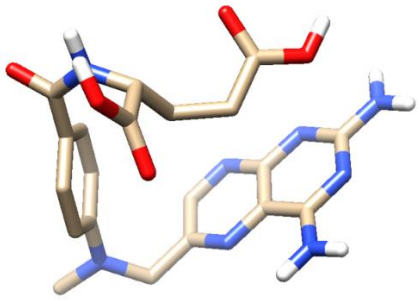
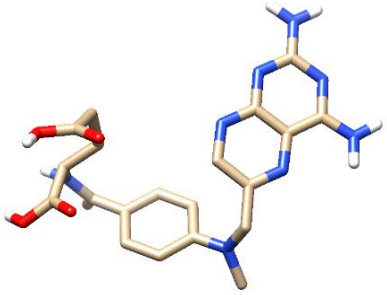
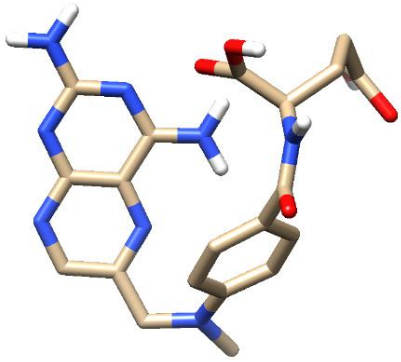
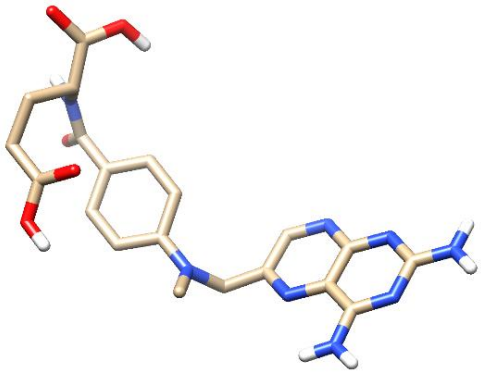
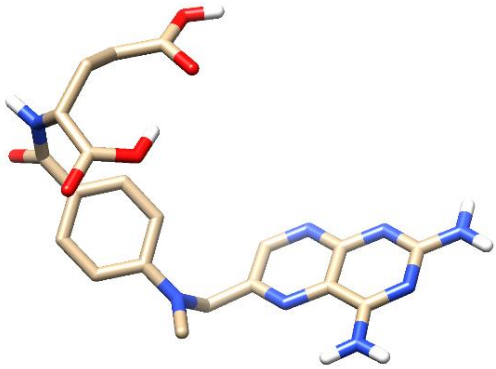
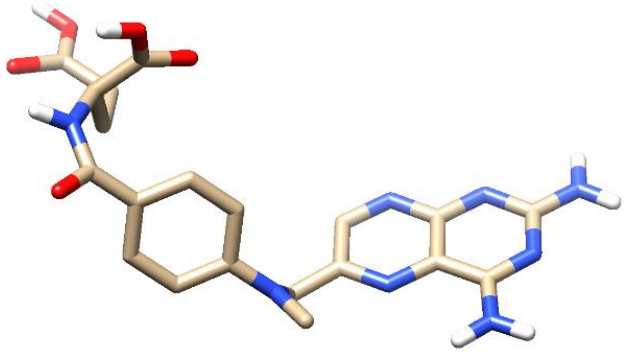
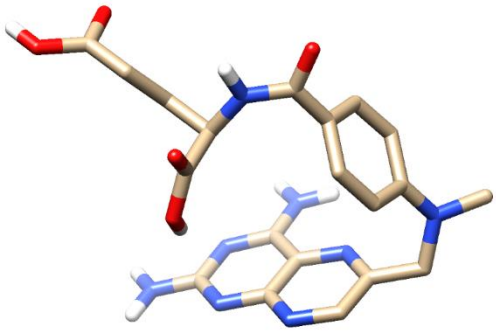
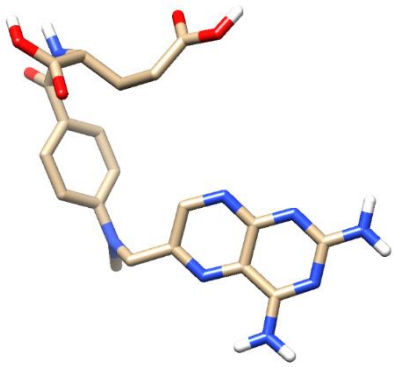
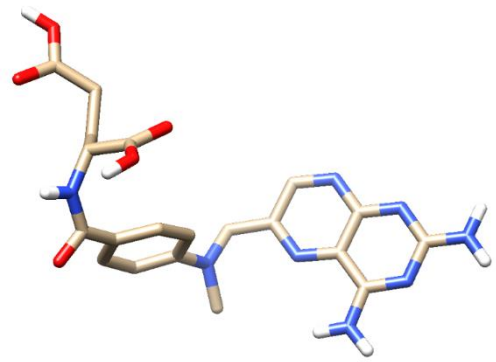
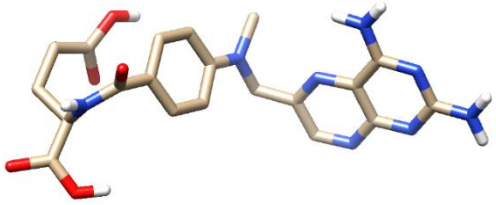
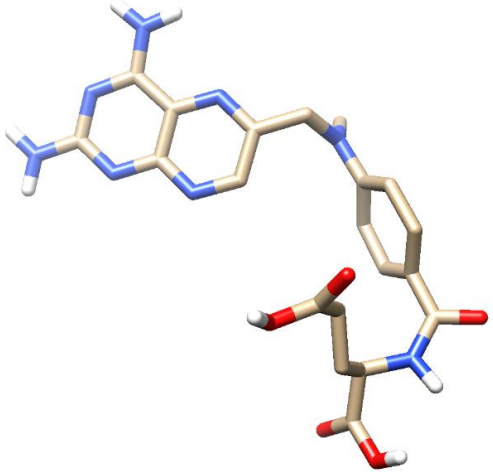
Addendum

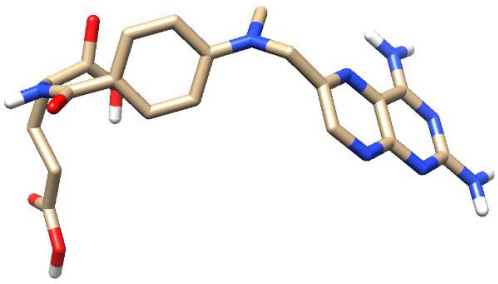
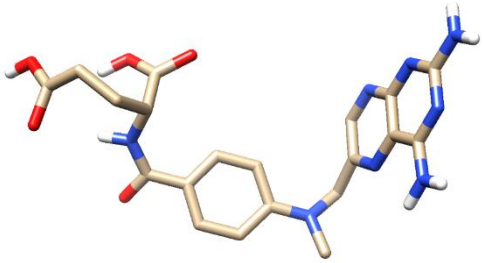
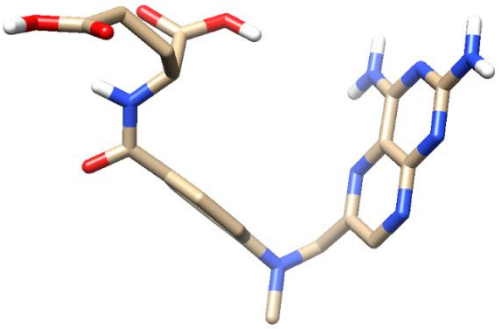
Conformers of MTX with their corresponding energy and affinity, obtained from conformational analysis. Image rendered in UCSF Chimera® v.1.12 (Petterson et al., 2004)

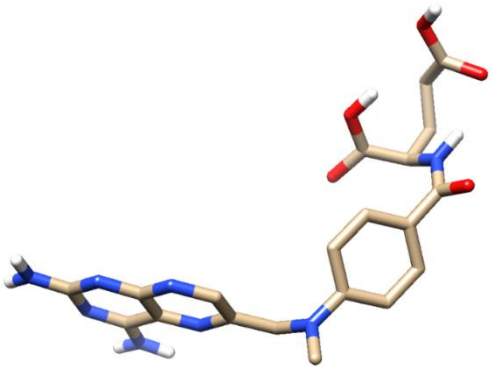
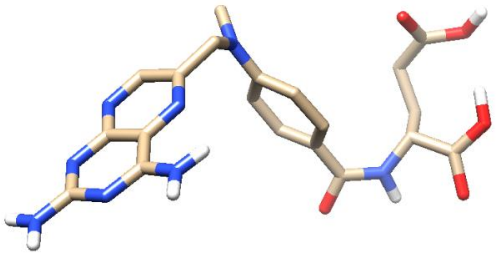
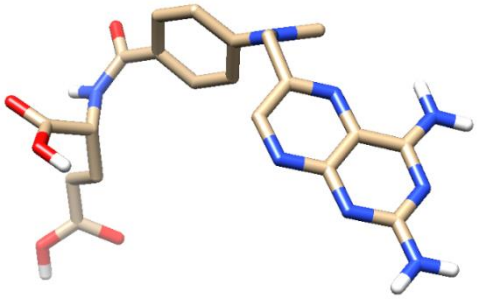
Conformer	LBA (pKd)	LBE ($kcalmol^{-1}$)
 Conformer 000	5.36	81.328
 Conformer 001	4.91	82.512

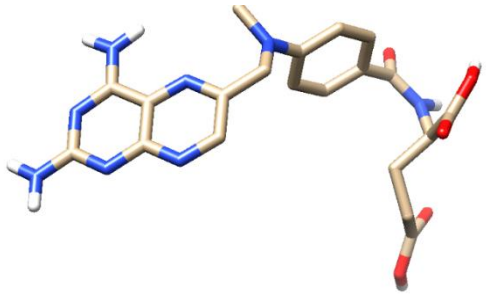
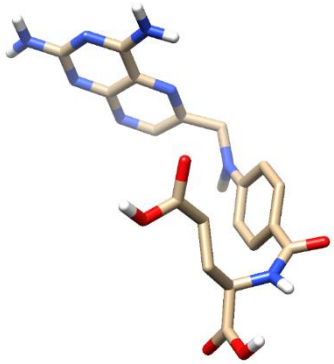
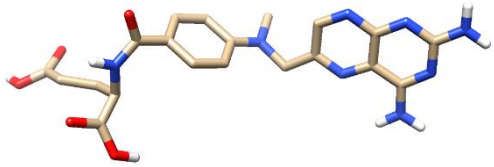
 Conformer 002	5.47	87.210
 Conformer 003	5.06	81.942
 Conformer 004	5.05	94.790

 Conformer 005	5.47	82.022
 Conformer 006	5.26	85.288
 Conformer 007	5.08	89.059

 Conformer 008	5.43	84.331
 Conformer 009	5.81	80.800
 Conformer 010	5.7	83.470

 Conformer 011	4.64	103.408
 Conformer 012	5.19	85.283
 Conformer 013	5.03	87.967

 Conformer 014	4.64	87.528
 Conformer 015	5.05	85.297
 Conformer 016	5.08	85.634

 Conformer 017	5.23	87.201
 Conformer 018	5.73	83.218
 Conformer 019	5.25	86.243

Raw Data extracted from X-Score® v1.3 (Wang et al,2002)

Energy for molecule 1:

Energy for molecule : methotrexate_drawn_000
Bond Stretching Energy : 52.451
Angle Bending Energy : 13.024
Torsional Energy : 18.414
Out of Plane Bending Energy : 0.855
1-4 van der Waals Energy : 6.140
van der Waals Energy : -9.556
==========
Total Energy : 81.328 kcals/mol

Avg. Number of van der Waals only pairs = 1154
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 48

Energy for molecule 2:

Energy for molecule : methotrexate_drawn_001
Bond Stretching Energy : 55.798
Angle Bending Energy : 12.564
Torsional Energy : 17.663
Out of Plane Bending Energy : 0.968
1-4 van der Waals Energy : 5.558
van der Waals Energy : -10.039
==========
Total Energy : 82.512 kcals/mol

Avg. Number of van der Waals only pairs = 1146
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 44

Energy for molecule 3:

Energy for molecule : methotrexate_drawn_002
Bond Stretching Energy : 57.434
Angle Bending Energy : 14.042
Torsional Energy : 12.659
Out of Plane Bending Energy : 3.522
1-4 van der Waals Energy : 5.306
van der Waals Energy : -5.751

==========
Total Energy : 87.210 kcals/mol

Avg. Number of van der Waals only pairs = 1162
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 52

Energy for molecule 4:

Energy for molecule : methotrexate_drawn_003
Bond Stretching Energy : 55.586
Angle Bending Energy : 13.408
Torsional Energy : 15.908
Out of Plane Bending Energy : 1.767
1-4 van der Waals Energy : 5.114
van der Waals Energy : -9.840
==========
Total Energy : 81.942 kcals/mol

Avg. Number of van der Waals only pairs = 1082
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 42

Energy for molecule 5:

Energy for molecule : methotrexate_drawn_004
Bond Stretching Energy : 55.296
Angle Bending Energy : 16.085
Torsional Energy : 19.058
Out of Plane Bending Energy : 2.925
1-4 van der Waals Energy : 6.889
van der Waals Energy : -5.463
==========
Total Energy : 94.790 kcals/mol

Avg. Number of van der Waals only pairs = 1146
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 44

Energy for molecule 6:

Energy for molecule : methotrexate_drawn_005
Bond Stretching Energy : 53.850
Angle Bending Energy : 14.009
Torsional Energy : 15.966
Out of Plane Bending Energy : 0.967
1-4 van der Waals Energy : 5.952
van der Waals Energy : -8.723
==========
Total Energy : 82.022 kcals/mol

Avg. Number of van der Waals only pairs = 1082
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 42

Energy for molecule 7:

Energy for molecule : methotrexate_drawn_006
Bond Stretching Energy : 57.890
Angle Bending Energy : 13.109
Torsional Energy : 14.905
Out of Plane Bending Energy : 1.155
1-4 van der Waals Energy : 4.860
van der Waals Energy : -6.631
==========
Total Energy : 85.288 kcals/mol
Avg. Number of van der Waals only pairs = 1154
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 48

Energy for molecule 8:

Energy for molecule : methotrexate_drawn_007
Bond Stretching Energy : 58.479
Angle Bending Energy : 13.025
Torsional Energy : 17.594
Out of Plane Bending Energy : 1.697
1-4 van der Waals Energy : 5.915
van der Waals Energy : -7.650
==========
Total Energy : 89.059 kcals/mol

Avg. Number of van der Waals only pairs = 1154

Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 48

Energy for molecule 9:

Energy for molecule : methotrexate_drawn_008
Bond Stretching Energy : 54.994
Angle Bending Energy : 14.197
Torsional Energy : 15.752
Out of Plane Bending Energy : 1.632
1-4 van der Waals Energy : 6.536
van der Waals Energy : -8.781
==========
Total Energy : 84.331 kcals/mol

Avg. Number of van der Waals only pairs = 1146
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 44

Energy for molecule 10:

Energy for molecule : methotrexate_drawn_009
Bond Stretching Energy : 56.501
Angle Bending Energy : 14.153
Torsional Energy : 11.056
Out of Plane Bending Energy : 1.022
1-4 van der Waals Energy : 5.210
van der Waals Energy : -7.143
==========
Total Energy : 80.800 kcals/mol

Avg. Number of van der Waals only pairs = 1082
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 42

Energy for molecule 11:

Energy for molecule : methotrexate_drawn_010
Bond Stretching Energy : 58.020
Angle Bending Energy : 13.944
Torsional Energy : 10.997
Out of Plane Bending Energy : 0.729

1-4 van der Waals Energy : 5.171
van der Waals Energy : -5.392
==========
Total Energy : 83.470 kcals/mol

Avg. Number of van der Waals only pairs = 1082
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 42

Energy for molecule 12:

Energy for molecule : methotrexate_drawn_011
Bond Stretching Energy : 63.963
Angle Bending Energy : 19.054
Torsional Energy : 18.597
Out of Plane Bending Energy : 2.248
1-4 van der Waals Energy : 6.278
van der Waals Energy : -6.733
==========
Total Energy : 103.408 kcals/mol

Avg. Number of van der Waals only pairs = 1002
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 34

Energy for molecule 13:

Energy for molecule : methotrexate_drawn_012
Bond Stretching Energy : 56.694
Angle Bending Energy : 14.607
Torsional Energy : 10.464
Out of Plane Bending Energy : 0.878
1-4 van der Waals Energy : 5.955
van der Waals Energy : -3.316
==========
Total Energy : 85.283 kcals/mol

Avg. Number of van der Waals only pairs = 1066
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 36

Energy for molecule 14:

Energy for molecule : methotrexate_drawn_013
Bond Stretching Energy : 55.500
Angle Bending Energy : 11.432
Torsional Energy : 20.423
Out of Plane Bending Energy : 2.172
1-4 van der Waals Energy : 5.333
van der Waals Energy : -6.893
==========
Total Energy : 87.967 kcals/mol

Avg. Number of van der Waals only pairs = 1074
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 40

Energy for molecule 15:

Energy for molecule : methotrexate_drawn_014
Bond Stretching Energy : 57.098
Angle Bending Energy : 14.945
Torsional Energy : 12.774
Out of Plane Bending Energy : 3.080
1-4 van der Waals Energy : 5.960
van der Waals Energy : -6.330
==========
Total Energy : 87.528 kcals/mol

Avg. Number of van der Waals only pairs = 1002
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 34

Energy for molecule 16:

Energy for molecule : methotrexate_drawn_015
Bond Stretching Energy : 56.706
Angle Bending Energy : 12.581
Torsional Energy : 14.651
Out of Plane Bending Energy : 1.203
1-4 van der Waals Energy : 5.797
van der Waals Energy : -5.641
==========
Total Energy : 85.297 kcals/mol

Avg. Number of van der Waals only pairs = 1082
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 42

Energy for molecule 17:

Energy for molecule : methotrexate_drawn_016
Bond Stretching Energy : 58.824
Angle Bending Energy : 10.575
Torsional Energy : 15.991
Out of Plane Bending Energy : 0.910
1-4 van der Waals Energy : 4.766
van der Waals Energy : -5.432
==========
Total Energy : 85.634 kcals/mol

Avg. Number of van der Waals only pairs = 1002
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 34

Energy for molecule 18:

Energy for molecule : methotrexate_drawn_017
Bond Stretching Energy : 55.280
Angle Bending Energy : 12.782
Torsional Energy : 20.633
Out of Plane Bending Energy : 0.582
1-4 van der Waals Energy : 6.507
van der Waals Energy : -8.583
==========
Total Energy : 87.201 kcals/mol

Avg. Number of van der Waals only pairs = 1146
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 44

Energy for molecule 19:

Energy for molecule : methotrexate_drawn_018
Bond Stretching Energy : 52.991
Angle Bending Energy : 13.005
Torsional Energy : 13.944

Out of Plane Bending Energy : 0.680
1-4 van der Waals Energy : 6.385
van der Waals Energy : -3.788
==========
Total Energy : 83.218 kcals/mol

Avg. Number of van der Waals only pairs = 1082
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 42

Energy for molecule 20:

Energy for molecule : methotrexate_drawn_019
Bond Stretching Energy : 58.108
Angle Bending Energy : 13.562
Torsional Energy : 11.692
Out of Plane Bending Energy : 0.688
1-4 van der Waals Energy : 5.008
van der Waals Energy : -2.815
==========
Total Energy : 86.243 kcals/mol

Avg. Number of van der Waals only pairs = 1002
Avg. Number of 1-4 van der Waals only pairs = 121
Avg. Number of scaled van der Waals only pairs = 34

Energy for 2b7a extract:

Energy for molecule : 2b7a_extract
Bond Stretching Energy : 91.702
Angle Bending Energy : 32.634
Torsional Energy : 0.375
Out of Plane Bending Energy : 0.036
1-4 van der Waals Energy : 1.130
van der Waals Energy : -2.012
==========
Total Energy : 123.864 kcals/mol

Avg. Number of van der Waals only pairs = 143
Avg. Number of 1-4 van der Waals only pairs = 43

Raw data extracted from LigBuilder® v1.2 (Wang et al, 2000)

The highlighted molecules indicated Lipinski Rule (Lipinski et al, 2001) compliant molecules.

Ligands Obtained from Seed 1

1st column: ID of the molecule

2nd column: name of the mol2 file

3rd column: family of the molecule

4th column: formula

5th column: molecular weight

6th column: calculated LogP

7th column: binding score (pKd)

8th column: chemical score

1	result_001.mol2	<1>	C34H45N7O2	583	4.85	9.60	-90
2	result_002.mol2	<1>	C35H41N5O3	579	5.75	9.17	-50
3	result_003.mol2	<1>	C33H41N6O4	585	5.99	9.16	-30
4	result_004.mol2	<1>	C31H33N5O2	507	5.73	8.86	-20
5	result_005.mol2	<1>	C32H33N5O3	535	5.22	8.77	-30
6	result_006.mol2	<1>	C32H35N5O6	585	5.66	8.67	-30
7	result_007.mol2	<1>	C31H34N6O4	554	4.20	8.52	-20
8	result_008.mol2	<1>	C35H37N5O3	575	5.69	8.48	-30
9	result_009.mol2	<1>	C31H35N5O2	509	5.86	8.38	-20
10	result_010.mol2	<1>	C35H39N5O4	593	5.74	8.36	-50
11	result_011.mol2	<1>	C29H31N6O3	511	3.51	8.35	-20
12	result_012.mol2	<1>	C31H32N5O4	538	5.23	8.31	-20
13	result_013.mol2	<1>	C30H33N5O2	495	5.88	8.28	-20
14	result_014.mol2	<1>	C31H33N5O3	523	5.27	8.26	-20
15	result_015.mol2	<1>	C32H32N6O5	580	5.23	8.22	0
16	result_016.mol2	<1>	C28H29N5O6	531	4.35	8.21	-20
17	result_017.mol2	<1>	C33H35N5O5	581	4.56	8.18	-40
18	result_018.mol2	<1>	C32H39N6O4	571	4.93	8.16	-20
19	result_019.mol2	<1>	C32H33N5O5	567	3.19	8.15	-60
20	result_020.mol2	<1>	C27H30N7O3	500	4.55	8.09	-20
21	result_021.mol2	<1>	C31H33N5O4	539	5.34	8.06	-20
22	result_022.mol2	<1>	C33H38N6O3	566	4.44	8.06	-80
23	result_023.mol2	<1>	C32H33N5O5	567	4.09	8.00	-20
24	result_024.mol2	<1>	C32H35N5O4	553	4.51	7.97	-60

25	result_025.mol2	<1>	C34H33N5O5	591	5.89	7.94	-10
26	result_026.mol2	<1>	C33H35N6O3	563	3.81	7.91	-140
27	result_027.mol2	<1>	C35H40N6O3	592	5.32	7.90	-50
28	result_028.mol2	<1>	C28H29N5O2	467	5.42	7.88	0
29	result_029.mol2	<1>	C33H33N6O4	577	3.97	7.87	0
30	result_030.mol2	<1>	C33H38N7O2	564	5.34	7.83	-40
31	result_031.mol2	<1>	C32H34N5O4	552	4.28	7.79	-40
32	result_032.mol2	<1>	C31H34N6O3	538	4.93	7.79	-20
33	result_033.mol2	<1>	C31H36N7O5	586	3.94	7.76	-40
34	result_034.mol2	<1>	C32H31N5O5	565	4.27	7.72	0
35	result_035.mol2	<1>	C35H43N6O2	579	5.71	7.68	-80
36	result_036.mol2	<1>	C30H33N5O3	511	5.17	7.67	0
37	result_037.mol2	<1>	C32H30N6O4	562	5.24	7.66	0
38	result_038.mol2	<1>	C30H29N5O3	507	4.81	7.64	-50
39	result_039.mol2	<1>	C32H37N8O3	581	3.69	7.63	-60
40	result_040.mol2	<1>	C32H39N6O5	587	5.24	7.50	-30
41	result_041.mol2	<1>	C33H39N6O3	567	5.09	7.42	-60
42	result_042.mol2	<1>	C31H34N6O5	570	3.25	7.39	-60
43	result_043.mol2	<1>	C30H31N5O6	557	3.71	7.37	-40
44	result_044.mol2	<1>	C31H39N6O2	527	5.16	7.25	0
45	result_045.mol2	<2>	C35H41N7O2	591	5.98	9.58	-20
46	result_046.mol2	<2>	C34H41N7O	563	5.74	9.37	-20
47	result_047.mol2	<2>	C34H41N7O	563	5.74	8.67	0
48	result_048.mol2	<2>	C33H40N7O3	582	5.73	8.61	-20
49	result_049.mol2	<2>	C31H35N7O5	585	4.20	8.49	-20
50	result_050.mol2	<2>	C32H43N7O2	557	5.11	8.42	-20
51	result_051.mol2	<2>	C31H31N7O6	597	3.31	8.24	0
52	result_052.mol2	<2>	C32H37N7O3	567	5.38	8.19	-50
53	result_053.mol2	<2>	C32H36N8O3	580	5.97	8.14	-20
54	result_054.mol2	<2>	C31H39N7O2	541	4.53	8.07	-20
55	result_055.mol2	<2>	C32H36N7O3	566	4.19	7.97	-50
56	result_056.mol2	<2>	C32H38N7O4	584	3.60	7.94	-60
57	result_057.mol2	<2>	C30H34N7O6	588	3.70	7.88	-20
58	result_058.mol2	<2>	C32H42N8O2	570	5.21	7.66	-40
59	result_059.mol2	<2>	C32H42N8O2	570	5.21	7.52	-40
60	result_060.mol2	<2>	C33H39N7O4	597	4.30	7.50	-70
61	result_061.mol2	<3>	C29H29N5O2	479	5.77	9.31	-50
62	result_062.mol2	<3>	C29H33N6O2	497	5.11	8.78	-70
63	result_063.mol2	<3>	C32H38N6O3	554	5.84	8.33	-20
64	result_064.mol2	<3>	C30H33N5O2	495	5.98	8.31	-70
65	result_065.mol2	<3>	C34H35N5O4	577	5.36	8.22	-50
66	result_066.mol2	<3>	C32H36N6O4	568	5.40	8.01	-30
67	result_067.mol2	<3>	C28H31N5O3	485	5.63	7.93	0
68	result_068.mol2	<3>	C31H33N5O3	523	5.80	7.84	-10
69	result_069.mol2	<3>	C34H41N5O4	583	5.99	7.81	-70
70	result_070.mol2	<3>	C31H34N7O3	552	4.44	7.63	-70
71	result_071.mol2	<3>	C33H37N5O4	567	5.37	7.62	-30
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73	result_073.mol2	<3>	C31H35N6O2	523	5.64	7.51	-60
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75	result_075.mol2	<3>	C29H33N6O3	513	3.26	7.41	-40
76	result_076.mol2	<3>	C34H39N5O4	581	5.10	7.41	-30
77	result_077.mol2	<3>	C32H37N7O4	583	3.97	7.31	-30
78	result_078.mol2	<3>	C33H39N5O4	569	5.74	7.21	-20
79	result_079.mol2	<4>	C35H34N8O2	598	5.62	9.18	-40
80	result_080.mol2	<4>	C33H35N8O2	575	5.96	8.94	-20
81	result_081.mol2	<4>	C34H43N9O	593	5.17	8.89	-30
82	result_082.mol2	<4>	C32H37N8O2	565	4.53	8.82	-30
83	result_083.mol2	<4>	C32H32N8O	544	5.91	8.72	-10
84	result_084.mol2	<4>	C34H34N8O2	586	4.89	8.66	0
85	result_085.mol2	<4>	C33H34N9O	572	4.30	8.59	-60
86	result_086.mol2	<4>	C34H35N8O2	587	5.43	8.56	-70
87	result_087.mol2	<4>	C32H32N8O2	560	5.50	8.56	-20
88	result_088.mol2	<4>	C33H33N7O3	575	5.44	8.54	0
89	result_089.mol2	<4>	C34H39N7O3	593	4.91	8.54	-20
90	result_090.mol2	<4>	C33H38N9O2	592	3.71	8.53	-10
91	result_091.mol2	<4>	C32H33N7O3	563	5.51	8.52	-30
92	result_092.mol2	<4>	C33H36N8O3	592	5.84	8.50	-20
93	result_093.mol2	<4>	C31H31N7O4	565	5.60	8.47	-20
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96	result_096.mol2	<4>	C35H36N8O2	600	5.41	8.44	0
97	result_097.mol2	<4>	C34H31N8O3	599	5.05	8.39	-30
98	result_098.mol2	<4>	C33H34N8O2	574	4.99	8.39	-40
99	result_099.mol2	<4>	C34H33N8O	569	5.79	8.28	-10
100	result_100.mol2	<4>	C35H34N8O2	598	5.23	8.27	-20
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102	result_102.mol2	<4>	C35H36N9O	598	4.85	8.24	-20
103	result_103.mol2	<4>	C35H34N8O2	598	5.23	8.22	-20
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105	result_105.mol2	<4>	C29H32N9O2	538	3.35	8.21	-30
106	result_106.mol2	<4>	C31H35N8O	535	5.13	8.21	-10
107	result_107.mol2	<4>	C32H33N7O2	547	5.60	8.21	0
108	result_108.mol2	<4>	C32H37N9O	563	5.05	8.20	-70
109	result_109.mol2	<4>	C33H39N8O	563	5.85	8.20	-20
110	result_110.mol2	<4>	C32H33N7O3	563	5.62	8.20	0
111	result_111.mol2	<4>	C32H36N8O3	580	4.56	8.20	-20
112	result_112.mol2	<4>	C32H36N8O2	564	5.67	8.19	-20
113	result_113.mol2	<4>	C33H36N8O3	592	5.12	8.19	0
114	result_114.mol2	<4>	C32H37N8O	549	5.39	8.18	-10
115	result_115.mol2	<4>	C34H35N7O3	589	5.79	8.18	-20
116	result_116.mol2	<4>	C33H36N9O2	590	4.58	8.17	-20
117	result_117.mol2	<4>	C32H34N8O4	594	3.79	8.16	-20
118	result_118.mol2	<4>	C32H33N7O5	595	5.91	8.15	-20
119	result_119.mol2	<4>	C32H33N7O3	563	4.78	8.13	-40
120	result_120.mol2	<4>	C29H27N7O4	537	5.75	8.13	-20
121	result_121.mol2	<4>	C30H35N8O	523	5.07	8.12	-20
122	result_122.mol2	<4>	C34H37N7O3	591	5.65	8.12	-70
123	result_123.mol2	<4>	C31H33N7O2	535	5.05	8.08	-20
124	result_124.mol2	<4>	C33H34N8O3	590	4.85	8.08	-20

125	result_125.mol2	<4>	C32H32N8O3	576	4.26	8.08	-20
126	result_126.mol2	<4>	C31H32N8O3	564	3.78	8.07	-20
127	result_127.mol2	<4>	C33H36N9O2	590	4.82	8.06	-20
128	result_128.mol2	<4>	C34H33N7O3	587	5.97	8.06	-20
129	result_129.mol2	<4>	C32H34N9O	560	4.63	8.06	-30
130	result_130.mol2	<4>	C32H31N8O4	591	4.18	8.05	-20
131	result_131.mol2	<4>	C36H39N8O	599	5.78	8.04	-90
132	result_132.mol2	<4>	C29H31N8O2	523	4.49	8.02	-30
133	result_133.mol2	<4>	C34H38N9O	588	5.63	8.00	-30
134	result_134.mol2	<4>	C34H29N7O3	583	5.78	8.00	0
135	result_135.mol2	<4>	C32H35N7O2	549	5.18	7.98	0
136	result_136.mol2	<4>	C34H33N8O2	585	5.22	7.96	-20
137	result_137.mol2	<4>	C30H29N7O4	551	4.46	7.95	0
138	result_138.mol2	<4>	C34H39N8O2	591	5.67	7.90	-50
139	result_139.mol2	<4>	C33H33N7O4	591	5.28	7.88	-40
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142	result_142.mol2	<4>	C32H34N8O3	578	4.13	7.83	-20
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144	result_144.mol2	<4>	C31H29N7O2	531	5.67	7.82	0
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146	result_146.mol2	<4>	C32H32N8O3	576	4.56	7.82	-40
147	result_147.mol2	<4>	C29H30N8O3	538	3.44	7.81	-10
148	result_148.mol2	<4>	C31H33N7O3	551	5.44	7.81	0
149	result_149.mol2	<4>	C32H32N8O	544	5.59	7.80	-10
150	result_150.mol2	<4>	C32H35N7O3	565	5.97	7.80	0
151	result_151.mol2	<4>	C33H35N7O3	577	4.72	7.77	-70
152	result_152.mol2	<4>	C34H35N7O2	573	5.87	7.76	0
153	result_153.mol2	<4>	C33H31N8O2	571	5.08	7.75	-10
154	result_154.mol2	<4>	C34H39N8O	575	5.38	7.75	-50
155	result_155.mol2	<4>	C30H31N7O	505	5.76	7.73	0
156	result_156.mol2	<4>	C31H35N8O2	551	4.52	7.73	-30
157	result_157.mol2	<4>	C31H34N8O2	550	5.16	7.72	-10
158	result_158.mol2	<4>	C30H31N7O2	521	4.98	7.71	0
159	result_159.mol2	<4>	C32H33N7O4	579	3.92	7.70	0
160	result_160.mol2	<4>	C31H31N8O5	595	5.18	7.69	-20
161	result_161.mol2	<4>	C32H35N7O4	581	4.80	7.68	-50
162	result_162.mol2	<4>	C32H34N8O3	578	4.96	7.64	0
163	result_163.mol2	<4>	C33H33N7O3	575	5.98	7.63	-20
164	result_164.mol2	<4>	C31H28N7O6	594	3.50	7.62	-40
165	result_165.mol2	<4>	C32H34N9O	560	4.63	7.61	-30
166	result_166.mol2	<4>	C33H32N9O2	586	4.48	7.60	-30
167	result_167.mol2	<4>	C31H36N9O2	566	4.02	7.59	-20
168	result_168.mol2	<4>	C34H38N8O2	590	5.96	7.59	-40
169	result_169.mol2	<4>	C31H31N7O4	565	5.09	7.57	-20
170	result_170.mol2	<4>	C32H34N8O3	578	4.13	7.57	-20
171	result_171.mol2	<4>	C33H38N9O2	592	4.73	7.56	-20
172	result_172.mol2	<4>	C32H32N7O4	578	4.22	7.56	-20
173	result_173.mol2	<4>	C34H39N8O2	591	5.81	7.55	-20

174	result_174.mol2	<4>	C33H34N8O3	590	4.79	7.53	-40
175	result_175.mol2	<4>	C32H32N8O	544	6.00	7.52	-40
176	result_176.mol2	<4>	C34H39N8O2	591	5.36	7.51	-20
177	result_177.mol2	<4>	C31H33N9O4	595	4.07	7.49	-20
178	result_178.mol2	<4>	C32H29N8O4	589	4.87	7.48	-20
179	result_179.mol2	<4>	C34H39N8O2	591	5.54	7.45	-30
180	result_180.mol2	<4>	C33H37N7O3	579	4.95	7.44	-70
181	result_181.mol2	<4>	C34H35N7O3	589	5.39	7.42	-20
182	result_182.mol2	<4>	C30H31N7O3	537	5.22	7.40	-20
183	result_183.mol2	<4>	C35H38N9O	600	5.40	7.38	-20
184	result_184.mol2	<4>	C32H35N8O3	579	3.98	7.38	-30
185	result_185.mol2	<4>	C34H37N8O2	589	5.92	7.36	-20
186	result_186.mol2	<4>	C34H36N8O2	588	5.69	7.34	-50
187	result_187.mol2	<4>	C35H39N7O2	589	5.26	7.32	-40
188	result_188.mol2	<4>	C32H34N8O3	578	5.12	7.30	-20
189	result_189.mol2	<4>	C33H32N8O3	588	5.12	7.27	-20
190	result_190.mol2	<4>	C33H37N8O	561	4.02	7.27	-50
191	result_191.mol2	<4>	C33H35N8O	559	5.19	7.24	-50
192	result_192.mol2	<4>	C30H29N7O4	551	4.43	7.23	-20
193	result_193.mol2	<4>	C33H38N9O2	592	4.73	7.21	-20
194	result_194.mol2	<4>	C33H35N8O3	591	5.39	7.20	-20
195	result_195.mol2	<4>	C32H36N9O3	594	3.62	7.20	-30
196	result_196.mol2	<4>	C33H34N8O3	590	3.07	7.19	-10
197	result_197.mol2	<5>	C26H34N6O3	478	3.86	8.38	0
198	result_198.mol2	<5>	C28H38N6O3	506	4.78	8.04	-10
199	result_199.mol2	<5>	C26H34N6O3	478	3.75	7.75	0
200	result_200.mol2	<5>	C27H34N6O3	490	4.14	7.34	0

Ligands Obtained from Seed 2

1st column: ID of the molecule

2nd column: name of the mol2 file

3rd column: family of the molecule

4th column: formula

5th column: molecular weight

6th column: calculated LogP

7th column: binding score (pKd)

8th column: chemical score

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2	result_002.mol2	<1>	C26H33N4O	417	5.05	5.90	0
3	result_003.mol2	<1>	C25H33N3O2	407	5.45	5.82	-20
4	result_004.mol2	<1>	C24H31N3O	377	4.50	5.73	0
5	result_005.mol2	<1>	C31H43N3O	473	5.54	5.49	0
6	result_006.mol2	<1>	C19H24N4O	324	3.85	5.35	0
7	result_007.mol2	<1>	C25H31N3O2	405	3.95	5.09	0
8	result_008.mol2	<2>	C21H27N3O	337	3.93	6.09	-20
9	result_009.mol2	<2>	C20H27N4	323	3.51	5.95	-20
10	result_010.mol2	<2>	C24H33N4O	393	3.65	5.92	-20
11	result_011.mol2	<2>	C21H27N3	321	5.39	5.91	0
12	result_012.mol2	<2>	C23H33N4	365	4.39	5.55	-20
13	result_013.mol2	<2>	C24H33N4O	393	3.93	5.40	-20
14	result_014.mol2	<2>	C24H30N4O2	406	4.23	5.31	0
15	result_015.mol2	<2>	C26H34N4O2	434	4.07	5.28	0
16	result_016.mol2	<2>	C22H27N3O	349	4.64	5.16	-20
17	result_017.mol2	<3>	C23H33N4	365	5.38	5.43	-20
18	result_018.mol2	<3>	C27H35N3O2	433	4.86	5.39	-40
19	result_019.mol2	<3>	C26H41N5	423	5.07	5.09	-20
20	result_020.mol2	<3>	C24H33N4O	393	4.05	5.07	-40

Ligands Obtained from Seed 3

1st column: ID of the molecule

2nd column: name of the mol2 file

3rd column: family of the molecule

4th column: formula

5th column: molecular weight

6th column: calculated LogP

7th column: binding score (pKd)

8th column: chemical score

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3	result_003.mol2	<2>	C27H27N4O4	471	4.15	5.22	-20
4	result_004.mol2	<2>	C30H33N4O	465	5.68	5.03	-40
5	result_005.mol2	<2>	C29H28N4O4	496	3.68	5.03	-20
6	result_006.mol2	<3>	C24H32N4O2	408	3.69	5.09	-20
7	result_007.mol2	<4>	C18H28N3O	302	3.16	5.09	-20