

**Chemometric design to explore pharmacophoric features of BACE
inhibitors for controlling alzheimer's disease**

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Supplementary Table 1 Observed and predicted activity of diverse compounds in different models

Comp No.	SMILES	Observed Activity (pIC ₅₀)	Predicted Activity through model				Dock Score
			1	2	3	4	
1 ¹	<chem>c1cccc1CN(CC)Cc2ccc(cc2)-c(c(o3)=O)cc(c34)cc(cc4)OCCNC(=O)Cc5cc(F)cc(F)c5</chem>	3.827	3.580	3.819	3.636	3.386	69.831
2 ¹	<chem>c1cccc1CN(CC)Cc2ccc(cc2)-c(c(o3)=O)cc(c34)cc(cc4)OCCNC(=O)/C=C/c5cc(F)cc(F)c5</chem>	4.004	4.331	3.669	3.566	4.045	67.789
3 ¹	<chem>c1cccc1CN(CC)Cc2ccc(cc2)-c(c(o3)=O)cc(c34)cc(cc4)OCCNC(=O)CCc5cc(F)c(F)c5</chem>	3.936	4.140	4.141	3.720	4.352	67.368
4 ¹	<chem>c1cccc1CN(CC)Cc2ccc(cc2)-c(c(o3)=O)cc(c34)cc(cc4)OCCNC(=O)/C=C/c5cc(Cl)c(Cl)c5</chem>	3.876	3.811	4.007	3.735	3.449	71.384
5 ¹	<chem>c1cccc1CN(CC)Cc2ccc(cc2)-c(c(o3)=O)cc(c34)ccc(c4)OCCNC(=O)Cc5cc(F)cc(F)c5</chem>	3.824	4.046	3.789	3.914	4.813	59.232
6 ¹	<chem>c1cccc1CN(CC)Cc2ccc(cc2)-c(c(o3)=O)cc(c34)ccc(c4)OCCNC(=O)/C=C/c5cc(F)cc(F)c5</chem>	3.917	3.604	3.887	3.861	3.498	57.466
7 ¹	<chem>c1cccc1CN(CC)Cc2ccc(cc2)-c(c(o3)=O)cc(c34)ccc(c4)OCCNC(=O)CCc5cc(F)c(F)c5</chem>	3.943	3.577	4.092	3.998	3.420	61.743
8 ¹	<chem>c1cccc1CN(CC)Cc2ccc(cc2)-c(c(o3)=O)cc(c34)ccc(c4)OCCNC(=O)/C=C/c5cc(Cl)c(Cl)c5</chem>	3.821	3.524	4.450	4.030	4.836	59.378
9 ¹	<chem>O=C(O)c(c1)cc(C(=O)O)cc1NC(=O)[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CCC(=O)O</chem>	4.260	5.078	4.690	4.742	4.501	59.261
10 ¹	<chem>c1ccc(C(=O)O)cc1NC(=O)[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)c3nn[nH]n3</chem>	5.086	5.039	5.136	5.329	4.960	65.744
11 ²	<chem>O=C(O)c(c1)cc(C(=O)O)cc1NC(=O)[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)c3nn[nH]n3</chem>	5.409	5.731	5.106	5.346	6.401	55.255
12 ²	<chem>n1n[nH]nc1-c(c2)cc(-c3n[nH]nn3)cc2NC(=O)[C@H](O)[C@H](Cc4ccccc4)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CCC(=O)O</chem>	5.194	5.081	5.280	5.192	5.296	62.357
13 ²	<chem>n1n[nH]nc1-c(ccc2)cc2NC(=O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)c4nn[nH]n4</chem>	5.319	5.501	5.267	5.129	5.853	62.281
14 ²	<chem>n1n[nH]nc1-c(c2)cc(-c3n[nH]nn3)cc2NC(=O)[C@H](O)[C@H](Cc4ccccc4)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)c5nn[nH]n5</chem>	5.921	5.768	5.868	5.795	5.415	48.823
15 ²	<chem>n1oc(=O)[nH]c1-c(ccc2)cc2NC(=O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)c4nn[nH]n4</chem>	5.180	5.055	5.355	5.477	5.786	52.241
16 ²	<chem>n1oc(=S)[nH]c1-c(ccc2)cc2NC(=O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)c4nn[nH]n4</chem>	5.194	5.323	5.409	5.477	4.865	53.229
17 ³	<chem>OC(=O)CC[C@@H](C(=O)O)NC(=O)[C@H](C)NC(=O)[C@H](CC(=O)O)NC(=O)[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)C(=O)O</chem>	4.076	4.318	5.120	4.920	4.467	64.265
18 ³	<chem>c1ccc(C(=O)O)cc1NC(=O)[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)C(=O)O</chem>	4.796	5.234	5.006	5.059	4.068	62.413
19 ³	<chem>O=C(O)c(c1)cc(C(=O)O)cc1NC(=O)[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)C(=O)O</chem>	5.328	5.095	5.975	5.075	6.142	59.635
20 ³	<chem>c1ccc(C(=O)O)cc1NC(=O)[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)c3[nH]nnn3</chem>	5.086	4.960	5.560	5.630	5.463	62.248
21 ³	<chem>O=C(O)c(c1)cc(C(=O)O)cc1NC(=O)[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)c3[nH]nnn3</chem>	5.409	5.835	5.460	5.647	6.167	54.353
22 ⁴	<chem>c1cccc1-c2n(CC(=O)N=C(N)N)c(cc2)-c3ccccc3</chem>	2.432	2.780	2.027	2.300	0.156	67.287
23 ⁴	<chem>c1cccc(Cl)c1-c2n(CC(=O)N=C(N)N)c(cc2)-c3ccc(cc3)Oc4ccc(cc4)C(=O)C</chem>	3.155	3.311	2.762	2.680	3.561	61.584

24 ⁴	c1cccc1-c2n(CC(=O)N=C(N)N)c(cc2)C34C[C@@H]5C[C@H](C3)C[C@H](C4)C5	3.222	2.976	3.040	3.152	3.255	73.896
25 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\N[C@H](CC4)CC[C@@H]4C(=O)O	4.108	4.443	3.794	3.646	4.152	66.648
26 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\N[C@H]4CC[C@H](O)CC4	3.903	3.764	4.213	3.596	3.236	73.708
27 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\NCCC(=O)O	3.886	4.124	4.119	3.260	3.230	66.608
28 ⁴	O=C(O)CCN/C(N)=N\C(=O)Cn(c1-c2cccc2Cl)c(cc1)-c3ccc(cc3)OCCC	3.556	3.338	3.402	3.203	3.584	68.159
29 ⁴	O=C(N)CCN/C(N)=N\C(=O)Cn(c1-c2cccc2Cl)c(cc1)-c3ccc(cc3)OCCC	3.764	3.776	4.001	3.293	3.347	66.544
30 ⁴	OCCCN/C(N)=N\C(=O)Cn(c1-c2cccc2Cl)c(cc1)-c3ccc(cc3)OCCC	3.917	3.815	3.397	3.373	3.629	67.101
31 ⁴	OC[C@H](O)CN/C(N)=N\C(=O)Cn(c1-c2cccc2Cl)c(cc1)-c3ccc(cc3)OCCC	3.907	3.440	4.023	3.503	3.226	69.544
32 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\NCCNC(=O)C	3.863	3.236	3.269	3.411	3.665	75.092
33 ⁴	OCC(C)(C)CN/C(N)=N\C(=O)Cn(c1-c2cccc2Cl)c(cc1)-c3ccc(cc3)OCCC	3.693	3.811	3.584	3.448	3.316	66.620
34 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\NCCCSC	3.493	4.256	4.090	3.288	3.637	79.265
35 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\NCCC4OCCO4	3.570	4.115	3.819	3.404	3.309	68.196
36 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\NCCCN4encc4	3.618	3.581	3.472	3.366	3.777	68.519
37 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\NCc4cccc4	3.124	3.175	3.015	3.308	3.434	70.784
38 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\NCc4occc4	3.253	3.420	3.363	3.085	3.444	79.727
39 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\NCc4c(F)c(F)c(F)cc4	3.693	3.366	3.752	3.367	3.428	66.278
40 ⁴	CCCOc(cc1)ccc1-c(cc2)n(c2-c3cccc3Cl)CC(=O)/N=C(N)\NCc4cc(OC)c(O)cc4	3.186	3.263	3.731	3.529	4.104	63.083
41 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\NCCCC#N	3.593	3.699	3.822	3.517	4.597	64.915
42 ⁴	OCCCN/C(N)=N\C(=O)Cn(c1-c2cccc2)c(cc1)C34C[C@@H]5C[C@H](C3)C[C@H](C4)C5	3.622	3.399	3.583	3.520	3.599	67.513
43 ⁴	OCCN/C(N)=N\C(=O)Cn(c1-c2cccc2)c(cc1)C34C[C@@H]5C[C@H](C3)C[C@H](C4)C5	3.167	3.292	2.863	3.241	3.229	66.798
44 ⁴	N#CCCN/C(N)=N\C(=O)Cn(c1-c2cccc2)c(cc1)C34C[C@@H]5C[C@H](C3)C[C@H](C4)C5	3.509	3.597	3.387	3.406	3.995	68.430
45 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\NCCCCO	3.593	3.914	3.672	3.421	3.076	70.327
46 ⁴	OC[C@H](O)CN/C(N)=N\C(=O)Cn(c1-c2cccc2)c(cc1)C34C[C@@H]5C[C@H](C3)C[C@H](C4)C5	3.271	3.426	3.445	3.685	3.656	70.396
47 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\NCCCn6encc6	2.767	2.825	3.083	3.492	2.198	66.098
48 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\N[C@H]6CC[C@H](O)CC6	3.548	3.656	3.363	3.804	3.531	71.046
49 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\NC6CCCC6	2.143	2.348	2.700	2.787	2.615	70.810
50 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\NCc6oc(nn6)C	3.177	3.088	3.487	3.421	3.736	70.855
51 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\NCc6sec(n6)C	3.559	3.247	3.458	3.153	3.276	74.226
52 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\NCCc6cccs6	3.253	2.931	3.019	3.578	3.540	71.607
53 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\NCc6cc(N)ccc6	3.128	3.229	3.172	3.404	3.406	62.578
54 ⁴	C1[C@H](C2)C[C@@H](C3)C[C@H]2CC13c(cc4)n(c4-c5cccc5)CC(=O)/N=C(N)\NCCc6sc6	3.248	2.777	3.199	3.443	4.212	66.144
55 ⁵	c1cccc(e12)ccc(c2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)C(=O)OC(C)(C)C	2.770	3.468	2.654	2.748	3.070	67.996
56 ⁵	c1cccc(e12)ccc(c2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)Cc5cccc5	2.284	2.712	2.756	3.226	2.586	69.074
57 ⁵	c1cccc(e12)oc(=O)c(c2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)C(=O)OC(C)(C)C	3.000	3.187	2.889	2.719	3.668	65.290
58 ⁵	c1cccc(e12)oc(=O)c(c2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)Cc5cccc5	3.119	3.310	3.125	3.172	3.369	71.943
59 ⁵	c1ccc(OC)c(c12)oc(=O)c(c2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)C(=O)OC(C)(C)C	2.620	3.369	2.907	3.005	3.604	65.903
60 ⁵	c1ccc(OC)c(c12)oc(=O)c(c2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)Cc5cccc5	2.260	2.437	2.589	2.457	2.113	73.836

61 ⁵	COc(c1)ccc(c12)c(cc(o2)=O)CC(=O)Nc3cc(Br)ccc3N4CCN(CC4)C(=O)OC(C)(C)C	4.032	4.187	4.812	3.432	4.447	66.704
62 ⁵	COc(c1)ccc(c12)c(cc(o2)=O)CC(=O)Nc3cc(Br)ccc3N4CCN(CC4)S(=O)(=O)c5cccs5	2.947	2.709	2.788	2.537	2.742	73.254
63 ⁵	c1cccc(c12)c(=O)cc(o2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)C(=O)OC(C)(C)C	2.721	2.927	2.920	2.329	2.078	63.487
64 ⁵	c1cccc(c12)c(=O)cc(o2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)S(=O)(=O)c5cccs5	2.585	2.563	2.485	2.594	2.840	72.495
65 ⁵	c1cccc(c12)ccc(n2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)C(=O)OC(C)(C)C	2.770	2.947	2.382	2.809	2.205	78.068
66 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(S(=O)(=O)C)ccc3	2.268	2.912	2.266	2.535	2.460	72.626
67 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(ccc3)N(S4(=O)=O)CCCC4	2.721	2.822	2.656	3.298	2.304	70.550
68 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(ccc3)N4C(=O)CCCC4	2.278	2.364	2.571	3.174	2.974	66.785
69 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc3)NC(=O)C	1.208	2.744	1.876	2.853	1.022	72.938
70 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(ccc3)S(=O)(=O)CCCC	2.745	2.768	2.195	2.506	3.769	66.594
71 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc(c3)OC)N4C(=O)CCCC4	3.128	3.145	3.779	3.607	3.657	60.513
72 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc(c3)OCC)N4C(=O)CCCC4	4.229	4.768	4.045	3.553	4.314	61.783
73 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc(c3)OC(C)C)N4C(=O)CCCC4	3.921	2.962	3.606	3.500	4.001	68.821
74 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(N4C(=O)CCCC4)cc(c3)OCCCC	4.495	4.900	4.025	3.684	4.326	73.226
75 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc(c3)OCC)N4CCCC4	2.839	2.937	2.033	3.319	3.300	65.683
76 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(N4C(=O)CCCC4)cc(c3)OCCC	3.218	3.506	3.749	3.598	3.461	74.318
77 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc(c3)NCC)N4C(=O)CCCC4	4.886	4.933	4.697	3.731	4.452	70.999
78 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc(c3)NC(C)C)N4C(=O)CCCC4	4.409	5.015	4.783	3.741	4.008	69.052
79 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(N4C(=O)CCCC4)cc(c3)NCC(C)C	3.745	3.866	3.410	3.780	4.268	65.071
80 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(N4C(=O)CCCC4)cc(c3)C5CCCC5	3.066	3.512	3.965	3.241	3.450	77.432
81 ⁶	C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc(c3)CCC)N4C(=O)CCCC4	4.143	4.182	3.998	3.354	3.802	66.116
82 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3c(F)c(cc(c3)NCC)N(S4(=O)=O)CCCC4	5.699	4.757	4.987	5.557	6.050	69.100
83 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3c(F)c(cc(c3)NCC)N4C(=O)CCCC4	5.046	4.430	4.963	4.304	5.331	69.870
84 ⁷	CCn(c1)nc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3cc(cc(c3)NC)N(S4(=O)=O)CCCC4	5.000	5.411	5.656	4.275	4.949	65.479
85 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc(c3)NCC)N4C(=O)CCCC4	4.310	3.624	5.107	4.254	5.313	69.197
86 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(c(C)j(c3)NCC)N4C(=O)CCCC4	4.201	3.418	3.656	4.159	4.318	77.509
87 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(c(OC)c(c3)NCC)N4C(=O)CCCC4	3.959	4.763	3.022	4.186	4.220	75.150
88 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc(c3)NCC)N(S4(=O)=O)CCCC4	5.301	5.382	5.410	4.459	5.622	70.802
89 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(c(C)j(c3)NCC)N(S4(=O)=O)CCCC4	4.638	4.572	4.293	4.450	4.532	68.485
90 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(c(OC)c(c3)NCC)N(S4(=O)=O)CCCC4	4.745	4.135	3.896	4.819	5.716	68.375
91 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c(cc(c34)jn(en4)CC)cc3N5C(=O)CCC5	4.721	4.915	4.794	5.121	4.344	69.468
92 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c(cc(c34)jn(nc4)CC)cc3N5C(=O)CCC5	4.638	4.540	4.316	4.248	4.369	67.021
93 ⁷	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c(cc(c34)j(c[nH]4)CC)cc3N5C(=O)CCC5	4.585	3.997	3.751	4.463	4.348	70.322

947	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c(cc(c34)j)c(CC)cn4C)cc3N5C(=O)CCCC5	4.398	3.803	4.037	4.426	4.367	69.253
957	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c(cc(c34)n(nc4)CC)cc3N5C(=O)CCCC5	4.553	3.954	3.919	4.537	4.667	71.398
967	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c(cc(c34)n(nn4)CC)cc3N5C(=O)CCCC5	4.469	4.603	4.629	4.080	3.817	69.098
977	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c(cc(c34)j)c(cc4)CC)cc3N5C(=O)CCCC5	4.060	4.172	4.363	4.358	4.340	71.488
987	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c(cc(c34)j)c(ccn4)CC)cc3N5C(=O)CCCC5	3.678	4.243	4.219	4.449	3.334	62.486
997	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c(cc(c34)n(c(=O)[nH]4)CC)cc3N5C(=O)CCCC5	3.377	3.901	3.423	3.825	4.371	73.675
1007	FC(F)(F)c(c1)cccc1C(C)(C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(cc(c3)NCC)N(S4(=O)=O)CCCC4	5.222	5.372	4.597	4.756	5.071	82.238
1017	c1cc(OC)cc(c12)[C@H](CC2)NC[C@@H](O)[C@H](Cc3ccccc3)NC(=O)c4ccc(cc(c4)NCC)N(S5(=O)=O)CCCC5	4.745	4.824	4.966	5.068	5.765	54.780
1027	N#Cc(c1)encc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(cc(c3)NCC)N(S4(=O)=O)CCCC4	4.398	3.966	4.362	4.456	3.854	57.513
103 ⁸	c1cccc1-c(n2OC)nc(c23)ncccc3	0.032	0.833	0.689	0.933	1.102	48.576
104 ⁸	n1c(N)[nH]e(c12)ccc(Cl)c2	0.136	-0.602	-0.499	0.565	1.511	56.310
105 ⁸	c1cc(Cl)ccc(c12)nc(N)n2CCCO	0.114	0.110	0.695	0.299	0.781	55.796
106 ⁸	c1ccnc(n12)nc2-c3ccc(Cl)c3	0.064	0.534	0.456	1.044	0.125	56.187
107 ⁸	c1ccnc(n12)nc2-c3cncnc3	-0.003	0.795	0.393	1.107	-0.115	56.244
108 ⁸	c1cccc(c12)C(=O)C(C2=O)(O)O	0.110	-0.055	0.392	0.265	1.127	58.395
109 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)NCc3ccccc3	-0.147	0.089	0.996	0.378	1.170	57.691
110 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)N(C)C3CCCCC3	1.585	1.234	1.420	0.599	1.480	48.108
111 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)NC(C)C	0.714	0.605	0.536	0.301	0.534	57.592
112 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)NCCN3CCOCC3	0.082	0.816	0.513	0.338	0.890	57.553
113 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)NCC[C@H]3CCNC3	0.353	1.485	0.907	0.451	1.388	64.265
114 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)NCc3ccccc3	0.371	0.881	1.020	0.343	0.137	63.882
115 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)NCC3CCCCC3	1.081	1.238	1.426	0.454	1.487	69.678
116 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)NC3CCN(C)CC3	0.488	1.005	1.578	0.425	0.344	58.204
117 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)NCc3cc(F)ccc3	0.604	0.268	0.514	0.647	0.647	51.833
118 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)NCC3CC3	-0.455	0.741	0.393	0.448	-0.334	49.457
119 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)N(C)Cc3cc(F)ccc3	0.712	1.376	1.673	0.861	0.502	74.233
120 ⁸	c1c(Cl)ccc(c12)n(c(n2)N)CCCC(=O)N(C)CC3CCCCC3	1.229	1.530	1.611	0.656	1.772	80.533
121 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cccc(c3)C(=O)N(CCC)CCC	3.721	3.767	3.719	3.970	3.635	63.063
122 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccc(F)cc(F)e2)NC(=O)c3cccc(c3)C(=O)N(CCC)CCC	4.745	3.984	4.472	4.371	4.684	63.082
123 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cn(C(=O)N(C)CC)j(c34)cccc4	2.824	3.372	3.366	3.879	2.503	53.764
124 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cn(c(c34)ccc4)C(=O)N(CCC)CCC	3.620	3.600	3.660	3.704	2.920	54.208
125 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cn(c(c34)ccc4)C(=O)N(CCCC)CCCC	4.027	4.210	4.377	3.734	4.197	59.936
126 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccc(F)cc(F)e2)NC(=O)c3cn(c(c34)cccc4)C(=O)N(CCCC)CCCC	4.347	4.572	4.586	4.136	4.404	54.023
127 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cn(CCCC)c(c34)cccc4	1.420	2.027	2.000	2.015	1.866	48.088
128 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cn(c(c34)ccc4)S(=O)(=O)CCCC	2.509	4.347	3.556	2.896	2.725	57.816
129 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccc(F)cc(F)e2)NC(=O)c3cn(c(c34)cccc4)C(=O)OCCCC	2.959	3.439	2.966	3.825	2.345	57.302
130 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccc(F)cc(F)e2)NC(=O)c3cn(c(c34)cccc4)C(=O)NCCCC	3.721	3.528	3.662	4.132	3.327	31.358
131 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccc(F)cc(F)e2)NC(=O)c3cn(c(c34)cccc4)C(=O)N(C)CCCC	5.131	4.949	5.119	4.341	5.349	57.525
132 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccc(F)cc(F)e2)NC(=O)c3cn(c(c34)ccc(F)cc4)C(=O)N(C)CCCC	4.180	4.236	3.569	4.318	4.409	71.900
133 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccc(F)cc(F)e2)NC(=O)c3cn(c(c34)ccc(C#N)cc4)C(=O)N(C)CCCC	3.921	3.567	3.782	4.332	3.737	64.717
134 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccc(F)cc(F)e2)NC(=O)c3cn(c(c34)ccc(F)cc4)C(=O)N(C)CCCC	4.886	4.464	4.314	4.339	4.362	67.957
	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccc(F)cc(F)e2)NC(=O)c3cn(c(c34)ccc(F)cc4)C(=O)N(C)CCCC	4.522	5.222	4.487	4.275	4.322	66.210

	34)ccc(Cl)c4)C(=O)N(C)CCCC								
136 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)ccc(c4)C#N)C(=O)N(C)CCCC	4.745	4.818	4.766	4.354	4.270	65.096		
137 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)ccc(c4)C(F)(F)C(=O)N(C)CCCC	3.796	3.870	3.879	4.385	3.406	64.072		
138 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(C(=O)N(C)CCCC)c(c34)ccc(c4)C(=O)OCc5ccccc5	3.066	2.880	3.641	4.719	3.211	61.632		
139 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)ccc(c4)C(=O)O)C(=O)N(C)CCCC	4.155	4.589	4.528	4.474	4.881	53.789		
140 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N(C)CCCC	4.481	4.181	3.458	4.255	4.738	67.282		
141 ⁹	c1e(Br)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cn(c(c34)nccc4)C(=O)N(C)CCCC	4.638	3.551	3.676	3.684	3.943	67.032		
142 ⁹	CCc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N(C)CCCC	5.066	4.324	4.638	3.943	5.640	65.714		
143 ⁹	CCc(c1)cccc1C2(CC2)NC[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)c4en(c(c45)nccc5)C(=O)N(C)CCCC	4.092	3.107	3.994	4.436	4.006	49.730		
144 ⁹	c1cccc1OC)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cn(c(c34)nccc4)C(=O)N(C)CCCC	2.187	2.383	2.940	3.765	2.610	53.443		
145 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N(C)CCCC	4.495	4.486	4.843	4.197	4.361	58.177		
146 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N(C)CCC(C)C	4.553	4.313	4.603	4.258	4.706	56.145		
147 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N(C)CCC)CC5CC5	3.678	3.449	3.707	3.763	3.305	51.523		
148 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N(C)CCOC	4.137	4.490	4.473	4.406	4.519	63.677		
149 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N5CCCC[C@@H]5COC	5.000	4.634	4.878	4.232	5.173	70.510		
150 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N5CCCC[C@@H]5COCC	4.921	4.599	4.200	4.159	4.684	75.738		
151 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N5CCCC[C@@H]5COC	4.523	4.365	4.676	4.105	4.247	65.897		
152 ⁹	COc(c1)cccc1CNC[C@@H](O)[C@H](Cc2cc(F)cc(F)c2)NC(=O)c3cn(c(c34)nccc4)C(=O)N5CCCC[C@@H]5COCC	4.585	4.691	4.957	4.067	4.843	51.433		
153 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H](CC(C)C)NC(=O)[C@H](C)CSC)NC(=O)CCC(C)C	2.854	3.002	3.593	2.595	2.492	46.159		
154 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H](CC(C)C)NC(=O)[C@H](C)NC(=O)CCC(C)C	2.432	2.846	2.619	2.499	2.966	46.159		
155 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H](CC(C)C)NC(=O)[C@H](C)N(C)C(=O)CCC(C)C	2.620	2.366	3.187	2.725	3.670	67.507		
156 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H]1NC(=O)[C@H](C)NC(=O)CCCCC[C@H](C1)C	2.796	2.755	3.031	2.659	3.055	60.083		
157 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H]1NC(=O)[C@H](C)NC(=O)CCCCC[C@H](C1)C	3.229	2.967	2.848	2.701	3.141	60.937		
158 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H]1NC(=O)[C@H](C)NC(=O)CCCCCCCC1	2.119	2.743	2.792	2.651	1.849	74.251		
159 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H]1NC(=O)[C@H](C)NC(=O)CCCCC[C@H](C1)C	3.602	3.391	3.312	2.720	3.239	61.496		
160 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H]1NC(=O)[C@H](C)NC(=O)CCCCC[C@H](C1)C	2.678	2.378	2.844	2.743	2.403	53.248		
161 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H]1NC(=O)[C@H](C)N(C)C(=O)CCCCC[C@H](C1)C	2.602	2.017	2.565	2.774	2.684	80.953		
162 ¹⁰	CCCCNC(=O)[C@H](C)C[C@H](O)[C@H]1NC(=O)[C@H](C)N(C)C(=O)CCCCC[C@H](C1)C	3.824	3.259	3.717	2.793	3.505	66.084		
163 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(N(C)S(=O)(=O)C)cc(c3)C(=O)N[C@H](C)c4cccc4	3.551	3.138	2.752	3.312	3.006	67.542		
164 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(O)cc(c3)C(=O)N[C@H](C)c4cccc4	2.801	2.751	2.402	2.964	2.854	58.644		
165 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(OC)cc(c3)C(=O)N[C@H](C)c4cccc4	2.601	2.806	3.367	3.061	2.793	65.871		
166 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(C#C)cc(c3)C(=O)N[C@H](C)c4cccc4	3.051	2.853	3.044	2.680	3.481	71.015		
167 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(-c4ccsc4)cc(c3)C(=O)N[C@H](C)c5cccc5	2.651	3.323	3.194	2.712	2.206	67.903		

168 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(-c4ccc(Cl)cc4)cc(c3)C(=O)N[C@H](C)c5cccc5	3.091	3.676	3.312	2.997	3.020	71.918
169 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(C#Cc4cccc4)cc(c3)C(=O)N[C@H](C)c5cccc5	2.951	2.728	2.846	2.822	2.620	64.715
170 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(cc(c3)C(=O)N[C@H](C)c4cccc4)-c5nnn(c5)C6cccc6	2.901	3.190	3.488	3.506	2.413	72.616
171 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(N(S4(=O)=O)CC(C4)cc(c3)C(=O)N[C@H](C)c5cccc5	2.751	2.285	2.689	3.804	2.896	69.155
172 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(N(S4(=O)=O)CC(C4)cc(c3)C(=O)N[C@H](C)c5cccc5	3.801	3.863	3.302	3.787	4.955	60.686
173 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c(c3)cc(c(c34)cc(o4)C)C(=O)N[C@H](C)c5cccc5	3.281	3.763	3.367	2.930	3.118	61.496
174 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c(c3)cc(c(c34)CCCCO4)C(=O)N[C@H](C)c5cccc5	4.201	3.594	3.406	3.343	4.365	50.051
175 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c(c3)cc(c(c34)CCCCO4)C(=O)N[C@H](C)c5cccc5	4.252	4.412	4.143	3.240	4.282	60.674
176 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c(c3)cc(c(c34)CCCCO4)C(=O)N[C@H](C)c5ccc(F)cc5	3.131	3.283	4.106	3.390	3.407	59.391
177 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c(c3)cc(c(c34)CCCCO4)C(=O)N[C@H](C)c5ccc(F)cc5	3.582	3.843	3.578	3.286	3.368	67.267
178 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(cc(c34)oc(c4)C)C(=O)N[C@H](C)c5cccc5	3.001	2.940	3.555	2.958	3.499	47.835
179 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(cc(c34)OCCC4)C(=O)N[C@H](C)c5cccc5	3.951	3.513	4.078	3.096	3.736	55.167
180 ¹¹	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c3cc(cc(c34)OCCC4)C(=O)N[C@H](C)c5cccc5	4.051	3.920	4.865	3.078	4.428	52.974
181 ¹²	n1cccc(c1F)-c(ccc2)cc2[C@@]3(C(=O)N(C)C(=N3)N)c4ccc(cc4)OC(F)F	5.000	4.319	4.031	4.385	4.926	54.733
182 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cccc3	3.770	3.040	3.390	3.200	3.373	55.551
183 ¹²	n1cccc(c1F)-c(ccc2)cc2[C@@]3(C(=O)N(C)C(=N3)N)c4ccc(cc4)OC	4.523	4.494	4.389	4.277	4.627	55.928
184 ¹²	n1cccc(c1F)-c(ccc2)cc2[C@@]3(C(=O)N(C)C(=N3)N)c4ccc(cc4)OC(F)F	4.222	4.184	4.232	4.512	4.631	53.847
185 ¹²	n1cccc(c1F)-c(ccc2)cc2[C@@]3(C(=O)N(C)C(=N3)N)c4ccc(cc4)OCCF	4.523	3.758	4.072	4.443	4.938	59.518
186 ¹²	FC(F)(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cccc3	2.848	1.927	1.912	2.267	2.433	59.018
187 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cccc3	2.907	3.074	3.159	4.069	2.583	63.822
188 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(CC)ccc3	3.046	3.693	3.430	4.182	2.995	59.682
189 ¹²	c1ccc(CCC)cc1[C@@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)OC(F)F	4.046	3.752	4.063	4.182	4.272	60.838
190 ¹²	CCCCc(ccc1)ccc1[C@@]2(C(=O)N(C)C(=N2)N)c3ccc(OC(F)F)cc3	4.523	4.266	4.105	4.200	4.237	60.036
191 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)CCCC	4.046	4.372	4.509	4.188	3.731	59.144
192 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)C[C@H](C)CC	3.959	4.115	4.448	4.248	4.279	60.280
193 ¹²	FC(F)(F)CCCc(ccc1)ccc1[C@@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)OC(F)F	4.222	4.294	4.116	4.189	4.014	64.851
194 ¹²	N#CCCCc(ccc1)ccc1[C@@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)OC(F)F	4.301	4.356	4.150	4.210	4.604	60.819
195 ¹²	FCCCC(=O)c(ccc1)ccc1[C@@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)OC(F)F	4.097	3.437	4.197	4.123	5.114	62.678
196 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)[C@H](F)CCCF	4.097	3.908	4.361	4.135	3.861	58.492
197 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C=C/CCF	4.398	4.410	4.537	4.309	4.314	64.554
198 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C=C/CC(F)F	4.523	4.385	4.339	4.296	4.318	62.817
199 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C=C/C4CC4	4.046	4.323	4.682	4.303	4.279	54.348
200 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C(F)=C/C4CC4	4.699	4.491	4.372	4.340	4.630	53.493
201 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C(F)=C4CC4	3.268	2.658	2.639	4.340	3.404	56.021
202 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C=C/COC	4.699	4.234	4.341	4.438	4.939	61.103
203 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C=C/CCOC	4.699	4.189	4.896	4.337	4.362	55.530
204 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C=C/CCOC	4.301	4.115	4.867	4.283	4.175	58.293
205 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C=C/CCO	4.301	3.869	4.406	4.339	4.357	61.685
206 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)/C=C/CCCO	4.398	4.477	4.435	4.290	5.396	57.601
207 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(C#C)ccc3	3.585	3.518	3.149	4.388	3.599	56.418
208 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)C#CC	4.699	4.469	4.250	4.413	4.625	64.559
209 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)C#CCC	4.398	4.530	4.544	4.399	4.622	59.274
210 ¹²	CCCC#Cc(ccc1)ccc1[C@@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)OC(F)F	4.523	4.494	4.172	4.406	4.071	61.652
211 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)C#CCF	5.000	4.281	4.455	4.405	4.669	61.140
212 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)C#CCCF	5.000	4.301	4.414	4.385	4.609	66.246
213 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccc(cc3)C#CCCCF	4.398	4.373	4.804	4.423	4.622	60.802

214 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)C#CC(C)C	4.699	4.622	4.451	4.397	4.372	59.386
215 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)C#CC4CC4	4.699	4.888	4.736	4.421	4.625	61.621
216 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)C#CC4CCCC4	3.481	3.247	3.580	4.414	3.213	60.835
217 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)C#CCOC	4.699	4.697	4.774	4.409	4.660	60.597
218 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)C#CCOC	4.699	4.634	4.825	4.409	4.327	57.187
219 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)C#CCCO	5.000	4.639	3.978	4.428	4.623	58.223
220 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)C#CCCCO	5.000	4.626	4.761	4.422	4.640	60.445
221 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)OCCF	3.921	4.296	4.512	4.469	4.234	61.256
222 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)OCCCF	5.000	4.399	4.467	4.462	5.107	63.807
223 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)OCCCF	4.000	4.611	4.572	4.434	4.139	59.829
224 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)OCC(F)(F)F	3.699	4.470	4.378	4.300	3.344	53.677
225 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)OCC4CC4	4.699	4.318	4.514	4.284	4.458	58.423
226 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(OC(F)F)ccc3	3.699	3.840	3.506	4.283	3.444	62.919
227 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)OCC(F)F	4.523	3.626	3.876	4.407	4.258	57.888
228 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)OCC(F)F	4.155	3.903	3.726	4.494	5.164	57.359
229 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)OCC(F)F	5.000	4.332	4.480	4.340	5.422	60.944
230 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)OCC=C(F)F	4.523	4.204	4.107	4.429	4.799	57.920
231 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)OCC=C(F)F	4.523	4.951	4.750	4.269	4.864	58.276
232 ¹²	FC(F)Oe(cc1)c(C)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3ccccc3	4.097	3.731	3.894	4.175	4.508	58.696
233 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)C#CC4CC4	4.699	4.223	4.524	4.544	4.137	57.999
234 ¹²	FC(F)Oe(cc1)c(C)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)C#CC4CC4	4.699	4.926	4.909	4.714	4.101	54.683
235 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)C#CCOC	4.921	4.490	4.628	4.523	4.861	68.460
236 ¹²	FC(F)Oe(cc1)c(C)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)C#CCOC	4.886	4.591	4.657	4.694	4.916	68.713
237 ¹²	FC(F)Oe(cc1)c(C)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)OCC(F)F	4.824	4.312	4.104	4.681	4.603	84.324
238 ¹²	FC(F)Oe(cc1)c(C)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)C#CC4CC4	4.658	4.657	4.719	4.588	4.544	91.882
239 ¹²	FC(F)Oe(cc1)c(C)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)C#CCF	4.699	4.719	4.489	4.693	4.664	69.089
240 ¹²	FC(F)Oe(cc1)c(C)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)C#CCCC	4.523	4.568	4.618	4.707	4.790	81.333
241 ¹²	FC(F)Oe(cc1)c(C)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(ccc3)C#CCCC	4.854	4.865	4.708	4.574	4.559	28.650
242 ¹²	FC(F)Oe(cc1)ccc1[C@]2(C(=O)N(C)C(=N2)N)c3cc(c(F)cc3)C#CC	4.387	4.273	4.392	4.545	4.049	50.124
243 ¹³	Oc1cc(O)ccc1O	1.438	0.499	0.648	1.367	1.605	52.860
244 ¹³	Oc1cc(O)cc(o2)c1oc(c23)cc(O)c4c3oc5e(o4)cc(O)cc5O	2.272	1.390	1.601	2.304	3.057	48.604
245 ¹³	c1e(O)cc(O)c(O2)c1Oe(c23)c(O)cc(O)c3Oe4cc(O)cc(e4)O	1.914	2.158	1.712	2.163	1.840	50.417
246 ¹³	c1e(O)cc(O)cc1Oe2c(O)cc(O)c(e23)Oe4c(O3)c(O)cc5e4e6c(o5)c(O)cc6(O)Oe7cc(O)cc(e7)O	2.672	3.156	3.207	3.745	2.441	55.093
247 ¹³	c1e(O)cc(O)cc1Oe2c(O)cc(O)c(e23)Oe4c(O3)c(O)cc(e4)Oe5c(O)cc(cc5O)Oe6c(O)cc(O)c(e67)Oe8c(O7)c(O)cc(e8)O	2.656	2.878	2.902	2.266	2.464	54.258
248 ¹³	Oc1cc(O)cc(O)c1Oe2cc(O)cc(O)c2Oe3cc(O)cc(e3)O	1.933	1.817	2.114	2.019	2.844	51.401
249 ¹³	c1e(O)cc(O)cc1Oe2c(O)cc(O)c(e23)Oe4c(O3)c(O)cc(e4)Oe5c(O)cc(O)cc5O	2.066	2.653	1.995	2.624	2.165	54.306
250 ¹⁴	n1[nH]nnc1-c(ccc2)cc2NC(=O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC4CC(C)C)NC(=O)[C@H](C(C)C)NC(=O)[C@@H](N)CNC(=O)c5[nH]c(=O)[nH]c(=O)c5F	5.252	5.308	4.979	5.410	4.698	42.601
251 ¹⁵	Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cccc(c3)C(C)C	4.328	3.570	4.247	3.746	4.204	45.868
252 ¹⁵	Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cccc(c3)-n4cccn4	4.229	3.266	3.597	2.987	4.544	46.774
253 ¹⁵	Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(COCC2)c3cccc(c3)C(C)C	4.215	3.203	4.103	3.318	4.503	45.476
254 ¹⁵	Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@]2(COCC2)c3cccc(c3)-n4cccn4	3.569	3.036	3.702	3.115	3.518	45.029
255 ¹⁵	Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CCCC2)c3cccc(c3)C(C)C	3.658	3.195	3.467	3.721	3.028	49.149
256 ¹⁵	Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@]2(COCC2)c3cccc(c3)-n4cccn4	2.620	2.743	2.967	2.925	2.438	47.748
257 ¹⁵	Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CNCC2)c3cccc(c3)C(C)C	2.328	2.335	2.087	2.684	2.756	43.893
258 ¹⁵	Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CCN(C2)C(=O)N)c3cccc(c3)C(C)C	3.420	4.100	3.674	3.456	3.197	44.953
259 ¹⁵	Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC(=O)NCC2)c3cccc(c3)C(C)C	4.745	4.747	4.727	4.412	4.541	43.020

260 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC(=O)NCC2)c3cccc(c3)C(C)(C)C</chem>	4.721	4.722	4.649	4.412	4.312	37.405
261 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CN(O)CCC2)c3cccc(c3)C(C)(C)C</chem>	3.398	4.310	3.658	3.674	3.037	38.503
262 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(c3cccc(c3)C(C)(C)C)CN(CCC2)C(=O)OCe4cccc4</chem>	3.066	3.975	3.993	4.178	3.524	44.454
263 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CN(C(=O)C)CC2)c3cccc(c3)C(C)(C)C</chem>	2.886	2.585	2.966	3.823	2.615	41.054
264 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CN(C(=O)N)CC2)c3cccc(c3)C(C)(C)C</chem>	3.481	3.508	3.797	3.920	3.634	46.150
265 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CNC(=O)CC2)c3cccc(c3)C(C)(C)C</chem>	4.328	4.204	3.963	3.833	4.160	41.542
266 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CCC(=O)CC2)c3cccc(c3)C(C)(C)C</chem>	3.921	3.434	4.144	4.027	3.520	71.442
267 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](O)CC2)c3cccc(c3)C(C)(C)C</chem>	2.036	2.755	2.412	3.640	2.124	46.693
268 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@@H](O)CC2)c3cccc(c3)C(C)(C)C</chem>	4.620	4.035	4.469	3.640	4.996	51.018
269 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)CO)c3cccc(c3)C(C)(C)C</chem>	4.420	4.216	4.949	3.781	4.746	41.552
270 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CCC(=C)CC2)c3cccc(c3)C(C)(C)C</chem>	4.319	4.687	4.534	4.106	4.867	41.981
271 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@@H](C)CC2)c3cccc(c3)C(C)(C)C</chem>	4.310	4.500	4.200	3.915	4.709	37.202
272 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)SC)c3cccc(c3)C(C)(C)C</chem>	4.620	4.136	4.208	3.980	4.481	42.139
273 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@@H](C(F)(F)F)CC2)c3cccc(c3)C(C)(C)C</chem>	4.481	4.188	4.372	3.538	4.904	48.727
274 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)OC)c3cccc(c3)C(C)(C)C</chem>	3.854	3.196	4.391	4.151	4.123	39.933
275 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@@H](C#N)CC2)c3cccc(c3)C(C)(C)C</chem>	3.420	3.810	3.189	3.761	3.912	45.929
276 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)S(=O)(=O)C)c3cccc(c3)C(C)(C)C</chem>	3.678	3.023	3.862	3.482	3.286	40.392
277 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CCC(CC2)=NO)c3cccc(c3)C(C)(C)C</chem>	5.056	4.482	5.036	4.607	5.398	41.317
278 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)NO)c3cccc(c3)C(C)(C)C</chem>	4.721	4.775	3.646	4.216	5.259	38.901
279 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)NOC)c3cccc(c3)C(C)(C)C</chem>	4.000	4.431	4.441	4.177	3.735	47.355
280 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(c3cccc(c3)C(C)(C)C)CC[C@H](CC2)NC(=O)OC</chem>	3.620	3.594	3.591	3.883	3.394	49.615
281 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)NC=O)c3cccc(c3)C(C)(C)C</chem>	3.678	3.580	3.535	3.912	3.210	48.767
282 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)NS(=O)(=O)C)c3cccc(c3)C(C)(C)C</chem>	3.398	4.392	3.861	4.402	3.670	66.477
283 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)N(O)C(=O)C)c3cccc(c3)C(C)(C)C</chem>	3.620	3.571	3.675	3.238	4.175	85.103
284 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(CC[C@H](CC2)NC(=O)C)c3cccc(c3)C(C)(C)C</chem>	3.456	3.904	3.870	4.106	3.355	76.055
285 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(c3cccc(c3)C(C)(C)C)CC[C@H](CC2)Nc4cccc4</chem>	4.137	4.048	4.330	3.951	4.452	80.425
286 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(c3cccc(c3)C(C)(C)C)CC[C@H](CC2)Nc4scn4</chem>	4.071	4.258	3.303	3.874	4.127	79.019
287 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@]2(c3cccc(c3)C(C)(C)C)CC[C@H](CC2)Nc4ence4</chem>	3.301	3.038	4.274	3.910	3.266	76.560
288 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@](C2)(CCc(c23)n[nH]c3)c4cccc(c4)C(C)(C)C</chem>	4.921	4.354	4.644	4.716	5.116	73.606
289 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@](C2)(c3cccc(c3)C(C)(C)C)CCc(c24)nc(N)nc4</chem>	4.854	3.885	4.097	4.809	5.127	69.392
290 ¹⁵	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@@](C2)(c3cccc(c3)C(C)(C)C)CCc(c24)nc(C)nc4</chem>	4.032	4.686	4.298	5.200	5.065	65.303
291 ¹⁶	<chem>c1cccc1C[C@H]([C@H](O)CNC2CC2)NC(=O)c(c3)cc(c4c35)c(C)cn4CCS(=O)(=O)N5C</chem>	4.699	4.653	4.999	4.470	4.916	82.047
292 ¹⁶	<chem>C1CCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2cccc2)NC(=O)c3ccc(cc3)N(S(=O)(=O)C)c4cccc4</chem>	4.824	4.561	4.225	3.904	4.273	80.395

293 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)Nc4ccccc4	2.201	2.730	2.831	3.011	2.793	66.770
294 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(C(=O)C)c4ccccc4	2.886	3.211	2.160	3.494	3.240	77.818
295 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)C4CCCCC4	3.523	2.792	3.291	3.570	3.479	69.009
296 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)C4c4ccccc4	3.745	3.701	3.916	2.921	3.659	77.863
297 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)NS(=O)(=O)c4ccccc4	2.102	2.417	2.287	2.885	2.583	74.844
298 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)NS(=O)(=O)C4c4ccccc4	2.260	2.977	2.667	3.079	3.729	78.770
299 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)OS(=O)(=O)C4c4ccccc4	1.886	2.451	2.726	2.074	1.716	73.518
300 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)CS(=O)(=O)c4ccccc4	1.357	1.643	2.244	1.730	1.556	69.344
301 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)S(=O)(=O)C4c4ccccc4	1.301	2.338	1.857	2.599	1.124	79.232
302 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)S(=O)(=O)N(C)C4c4ccccc4	1.387	3.996	2.048	2.162	1.337	81.052
303 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccccc4	4.638	4.520	4.728	4.425	4.836	69.981
304 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccccc4OC	3.900	3.517	3.780	3.905	4.801	79.210
305 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccccc4C#N	3.509	2.893	3.564	4.016	4.512	76.316
306 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4cccc(c4)OC	4.745	5.122	5.176	4.006	4.584	76.728
307 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4cccc(c4)C#N	5.097	4.943	4.619	4.663	5.393	77.592
308 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4cccc(c4)OC	4.959	4.476	4.618	4.688	4.675	73.430
309 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccc(C(F)(F)F)c4	4.699	4.608	4.436	3.951	4.657	80.166
310 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccc(Cl)cc4	5.000	4.156	5.878	4.685	4.671	77.662
311 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccc(C#N)cc4	3.721	3.839	3.501	3.807	3.982	77.650
312 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4cc(Cl)cc(Cl)c4	4.959	4.589	4.403	3.915	4.840	78.996
313 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)N(S(=O)(=O)C)c45ccccc5	3.041	3.152	3.208	2.629	2.861	79.451
314 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4cccn4	3.538	3.573	4.399	4.004	3.799	80.001
315 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccncc4	4.602	4.427	4.579	4.284	4.886	69.181
316 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccncc4	3.678	4.228	4.719	3.655	4.825	68.228
317 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3c(C)c(c3)N(S(=O)(=O)C)c4ccncc4	4.585	4.499	4.313	3.922	4.343	69.500
318 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccncc4	3.032	3.272	2.910	3.753	2.867	79.453
319 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(c3)N(S(=O)(=O)C)c4ccncc4	2.460	2.708	2.514	3.578	2.711	85.255
320 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3nc(c3)N(S(=O)(=O)C)c4ccncc4	2.440	2.806	3.074	2.458	2.859	67.018
321 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(ncc3)N(S(=O)(=O)C)c4ccncc4	4.824	4.516	4.430	4.395	4.731	70.287
322 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(ene3)N(S(=O)(=O)C)c4ccncc4	4.678	4.046	4.360	3.764	4.894	69.434
323 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(cen3)N(S(=O)(=O)C)c4ccncc4	2.340	2.450	2.974	2.292	2.853	74.855
324 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(cc3)NCCN4C(=O)CCC4	4.886	4.333	4.346	3.731	5.015	71.559
325 ¹⁶	C1CCCCC1NC(=O)[C@H](C)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cc(cc3)NCCN(S(=O)(=O)C)c4ccccc4	5.523	5.554	4.726	4.566	5.220	68.715

326 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(cc3)OCC)N(S(=O)(=O)C)c4cccc4	5.523	5.336	5.513	4.939	5.419	61.012
327 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(cc3)C(C)C)N(S(=O)(=O)C)c4cccc4	5.301	4.902	5.092	4.539	5.322	51.708
328 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(N(S(=O)(=O)C)c4cccc4)cc(c3)-c5cccc5	4.886	4.778	5.262	4.269	4.308	64.923
329 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(cc3)N4C(=O)CCC4)N(S(=O)(=O)C)c5cccc5	5.222	5.807	5.356	5.972	5.102	72.702
330 ¹⁶	FC(F)(F)c(c1)cccc1CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(cc3)S(=O)(=O)CC)N(S(=O)(=O)C)c4cccc4	4.854	4.980	4.693	4.372	4.332	70.107
331 ¹⁶	CC(C)CCC[C@@H](C)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c2ccc(cc2)N(S(=O)(=O)C)c3cccc3	4.495	3.993	4.156	3.695	4.314	69.280
332 ¹⁶	C1CCCCC1NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(cc3)N(S(=O)(=O)C)c4cccc4	3.614	3.772	3.918	3.719	3.481	70.462
333 ¹⁶	c1cccc1C[C@@H]([C@H](O)C)N2C2)NC(=O)c3ccc(cc3)N(S(=O)(=O)C)c4cccc4	3.357	3.976	3.732	3.500	3.751	63.938
334 ¹⁷	C1CCCN[C@H]1[C@@H](O)[C@H](C[C@@H]2C=C(F)C=C(F)C2)NC(=O)c3ccc(C)cc(c3)C(=O)N(CCC)CCC	3.886	3.798	4.148	3.900	4.174	65.574
335 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCC[C@H](C3)Cc4cccc4	4.854	4.893	4.595	4.187	4.345	56.741
336 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCC[C@H](C3)OCC	5.155	4.615	4.365	4.148	5.315	69.310
337 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4	5.523	5.630	4.682	4.981	5.162	74.025
338 ¹⁷	C1CC[C@H](COC)N1C(=O)c(c2)ccc(C)cc2C(=O)N[C@@H](C[C@@H]3C=C(F)C=C(F)C3)[C@H](O)[C@@H]4NCCN(C4=O)Cc5cccc5	6.000	4.953	5.315	5.787	5.677	68.945
339 ¹⁷	C1CC[C@H](COC)N1C(=O)c(c2)ccc(OC)cc2C(=O)N[C@@H](C[C@@H]3C=C(F)C=C(F)C3)[C@H](O)[C@@H]4NCCN(C4=O)Cc5cccc5	5.398	5.429	5.388	5.909	4.989	68.488
340 ¹⁷	C1CC[C@H](COC)N1C(=O)c(c2)ccc2C(=O)N[C@@H](C[C@@H]3C=C(F)C=C(F)C3)[C@H](O)[C@@H]4NCCN(C4=O)Cc5cccc5	5.699	4.548	4.800	4.575	5.386	63.555
341 ¹⁷	CCCN(C1)C(=O)C[C@@H]1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4	5.046	4.708	4.740	4.897	5.497	63.015
342 ¹⁷	CCCN(C1)C(=O)C[C@@H]1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4	5.301	4.143	5.107	5.008	5.891	71.797
343 ¹⁷	CCCN(C1)C(=O)C[C@@H](CC)[C@H]1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4	5.523	4.401	5.240	4.250	4.997	68.261
344 ¹⁷	C1=CC=CC[C@@H]1C[C@@H](C(=O)N(C2)CCCC)[C@H]2C(=O)N[C@@H](C[C@@H]3C=C(F)C=C(F)C3)[C@H](O)[C@@H]4NCCN(C4=O)Cc5cccc5	4.796	4.488	4.807	4.455	4.860	64.718
345 ¹⁷	C1CC1CN(C2)C(=O)C[C@@H]2C(=O)N[C@@H](C[C@@H]3C=C(F)C=C(F)C3)[C@H](O)[C@@H]4NCCN(C4=O)Cc5cccc5	5.000	4.997	5.117	4.245	4.931	55.498
346 ¹⁷	C1=CC=CC[C@@H]1CN(C2)C(=O)C[C@@H]2C(=O)N[C@@H](C[C@@H]3C=C(F)C=C(F)C3)[C@H](O)[C@@H]4NCCN(C4=O)Cc5cccc5	4.658	4.571	4.361	3.975	4.758	46.806
347 ¹⁷	COCCN(C1)C(=O)C[C@@H]1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4	4.886	4.413	4.798	4.020	5.898	54.270
348 ¹⁷	CCCN(C1)C(=O)N(CC)[C@H]1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4	5.046	4.195	4.543	4.920	4.956	60.689
349 ¹⁷	CCCN(C1)C(=O)N(C)C(C)[C@H]1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4	4.959	5.075	4.084	5.273	5.931	82.016
350 ¹⁷	CCCN(C1)C(=O)N(CCC)CC1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4	4.658	4.754	4.382	4.997	4.336	60.638
351 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H]([C@H](O)[C@@H]2NCCN2=O)C[C@@H]3C=C(F)C=C(F)C3	3.578	4.222	4.015	4.363	3.439	65.561
352 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H]([C@H](O)[C@@H]2NCCN(C2=O)C)C[C@@H]3C=C(F)C=C(F)C3	3.629	2.946	2.565	4.435	3.734	60.183
353 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)CC	3.757	3.680	4.144	4.549	4.086	67.011
354 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)CCC	4.357	4.590	4.543	4.515	4.869	69.794
355 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)CC(C)C	4.886	4.885	4.867	4.504	4.842	65.724
356 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)CC4CC4	5.000	4.993	4.452	4.533	5.488	70.759
357 ¹⁷	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4c(OC)cccc4	5.301	4.468	5.047	4.706	5.421	51.744
	CCCN(CCC)C(=O)c(c1)ccc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)[C@H](O)[C@@H]3NCCN(C3=O)Cc4c(OC)cccc4	4.600	4.648	3.658	4.702	4.255	42.246

	<chem>=C(F)C2)C@H](O)[C@@H]3NCCN(C3=O)Cc4c(C#N)cccc4</chem>								
359 ¹⁷	<chem>CCCN(CCC)C(=O)c(c1)cc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)C@H](O)[C@@H]3NCCN(C3=O)Cc4c(Cl)cccc4</chem>	4.569	4.806	4.910	4.976	4.494	45.245		
360 ¹⁷	<chem>CCCN(CCC)C(=O)c(c1)cc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)C@H](O)[C@@H]3NCCN(C3=O)c4cccc4</chem>	3.462	3.322	3.391	4.291	3.785	60.428		
361 ¹⁷	<chem>CCCN(CCC)C(=O)c(c1)cc(C)cc1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4</chem>	5.301	4.572	5.101	4.779	5.743	59.649		
362 ¹⁷	<chem>C1CC[C@H](COC)N1C(=O)c(c2)cc(C)cc2C(=O)N[C@@H](C[C@@H]3C=C(F)C=C(F)C3)C@H](O)[C@@H]4NCN(C4=O)Cc5cccc5</chem>	5.699	5.765	5.132	5.586	6.712	64.053		
363 ¹⁷	<chem>CCCN(C1)C(=O)C[C@@H]1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4</chem>	3.043	2.877	3.010	3.256	2.852	66.154		
364 ¹⁷	<chem>CCCN(C1)C(=O)C[C@@H]1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4</chem>	3.854	3.521	3.638	3.368	3.322	65.615		
365 ¹⁷	<chem>CCCN(C1)C(=O)[C@H](CC)[C@H]1C(=O)N[C@@H](C[C@@H]2C=C(F)C=C(F)C2)C@H](O)[C@@H]3NCCN(C3=O)Cc4cccc4</chem>	4.056	4.013	4.752	3.575	4.222	62.962		
366 ¹⁸	<chem>Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc2)N(C)S(=O)(=O)C)NC(=O)[C@@](O)(Cc3cccc3)CCC(=O)N[C@@H](C(C)C)C(=O)NC4cccc4</chem>	2.229	2.722	3.090	3.169	2.677	66.167		
367 ¹⁸	<chem>c1cccc1[C@@H](C)NC(=O)c2cc(cc2)N(C)S(=O)(=O)C)NC(=O)[C@@](O)(Cc3cccc3)CCC(=O)N[C@@H](C(C)C)C(=O)NC4cccc4</chem>	2.252	2.466	2.992	3.830	2.690	57.166		
368 ¹⁸	<chem>Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc2)N(C)S(=O)(=O)C)NC(=O)[C@@](O)(Cc3cccc3)CCC(=O)N[C@@H](C(C)C)C(=O)NC4ccc(cc4)C(=O)OC</chem>	2.398	2.798	2.435	2.456	2.151	41.580		
369 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@H]2C[C@H](CCC2)c3cccc(c3)C(C)C</chem>	4.328	4.158	4.057	4.886	4.256	58.006		
370 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@H]2C[C@H](COC2)c3cccc(c3)C(C)C</chem>	4.215	3.213	3.433	3.881	5.216	58.866		
371 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@H]2C[C@H](CCC2)c3nncn(c3)C(C)C</chem>	2.620	2.644	2.485	2.909	2.338	70.279		
372 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@H]2C[C@H](CCC2)c3cccc(c3)-n4nccc4</chem>	4.229	3.761	4.408	4.586	4.033	67.745		
373 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@H]2C[C@H](CCC2)c3cccc(c3)[C@@H]4COCC4</chem>	4.056	3.583	3.472	3.844	4.138	63.195		
374 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@H]2C[C@H](COC2)c3cccc(c3)-n4nccc4</chem>	3.959	3.800	3.400	3.731	4.066	59.628		
375 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@H]2C[C@H](COC2)c3cccc(c3)[C@H]4COCC4</chem>	3.538	3.955	2.892	2.870	4.087	61.059		
376 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNCc2cccc(c2)C(C)C</chem>	2.886	2.950	2.970	2.373	2.271	59.369		
377 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC(C)C)c2cccc(c2)C(C)C</chem>	3.699	2.929	2.731	2.952	3.311	47.216		
378 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cccc(c3)C(C)C</chem>	3.854	3.792	3.173	3.713	3.963	55.600		
379 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cnn(c3)CC(C)C</chem>	3.456	2.980	2.856	3.183	3.811	64.542		
380 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cccc(c3)-n4cccn4</chem>	3.009	2.954	2.787	2.973	2.795	67.485		
381 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cccc(c3)[C@@H]4CCOC4</chem>	3.119	1.719	2.666	3.718	2.666	66.275		
382 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cccc(c3)C(=C)C(F)F</chem>	2.886	2.829	3.000	3.062	3.156	66.367		
383 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cccc(c3)C(C)C</chem>	3.538	2.754	3.307	3.648	3.223	62.356		
384 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cccc(c3)C(C)F)C</chem>	3.638	2.712	3.473	3.581	3.327	63.550		
385 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cccc(c3)C(C)F)CF</chem>	3.409	3.181	3.789	3.564	3.468	65.377		
386 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CNC2(CCC2)c3cccc(c3)C(C)C</chem>	3.215	2.738	2.801	3.772	3.488	70.034		
387 ¹⁹	<chem>Fc1cc(F)cc(c1)C[C@H](NC(=O)C)[C@H](O)CN[C@]2([C@@H](C2)C)c3cccc(c3)C(C)F)C</chem>	2.770	3.286	2.824	2.893	3.075	74.665		
388 ²⁰	<chem>c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)NC(=O)c4cc(Br)ccc4</chem>	3.222	3.708	3.743	3.045	4.172	51.359		
389 ²⁰	<chem>c1ccoc1C(=O)Nc2cccc(c2)[C@@]3(C(=O)N(C)C(=N3)N)C4CCCC4</chem>	4.000	3.295	4.814	3.059	3.962	64.657		
390 ²⁰	<chem>Cc1ccoc1C(=O)Nc2cccc(c2)[C@@]3(C(=O)N(C)C(=N3)N)C4CCCC4</chem>	4.398	4.066	4.018	4.080	3.991	71.210		
391 ²⁰	<chem>c1ccn(C)c1C(=O)Nc2cccc(c2)[C@@]3(C(=O)N(C)C(=N3)N)C4CCCC4</chem>	3.066	2.952	3.760	2.737	2.774	53.932		
392 ²⁰	<chem>CCCC(=O)Nc1cccc(c1)[C@@]2(C(=O)N(C)C(=N2)N)C3CCCC3</chem>	2.545	2.521	2.805	2.676	2.576	56.095		
393 ²⁰	<chem>COCC(=O)Nc1cccc(c1)[C@@]2(C(=O)N(C)C(=N2)N)C3CCCC3</chem>	3.678	3.125	3.282	3.582	3.898	55.700		

394 ²⁰	COCCC(=O)Ne1cccc(e1)[C@@]2(C(=O)N(C)C(=N2)N)C3CCCCC3	2.105	2.854	2.939	2.727	1.820	54.137
395 ²⁰	COc(e1)cccc1C(=O)Ne2cccc(e2)[C@@]3(C(=O)N(C)C(=N3)N)C4CCCCC4	2.866	2.830	2.995	3.195	2.407	76.921
396 ²⁰	O1COc(e12)cc(cc2)C(=O)Ne3cccc(e3)[C@@]4(C(=O)N(C)C(=N4)N)C5CCCCC5	3.420	3.473	2.948	3.494	3.150	72.359
397 ²⁰	c1cccc1[C@]2(C3CCCCC3)C(=O)N(C(=N2)N)CCCCC	2.857	2.409	2.863	2.466	2.966	51.188
398 ²⁰	c1cccc1[C@]2(C3CCCCC3)C(=O)N(C(=N2)N)CCCCC(=O)O	3.022	2.677	2.935	2.467	3.182	52.756
399 ²⁰	c1cccc1[C@]2(C3CCCCC3)C(=O)N(C(=N2)N)C[C@H]4CC[C@H](CC4)C(=O)O	3.409	3.061	3.397	2.679	3.309	57.706
400 ²⁰	c1cccc1[C@]2(C3CCCCC3)C(=O)N(C(=N2)N)Cc4cccc4	2.907	2.439	2.928	2.919	3.243	61.498
401 ²⁰	c1cccc1[C@]2(C3CCCCC3)C(=O)N(C(=N2)N)Cc4cc(F)cc(F)c4	2.967	2.341	2.988	3.022	3.255	60.241
402 ²⁰	c1cccc1[C@]2(C3CCCCC3)C(=O)N(C(=N2)N)C[C@H]4CCCO4	2.983	2.858	2.966	2.517	3.182	61.917
403 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(cc(e3)N(C)S(=O)(=O)C)C(=O)N[C@H](CC2)c4cccc4	5.699	5.207	5.194	5.549	5.369	60.696
404 ²¹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)-c(nn3)oc3[C@](C)(N)Cc4cccc4	5.046	4.492	5.507	4.173	4.729	58.444
405 ²¹	c1cc(F)ccc1[C@@H](C)N[C@H](C(F)(F)F)c2cc(cc(e2)N(C)S(=O)(=O)C)-c(nn3)oc3[C@](C)(N)Cc4cc(F)cc4	1.824	2.353	1.343	2.479	1.438	60.179
406 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(cc(e3)N(C)S(=O)(=O)C)[C@@H](C(F)(F)F)N[C@H](CC2)c4cccc4	2.432	2.832	2.489	2.349	2.798	69.236
407 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(NCCCC2)nc(e3)N(C)S(=O)(=O)C	3.398	2.395	3.274	3.082	3.322	73.380
408 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(nc(e3)N(C)S(=O)(=O)C)N(CC2)Cc4cccc4	1.886	3.847	2.016	2.192	1.644	65.309
409 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(N(C)C)CCCC2nc(e3)N(C)S(=O)(=O)C	1.658	2.584	2.735	2.140	1.855	72.792
410 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(N(C)C)CC4CC4nc(e3)N(C)S(=O)(=O)C	2.222	2.951	2.745	2.898	3.193	69.156
411 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(CC[C@@H](C)CC2)cc(e3)N(C)S(=O)(=O)C	2.770	3.568	2.721	2.802	2.563	72.262
412 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(CC[C@@H](C)CC2)nc(e3)N(C)S(=O)(=O)C	2.745	2.513	2.640	2.607	2.696	70.611
413 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(nc(e3)N(C)S(=O)(=O)C)CC[C@@H](CC2)c4cccc4	2.155	2.442	2.119	3.034	2.305	72.381
414 ²¹	c12cccc(e1)C[C@@](C)(N)C(=O)OCc3cc(CCCCC2)nc(e3)N(C)S(=O)(=O)C	1.824	2.497	2.016	2.581	2.049	64.269
415 ²²	C1CCC(=O)N1e2cc(OCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)C(F)(F)F	3.420	3.973	4.244	4.081	4.398	68.839
416 ²²	O=C1CCC(C)=C1e2cc(OCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)C(F)(F)F	3.602	4.388	4.246	3.397	3.522	70.738
417 ²²	c1cccc(C(=O)C)c1-e2cc(OCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)C(F)(F)F	3.553	3.178	3.681	3.431	3.785	72.440
418 ²²	c1cccc(C#N)c1-e2cc(OCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)C(F)(F)F	3.796	3.201	3.378	3.539	3.582	76.122
419 ²²	C1CCN(S1(=O)=O)e2cc(OCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)C(F)(F)F	4.301	4.256	4.156	4.435	4.834	70.519
420 ²²	C1CCCN(S1(=O)=O)e2cc(OCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)C(F)(F)F	5.222	4.703	4.973	4.392	5.322	71.775
421 ²²	C1CCCN(S1(=O)=O)e2cc(CCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)C(F)(F)F	5.301	4.814	4.215	4.282	6.307	72.945
422 ²²	C1CCCN(S1(=O)=O)e2cc(NC(C)C)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)C(F)(F)F	4.959	4.278	5.395	4.455	4.598	70.571
423 ²²	C1CCCN(S1(=O)=O)e2cc(OCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)OC(F)(F)F	5.301	5.068	5.279	4.727	5.267	70.681
424 ²²	C1CCCN(S1(=O)=O)e2cc(NCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc(e4)OC(F)(F)F	5.301	4.420	5.446	4.800	5.016	70.593
425 ²²	C1CCCN(S1(=O)=O)e2cc(NCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc4	3.921	3.424	4.520	4.467	3.700	75.086
426 ²²	C1CCCN(S1(=O)=O)e2cc(NCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNC[C@@H]4CCc(e45)cccc5	4.469	5.096	4.715	4.777	4.122	73.476
	C1CCCN(S1(=O)=O)e2cc(NCC)cc(e2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCe4cccc4	4.745	4.748	3.656	5.068	4.666	69.036

	H](O)CN[C@@H]4CCc(c45)ccc(c5)OC							
428 ²²	C1CCCN(S1(=O)=O)c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4cccc(c4)OC	5.097	4.954	4.698	4.602	4.935	68.501	
429 ²²	C1CCCN(S1(=O)=O)c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cccc(c4)OC	5.301	4.542	4.681	5.002	5.128	69.909	
430 ²²	C1CCCN(S1(=O)=O)c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4cccc(c4)OC	4.398	3.679	3.697	4.299	4.754	71.132	
431 ²²	C1CCCN(S1(=O)=O)c2cc(NCC)cc(c2)C(=O)N[C@@H](Cn3nccc3)[C@H](O)CNCc4cccc(c4)OC	2.570	3.342	3.484	2.653	2.737	81.816	
432 ²²	C1CCCN(S1(=O)=O)c2cc(NCC)cc(c2)C(=O)N[C@@H](CC(C)C)[C@H](O)CNCc3cccc(c3)OC	2.240	2.719	2.902	3.943	2.596	70.562	
433 ²²	C1CCCN(S1(=O)=O)c2cc(NCC)cc(c2F)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4cccc(c4)OC	5.398	4.484	4.910	4.693	5.608	78.502	
434 ²²	C1CCCN(S1(=O)=O)c2cc(NCC)cc(c2F)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4cnn(c4)CC	5.222	5.143	4.333	4.552	5.471	84.273	
435 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CC	2.155	2.507	2.785	2.703	2.444	72.227	
436 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCC	3.046	3.131	2.272	3.719	3.447	71.737	
437 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)C(C)C	2.523	2.660	3.354	2.752	2.464	69.079	
438 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCCC	3.432	3.873	4.648	3.831	3.607	74.167	
439 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCCCC	4.347	4.494	4.968	3.847	4.447	72.615	
440 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCCCC	4.000	3.627	3.893	3.843	4.456	76.042	
441 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCCCC	4.149	4.533	3.955	3.861	4.414	73.249	
442 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CC5CC5	3.810	2.847	3.066	4.068	4.485	74.269	
443 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCOCC	2.699	2.716	3.502	3.742	2.495	79.169	
444 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCOC	2.530	2.827	3.475	2.701	2.741	75.973	
445 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCOCC	3.569	4.201	3.858	3.843	3.205	72.761	
446 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCOCCC	3.071	3.127	3.474	3.854	3.290	75.344	
447 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5ccccc5	3.538	3.097	3.035	3.681	3.439	75.484	
448 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5ccc(F)cc5	2.553	2.973	3.094	3.737	2.504	73.002	
449 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5ccc(Cl)cc5	1.726	1.975	1.208	1.726	1.496	70.173	
450 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5ccc(C(F)F)cc5	1.337	1.804	1.363	1.729	1.519	65.821	
451 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5cc(F)ccc5	3.471	2.714	3.114	3.728	4.504	73.213	
452 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5cc(C)ccc5	3.456	3.483	2.791	3.725	4.440	60.476	
453 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5ccccc5F	3.438	3.197	3.187	3.869	3.490	72.373	
454 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5cccn5	3.506	3.430	3.793	3.641	4.493	60.714	
455 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5enccc5	3.660	2.893	2.964	3.794	3.435	68.409	
456 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5ccc5	3.648	3.782	3.533	3.758	3.495	56.323	
457 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)Cc5ccc5	3.519	3.185	3.124	3.887	3.422	63.235	
458 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](NC(=O)[C@@H]3[C@@H](C(=O)NC3)CCC)Cc4cc(F)cc(F)c4	2.921	3.258	3.007	3.695	2.495	61.629	
459 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4[C@@H](CCC)C(=O)N(C4)CCCC	3.848	4.558	3.408	4.122	4.394	67.001	
	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@@H]4CC(=O)N(C4)CCCC	3.050	4.044	3.640	4.137	3.638	69.121	

	F)c3)NC(=O)[C@@H]4[C@H](CCCC)C(=O)N(C4)CCCC								
461 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@H]4[C@H](CC(C)C)C(=O)N(C4)CCCC	4.244	4.347	4.137	4.112	4.477	64.653		
462 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@H]4[C@H](C(=O)N(C4)CCCC)Cc5ccccc5	4.108	4.325	4.436	4.420	4.493	63.814		
463 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@H]4[C@H](C5CC5)C(=O)N(C4)CCCC	3.244	4.261	3.589	4.063	3.407	61.269		
464 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@H]4[C@H](C5CCCC)C(=O)N(C4)CCCC	3.530	3.949	3.207	3.957	3.428	64.124		
465 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@H]4[C@H](CC(C)C)C(=O)N(C4)CCCC	3.438	3.633	3.876	4.117	4.440	57.413		
466 ²³	c1cccc1CO[C@@H](CN2)C[C@@H]2[C@H](O)[C@H](Cc3cc(F)cc(F)c3)NC(=O)[C@H]4[C@H](C(=O)N(C4)CCCC)Cc5ccccc5	3.533	3.865	4.041	4.419	3.417	60.920		
467 ²⁴	Fc1cc(F)cc(c1)C[C@H]([C@H](O)[C@@H]2NCC2)NC(=O)c3cc(cc(c3)C)C(=O)N(CCC)CCC	3.114	3.288	2.858	3.448	3.250	51.197		
468 ²⁴	Fc1cc(F)cc(c1)C[C@H]([C@H](O)[C@H]2CCCN2)NC(=O)c3cc(cc(c3)C)C(=O)N(CCC)CCC	4.187	3.522	3.907	4.174	4.292	57.616		
469 ²⁴	Fc1cc(F)cc(c1)C[C@H]([C@H](O)[C@H]2C[C@@H](O)CN2)NC(=O)c3cc(cc(c3)C)C(=O)N(CCC)CCC	4.051	3.943	3.949	3.989	3.897	63.964		
470 ²⁴	Fc1cc(F)cc(c1)C[C@H]([C@H](O)[C@H]2C[C@@H](CN2)OC)NC(=O)c3cc(cc(c3)C)C(=O)N(CCC)CCC	3.728	4.732	3.925	4.358	3.467	68.891		
471 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3C[C@H](CN3)OCc4ccccc4	5.301	5.158	4.585	4.883	5.212	61.236		
472 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3C[C@H](CN3)OCc4ccccc4	5.523	4.373	4.685	5.276	5.320	65.112		
473 ²⁴	Fc1cc(F)cc(c1)C[C@H]([C@H](O)[C@@H]2NCCC2)NC(=O)c3cc(cc(c3)C)C(=O)N(CCC)CCC	3.886	4.328	3.838	4.324	3.434	63.162		
474 ²⁴	CCC[C@H](C1)CCN[C@H]1[C@@H](O)[C@@H](Cc(c2)cc(F)cc2F)NC(=O)c3cc(cc(c3)C)C(=O)N(CCC)CCC	4.155	3.680	3.270	4.474	4.053	65.179		
475 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)Cc4ccccc4	4.854	4.480	4.753	4.576	4.707	56.316		
476 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)Cc4c(OC)cccc4	2.870	3.091	2.968	3.582	3.869	61.635		
477 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)Cc4cc(OC)cccc4	3.481	4.617	3.743	4.560	3.210	61.866		
478 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)Cc4ccc(cc4)OC	3.357	3.397	3.669	4.680	3.302	50.306		
479 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)CCc4ccccc4	3.719	3.889	4.053	4.478	4.731	50.410		
480 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)C4CCCC4	3.215	3.632	3.627	3.665	3.162	62.021		
481 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)CC4CCCC4	3.201	3.623	4.071	3.775	3.426	68.704		
482 ²⁴	O=C(C)O[C@H](C1)CCN[C@H]1[C@@H](O)[C@@H](Cc(c2)cc(F)cc2F)NC(=O)c3cc(cc(c3)C)C(=O)N(CCC)CCC	2.699	3.267	2.590	3.690	2.457	63.236		
483 ²⁴	CCO[C@H](C1)CCN[C@H]1[C@@H](O)[C@@H](Cc(c2)cc(F)cc2F)NC(=O)c3cc(cc(c3)C)C(=O)N(CCC)CCC	5.097	5.084	5.225	4.605	4.817	61.737		
484 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)OCCCC	5.155	4.353	4.291	4.570	5.418	61.297		
485 ²⁴	CC(C)O[C@H](C1)CCN[C@H]1[C@@H](O)[C@@H](Cc(c2)cc(F)cc2F)NC(=O)c3cc(cc(c3)C)C(=O)N(CCC)CCC	3.921	3.860	4.712	4.551	3.825	59.839		
486 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)OCC4CC4	5.222	4.418	4.878	4.480	5.700	66.449		
487 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)OCCOC	5.398	4.904	5.512	4.556	5.014	59.382		
488 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)OCCN(C)C	4.585	4.659	4.358	4.607	4.871	61.651		
489 ²⁴	CCCN(CCC)C(=O)c(cc(c1)C)cc1C(=O)N[C@H](Cc(c2)cc(F)cc2F)[C@H](O)[C@H]3NCC[C@H](C3)OCC4CCCC4	4.921	4.537	4.350	4.575	4.977	60.673		
490 ²⁵	c1c(F)cc(F)cc1C[C@@H](CO)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC[C@H]3[C@H](C3)C	4.131	3.929	3.373	4.322	4.750	64.954		
491 ²⁵	c1c(F)cc(F)cc1C[C@@H]([C@@H](O)CCCC)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC[C@H]3[C@H](C3)C	4.886	4.776	5.077	4.867	5.048	58.203		
492 ²⁵	c1c(F)cc(F)cc1C[C@@H]([C@@H](N)CCCC)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC[C@H]3[C@H](C3)C	5.046	4.814	4.726	4.788	5.676	72.576		
	c1cccc1C[C@H](CN)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC[C@H]3[C@H](C3)C	4.460	3.746	4.463	4.038	5.442	54.743		

	3[C@H](C3)C						
494 ²⁵	c1cccc1C[C@@H]([C@@H](N)CCCC)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC[C@H]3[C@H](C3)C	4.699	4.372	4.226	4.570	4.092	65.636
495 ²⁵	c1cccc1C[C@@H]([C@@H](N)CCCF(F)F)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC[C@H]3[C@H](C3)C	5.699	5.693	5.750	4.380	4.926	41.019
496 ²⁵	c1cccc1C[C@@H]([C@@H](N)CCCC)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC[C@H]3[C@H](C3)C	4.959	4.704	4.167	4.224	4.231	58.454
497 ²⁵	c1cccc1C[C@@H]([C@@H](C)N)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC[C@H]3[C@H](C3)C	4.495	4.756	4.242	3.972	5.457	63.652
498 ²⁵	c1cccc1C[C@@H]([C@@H](N)CCCC)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC[C@H]3[C@H](C3)C	4.509	5.222	4.667	4.437	3.964	63.569
499 ²⁵	c1cccc1C[C@@H]([C@@H](N)CCCC)NC(=O)c2cc(N(C)S(=O)(=O)C)CC(C)nc(c2)NC(C)C[C@H]3[C@H](C3)C	4.409	4.689	4.375	4.476	3.954	63.365
500 ²⁵	c1cccc1C[C@@H]([C@@H](C)N)NC(=O)c2cc(N(S(=O)(=O)C)CCC)nc(c2)NC(C)C[C@H]3[C@H](C3)C	4.174	4.627	4.459	4.207	4.081	64.265
501 ²⁵	c1cccc1C[C@@H]([C@@H](N)COC)NC(=O)c2cc(N(C)S(=O)(=O)C)nc(c2)NC(C)C[C@H]3[C@H](C3)C	4.921	4.143	4.327	4.193	5.043	67.375
502 ²⁵	c1cccc1C[C@@H]([C@@H](N)COC)NC(=O)c2cc(N(C)S(=O)(=O)C(C)C)nc(c2)NC(C)C[C@H]3[C@H](C3)C	4.620	3.997	4.288	4.224	3.934	62.418
503 ²⁵	c1cccc1C[C@@H]([C@@H](N)COCC)NC(=O)c2cc(N(C)S(=O)(=O)C(C)C)nc(c2)NC(C)C[C@H]3[C@H](C3)C	4.620	4.543	4.165	4.213	4.186	63.699
504 ²⁵	c1cccc1C[C@@H]([C@@H](N)COC)NC(=O)c2cc(N(C)S(=O)(=O)C(C)C)nc(c2)NC(C)C[C@H]3[C@H](C3)C)CCOC	5.222	4.850	5.285	4.525	5.045	64.528
505 ²⁶	c1cccc1-c2ccc(-c3cccc3)n2Cc4cccc(n4)N	2.284	2.244	1.755	2.286	3.272	63.844
506 ²⁶	c1cc(OC)ccc1-c2ccc(-c3c(Cl)cccc3)n2Cc4cccc(n4)N	2.611	2.879	2.105	2.825	2.204	63.068
507 ²⁶	CCCOc(cc1)ccc1-c2ccc(-c3c(Cl)cccc3)n2Cc4cccc(n4)N	2.939	3.650	2.894	2.875	2.518	64.279
508 ²⁶	CCCCOe(cc1)ccc1-c2ccc(-c3c(Cl)cccc3)n2Cc4cccc(n4)N	2.783	2.794	2.499	2.891	2.278	61.984
509 ²⁶	CCCCOe(cc1)ccc1-c2ccc(-c3c(Cl)cccc3)n2Cc4cccc(n4)N	3.260	2.761	3.158	2.900	3.727	65.596
510 ²⁶	N#CCCCOe(cc1)ccc1-c2ccc(-c3c(Cl)cccc3)n2Cc4cccc(n4)N	3.377	3.350	3.497	2.915	3.532	68.834
511 ²⁶	CCNC(=O)c(cc1)ccc1-c2ccc(-c3cccc3)n2Cc4cccc(n4)N	2.648	3.006	2.304	2.561	1.690	65.831
512 ²⁶	CCNC(=O)c(cc1)ccc1-c2ccc(-c3cccc3)n2Cc4cccc(n4)N	2.523	2.667	2.672	2.622	3.479	65.563
513 ²⁶	CCCCNC(=O)c(cc1)ccc1-c2ccc(-c3cccc3)n2Cc4cccc(n4)N	2.523	2.905	2.742	2.653	3.686	67.993
514 ²⁶	C=CCNC(=O)c(cc1)ccc1-c2ccc(-c3cccc3)n2Cc4cccc(n4)N	3.229	2.967	2.816	2.494	2.524	66.720
515 ²⁶	CC(C)NC(=O)c(cc1)ccc1-c2ccc(-c3cccc3)n2Cc4cccc(n4)N	2.750	2.728	2.738	3.055	3.417	66.769
516 ²⁶	C1CC1NC(=O)c(cc2)ccc2-c3ccc(-c4cccc4)n3Cc5cccc(n5)N	2.921	3.073	3.033	3.121	2.841	67.624
517 ²⁶	C1CCC1NC(=O)c(cc2)ccc2-c3ccc(-c4cccc4)n3Cc5cccc(n5)N	2.469	2.841	3.110	3.342	1.708	69.846
518 ²⁶	c1cccc1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5cccc(n5)N	3.071	3.303	2.784	3.124	4.086	69.408
519 ²⁶	c1cccc1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5cccc(n5)N	3.229	2.825	2.616	3.066	3.575	67.849
520 ²⁶	c1cccc1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5cccc(n5)N	3.387	2.362	3.193	3.252	3.245	64.961
521 ²⁶	n1cccc1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5cccc(n5)N	3.092	3.028	2.908	3.282	3.004	70.497
522 ²⁶	N1C=CC=N[C@@H]1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5cccc(n5)N	4.000	4.420	4.290	3.334	3.635	73.661
523 ²⁶	C1=NC=CN[C@@H]1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5cccc(n5)N	3.337	3.037	2.795	3.509	4.041	87.015
524 ²⁶	C1=CC=NN[C@@H]1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5cccc(n5)N	3.387	2.392	2.514	3.473	2.913	79.455
525 ²⁶	n1ccsc1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5cccc(n5)N	3.538	3.081	3.374	3.346	3.589	73.190
526 ²⁶	N1C=CC=N[C@@H]1Ne(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5cccc(n5)N	3.009	2.922	2.119	3.758	3.351	77.942
527 ²⁶	CCCCOe(cc1)ccc1-c2ccc(-c3c(Cl)cccc3)n2Cc4ccc(c(n4)N)OCCO	3.959	3.482	3.852	3.805	4.797	79.835
528 ²⁶	CCCCOe(cc1)ccc1-c2ccc(-c3c(Cl)cccc3)n2Cc4ccc(c(n4)N)NCCO	3.770	3.015	2.696	3.435	4.667	79.223
529 ²⁶	CCCCOe(cc1)ccc1-c2ccc(-c3c(Cl)cccc3)n2Cc4ccc(c(n4)N)NCCCO	3.658	3.532	3.608	3.460	4.885	81.023
530 ²⁶	N1C=CC=N[C@@H]1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5ccc(c(n5)N)OCCO	4.398	4.624	3.876	3.788	5.449	81.256
531 ²⁶	N1C=CC=N[C@@H]1Oe(cc2)ccc2-c3ccc(-c4c(Cl)cccc4)n3Cc5ccc(c(n5)N)NCCO	4.155	4.196	3.193	3.418	5.572	69.662
532 ²⁷	C1CCCCN1c(n2)nc(N3CCCC3)n2Nc(c4)ccc(c45)nc(s5)SCCC(=O)NCc6ccc(OC)c(c6)OC	2.553	2.334	3.016	2.585	2.037	66.300
533 ²⁷	c1cccc1CNC(=O)CCSc(s2)nc(c23)ccc(c3)Nc4nc(N5CCCC5)nc(n4)N6C	2.770	2.293	2.682	2.452	3.258	65.169
534 ²⁷	CCOC(=O)CCSc(s1)nc(c12)ccc(c2)Nc3nc(N4CCCC4)nc(n3)N5CCCC5	2.752	2.372	2.703	2.404	1.757	62.407
535 ²⁷	c1cccc1NC(=O)CCSc(s2)nc(c23)ccc(c3)Nc4nc(N5CCCC5)nc(n4)N6C	3.921	3.312	2.920	3.665	4.953	64.967
536 ²⁷	C1CCCN1c(n2)nc(N3CCCC3)n2Nc(c4)ccc(c45)nc(s5)SCCC(=O)NCCO	2.523	2.945	2.622	2.624	2.690	66.092
537 ²⁷	c1ccc1CNC(=O)CCSc(s2)nc(c23)ccc(c3)Nc4nc(N5CCCC5)nc(n4)N6C	3.161	3.209	3.370	2.493	3.375	63.356
	c1ccc(C)c(C)1NC(=O)CCSc(s2)nc(c23)ccc(c3)Nc4nc(N5CCCC5)nc(n4)	2.548	2.756	2.242	2.772	2.138	68.675

	N6CCCC6						
539 ²⁷	CCOc(c1)ccc1NC(=O)CCSc(s2)nc(e23)ccc(c3)Nc4nc(N5CCCC5)nc(n4)N6CCCC6	1.764	2.207	1.825	2.290	2.653	71.019
540 ²⁷	C1COCCN1c(n2)nc(N3CCOCC3)nc2Nc(c4)ccc(c45)nc(s5)SCCC(=O)N6c(cccc7)c7CCc(c68)cccc8	1.833	1.751	2.454	2.646	3.324	66.483
541 ²⁸	CN(C)c1cccc1-c2nnc(c2)Nc3cc(c(C)cc3)NS(=O)(=O)C	0.499	1.123	1.474	1.659	0.262	65.152
542 ²⁸	c1cccc1-c2nnc(c2)Nc3cc(c(C)cc3)NS(=O)(=O)C	1.620	1.855	1.549	1.137	0.796	68.428
543 ²⁸	c1cccc1-c2nnc(c2)Nc3cc(ccc3)NS(=O)(=O)C	0.398	0.545	0.416	1.148	0.912	67.627
544 ²⁸	c1cccc1-c2nnc(c2)Nc3cc(c(Cl)cc3)NS(=O)(=O)C	1.796	1.871	1.588	1.404	1.541	70.396
545 ²⁸	c1cccc1-c2nnc(c2)Nc3cc(c(Br)cc3)NS(=O)(=O)C	1.523	1.613	1.326	1.076	1.061	49.048
546 ²⁸	c1cccc1-c2nnc(c2)Nc3cc(c(F)cc3)NS(=O)(=O)C	0.959	0.681	0.518	1.183	1.029	45.381
547 ²⁸	c1cccc1-c2nnc(c2)Nc3cc(c(cc3)OC)NS(=O)(=O)C	1.161	1.625	1.491	0.807	1.497	49.374
548 ²⁸	c1cccc1-c2nnc(c2)Nc3cc(NS(=O)(=O)C)c(cc3)CC=C	0.244	1.129	0.220	1.263	1.555	52.282
549 ²⁸	c1cc(N(C)C)ccc1-c2nnc(c2)Nc3cc(c(C)cc3)NS(=O)(=O)C	1.824	1.099	1.770	1.248	1.396	50.370
550 ²⁸	c1cccc(C)c1-c2nnc(c2)Nc3cc(c(C)cc3)NS(=O)(=O)C	0.660	1.615	1.176	1.249	0.561	29.197
551 ²⁸	c1cccc1-c(cc2)ccc2-c3nnc(c3)Nc4cc(c(C)cc4)NS(=O)(=O)C	1.721	1.561	2.060	1.356	1.415	16.530
552 ²⁸	OCCc(c1)ccc1-c2nnc(c2)Nc3cc(c(C)cc3)NS(=O)(=O)C	1.432	1.633	1.789	1.382	1.872	23.558
553 ²⁸	O1CCOc(c12)ccc(c2)-c3nnc(c3)Nc4cc(c(C)cc4)NS(=O)(=O)C	1.678	1.654	2.033	1.740	1.338	27.731
554 ²⁹	CC(C)c(c1)ccc1C2(CC2)NC[C@@H](O)[C@@H](NC(=O)c(c3)cc(cc34)COC)C5cccc(c5)OCCCCN4	4.770	4.666	3.775	4.853	4.053	30.868
555 ²⁹	CC(C)c(c1)ccc1CNC[C@@H](O)[C@@H](NC(=O)c(c2)ccc23)C4ccc(c4)OCCCCN3	3.535	3.596	3.427	3.878	3.837	59.710
556 ²⁹	CC(C)c(c1)ccc1CNC[C@@H](O)[C@@H](NC(=O)c(c2)cc(nc23)C)C4cccc(c4)OCCCCO3	4.377	4.346	3.873	3.738	4.130	24.479
557 ²⁹	CC(C)c(c1)ccc1CNC[C@@H](O)[C@@H](NC(=O)c(c2)cc(nc23)C)C4cccc(c4)OCCCCN3	4.569	4.213	4.263	4.966	4.760	16.213
558 ²⁹	CC(C)c(c1)ccc1CNC[C@@H](O)[C@@H](NC(=O)c(c2)cc(cc23)COC)C4cccc(c4)OCCCCN3	4.222	4.367	3.978	4.269	4.126	26.042
559 ²⁹	CC(C)c(c1)ccc1CNC[C@@H](O)[C@@H](NC(=O)c(c2)cc(cc23)N4COC)C4cccc(c5)OCCCCN3	4.721	4.266	4.806	4.881	4.158	33.235
560 ²⁹	CC(C)c(c1)ccc1CNC[C@@H](O)[C@@H](NC(=O)c(c2)cc(cc23)N(C)S(=O)(=O)CCC)C4cccc(c4)OCCCCN3	6.000	5.650	6.096	5.013	5.753	32.385
561 ²⁹	CC(C)(C)c(c1)ccc1[C@@H](COC)NC[C@@H](O)[C@@H](NC(=O)c(c2)cc(cc23)COC)C4cccc(c4)OCCCCN3	3.175	3.589	4.266	4.050	4.203	44.460
562 ²⁹	CC(C)c(c1)ccc1[C@@H](C)NC[C@@H](O)[C@@H](NC(=O)c(c2)cc(nc23)C)C4cccc(c4)OCCCCO3	4.081	4.230	4.215	3.867	4.305	73.605
563 ²⁹	CC(C)(C)c(c1)ccc1[C@@H](CF)NC[C@@H](O)[C@@H](NC(=O)c(c2)cc(cc23)COC)C4cccc(c4)OCCCCN3	3.752	3.971	3.863	4.295	3.683	73.202
564 ²⁹	CC(C)c(c1)ccc1C2(CC2)NC[C@@H](O)[C@@H](NC(=O)c(c3)cc(nc34)C)C5cccc(c5)OCCCCO4	4.770	4.271	4.176	4.322	5.767	76.426
565 ²⁹	CC(C)c(c1)ccc1C2(CC2)NC[C@@H](O)[C@@H](NC(=O)c(c3)cc(nc34)COC)C5cccc(c5)OCCCCO4	5.046	4.720	4.450	4.680	4.028	65.743
566 ²⁹	CC(C)c(c1)ccc1C2(CC2)NC[C@@H](O)[C@@H](NC(=O)c(c3)cc(cc34)N5C(=O)CCC5)C6cccc(c6)OCCCCO4	6.000	5.819	5.424	5.431	6.081	63.658
567 ²⁹	CC(C)c(c1)ccc1C2(CC2)NC[C@@H](O)[C@@H](NC(=O)c(c3)cc(cc34)N(C)S(=O)(=O)CCC)C5cccc(c5)OCCCCN4	5.699	5.888	5.364	5.597	6.021	69.212
568 ²⁹	CC(C)c(c1)ccc1C(C)NC[C@@H](O)[C@@H](NC(=O)c(c2)cc(cc23)COC)C4cccc(c4)OCCCCN3	4.301	3.838	4.712	4.394	5.131	74.838
569 ²⁹	CC(C)(C)c(c1)ccc1C2(CCC2)NC[C@@H](O)[C@@H](NC(=O)c(c3)cc(cc34)COC)C5cccc(c5)OCCCCN4	4.174	3.603	4.306	5.083	4.514	65.231
570 ²⁹	CC(C)(C)c(c1)ccc1C2(CCCC2)NC[C@@H](O)[C@@H](NC(=O)c(c3)cc(cc34)COC)C5cccc(c5)OCCCCN4	4.301	4.374	4.204	5.032	5.182	74.486
571 ³⁰	COc1ccc(cc1Br)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3	2.553	2.911	2.731	2.500	2.684	74.626
572 ³⁰	c1cccc1C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3	2.959	2.902	2.990	2.458	3.610	68.379
573 ³⁰	c1c(Br)cccc1C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3	3.119	3.471	2.635	2.450	3.613	69.838
574 ³⁰	CCCOc(c1)ccc1C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3	2.638	3.700	3.555	2.702	2.974	71.283
575 ³⁰	CCCOc(c1)ccc1C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3	2.959	2.725	2.721	2.607	2.729	68.841
576 ³⁰	Oc1ccc(cc1)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3	2.745	2.349	2.420	2.453	2.635	64.003
	c1ccc(C)cc1Cc2cc(ccc2O)C[C@@H](C3)[C@H](O)[C@H](CS3(=O)=O)	2.208	2.822	2.055	2.627	2.701	69.618

	<chem>NCc4cc(C(C)C)ccc4</chem>						
578 ³⁰	<chem>Oc1ccc(cc1CO)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3</chem>	2.921	2.695	2.591	2.382	2.677	70.060
579 ³⁰	<chem>OCCc1cc(ccc1O)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3</chem>	3.004	3.043	2.886	2.564	3.717	68.843
580 ³⁰	<chem>CCCCc1cc(ccc1O)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3</chem>	3.824	3.554	2.803	3.566	4.727	68.477
581 ³⁰	<chem>CCCc1cc(ccc1O)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3</chem>	3.721	1.488	2.692	2.584	4.714	80.737
582 ³⁰	<chem>Oc1ccc(cc1CC)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3</chem>	3.432	3.852	4.171	2.564	3.679	59.149
583 ³⁰	<chem>Oc1ccc(cc1Br)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3</chem>	3.523	3.723	3.339	2.457	3.623	53.631
584 ³⁰	<chem>CNC(=O)Oc1ccc(cc1Br)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3</chem>	4.222	4.748	3.684	3.583	4.719	55.277
585 ³⁰	<chem>Oc1ccc(cc1Br)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3ccccc3</chem>	1.180	1.893	0.847	2.038	1.462	56.944
586 ³⁰	<chem>Oc1ccc(cc1Br)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(ccn3)C(C)C</chem>	2.367	2.497	2.233	2.542	2.634	52.166
587 ³⁰	<chem>Oc1ccc(cc1Br)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(C(C)C)ccc3</chem>	4.260	4.292	3.662	3.346	4.614	54.637
588 ³⁰	<chem>Oc1ccc(cc1Br)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(ccc3)OC(C)C</chem>	2.854	2.335	2.432	2.423	2.416	52.082
589 ³⁰	<chem>Oc1ccc(cc1Br)C[C@@H](C2)[C@H](O)[C@H](CS2(=O)=O)NCc3cc(Cl)cc(Cl)e3</chem>	2.377	2.433	2.192	2.989	3.513	58.976
590 ³⁰	<chem>CCCN1C(=O)OC[C@H]1Cc2cc(ccc2O)C[C@@H](C3)[C@H](O)[C@H](CS3(=O)=O)NCc4cc(C(C)C)ccc4</chem>	3.824	3.322	3.069	3.300	3.641	52.115
591 ³⁰	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNCc2cc(C(C)C)ccc2</chem>	2.495	2.691	1.559	2.491	2.922	53.654
592 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3ccccc3C(C)C(C)C</chem>	4.328	3.798	3.919	3.746	5.239	51.541
593 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cc1cc(c3)C(C)C(C)C</chem>	3.652	4.105	3.482	3.719	3.782	57.605
594 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3ccccc3CC(C)C(C)C</chem>	2.678	2.434	2.320	3.801	2.902	48.960
595 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cc(F)cc(c3)C(C)C(C)C</chem>	4.337	3.925	4.196	4.162	5.298	59.745
596 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cc(Br)cc(c3)C(C)C(C)C</chem>	3.759	4.439	4.236	3.728	4.720	60.988
597 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cc(C)cc(c3)C(C)C(C)C</chem>	3.745	3.603	3.830	3.974	3.549	65.381
598 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cc(OC)c(c3)C(C)C(C)C</chem>	4.114	3.931	4.384	4.170	4.577	63.495
599 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cc(O)cc(c3)C(C)C(C)C</chem>	3.770	3.626	3.802	4.481	3.238	64.870
600 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cc(N)cc(c3)C(C)C(C)C</chem>	3.498	3.771	3.664	3.899	3.009	67.713
601 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cc(NS(=O)(=O)C)cc(c3)C(C)C(C)C</chem>	4.032	4.238	4.325	3.846	4.404	64.274
602 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cc(C(=O)C)cc(c3)C(C)C(C)C</chem>	3.796	3.910	4.340	3.655	3.188	63.727
603 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3ccc(Br)c(c3)C(C)C(C)C</chem>	2.161	2.840	2.155	3.756	2.034	59.209
604 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3scc(c3)CC(C)C(C)C</chem>	3.883	2.646	3.155	2.934	4.969	61.390
605 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3ccc(s3)C(C)C</chem>	2.397	2.902	4.374	2.627	2.148	65.148
606 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3csc(c3)C(C)C</chem>	3.495	2.614	3.468	3.418	3.594	67.276
607 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3scc(c3)C(C)C</chem>	3.453	4.077	3.137	3.079	3.689	64.177
608 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3scc(c3)C(C)C(C)C</chem>	3.983	3.198	4.259	3.293	3.014	53.927
609 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3scc(c3)C#C</chem>	2.365	2.046	1.922	2.703	2.938	67.090
610 ³¹	<chem>c1c(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3scc(c3)CC</chem>	2.759	3.617	2.878	2.886	3.581	65.289

611 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3onc(e3)C(C)(C)C	2.351	3.084	3.211	3.476	2.475	60.096
612 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3onc(e3)CC(C)(C)C	3.857	3.367	3.151	3.850	4.120	63.379
613 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3nnn(e3)C[Si](C)(C)C	3.812	3.870	3.269	3.545	4.872	59.873
614 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3nnn(e3)C45C[C@@H]6C[C@H](C5)C[C@H](C4)C6	3.407	3.280	3.191	4.180	4.122	63.633
615 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3occ(n3)C(C)(C)C	0.861	1.447	1.119	1.215	1.568	70.501
616 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cnn(e3)C(C)(C)C	2.735	2.807	3.654	3.013	3.557	54.567
617 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3cnn(e3)CC(C)(C)C	3.678	3.442	3.678	3.151	3.097	66.256
618 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3ncc(o3)C(C)(C)C	2.801	2.321	3.023	2.636	3.463	64.829
619 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3scc(e3)CC(C)(C)C	3.328	3.420	3.219	2.805	4.001	66.292
620 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cccc(e3)C(C)(C)C	3.854	3.655	3.793	3.713	2.982	66.188
621 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3cccc(e3)CC(C)(C)C	3.467	3.037	3.176	3.824	3.946	65.910
622 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3nccc(e3)C(C)(C)C	3.194	3.251	3.401	3.676	3.981	61.659
623 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3encc(e3)CC(C)(C)C	3.108	2.978	3.290	4.262	3.484	62.824
624 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3e[n+](O)cc(e3)CC(C)(C)C	3.143	3.055	3.637	3.785	3.026	64.332
625 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CCCCC2)c3ncnc(e3)C(C)(C)C	2.614	2.675	3.647	3.709	2.840	63.036
626 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3ccc(s3)CC(C)(C)C	2.790	3.690	3.108	2.134	3.790	64.939
627 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3ncc(o3)C(C)(C)C	2.310	2.358	2.317	2.073	2.861	60.571
628 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3occ(n3)C(C)(C)C	1.368	2.014	1.859	1.724	2.233	55.664
629 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3scc(n3)CC(C)(C)C	2.029	1.983	2.144	2.527	2.602	41.690
630 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3esc(n3)CC(C)(C)C	2.516	2.056	2.957	2.593	2.885	40.830
631 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3enn(e3)CC(C)(C)C	3.461	3.595	2.528	3.183	3.215	42.602
632 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3ecn(n3)CC(C)(C)C	3.060	3.211	2.978	3.735	2.846	46.419
633 ³¹	c1e(F)cc(F)cc1C[C@H](NC(=O)C)[C@H](O)CNC2(CC2)c3nnn(e3)CC(C)(C)C	3.347	3.134	3.546	2.810	3.823	51.607
634 ³²	CCCN(CCC)C(=O)c1cc(cc(e1)C)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@H](O)CNCc3cc(OC)ccc3	4.699	4.878	3.942	4.868	4.873	53.547
635 ³²	CCCN(CCC)C(=O)c1cc(cc(e1)C)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@H](O)CNCc3cc(OC)ccc3	4.699	4.098	4.588	4.773	5.697	60.398
636 ³²	CCCN(CCC)C(=O)c1cc(cc(e1)CC(=O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@H](O)CNCc3cc(OC)ccc3	5.398	5.415	4.704	4.789	5.087	55.139
637 ³²	CCCN(CCC)C(=O)c1cc(cc(e1)C/C(C)=N/O)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@H](O)CNCc3cc(OC)ccc3	5.523	5.140	5.196	4.808	5.029	58.077
638 ³²	CCCN(CCC)C(=O)c1cc(cc(e1)C/C(C)=N/OC)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@H](O)CNCc3cc(OC)ccc3	6.000	5.138	5.757	4.529	5.366	73.769
639 ³²	C=CCO\N=C(C)Cc(e1)cc(cc1C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@H](O)CNCc3cc(OC)ccc3	5.000	5.105	4.850	4.737	4.196	64.267
640 ³²	CC(C)CO\N=C(C)Cc(e1)cc(cc1C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@H](O)CNCc3cc(OC)ccc3	4.260	4.326	4.630	4.525	3.846	68.978
641 ³²	e1cccc1CO\N=C(C)Cc(e2)cc(cc2C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc3cc(F)cc(F)e3)[C@H](O)CNCc4cc(OC)ccc4	4.174	4.087	4.395	4.713	3.285	55.012
642 ³²	CCCN(CCC)C(=O)c1cc(cc(e1)C[C@H](O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@H](O)CNCc3cc(OC)ccc3	5.699	5.864	5.528	4.576	5.079	53.802
643 ³²	CCCN(CCC)C(=O)c1cc(cc(e1)CC[C@H](C)O)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@H](O)CNCc3cc(OC)ccc3	4.796	4.758	4.686	4.821	5.228	72.616

644 ³²	CCCN(CCC)C(=O)c1cc(cc(c1)CCCO)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	5.000	5.445	4.760	4.751	5.460	70.307
645 ³²	CCCN(CCC)C(=O)c1cc(cc(c1)C[C@@H](N)C)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	3.910	4.296	4.454	4.578	4.661	68.702
646 ³²	CCCN(CCC)C(=O)c1cc(cc(c1)C[C@H](C)NC(=O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	4.699	5.168	5.182	4.731	4.413	63.211
647 ³²	c1cccc1[C@@H](C)NC(=O)c2cc(ccc2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.051	3.638	3.560	4.193	3.836	56.278
648 ³²	c1cccc1[C@@H](C)NC(=O)c2cc(cc(c2)CC(=O)C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.699	4.487	4.536	4.401	4.365	76.437
649 ³²	c1cccc1[C@@H](C)NC(=O)c2cc(cc(c2)C[C@H](O)C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.538	4.872	4.606	4.198	5.493	76.461
650 ³²	c1cccc1[C@@H](C)NC(=O)c2cc(cc(c2)C/C(C)=N/OC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.495	3.980	4.083	4.386	4.369	70.161
651 ³²	c1cccc1[C@@H](C)NC(=O)c2cc(cc(c2)C/C(C)=N/OCC=C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.066	4.259	3.783	4.310	4.389	60.846
652 ³²	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(ccc2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	3.780	4.459	4.193	4.239	3.408	60.682
653 ³²	c1cc(F)ccc1[C@H](C)NC(=O)c2cc(cc(c2)CC(=O)C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.292	4.109	4.092	4.447	4.140	55.170
654 ³²	c1cc(F)ccc1[C@H](C)NC(=O)c2cc(cc(c2)C[C@H](O)C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.432	4.368	4.339	4.245	4.533	65.224
655 ³²	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(c2)C/C(C)=N/OC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.620	4.959	4.843	4.433	4.395	60.704
656 ³²	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(c2)C/C(C)=N/OCC=C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	3.775	3.950	4.031	4.357	3.365	66.174
657 ³²	C1CCCN(S1(=O)=O)c2cc(ccc2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.131	3.890	3.148	3.468	4.939	69.172
658 ³²	C1CCCN(S1(=O)=O)c2cc(cc(c2)CC(=O)C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.046	3.720	3.883	4.539	4.669	71.171
659 ³²	C1CCCN(S1(=O)=O)c2cc(cc(c2)C[C@H](O)C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.367	4.376	3.688	4.579	4.683	69.704
660 ³²	C1CCCN(S1(=O)=O)c2cc(cc(c2)C/C(C)=N/OC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.420	4.024	4.704	4.273	4.121	64.206
661 ³²	C1CCCN(S1(=O)=O)c2cc(cc(c2)C/C(C)=N/OC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.284	4.544	4.388	4.223	4.596	68.409
662 ³²	CCCO\N=C(C)Cc(c1)cc(cc1N(S2(=O)=O)CCCC2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.602	4.498	4.447	4.227	5.671	62.955
663 ³²	C=CCO\N=C(C)Cc(c1)cc(cc1N(S2(=O)=O)CCCC2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	3.955	3.888	3.084	4.152	3.708	67.251
664 ³²	CC(C)CO\N=C(C)Cc(c1)cc(cc1N(S2(=O)=O)CCCC2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	3.369	3.800	3.690	4.236	3.171	64.813
665 ³²	c1cccc1CO\N=C(C)Cc(c2)cc(cc2N(S3(=O)=O)CCCC3)C(=O)N[C@@H](Cc4cc(F)cc(F)c4)[C@H](O)CNCc5cc(OC)ccc5	4.509	4.064	3.512	4.393	4.959	67.451
666 ³²	CS(=O)(=O)N(C)C)c1cc(ccc1)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	4.125	3.476	3.055	4.220	4.715	82.532
667 ³²	CS(=O)(=O)N(C)C)c1cc(cc(c1)CC(=O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	3.907	3.268	4.117	4.180	3.601	76.575
668 ³²	CS(=O)(=O)N(C)C)c1cc(cc(c1)C[C@@H](O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	4.367	3.585	4.185	4.206	4.526	60.982
669 ³²	O\N=C(C)Cc(c1)cc(cc1N(C)S(=O)(=O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	4.119	4.364	4.515	3.916	4.728	63.729
670 ³²	CO\N=C(C)Cc(c1)cc(cc1N(C)S(=O)(=O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	4.222	4.794	4.215	3.866	4.639	66.271
671 ³²	CCCO\N=C(C)Cc(c1)cc(cc1N(C)S(=O)(=O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	4.229	3.731	3.505	3.869	4.532	63.712
672 ³²	C=CCO\N=C(C)Cc(c1)cc(cc1N(C)S(=O)(=O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	3.821	3.415	4.239	3.794	4.244	42.599
673 ³²	CC(C)CO\N=C(C)Cc(c1)cc(cc1N(C)S(=O)(=O)C)C(=O)N[C@@H](Cc2cc(F)cc(F)c2)[C@H](O)CNCc3cc(OC)ccc3	3.762	3.818	4.249	3.878	3.322	61.321
674 ³²	c1cccc1CO\N=C(C)Cc(c2)cc(cc2N(C)S(=O)(=O)C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	5.046	5.803	4.655	4.036	5.376	59.844
675 ³²	c1cccc1N(S(=O)(=O)C)c2cc(ccc2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.959	4.650	4.651	4.962	5.280	55.366
676 ³²	c1cccc1N(S(=O)(=O)C)c2cc(cc(c2)CC(=O)C)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.770	4.832	4.906	5.088	4.385	63.341

677 ³²	c1cccc1N(S(=O)(=O)C)c2cc(cc(e2)C/C(C)=N/O)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	5.046	5.793	5.404	4.821	6.067	43.705
678 ³²	c1cccc1N(S(=O)(=O)C)c2cc(cc(e2)C/C(C)=N/O)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	5.000	4.569	4.424	4.781	6.096	56.498
679 ³²	CCCO\N=C(C)\Cc(c1)cc(cc1N(S(=O)(=O)C)c2cccc2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	5.222	4.858	5.030	4.785	4.931	41.320
680 ³²	C=CCO\N=C(C)\Cc(c1)cc(cc1N(S(=O)(=O)C)c2cccc2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.569	5.110	4.310	4.709	5.624	56.121
681 ³²	CC(C)CO\N=C(C)\Cc(c1)cc(cc1N(S(=O)(=O)C)c2cccc2)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	3.616	4.523	4.188	3.793	3.406	43.909
682 ³²	c1cccc1CO\N=C(C)\Cc(c2)cc(cc2N(S(=O)(=O)C)c3cccc3)C(=O)N[C@@H](Cc4cc(F)cc(F)c4)[C@H](O)CNCc5cc(OC)ccc5	4.921	5.342	4.927	4.951	5.191	70.407
683 ³²	c1cccc1O(c2)cc(cc2C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	5.000	5.015	4.727	4.735	5.605	66.736
684 ³²	c1cc(OC)ccc1O(c2)cc(cc2C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	5.000	5.008	4.774	4.633	5.408	64.021
685 ³²	c1cccc(OC)c1O(c2)cc(cc2C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.268	4.625	4.391	4.761	3.996	65.986
686 ³²	c1cc(F)ccc1O(c2)cc(cc2C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.658	4.527	4.992	4.701	4.414	58.279
687 ³²	c1cccc1Se(c2)cc(cc2C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.886	4.651	4.501	4.846	4.383	60.995
688 ³²	c1cc(OC)ccc1Se(c2)cc(cc2C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.569	4.569	4.763	4.556	5.596	36.679
689 ³²	c1cccc1S(=O)(=O)c(c2)cc(cc2C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.959	5.383	5.166	4.898	5.140	60.603
690 ³²	c1cc(OC)ccc1S(=O)(=O)c(c2)cc(cc2C(=O)N(CCC)CCC)C(=O)N[C@@H](Cc3cc(F)cc(F)c3)[C@H](O)CNCc4cc(OC)ccc4	4.921	4.842	4.513	4.908	5.130	49.163
691 ³³	c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)NC(=O)c4c(Cl)cc(Cl)cc4	2.921	2.993	3.728	3.143	3.833	66.006
692 ³³	c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)NC(=O)c4cc(C)ccc4	3.222	3.332	3.246	2.998	3.601	73.603
693 ³³	c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)NC(=O)c4cc(OC)ccc4	2.745	3.015	2.792	3.072	3.247	64.261
694 ³³	c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)NC(=O)c4ccc(Br)cc4	2.854	2.772	2.861	3.139	3.057	73.852
695 ³³	c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)OCC	2.796	3.045	3.097	2.879	2.937	52.620
696 ³³	c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)OCC=C	2.770	2.390	2.211	2.799	2.179	60.552
697 ³³	c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)OCCCC#N	3.046	3.221	3.130	2.864	3.299	30.027
698 ³³	c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)OCCCC	2.745	3.214	3.094	2.840	2.241	68.015
699 ³³	c1cccc1-c2n(CC(=O)N/C(N)=N/[H])c(cc2)-c3ccc(cc3)OCC4ccc(C#N)cc4	2.721	2.201	2.675	2.833	2.793	42.904
700 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNC4CCCCC4	3.745	3.179	3.599	3.777	4.334	47.518
701 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNC4CCCCC4	2.951	4.078	3.012	3.854	3.025	68.069
702 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNC4CCCCC4	2.611	2.727	3.502	3.803	2.940	64.042
703 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNC4CCSCC4	3.187	3.786	3.081	3.746	3.338	62.396
704 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CN[C@@H](C)C(=C)CC4CCCCC4	2.230	2.742	2.619	3.036	2.657	66.649
705 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CN[C@H](C)CCCC(C)C	4.481	3.950	4.479	3.792	4.638	65.455
706 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNC(C)(C)CCCC(C)C	4.481	4.304	4.668	3.805	4.313	74.593
707 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNC(C)(C)CCCC(C)C	3.516	3.209	2.590	3.780	3.214	67.426
708 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNC(C)(C)CCCC	3.260	3.478	3.774	3.780	4.208	70.034
709 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNC(C)(C)COCC(C)C	3.102	3.963	4.066	3.606	2.821	68.160
710 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCc4cccc(c4)OC	4.367	4.363	4.016	4.390	3.892	52.790
711 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)CNCc4cccc4	3.119	3.379	3.372	3.255	3.881	71.994
	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3cccc3)[C@H](O)	4.770	3.640	4.218	4.551	4.182	73.056

	CNC(C)(C)c4ccce(c4)C(F)(F)F						
713 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4ccccc4OC	2.870	3.839	3.740	3.369	2.535	67.089
714 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4ccc(cc4)OC	2.680	2.917	3.424	3.258	2.881	71.033
715 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4ccccc4	2.770	3.663	3.452	3.653	3.173	71.587
716 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4ccccc4	3.222	3.258	3.824	4.038	3.859	68.973
717 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN[C@@H]4CCc(c45)cccc5	3.796	3.627	3.409	4.564	4.747	68.325
718 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN[C@@H]4CCc(c45)cccc5	1.460	1.353	2.376	1.564	1.397	70.460
719 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNC4(CCCCC4)c5cccc(c5)OC	4.854	5.376	5.213	4.856	5.501	75.113
720 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4cccc(c4)OC(F)(F)F	4.699	4.325	3.862	4.587	5.348	73.522
721 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4cccc(Cl)c4	4.081	3.913	3.627	4.244	4.041	80.114
722 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4cc(OC)cc(c4)OC	4.000	4.414	3.998	4.671	4.687	72.932
723 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4cccc(n4)OC	3.481	3.672	4.468	4.154	4.419	73.951
724 ³⁴	C1CCC(=O)N1c2cc(NCC)cc(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CNCc4enn(c4)CC	3.638	3.193	3.807	4.248	3.177	69.779
725 ³⁵	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H](Cc4ccccc4)[C@H](O)CNC5CCOCC5	5.301	5.568	4.681	4.253	6.220	69.602
726 ³⁵	C1CS(=O)(=O)N(C)C(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H](Cc4ccccc4)[C@H](O)CNC5CCOCC5	4.824	4.619	4.685	4.851	5.064	68.366
727 ³⁵	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCCC(F)(F)Fc4ccccc4	5.398	5.777	4.415	5.152	4.443	81.346
728 ³⁵	C1CS(=O)(=O)N(C)C(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCCC(F)(F)Fc4ccccc4	5.155	5.562	4.523	4.750	5.457	90.827
729 ³⁵	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H]([C@H](O)C)N[C@@H](C)CCc4ccccc4	5.000	4.248	4.222	4.222	5.798	70.541
730 ³⁵	C1CS(=O)(=O)N(C)C(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H]([C@H](O)C)N[C@@H](C)CCc4ccccc4	4.658	4.464	4.633	4.820	4.813	83.230
731 ³⁵	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCC#C)c4ccccc4	4.959	4.049	4.054	4.413	5.870	78.811
732 ³⁵	C1CS(=O)(=O)N(C)C(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCC#C)c4ccccc4	4.137	3.430	3.140	5.011	4.957	69.383
733 ³⁵	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCC)c4ccccc4	4.638	4.644	4.438	4.269	4.882	70.437
734 ³⁵	C1CS(=O)(=O)N(C)C(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCC)c4ccccc4	4.319	3.455	3.721	4.867	4.726	71.110
735 ³⁵	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H]([C@H](O)C)NC4CC4)c5ccccc5	5.046	4.531	4.778	4.222	5.907	75.456
736 ³⁵	C1CS(=O)(=O)N(C)C(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H](Cc4ccccc4)[C@H](O)CNCc5cccc(c5)C(F)(F)F	5.699	5.326	5.225	5.359	5.119	72.742
737 ³⁵	C1CS(=O)(=O)O(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H](Cc4ccccc4)[C@H](O)CNCc5cccc(c5)C(F)(F)F	5.097	5.533	4.638	4.141	5.464	68.651
738 ³⁵	C1CS(=O)(=O)O(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H](Cc4ccccc4)[C@H](O)CNC5CCOCC5	4.066	3.936	3.976	3.620	4.570	77.455
739 ³⁵	C1CS(=O)(=O)O(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCC#C)c4ccccc4	3.444	3.278	3.514	3.779	3.755	55.520
740 ³⁵	C1CS(=O)(=O)O(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCC4CC4)c5ccccc5	3.602	3.302	3.668	3.588	3.911	52.380
741 ³⁵	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCCC)c4ccccc4	5.097	5.031	4.386	4.248	5.979	52.201
742 ³⁵	C1CS(=O)(=O)N(C)C(c2n13)cc(cc2c(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCCF)c4ccccc4	4.301	3.938	4.164	5.089	4.940	57.920
743 ³⁵	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCCF)c4ccccc4	4.398	3.694	3.927	4.469	4.729	64.153
744 ³⁵	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCC(F)Fc4ccccc4	4.699	4.115	4.565	4.539	4.826	58.682
	C1CS(=O)(=O)N(C)C(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H]([C@H](O)C)NCC(F)Fc4ccccc4	4.495	4.222	4.071	4.334	4.571	56.647

	NCC(F)(F)C(F)(F)F)Ce4cccc4								
746 ³⁵	C1CS(=O)(=O)N(C)c(c2c13)cc(cc2n(c3)CC)C(=O)N[C@H]([C@H](O)C NCC(F)(F)F)Ce4cccc4	4.102	4.204	3.973	4.595	4.918	50.205		
747 ³⁵	C1CS(=O)(=O)N(C)c(c2c13)cc(cc2n(c3)CC)C(=O)N[C@@H](Ce4cccc4)C@H](O)CNc5cccc5	5.301	5.381	4.428	5.097	5.548	54.888		
748 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(cc(c3)N(S(=O)(=O)C)CCC)C(=O) N[C@H](CC2)c4cccc4	4.770	4.557	4.831	4.327	5.529	48.057		
749 ³⁶	c12cccc(c1)C[C@@](C)(N)C(=O)OCc3cc(cc(c3)N(S(=O)(=O)C)CCC)C(=O) N[C@H](CC2)c4cccc4	5.699	4.893	4.840	4.578	5.294	34.132		
750 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(cc(c3)N(C)S(=O)(=O)C)C(=O)N[C @H](CC2)c4cccc4	4.310	4.462	4.635	4.341	5.446	43.237		
751 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(C(=O)N[C@H](CC2)c4cccc4)cc(c 3)N(S(=O)(=O)C)c5cccc5	4.921	4.455	4.965	4.726	2.834	60.301		
752 ³⁶	c12cccc(c1)C[C@@](C)(N)C(=O)OCc3cc(C(=O)N[C@H](CC2)c4cccc4)cc(c3)N(S(=O)(=O)C)c5cccc5	6.000	5.904	5.285	5.458	5.826	56.447		
753 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(cc(c3)N(C)S(=O)(=O)CC)C(=O)N[C@H](CC2)c4cccc4	4.252	4.806	4.537	4.453	4.562	61.063		
754 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(cc(c3)N(C)S(=O)(=O)C(C)C)C(=O) N[C@H](CC2)c4cccc4	3.708	3.483	3.187	4.649	4.459	47.888		
755 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(cc(c3)N(S(=O)(=O)C)CCC)C(=O) N[C@H](CC2)c4ccc(F)cc4	5.000	5.062	4.973	4.521	5.799	57.144		
756 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(C(=O)N[C@H](C)CC2)cc(c3)N(S(=O)(=O)C)CCC	3.538	3.706	2.858	3.482	4.707	54.646		
757 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(C(=O)N[C@H](CC2)CC)cc(c3)N(S (=O)(=O)C)CCC	4.071	3.059	3.963	3.610	4.248	54.646		
758 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(C(=O)N[C@H](CC2)C(C)C)cc(c3) N(S(=O)(=O)C)CCC	3.757	3.844	3.890	3.805	4.755	54.646		
759 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(C(=O)N[C@H](CC2)C#C)cc(c3)N(S(=O)(=O)C)CCC	4.276	4.514	3.434	3.298	4.594	54.646		
760 ³⁶	c12cccc(c1)C[C@@](C)(N)COCc3cc(C(=O)N[C@H](CC2)C4CC4)cc(c3) N(S(=O)(=O)C)CCC	2.959	3.287	3.217	3.977	2.661	54.646		
761 ³⁶	c12cccc(c1)C[C@@](C)(N)C(=O)OCc3cc(cc(c3)N(C)S(=O)(=O)CC(F)(F)F)C(=O)N[C@H](CC2)c4cccc4	4.796	4.887	5.048	4.968	5.276	77.147		
762 ³⁶	c12cccc(c1)C[C@@](C)(N)C(=O)OCc3cc(cc(c3)N(C)S(=O)(=O)C(F)(F)F)C(=O)N[C@H](CC2)c4cccc4	4.420	3.862	4.456	4.635	5.121	76.838		
763 ³⁶	c12cccc(c1)C[C@@](C)(N)C(=O)OCc3cc(cc(c3)N(C)S(=O)(=O)N(C)C) C(=O)N[C@H](CC2)c4cccc4	5.398	5.478	4.875	5.137	5.531	79.855		
764 ³⁶	c12cccc(c1)C[C@@](C)(N)C(=O)OCc3cc(cc(Br)c3)C(=O)N[C@H](CC2) c4cccc4	3.569	3.679	3.309	3.799	3.664	81.137		
765 ³⁶	c12cccc(c1)C[C@@](C)(N)C(=O)OCc3cc(cc(c3)- c4ncco4)C(=O)N[C@H](CC2)c5cccc5	3.108	3.017	3.147	3.584	3.690	79.351		
766 ³⁶	c12cccc(c1)C[C@@](C)(N)C(=O)OCc3cc(C(=O)N[C@H](CC2)c4cccc4)cc(c3)-c5cccc5C#N	4.569	4.866	4.711	4.000	4.833	80.135		
767 ³⁶	c12cc(F)cc(c1)C[C@@](C)(N)C(=O)OCc3cc(C(=O)N[C@H](CC2)c4ccc (F)cc4)cc(c3)-c5cccc5C#N	3.886	3.696	3.763	4.148	3.776	67.303		
768 ³⁶	c12c(F)ccc(c1)C[C@@](C)(N)C(=O)OCc3cc(C(=O)N[C@H](CC2)c4ccc (F)cc4)cc(c3)-c5cccc5C#N	4.337	4.697	3.526	3.975	4.720	78.518		
769 ³⁶	c12cccc(c1F)C[C@@](C)(N)C(=O)OCc3cc(C(=O)N[C@H](CC2)c4ccc(F)cc4)cc(c3)-c5cccc5C#N	4.108	4.779	3.405	4.203	3.765	71.234		
770 ³⁶	c12cccc(c1)C[C@@](C)(N)C(=O)OCc3cc(cc(c3)- c4c(C#N)c(F)ccc4)C(=O)N[C@H](CC2)c5ccc(F)cc5	4.658	5.158	4.958	4.228	4.746	70.573		
771 ³⁶	c12c(F)ccc(c1)C[C@@](C)(N)C(=O)OCc3cc(cc(c3)- c4c(C#N)c(F)ccc4)C(=O)N[C@H](CC2)c5ccc(F)cc5	4.337	4.978	3.443	3.900	4.717	66.155		
772 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)C(=O)OC[C@@](N)(CO)Cc3cccc3	3.714	3.478	3.163	2.576	3.634	69.475		
773 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)C(=O)NC[C@@](N)(CO)Cc3cccc3	1.967	2.454	2.218	2.839	2.987	70.497		
774 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)C(=O)OC[C@@](O)(CN)Cc3cccc3	1.654	2.683	2.417	2.282	1.709	72.078		
775 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)C(=O)NC[C@@](O)(CO)Cc3cccc3	1.604	1.893	2.584	1.825	1.844	71.499		
776 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)COC[C@ @](N)(CO)Cc3cccc3	2.863	2.436	3.030	2.691	2.967	75.533		
777 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)CNC[C@ @](N)(CO)Cc3cccc3	1.996	2.544	2.108	1.889	2.884	75.214		
	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)CCC[C@	1.650	2.450	2.327	2.418	0.737	70.201		

	@](N)(CO)Ce3ceccc3						
779 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)OCC[C@@](N)(CO)Ce3ceccc3	1.152	1.750	1.180	1.730	1.887	78.682
780 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)COC[C@@H](N)Ce3ceccc3	1.996	2.096	2.797	2.577	2.848	78.597
781 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)COC[C@@](C)(N)Ce3ceccc3	3.463	3.879	3.704	2.692	3.872	78.612
782 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)COC[C@@](N)(CC)Ce3ceccc3	1.658	1.348	2.473	2.686	1.937	79.038
783 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)COC[C@@](CF)(N)Ce3ceccc3	3.001	3.107	2.745	2.796	3.385	78.515
784 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)COC[C@@](C(F)F)(N)Ce3ceccc3	3.034	2.515	2.954	3.281	3.466	78.393
785 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)COC(=O)[C@@](N)(CO)Ce3ceccc3	3.509	3.874	1.705	2.886	3.700	79.973
786 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)COC(=O)[C@@](C)(N)Ce3ceccc3	4.721	4.370	3.956	4.604	5.334	68.580
787 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)CNC(=O)[C@@](N)(CO)Ce3ceccc3	1.742	1.739	1.986	2.448	2.701	68.320
788 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)CNC(=O)[C@@](C)(N)Ce3ceccc3	2.243	3.017	2.512	2.254	1.467	63.226
789 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)-c3oc(nn3)[C@@](C)(N)Ce4ceccc4	4.921	4.373	3.931	4.415	4.883	65.107
790 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)-c3nc(no3)[C@@](C)(N)Ce4ceccc4	2.738	3.383	2.391	2.364	3.146	71.994
791 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)-c3nc(on3)[C@@](C)(N)Ce4ceccc4	2.686	2.815	2.815	3.272	3.328	69.227
792 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)-c3sc(nn3)[C@@](C)(N)Ce4ceccc4	1.524	1.296	1.854	1.708	1.766	65.596
793 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)-c3oc(cn3)[C@@](C)(N)Ce4ceccc4	5.155	4.946	5.829	4.682	5.596	66.354
794 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)-c3oc(cc3)[C@@](C)(N)Ce4ceccc4	4.699	4.385	3.959	3.776	4.801	78.881
795 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)-c3nc([nH]n3)[C@@](C)(N)Ce4ceccc4	3.085	2.686	2.801	3.116	4.487	81.541
796 ³⁷	Fc1ccc(cc1)[C@@H](C)NC(=O)c2cc(cc(c2)N(C)S(=O)(=O)C)-n3cc(nn3)[C@@](C)(N)Ce4ceccc4	1.788	1.389	1.908	2.160	1.565	52.754
797 ³⁸	CN1S(=O)(=O)CCN2CCN(CC)C([C@@H]2[C@@H]13)=CC(=C3)C(=O)N[C@@H](C)C4CCCC4[C@@H](O)CNC5CCCC5C(F)F	4.585	4.567	4.791	5.219	4.403	35.316
798 ³⁸	CN1S(=O)(=O)CCC(c12)c(NCC)cc(c2)C(=O)N[C@@H](C)C3CCCC3[C@@H](O)CNC4CCCC4C(F)F	4.721	3.797	4.116	4.841	4.252	72.258
799 ³⁸	C1CCCN(S1(=O)=O)c(cc(c2)NCC)cc2C(=O)N[C@@H](C)C3CCCC3[C@@H](O)CNC4CCOCC4	4.041	4.229	3.358	3.937	5.048	69.168
800 ³⁸	CN1S(=O)(=O)CCC(c12)c(NCC)cc(c2)C(=O)N[C@@H](C)C3CCCC3[C@@H](O)CNC4CCOCC4	3.721	3.640	3.622	4.319	3.367	73.488
801 ³⁸	CN1S(=O)(=O)CCC(c12)c(NCC)cc(c2)C(=O)N[C@@H](C)C3CCCC3C(F)F	4.585	3.533	4.091	4.218	5.405	70.111
802 ³⁸	C1CCCN(S1(=O)=O)c(cc(c2)NCC)cc2C(=O)N[C@@H](C)C3CCCC3C3)C4CCCC4	3.921	3.229	3.369	3.906	3.365	77.996
803 ³⁸	c1cccc1[C@@H]([C@@H](O)CNC2CC2)NC(=O)C(=C3)C=C([C@@H]4[C@@H]35)N(CCC)CCN4CCS(=O)(=O)N5C	3.260	3.815	3.261	3.691	3.339	71.941
804 ³⁸	CN1S(=O)(=O)CCC(c12)c(NCC)cc(c2)C(=O)N[C@@H](C)C3CCCC3C3)C4CCCC4	3.824	3.662	3.621	4.287	4.881	80.381
805 ³⁸	CN1S(=O)(=O)Cn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](C)C4CCCC4[C@@H](O)CNC5CCCC5OC	5.097	4.544	4.222	5.215	5.345	69.879
806 ³⁸	CN1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](C)C4CCCC4[C@@H](O)CNC5CCCC5OC	5.699	5.147	5.528	5.516	6.386	56.499
807 ³⁸	CN1S(=O)(=O)Cn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](C)C4CCCC4[C@@H](O)CNC(C)C(C)CCCC(C)C	4.638	4.088	4.128	4.631	5.645	65.346
808 ³⁸	CN1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](C)C4CCCC4[C@@H](O)CNC(C)C(C)CCCC(C)C	5.301	5.842	4.331	4.931	5.701	68.755
809 ³⁸	CN1S(=O)(=O)Cn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](C)C4CCCC4[C@@H](O)CNC5CCCC5	4.222	4.147	3.343	4.603	4.379	69.114
810 ³⁸	CN1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](C)C4CCCC4[C@@H](O)CNC5CCCC5	5.046	4.173	4.004	4.904	5.150	68.989
	CN1S(=O)(=O)Cn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](C)C4CCCC4[C@@H](O)CNC	4.041	3.254	3.506	4.560	2.757	62.390

)Ce4cccc4							
812 ³⁸	CN1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@H]([C@H](O)CN)C)Ce4cccc4	4.824	5.120	4.602	4.860	5.818	64.857	
813 ³⁸	CN1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](Ce4cccc4)[C@H](O)CNCe5cccc(e5)OC	4.553	3.332	3.814	5.168	4.882	56.831	
814 ³⁸	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c(c3)cc(c4c35)c(CC)c n4CCCS(=O)(=O)N5C	3.310	2.981	3.224	3.471	3.879	65.444	
815 ³⁸	N1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](Ce4cccc4)[C@H](O)CNCe5cccc(e5)OC	4.854	4.781	4.043	5.238	4.461	51.007	
816 ³⁸	CCN1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](Ce4cccc4)[C@H](O)CNC5CCOCC5	5.301	4.717	5.971	4.855	5.553	67.561	
817 ³⁸	CC(C)N1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](Ce4cccc4)[C@H](O)CNC5CCOCC5	4.638	4.477	5.069	4.871	4.546	71.877	
818 ³⁸	FC(F)(F)CN1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](Ce4cccc4)[C@H](O)CNC5CCOCC5	4.538	4.477	4.316	4.735	5.542	74.956	
819 ³⁸	CCN1S(=O)(=O)CCn2cc(CC)c(c2c13)cc(c3)C(=O)N[C@@H](Ce4cccc4)[C@H](O)CNC5CCCC5	5.155	3.826	4.336	4.908	5.550	85.671	
820 ³⁸	c1cccc1C[C@@H]([C@H](O)CNC2CC2)NC(=O)c(c3)cc(c4c35)c(CC)c n4CCS(=O)(=O)N5CC	4.699	4.010	4.426	4.824	5.485	45.492	
821 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](Ce3cccc3)CNCC(=O)NCC(C)C	3.932	3.649	3.531	4.319	4.355	43.234	
822 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](Ce3cccc3)CN[C@@H](C)C(=O)NCC(C)C	5.097	4.956	5.083	4.234	6.270	74.461	
823 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](Ce3cccc3)CN[C@@H](CC)C(=O)NCC(C)C	5.155	4.359	4.523	4.475	6.176	70.893	
824 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](Ce3cccc3)CN[C@@H](CCC)C(=O)NCC(C)C	5.398	5.165	5.416	4.571	5.023	69.907	
825 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](Ce3cccc3)CN[C@@H](CCO)C(=O)NCC(C)C	4.886	4.557	4.434	4.470	4.648	66.396	
826 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](Ce3cccc3)CN[C@@H](CCS(=O)(=O)C)C(=O)NCC(C)C	4.886	5.006	4.912	4.519	4.806	76.879	
827 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](CN[C@@H](C)C(=O)NCC)Ce3cccc3	4.284	4.398	3.738	4.087	4.225	81.124	
828 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](Ce3cccc3)CN[C@@H](C)C(=O)NC4CC4	4.620	3.882	4.096	4.277	5.238	77.646	
829 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](Ce3cccc3)CN[C@@H](C)C(=O)NC4cccc4	3.857	3.728	4.327	4.152	3.523	72.125	
830 ³⁹	c1cc(F)ccc1[C@@H](C)NC(=O)c2cc(cc(e2)N(C)S(=O)(=O)C)C(=O)N[C@@H](Ce3cccc3)CN[C@@H](C)C(=O)[C@@H](C4)CN[C@@H]4C(=O)O	1.764	2.555	2.447	1.958	1.410	87.237	
831 ⁴⁰	c1cccc(S2)c1N(c(c23)cccc3)C(=O)/N=C(\Nc4nc(C)cc(n4)C)Nc5cccc(c5)[N+](=O)[O-]	1.544	2.553	2.599	1.570	1.492	76.979	
832 ⁴⁰	c1cc(F)ccc1-c(c2C#N)cc(-c3cccc3)nc2SCC(=O)NC45C[C@H]6C[C@@H](C4)C[C@H](C6)C5	0.928	1.641	1.648	1.523	0.613	81.576	
833 ⁴⁰	c1cc(F)ccc1-c2cc(-c3cccc3)c(C#N)c(n2)SCC(=O)Nc4sc(nn4)CC	1.301	1.652	1.721	1.638	1.389	74.478	
834 ⁴⁰	c1cccc(c12)ccc(c2)N(c3cccc3)C(=O)CSc4nc(-c5ccc(cc5)OC)cc(c4C#N)-c6ccc(Cl)cc6	1.301	1.235	2.030	2.097	0.774	60.773	
835 ⁴⁰	c1cccc1CSc(nn2)nc(c2c(c34)cccc3)O[C@H](N4)c5c(C)nn(c5Cl)-c6cccc6	1.000	1.009	1.480	1.960	0.585	36.121	
836 ⁴⁰	c1cccc1NC(=O)/N=C(/NC(=O)Nc2cccc2)Nc(n3)nc(C)c(c34)cccc4	2.523	2.907	2.267	2.159	2.235	48.078	
837 ⁴⁰	c1cccc(c12)[nH]cc2C(=O)CSc3n(Ce4cccc4)c(nn3)Cc5c[nH]c(c56)cccc6	1.000	1.634	0.931	1.733	1.236	57.720	
838 ⁴⁰	c1cc(Br)ccc1S(=O)(=O)N(S(=O)(=O)c(c2)ccc2Br)c3nn(c3)Cc4cc(Cl)c(Cl)cc4	1.046	1.507	1.499	2.769	2.022	25.626	
839 ⁴⁰	c1cccc1-c2nc(c(C#N)c(e2)-c3cccc3)SCC(=O)Nc4cccc(c4)[N+](=[O-])=O	1.699	2.160	2.484	2.028	1.901	42.555	
840 ⁴⁰	c1cccc1-c2esc(n2)NC(=O)CSc3n(C)c(nn3)CC(=O)Nc4cccc(C)cc4	1.678	1.915	1.745	1.846	1.736	60.550	
841 ⁴⁰	C1CCCCN1c2nc(nc(n2)N3CCCC3)Nc(cc4)cc(c45)sc(n5)SCC(=O)NCCc6cc(OC)c(cc6)OC	2.553	3.019	2.655	2.537	2.480	53.488	
842 ⁴⁰	C1CCCCN1c2nc(N3CCCC3)nc(n2)Nc(cc4)cc(c45)sc(n5)SCC(=O)Nc6cccc6F	1.991	2.043	2.061	2.145	2.324	49.912	
843 ⁴⁰	c1cccc1-c2cc(-c3cccc3)nc(n2)SCC(=O)OCC(=O)Nc(s4)c(C#N)c(c45)CCCC5	1.462	2.337	1.708	1.791	1.367	54.979	
844 ⁴⁰	C1CCCCc(c12)sc(c2C#N)NC(=O)C(F)(F)C(F)(F)C(F)(F)C(=O)Nc(s3)c(C#N)c(c34)CCCCC4	1.914	2.059	1.894	1.992	1.808	48.888	
845 ⁴¹	CC(C)[C@H](O)C(=O)N[C@@H](C)C(=O)N[C@@H](Ce1cccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C)C(=O)Nc2cccc2	3.886	3.500	3.975	3.626	4.366	44.334	
	CC(C)[C@H](O)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](Ce1cccc1)[2.456	2.820	2.004	2.886	2.260	22.740	

	(CC(C)C)[C@@H](O)CC(=O)N[C@@H](CC(C)C)C(=O)NCc1cc(C(=O)O)ccc1							
873 ⁴²	O=C(C)N[C@@H]([C@H](C)CC)C(=O)N[C@@H](C)C(=O)N[C@@H](CC(C)C)[C@@H](O)CC(=O)N[C@@H](Cc1ccccc1)C(=O)NCc2cc(C(=O)O)ccc2	3.602	4.208	4.423	2.799	3.472	68.348	
874 ⁴²	O=C(C)N[C@@H]([C@H](C)CC)C(=O)N[C@@H](C)C(=O)N[C@@H](CC(C)C)[C@@H](O)CC(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)NCc2cc(C(=O)O)ccc2	3.959	3.881	3.289	3.808	3.615	75.454	
875 ⁴³	CNC(=O)c1cc(N(C)S(=O)(=O)C)cc(c1)C(=O)N[C@@H]([C@H](O)CNC2CC2)Cc3ccccc3	3.009	2.461	3.038	3.749	3.316	73.557	
876 ⁴³	CCC(=O)c1cc(N(C)S(=O)(=O)C)cc(c1)C(=O)N[C@@H]([C@H](O)CNC2CC2)Cc3ccccc3	2.824	3.597	2.589	3.532	3.047	66.999	
877 ⁴³	c1ccccc1CC(=O)c2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	2.854	2.759	2.097	3.523	2.295	70.220	
878 ⁴³	c1ccccc1C[C@@H](O)c2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	2.260	2.532	3.082	2.907	2.355	55.352	
879 ⁴³	c1ccccc1C(=O)c2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	4.009	4.005	4.182	3.496	4.910	37.054	
880 ⁴³	c1ccccc1[C@@H](O)c2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	2.229	4.966	2.688	2.457	2.856	8.475	
881 ⁴³	c1ccccc1C(=C)c2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	2.886	2.987	3.444	3.511	2.937	21.469	
882 ⁴³	c1ccccc1Cc2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	2.334	3.219	2.740	2.835	2.095	48.316	
883 ⁴³	C1CCCCC1C(=O)c2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	3.347	3.757	3.728	3.536	3.373	24.599	
884 ⁴³	CC(C)C(=O)c1cc(N(C)S(=O)(=O)C)cc(c1)C(=O)N[C@@H]([C@H](O)CNC2CC2)Cc3ccccc3	3.620	4.005	3.708	3.608	3.348	46.033	
885 ⁴³	C1CCCCC1C(=O)c2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	3.745	3.901	3.545	3.440	4.050	26.626	
886 ⁴³	C1CC1C=Cc2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	3.137	3.834	3.563	3.442	6.293	37.936	
887 ⁴³	C1CC1C=Cc2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	4.456	4.414	3.863	3.442	4.253	58.042	
888 ⁴³	C1CC1CCc2cc(N(C)S(=O)(=O)C)cc(c2)C(=O)N[C@@H]([C@H](O)CNC3CC3)Cc4ccccc4	3.377	3.939	3.375	3.594	3.597	43.960	
889 ⁴⁴	CC(C)C)OC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	4.155	4.354	4.596	4.523	4.721	45.848	
890 ⁴⁴	CC(C)C)OC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	4.086	4.704	4.221	3.976	4.342	34.268	
891 ⁴⁴	CC(C)C)OC(=O)N[C@@H](CCC)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	4.222	4.533	4.435	4.278	4.370	56.217	
892 ⁴⁴	CC(C)C)OC(=O)N[C@@H](CCC)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	4.387	4.684	4.415	3.702	4.278	71.300	
893 ⁴⁴	CC(C)C)OC(=O)N[C@@H](CC)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	4.125	3.869	4.161	3.568	4.307	64.914	
894 ⁴⁴	CC(C)C)OC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	4.201	5.255	4.750	3.791	3.589	61.112	
895 ⁴⁴	CC(C)C)OC(=O)N[C@@H]([C@H](C)CC)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	4.377	4.393	4.523	4.009	4.279	61.170	
896 ⁴⁴	CC(C)C)OC(=O)N[C@@H](CN(C)C)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	2.597	2.706	3.521	2.978	4.503	58.922	
897 ⁴⁴	CC(C)C)OC(=O)N[C@@H](CCN(C)C)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	1.051	1.553	1.866	1.839	1.326	63.986	
898 ⁴⁴	CC(C)C)OC(=O)N[C@@H](COC)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2	3.928	4.031	4.925	3.494	4.295	67.633	
	CC(C)C)OC(=O)N[C@@H](CCOC)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)NCc2ccccc2							

	H][Cc1cccc1][C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)Nc2cnc2								
900 ⁴⁴	CC(C)(C)OC(=O)N[C@@H](CC(F)F)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1cccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)Nc2cnc2	4.347	3.947	4.308	3.695	4.386	62.285		
901 ⁴⁴	CC(C)(C)OC(=O)N[C@@H](CC(F)F)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1cccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)Nc2cnc2	3.551	4.536	4.439	3.685	3.305	69.207		
902 ⁴⁴	CC(C)(C)OC(=O)N[C@@H](CCCC(F)F)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1cccc1)[C@@H](O)C[C@@H](C)C(=O)N[C@@H](C(C)C)C(=O)Nc2cnc2	3.378	3.932	4.112	3.691	3.401	64.541		
903 ⁴⁵	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C)C(=O)N[C@@H](O)CC(=O)N[C@@H](Cc1cccc1)[C@@H](O)CC(=O)N[C@@H](C(C)C)C(=O)Nc2cnc2	4.678	4.648	4.396	3.820	5.627	67.418		
904 ⁴⁵	c1cccc1C[C@H](NC(=O)[C@@H](NC(=O)C)CC(C)C)[C@@H](O)CC(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)Nc2cnc2	3.187	3.233	3.773	3.876	3.674	65.280		
905 ⁴⁵	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C)C(=O)N[C@@H](O)CC(=O)N[C@@H](CCSC)[C@@H](O)CC(=O)N[C@@H](C(C)C)C(=O)Nc2cnc2	3.337	3.477	3.652	3.432	3.737	65.139		
906 ⁴⁵	c1cccc1C[C@H](NC(=O)[C@@H](NC(=O)C)CC(C)C)[C@@H](O)CC(=O)N[C@@H](CC2CCCC2)[C@@H](O)CC(=O)N[C@@H](C(C)C)C(=O)Nc2cnc2	4.301	3.804	4.582	3.987	5.013	67.985		
907 ⁴⁵	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C)C(=O)N[C@@H](O)CC(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)Nc2cnc2	1.469	1.644	1.774	2.390	1.693	64.805		
908 ⁴⁶	c1cccc1-c2sec(c2CC(=O)N=C(N)N)-c3cccc3	2.081	2.015	2.526	2.908	2.290	63.067		
909 ⁴⁶	NC(N)=NC(=O)Cc1c(-c2c(Cl)cccc2)csc1-c3ccc(cc3)Oe4ccc(cc4)C(=O)C	3.125	3.327	3.358	2.839	3.465	70.790		
910 ⁴⁶	NC(N)=NC(=O)Cc1c(-c2c(Cl)cccc2)csc1-c3ccc(cc3)OCCe4cn[nH]e4	2.161	2.775	2.676	3.128	2.312	63.110		
911 ⁴⁶	CCCOc(c1)ccc1-c2sec(c2CC(=O)N=C(N)N)-c3cccc3	3.167	3.141	2.749	3.176	3.152	62.137		
912 ⁴⁶	c1cccc1-c2sec(c2CC(=O)N=C(N)N)-c3ccc(cc3)OCCC	2.724	3.220	2.641	3.117	2.419	61.247		
913 ⁴⁶	CCCOc(c1)ccc1-c2sec(c2CC(=O)N=C(N)N)-c3c(Cl)cccc3	3.201	3.257	2.867	3.177	-1.736	48.240		
914 ⁴⁶	Clc1cccc1-c2sec(c2CC(=O)N=C(N)N)-c3ccc(cc3)OCCC	3.229	3.139	2.366	3.264	3.394	47.638		
915 ⁴⁶	CCCOc(c1)ccc1-c2sec(-c3c(Cl)cccc3)e2CC(=O)N=C(N)NCCCO	3.824	3.651	3.430	3.388	3.680	61.468		
916 ⁴⁶	CCCOc(c1)ccc1-c2sec(-c3c(Cl)cccc3)e2CC(=O)N=C(N)NCCCO	3.268	3.605	3.080	3.410	3.965	65.561		
917 ⁴⁶	CCCOc(c1)ccc1-c2sec(-c3c(Cl)cccc3)e2CC(=O)N=C(N)NCCCO	2.810	2.626	2.871	3.466	2.678	63.267		
918 ⁴⁶	FC(F)CNC(=O)c(c1)ccc1-c2sec(-c3c(Cl)cccc3)e2CC(=O)N=C(N)NCCCO	3.699	3.734	3.267	3.151	4.329	53.535		
919 ⁴⁶	CCNC(=O)c(c1)ccc1-c2sec(-c3c(Cl)cccc3)e2CC(=O)N=C(N)NCCCO	3.585	3.285	3.079	3.312	3.641	54.806		
920 ⁴⁶	C1CC1CNC(=O)c(c2)ccc2-c3sec(-c4c(Cl)cccc4)e3CC(=O)N=C(N)NCCCO	3.854	3.847	3.561	3.447	3.633	59.318		
921 ⁴⁶	CCCCNC(=O)c(c1)ccc1-c2sec(-c3c(Cl)cccc3)e2CC(=O)N=C(N)NCCCO	3.553	3.361	4.380	3.342	3.687	57.697		
922 ⁴⁶	CCC(CC)NC(=O)c(c1)ccc1-c2sec(-c3c(Cl)cccc3)e2CC(=O)N=C(N)NCCCO	3.032	3.885	3.262	3.570	3.712	57.597		
923 ⁴⁷	CC(C)C[C@@]1(C)NC(=N/[H])N(C1=O)Cc2ccc(cc2)CCNC(=O)Nc3ccc(C#N)cc3	2.155	2.446	2.170	1.776	2.312	61.380		
924 ⁴⁷	CCCCNC(=O)NCCc(c1)ccc1CN(C2=O)/C(=N/[H])N[C@@]2(CC)CC3CCC3	2.301	2.543	3.298	2.277	2.030	58.354		
925 ⁴⁷	CCCCNC(=O)NCCc(c1)ccc1CN(C2=O)/C(=N/[H])N[C@@]2(CC3CCCC3)CC4CCCC4	2.678	3.449	3.089	2.918	2.650	62.763		
926 ⁴⁷	CCCCNC(=O)NCCc(c1)ccc1CN(C2=O)/C(=N/[H])N[C@@]2(CC(C)C)CC3CCCC3	1.301	1.485	1.793	2.249	1.216	64.752		
927 ⁴⁷	CCCCNC(=O)NCCc(c1)ccc1CN(C2=O)/C(=N/[H])N[C@@]2(CC(C)C)CC3CCCC3	2.523	2.715	2.489	2.476	1.915	64.269		
928 ⁴⁷	CCCCNC(=O)NCCc(c1)ccc1CN(C2=O)/C(=N/[H])N[C@@]2(CC3CCC3)CC4CCCC4	3.456	3.962	4.212	3.041	3.483	64.055		
929 ⁴⁷	CCC[C@H](C1)NC(=O)N1CCc(cc2)ccc2CN(C3=O)/C(=N/[H])N[C@@]3(CC4CCCC4)CC5CCCC5	4.569	4.034	4.934	3.792	4.810	59.574		
930 ⁴⁸	c1cccc1C2(c3cccc3)N=C(N)N(C2=4)CCCN4	1.420	1.747	1.680	1.113	1.760	61.800		
931 ⁴⁸	FC(F)Fc1cccc(c1)[C@@]2(c3cccc3)N=C(N)N(C2=4)CCCN4	1.660	1.630	1.627	1.681	1.117	62.862		
932 ⁴⁸	COc1cccc(c1)[C@@]2(c3cccc3)N=C(N)N(C2=4)CCCN4	1.693	2.342	1.889	2.007	1.945	61.247		
933 ⁴⁸	CC(C)(C)c1cccc(c1)[C@@]2(c3cccc3)N=C(N)N(C2=4)CCCN4	1.520	2.541	3.061	1.734	1.931	39.555		
934 ⁴⁸	c1cccc1Cc2ccc(c2)[C@@]3(c4cccc4)N=C(N)N(C3=5)CCCN5	2.276	2.625	1.922	2.381	2.670	52.077		
935 ⁴⁸	c1cc(OC)ccc1Cc2ccc(c2)[C@@]3(c4cccc4)N=C(N)N(C3=5)CCCN5	2.149	2.609	2.264	2.495	1.919	11.030		

936 ⁴⁸	c1cc(F)ccc1Cc2cccc(e2)[C@@]3(c4cccc4)N=C(N)N(C3=5)CCCN5	2.086	2.626	1.922	2.365	2.352	30.217
937 ⁴⁸	FC(F)(F)Oc(cc1)ccc1[C@@]2(c3cccc3Br)N=C(N)N(C2=4)CCCN4	2.585	2.565	3.097	3.108	2.847	3.242
938 ⁴⁸	CCCc1cccc(c1)[C@@]2(c3cccc3)OC(F)(F)F)N=C(N)N(C2=4)CCCN4	2.845	3.450	3.348	2.974	3.250	14.837
939 ⁴⁸	C1CC1CCc2cccc(e2)[C@@]3(c4ccc(cc4)OC(F)(F)F)N=C(N)N(C3=5)CCCN5	3.678	4.351	3.940	3.024	3.307	33.698
940 ⁴⁸	c1ncnc1-c2cccc(e2)[C@@]3(c4ccc(cc4)OC)N=C(N)N(C3=5)CCCN5	4.000	3.823	3.891	3.551	3.726	58.351
941 ⁴⁸	c1ncnc1-c2cccc(e2)[C@@]3(c4ccc(cc4)OC(F)(F)F)N=C(N)N(C3=5)CCCN5	4.000	3.664	3.902	3.815	3.870	67.723
942 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(c4ccc(cc4)OC)N=C(N)N(C3=5)CCCN5	4.155	4.607	3.855	3.658	3.803	53.640
943 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(c4ccc(cc4)OC(F)(F)F)N=C(N)N(C3=5)CCCN5	4.222	4.153	3.987	3.922	4.389	54.254
944 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(c(c4)ccc(c45)OCO5)N=C(N)N(C3=6)CCCN6	3.796	3.631	3.455	3.959	3.474	57.740
945 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(N=C(N)N(C3=4)CCCN4)c(c5)ccc(c56)OCCO6	3.721	3.501	3.543	3.829	3.473	59.489
946 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(c(c4)ccc(c45)OC(O5)(F)F)N=C(N)N(C3=6)CCCN6	3.131	3.625	3.551	4.107	3.465	64.656
947 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(N=C(N)N(C3=4)CCCN4)c5cc(OCC)c(cc5)OCC	4.097	3.475	3.727	4.028	3.574	69.300
948 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(N=C(N)N(C3=4)CCCN4)c5ccc(cc5)OC(F)(F)F	4.097	4.326	3.933	4.566	4.157	66.249
949 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(c4ccc(cc4)OC(F)(F)F)N=C(N)N(C3=5)CCCN5	4.097	3.858	3.850	3.861	4.526	63.373
950 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(c4ccc(cc4)OC(F)(F)F)N=C(N)N(C3=5)CCCN5	3.886	3.652	3.930	3.927	4.298	69.478
951 ⁴⁸	Fc1ncnc1-c2cccc(e2)[C@@]3(c4ccc(cc4)OC(F)(F)F)N=C(N)N(C3=5)CC(N5)(C)C	3.721	4.164	4.085	3.335	3.764	74.102
952 ⁴⁹	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](CC(C)C)[C@@H](O)[C@@H]1[C@@H](CC(=O)C1)C(=O)N[C@@H](C)C(=O)O	3.143	2.843	2.804	3.894	4.483	67.657
953 ⁴⁹	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](CC(C)C)[C@@H](O)[C@@H]1[C@@H](CCC1)C(=O)N[C@@H](C)C(=O)O	3.222	3.623	4.182	4.107	3.630	68.630
954 ⁴⁹	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](CC(C)C)[C@@H](O)[C@@H]1[C@@H](CC(=O)C1)C(=O)N[C@@H](C)C(=O)NCCCC	5.000	5.224	4.992	4.623	6.003	69.864
955 ⁴⁹	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](CC(C)C)[C@@H](O)[C@@H]1[C@@H](CCC1)C(=O)N[C@@H](C)C(=O)NCCCC	4.602	4.867	4.516	4.629	4.487	65.333
956 ⁴⁹	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](CC(C)C)[C@@H](O)[C@@H]1[C@@H](CN(C1)C)C(=O)N[C@@H](C)C(=O)NCCCC	2.463	3.020	2.636	2.664	2.746	69.862
957 ⁴⁹	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](CC(C)C)[C@@H](O)[C@@H]1[C@@H](C(=O)N(C1)CC)C(=O)N[C@@H](C)C(=O)NCCCC	2.475	3.271	2.958	2.212	2.668	68.605
958 ⁴⁹	CC(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](CC(C)C)[C@@H](O)[C@@H]1[C@@H](OCC1)C(=O)N[C@@H](C)C(=O)NCCCC	2.020	2.480	2.489	2.901	2.298	65.653
959 ⁵⁰	CCCN(CCC)C(=O)c1ccc(cc1)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@@H](O)CN[C@@H](C)C(=O)NCCC(C)C	3.886	3.536	3.329	4.211	3.735	66.812
960 ⁵⁰	CCCN(CCC)C(=O)c1ccc(cc1)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@@H](O)CN[C@@H](C)C(=O)NCCC(C)C	3.301	4.385	3.931	4.211	4.056	65.510
961 ⁵⁰	CCCN(CCC)C(=O)c1ccc(cc1)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@@H](O)CN[C@@H](C)C(=O)NCCC(C)C	4.155	4.095	3.682	4.453	4.848	70.992
962 ⁵⁰	CCCN(CCC)C(=O)c1ccc(cc1)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@@H](O)CNC(C)C(=O)NCCC(C)C	3.699	3.720	3.337	4.578	4.206	62.859
963 ⁵⁰	CCCN(CCC)C(=O)c1ccc(cc1)C(=O)N[C@@H](Cc2cc(F)cc(F)e2)[C@@H](O)CNCc3cccc3	3.886	4.216	4.343	4.734	2.121	45.665
964 ⁵¹	C1CNCCN1c2ccc(Br)cc2NC(=O)c3cccc(c34)cccc4	3.000	2.385	2.629	2.208	3.545	54.223
965 ⁵¹	OCCN(CC1)CCN1c2ccc(Br)cc2NC(=O)c3cccc(c34)cccc4	4.102	3.505	3.949	3.356	4.568	63.879
966 ⁵¹	c1cccc(e12)cccc2C(=O)Nc3ccc(-c4cccc4)ccc3N5CCN(CC5)C6c6cccc6	2.903	3.589	2.955	3.920	3.976	57.645
967 ⁵¹	C1CNCCN1c2ccc(-c3cccc3)cc2NC(=O)c4cccc(c45)cccc5	3.523	2.370	3.031	2.795	3.303	52.331
968 ⁵¹	OCCN(CC1)CCN1c2ccc(-c3cccc3)cc2NC(=O)c4cccc(c45)cccc5	3.959	3.576	3.837	3.697	3.549	61.423
969 ⁵¹	c1cccc(e12)cccc2C(=O)Nc3ccc(-c4cccc4)ccc3N5CCN(CC5)CC(=O)OCC	4.046	3.674	3.437	3.589	3.832	51.745
	c1cccc(e12)cccc2C(=O)Nc3ccc(-	4.000	2.840	4.102	4.504	2.705	58.248

	c4cccc4)ccc3N5CCN(CC5)CCCCN(C6=O)C(=O)c(c67)cccc7						
971 ⁵¹	c1cccc(c12)cccc2C(=O)Nc3cc(-c4cccc4)ccc3N5CCN(CC5)CCCCCN	4.167	4.421	4.069	3.525	4.310	68.156
972 ⁵¹	c1cccc(c12)cccc2C(=O)Nc3cc(-c4cccc4)ccc3N5CCN(CC5)CC[C@@H](O)c6cccc6	4.161	3.722	3.836	3.898	4.171	57.320
973 ⁵¹	c1cccc(c12)cccc2C(=O)Nc3cc(-c4cccc4)ccc3N5CCN(CC5)C(=O)c6cccc6	4.102	4.104	3.851	3.933	3.844	64.248
974 ⁵¹	c1cccc(c12)cccc2C(=O)Nc3cc(-c4cccc4)ccc3N5CCN(CC5)C(=O)CCCCC6SCCS6	2.420	3.488	3.062	3.326	2.839	36.470
975 ⁵¹	c1cccc(c12)oc(=O)c(c2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)C(=O)OC(C)(C)C	3.000	3.411	3.076	2.719	3.020	48.654
976 ⁵¹	c1cccc(c12)oc(=O)c(c2)C(=O)Nc3cc(Br)ccc3N4CCN(CC4)Cc5cccc5	3.119	3.292	2.732	3.172	3.692	56.221
977 ⁵¹	OCCN(CC1)CCN1c2ccc(Br)cc2NC(=O)c(c3)c(=O)oc(c34)cccc4	3.201	3.227	2.949	3.323	3.373	59.741
978 ⁵¹	OCCN(CC1)CCN1c2ccc(Br)cc2NC(=O)c(c3)c(=O)oc(c34)c(OC)ccc4	3.000	2.874	2.630	3.609	3.054	64.412
979 ⁵¹	c1cccc(c12)oc(=O)c(c2)C(=O)Nc3cc(-c4cccc4)ccc3N5CCN(CC5)C(=O)OC(C)(C)C	2.000	1.883	1.964	2.264	1.829	62.697
980 ⁵¹	c1cccc(c12)oc(=O)c(c2)C(=O)Nc3cc(-c4cccc4)ccc3N5CCN(CC5)Cc6cccc6	3.821	2.780	2.781	3.704	4.097	58.405

Name	Structure	1: COEFFICIENT	Name	Structure	1: COEFFICIENT	Name	Structure	1: COEFFICIENT	Name	Structure	1: COEFFICIENT
frag1024641		0.01	frag567248		0.01	frag1016021		-0.01	frag1210351		-0.01
frag257809		0.01	frag389092		0.01	frag1015983		-0.01	frag710502		-0.01
frag37219		0.01	frag1032956		0.01	frag219767		-0.01	frag219564		-0.01
frag1228108		0.01	frag379514		0.01	frag670006		-0.01	frag492790		-0.01

A

B

Figure S1: (A) Favorable and (B) unfavorable fragments for BACE inhibitory activity

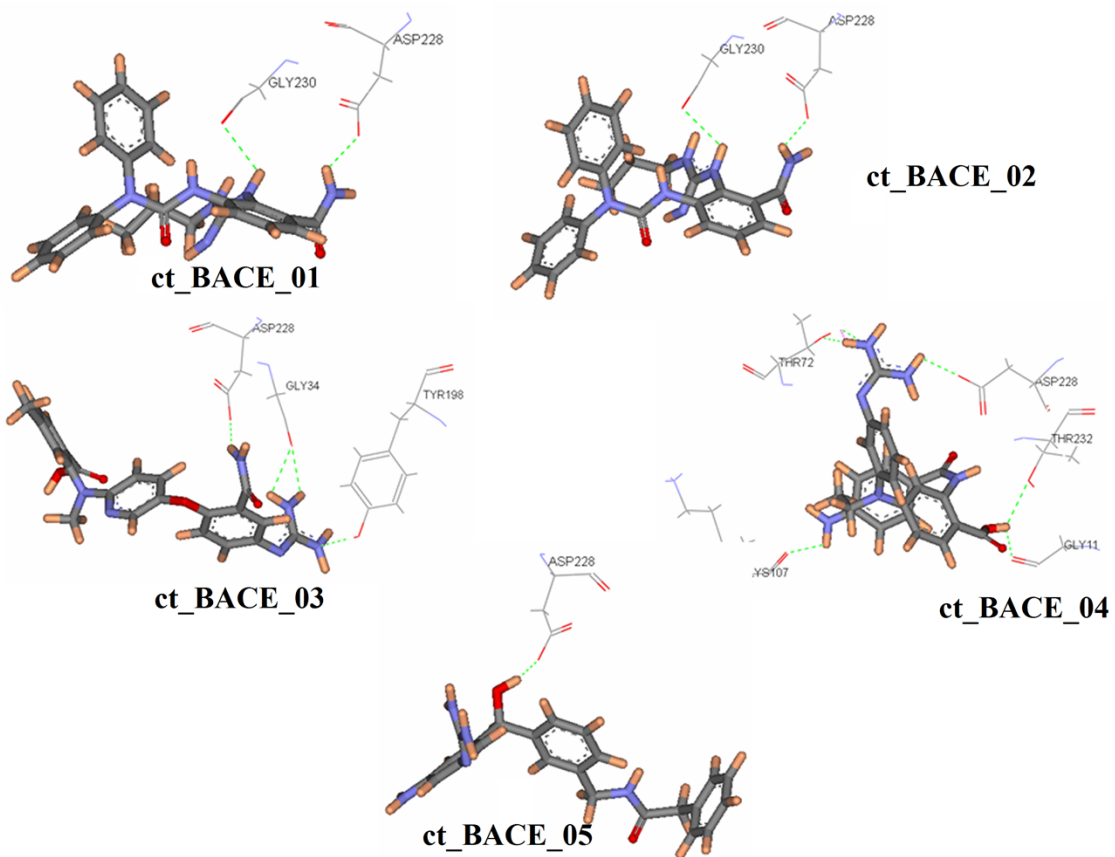


Figure S2: Hit molecules from *de novo* design showing interactions at the catalytic site of the receptor

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