1cc(O)c(F)cc1NC(=S)N	C16125760	-10.49	-1.95	-17.45	11.48	-2.58
8807	CC(=O)C(=O)C	C17157292	-10.49	-2.16	-11.12	4.18	-1.39
8808	c1ccc(O)c1	C19045764	-10.49	-0.94	-10.82	4.74	-3.48
8809	c1ccc(O)c1	C19689129	-10.49	1.33	-17.43	9.42	-3.81
8810	CC1(C)C@H(C)C1	C20357970	-10.49	0.11	-9.46	2.37	-3.51
8811	Cc1ccc(O)c1	C20443719	-10.49	-2.66	-14.29	6.43	0.03
8812	c1ccc(O)c1	C20534453	-10.49	-3.78	-14.36	8.65	-1
8813	CC(C)C=C(=O)O	C21304287	-10.49	0.53	-11.46	4.28	-3.83
8814	CC(C)c1ccc(O)c1	C32005426	-10.49	1.85	-13.09	4.07	-3.32
8815	COC(=O)c1ccc(O)c1	C00082364	-10.48	-2.9	-10.05	4.08	-1.61
8816	COCC2(O)C#C	C01564788	-10.48	-1.62	-12.81	5.88	-1.94

8817	CC(C)CCCO	C01592388	-10.48	-3.08	-8.18	1.83	-1.04
8818	C=CC(CC=C)O	C01632707	-10.48	-1.01	-9.32	1.7	-1.86
8819	CC[C@H](C#C)O	C01690299	-10.48	-0.94	-10.93	2.14	-0.74
8820	CCCC#CCO	C01845729	-10.48	-1.84	-11.58	4.11	-1.17
8821	CC(=O)Nn1cncn1	C02037314	-10.48	-1.95	-18.7	10.78	-0.61
8822	C1CCC(CC1)OC(=O)Cl	C02243070	-10.48	0.31	-8.48	1.8	-4.12
8823	Cc1ccc(c(c1)F)CO	C02243230	-10.48	-1.75	-9.8	3.05	-1.98
8824	C[C@H]1C(=O)N(C(=S)S1)N	C02798507	-10.48	0.03	-14.52	5.49	-1.48
8825	C1CCOC1	C03593622	-10.48	-0.34	-10.49	1.58	-1.24
8826	CC[C@H](C)SC#N	C04290565	-10.48	0.04	-10.19	2.86	-3.19
8827	C1C=C[C@H](C)C(F)(F)F	C05004377	-10.48	-0.43	-10.09	1.54	-1.5
8828	c1ccc(cc1)F)NC(=O)NN	C05226052	-10.48	-1.43	-16.85	8.49	-0.68
8829	Cc1cccn1CC=C	C05885712	-10.48	-1.35	-9.9	2.73	-1.96
8830	c1ccc(c(c1)c2[nH]c(nn2)N)O	C12404747	-10.48	-1.48	-16.64	9.61	-1.96
8831	c1[nH]c(c(n1)C(F)(F)F)C(F)(F)F	C13283503	-10.48	-2.19	-11.69	6.35	-2.95
8832	Cc1c(nc(s1)N)N(=O)[O-][N+](=O)[O-]	C15783911	-10.48	-2.43	-13.89	10.4	-4.55
8833	C=C(C=O)C=O	C17060229	-10.48	-1.86	-13.99	6.52	-1.15
8834	C1CCC(=N)C(=S)N)C1	C17730060	-10.48	2.62	-18.06	7.56	-2.59
8835	c1cc(ncc1C(F)(F)F)CO	C22200556	-10.48	-4.08	-10.19	4.49	-0.69
8836	c1cnoc1CO	C26547716	-10.48	-4.48	-13.06	6.56	0.49
8837	Cc1nccc(n1)N	C00333686	-10.47	-1.42	-14.91	4.42	1.44
8838	CCNc1c(cncn1)N	C01592097	-10.47	-5.94	-11.39	4.62	2.25
8839	c1ccc(cc1)C2=CCC(=O)O2	C01723799	-10.47	-1.01	-14.23	6.79	-2.03
8840	CCCCSSC	C02038818	-10.47	-0.49	-10.48	1.62	-1.12
8841	Cc1n[nH]c(c=s)n1C	C02566750	-10.47	-2.58	-12.71	7.44	-2.62
8842	c1nncn1N=C(C)C(F)(F)F)O	C03164721	-10.47	-3.02	-13.34	8.14	-2.25
8843	c1cc(c([nH+]c1)CSC(=[NH2+])N)O	C03877581	-10.47	-1.51	-15.59	5.87	0.76
8844	c1cc(=S)[nH]cc1Cl	C05426296	-10.47	-3.76	-15.3	11.68	-3.09
8845	COC(=O)n1cccn1	C05526484	-10.47	0.17	-15.38	6.21	-1.47
8846	CCO[C@H]1OCCS1	C05718331	-10.47	-0.6	-13.94	3.37	0.7
8847	Cc1ccnc(c1)C	C08294954	-10.47	-1.16	-9.27	3.08	-3.12
8848	c1c(c[nH]c(c=O)c1[N+](=O)[O-])Br	C08698072	-10.47	-2.57	-11.93	4.62	-0.59
8849	c1cnc(c(c1O)N)N(=O)[O-]O	C12360011	-10.47	-3.45	-18.02	8.42	2.57
8850	c1cc(ncc1CC#N)Br	C15042693	-10.47	-2.9	-12.89	8.66	-3.35
8851	Cc1cnc(nc1)Cl	C19091751	-10.47	0.68	-11.94	3.6	-2.81
8852	CNc1[nH]c(c=s)[nH]n1	C19476926	-10.47	-4.55	-14.85	11.45	-2.52
8853	CC(=O)c1ccc(c(c1)F)F	C00152902	-10.46	-1.46	-13.97	7.3	-2.33
8854	c1ccc2c(c1)NCS2	C00397013	-10.46	-1.59	-9.83	3.54	-2.58
8855	c1(c(nsc1)Cl)C(=O)N)Cl	C00978058	-10.46	-2.86	-12.21	4.46	0.15
8856	CCCC=O	C01529195	-10.46	-0.4	-11.7	3.62	-1.98
8857	C1[C@H]2C=C[C@H]2CC1=O	C01570420	-10.46	-1.05	-9.14	3.03	-3.29
8858	c1c(=O)[nH]c(c=O)n(n1)C/C=C/O	C01647361	-10.46	-0.75	-19.51	6.97	2.84
8859	CCOC(=S)SC	C01665538	-10.46	-0.78	-10.91	3.89	-2.66
8860	C=C(C)C(C)C(F)(F)F)Br	C01673696	-10.46	2.63	-14.7	3.36	-1.75
8861	CC(=O)O[C@H]1CC(=O)OC1	C04283640	-10.46	1.1	-15.51	6.68	-2.73
8862	c1cc2nncn2nc1NN	C04785566	-10.46	-5.57	-13.68	10.63	-1.85
8863	Cc1c(=O)nc([nH]n1)NC	C05009525	-10.46	-4.88	-11.38	6.87	-1.07
8864	Cc1c(c([nH]n1)C(F)(F)F)Cl	C08996181	-10.46	-1.38	-9.08	2.32	-2.32
8865	c1c[nH]c2c1[nH]cnc2=O	C12504135	-10.46	-2.48	-18.21	11.21	-0.98
8866	c1(nc(nc(n1)N)N)N(=O)[N-]N(=[N+]=[N-])N	C13763906	-10.46	-2.5	-10.15	3.09	-0.9
8867	Cc1ccc(cc1)n2c(nnn2)N	C16953783	-10.46	-0.25	-15.55	9.08	-3.75
8868	Cc1nc(nn1)C)N	C17024971	-10.46	-1.77	-13.31	7.01	-2.38
8869	c1cc(nc(c1)N)C(F)(F)F	C19616464	-10.46	-4.97	-9.1	5.42	-1.81
8870	C#CCN[C@@H]1CCSC1	C19875380	-10.46	0.98	-11.82	2.87	-2.49
8871	C1[C@H](C)C1(C)Cl)C(=O)Cl	C20357969	-10.46	-0.65	-9.36	2.84	-3.29
8872	c1cc(ccc1CO)O	C21994423	-10.46	1.25	-18.43	6.26	0.46
8873	Cc1nccc(n1C)N(=O)[O-]	C00001307	-10.45	-3.51	-8.76	5.9	-4.09
8874	Cc1c(nnc(n1)N)C	C00154796	-10.45	-2.51	-12.59	6.19	-1.54
8875	c1c(csc1CO)Br	C00159064	-10.45	-3.05	-9.49	3.24	-1.15
8876	Cc1ccc(cc1N=C=O)F	C00164861	-10.45	-0.68	-10.4	2.41	-1.78
8877	C1COCCN1C#N	C00407026	-10.45	-0.01	-11.34	4.08	-3.18
8878	COC(=O)/C=C/N)C(=O)N	C01604054	-10.45	-2.67	-16.83	7.38	1.68
8879	Cn1c2c(cncn2)cn1	C01718409	-10.45	-2.51	-11.13	6.14	-2.96
8880	Cc1ccc(o1)CC=O	C01762800	-10.45	-1.72	-11.35	6.16	-3.54
8881	C[C@H](C)C(C)Cl)O	C01762873	-10.45	-0.82	-10.12	1.36	-0.87
8882	CCCON	C02388227	-10.45	-1.92	-10.05	1.83	-0.31
8883	C[C@H](CCC(=O)C)O	C02526567	-10.45	1.3	-15.98	3.73	0.51
8884	CC1CCC(=O)CC1	C03861284	-10.45	-0.88	-9.58	3.32	-3.32
8885	Cc1cnc(n1)C)Br	C04352757	-10.45	-1.04	-11.08	4.82	-3.15
8886	C/C(=N)NC(=O)N)C(F)(F)F	C04897004	-10.45	-1.71	-14.1	4.82	0.53
8887	C(CC#N)CN=N)N(=O)[O-]	C04984167	-10.45	-1.71	-14.41	6.99	-1.33
8888	C(OC(F)(F)F)F	C05178907	-10.45	-1.72	-10.74	2.85	-0.84
8889	Cc1c(nc(nn1)S)O	C11914473	-10.45	-4.36	-13.35	5.41	1.85
8890	Cn1c(cnc1[N+](=O)[O-])C(=O)OC	C13282292	-10.45	-0.72	-10.06	5.49	-5.17
8891	CC(C)N)H2+CC(F)(F)F	C19263191	-10.45	-0.15	-10.22	1.67	-1.74
8892	CNc1ccc(cn1)C#N	C19487183	-10.45	-1.47	-12.05	5.17	-2.09
8893	#CCOCc1ccc(cc1)Br	C19510323	-10.45	0.76	-10.47	3.74	-4.5
8894	c1cc([nH]c1)CO	C22011165	-10.45	-4.24	-13.25	6.82	0.23
8895	c1cc2c(cc1C)nn[nH]2	C32600123	-10.45	-2.46	-13.35	7.51	-2.16
8896	CCCCc1ccccc1	M1995A047	-10.45	-0.64	-5.33	1.17	-5.65
8897	Cc1c([nH]c(=O)[nH]c1=O	C00157062	-10.44	-4.5	-15.93	9.68	0.31
8898	c1ccc(cc1)C[C@@H](C2c2c(nnn2)N)O	C00368799	-10.44	-1.17	-17.18	8.53	-0.63
8899	Cc1c(cc(cc1O)O)O	C00394377	-10.44	-2.45	-15.15	4.79	2.37
8900	c1cc(ccc1)F)C(=O)N	C00406944	-10.44	-2.31	-12.73	5.51	-0.92
8901	CC(=O)CCCCI	C01586735	-10.44	-0.53	-12	5.22	-3.13
8902	C(=O)c1c(c(c(c1F)F)F)F	C01627094	-10.44	-2.08	-8.25	3.73	-3.84
8903	CCN(C)N(=[N+]=[O-])O	C01668618	-10.44	-1.43	-12.24	5.92	-2.69
8904	C(CO)CBr	C02031639	-10.44	-2.46	-10.61	2.75	-0.12
8905	CO[C@H](C(F)F)O	C02040621	-10.44	-1.87	-11.27	2.43	0.27
8906	COC(=O)CSCC#N	C02169247	-10.44	-1.68	-12.93	7.73	-3.56

8907	c1nc([nH]n1)/N=C(/CC1)[O-]	C03099659	-10.44	-0.69	-18.81	9.11	-0.04
8908	Cc1nc(cs1)C#N	C03190898	-10.44	-2.39	-13.56	8.2	-2.69
8909	CC(=O)CC(=O)n1cncn1	C03203246	-10.44	-3.77	-13.28	8.46	-1.85
8910	C=C=OCCCO	C05377559	-10.44	-1.41	-13.42	3.77	0.63
8911	C1CC(=O)O[C@H]1CCl	C05413209	-10.44	-0.68	-16.37	7.5	-0.89
8912	C1CCNC(=O)[C@H](C1)Cl	C05566898	-10.44	2.22	-15.36	4.02	-1.32
8913	CO[C@H]1C=O	C05734707	-10.44	-1.59	-14.34	3.5	1.99
8914	c1cc(ccc1C(=S)N)Cl	C05839325	-10.44	-1.69	-14.27	8.67	-3.15
8915	CNC(=S)NCC(=O)C(F)F	C07058659	-10.44	-0.05	-18.34	9.22	-1.27
8916	C1CCNC(=O)[C@H](C1)Br	C09256648	-10.44	2.39	-15.43	3.98	-1.38
8917	CCOc1ccc(c1F)[N+](=O)[O-]	C12471368	-10.44	-1.5	-10.67	5.79	-4.06
8918	c1cc(ccc1NC(=S)NN)Cl	C13684747	-10.44	-1.06	-9.8	3.13	-2.71
8919	c1c(cc(c2c1[nH]nc2O)F)F	C14983968	-10.44	-1.99	-14	4.64	0.9
8920	C/C(=[NH+]/N)/N	C16082795	-10.44	-2.72	-11.83	3.5	0.62
8921	C(CC)OCC(F)F	C16158943	-10.44	-1.78	-10.51	4.36	-2.51
8922	CCc1c(non1)N	C16752464	-10.44	-2.84	-14.41	7.58	-0.78
8923	COc1nc(non1)C=O	C16944199	-10.44	-2.87	-15.41	7.24	0.59
8924	c1ccnc(c1)CNCC(F)F	C19481082	-10.44	-1.24	-12.16	5.07	-2.1
8925	COc(=O)[C@H](CF)Br	C19735921	-10.44	-0.93	-10.09	3.43	-2.84
8926	c1ccc2c(c1)ncn2O	C25559332	-10.44	-4.26	-13.46	9.64	-2.36
8927	c1c(nc(c1Br)Cl)C#N	C29753708	-10.44	-1.49	-9.18	3.34	-3.1
8928	c1ccc2c(c1)nnn2Cl	C01731575	-10.43	2.03	-14.83	4.97	-2.6
8929	c1ccc2c(c1)ccs2=O	C01735943	-10.43	-2.53	-13.57	8.13	-2.47
8930	c1[nH]c2c(n1)c(ncn2)NN	C02383126	-10.43	-0.68	-15.81	7.68	-1.61
8931	C[C@H](CC#C)O	C02504416	-10.43	-1.3	-11.7	3.16	-0.6
8932	Cc1c(ccc1)C#N	C02537519	-10.43	-0.54	-13.32	6.13	-2.7
8933	Cc1c(ccc1Cl)F	C02540184	-10.43	-0.84	-11.15	2.49	-0.94
8934	c1cc(oc1)Cn2c(ccn2)N	C03426796	-10.43	0.49	-15.63	7.09	-2.38
8935	c1ccc2c(nc1)nc(o2)Cl	C03880831	-10.43	-1.96	-15.52	8.85	-1.81
8936	c1ccc(sc1)/C=N/N(=O)N	C04538806	-10.43	0.12	-19.13	8.67	-0.09
8937	C=C/C=N/NC(=O)N	C06261988	-10.43	-3.96	-14.9	6.06	2.36
8938	CC1c(ccc1F)Br	C15443750	-10.43	-1.12	-9.93	3.41	-2.79
8939	c1cc(ccc1Cl)Nc2nc([nH]n2)N	C15924287	-10.43	0.71	-13.12	7.2	-5.21
8940	C1CN=[C@H]1C(=O)C=[N+]=[N-]	C17375770	-10.43	-0.48	-20.23	8.39	1.89
8941	c1ccc2c(nc1)nc(o2)N	C20136404	-10.43	-4.2	-17.62	10.45	0.93
8942	Cn1c(=O)[nH]nc1OC	C22013429	-10.43	-2.81	-14.99	6.23	1.14
8943	C1CCC(=C(C1)[N+](=O)[O-])O	C25695929	-10.43	0.57	-14.07	6.42	-3.35
8944	CCOC(=O)N(C)OC	C00389791	-10.42	-1.5	-11.97	4.57	-1.53
8945	c1c(nc(=O)[nH]c1F)N	C00967447	-10.42	-4.62	-16.29	8.82	1.67
8946	C1(=NC(=O)N=C1[NH-])(C(=O)N	C01723627	-10.42	-3.05	-20.15	7.61	5.17
8947	COc(=O)C=O	C01845566	-10.42	-2.86	-12.66	7.08	-1.99
8948	CC(C)CC(=O)Cl	C02015931	-10.42	-0.65	-11.03	2.5	-1.23
8949	c1nnc(o1)OCC#N	C02381232	-10.42	-3.4	-17.31	7.59	2.7
8950	c1cc2c(cc1F)sc(n2)Cl	C02455703	-10.42	-1.29	-11.48	2.43	-0.08
8951	Cc1ccc(o1)CCC=C	C02518858	-10.42	-1.18	-9.53	2.49	-2.2
8952	c1cc(ccc1F)CNC(=O)NF	C03631554	-10.42	0.94	-21.34	10.4	-0.42
8953	c1cc(ccc1/C(=C/C(=O)[O-])F	C03887805	-10.42	-4.49	-10.43	6.47	-1.97
8954	C1C=CC=CCC1O	C05004691	-10.42	-0.83	-12.56	1.93	1.04
8955	CC[C@H](C#CC)O	C05227164	-10.42	0.23	-11.63	2.56	-1.59
8956	CN1C(=O)CNC1=O	C05965961	-10.42	-2.88	-15.35	7.04	0.77
8957	COC(=S)Nc1ccccc1	C06379025	-10.42	0.88	-16.46	7.67	-2.5
8958	COCCNc1[nH]ncn1	C08206217	-10.42	-0.98	-16.91	5.54	1.92
8959	C[C@H](Cc1ncnc1)O	C12397659	-10.42	-4.08	-11.44	4.86	0.25
8960	CC(=O)Oc1ccc[nH]c1=O	C17000747	-10.42	-0.52	-18.95	9.4	-0.34
8961	[H]/N=C(C(F)(F)F)OCC(F)F	C17005395	-10.42	-2.83	-10.4	3.17	-0.35
8962	COCc1nc(on1)CCl	C21953353	-10.42	-1.32	-12.87	4.72	-0.95
8963	CC(=O)c1ccc(s1)Br	C00096540	-10.41	-0.43	-13.24	3.19	0.07
8964	Cc1cncc1C#N	C00330972	-10.41	-2.1	-10	4.33	-2.64
8965	CC(=O)Nc1ncccn1	C00397441	-10.41	-2.92	-13.93	9.14	-2.7
8966	Cc1cncc1CO	C01435953	-10.41	-1.82	-12.87	4.74	-0.45
8967	Cc1nnc2n1ncs2	C01657455	-10.41	-1.08	-17.19	10.41	-2.54
8968	c1c(c(=O)[nH]c(=O)[nH]1)C(F)F	C01713949	-10.41	-5.35	-14.12	8.93	0.13
8969	C[C@H]1(CO1)C=C	C02044857	-10.41	-0.4	-11.53	2.84	-1.32
8970	c1cc(ccc1O)[N+](=O)[O-]	C02525422	-10.41	-4.75	-12.27	8.37	-1.76
8971	c1coc(n1)C=O	C02530178	-10.41	-2.42	-16.05	7.98	0.08
8972	C1COc(=O)[C@H]1Br	C03860233	-10.41	-1.52	-11.94	5.55	-2.5
8973	[H]/N=C(C(=O)N)OC=C(C)C	C05187801	-10.41	-1.98	-17.27	7.23	1.6
8974	CC(=O)CSc1nnn1C	C05480863	-10.41	-0.39	-16.25	7.55	-1.33
8975	CCNC(=S)[S-]	C05650405	-10.41	-2.08	-12.09	1.75	2.01
8976	c1ccc2c(c1)[nH]c(n2)CB	C13284914	-10.41	-3.68	-8.99	5.94	-3.67
8977	C[C@H](COC(F)F)O	C16159291	-10.41	-2.41	-11.17	2.82	0.35
8978	c1cc(c(nc1)/C=N/O)O	C17355132	-10.41	-1.85	-17.02	7.11	1.35
8979	c1cc(nc(c1N)N)C(F)F	C26461755	-10.41	-6.83	-10.68	7.42	-0.33
8980	Cc1ccc(c(c1)N)OCC=C	C32006204	-10.41	-2.32	-8.2	3.21	-3.1
8981	c1ccc(cc1Cl)OCC(F)F	C00153363	-10.4	-1.98	-8.55	2.19	-2.07
8982	COc1ccc(c1)N	C00157624	-10.4	-1.61	-9.96	3.15	-1.99
8983	Cc1cncc([nH]c1=O)CS	C00330944	-10.4	-2.92	-12.76	7.21	-1.93
8984	C/C(=N/N)/C(=C)NN	C01570042	-10.4	-0.85	-13.36	3.01	0.8
8985	c1ccc(c(c1N)O)O	C01598464	-10.4	-3.51	-15.89	5.59	3.42
8986	C(C(C#N)(Cl)Cl)Cl	C01641016	-10.4	0.47	-10.25	2.44	-3.06
8987	C[C@H](C(F)(F)F)O	C02040700	-10.4	-1.95	-10.62	2.21	-0.03
8988	C(CP)C#N	C02560453	-10.4	-2.01	-10.57	4.06	-1.86
8989	C[C@H](C(C(F)F)F)O	C02584331	-10.4	-0.8	-10.66	1.95	-0.88
8990	C1CSC(=O)NC1=O	C03102095	-10.4	0.78	-17.94	6.63	0.12
8991	C1COCC[C@H]1C=O	C04979101	-10.4	-1.24	-12.91	4.66	-0.92
8992	CC1=NOC(=O)C12CC2	C05080409	-10.4	-0.36	-13.71	7.05	-3.38
8993	CCSCC#N	C19870242	-10.4	0.47	-12.61	5.28	-3.55
8994	COc1nc(on1)CCl	C21953090	-10.4	0.01	-15.81	5.88	-0.47
8995	Cc1nc(on1)N	C32625168	-10.4	-4.57	-13.77	6.65	1.3
8996	c1cc(oc1)C(=O)NN	C00153131	-10.39	-1.42	-15.94	6.65	0.33

8997	COC(=O)Cc1ccc(cc1)C#N	C00257225	-10.39	-1.59	-10.19	5.84	-4.45
8998	CCc1c(cc(=O)[nH]c1=O)N	C00401339	-10.39	-4.53	-14.75	9.6	-0.71
8999	c1c2c(cs1)OCCO2	C00403256	-10.39	-1.16	-13.39	3.49	0.66
9000	C=C1COOC(=C)CO1	C01684621	-10.39	-1.2	-11.26	3.11	-1.05
9001	Cc1ccnc(n1)SC#N	C01698027	-10.39	-0.69	-14.7	5.88	-0.87
9002	CN(C)C(=S)[O-]	C02557686	-10.39	-0.86	-14.02	4.33	0.16
9003	CC/C=C/C[C@H](C)O	C04283840	-10.39	-3.14	-7.1	1.7	-1.86
9004	Cc1[nH]c(c(n1)Cl)[N+](=O)[O-]	C04632347	-10.39	-2.48	-10.58	5.95	-3.28
9005	C/C=C/C=O	C04726476	-10.39	-1.16	-12.38	4.43	-1.28
9006	c1(c(nH)n1)BrBr	C04771904	-10.39	-0.72	-14.91	3.35	1.89
9007	c1ccc(cc1)S(=O)=O	C06581647	-10.39	-2.04	-15.14	7.36	-0.56
9008	c1c(c([nH]n1)N)C(=S)N	C06658020	-10.39	-5.71	-14.12	8.65	0.78
9009	c1c[nH]c(=O)cc1[O-]	C08637458	-10.39	-2.86	-15.87	5.19	3.15
9010	c1cc(c(cc1O)OC(F)F)F	C12359285	-10.39	0.85	-13.86	3.88	-1.24
9011	[C@H](C(F)F)F(OC(F)F)Cl)Cl	C14628421	-10.39	-0.59	-8.71	1.22	-2.31
9012	c1cc(oc1)/C=N/NC(=O)N	C17146950	-10.39	-0.59	-19.14	8.88	0.46
9013	C1CS[C@H](N1)C(F)F	C19441091	-10.39	-1.38	-10.55	2.65	-1.11
9014	c1cc(ccc1C(=O)N=[N+]=[N-])Cl	C19872840	-10.39	0.7	-13.06	2.73	-0.77
9015	c1cc(c(c1N)CO)F	C21985431	-10.39	-4.05	-14.85	8.24	0.27
9016	c1cncoc1NC=O	C23993715	-10.39	-2.61	-16.38	9.27	-0.66
9017	#CCc1c2ccccc2nn1	C00135742	-10.38	1.55	-15.97	7.49	-3.46
9018	c1c(c(n1)CC#N)I	C01432444	-10.38	-0.23	-15.93	8.9	-3.12
9019	C=CCNC(=O)C=C	C01577262	-10.38	-0.64	-13.67	5.31	-1.38
9020	CCCCC#N	C01587817	-10.38	-1.77	-9.41	4.51	-3.7
9021	CC(=O)CCc1ccccc1O	C01672065	-10.38	-1.77	-13.4	4.89	-0.1
9022	c1ccc(cc1)C(=O)C(F)F	C01708231	-10.38	0.89	-13.91	4.82	-2.18
9023	c1cc(ccc1C(=O)C=O)O	C01728403	-10.38	0.97	-19.62	9.96	-1.69
9024	[C@H]1CC[C@@H](C1)O	C02242640	-10.38	-1.53	-9.61	1.71	-0.96
9025	c1cc(c(cc1C=O)OC(F)F)	C02532881	-10.38	-1.76	-15.59	8.21	-1.24
9026	Cc1c(c(nHn1)C)N=O	C04644856	-10.38	-0.06	-15.26	5.71	-0.76
9027	CNC(=S)C#N	C05187276	-10.38	-1.94	-11.66	2.75	0.47
9028	CCOC(=O)/C(=N[O-])C(=O)C	C12345800	-10.38	-1.71	-14.87	8.14	-1.94
9029	CC(=O)NC1=NC(=O)CS1	C12364192	-10.38	1.79	-19.02	7.09	-0.25
9030	c1cc(c(cc1N)Cl)SC#N	C16385315	-10.38	-1.54	-9.67	3.33	-2.51
9031	C1CCN(C1)CC#N	C19488582	-10.38	-0.94	-12.57	4.5	-1.36
9032	CSCCC#N	C20232204	-10.38	0.77	-12.28	4.1	-2.96
9033	c1nc(n1)C=O	C20443641	-10.38	-3.32	-15.5	7.98	0.47
9034	c1cc(c(cc1F)[C@H]2CO2)F	C22215711	-10.38	0.41	-11.48	3.43	-2.75
9035	c1cc2c(c[nH]c2nc1)C(F)F	C32914955	-10.38	-5.45	-7.97	6.57	-3.53
9036	c1ccc(c(c1)[C@@H](CO)O)Cl	C00403281	-10.37	-5.52	-9.72	4.93	-0.06
9037	CCSc1ccccc1	C01671802	-10.37	-1.7	-11.8	3.34	-0.22
9038	COC(=O)OC	C01699944	-10.37	-0.85	-11.91	3.82	-1.44
9039	C1CCC(C1)NC=O	C01702555	-10.37	-1.34	-13.29	5.75	-1.49
9040	c1cc(c(cc1Cl)F)N=C=O	C02509914	-10.37	1.56	-13.06	2.31	-1.19
9041	COC(=O)/C=C/C(=O)OC	C03843378	-10.37	0.31	-12.59	4.54	-2.63
9042	CCOC(=O)c1ccccc1N	C03861699	-10.37	-1.65	-9.25	3.81	-3.29
9043	C=CCOC1ccccc1N	C04124227	-10.37	-1.27	-11.85	2.66	0.1
9044	C/C=C/C=N/NC(=O)N	C04782860	-10.37	-2.49	-15.06	6.69	0.49
9045	C(C(C(F)F)F)F(O)O	C05178437	-10.37	-5.39	-9.61	3.26	1.38
9046	C1C[C@@H](C1)OC1CS	C05282940	-10.37	0.17	-13.86	2.55	0.78
9047	CCc1ccc(o1)C=O	C06678069	-10.37	-1.85	-10.72	4.02	-1.82
9048	CCc1nc(on1)[C@H](C)Cl	C12505710	-10.37	-0.25	-11.25	3.55	-2.42
9049	CCOC(=O)[C@H](C#C)O	C12955464	-10.37	-2.11	-11.33	4.47	-1.39
9050	Cc1cc(ncc1Br)F	C16159658	-10.37	-0.82	-9.49	2.77	-2.83
9051	c1cc2c(c(c1)F)CC[C@H]2O	C19727087	-10.37	-0.57	-12.23	4.76	-2.33
9052	c1c(cnc(c1C#N)N)C#N	C20436862	-10.37	-0.81	-14.22	6.28	-1.62
9053	C1C=C[C@H](CO1)O	C22002567	-10.37	-1.92	-13.2	4.01	0.74
9054	CCN1CSCSC1	C32599205	-10.37	-1.31	-9.13	2.13	-2.06
9055	c1cc(ccc1C=O)OC(F)F	C00165235	-10.36	-0.29	-13.09	5.52	-2.5
9056	Cc1cc(ccc1O)SC#N	C00409898	-10.36	-1.83	-12.54	4.41	-0.39
9057	C([C@H](C(S)S)O)	C00901552	-10.36	-2.89	-9.99	2.29	0.22
9058	CC(C)CCNO	C01677567	-10.36	-2.77	-10.03	2.3	0.15
9059	Cc1[nH]c(c(n1)Cl)Cl	C01756169	-10.36	-2.99	-9.67	4.57	-2.28
9060	#CCCCCO	C01845543	-10.36	0.47	-12.54	2.87	-1.16
9061	c1cccc(c(c1)c2nsc(=O)o2)O	C01849864	-10.36	0.54	-14.59	4.7	-1.01
9062	[C@H]1[C@H](C[N+](=O)[O-])O	C02042096	-10.36	-1.74	-13.69	5.74	-0.66
9063	c1cc(c(cc1C#N)Cl)O	C02380632	-10.36	-1.21	-13.5	4.73	-0.39
9064	Cc1cc(ccc1F)N=C=O	C02585389	-10.36	-0.55	-10	1.86	-1.66
9065	Cc1csc(n1)Br	C04198760	-10.36	-0.62	-13.57	3.1	0.73
9066	c1ccc(cc1)c2nc(nc(n2)N)N	C04428660	-10.36	-1.28	-11.56	7.12	-4.64
9067	[H]N=C(\C)/OCC	C04974301	-10.36	-0.78	-12.86	2.64	0.62
9068	C(=O)C(F)Cl	C05112661	-10.36	-0.21	-12.72	4.09	-1.53
9069	[C@H]1/C(=N/O)CCO1	C15022664	-10.36	-1.27	-13.16	3.57	0.5
9070	c1nc(c(c(n1)Cl)[N+](=O)[O-])[O-]	C17300083	-10.36	-2.31	-13.44	5.16	0.23
9071	C=CCNCC#N	C20033611	-10.36	-1.48	-12.31	4.54	-1.12
9072	CN(C=O)OC	C21304109	-10.36	-1.36	-12.98	4.54	-0.56
9073	COCc1cc([nH]n1)N	C26511567	-10.36	-0.97	-16.87	7.27	0.21
9074	CC(=O)[C@H]1CCOC1=O	C00519771	-10.35	0.68	-15.6	6.98	-2.42
9075	CC(=O)NC(=O)/C(=N[O-])/C#N	C01039313	-10.35	-4.04	-19.7	13.38	0.01
9076	Cn1cc(c(=O)[nH]c1=O)F	C01639707	-10.35	-2.46	-17.54	9.44	0.2
9077	CCOC(=O)c1cc([nH]1)O	C01653144	-10.35	-0.19	-16.27	4.66	1.45
9078	C1CCN(C1)C=O	C01675320	-10.35	0.26	-14.75	5.78	-1.63
9079	CCOC(=O)/C=C(\C)/Cl	C01722721	-10.35	0.36	-11	1.93	-1.63
9080	[C@H]1[C@H](C(=O)C)Br	C02031004	-10.35	-0.5	-11.83	4.49	-2.51
9081	[C@H]1C=C(C(=O)O1)C	C02031908	-10.35	-1.85	-14.59	7.51	-1.42
9082	c1ccc2c(c1)C=C[C@H]2O	C02032278	-10.35	-2.55	-13.14	4.21	1.14
9083	CC(=O)CBr	C02034519	-10.35	-0.84	-12.45	4.98	-2.04
9084	C1CCC(=CC1)[N+](=O)[O-]	C04528664	-10.35	-2.13	-11.66	4.6	-1.16
9085	c1nnc2n1[nH]c(=S)n2N	C04995303	-10.35	-2.28	-19.67	8.43	3.16
9086	Cc1ccnc(n1)NN=O	C06523327	-10.35	-0.04	-13.92	5.74	-2.13

9087	c1cc2c(nc1)sc(n2)N	C08251251	-10.35	-1.84	-14.53	7.06	-1.05
9088	c1c2c([nH]c(=O)[nH]2)[nH]c(=S)n1	C16970394	-10.35	-6.59	-10.16	6.23	0.17
9089	C(C(=O)C=N)OCl	C16972747	-10.35	-3.46	-14.65	7.49	0.27
9090	Cc1cccc1CON	C19733267	-10.35	0.8	-12.36	3.56	-2.35
9091	c1ccc(ccc1SC(F)F)Br	C20268463	-10.35	-0.29	-7.83	2.6	-4.84
9092	CC(C)N=C(C)C	C31426676	-10.35	-0.85	-9.31	1.98	-2.17
9093	c1(c([nH]c(=O)n1)Br)[O-]	C32497008	-10.35	-1.47	-19.1	4.32	5.89
9094	c1ccc(cc1)OC(C(F)F)(F)F	C00163973	-10.34	-0.51	-11	3.99	-2.83
9095	CC1=COC(=O)[C@H]1C(=O)C	C00501649	-10.34	-1.72	-11.49	5.96	-3.09
9096	CCN1C(=O)C=CC1=O	C00901367	-10.34	1.03	-15.25	5.77	-1.89
9097	c1cncnc1c2csnn2	C01383115	-10.34	-2.81	-12.58	6.93	-1.88
9098	CSC(=O)NCC=C	C01583570	-10.34	-1.21	-10.59	3.41	-1.95
9099	C[C@H](CC)C#N	C01632615	-10.34	-0.48	-10.47	3.44	-2.83
9100	C1(C(=O)NC(=O)NC1=O)Br	C01716694	-10.34	1.24	-19.56	4.79	3.18
9101	CC(=O)[C@H]1CCCC1=O	C01726108	-10.34	-0.59	-11.68	4.75	-2.82
9102	CC#CC(=O)OC	C01765591	-10.34	-0.17	-12.95	5.55	-2.77
9103	c1ccc(cc1)OC(=O)C(F)F	C01846603	-10.34	-0.25	-9.55	3	-3.54
9104	CC[C@H](C)OC	C02029845	-10.34	0.08	-10.68	1.19	-0.93
9105	C[C@@H](c1ccc(O)OC(=O)C	C02389351	-10.34	-0.46	-11.43	5.46	-3.91
9106	C[C@H](C(=O)C)SC	C03861605	-10.34	-1.35	-11.58	5.41	-2.82
9107	c1c([n+](c2cn[nH]c2n1)[O-]	C04772449	-10.34	-3.18	-18.72	12.21	-0.64
9108	C1C(=O)NC(=O)N1	C05133259	-10.34	-6.13	-14.28	4.71	5.36
9109	CC(=O)CCS	C05196560	-10.34	-0.3	-13.19	3.47	-0.32
9110	c1ccc(cc1O)CO	C06092100	-10.34	-1.23	-18.04	5.06	3.88
9111	c1cnc(c1C#N)Br	C12359347	-10.34	-3.14	-8.75	4.2	-2.65
9112	c1c([nH]nc1N)C2CCC2	C12359806	-10.34	-3.73	-9.38	4.61	-1.84
9113	[H]N=C(N)/SCc1c(ccc1F)F	C12368553	-10.34	0.32	-12.55	4.6	-2.71
9114	CCOC(=O)c1csnc1C	C16124743	-10.34	1.85	-12.99	4.01	-3.2
9115	C[C@@H](CN/C(=N)/N(=O)[O-])/N	C17300035	-10.34	-3.88	-16.39	9.98	-0.05
9116	CCNC#N	C20033303	-10.34	-1.11	-14.76	6.3	-0.77
9117	CCNC1cncs1	C20566285	-10.34	-2.26	-9.36	4	-2.72
9118	CC(=O)C(C(=O)C)F	C22004319	-10.34	-1.35	-12.76	5.8	-2.02
9119	C1=CC(=O)[C@H]2[C@H]1C(=O)C=C2	C00158288	-10.33	1.11	-13.86	5.25	-2.83
9120	CCN(CC)C=O	C00388483	-10.33	-1.59	-11.73	5.2	-2.21
9121	COC(=O)C1CCCC1	C00404439	-10.33	-1.86	-11.45	6.92	-3.94
9122	CCCC(=O)CC	C01586745	-10.33	-0.27	-12.09	3.52	-1.5
9123	CC[C@H](C)O	C01622055	-10.33	-0.97	-10.59	1.61	-0.39
9124	c1ccc(cc1[N+](=O)[O-])Br	C01666827	-10.33	-1.59	-11.45	3.4	-0.68
9125	CN(C)C#N	C01688358	-10.33	-1.48	-9.44	4.08	-3.49
9126	C/C=C/C(=O)C	C01716739	-10.33	-0.12	-9.85	3.48	-3.83
9127	C/C=C/C(C)[C@H](C)O	C01730157	-10.33	-0.44	-10.27	1.64	-1.26
9128	CC(C)N=C=S	C01841344	-10.33	0.28	-12.44	1.38	0.46
9129	CC(=O)N(C)CCC#N	C02381335	-10.33	-1.4	-15.38	8.74	-2.29
9130	c1c(cnc1Br)CO	C02507201	-10.33	-2.01	-11.56	3.8	-0.55
9131	CCc1ccc(s1)C	C02510291	-10.33	-0.5	-10.8	1.77	-0.8
9132	Cc1ccn(c(n1)N)Cl	C02537813	-10.33	-0.09	-12.74	4.52	-2.02
9133	c1ccc2c(c1)CC(=C2)C#N	C04273543	-10.33	-1.34	-10.91	3.9	-1.99
9134	Cn1c(=O)cccc1Cl	C05423926	-10.33	-2.2	-11.62	6.02	-2.53
9135	Cn1c(=O)[nH]c(=O)[nH]1	C06072277	-10.33	-3.32	-17	8.48	1.51
9136	c1cc2c(cc1Br)nc[nH]2	C06667027	-10.33	-2.08	-10.93	6.28	-3.6
9137	CCc1nc(on1)[C@@H](C)Cl	C12505709	-10.33	2.44	-14.05	3.57	-2.29
9138	C/C=C/[C@@H](O)[C@H](O)/C=C/C	C17046406	-10.33	-1.35	-10.97	2.37	-0.37
9139	c1ccc(cc1)/C=C/C(=O)Cl	C21304307	-10.33	1.03	-11.97	5.05	-4.44
9140	c1cnc(nc1)NCC(=O)N	C21517217	-10.33	-3.43	-15.93	8.99	0.04
9141	CC(C(=O)C)C(=O)N	C24717448	-10.33	-2.32	-10.43	4.07	-1.66
9142	c1c(c(nc(=O)[nH]1)N)I	C00967457	-10.32	-4.16	-16.58	9.72	0.69
9143	C1=CC(=O)OC1=C(C)Cl	C01581213	-10.32	-1.51	-10.34	5.02	-3.48
9144	CCOC(=O)C(=C)Cl	C01608903	-10.32	-0.08	-11.68	3.27	-1.84
9145	CCC(=O)c1cccnc1	C01663885	-10.32	-2.54	-10.16	5.37	-2.99
9146	CCc1ncnc(=O)[nH]c1=O	C01696276	-10.32	-2.63	-15.45	9.38	-1.63
9147	c1ccc(cc1)S(=O)(=O)NC#N	C01703100	-10.32	-3.09	-11.28	7.14	-3.09
9148	CC(=C/C=C/C(=O)C)C	C02018343	-10.32	0.68	-13.16	4.1	-1.94
9149	c1nnc(n1)N	C04152201	-10.32	-3.91	-15.8	7.37	2.02
9150	C(=O)(C(F)F)(F)F)N	C05177760	-10.32	-1.29	-12.94	3.64	0.27
9151	C=CCSC1=NCSS1	C05185842	-10.32	-0.4	-14.45	2.87	1.66
9152	c1cc(ccc1)Cl)C=N/O	C08637842	-10.32	-2.35	-10.9	5.03	-2.11
9153	c1cc(sc1)C(=O)NO	C12504622	-10.32	-5.18	-13.44	8.81	-0.51
9154	c1ccc(cc1)SCC=O	C19686055	-10.32	-1.45	-9.39	4.59	-4.08
9155	CNc1cc(ccn1)Cl	C21303251	-10.32	-2.24	-8.92	3.1	-2.26
9156	Cc1c[nH]c(n1)I	C01563468	-10.31	-1.97	-13.44	4.24	0.87
9157	COC(=O)CC(=O)C(=O)OC	C01621874	-10.31	-0.95	-13.78	7.53	-3.1
9158	C[C@@H]1(CO1)C=C	C01679929	-10.31	-0.44	-11.2	2.74	-1.42
9159	Cc1c(ccs1)Br	C01695822	-10.31	-0.55	-11.43	1.66	0.01
9160	COC(=O)NCCC	C01698370	-10.31	-0.2	-14.92	5.24	-2.42
9161	CC1=CCOC1=O	C02015746	-10.31	-1.81	-14.1	8.03	-0.43
9162	CC(C)ON	C02388228	-10.31	-1.57	-10.34	1.89	-0.29
9163	c1nc(c(n1)C)N)N	C02523006	-10.31	-2.63	-12.75	4.94	0.12
9164	COC(=O)c1ccc(c[nH]1)C=O	C02577863	-10.31	-1.23	-13.74	6.74	-2.09
9165	CC[C@H](C)C(=O)Cl	C02584245	-10.31	0.06	-11.45	2.32	-1.24
9166	C[C@H]1CCCCO1	C05211760	-10.31	0.24	-11.74	1.27	-0.08
9167	CC(=C)OC1CCC1	C05283281	-10.31	0.02	-10.43	1.38	-1.28
9168	CCOC(=O)OCC(C(F)F)(F)F	C15443008	-10.31	-0.22	-9.34	3.2	-3.94
9169	C/C(=N)O)N/C(=N)O)/N	C16082792	-10.31	-5.14	-17.03	7.78	4.08
9170	c1c(c([nH]c1=O)C(=O)N=[N+]=[N-])[O-]	C17288490	-10.31	0.33	-21.07	5.49	4.94
9171	c1c(nc[nH]1)C/C=C(C(=O)Cl	C21987274	-10.31	0.02	-15.21	8.28	-3.4
9172	COCNC(=O)n1ccnc1	C32628597	-10.31	-0.66	-15.77	7.96	-1.83
9173	c1cn(cn1)C(=O)NCC(F)(F)F	C32628638	-10.31	-2.67	-11.54	6.85	-2.95
9174	c1ccc(cc1N)C#N)O	C00331906	-10.3	-0.29	-16.68	5.63	1.03
9175	CC(=O)c1cccc1	C00896628	-10.3	-1.45	-10.14	4.99	-3.71
9176	COc1ccc(cc1)N)O	C01304689	-10.3	-1.78	-13.29	3.91	0.86

9177	Cn1c(c(nn1)C(=O)N)N	C01417949	-10.3	-5.46	-13.99	6.79	2.36
9178	C[C@@]12[C@@@H](O1)C(=O)C=CC2=O	C01559090	-10.3	0.11	-15.07	4.29	0.36
9179	C/C=C/CCCO	C01601235	-10.3	-0.58	-10.56	2.11	-1.28
9180	CCO[C@@@H](C(=O)OCC)O	C01621875	-10.3	0.39	-13.85	4.59	-1.43
9181	CCCCC(=O)N	C01641410	-10.3	-0.03	-9.95	1.94	-2.26
9182	CC[C@@H](C(=O)OCC)F	C02147435	-10.3	-0.15	-11.4	3.6	-2.34
9183	c1cc(c(cc1N)C(=O)Cl)F	C02243176	-10.3	0.56	-14.46	5.66	-2.07
9184	CCC[C@@@H](C)O	C02504420	-10.3	-0.26	-10.5	1.37	-0.92
9185	c1cc(c(cc1Br)F)CO	C02512504	-10.3	-1.08	-12.47	2.31	0.94
9186	c1cc(ccc1NCCO)Cl	C03210880	-10.3	-3.5	-9.6	3.53	-0.72
9187	c1nc(c(n1C(=O)N)N(=O)[O-])	C04125317	-10.3	-5.9	-14.92	11.83	-1.32
9188	C1CCC(=NN)C1	C04887228	-10.3	-1.13	-13.34	2.19	1.98
9189	COc1ccc(cc1)/C=N/O	C12341485	-10.3	-2.72	-13.14	6.65	-1.1
9190	C1CC(=O)N(C1)N	C13550143	-10.3	-1.54	-14.56	6.09	-0.3
9191	CCO[C@@@](C(F)F)(F)Br	C14611376	-10.3	-1.46	-8.61	2.24	-2.47
9192	C[C@@H](C(=N)O)N	C16082781	-10.3	-3.9	-13.93	4.36	3.17
9193	C[C@@H](O)OC(F)F	C16159295	-10.3	-1.79	-12.12	3.35	0.26
9194	c1cc(ccc1C(=O)N=C=O)Cl	C19408021	-10.3	1.56	-13.42	2.86	-1.3
9195	c1(nc([nH]n1)N)C(=O)N	C19505675	-10.3	-6.16	-19.59	14.01	1.44
9196	c1cnc(c1n2cncn2)N	C20370479	-10.3	-0.72	-13.25	6.57	-2.91
9197	COc1cc(c(n1nH)O)F	C26896783	-10.3	-2.48	-16.79	9.98	-1.01
9198	c1(c(c(c1F)F)O)F	C00395548	-10.29	-1.74	-13.26	3.92	0.8
9199	c1ccc(cc1)[C@H](CNO)O	C00397119	-10.29	-3.36	-14.55	4	3.62
9200	C=COCCNC=O	C01603470	-10.29	0.33	-17.16	6.48	0.06
9201	CCN(CC)O	C01698912	-10.29	-1.25	-11.02	2.07	-0.08
9202	Cc1c(ocn1)C#N	C02004545	-10.29	-1.74	-13.05	4.87	-0.37
9203	C/C=C/C[C@H](C)O	C02039433	-10.29	-0.71	-10.15	1.41	-0.83
9204	C1CC(=O)C2=C1OCOC2	C02149591	-10.29	-1.18	-13.99	6.67	-1.79
9205	Cc1nnc(n1)N	C02511426	-10.29	-5.29	-15.22	7.73	2.5
9206	Cc1ccnc(n1)Cl	C02515987	-10.29	0.53	-13.47	5.02	-2.36
9207	c1cc2c(c1)cc([nH]2)N	C02576352	-10.29	-2.96	-12.93	4.2	1.4
9208	C1CC(=C(C(=O)C1)Br)[O-]	C03865375	-10.29	-1.35	-13.74	6.33	-1.53
9209	c1(c(non1)NNc2c(non2)N)N	C03898323	-10.29	-4.43	-16	9.96	0.18
9210	C1CN(NC1=O)C(=O)CCl	C04038567	-10.29	0.64	-18.18	7.83	-0.58
9211	c1cc(c(c1)F)N=C=S)F	C04255362	-10.29	0	-11.38	5.09	-4
9212	c1cnc(cn1)C(=O)NO	C04429661	-10.29	0.06	-21.23	9.32	1.55
9213	c1ccc(cc1)C(=O)/C=N/O	C04536813	-10.29	-2.63	-12.85	6.53	-1.35
9214	C[C@@@H](Cn1ccnc1)O	C05115865	-10.29	-1.13	-14.42	6.67	-1.41
9215	c1nc(no1)/C(=N)O/Cl	C05705310	-10.29	-3.13	-16.13	7.52	1.44
9216	CS/C(=[NH+]/N=C(N)/[S-])/N	C06259690	-10.29	-0.89	-18.69	10.6	-1.32
9217	c1ccc2c(c1)nc(n2[O-])C#N	C13219726	-10.29	-2.95	-11.12	5.85	-2.07
9218	Cn1ccc(n1)C(=O)N	C13466603	-10.29	-4.85	-13.91	7.91	0.56
9219	COc1cc(ccn1)C(F)F	C19616188	-10.29	-0.45	-11.05	3.07	-1.86
9220	c1cc(c(cc1Br)F)C#N	C00155137	-10.28	-1.78	-10.61	3.96	-1.85
9221	c1cc(c(cc1N)C(F)F)F	C00164786	-10.28	-2.76	-9.03	3.97	-2.47
9222	c1cc(sc1CC#N)Br	C00334102	-10.28	-3	-12.7	6.31	-0.88
9223	CCOc1ccc(on1)[N+](=O)[O-]	C00335039	-10.28	2.3	-14.09	3.75	-2.24
9224	CC(=O)OCC#N	C01555375	-10.28	-2.28	-13.08	7.8	-2.72
9225	CNc1cc(ncn1)Cl	C01749496	-10.28	-1.67	-13.85	3.85	1.39
9226	CC(C#C)/C(=O)C	C02039894	-10.28	-0.5	-11.82	3.7	-1.66
9227	c1cnc(nc1)SCC#N	C02171569	-10.28	-2.09	-12.23	6.92	-2.89
9228	CC[C@@H](CC(=C)C)O	C02508080	-10.28	-0.76	-11.09	1.56	0.02
9229	CN(C(=O)C(F)F)OC	C02555201	-10.28	1.66	-13.87	3.37	-1.44
9230	Cc1c(ocn1)N	C03407837	-10.28	-2.06	-14.06	4.96	0.89
9231	C[C@H]1CCCCC1=O	C03860605	-10.28	1.68	-11.7	3.12	-3.38
9232	C1C(CSCS1)O	C05085555	-10.28	-1.09	-10.95	2.38	-0.62
9233	C(Oc1c(non1)N)Oc2c(non2)N	C05380685	-10.28	-4.52	-17.5	8.19	3.55
9234	C/C=C/[C@@@H]1OC[C@@H](O1)C	C05539417	-10.28	0.01	-12.86	2.63	-0.06
9235	C1[C@@@H]2[C@@@H](CS1)OC(=O)O2	C05574446	-10.28	1.39	-14	4.68	-2.35
9236	CNC(=O)OCC(F)F	C08037175	-10.28	-2.21	-12.33	4.48	-0.22
9237	C([N])C[C@@H](F)Br	C08698382	-10.28	-0.11	-11.88	3.76	-2.05
9238	c1cnc(nc1)/C(=N)O/N	C15828506	-10.28	-3.79	-14.98	7.57	0.92
9239	CC(=O)Nc1ccncc1	C16102283	-10.28	-1.19	-15.29	7.47	-1.27
9240	c1cnn(c1)c2cncn2N	C20370482	-10.28	-2.02	-12.33	5.93	-1.86
9241	C1CCN(C(=O)C1)N	C21298954	-10.28	0.07	-14.78	5.31	-0.88
9242	C[C@@@H]1[C@H](C(=O)N)N=C=S	C22141575	-10.28	-0.46	-10.9	3.71	-2.64
9243	C[C@@@H]1CCOC1=O	C00388119	-10.27	-0.48	-13.11	5.81	-2.49
9244	Cc1ccc(s1)	C00403123	-10.27	-0.4	-11.57	1.47	0.23
9245	Cc1ccc(cc1Cl)O	C00407449	-10.27	-1.32	-9.87	2.86	-1.94
9246	Cc1cc(=O)c(cc1)O	C01395450	-10.27	-3.3	-16.37	10.23	-0.82
9247	CCCCCO	C01687154	-10.27	-2.92	-8.54	1.89	-0.71
9248	CCc1nnc(s1)Cl	C01701726	-10.27	-1.81	-12.39	4.17	-0.24
9249	COc(=O)C1=CC=CC1	C01730116	-10.27	1.71	-15	4.61	-1.6
9250	CCNOCC	C01756760	-10.27	-0.63	-11.75	1.91	0.21
9251	C1CC1C(C2CC2)O	C02162270	-10.27	-0.38	-8.71	1.17	-2.35
9252	COc(=O)C(=O)c1cccc1	C02166852	-10.27	-0.88	-9.3	4.03	-4.11
9253	CNc1ccc(nn1)Cl	C02391440	-10.27	-1.4	-12.92	5.55	-1.5
9254	c1c(ccc1Br)C=O	C02507202	-10.27	-0.25	-13.06	5.41	-2.37
9255	Cc1c(non1)CCC=C	C02522331	-10.27	-0.13	-13.41	6.21	-2.94
9256	CCO[P@@]1CC=C(C1)C	C03957835	-10.27	0	-8.82	1.86	-3.31
9257	C1=CC(=O)N(C1=O)CCC#N	C05372810	-10.27	0.35	-17.24	8.3	-1.68
9258	C([C@H]1C(=O)NC(=O)N1)S	C05411549	-10.27	0.29	-17.1	5.12	1.41
9259	CNC(=O)C(=O)N	C05700330	-10.27	-3.43	-14.5	4.69	2.97
9260	CC(=O)N(C=O)C=O	C06731774	-10.27	-2.55	-17.76	12.01	-1.97
9261	c1cnc(c1)SCCO	C11535633	-10.27	-5.05	-9.19	4.99	-1.02
9262	CCN/C(=[NH+](=O)[O-])/N	C16033785	-10.27	-4.24	-14.6	10.46	-1.89
9263	c1cc2c(nc1)SCC2	C19801135	-10.27	-1.95	-11.3	6.22	-3.23
9264	c1cc(ccc1)F)CNC(=S)NN	C20473713	-10.27	0.42	-18.35	10.43	-2.76
9265	CCC1=NN(C(=O)C1)C	C26515269	-10.27	-0.55	-14.54	6.69	-1.86
9266	CC(C)c1[n-]cc(n1)[N+](=O)[O-]	C00157584	-10.26	-0.27	-10.71	4.6	-3.88

9267	c1cc(c(cc1O)C(F)F)F	C00164785	-10.26	-5.4	-7.28	4.01	-1.58
9268	c1csc(c1[N+](=O)[O-])Cl	C01513509	-10.26	-1.87	-13.11	5.37	-0.64
9269	c1ccc(cc1)Nc2nc([nH]n2)N	C01575013	-10.26	2.94	-18.22	9.91	-4.89
9270	CCCCSCC=C	C01587859	-10.26	-0.71	-9.41	1.15	-1.29
9271	C[C@@H]1C[C@@H](C(=O)O1)Br	C01592385	-10.26	-1.16	-11.57	5.57	-3.1
9272	C(C[N+](=O)[O-])C(Cl)C	C01758979	-10.26	-0.97	-11.32	4.95	-2.93
9273	CC(=O)Nc1cc(cc(c1)F)F	C02243414	-10.26	-1.46	-12.59	6.48	-2.69
9274	c1cc(c(cc1OC(F)F)F)Cl)N	C02382405	-10.26	-0.6	-11.08	1.96	-0.55
9275	c1cc(c(cc1C=O)F)Br	C02383961	-10.26	-0.49	-10.68	4.55	-3.64
9276	Cc1cc(oc1C)C	C02518855	-10.26	-0.91	-8.72	2.98	-3.62
9277	CO[C@H](C(C(F)F)F)F)O	C02579122	-10.26	-2.4	-9.56	2.21	-0.51
9278	Cc1cc(ncn1)Cl	C02581590	-10.26	-2.01	-11.54	3.32	-0.03
9279	C1C[C@@H](C=C)C@H]1O)O	C03860563	-10.26	-1.99	-13.36	3.67	1.42
9280	C[C@H]1(C@H)1CCC(C@H)1O)O	C05031337	-10.26	-0.69	-11.3	2.39	-0.66
9281	c1[nH]c2c(n1)c(=O)n(c2)O	C05425242	-10.26	-4.3	-19.24	14.87	-1.58
9282	C1233855CC(=O)C=N/Nc1cccc1	C12338552	-10.26	-0.72	-11.12	5.13	-3.55
9283	c1c[nH]c2c1ncc(c2)Cl	C14401120	-10.26	-0.61	-12.5	5.37	-2.51
9284	Cc1c(ccc(n1)N)Cl	C15423947	-10.26	-2.29	-9.15	3.06	-1.87
9285	c1c(c(c(=O)[nH]n1)Cl)N	C17300623	-10.26	-3.89	-15.49	6.17	2.95
9286	CCOC(=O)c1csc(n1)N	C18210877	-10.26	1.25	-12.21	2.89	-2.18
9287	c1cc(c(c(c1)F)C@H]2CO2)F	C18344987	-10.26	-1.6	-10.58	4.84	-2.93
9288	C[P@H](=O)OCc1cccc1	C21993426	-10.26	-1.81	-12.48	7.49	-3.46
9289	C1[C@H](O1)CN2C(=O)CSC2=O	C22223265	-10.26	-0.38	-15.99	6.74	-0.64
9290	c1cnc(c(n1)CO)Cl	C32915065	-10.26	-2.13	-15.93	6.74	1.07
9291	COc1ccnc(n1)N	C00332004	-10.25	-0.47	-13.66	4.27	-0.39
9292	C1CCN(CC1)C#N	C00407019	-10.25	1.66	-10.57	3.54	-4.89
9293	C1[C@H](OC1)Cl	C01622487	-10.25	0.03	-9.57	2.06	-2.77
9294	CC(=O)CCC#N	C01653073	-10.25	0.2	-14.24	5.97	-2.18
9295	C1=CC(=O)C=CC1=NBr	C01762858	-10.25	1.65	-12.96	3.71	-2.65
9296	COc1cccc1	C05701055	-10.25	-0.99	-10.05	1.65	-0.86
9297	C[C@H]1N=NNN1C	C06481676	-10.25	-1.43	-13.28	2.59	1.86
9298	c1csc(c1)P@H](=O)O	C06599421	-10.25	-5.57	-12.23	8.04	-0.48
9299	c1cc(c(cc1O)O)CCO	C13340461	-10.25	-2.5	-14.98	4.99	2.25
9300	C1[C@H]2[C@@H]1CC(C2)O	C16698377	-10.25	-2.35	-8.88	2.06	-1.08
9301	C(=C)SC#N(C=O)N	C16955772	-10.25	-0.75	-16.68	6.86	0.32
9302	Cc1ccc(o1)C(=O)N=[N+]=[N-]	C17108604	-10.25	-0.56	-14.2	4.18	0.33
9303	C/N=C(C#N)/C1CCCC1	C17174700	-10.25	0.43	-10.6	2.69	-2.77
9304	C[C@H]1C=C(C(=O)O1)CO	C17299098	-10.25	-3.07	-13.36	6.77	-0.58
9305	CC[C@@H]1[C@H](O)C	C19260482	-10.25	-0.36	-10.9	2.75	-1.74
9306	c1ccc(c(c1)C)C(F)F	C19729345	-10.25	-0.29	-12.95	5.27	-2.28
9307	c1ccc(c(c1)C)C(=O)O	C19730647	-10.25	1.34	-11.95	3.11	-2.75
9308	CC(=O)COC(C(F)F)F	C20439919	-10.25	-1.04	-11.58	4.8	-2.43
9309	Cc1ccc([nH]c1)NC	C21505277	-10.25	-2.16	-9.23	3.52	-2.39
9310	C1CC1(C(=O)C)Cl	C22112864	-10.25	-0.19	-9.53	3	-3.54
9311	c1cnccc1C(=C)C=O/[O-]	C26515431	-10.25	-0.17	-15.37	7.23	-1.94
9312	Cc1c(c(=O)[nH]c(=O)[nH]1)O	C00013352	-10.24	-3.45	-15.14	6.53	1.83
9313	CCC[C@H]1CC(C(=O)O1)	C00388712	-10.24	-0.82	-11.25	5.58	-3.74
9314	CC1=C(C(=CC1=O)O)O	C00389481	-10.24	-5.41	-15.92	10.51	0.58
9315	Cn1cc(nc1)CC=O	C00895896	-10.24	-2.42	-15.08	8.69	-1.43
9316	c1cc2ccsc2nc1	C01555982	-10.24	-2.49	-13.26	5.33	0.18
9317	CC(=C)Cl(=O)OCCO	C01608929	-10.24	-1.55	-13.82	5.85	-0.73
9318	C(C(=O)C)Cl	C01648213	-10.24	-0.5	-13.74	6.47	-2.47
9319	c1nc2c(o1)CCC2	C01734291	-10.24	-1.46	-13.67	4.44	0.45
9320	C[C@H]1(C@H)(C)Cl)O	C01762876	-10.24	-0.93	-10.23	1.55	-0.63
9321	CN(C)C1CCCC1	C02569844	-10.24	-2	-7.33	2.38	-3.29
9322	C[C@@H]1C[C@@H](O)O	C04212241	-10.24	-1.88	-13.75	6.21	-0.83
9323	CCCC(=O)CC(=O)C	C04552332	-10.24	-0.83	-12.88	4.34	-0.87
9324	c1ccc(cc1)NCCO	C04806325	-10.24	-2.89	-10.28	3.48	-0.55
9325	c12c(nc(nc1[nH]n2)[O-])N	C05479634	-10.24	-4.34	-17.62	8.87	2.86
9326	C[C@H](CC(F)F)F)O	C16082634	-10.24	-1.07	-11.6	3.28	-0.85
9327	c1cc(ccc1C/C(=N/O)N)Cl	C16082778	-10.24	-3.23	-10.61	5.17	-1.57
9328	COCCNCC#C	C20033344	-10.24	0.57	-13.1	2.77	-0.47
9329	CCc1c([nH]c1N)C(F)F)F	C26511521	-10.24	-4.55	-11.2	6.94	-1.42
9330	C1[C@H]2C=CC(=O)C@H](O1)O2	C00078172	-10.23	-0.75	-15.38	6.73	-0.82
9331	C1[C@H]2[C@@H]2[C@@H](C1)O2	C01639894	-10.23	-0.94	-11.18	3.2	-1.3
9332	CC1(OCCC1)C=C	C01639928	-10.23	-1.44	-10.87	2.42	-0.35
9333	c1cc(c(cc1C(=O)C=O)F)F	C02507504	-10.23	-1.51	-16.23	11.44	-3.94
9334	c1cc(c(c(c1)F)O)C(F)F)F	C02560194	-10.23	-2.39	-10.47	4.28	-1.66
9335	CC(=O)OCCCC#C	C02567252	-10.23	0.62	-11.58	4.71	-3.99
9336	c1cnc2c(n1)c([nH]n2)[O-]	C04714875	-10.23	-2.24	-19.25	7.43	3.83
9337	C/C(=C)/C(=O)C1CCCC1/[O-]	C04876957	-10.23	-1.21	-12.19	5.16	-1.98
9338	CS(=O)(=O)Nn1cnnc1	C05515275	-10.23	-1.17	-21.69	10.86	1.77
9339	CN1CC(=O)NC1=O	C05966178	-10.23	-2.08	-16.37	7.47	0.76
9340	C1[C@H]2C=C[C@@H](C@H)(O1)O2)O	C06658001	-10.23	-1.31	-14.15	4.23	0.99
9341	Cc1c(sc1n1)CO	C13539621	-10.23	-1.77	-14.2	5.38	0.36
9342	Cc1cc(c(nc1)F)N+=[O-][O-]	C14982834	-10.23	-2.11	-12.04	6.92	-2.99
9343	c1c(c(=O)[nH]c(=O)[nH]1)NC(=O)N	C16857705	-10.23	-3.35	-24	11.78	5.35
9344	c1c(c(c(nc1O)N)N)O	C16980118	-10.23	-4.74	-17.03	6.02	5.51
9345	c1c(o[nH]c1=O)C(=O)NO	C16983356	-10.23	-4.99	-18.08	10.59	2.24
9346	C1=CC(=O)[C@@H]2[C@@H](C@H](C@H)1O)O2	C17061956	-10.23	-2.42	-14.95	5.88	1.27
9347	CCOCN=C=O	C20252602	-10.23	-1.44	-13.44	2.74	1.9
9348	C[C@H](c1cncc1)[NH3+]	C20441648	-10.23	-0.53	-12.3	3.35	-0.75
9349	c1cnc(cc1Br)C(F)F)F	C21985271	-10.23	-2.81	-7.23	3.12	-3.32
9350	CC(=O)OCC(=S)N	C32627844	-10.23	-1.42	-17.32	9.82	-1.31
9351	c1cc(c(cc1Cl)F)CC#N	C00161645	-10.22	-0.55	-13.73	6.64	-2.58
9352	c1cc(c(nc1)C#N)Cl	C00332990	-10.22	-2.86	-10.82	6.12	-2.65
9353	C1[C@H]2[C@@H](C(=O)C1)Cl	C02031398	-10.22	1.01	-12.66	4.21	-2.79
9354	CCC[C@H](C#C)O	C02041127	-10.22	-1.29	-9.71	2.17	-1.39
9355	C[C@H](c1cc(cc(c1)F)F)O	C02525259	-10.22	-4.6	-6.05	2.66	-2.24
9356	CO=C/C(Cl=O)OC	C02582018	-10.22	-1.3	-11.7	4.41	-1.64

9357	c1cc(ccc1/C=C/C=O)Cl	C03080768	-10.22	-2.31	-12.8	6.31	-1.42
9358	C(C(S)O)S	C04362873	-10.22	-1.13	-12.43	3.54	-0.2
9359	C(=O)NNc1c(non1)N	C05368746	-10.22	-5.54	-19.56	12.6	2.27
9360	C[C@H]1[C@@H](C(=O)C1)C	C06037927	-10.22	-0.62	-11.44	2.98	-1.14
9361	Cc1ccc(s1)CO	C08727914	-10.22	-1.9	-10.96	3.84	-1.2
9362	Cn1cc(c(n1)N)C=O	C12370883	-10.22	-5.58	-11.19	7.12	-0.57
9363	c1c(cc(cc1F)CC(=O)NN	C16158280	-10.22	-6.02	-11.54	8.81	-1.47
9364	C1C(=CN=NC1=O)O	C17063634	-10.22	-4.61	-16.05	6.42	4.01
9365	CC1=NCC(=O)C(=O)N1	C17378515	-10.22	-3.2	-15.79	5.98	2.79
9366	Cc1c(snn1)CCI	C19093023	-10.22	-1.65	-11.46	5	-2.11
9367	C1C=C[C@@H]2[C@H]1CC2=O	C19230143	-10.22	-0.76	-10.36	4.08	-3.17
9368	c1cc(oc1)CNCC(F)F	C19505158	-10.22	-1.08	-11.9	4.81	-2.05
9369	c1c(cn[nH]1)c2c(c[nH]n2)N	C19737402	-10.22	-6.21	-13.74	8.82	0.9
9370	C[C@H]([C@@](C(F)F)(O-))F	C20232452	-10.22	-2.43	-10.42	3.42	-0.79
9371	Cc1cccc(n1)Cl	C00388111	-10.21	-1.39	-9.77	3.86	-2.92
9372	C[C@H]1[C@@H](C(=O)OC(=O)C	C01095299	-10.21	-0.66	-12.16	4.49	-1.88
9373	c1(c([nH]c(=O)[nH]c1=O)[O-])O	C01847417	-10.21	-6.33	-17.72	9.01	4.83
9374	c1cc(c(cc1F)[N+](=O)[O-])Cl	C01847554	-10.21	-2.96	-10.35	4.79	-1.7
9375	Cc1cc(oc1)FBr	C02384021	-10.21	-0.41	-12.06	2.64	-0.38
9376	C[C@H](C(=O)OCC(=O)C)O	C02508059	-10.21	0.14	-12.66	3.88	-1.58
9377	Cc1c(cnn1)CC#N)Cl	C02537505	-10.21	-1.2	-13.79	7.86	-3.07
9378	C=CCOc1ccc(c1)C=O	C03764991	-10.21	-2.54	-13.13	7.11	-1.65
9379	CCCc1c([nH+]c(nc1)N)N	C04771750	-10.21	-3.18	-10.49	4.91	-1.44
9380	c1cc(sc1)/C(=C/[N+](=O)[O-])[O-]	C06829208	-10.21	-1.5	-16.01	7.99	-0.69
9381	c1cc(nc1)COBr	C14989372	-10.21	-1.2	-13.36	4.82	-0.47
9382	C/C(=NO)/C(=O)c1cccc1	C15221905	-10.21	-2.39	-12.39	5.25	-0.68
9383	CCOC(=O)[C@H]1[C@@H](O)F	C15442310	-10.21	0.07	-9.8	3.21	-3.68
9384	CNc1cc(=O)nc[nH]1	C17040194	-10.21	-2.04	-14.95	5.34	1.44
9385	COCCNc1ccc(cc1)F	C20051948	-10.21	-0.3	-10.97	3.56	-2.49
9386	Cc1cc(ns1)C=O	C20443679	-10.21	-1.99	-14.6	8.2	-1.82
9387	Cc1cnc(n1)C=O	C20443702	-10.21	-2.96	-10.11	5.22	-2.35
9388	Cc1cnc(c(n1)Cl)N	C21300754	-10.21	-1.33	-13.13	4.85	-0.6
9389	CCNc1nc(cc(n1)F)F	C00039511	-10.2	-1.91	-7.8	2.53	-3.02
9390	Cc1ccc(cc1)N	C00388037	-10.2	-1.62	-8.32	2.23	-2.49
9391	c1c(c(=O)[nH]c(n1)[O-])[N+](=O)[O-]	C00967347	-10.2	-6.45	-17.26	13.93	-0.42
9392	CN(C)C(=O)C(F)F	C01603497	-10.2	-1.53	-11.37	4.06	-1.37
9393	c1cc(ccc1)NNC(=S)N)O	C01657381	-10.2	-1.9	-17.99	10.31	-0.63
9394	CN1C(=O)CSCC1=O	C01676218	-10.2	1.06	-16.68	5.15	0.26
9395	c1c(c2c([nH]c(=S)[nH]2)nn1)Cl	C01713791	-10.2	-1.55	-12.73	6.37	-2.29
9396	C(=O)C(C(F)F)F	C01847431	-10.2	-2.45	-9.89	3.99	-1.84
9397	CCOC(=O)[C@@H](C)[N+](=O)[O-]	C02043884	-10.2	0	-12.96	6.26	-3.5
9398	Cc1ccnc(n1)Br	C02525097	-10.2	0.4	-13.07	4.91	-2.44
9399	c1cc(c(cc1F)C(=O)NN)F	C02578079	-10.2	-1.14	-16.27	8.18	-0.98
9400	c1nccc1C(=O)NO	C04362829	-10.2	-0.57	-19.99	10.04	0.32
9401	CNC(=O)Cl	C04963934	-10.2	-2.33	-12.85	4.1	0.88
9402	Cc1ccc2c(c1)cn[nH]2	C05612486	-10.2	-1.4	-10.02	4.03	-2.82
9403	C1[C@H]2[C@H](C1)O2	C12358906	-10.2	-0.97	-11.12	3.19	-1.3
9404	Cc1cc(=O)n([nH]1)C(=[NH2+])N	C12416814	-10.2	-3.41	-14.93	9.71	-1.57
9405	CCOC(=O)C[NH2+]	C19168190	-10.2	-0.53	-14.2	4.47	0.06
9406	CC(=O)c1cnoc1[N+](=O)[O-]	C20311077	-10.2	-0.12	-15.05	7.94	-2.97
9407	C(#N)Sc1c(nc([nH]c1=O)N)N	C22056681	-10.2	-5.12	-20.22	15.38	-0.24
9408	c1cnc(c(n1)C=O)Cl	C26897747	-10.2	-2.46	-13.37	6.51	-0.87
9409	COC(=O)c1cc(c(=O)[nH]c1)N	C32628217	-10.2	-2.15	-15.93	7.9	-0.03
9410	c1ncccc1c2cc([nH]2)O	C00129538	-10.19	-3.76	-14.08	5.83	1.81
9411	c1c(c(cs1)Cl)C=O	C00334485	-10.19	-2.22	-13.82	6.52	-0.67
9412	c1(c(c(c(c1F)F)O)F)O	C00388051	-10.19	-1.57	-13.31	3.94	0.76
9413	c1c(cc(c1)O)O	C00391883	-10.19	-2.55	-15.64	4.92	3.09
9414	Cc1ccc(c(c1)O)C(=O)OC	C00395010	-10.19	-0.92	-14.21	5.95	-1.01
9415	Oc1c(cccc1)N	C00403404	-10.19	-1.43	-11.5	4.11	-1.38
9416	c1cc(c(cc1O)C#N)O	C00405075	-10.19	0.25	-17.37	6.27	0.65
9417	Cc1ccc(cc1)I	C01003750	-10.19	-0.24	-10.77	1.3	-0.48
9418	COC(=O)c1c(no[nH]1[O-])N	C01062353	-10.19	-4.54	-11.29	7.44	-1.81
9419	C/C=C/C(=O)OCC=C	C01561516	-10.19	0.27	-10.1	3.56	-3.91
9420	CC(=O)OC	C01597766	-10.19	-1.3	-11.26	3.94	-1.57
9421	C=CCSC1=NCCN1	C01605548	-10.19	-0.93	-14.65	2.67	2.73
9422	CC/C=C(C)C#N	C01765460	-10.19	-1.27	-10.06	3.7	-2.55
9423	CCOC(=O)N(C)O	C05463729	-10.19	-2.14	-14.57	6.34	0.19
9424	CN(C)S(=O)(=O)NC#N	C05524996	-10.19	-2.05	-15.27	6.22	0.92
9425	CCOc1ncc(c(n1)Cl)F	C14982379	-10.19	-0.88	-12.27	3.69	-0.73
9426	c1cc(oc1)C(=O)c2nccs2	C15441685	-10.19	-0.07	-14.09	6.59	-2.62
9427	c1cc(ncc1/C(=N/O)/N)C(F)F	C15445959	-10.19	-3.15	-12.45	5.67	-0.26
9428	CCOC(=O)c1c([nH]cnc1=O	C17003049	-10.19	-0.09	-14.95	5.62	-0.78
9429	c1cc(nc2c1nsn2)N	C17061570	-10.19	-6.28	-13.28	9.47	-0.1
9430	c1ccc(c(c1)NC(=S)C(=O)N)O	C20508137	-10.19	-6.31	-13.18	8.27	1.03
9431	COc1ccc(cc1)OC(=O)OC	C30836142	-10.19	-1.36	-10.74	5.51	-3.61
9432	CCOC(=O)c1nccn1	C31776762	-10.19	1.25	-18.22	8.77	-2
9433	c1cc2c(cc1F)C(no2)N	C33358877	-10.19	-1.64	-13.33	7.01	-2.22
9434	C1[C@H]2C=CC(=O)[C@H](O1)O2	C00078169	-10.18	-1.98	-14.31	6.81	-0.71
9435	COc1c1ccc(s1)Br	C00153666	-10.18	0.16	-11.68	4.53	-3.19
9436	Cc1cccc(n1)Br	C00396090	-10.18	-1.3	-9.71	3.8	-2.97
9437	c1ccc(cc1)NNC(=S)NN	C01555391	-10.18	-1.65	-14.28	8.32	-2.56
9438	c1coc(=O)1	C01577290	-10.18	-2.11	-13.28	7.08	-1.88
9439	CCCC(=O)OC=C	C01665007	-10.18	2.35	-13.29	3.55	-2.79
9440	C[C@H]1C=CC(=O)O1	C01718609	-10.18	-2.28	-13.31	7.89	-2.49
9441	c1cc(c(c2c1[nH]cc2)F)F	C02386969	-10.18	-1.96	-13.57	6.52	-1.17
9442	C[C@@H](C(=O)C(=O)OC	C03848374	-10.18	-1.22	-11.98	4.97	-1.95
9443	COC1OCCO1	C03861532	-10.18	-1.07	-12.39	3.58	-0.31
9444	C[C@H]1CC=C[C@@H](C1)O	C05809801	-10.18	-0.69	-9.88	1.81	-1.42
9445	C[C@H](C(=O)C(=O)OC	C06036071	-10.18	-0.13	-13.08	4.99	-1.97
9446	c1[nH]c(=O)c(c(n1)[O-])Br	C15021880	-10.18	-2.56	-16.44	5.09	3.73

9447	c1cncc2c1[nH]c(=S)[nH]2	C19878153	-10.18	-3.16	-16.92	11.99	-2.09
9448	C#CCOCC#N	C20519005	-10.18	-1.53	-14.48	7.76	-1.93
9449	c1cc(c(c(c1)Cl)C=O)F	C00151783	-10.17	-2.65	-11.49	5.52	-1.54
9450	c1cccc1C(=S)N	C00161816	-10.17	-1.81	-17.97	10.98	-1.37
9451	Cc1cccc(c1)NC(=O)OC	C00395292	-10.17	0.34	-15.41	5.26	-0.37
9452	C1CN2C(=O)CSC2=N1	C01235980	-10.17	-1.07	-14.09	5.69	-0.7
9453	CCCCSC	C01644625	-10.17	-0.31	-10.01	1.15	-1
9454	c1cc(ccc1CC(=O)N)N	C01675015	-10.17	-1.38	-16.49	7.54	0.16
9455	CCNC(=O)c1csnn1	C01709778	-10.17	-2.32	-12.5	4.83	-0.19
9456	C[C@@H](C#C)O	C01756137	-10.17	-1.02	-11.44	2.4	-0.11
9457	C=Cc1ccc(cc1)C=C	C02015938	-10.17	-0.33	-6.75	1.94	-5.02
9458	C(C#CCC)O	C02383013	-10.17	-1.79	-12.18	4.46	-0.67
9459	c1c(c(cc(c1F)N)F)C(F)(F)F	C02556415	-10.17	-1.97	-9.23	2.97	-1.95
9460	COc1ccc(cc1F)Cl	C02567850	-10.17	2.06	-14.15	3.28	-1.37
9461	COCC/C(=C/C(=O)C(F)(F)F)/[O-]	C03885152	-10.17	-0.93	-10.12	2.94	-2.06
9462	c1ccc(cc1)c2ccc([nH]n2)N	C03887184	-10.17	-0.13	-12.73	5.01	-2.32
9463	c1cncc(c1Br)C=O	C04208984	-10.17	-2.5	-9.32	3.85	-2.19
9464	C(C([C@H](C(F)(F)F)F)F)F)O	C04262388	-10.17	-2.14	-11.29	3.84	-0.57
9465	CCOC(=O)CO	C04284427	-10.17	-3.78	-12.6	6.65	-0.44
9466	CCOC(=O)c1c(n[n-]n1)Cl	C04817834	-10.17	0.4	-13.53	4.27	-1.31
9467	CC(C)OP@[C@H](O)O	C05381386	-10.17	-4.05	-12.33	6.67	-0.46
9468	COC(=O)[C@H]1CCCO1	C06658150	-10.17	0.26	-13.77	6.02	-2.69
9469	CC(C)OC(=[N-])C(F)(F)F	C12417434	-10.17	-0.69	-10.01	1.25	-0.73
9470	Cc1c(scn1)C=O	C12959076	-10.17	0.75	-15.71	6.35	-1.55
9471	c1cc(c(nc1)C=O)Cl	C14982472	-10.17	-0.33	-14.01	6.37	-2.2
9472	CC(C(=O)N)(F)F	C16158444	-10.17	-1	-13.36	3.5	0.68
9473	CCc1c(c(ncn1)Cl)F	C19615494	-10.17	-0.99	-8.31	2.43	-3.31
9474	c1cc(ccc1NCC#N)Br	C20051713	-10.17	-2.3	-10.46	5.9	-3.31
9475	C[C@H](C(=O)Cl)N	C20216997	-10.17	-0.03	-14.12	3.74	0.24
9476	CC/C=C/C=O	C20231649	-10.17	-1.14	-10.82	3.35	-1.56
9477	CCOC(=O)CCO	C20232648	-10.17	-2.92	-11.28	4.81	-0.77
9478	C[C@@H]1C=NN([C@H]1C)C	C22205954	-10.17	-1.23	-9.91	3.23	-2.26
9479	Cn1c(nnn1)c2cccc2	C00039506	-10.16	-1.65	-14.04	7.23	-1.71
9480	c1cc(c(cc1F)NC(=S)N)F	C00156320	-10.16	-0.84	-15.72	9.2	-2.81
9481	c1cc2c(cc1N)ocn2	C00168382	-10.16	-3.42	-13.77	6.33	0.7
9482	c1cc(c(cc1Cl)O)NC(=O)NN	C00369954	-10.16	-1.59	-15.7	6.09	1.04
9483	Cc1c(sc(n1)Cl)C	C00407028	-10.16	-0.7	-10.22	3.75	-2.99
9484	C(c1nc(no1)c2c(non2)N)Cl	C01084794	-10.16	0.85	-16.65	6.04	-0.39
9485	CCSCC(=C)Cl	C01639899	-10.16	-0.89	-10.29	2.09	-1.07
9486	Cn1c(=O)[nH]c(=O)c(n1)C(=O)Cl	C01686835	-10.16	1.1	-17.16	6.32	-0.42
9487	CC/C=C/C=O	C01752910	-10.16	-0.72	-12.31	6.46	-3.58
9488	Cc1c(c(nc(n1)F)F)Cl	C02243611	-10.16	0.93	-11.12	2.34	-2.31
9489	c1(c(n[n-]n1)Br)C(=O)NN	C04115061	-10.16	0.31	-18.89	6.12	2.3
9490	C1CC(C1)/C(=NH+)[N-]/N	C04202552	-10.16	-1.07	-11.17	2.93	-0.86
9491	c1c(cnc(n1)C(=O)N)Cl	C04228199	-10.16	-2.7	-14.31	6.54	0.31
9492	COC(=O)c1cscn1	C04368835	-10.16	1.2	-15.79	6.16	-1.73
9493	c1ccc2c(c1)CCN=C2	C04403871	-10.16	-0.7	-9.94	3.14	-2.67
9494	COC(=O)[C]C@H([C(=O)OC])S	C05138610	-10.16	0.22	-13.12	4.7	-1.96
9495	Cc1c(nc[nH]c1=O)C	C08700020	-10.16	-2.46	-13.08	5.07	0.31
9496	COC(=O)c1c(ncs1)N	C08764165	-10.16	-2.65	-12.59	6.09	-1.01
9497	CCOC(=O)C=C	C17161119	-10.16	0.3	-9.78	3.33	-4
9498	[C@H-]([C(=NH2+)]N)Cl	C19735101	-10.16	-5.24	-12.43	7.32	0.19
9499	CCc1[nH]c(c(n1)C=O)Cl	C20357664	-10.16	-3.12	-11.3	6.48	-2.22
9500	c1ccnc(c1)/C(=C/C(=O)C(F)F)/[O-]	C20369428	-10.16	-2.39	-9	6.37	-5.14
9501	C(C#N)OCC(C(F)F)F	C20518189	-10.16	-2.07	-13.9	8.28	-2.47
9502	c1cc2c(c1)c(n2)O	C29865984	-10.16	-2.5	-15.25	6.44	1.15
9503	c1ccc(cc1)CNS(=O)(=O)C(F)(F)F	C00057550	-10.15	-1.83	-15.51	5.06	2.14
9504	C(#N)c1c(c(c(c1F)F)N)F	C00120149	-10.15	1.59	-13.65	4.06	-2.15
9505	C[C@@H]1CCCN=C1=O	C00158406	-10.15	-2.59	-11.62	5.2	-1.15
9506	c1c(csc1Cl)C(=O)N	C00334077	-10.15	-2.02	-17.2	7.19	1.88
9507	CCOC(=O)NCC(=O)N	C01571298	-10.15	-4.99	-14.58	6.99	2.42
9508	Cn1nc(nn1)C(=O)N	C01742190	-10.15	-2.69	-16.18	7.64	1.08
9509	COC(=O)CC(=O)C(F)(F)F	C02168480	-10.15	0.03	-14.18	7.16	-3.15
9510	c1c(c(c([nH]1)C(=O)C(F)(F)F)C(F)(F)F)	C02519460	-10.15	-0.99	-11.3	5.35	-3.22
9511	CC1([C@H](O)OC)C	C02539384	-10.15	-1.42	-11.41	3.87	-1.18
9512	CN1[C@H](C(=O)NC1=O)O	C03788800	-10.15	-2.98	-18.1	6.91	4.02
9513	c1cc(cnc1)c2cc([nH]2)O	C04626320	-10.15	-3.11	-14.83	6.14	1.65
9514	C(=O)(C(=O)N)N	C05177750	-10.15	-8.48	-10.33	4.76	3.9
9515	CCNc1c(cc(=O)[nH]c1=O)[O-]	C05346174	-10.15	-3.66	-15.39	8.3	0.59
9516	c1cc(nc(c1)Cl)C#N	C06093447	-10.15	-1.83	-12.01	6.34	-2.64
9517	CC[C@H](C(=O)C(F)(F)F)Br	C08700958	-10.15	-0.07	-8.78	5.03	-3.33
9518	C1COC(O)CC[N+](=O)[O-]	C15021206	-10.15	-2.55	-11	2.08	-1.68
9519	C[C@@H]1C(=O)NC(=S)N=N1	C16039605	-10.15	-2.22	-14.91	5.63	1.37
9520	c1c(c(=O)[nH]c(n1)N)CCO	C17174414	-10.15	-3.84	-15.14	5.92	2.91
9521	Cc1ccn(n1)CCO	C19092107	-10.15	-2.9	-11.67	4.84	-0.43
9522	COC(=O)C1=CCCC1N	C19942855	-10.15	-2	-10.33	4.43	-2.26
9523	c1c(c(cc1Cl)F)F)C#N	C22001384	-10.15	0.57	-9.78	3.13	-4.06
9524	CN1CSCSC1	C31308455	-10.15	-0.61	-10.26	2.32	-1.59
9525	C(CCC)CC=O	C32302927	-10.15	-0.22	-11.84	4.97	-3.06
9526	c1ccc(cc1)C(=O)NN	C00115752	-10.14	-2.76	-13.76	7.3	-0.91
9527	CC(=O)Nc1ccc(cc1)N	C00152946	-10.14	-1.01	-15.43	7.26	-0.95
9528	C[C@H](C=C)OC(=O)C	C00394373	-10.14	-0.32	-11.39	3.88	-2.31
9529	c1ccc(cc1)OC2=NC(=O)C(=O)S2	C01568197	-10.14	-0.23	-12.86	4.61	-1.66
9530	C=Nc1cccc1O	C01596247	-10.14	-2.88	-13.34	5.61	0.47
9531	CCOC(=O)NCCO	C01718597	-10.14	-3.69	-14.21	5.94	1.82
9532	c1cncc(c1Br)Cl	C02526750	-10.14	-2.2	-10.52	2.2	0.38
9533	c1cc(c(c(c1)O)F)C(F)(F)F	C02575080	-10.14	-3.76	-10.11	5.2	-1.47
9534	C1CC1N2C(=O)C(=O)NC2=O	C04218315	-10.14	-4.81	-11.11	4.27	1.51
9535	CC(=Nn1cc(cn1)[N-](=O)[O-])C	C05003193	-10.14	-0.93	-12.88	7.09	-3.42
9536	CCc1cnc(o1)CC	C05341800	-10.14	-1.15	-12.71	3.83	-0.12

9537	c1nnc(s1)NCC(=O)NO	C05497622	-10.14	-7.05	-15.78	11.19	1.51
9538	c1ccnc(c1)[C@@H](O)OS@=(O)O	C05572597	-10.14	-8.46	-17.93	13.77	2.49
9539	c1c(nc2n1CCS2)Cl	C05641908	-10.14	-0.75	-17.81	7.76	0.66
9540	COCC/C=C/CO	C06385258	-10.14	-0.82	-10.67	2.56	-1.22
9541	C=CC[C@@H]1C(=O)N=C(S1)N	C08615002	-10.14	-0.02	-12.04	3.33	-1.41
9542	C1CC1C(=S)N	C12394934	-10.14	-2.28	-11.94	5.66	-1.58
9543	Cc1ccc(cc1)/C=C/CO	C13542659	-10.14	-0.97	-9.87	3.25	-2.56
9544	c1cc2c(cc1F)c(nH)2O	C14983573	-10.14	-4.6	-11.77	5.19	1.04
9545	c1ccc2c(c1)cc(=O)[nH]n2	C15767326	-10.14	-1.94	-14.01	7.51	-1.7
9546	Cc1cc(ncc1F)Cl	C16159659	-10.14	1.11	-10.68	2.4	-2.97
9547	Cc1ccncc1Br	C20358063	-10.14	-1.17	-11.07	4.91	-2.82
9548	c1cn(cn1)C[C@@H]2CO2	C22178511	-10.14	-0.05	-15.27	7.47	-2.29
9549	Cc1ccnc(c1)Cl	C00388110	-10.13	-0.04	-10.55	3.47	-3
9550	COCC(=O)c1ccncc1	C00391131	-10.13	-1.17	-10.86	4.4	-2.5
9551	CCSc1[n-]nc(n1)C(F)(F)F	C01047355	-10.13	1.75	-12.53	3.53	-2.89
9552	c1cc(ccc1)CONC(=O)N	C01398289	-10.13	-3.58	-16.11	10.82	-1.26
9553	CG(=Cc1ccn1)C	C01703390	-10.13	0.24	-11.96	3.46	-1.88
9554	CCC[C@H]([N+](=O)[O-])Br	C01758989	-10.13	-0.64	-11.43	2.41	-0.48
9555	CCOC(=O)C[C@H](C(F)(F)F)O	C02168466	-10.13	-1.08	-12.27	5.01	-1.79
9556	C(C(=O)Cl)S[C@H](C(F)(F)F)Cl	C04204957	-10.13	-2.28	-9.68	3.67	-1.84
9557	Cc1cnn(c1)CO	C04290890	-10.13	-0.98	-14.68	4.96	0.57
9558	C1COP(=O)O1	C04803593	-10.13	-1.28	-13.49	3.94	0.71
9559	Cc1ccc(cc1)C(=S)N	C06070792	-10.13	-0.95	-15.01	9.12	-3.29
9560	c1c(c[n1]C(=O)CC)Cl	C06328676	-10.13	0.02	-11.58	4.18	-2.76
9561	C1C=CC(=O)NC1=O	C13546090	-10.13	-1.92	-16.64	8.28	0.15
9562	C1Cc2c(n[nH]c2C=O)C1	C20270526	-10.13	-2.86	-14.34	8.97	-1.9
9563	C[C@@H]1CC(=C(C1=O)O)C	C25695707	-10.13	0.79	-13.97	4.98	-1.93
9564	Cc1cccnc1N[N+](=O)[O-]	C00053412	-10.12	1.81	-15.29	7.02	-3.65
9565	c1cc2c(cc1Cl)nsn2	C00168246	-10.12	-2.9	-11.96	3.16	1.59
9566	COCC1cc[nH]1O	C00335575	-10.12	-2.22	-16.62	5.93	2.8
9567	c1ccc(cc1)CC(=O)N	C00394644	-10.12	-4.85	-10.79	6.85	-1.32
9568	Cc1ccc(c1)C=O	C00896726	-10.12	-1.53	-9.17	4.26	-3.68
9569	CC[C@@H](CC=C)O	C01766031	-10.12	-0.19	-11.53	1.49	0.12
9570	C1[C][C@@H](OC)COC(=O)C(F)(F)F	C02155893	-10.12	2.34	-13.46	3.18	-2.18
9571	Cn1ccc(c1)CO	C02383102	-10.12	-3.16	-11.36	5.38	-0.97
9572	c1c(cc(c(c1C(=O)C)F)F)F	C02575067	-10.12	1.41	-12.63	3.63	-2.53
9573	c1ccc2c(c1)c(ns2)[O-]	C02581983	-10.12	-3.96	-12	5.87	-0.03
9574	CC(=O)COCC#C	C03121853	-10.12	-0.06	-16.11	8.05	-2
9575	C(S)C#N	C04501379	-10.12	-1.27	-10.93	4.21	-2.14
9576	C=C[N+](=O)[O-]	C05194331	-10.12	-1.35	-12.84	5.8	-1.74
9577	C(=O)C(C(C(F)(F)Cl)(F)(F)F)N	C05287059	-10.12	-2.78	-10.41	3.58	-0.51
9578	c1ccc(cc1)OC(=O)NCO	C05484624	-10.12	0.11	-19.54	8.11	1.2
9579	c1cc(ccc1[C@@H]2CO2)O	C06093218	-10.12	-1.86	-14.62	4.73	1.64
9580	c1cc(ccc1C(=O)CO)O	C13542648	-10.12	-4.05	-12.54	6.57	-0.09
9581	COCC/C=C/C(=O)C	C13544952	-10.12	0.42	-10.37	4.2	-4.37
9582	c1csc(c1C)Cl	C16123946	-10.12	-0.4	-7.88	2.14	-3.98
9583	C1COCC[C@H]1CCl	C20078002	-10.12	0.42	-10.43	1.99	-2.1
9584	C[C@H](C1CC1)S	C20476538	-10.12	-0.63	-7.47	1.18	-3.19
9585	CNc1ccc(cn1)Br	C21516533	-10.12	-0.68	-10.03	2.99	-2.39
9586	C[C@H](c1cnn(c1)C)O	C26546637	-10.12	-3.41	-12.36	5.97	-0.32
9587	CCOC(=O)c1ccc[nH]1	C00165736	-10.11	0.99	-13.36	5.39	-3.14
9588	CCCOCC(=S)S	C01562478	-10.11	-3.04	-11.98	4	0.9
9589	c1cnc2nncn2c1	C01597159	-10.11	-2.68	-19.73	13.85	-1.55
9590	CC(C)N[N+](=O)[O-]	C01668640	-10.11	-1.49	-11.4	4.47	-1.68
9591	COc1ccc(cc1)C=C	C01675020	-10.11	-0.42	-10.84	2.68	-1.53
9592	CC(=O)OC[C@H](CC)O	C01699458	-10.11	-0.48	-15.91	5.94	0.34
9593	CCSCC#N	C01700241	-10.11	0.34	-10.92	3.99	-3.52
9594	COc1ccc(cc1N)F	C01706177	-10.11	-2.32	-9.32	2.93	-1.39
9595	CCOC(=O)[C@H](C#N)Br	C01708352	-10.11	-0.01	-11.88	5.02	-3.23
9596	CC[C@H](C)O	C02539567	-10.11	-0.39	-10.18	1.38	-0.92
9597	C=COCCCO	C02572050	-10.11	-0.23	-12.43	3	-0.45
9598	Cc1cc(cen1)C#N	C04099779	-10.11	-1.85	-10.85	4.05	-1.46
9599	C[C@@H]1[C@@H](CCO1)S	C04262494	-10.11	0.33	-10.78	2.02	-1.68
9600	C=CN1CCOC1=O	C05048437	-10.11	-0.93	-15.42	7.72	-1.49
9601	c1cc(ccc1/C=C/O)[N+](=O)[O-]	C08579449	-10.11	-2.38	-14.72	8.77	-1.77
9602	c1c(ncnc1O)C(F)F	C12958923	-10.11	-1.36	-13.53	4.43	0.36
9603	C1CC(=O)N(C1)C/C(=N/O)/N	C131116400	-10.11	-3.91	-15.8	9.26	0.34
9604	c1cc2c(c(c1)N)C(=N)non2	C15909741	-10.11	-1.68	-12.49	5.59	-1.54
9605	C/C(=N/O)/C=N/O	C17300243	-10.11	-5.45	-14.71	7.8	2.25
9606	CCc1cnn1N	C19089908	-10.11	-3.25	-11.82	6.33	-1.38
9607	c1c(cc1)Br)CO	C30678085	-10.11	-2.65	-15.7	6.23	2
9608	Cc1ccc(c1)NN	C00085252	-10.11	-2.12	-8.33	2.63	-2.28
9609	c1ccc2c(c1)CCN2N	C00153910	-10.1	-2.15	-8.58	2.92	-2.28
9610	c1cc(ncc1Cl)Cl	C00336169	-10.1	-2.12	-11.9	4.04	-0.12
9611	CC1(CCCC1)O	C01602491	-10.1	-1.72	-8.95	1.66	-1.09
9612	c1ccc2c(c1)c(c[nH]2)O	C01628352	-10.1	-3.88	-13.25	8.18	-1.14
9613	c1cc(oc1CO)CO	C01672225	-10.1	-4.89	-14.76	6.79	2.77
9614	C[C@@H](CO)C(=O)C	C01690992	-10.1	-1.6	-12.29	3.78	0.01
9615	CC(C)OCC#N	C01847865	-10.1	-0.25	-11.31	4.11	-2.65
9616	CCO[C@H](C(F)(F)F)O	C02040616	-10.1	-2.19	-9.78	2.41	-0.54
9617	c1c([nH]nc1CO)CO	C02518933	-10.1	-6.06	-16.25	7.54	4.67
9618	C[C@H](CO)C=C	C02539288	-10.1	-0.7	-11.65	1.8	0.45
9619	CCOC(=O)[C@H](C(F)(F)F)O	C02548173	-10.1	-0.68	-11.54	3.65	-1.53
9620	Cn1ccc(cn1)/C=N/O	C02578418	-10.1	-3.03	-14.39	7.18	0.14
9621	c1ccnc(c1)NC(=O)C(=O)N	C03043690	-10.1	-2.07	-18.28	7.72	2.52
9622	c1c(nc2nncn2n1)[O-]	C03070866	-10.1	-2.85	-18.62	10.06	1.3
9623	C[C@H](CCS)O	C04533097	-10.1	-1.09	-12.73	2.1	1.62
9624	CCO[C@H]1OCCS1	C05718367	-10.1	-0.36	-14.03	3.56	0.74
9625	CC(=C/C=C/C(=O)C)C	C14591922	-10.1	-0.55	-9.43	3.82	-3.94
9626	C[C@H]1C(=O)[C@H](S1)C	C17141873	-10.1	0.03	-10.17	2.85	-2.8

9627	C1C(=O)N=C(O)N	C17173516	-10.1	-2.04	-15.35	4.23	3.06
9628	C1CC(C1)CC#N	C19093253	-10.1	-0.56	-10.54	4.48	-3.49
9629	CC[C@H](C)SCCC#N	C19870152	-10.1	-0.78	-8.67	3.89	-4.55
9630	c1cnc(cn1)NCCO	C21796689	-10.1	-2.07	-15.9	6.43	1.44
9631	c1ccc(c(c1)O)OC2CC2	C21991259	-10.1	-0.92	-13.4	6.84	-2.62
9632	Cc1ccc(nc1)Br	C00409192	-10.09	-0.7	-12.84	3.33	0.11
9633	C=CCNC1=CCO1	C01673732	-10.09	-0.24	-16.92	3.33	3.75
9634	C[C@H](CC#N)CCI	C01707957	-10.09	-1.78	-11.19	6.11	-3.23
9635	Cc1cc(c(c1)C)S	C02002624	-10.09	-0.44	-9.15	2.63	-3.13
9636	C[C@H](CC(=O)OC)Cl	C02162125	-10.09	-2.41	-10.69	4.69	-1.68
9637	c1csc(n1)NC(=S)NN	C02275347	-10.09	-3.59	-15.69	11.28	-2.09
9638	CCc1nnc(n1)NN	C03133970	-10.09	-2.71	-13.37	8.24	-2.24
9639	CC[C@H](C(=O)Cl)Cl	C05227378	-10.09	0.59	-11.81	1.97	-0.83
9640	CN(C)C/C(=N/O)N	C19424528	-10.09	-4.17	-13.69	5.67	2.1
9641	C1CCC(C1)ON	C19779147	-10.09	-1.55	-9.53	2.23	-1.25
9642	c1ccc(cc1)COP@H(=O)ON	C19910525	-10.09	-1.22	-14.64	8.19	-2.42
9643	c1cc(oc1)c2cc(sc2)C=O	C22200606	-10.09	0.31	-12.6	6.05	-3.84
9644	C/C=C/[C@H]1CCC(=O)C1=C	C01575071	-10.08	-1.29	-10.68	3.64	-1.75
9645	CC=CCCO	C01680814	-10.08	-0.5	-12.38	3.39	-0.6
9646	CSCc1ccc(cc1)N	C01729092	-10.08	-1.41	-12.18	2.87	0.65
9647	C/C=C(C)CCO	C01995218	-10.08	-0.75	-11.91	1.92	0.67
9648	CC(=O)[C@H](OC)F	C02032483	-10.08	-0.73	-12.16	4.36	-1.55
9649	CCOC(=O)CCC(=O)Cl	C02242610	-10.08	0.22	-10.74	3.74	-3.29
9650	c1c(c[nH]1)CCCO	C02385076	-10.08	-4.03	-14.38	5.73	2.6
9651	COCc1c(ccc1)F)N	C02527852	-10.08	0.69	-14.22	4.88	-1.42
9652	CC(=C)(C)(C)O	C02579181	-10.08	-0.74	-10.66	1.52	-0.19
9653	C1C=C[C@@H]2[C@@H]1C(=O)C2	C05046473	-10.08	-0.58	-9.25	3.05	-3.3
9654	CC(=NOC)C	C05048375	-10.08	-0.05	-11.76	3.48	-1.74
9655	C1CC(=NNC(=O)N)C1	C05081169	-10.08	-1.48	-14.7	5.81	0.29
9656	C1CCc2c(c(on2)N)C1	C05175401	-10.08	0.63	-14.35	4.49	-0.86
9657	C[C@H]1[C@@H](C(=O)OC)1	C06030659	-10.08	-0.87	-12.7	5.97	-2.48
9658	CNC(=S)Nc1cc(coc1)F	C07571141	-10.08	0.33	-15.63	8.83	-3.61
9659	Cc1ccc(cn1)C=O	C08698167	-10.08	-2.15	-12.52	5.44	-0.85
9660	c1cc(ncc1C(F)(F)F)OCC#N	C11535916	-10.08	-0.52	-12.35	5.1	-2.31
9661	CC(=O)Nc1cc(coc1)F)N	C12505819	-10.08	-1.37	-13.56	5.98	-1.12
9662	c1csc2c1nc[nH]c2=O	C13598177	-10.08	-4.58	-12.28	6.28	0.5
9663	c1c2c(cc1c1)C[nH]2	C13656634	-10.08	-4.95	-7.75	6.34	-3.71
9664	Cc1cccc(n1)CBr	C15932735	-10.08	-0.35	-9.69	3.54	-3.58
9665	Cc1c(cc(cn1)Br)[N+]([O-])	C21303269	-10.08	-1.58	-7.86	2.51	-3.15
9666	C1COCC(=O)[C@H]1ON	C22006360	-10.08	-1.76	-14.44	6.29	-0.17
9667	c1cc(ncc1Br)C(=O)N	C00151257	-10.07	-2.68	-11.32	4.11	-0.18
9668	Cc1ccc(n1)NC	C00330652	-10.07	-3.48	-9.02	4.2	-1.77
9669	CC1=CCS(=O)(=O)C1	C00394514	-10.07	-1.07	-15.8	7.32	-0.52
9670	c1ccc2c(c1)CC[C@H]2O	C00901099	-10.07	-1.41	-9.49	3.07	-2.24
9671	c1cn2cnnc2c(=O)[nH]1	C01566214	-10.07	-3.95	-19.14	15.2	-2.18
9672	Cc1cc2ncnn2cn1	C01571373	-10.07	-1.33	-13.58	5.71	-0.87
9673	c1cc([nH]c1)c2ccc[nH]2	C01581224	-10.07	1.36	-15.74	4.1	0.21
9674	CNc1ncc(c(n1)N)N	C01639691	-10.07	-2.5	-12.74	5.29	-0.12
9675	C=CCSCCO=C	C01729233	-10.07	-2.25	-11.56	5.09	-1.36
9676	COCC1nnc(s1)[S-]	C02511075	-10.07	-2.52	-12.11	5.07	-0.52
9677	CCCOCC=C	C02539247	-10.07	-0.29	-9.91	1.29	-1.17
9678	c1cc(oc1)C(=O)C(O)O	C02559764	-10.07	-4.75	-16.69	10.78	0.59
9679	c1cc(c(c1)CC#N)O	C03133991	-10.07	-3.05	-17.3	9.72	0.57
9680	C[C@H]1CCNC1=O	C05226936	-10.07	-2.25	-13.19	5.78	-0.41
9681	[C@H](C)C(O)C@H(F)(Cl)(F)C(F)(F)F	C08698274	-10.07	-2.01	-8.94	4.07	-3.2
9682	Cc1c(=O)nc([nH]1)NN	C08951610	-10.07	-2.78	-15.93	6.55	2.08
9683	Cc1cc([nH]1)OCC#N	C12398527	-10.07	-3.43	-12.53	7.31	-1.42
9684	c1c[nH]c2c1cnc(c2)Br	C14985684	-10.07	1.84	-14.43	5.12	-2.59
9685	c1ccc(cc1)Cc2nc([nH]2)N	C15635599	-10.07	0.2	-12.02	6.11	-4.35
9686	C/C(=N)N/C(=N)N/C	C16978810	-10.07	-2.14	-12.92	4.11	0.88
9687	C[C@H](c1cccnc1)O	C21985760	-10.07	-2.42	-13.06	5.24	0.18
9688	c1c(c[nH]c(=O)c1)C#N	C22995856	-10.07	-5.54	-17.68	14.14	-0.99
9689	Cc1nc(cot1)C(=S)N	C30677881	-10.07	-1.81	-17.07	8.51	0.31
9690	c1cnc(c1)C(=O)NCC(F)(F)F	C33029006	-10.07	0.63	-14.01	5.34	-2.03
9691	c1cc(c(c1)F)NC(=O)NN)F	C00167739	-10.06	0.16	-18.1	8.67	-0.79
9692	COCc1ccc(cnn1)[O-]	C00337143	-10.06	-2.19	-16.55	8.05	0.63
9693	Cc1c(c([nH]1)NN)Cl	C01233068	-10.06	-4.43	-9.14	3.87	-0.36
9694	C(#N)c1c([n+](on1)[O-])C#N	C01304684	-10.06	-1.97	-11.12	5.51	-2.48
9695	C1C(=O)CC(=O)NC1=O	C01556431	-10.06	0.79	-18.83	7.05	0.93
9696	C1C(=O)OCCO1=O	C01682843	-10.06	-2.27	-12.84	6.7	-1.65
9697	c1c(c(=O)[nH]c(=O)[nH]1)C=N/NC=O	C01702911	-10.06	-4.99	-19.92	11.68	3.17
9698	c1cc(coc1)OCC#N)Cl	C01738561	-10.06	0.07	-14.85	6.43	-1.72
9699	CCc1ccc2c(c1)[nH]nn2	C02534162	-10.06	-4.63	-12.01	4.88	1.7
9700	c1cc(c(c1)OC(F)(F)Cl)O	C02540209	-10.06	-1.18	-10.74	2.41	-0.55
9701	c1cc(c(c1)C(=O)Cl)F)F	C02545325	-10.06	1	-14.3	5.75	-2.51
9702	C=CCCOCCBr	C04203465	-10.06	-1.7	-9.84	1.83	-0.35
9703	CC[C@H](C)N=C=O	C04979173	-10.06	-0.34	-10.81	1.81	-0.72
9704	[H]/N=C\C#N)/C(C#N)C#N	C05012752	-10.06	-2.6	-14.44	7.85	-0.87
9705	C(Br)[C@@H](CO)O	C05410102	-10.06	-3.94	-11.49	3.84	1.52
9706	CC1=CC(=O)O[C@H]1O	C05766771	-10.06	-2.26	-15.6	7.21	0.59
9707	CCOC(=O)/C=C/C=C/C	C08602915	-10.06	-0.48	-8.88	3.75	-4.44
9708	Cc1cn(c(=O)[nH]1)S(=O)(=O)C	C09193603	-10.06	-2.49	-20.02	12.63	-0.18
9709	c1cc(c(c1)O)F)C#N)F	C10336047	-10.06	0.94	-16.75	7.27	-1.52
9710	c1cnc1[C@H]2C[C@H]2C=O	C12370897	-10.06	-0.88	-13.36	7.54	-3.36
9711	Cc1cccc2c1[nH]nc2	C13497059	-10.06	-2.32	-8.93	4.08	-2.89
9712	CC[N+](=O)[O-]	C13507190	-10.06	-0.85	-11.23	3.89	-1.87
9713	CCCN1C(=O)CSC1=O	C15014963	-10.06	1.25	-13.47	4.55	-2.39
9714	CC(=O)OCC(C(F)(F)F)F	C16158746	-10.06	-0.15	-10.18	3.68	-3.4
9715	c1cc(coc1c2cn[nH]2)F	C16429384	-10.06	0.11	-13.74	5.92	-2.35
9716	Cc1nc([nH]1)SCCO	C18039857	-10.06	-4.24	-15.48	9.87	-0.21

9717	CScc1nc(on)1CCl	C19090818	-10.06	-0.57	-13.13	5.75	-2.11
9718	CC[C@H]1[C@@H](O)1C	C19260485	-10.06	-0.62	-10.55	2.78	-1.66
9719	c1ccc2c(c1)C[C@H](O2)N=C=O	C19428276	-10.06	-0.95	-12.85	3.96	-0.22
9720	CCNc1nc(cs1)C	C21518939	-10.06	-0.63	-10.95	3.99	-2.47
9721	c1c(c[nH]c(=O)c1F)Cl	C21981711	-10.06	-3.17	-18.76	12.53	-0.67
9722	c1ccc2c(c1)cc(o2)C=O	C00158629	-10.05	-3.82	-9.88	5.01	-1.35
9723	CN1CC1=C	C01600530	-10.05	-1.25	-11.15	2.12	0.23
9724	CCN(C)C=O	C01603722	-10.05	-1.12	-13.41	5.32	-0.85
9725	c1c(cnc2c1nns2)Br	C01617946	-10.05	-2.12	-15.45	4.66	2.86
9726	CC(=O)C#C	C02039581	-10.05	-1.7	-11.56	5.03	-1.81
9727	c1c(cnc1N)ClBr	C02582882	-10.05	-2	-12.79	2.79	1.95
9728	C/C(=C/c1cccc1)/[N+](=O)[O-]	C04777940	-10.05	0.26	-13.34	5.21	-2.18
9729	C1COC(=S)N1	C05190638	-10.05	-1.05	-13.83	2.89	1.95
9730	CN1CCC(=O)N1	C05758016	-10.05	-1.79	-14.05	5.34	0.44
9731	C1COCC1=O	C12495988	-10.05	-0.4	-12.73	3.56	-0.48
9732	CCOCC(=S)S	C13763871	-10.05	-1.15	-10.41	3.99	-2.48
9733	C/C=C/C=C(C=O)N	C15274137	-10.05	-0.19	-14.49	5.33	-0.69
9734	Cc1cc(ccc1F)OC(F)F	C16125803	-10.05	-0.77	-7.06	1.52	-3.74
9735	c1cc(cnc1)C(=O)C=N/O	C17163781	-10.05	-0.2	-16.79	8.03	-1.1
9736	CC(C)c1nc(no1)CCl	C19089866	-10.05	1.59	-13.1	3.76	-2.31
9737	CSc1ccc(cn1)N	C19951408	-10.05	0.05	-13.85	4.98	-1.22
9738	Cc1c(cncn1)C=O	C20443760	-10.05	-0.45	-13.47	5.94	-2.07
9739	c1ccc(c(c1)NC(=O)NN)Cl	C00167741	-10.04	-1.48	-13.06	5.55	-1.06
9740	c1ccc2c(c1)ncnn2	C00394801	-10.04	-3.05	-13.37	6.49	-0.11
9741	CC[C@@H]1[C@@H](c1cccc1)O	C00403955	-10.04	-1.39	-10.1	2.88	-1.44
9742	c1c(c(=O)[nH]c(=O)[nH]1)C(F)(F)F	C01036885	-10.04	-5.76	-14.55	10.23	0.04
9743	CC(=O)Nc1cc(c(c1)F)NF	C01574360	-10.04	-1.41	-14.44	6.88	-1.08
9744	CC(C)[C@@H](C=C)O	C01615748	-10.04	-0.27	-9.3	1.03	-1.5
9745	C[C@H]([C@H]([C@H](C)Cl)O	C01762872	-10.04	-1.49	-9.59	1.71	-0.66
9746	c1c(cc(c(c1)C#N)F)Cl	C02243325	-10.04	-0.83	-10.72	4.58	-3.67
9747	c1cc2ccc2c(c1)O	C02510646	-10.04	-2.63	-13.24	5.61	0.22
9748	CCc1c(c[nH]1)C=O	C04243076	-10.04	-2.34	-14.44	8.29	-1.55
9749	Cc1c(c([nH]1)N)C#N	C04353708	-10.04	-5.18	-12.57	8.1	-0.39
9750	CC1SCCCS1	C04521671	-10.04	0	-8.2	1.95	-3.79
9751	c1c(c(nc(n1)NN)N)C(=O)NN	C05580295	-10.04	-5.73	-13.96	7.94	1.71
9752	C{[C@](OC(F)(F)F)(F)Br}(F)F	C08698309	-10.04	0.39	-10.35	1.98	-2.05
9753	CC(C)NC(=O)c1cn[nH]c1N	C14608624	-10.04	-4.31	-12.07	6.4	-0.07
9754	CC(=O)c1ccc(nc1)C#N	C14981999	-10.04	1.3	-15.33	6.59	-2.6
9755	c1ncccc1[C@@H]2CO2	C19730644	-10.04	-3.26	-10.64	5.19	-1.32
9756	c1cncc2c1ncc(c2)Cl	C00331567	-10.03	-0.6	-10.56	3.89	-2.75
9757	Cc1cc2ccc2c(c1)F	C00403325	-10.03	-3.23	-6.86	4.03	-3.97
9758	c1c(c(ncn1Cl)Cl)Cl	C01020140	-10.03	1.98	-14.16	2.32	-0.17
9759	c1cnc(nc1)N[C@@H](C(F)(F)F)O	C01558269	-10.03	-4.05	-10.21	4.94	-0.71
9760	Cc1nnc(s1)C	C01609484	-10.03	-1.58	-12.43	5.68	-1.7
9761	CC(=O)C(C=O)C(=O)OC	C01667224	-10.03	0.29	-14.88	7.53	-2.98
9762	C1[C@@H]([C@H]([C@H]1)Cl)Cl	C01677878	-10.03	1.2	-13.58	3.39	-1.04
9763	Cc1cc(ncn1)SC#N	C01680097	-10.03	-1.34	-13.91	6.26	-1.05
9764	C(CCl)OC(=O)N	C01865419	-10.03	-1.26	-14.92	5.33	0.81
9765	c1ccn2cc(nc2c1)Cl	C02650735	-10.03	-1.77	-14.43	6.9	-0.74
9766	C1CCC(=O)[C@@H](C1)Cl	C03860268	-10.03	2.69	-13.64	4.24	-3.32
9767	c1(c(nc([n+](c1N)[O-])N)N)[N+](=O)[O-]	C04824732	-10.03	-2.73	-14.26	7.76	-0.8
9768	Cc1c[nH]c2c1nccn2	C06491788	-10.03	-4.46	-12.2	8.49	-1.87
9769	c1c(=O)[nH]c(=S)[nH]n1	C08100917	-10.03	-3.01	-14.57	7.8	-0.25
9770	c1cc2c(cc1Cl)oc(n2)N	C08614805	-10.03	-7.36	-6.15	3.67	-0.18
9771	C1[C@@H]([C@H]([C@H]1)N)Br	C08614815	-10.03	-0.26	-10.59	2.06	-1.25
9772	C(c1nnc(o1)C(F)F)Cl	C08731344	-10.03	-2	-12.46	4.09	0.34
9773	C{[C@H]([C@H]([C@H]1)O)S	C12341762	-10.03	-2.33	-12.86	3.54	1.62
9774	c1cnc(cc1[N+](=O)[O-])C#N	C14982541	-10.03	-0.46	-13	6.28	-2.85
9775	CNc1ncc(c1)Cl	C16124195	-10.03	-1.55	-11.43	3.74	-0.79
9776	c1ccc(cc1)FNCCO	C20051177	-10.03	-2.98	-11.49	4.95	-0.51
9777	c1cnc(nc1)SC#N	C00334397	-10.02	-1.99	-12.04	6.11	-2.1
9778	c1c(c(n1)CCO)N(C(=O)N	C00399507	-10.02	-5.74	-16.62	7.62	4.72
9779	Cc1ccccc1OC(=O)C	C01095311	-10.02	-0.55	-10.42	5.76	-4.81
9780	c1c(=O)[nH]c(=O)[nH]c1Br	C01597571	-10.02	-1.25	-16.7	5.25	2.69
9781	c1cc2c(cc1Cl)scn2	C01605362	-10.02	-2.24	-12.03	3.85	0.61
9782	C=CCC#N	C01641012	-10.02	-0.65	-11.49	4.53	-2.4
9783	CC[C@H]1(C(=O)O1)Br	C01729752	-10.02	-0.43	-9.2	1.94	-2.34
9784	Cn1cc(ccc1=O)C#N	C01845712	-10.02	-1.84	-14.7	8.38	-1.86
9785	C[C@@H]([C@H]([C@H]1)Cl)O	C01850593	-10.02	-1.56	-8.78	3.1	-2.78
9786	COCCSC	C02167500	-10.02	-0.79	-10.61	1.7	-0.32
9787	CCOcn1ccnc1Cl	C02510763	-10.02	-2.27	-9.3	4.13	-2.58
9788	COCCc1ccc(cc1)O	C02566176	-10.02	0.11	-11.81	3.25	-1.57
9789	Cc1ccc(c(c1F)O)Cl	C02574987	-10.02	0.69	-14.27	3.68	-0.11
9790	CC[C@@H](C(=O)C)S	C04802621	-10.02	-0.49	-11.04	4.15	-2.65
9791	C1=C[C@@H]([C@@H]([C@H]1)Cl)O	C04978595	-10.02	-1.83	-15.06	4.07	2.8
9792	CC(=O)NCCSC(=NH2+)N	C05378213	-10.02	-0.57	-19.33	6.52	3.36
9793	c1[nH]c2c(n1)c(ncn2)Br	C05783717	-10.02	-4.47	-10.38	7.72	-2.89
9794	CC(C)OCCCl	C06645507	-10.02	0.14	-9.67	2.31	-2.78
9795	Cc1ccc(ccn1)Br	C12359508	-10.02	1.41	-10.68	2.3	-3.05
9796	c1ccnc(c1)[C@@H]([C@@H]2[C@H](O2)C#N	C13213068	-10.02	-4.24	-9.08	5.19	-1.89
9797	C1COC[C@H]1Cl	C14983073	-10.02	0.45	-9.54	1.68	-2.6
9798	CS/C(=N/O)/C=N/O	C17125528	-10.02	-0.54	-15.08	3.86	1.73
9799	COC(=O)Cn1c(ncn1)N	C18192103	-10.02	-1.63	-17.96	11.35	-1.78
9800	c1ccc(ccc1)C(=O)F	C19729346	-10.02	-1.95	-10.59	4.87	-2.3
9801	CN(C)c1cc[nH+]c(c1)F	C21990753	-10.02	-1.82	-10.26	4.42	-2.42
9802	c1cc2c(cc1CO)CC2	C22013201	-10.02	-2.28	-10.74	5.21	-2.22
9803	C1[C@H]([C@H]([C@H]1)Cl)CS	C32628463	-10.02	1.08	-9.64	2.21	-3.68
9804	c1ccc(c(c1)F)C(=O)N)N	C00154077	-10.01	-2.32	-15.86	7.33	0.83
9805	CCOC(=O)CC#N	C00164473	-10.01	-1.47	-14.8	8.93	-2.66
9806	COC(=O)Cc1ccc(cc1)Cl	C00398512	-10.01	-2.16	-11.23	5.31	-1.93

9807	c1c(cc(c(c1O)Br)O)O	C01609435	-10.01	-2.19	-15.04	4.78	2.44
9808	C(C(CCI)O)Cl	C01696572	-10.01	-0.34	-12.92	4.08	-0.83
9809	CCCC(=O)[C@@H](C)O	C02527911	-10.01	-1.69	-10.46	3.81	-1.67
9810	CCCC#CCCC	C02579172	-10.01	-1.86	-8.91	2.72	-1.96
9811	C1[C@@@H](S[C]C@H)(S1)O)O	C03861336	-10.01	-3.51	-11.17	2.81	1.87
9812	c1nc2c(c(n1)[O-])n[nH]n2	C04429559	-10.01	-5.23	-20.19	14.69	0.72
9813	c1nc(no1)c2c(non2)[N+](=O)[O-]	C04844055	-10.01	-0.56	-14.42	6.49	-1.52
9814	C[C@@@H]1CC=C[C@H](C1)O	C05809803	-10.01	-1.11	-9.15	1.78	-1.53
9815	CCCCOP(O)O	C05973697	-10.01	-3.03	-13.21	5.12	1.11
9816	CC(C)CNC(=O)O	C15894359	-10.01	-3.34	-12.03	4.58	0.78
9817	C[C@@@H]1[C@H](O1)[C@H]2[C@H](O)C2	C17003126	-10.01	0.61	-13.13	3.04	-0.53
9818	Cc1cc(cnc1N)Br	C19735096	-10.01	0.29	-12.04	3.83	-2.09
9819	Cc1ccc(c(c1)F)Nc	C20359878	-10.01	-1.91	-7.68	2.64	-3.06
9820	c1cc(cc(c1)Cl)OC(=O)N	C32603037	-10.01	-1.37	-15.73	7.79	-0.7
9821	CCC/C=C/O	C01531148	-10	-0.48	-12.46	4.55	-1.61
9822	COc1ccc(o1)[N+](=O)[O-]	C01591770	-10	0.32	-14.92	6.87	-2.27
9823	CCc1c(coc1[O-])O	C02046320	-10	1.05	-13.45	4.7	-2.29
9824	CO[C@@@](C(=O)N)(C(F)F)F	C03123722	-10	-1.94	-12.33	3.86	0.41
9825	CCSc1nc(ns1)N	C04290487	-10	-3.39	-9.31	4.81	-2.11
9826	COC(F)F	C05701046	-10	-0.6	-10.27	1.36	-0.49
9827	c1cn(c(n1)C)C(F)F	C09200828	-10	-2.21	-11.04	6.38	-3.14
9828	c1cc2c(cc1Cl)oc(n2)[O-]	C13463739	-10	-6.93	-8.56	7.35	-1.87
9829	Cc1cc2c(ccnH2)cn1	C15021972	-10	1.43	-13.88	5.11	-2.67
9830	c1cc(cc(c1O)/C=N/O)O	C15046774	-10	-1.4	-17.03	5.86	2.57
9831	C1C[C@H](C)C[C@H]2[C@H]1C2)O	C17059382	-10	-0.86	-9.07	1.62	-1.69
9832	c1cn2ccc2cc1O	C18559358	-10	-3.78	-12.38	7.79	-1.63
9833	c1cn(c[nH]1)CCO	C19926709	-10	-5.13	-13.27	7.75	0.66
9834	CNC(=O)c1ccc(c(c1)N)F	C21953393	-10	-2.74	-15.15	8.39	-0.5
9835	COC(=O)C(=O)NN	C31775914	-10	-2.14	-15.59	6.85	0.88
9836	C[C@H](C)C(=O)c1cccs1	C32005445	-10	-0.49	-9.58	3.58	-3.51
9837	Cn1cc(c(n1)C(=O)OC	C32777199	-10	0.27	-14.31	6.31	-2.28
9838	Cc1c(ccc1)CO	C00159615	-9.99	-1.29	-12.72	4.55	-0.53
9839	C1CC(=O)C(=C1)CO	C01568570	-9.99	-1.98	-14.42	5.32	1.09
9840	CN(C)C=S	C01594591	-9.99	-2.6	-11.48	6.02	-1.93
9841	C=CN1C(=O)CCC1=O	C01596359	-9.99	-2.02	-13.03	6.97	-1.91
9842	C(Cl)OC(=O)N	C01669927	-9.99	-3.35	-13.97	4.94	2.4
9843	Cc1ccc(c(c1)OCC=C	C01679842	-9.99	-1.36	-9.68	2.64	-1.59
9844	c1cc(ccc1NS(=O)(=O)O)Cl	C01732183	-9.99	-7.2	-12.26	8.49	0.99
9845	CCOC1cc(ccc1N)F	C02527708	-9.99	-1.6	-9.12	2.86	-2.14
9846	c1c(cc(c(c1F)F)C=O	C02575049	-9.99	-2.8	-10.62	6.29	-2.86
9847	C(CBr)C#N	C03860883	-9.99	0.11	-11.91	4.28	-2.47
9848	c1c(cnc2c1[nH](c2)N)Cl	C03908916	-9.99	-3.62	-9.45	5.76	-2.68
9849	C1C[C@@@H](CC=C1)C#N	C04411093	-9.99	-0.12	-11.07	4.8	-3.59
9850	C1C[C@H](OC=C1)C#N	C05191551	-9.99	1.18	-13.52	4	-1.66
9851	Cc1c(oc(=S)[nH]1)C	C06069108	-9.99	-1.3	-13.67	4.11	0.88
9852	Cc1c(c(ncn1)NN)N	C08615123	-9.99	-2.28	-13.33	5.67	-0.05
9853	CC(=O)Oc1ccc(nn1)[O-]	C08617519	-9.99	-1.53	-21.49	11.57	1.47
9854	CC(=O)[C@H]1[C@@@H](O1)c2cccnc2	C13213330	-9.99	-2.85	-13.62	8.8	-2.31
9855	c1cc(ccc1C(=NH2+)NO)Br	C16082759	-9.99	-1.68	-11.9	4.74	-1.15
9856	CCc1nnc(o1)N	C17289973	-9.99	-2.44	-13.78	3.96	2.26
9857	c1c(nc(s1)N)CCC	C19091546	-9.99	-3.21	-12.79	4.87	1.14
9858	c1cc(cc(c1F)F)C#CCO	C22203395	-9.99	-1.03	-13.45	6.8	-2.31
9859	c1cc(cc(c1)OC(F)F)F)F)F)N	C31176446	-9.99	-0.52	-12.19	4.44	-1.73
9860	c1ccc(cc1)C(=O)N)F	C00039562	-9.98	-4.15	-14.44	9.6	-0.99
9861	Cc1cccc(n1)C	C00967330	-9.98	-1.85	-8.45	3.36	-3.04
9862	CC(=O)C1CC1	C01577097	-9.98	-0.68	-10.43	3.76	-2.61
9863	c1c(onc1[N+](=O)[O-])C=O	C01618618	-9.98	-4.98	-12.29	10.16	-2.87
9864	CCOP@@@1OC[C@H](O1)C	C01667514	-9.98	0.77	-12.46	4.09	-2.38
9865	COc1ccc(c(c1)C=O	C01676373	-9.98	-3.22	-9.02	4.92	-2.67
9866	CCC(=O)NCCO	C01687366	-9.98	-3.15	-14.92	6.58	1.51
9867	CCC#CCCO	C02015917	-9.98	-2.08	-9.45	2.87	-1.33
9868	C[C@H](C)SC)O	C02043068	-9.98	-0.7	-11.51	2.85	-0.61
9869	c1ccc(cc1)OCC=C(C(F)F)F	C02530942	-9.98	-2.86	-4.75	2.56	-4.93
9870	Cn1ccc(n1)C=O	C02731920	-9.98	-2.32	-15.45	9.36	-1.56
9871	c1c(n(cn1)C)CO[N+](=O)[O-]	C03091270	-9.98	-2.89	-14.64	6.87	0.67
9872	c1cc2c(nc1)onc2Br	C03852685	-9.98	0.86	-16.57	6.75	-1.02
9873	c1cnccc1C(=O)c2[nH]cn2	C04243446	-9.98	-0.38	-13.26	6.4	-2.73
9874	c1cc(oc1)[C@@@H](C(F)F)F)O	C04290173	-9.98	-1.04	-11.65	3.7	-1
9875	CC1=C[P@@@](=O)(CC1)O	C05767716	-9.98	-2.89	-13.3	6.42	-0.21
9876	c1(=S)[nH]nc2n1nc(s2)[S-]	C06494853	-9.98	-3.73	-13.21	5.92	1.04
9877	C1CC(=O)NCC1=O	C16698297	-9.98	0.28	-16.49	6.27	-0.05
9878	C(=S)(N)NNC(=S)S	C16911639	-9.98	-3.04	-15.3	9.64	-1.27
9879	CC(C)NCC#N	C19404245	-9.98	-0.57	-12.54	4.26	-1.13
9880	c1cc(oc1)CNCC(F)F)F	C20268151	-9.98	-1.42	-10.94	4.38	-2.01
9881	c1cc(cc(c(c1)F)Nc(=O)N)F	C20476338	-9.98	-0.9	-19.27	10.82	-0.62
9882	c1cc(cc(c1)Br)Cl)O	C26896114	-9.98	-3.4	-7.51	2.97	-2.04
9883	c1cncc(c1Br)C(F)F)F	C30714826	-9.98	-2.77	-6.93	2.84	-3.12
9884	c1ccc2c(c1)NC(N2)CO	C00406149	-9.97	-4.98	-14.1	4.67	4.44
9885	CC(=O)Nc1ccc(c(c1)N)F	C01595336	-9.97	-1.03	-15.03	7.14	-1.04
9886	c1c(nc([nH]c1=O)[O-])C(F)F)F	C01665341	-9.97	-2.45	-12.88	5.2	0.17
9887	c1ccc(cc1)CC(=O)CCI	C01670907	-9.97	0.17	-15.55	6.58	-1.18
9888	Cn1cc(c(=O)[nH]c1=O)N	C01674640	-9.97	-0.52	-19.11	7.56	2.1
9889	C=CCNC(=S)NN	C01701820	-9.97	-1.5	-15.15	7.86	-1.18
9890	CCCCS(=O)N	C01737529	-9.97	-0.63	-12.4	3.78	-0.72
9891	c1cc(cc(c1SC#N)[N+](=O)[O-])N	C04014529	-9.97	-3	-9.3	5.15	-2.83
9892	C(=O)(C(F)F)N	C04290136	-9.97	-3.42	-13.49	6.67	2.26
9893	C1CC(=O)NCC1=O	C04428982	-9.97	-4.72	-15.01	6.41	3.35
9894	C([C@@@H])([N+](=O)[O-])Br)O	C05131846	-9.97	-1.31	-13.51	5.21	-0.36
9895	C(C#N)N=[N+]=[N-]	C05188385	-9.97	-3.03	-11.47	5.49	-0.96
9896	C[C@H](C=C)n1ccnc1	C05503517	-9.97	-1.75	-8.27	4.23	-4.18

9897	c1c(c([nH]n1)[n+]2nc(on2)[O-])[N+](=O)[O-]	C06188121	-9.97	-2.07	-18.48	9.77	0.8
9898	C(COCC(F)F)C#N	C08698325	-9.97	-0.51	-12.94	5.9	-2.43
9899	CCO/C=C/C(=O)C(F)F	C08698358	-9.97	-0.77	-12.06	6.57	-3.71
9900	C[C@H](C[C@H](C)O)O	C12359922	-9.97	-1.17	-11.77	2.5	0.47
9901	COC(=O)Cn1cc(cn1)N	C19810522	-9.97	-0.98	-17.7	9.69	-0.98
9902	CC[C[NH2+]]CC(=O)OC	C19885652	-9.97	-1.37	-10.89	3.9	-1.6
9903	C(C(F)F)F)NN	C20518386	-9.97	-1.72	-12.47	4.39	-0.17
9904	c1cc(cc(c1)O)CCO	C00395670	-9.96	-2.81	-11.5	3.93	0.4
9905	C#CCOC(=O)c1ccccc1	C01581468	-9.96	2.32	-12.57	5.42	-5.13
9906	CCOC#C[C@@H](C)O	C01605344	-9.96	-1.92	-12.98	4.84	0.1
9907	c1cc(c(cc1C(F)F)N)F	C01706172	-9.96	-3.43	-7.14	2.16	-1.56
9908	c1(c(nc([nH]1)Br)Cl)Cl	C01757466	-9.96	-2.58	-11.42	2.65	1.39
9909	C1C[C@@H](C=C1)C#N	C02032340	-9.96	0.78	-12.85	3.93	-1.81
9910	c1c(con1)CCCO	C02559655	-9.96	-3.36	-11.51	5.34	-0.43
9911	CC(=O)[C@H](C(=O)OC)Cl	C02568011	-9.96	-1.64	-12.4	6.61	-2.53
9912	c1ccc(cc1)[C@@H]2[C@H](O2)CO	C02597084	-9.96	-2.77	-11.81	5.42	-0.79
9913	C(#N)C(Cl)Cl	C03860796	-9.96	0.01	-8.25	0.87	-2.6
9914	CC(CS)CS	C04353093	-9.96	-0.46	-8.11	1.41	-2.8
9915	c1cc(nc2c1[nH]c(=O)[nH]2)N	C05818840	-9.96	-5.24	-14.86	9.67	0.46
9916	Cc1cccn1CCO	C05885732	-9.96	-4.07	-10.11	3.43	0.78
9917	c1cc(c(c(c1)F)F)C(=NH2+)NO	C06234852	-9.96	-3.15	-15.82	8.68	0.32
9918	C(=O)(C(F)F)NNC(=S)N	C08731348	-9.96	-0.4	-19.24	10	-0.32
9919	c1cc(ccc1/C(=N)O)/N)N	C12647936	-9.96	-4.16	-12.2	5.56	0.84
9920	C(C(F)F)F(C(F)F)N	C16082651	-9.96	-1.71	-10.28	2.52	-0.49
9921	c1cnccc1/C(=N)O)/C#N	C17328107	-9.96	-1.12	-13.15	4.84	-0.53
9922	c1(c(=O)[nH]c(nc1[O-])N)N	C18156496	-9.96	-5.66	-16.69	8.39	4
9923	COC(=O)Nc1ccc(cc1)O	C20212818	-9.96	0.03	-19.84	9.71	0.14
9924	C1C[NH2+][C@@H]1C(F)F	C20380768	-9.96	0.07	-11.69	1.89	-0.22
9925	c1cnccc1C#CCO	C22203546	-9.96	-1.18	-15.09	7.14	-0.83
9926	Cn1c(cc(n1)COC)N	C26512024	-9.96	-2.3	-14.41	7.2	-0.45
9927	c1ccc2c(c1)nc(s2)Cl	C00152274	-9.95	-0.97	-13.73	4.24	0.52
9928	Cn1cc2cccc2n1	C00331078	-9.95	-2.67	-11.09	7.23	-3.42
9929	C1CCN(C1)C(=O)Cl	C00407001	-9.95	2.81	-15.02	4.14	-1.87
9930	COC(=C)C(=C)OC	C00409235	-9.95	-0.49	-10.43	2.73	-1.76
9931	c1(c(c(nc1Cl)Cl)Cl)N	C00967313	-9.95	-4.99	-9.1	3.02	1.12
9932	Cn1c(c(cn1)Br)[N+](=O)[O-]	C00987400	-9.95	-1.19	-8.79	3.47	-3.45
9933	COC(=O)Cn1cnc(n1)[N+](=O)[O-]	C01085585	-9.95	-5.85	-14.29	15.95	-5.76
9934	CNc1cccc1O	C01672894	-9.95	-2.31	-10.24	3.07	-0.48
9935	C[C@@H](C(=O)S)O	C02043774	-9.95	-2.49	-12.85	5.37	0.02
9936	CNC(=S)C(=S)NC	C02274048	-9.95	-2.08	-10.41	1.96	0.58
9937	c1cnccc1C=O	C02511465	-9.95	-2.33	-16.52	9.14	-0.23
9938	c1cc(c(c(c1N)F)Cl)Cl	C02525756	-9.95	-2.7	-8.27	3.47	-2.45
9939	CCOCC/C(=N)O)/N	C02547259	-9.95	-2.93	-12.67	4.79	0.85
9940	C[C@@H](CCS)O	C04533096	-9.95	-1.4	-11.81	1.71	1.55
9941	CC(=O)S/C=C/C(=O)C	C04721537	-9.95	-0.36	-12.01	5.45	-3.02
9942	CC[C@H](C=C)C(O)O	C04934049	-9.95	-0.15	-9.92	1.5	-1.38
9943	CCc1cnc([nH]c1=O)N	C05115181	-9.95	-2.97	-16.21	6.45	2.78
9944	C1C2c2c(sc(n2)NN)C1	C07881333	-9.95	-2.66	-10.94	5.46	-1.81
9945	c1cnc(c(c1)F)F)N)Cl	C11919470	-9.95	1.22	-12.16	2.81	-1.82
9946	c1c2c(cc(c1F)F)[nH]c(=O)[nH]2	C12505871	-9.95	-2.16	-12.08	5.52	-1.24
9947	C1[C@@H]2C=C[C@H](C@@H)(O1)O2)O	C14987555	-9.95	-1.79	-13.63	4.35	1.11
9948	CCOC(=O)c1cccn1	C16697860	-9.95	3.08	-14.61	4.85	-3.27
9949	c1cc(ccc1C2c2cnc2N)F	C19785804	-9.95	-0.41	-13.43	7.77	-3.88
9950	c1csc1CNC#N	C22076644	-9.95	-2.24	-11.83	6.11	-1.99
9951	c1cc(nc(c1)Cl)NN	C00168495	-9.94	-4.04	-9.62	4.96	-1.25
9952	Cc1c(c(=O)cc([nH]1)[O-])	C00494717	-9.94	-3.26	-13.24	5.33	1.22
9953	CC[C@H](C(=O)CC)O	C00901574	-9.94	-2.45	-9.56	3.88	-1.81
9954	CC1=C(C(=O)OC)1C	C01585192	-9.94	-1.43	-13.12	7.52	-2.92
9955	CCOC[C@H](C)O	C01640885	-9.94	-0.22	-12.73	3.15	-0.13
9956	c1ccc(cc1)OCC=O	C01681320	-9.94	1.02	-12.87	4.79	-2.88
9957	c1cc(cc2c1ccnn2)F	C01704364	-9.94	-1.73	-12.39	7.07	-2.89
9958	C(C(F)F)OC(F)F	C02576918	-9.94	-0.37	-12.21	4.03	-1.4
9959	c1cc(cnc1)C(=O)c2[nH]ccn2	C04243445	-9.94	1.31	-15.26	6.82	-2.8
9960	c1c[nH]c(nc1=S)[O-]	C05117659	-9.94	-2.26	-16.43	5.05	3.71
9961	c1cc(oc1)/C=C/C(=O)NN	C05676645	-9.94	0.1	-21.06	7.45	3.57
9962	COc1ccc(nn1)NN	C10151793	-9.94	-3.61	-14.47	7.02	1.12
9963	c1ccc(cc1)NCCC#N	C12376742	-9.94	-1.55	-10.93	6.21	-3.67
9964	c1c(cnc(c1N)N)I	C14007799	-9.94	-0.4	-14.23	5.29	-0.59
9965	Cc1cc(cnc1)C=O	C14983272	-9.94	-0.7	-13.13	6.26	-2.37
9966	C/[NH+]=C/c1ccccc1[O-]	C16991557	-9.94	-1.81	-11.04	3.98	-1.07
9967	c1ccc(c(c1)O)[C@@H](C(=O)[NH2+])N)F	C19437723	-9.94	0.85	-19.12	9.71	-1.37
9968	c1cc(nc(c1N)Sc2[nH]cn2	C19845527	-9.94	-1.52	-14.35	8.16	-2.23
9969	COC(=O)c1[nH]ccn1	C22011174	-9.94	-1.38	-14.04	7.08	-1.6
9970	CN(C)c1ncc(s1)CCl	C32006952	-9.94	0.02	-10.64	4.27	-3.59
9971	C1[C@@H]2C=CC(=O)[C@H]1C=CC2=O	C00164014	-9.93	-0.05	-12.02	5.23	-3.1
9972	C1C(=O)N(C(=S)S)1N	C01083111	-9.93	-0.6	-15.2	6.81	-0.95
9973	C1COCOCO1	C01603521	-9.93	-0.59	-13.26	3.07	0.85
9974	C1=C/C=C[C@H]2[C@H](O2)/C=C1	C01646309	-9.93	-1.6	-11.19	2.51	0.34
9975	CCCC[N+](=O)[O-]	C01666924	-9.93	-0.38	-11.8	3.36	-1.11
9976	C1(=[N+]([O-])[O-])C(=O)NC(=O)N=C1[O-]	C01680671	-9.93	2.06	-20.4	6.56	1.86
9977	C[C@@H]1CC=C(C1=O)C	C02038157	-9.93	-0.97	-10.77	5.15	-3.34
9978	Cc1cc(nn1C)N	C02537814	-9.93	-2.48	-11.73	5.44	-1.16
9979	c1ccc(cc1)/C=C/[P@@H](=O)[O-]	C03958322	-9.93	-3.53	-13.19	8.76	-1.98
9980	C1CC1C(=O)O)/N=C/c2c(non2)N)N	C04349472	-9.93	-2.24	-10.38	5.43	-2.74
9981	CO[C@H]1CCCC=C1	C05124667	-9.93	-1.42	-9.53	1.51	-0.49
9982	c1ccc(cc1)C=NNC(=O)N	C08579559	-9.93	-0.16	-16.09	7.33	-1.02
9983	CNC(=O)[C@H](F)I	C08698290	-9.93	0.16	-13.77	4.36	-0.67
9984	c1ccc(cc1)/C(=N)O)/N	C12375727	-9.93	-0.69	-15.71	7.2	-0.72
9985	c1c(c([nH]n1)C(=O)NN)[N+](=O)[O-]	C18166902	-9.93	-4.55	-17.19	11.44	0.37
9986	CC(=O)Cc1cnccc1	C19088351	-9.93	-1.77	-14.53	8.17	-1.8

9987	<chem>CCC[C@H](C=C)O</chem>	C20231667	-9.93	-0.49	-9.7	2.27	-2.01
9988	<chem>c1cc(nc(c1)Cl)CCl</chem>	C21985748	-9.93	-0.49	-10.48	4.42	-3.37
9989	<chem>CCOC(=O)N1C(=O)CSC1=O</chem>	C32594599	-9.93	2.33	-18.06	8.86	-3.06
9990	<chem>CC(=C)C(=O)NCO</chem>	C01641091	-9.92	-3.95	-15.57	7.04	2.56
9991	<chem>c1ccc(c(c1)N)NCC#N</chem>	C01675044	-9.92	-3.83	-9.63	5.07	-1.53
9992	<chem>CCOC(=O)C1=CCCC1</chem>	C01711930	-9.92	2.78	-12.1	3.81	-4.41
9993	<chem>C/C=C/C=C/O</chem>	C01733897	-9.92	0.11	-12.49	5.49	-3.02
9994	<chem>C=C[C@@H]1CO1</chem>	C02040168	-9.92	-0.48	-11.49	2.83	-0.78
9995	<chem>c1c(cc(c(c1F)C=O)F)Cl</chem>	C02243321	-9.92	-0.17	-11.5	3.85	-2.1
9996	<chem>COCN=C=S</chem>	C02528107	-9.92	-1.39	-11.44	2.19	0.72
9997	<chem>c1ccn(c1)CC/C(=N\O)/N</chem>	C02547394	-9.92	-2.91	-12.06	6.07	-1.02
9998	<chem>C=CCOCC(C(F)(F)F)(F)F</chem>	C02576922	-9.92	-1.17	-7.66	2.52	-3.61
9999	<chem>C1C(C(CO1)(F)F)(F)F</chem>	C02576928	-9.92	-0.49	-11.12	3.18	-1.5
10000	<chem>CC(=O)N(C)C=C</chem>	C03860745	-9.92	-1.12	-12.74	5.76	-1.82

SI Table 4: The top 10,000 molecule docking list for used for hit picking in this report. The molecules are listed by their rank, SMILES string, ZINC ID and total docking score. The individual components of the docking score (electrostatics, van der Waals, polar desolvation and non-polar desolvation scores) are also provided. SMILES are given of the molecule at pH 7.0, although docking was performed using species present from pH 4.0 – 8.0 and the scored tautomer may not be the one present at pH 7.0.

SI References:

1. Merski, M.; Shoichet, B. K., Engineering a model protein cavity to catalyze the Kemp elimination. *P Natl Acad Sci USA* **2012**, *109* (40), 16179-16183.
2. Morton, A.; Matthews, B. W., Specificity of Ligand-Binding in a Buried Nonpolar Cavity of T4 Lysozyme - Linkage of Dynamics and Structural Plasticity. *Biochemistry* **1995**, *34* (27), 8576-8588.
3. Liu, L. J.; Marwitz, A. J. V.; Matthews, B. W.; Liu, S. Y., Boron Mimetics: 1,2-Dihydro-1,2-azaborines Bind inside a Nonpolar Cavity of T4 Lysozyme. *Angew Chem Int Edit* **2009**, *48* (37), 6817-6819.
4. Graves, A. P.; Shivakumar, D. M.; Boyce, S. E.; Jacobson, M. P.; Case, D. A.; Shoichet, B. K., Rescoring docking hit lists for model cavity sites: Predictions and experimental testing. *J Mol Biol* **2008**, *377* (3), 914-934.
5. <http://www.molinspiration.com>.