Supporting Information

Discovery of Inhibitors of Four Bromodomains by Fragment-Anchored Ligand Docking

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Supplementary information 1. Detailed description of the screening library.

The library was compiled from the Lausanne Bioscreening Facility chemical library

It is an assembly of five sets from seven vendors, detailed on their website at http://bsf.epfl.ch/collections#faq-568582. In details, it contains the following libraries:

- Chemically Diverse Collection (CDC). 53'929 molecules from Enamine, ChemDiv, Life Chemicals. Those are representing the commercially available chemical space, covered with an average redundancy of six compounds per cluster enriched with 3D structures and sp3 centers.
- Natural products-inspired set (CDC extension). 13'433 molecules from Enamine, ChemBridge, Life Chemicals. Those are synthetic molecules designed and selected by using all commercially available natural products and derivatives as reference.
- Protein-Protein Interaction (PPi). 5'441 molecules from Life Chemicals. Compounds chosen by PPi machine learning method (895) and PPI rule of four (4'546)
- Natural Products (NPs). 2'649 molecules from Analyticon and InterBioscreen. Purified organic molecules from fractionated extracts of two sources, plants and bacteria.
- The Prestwick Chemical Library (PCL). 1'280 compounds from Prestwick Chemicals. Set of known bioactive molecules, approved drugs.

Our library did not include their Maybridge HitFinder set nor Kinases inhibitors.

In total, that represents 76'731 molecules

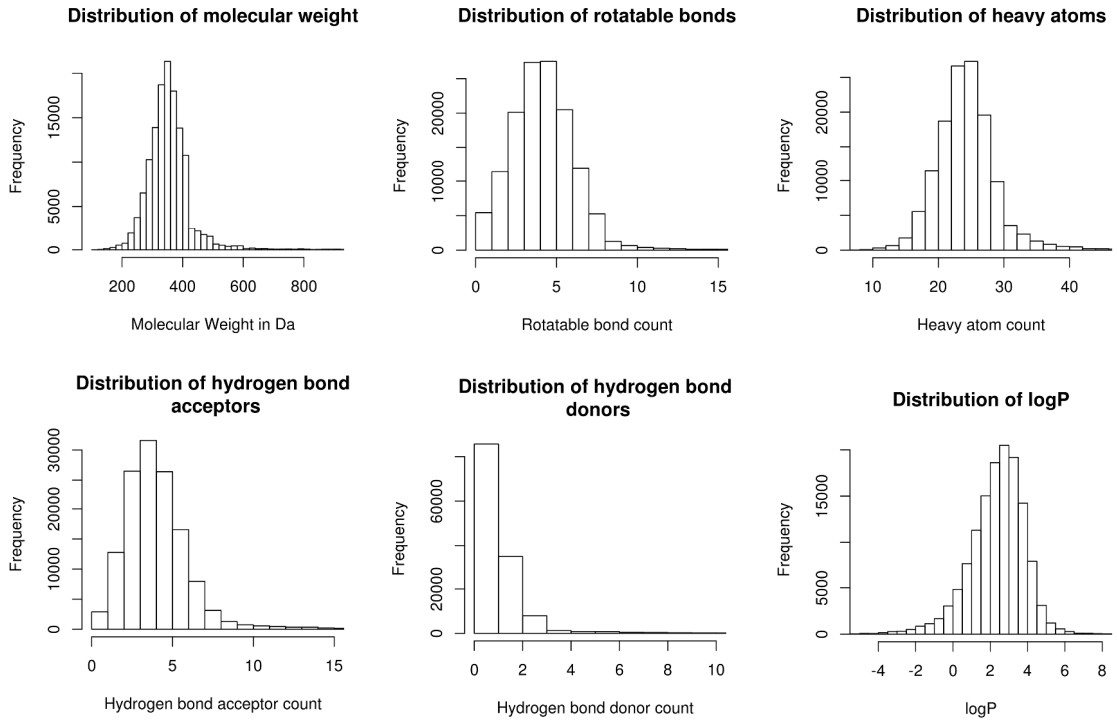


Figure S1. Distribution of miscellaneous properties of the chemical library: molecular weight, rotatable bonds, heavy atom, hydrogen bond donor and acceptor counts, logP (as calculated with the Wildman-Crippen logP calculator of the RDKit).

Supplementary information 2. Statistics of docking scores with respect to experimental results.

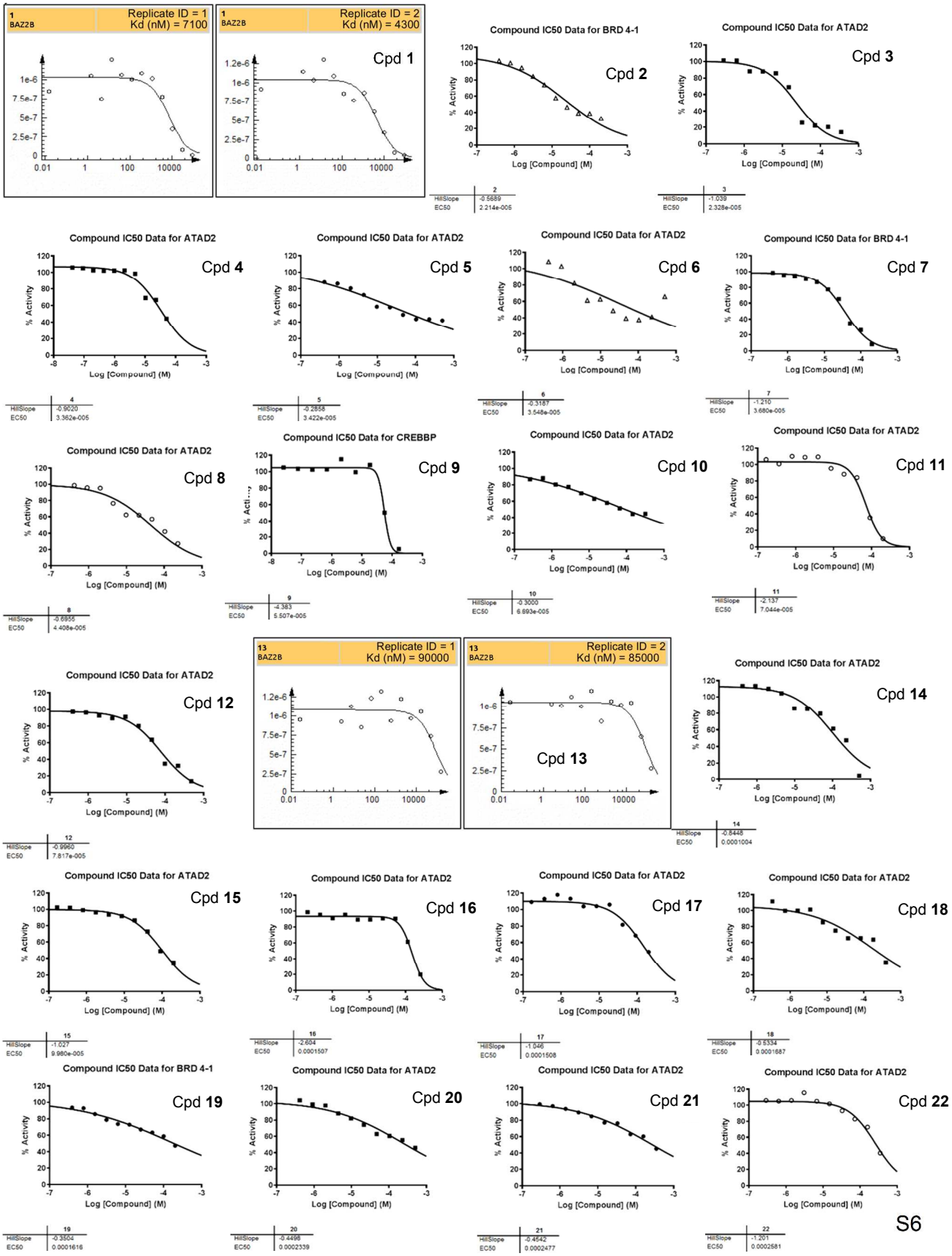
Table S1. Distribution of individual energy terms for the 260 molecules tested *in vitro*.

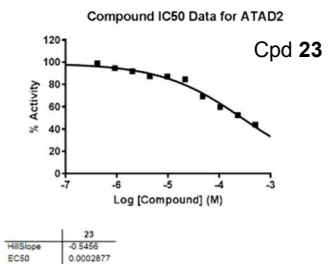
Bromodomain	Delta electr. < 0	Total efficiency < -1.0 kcal/mol	Electr. efficiency < -1.0 kcal/mol
ATAD2	121/142 (unique: 74)	67/142 (unique: 21)	2/142 (unique: 0)
	< 65%: 37/142 (unique: 21)	< 65%: 23/142 (unique: 7)	< 65%: 1/142 (unique:0)
	KD: 14/19 (unique: 9)	KD: 10/19 (unique: 5)	KD: 0/19 (unique: 0)
BAZ2A	20/30 (unique: 20)	19/30 (unique: 10)	0/30 (unique: 0)
	< 65%: 3/3 (unique: 0)	< 65%: 3/3 (unique: 0)	< 65%: 0/3 (unique: 0)
	KD: 0/0 (unique: 0)	KD: 0/0 (unique: 0)	KD: 0/0 (unique: 0)
BAZ2B	8/25 (unique:2)	23/25 (unique:17)	0/25 (unique:0)
	< 65%: 4/10 (unique: 1)	< 65%: 9/10 (unique: 5)	< 65%: 0/10 (unique: 0)
	KD: 0/2 (unique: 0)	KD: 2/2 (unique: 2)	KD: 0/2 (unique: 0)
BRD4(1)	10/38 (unique:0)	38/38 (unique:20)	0/38 (unique:0)
	< 65%: 2/9 (unique: 0)	< 65%: 9/9 (unique: 7)	< 65%: 0/9 (unique: 0)
	KD: 1/3 (unique: 0)	KD: 3/3 (unique: 2)	KD: 0/3 (unique: 0)
CREBBP	19/25 (unique:2)	23/25 (unique:6)	0/25 (unique:0)
	< 65%: 1/2 (unique: 1)	< 65%: 1/2 (unique: 1)	< 65%: 0/2 (unique: 0)
	KD: 1/2 (unique: 1)	KD: 1/2 (unique: 1)	KD: 0/2 (unique: 0)

Table S2. Distribution of individual energy terms for the 192 inactive compounds.

Bromodomain	Delta electr. < 0	Total efficiency < -1.0 kcal/mol	Both	Electr. efficiency < -1.0 kcal/mol	Total
ATAD2	84/98 (unique: 53)	44/98 (unique: 14)	31/98	1/98 (unique: 0)	98/142
BAZ2A	18/27 (unique: 11)	16/27 (unique: 9)	7/98	0/27 (unique: 0)	27/30
BAZ2B	4/15 (unique:1)	14/15 (unique:11)	3/15	0/15 (unique: 0)	15/25
BRD4(1)	8/29 (unique: 0)	29/29 (unique:21)	8/29	0/29 (unique: 0)	29/38
CREBBP	18/23 (unique:1)	22/23 (unique:5)	17/23	0/23 (unique: 0)	23/25

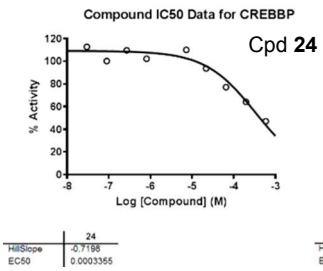
Supplementary information 3. Alphascreen dose-response curves for compounds **2-12** and **14-26**, and BROMOscan dose-response curves for compounds **1** and **13** (in duplicates).





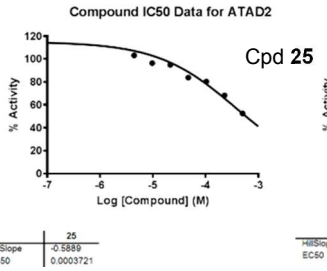
Cpd **23**

	23
HillSlope	-0.5456
EC50	0.0002877



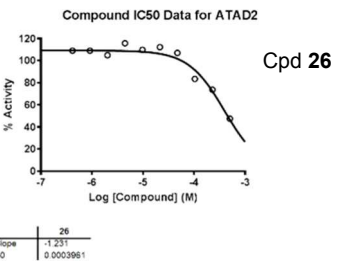
Cpd **24**

	24
HillSlope	-0.7198
EC50	0.0003355



Cpd **25**

	25
HillSlope	-0.5889
EC50	0.0003721



Cpd **26**

	26
HillSlope	-1.231
EC50	0.0003961

Supplementary information 4. X-ray crystallization data

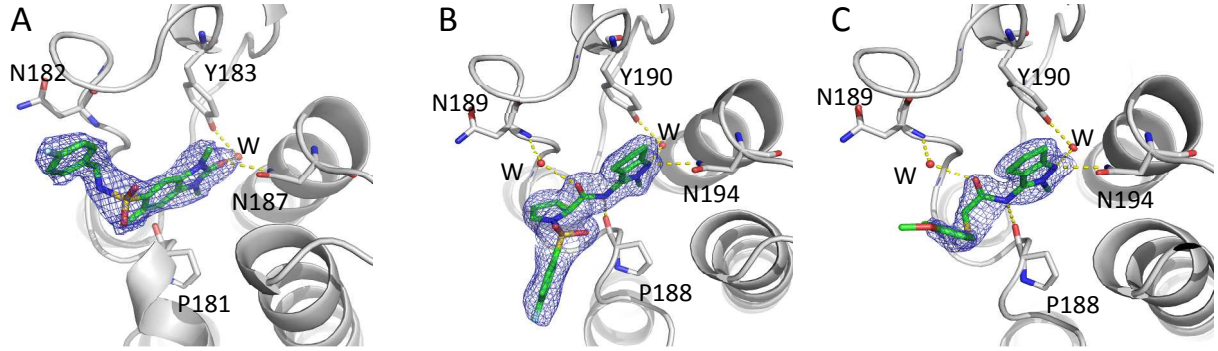


Figure S2. $2F_O$-F_C map, contoured at 1σ, showing electron density for compounds **1** (in complex with BAZ2A, PDB code 5OR8, panel **A**), **13** (in complex with BAZ2B, PDB code 5OR9, panel **B**) and **30** (in complex with BAZ2B, PDB code 5ORB, panel **C**). Protein matrices are shown in white with relevant amino acids as sticks, bound compounds are shown as green sticks, hydrogen bonds as yellow dashed lines and bridging water molecule as red spheres.

Table S3. Data collection and refinement statistics

	BAZ2A/cmp**1**	BAZ2B/cmp**13**	BAZ2B/cmp**30**
Data Collection			
Space group	$P3_121$	$C222_1$	$C222_1$
Unit-cell parameters (Å)	a = 95.14 b = 95.14 c = 32.65	a = 81.44, b = 96.65, c = 57.58	a = 80.91, b = 96.79, c = 57.82
Wavelength (Å)	1.00	1.00	1.00
Resolution (Å)	47.57-2.40 (2.49-2.40)	48.32-2.00 (2.05-2.00)	48.39-2.10 (2.17-2.10)
R_{merge} (%)	25.8 (140.7)	7.8 (66.8)	8.2 (54.2)
R_{meas} (%)	27.2 (148.0)	8.4 (71.7)	9.3 (57.9)
R_{pim} (%)	8.6 (45.7)	3.1 (25.8)	3.3 (21.0)
$\langle I/\sigma(I)\rangle$	8.3 (2.0)	14.5 (3.0)	12.7 (3.9)
$CC^{1/2}$	0.991 (0.723)	0.999 (0.953)	0.996 (0.937)
Completeness (%)	99.9 (99.9)	99.7 (99.3)	72.1 (41.6), spherical 94.7 (96.0), ellipsoidal
Multiplicity	9.9 (10.2)	7.2 (7.5)	7.5 (7.2)
Refinement			
Resolution (Å)	41.20-2.40	40.73-2.00	48.39-2.10
R_{work}/R_{free} (%)	20.5/24.3	18.7/20.8	18.8/21.8
R.m.s. deviations			
Bond lengths (Å)	0.008	0.006	0.006
Bond angles (°)	0.9	0.8	0.8
PDB entry	5OR8	5OR9	5ORB

Supplementary information 5. Docking and experimental data for all tested molecules.

Table S4. Experimental data. Compounds are sorted first according to potency in dose-response measurements irrespective of the target, and the remaining ones according to bromodomain target.

Cpd	Target	Vendor	Code	Single dose at [μM]	% remnant inhibition of competitor	IC_{50} or K_D(μM)	HAC
1	BAZ2B	ChemDiv	g801-0410	90	0.75	6	25
2	BRD4(1)	Life Chem	F1740-0340	200	38	22	17
3	ATAD2	Life Chem	F3098-8183	350	10	23	21
4	ATAD2	Enamine	T5701955	50	38	34	22
5	ATAD2	Enamine	T5903382	504	40	34	26
6	ATAD2	ChemDiv	c216-0021	504	48	35	23
7	BRD4(1)	ChemDiv	8016-9131	201	23	37	26
8	ATAD2	Enamine	T6869430	503	4	44	20
9	CREBBP	ChemBridge	78636485	503	0	55	25
10	ATAD2	Enamine	T6948910	318	48	67	25
11	ATAD2	Enamine	T6325318	200	48	70	26
12	ATAD2	Enamine	T6068544	479	12	78	24
13	BAZ2B	Life Chemicals	F5323-0167	160	18	88	27
14	ATAD2	Enamine	T6371051	503	6	100	18
15	ATAD2	Enamine	T6190878	200	29	100	28
16	ATAD2	ChemDiv	g890-0613	254	37	151	26
17	ATAD2	Enamine	T6680820	200	42	151	20
18	BRD4(1)	ChemDiv	g856-1818	201	40	167	25
19	ATAD2	Enamine	T6323310	399	37	169	28
20	ATAD2	Enamine	T6108302	504	45	234	21
21	ATAD2	Enamine	T6977231	350	47	248	23
22	ATAD2	Enamine	T5612469	350	45	258	26
23	ATAD2	Enamine	T5731299	505	43	288	23
24	CREBBP	ChemDiv	m950-0467	588	31	336	26
25	ATAD2	Enamine	T7007608	504	49	372	25
26	ATAD2	Enamine	T6387312	504	49	396	20
27	BAZ2B	Enamine	T6242932	130	7.3	> 130	30
28	BAZ2A	IBScreen	STOCK1N-74248	420	38	> 420	20
29	ATAD2	Enamine	T5856373	504	47	> 504	24
30	BAZ2B	Life Chemicals	F5323-0135	50	41	> 51	22
31	BAZ2B	Enamine	T6248176	100	50	>100	22
32	ATAD2	Life Chem	F2978-0107	504	40	>504	23
33	ATAD2	Enamine	T5900669	504	31	> 504	23

34	ATAD2	Enamine	T6346086	503	35	> 503	19
35	ATAD2	Enamine	T5918987	50	50	> 50	29
36	ATAD2	Enamine	T6590056	504	53	> 504	24
37	ATAD2	ChemDiv	c276-0027	446	53	> 446	22
38	ATAD2	ChemDiv	c276-0058	350	55	> 350	21
39	BRD4(1)	ChemDiv	8341-0732	201	45	> 201	29
40	ATAD2	Enamine	T6813230	446	52	Not Evaluated	26
41	ATAD2	Enamine	T5967282	422	52	Not Evaluated	27
42	ATAD2	Enamine	T5609622	340	53	Not Evaluated	29
43	ATAD2	Enamine	T7017679	500	54	Not Evaluated	25
44	ATAD2	Enamine	T6130730	398	55	Not Evaluated	29
45	ATAD2	Enamine	T7022384	200	57	Not Evaluated	24
46	ATAD2	Enamine	T6012391	504	58	Not Evaluated	23
47	ATAD2	Enamine	T5740325	481	58	Not Evaluated	23
48	ATAD2	Enamine	T6153138	50	59	Not Evaluated	25
49	ATAD2	ChemDiv	e465-0641	133	59	Not Evaluated	25
50	ATAD2	ChemDiv	e465-0503	150	60	Not Evaluated	26
51	ATAD2	ChemDiv	j016-0086	350	61	Not Evaluated	24
52	ATAD2	Enamine	T6611114	200	62	Not Evaluated	25
53	ATAD2	Enamine	T6537283	430	63	Not Evaluated	24
54	ATAD2	ChemDiv	g805-0567	504	63	Not Evaluated	26
55	ATAD2	Enamine	T6380095	415	65	Not Evaluated	23
56	ATAD2	ChemDiv	p041-1724	100	65	Not Evaluated	28
57	ATAD2	Enamine	T6561246	504	66	Not Evaluated	22
58	ATAD2	Enamine	Z749560420	425	66	Not Evaluated	23
59	ATAD2	Enamine	Z818987068	350	66	Not Evaluated	19
60	ATAD2	Life Chem	F5834-3747	503	67	Not Evaluated	24
61	ATAD2	Life Chem	F6350-0082	100	67	Not Evaluated	23
62	ATAD2	Enamine	T5718402	50	67	Not Evaluated	22
63	ATAD2	Life Chem	F2487-0218	503	68	Not Evaluated	19
64	ATAD2	Life Chem	F2145-0396	503	68	Not Evaluated	20
65	ATAD2	Enamine	T5787308	200	69	Not Evaluated	26
66	ATAD2	Enamine	T6646435	416	69	Not Evaluated	26
67	ATAD2	Enamine	T6348957	100	69	Not Evaluated	21
68	ATAD2	Enamine	T6776139	350	69	Not Evaluated	27
69	ATAD2	ChemDiv	k906-3851	200	70	Not Evaluated	24
70	ATAD2	ChemDiv	L347-0193	332	70	Not Evaluated	28
71	ATAD2	Life Chem	F2688-0076	504	71	Not Evaluated	24
72	ATAD2	Enamine	T6551397	503	71	Not Evaluated	21
73	ATAD2	Enamine	T6630026	503	71	Not Evaluated	16
74	ATAD2	Enamine	T6131977	532	72	Not Evaluated	26

75	ATAD2	Enamine	T6718420	467	72	Not Evaluated	22
76	ATAD2	ChemDiv	e245-0412	370	73	Not Evaluated	23
77	ATAD2	ChemDiv	e511-0114	200	73	Not Evaluated	28
78	ATAD2	Enamine	T5946915	410	73	Not Evaluated	27
79	ATAD2	Enamine	T5275295	100	74	Not Evaluated	26
80	ATAD2	Enamine	T6913629	504	74	Not Evaluated	22
81	ATAD2	Enamine	T6666547	463	76	Not Evaluated	27
82	ATAD2	Enamine	T6566814	504	76	Not Evaluated	18
83	ATAD2	ChemDiv	k786-8251	127	76	Not Evaluated	24
84	ATAD2	Enamine	Z434087574	452	77	Not Evaluated	24
85	ATAD2	Life Chem	F6350-0206	503	77	Not Evaluated	17
86	ATAD2	ChemDiv	e667-1070	401	79	Not Evaluated	28
87	ATAD2	ChemDiv	d479-0280	503	80	Not Evaluated	20
88	ATAD2	Enamine	T6221649	469	80	Not Evaluated	29
89	ATAD2	Enamine	T6783260	422	81	Not Evaluated	25
90	ATAD2	Enamine	T6302427	503	81	Not Evaluated	24
91	ATAD2	ChemDiv	c209-0350	265	81	Not Evaluated	24
92	ATAD2	Enamine	T6584114	504	83	Not Evaluated	23
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94	ATAD2	Enamine	T6583582	473	84	Not Evaluated	25
95	ATAD2	Enamine	T6506747	504	84	Not Evaluated	23
96	ATAD2	Enamine	T5713602	504	85	Not Evaluated	21
97	ATAD2	Enamine	T6471416	476	85	Not Evaluated	23
98	ATAD2	ChemDiv	e511-0324	401	85	Not Evaluated	28
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100	ATAD2	Enamine	T6847905	503	86	Not Evaluated	20
101	ATAD2	ChemDiv	6865-4077	148	87	Not Evaluated	21
102	ATAD2	Enamine	T6997824	478	88	Not Evaluated	23
103	ATAD2	Life Chem	F1838-1766	503	89	Not Evaluated	25
104	ATAD2	ChemDiv	L553-1646	50	89	Not Evaluated	30
105	ATAD2	ChemDiv	e245-0420	247	89	Not Evaluated	22
106	ATAD2	Life Chem	F5142-0437	350	89	Not Evaluated	22
107	ATAD2	Enamine	T6312803	503	89	Not Evaluated	19
108	ATAD2	Enamine	T6323732	409	90	Not Evaluated	29
109	ATAD2	ChemDiv	e465-0643	425	90	Not Evaluated	21
110	ATAD2	ChemDiv	e667-1162	504	91	Not Evaluated	28
111	ATAD2	ChemDiv	e511-1404	130	92	Not Evaluated	25
112	ATAD2	Enamine	T6786646	350	92	Not Evaluated	25
113	ATAD2	Enamine	T6901093	503	92	Not Evaluated	21
114	ATAD2	Enamine	T6524872	150	92	Not Evaluated	23
115	ATAD2	ChemDiv	e245-0086	461	93	Not Evaluated	19

116	ATAD2	Enamine	T6931358	100	93	Not Evaluated	19
117	ATAD2	Enamine	T6913080	200	94	Not Evaluated	26
118	ATAD2	Enamine	T5820836	504	94	Not Evaluated	23
119	ATAD2	ChemDiv	c205-0146	302	94	Not Evaluated	21
120	ATAD2	ChemDiv	e465-0733	504	95	Not Evaluated	24
121	ATAD2	ChemDiv	e465-0587	200	96	Not Evaluated	27
122	ATAD2	Enamine	T6642712	200	96	Not Evaluated	27
123	ATAD2	Enamine	T6386275	360	96	Not Evaluated	25
124	ATAD2	Enamine	T6971525	50	96	Not Evaluated	23
125	ATAD2	Enamine	T6971778	504	97	Not Evaluated	18
126	ATAD2	Life Chem	F6350-0211	200	98	Not Evaluated	22
127	ATAD2	Enamine	T5950805	504	98	Not Evaluated	26
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129	ATAD2	Enamine	Z812826508	462	99	Not Evaluated	25
130	ATAD2	Life Chem	F2688-0093	504	100	Not Evaluated	28
131	ATAD2	Life Chem	F0417-1543	50	101	Not Evaluated	23
132	ATAD2	Life Chem	F0862-0087	502	101	Not Evaluated	18
133	ATAD2	ChemDiv	g938-0141	200	101	Not Evaluated	29
134	ATAD2	Enamine	T6791666	200	102	Not Evaluated	25
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143	ATAD2	Life Chem	F5094-0286	504	108	Not Evaluated	24
144	ATAD2	ChemDiv	e511-0280	342	109	Not Evaluated	27
145	ATAD2	ChemDiv	d437-0225	50	110	Not Evaluated	24
146	ATAD2	ChemDiv	e667-1084	200	112	Not Evaluated	26
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148	ATAD2	Enamine	Z1275600959	504	114	Not Evaluated	23
149	ATAD2	ChemBridge	96992714	144	118	Not Evaluated	25
150	ATAD2	ChemDiv	e511-0552	200	119	Not Evaluated	26
151	ATAD2	Life Chem	F2487-0355	350	121	Not Evaluated	25
152	ATAD2	ChemDiv	k786-6644	145	122	Not Evaluated	23
153	ATAD2	ChemDiv	k786-5006	430	122	Not Evaluated	23
154	ATAD2	Enamine	T6940994	384	128	Not Evaluated	26
155	BAZ2A	Life Chem	F2833-0189	500	52	Not Evaluated	17
156	BAZ2A	Life Chem	F3296-0443	100	100	Not Evaluated	19

157	BAZ2A	Life Chem	F3309-0741	190	78	Not Evaluated	30
158	BAZ2A	Life Chem	F5959-0116	120	91	Not Evaluated	21
159	BAZ2A	Life Chem	F6021-1860	100	96	Not Evaluated	22
160	BAZ2A	Enamine	T5344099	280	88	Not Evaluated	26
161	BAZ2A	Enamine	T5550503	200	69	Not Evaluated	18
162	BAZ2A	Enamine	T5817038	150	93	Not Evaluated	23
163	BAZ2A	Enamine	T5830455	250	87	Not Evaluated	20
164	BAZ2A	Enamine	T5844783	200	93	Not Evaluated	26
165	BAZ2A	Enamine	T6136508	230	90	Not Evaluated	20
166	BAZ2A	Enamine	T6149976	50	96	Not Evaluated	21
167	BAZ2A	Enamine	T6361888	240	100	Not Evaluated	22
168	BAZ2A	Enamine	Z1451206848	220	87	Not Evaluated	22
169	BAZ2A	Enamine	Z57009636	240	74	Not Evaluated	23
170	BAZ2A	ChemDiv	1488-1629	80	97	Not Evaluated	24
171	BAZ2A	ChemDiv	1711-1374	200	100	Not Evaluated	21
172	BAZ2A	ChemDiv	3049-0070	80	100	Not Evaluated	21
173	BAZ2A	ChemDiv	D221-0093	100	91	Not Evaluated	17
174	BAZ2A	ChemDiv	D416-0430	330	95	Not Evaluated	17
175	BAZ2A	ChemDiv	G008-1537	200	100	Not Evaluated	25
176	BAZ2A	ChemDiv	J015-0004	290	57	Not Evaluated	20
177	BAZ2A	ChemDiv	m030-0196	170	77	Not Evaluated	24
178	BAZ2A	ChemDiv	P029-0047	50	92	Not Evaluated	17
179	BAZ2A	ChemBridge	58738461	170	88	Not Evaluated	26
180	BAZ2A	ChemBridge	80931327	280	79	Not Evaluated	20
181	BAZ2A	ChemBridge	89912227	280	92	Not Evaluated	22
182	BAZ2A	ChemBridge	92117250	100	79	Not Evaluated	24
183	BAZ2A	ChemBridge	99620140	50	97	Not Evaluated	23
184	BAZ2B	Enamine	T5920293	50	65	Not Evaluated	26
185	BAZ2B	Enamine	T6281001	50	67	Not Evaluated	24
186	BAZ2B	Enamine	T6402776	190	63	Not Evaluated	19
187	BAZ2B	Enamine	T6515391	200	51	Not Evaluated	30
188	BAZ2B	Enamine	T6629993	50	75	Not Evaluated	26
189	BAZ2B	Enamine	T6648477	50	70	Not Evaluated	25
190	BAZ2B	Enamine	T6667014	180	70	Not Evaluated	26
191	BAZ2B	Enamine	T6996555	200	89	Not Evaluated	23
192	BAZ2B	Enamine	T7030147	240	67	Not Evaluated	25
193	BAZ2B	Enamine	Z222977452	230	65	Not Evaluated	21
194	BAZ2B	Enamine	Z647682662	50	70	Not Evaluated	25
195	BAZ2B	ChemDiv	8016-6500	100	74	Not Evaluated	24
196	BAZ2B	ChemDiv	c176-0448	100	100	Not Evaluated	22
197	BAZ2B	ChemDiv	c280-1087	50	90	Not Evaluated	24

198	BAZ2B	ChemDiv	e570-2241	50	89	Not Evaluated	29
199	BAZ2B	ChemDiv	L228-0600	230	64	Not Evaluated	24
200	BAZ2B	ChemDiv	p181-0836	50	82	Not Evaluated	25
201	BAZ2B	ChemDiv	p634-0351	190	71	Not Evaluated	30
202	BAZ2B	ChemBridge	50508712	100	74	Not Evaluated	22
203	BAZ2B	ChemBridge	53864409	200	89	Not Evaluated	22
204	BRD4(1)	IBScreen	STOCK1N-00949	200	95	Not Evaluated	21
205	BRD4(1)	Life Chem	F1016-0301	201	103	Not Evaluated	18
206	BRD4(1)	Life Chem	F1065-0396	201	108	Not Evaluated	27
207	BRD4(1)	Life Chem	F1736-0124	200	69	Not Evaluated	19
208	BRD4(1)	Life Chem	F3316-0138	200	106	Not Evaluated	19
209	BRD4(1)	Enamine	T5447902	201	93	Not Evaluated	19
210	BRD4(1)	Enamine	T5551560	201	48	Not Evaluated	25
211	BRD4(1)	Enamine	T5743717	100	95	Not Evaluated	20
212	BRD4(1)	Enamine	T5839262	201	116	Not Evaluated	22
213	BRD4(1)	Enamine	T5920017	200	84	Not Evaluated	19
214	BRD4(1)	Enamine	T6013245	201	101	Not Evaluated	18
215	BRD4(1)	Enamine	T6023829	201	114	Not Evaluated	21
216	BRD4(1)	Enamine	T6254506	50	114	Not Evaluated	18
217	BRD4(1)	Enamine	T6332725	201	108	Not Evaluated	20
218	BRD4(1)	Enamine	T6406520	201	66	Not Evaluated	28
219	BRD4(1)	Enamine	T6567836	100	97	Not Evaluated	22
220	BRD4(1)	Enamine	T6572366	201	107	Not Evaluated	22
221	BRD4(1)	Enamine	T6673024	201	80	Not Evaluated	28
222	BRD4(1)	Enamine	T6851965	201	97	Not Evaluated	24
223	BRD4(1)	Enamine	T6887081	201	76	Not Evaluated	24
224	BRD4(1)	Enamine	T6910403	201	65	Not Evaluated	25
225	BRD4(1)	ChemDiv	3993-2206	200	79	Not Evaluated	25
226	BRD4(1)	ChemDiv	4507-0165	201	75	Not Evaluated	26
227	BRD4(1)	ChemDiv	5941-1280	201	115	Not Evaluated	21
228	BRD4(1)	ChemDiv	c202-3849	150	86	Not Evaluated	22
229	BRD4(1)	ChemDiv	d319-0671	200	102	Not Evaluated	16
230	BRD4(1)	ChemDiv	d718-1640	100	87	Not Evaluated	24
231	BRD4(1)	ChemDiv	e922-1685	201	106	Not Evaluated	28
232	BRD4(1)	ChemDiv	g805-0501	201	43	Not Evaluated	26
233	BRD4(1)	ChemBridge	19472033	201	59	Not Evaluated	24
234	BRD4(1)	ChemBridge	36076738	200	46	Not Evaluated	21
235	BRD4(1)	ChemBridge	40759875	201	85	Not Evaluated	25
236	BRD4(1)	ChemBridge	81557742	201	104	Not Evaluated	27
237	BRD4(1)	ChemBridge	89859923	201	109	Not Evaluated	24
238	CREBBP	Life Chemicals	F2227-0245	15	78	Not Evaluated	34

239	CREBBP	Life Chemicals	F5115-0065	61	109	Not Evaluated	25
240	CREBBP	Enamine	T5272194	200	112	Not Evaluated	23
241	CREBBP	Enamine	T5348117	50	105	Not Evaluated	21
242	CREBBP	Enamine	T5718196	200	73	Not Evaluated	26
243	CREBBP	Enamine	T6391914	483	101	Not Evaluated	25
244	CREBBP	Enamine	T6417299	351	120	Not Evaluated	21
245	CREBBP	Enamine	T6513277	383	92	Not Evaluated	25
246	CREBBP	Enamine	T6517118	200	109	Not Evaluated	22
247	CREBBP	Enamine	T6535493	200	109	Not Evaluated	29
248	CREBBP	Enamine	T6537565	75	96	Not Evaluated	24
249	CREBBP	Enamine	T6671747	503	101	Not Evaluated	20
250	CREBBP	Enamine	T6740924	100	96	Not Evaluated	20
251	CREBBP	Enamine	T6754606	28	103	Not Evaluated	26
252	CREBBP	Enamine	T6806811	848	100	Not Evaluated	20
253	CREBBP	Enamine	T6869299	608	116	Not Evaluated	19
254	CREBBP	Enamine	T6984532	347	100	Not Evaluated	24
255	CREBBP	Enamine	T6994049	430	91	Not Evaluated	20
256	CREBBP	Enamine	Z1508720959	363	81	Not Evaluated	27
257	CREBBP	ChemDiv	4025-0104	242	100	Not Evaluated	26
258	CREBBP	ChemDiv	d370-0066	504	98	Not Evaluated	17
259	CREBBP	ChemDiv	d386-1090	505	74	Not Evaluated	22
260	CREBBP	ChemBridge	82196858	503	84	Not Evaluated	25

Table S5. Docking data. All energy values are in kcal/mol. Compounds are sorted as in Table S3.

Cpd	Electrost. Diff.	Total Eff.	Total Energy	Smiles
1	2.7	-1.1	-27.5	c1(=O)n(c2c(n1C)cc(c(S(=O)(=O)NCc1ccc(F)cc1)c2)C)C
2	0.9	-1.3	-21.4	N1=C(/C(=C/c2cc(c(cc2)O)OC)/SC1=O)N
3	-2.0	-0.9	-19.5	c1(nc(c(s1)C)C)NC(=O)CCCOc1ccc(cc1)C
4	-1.6	-0.8	-17.8	c1(nc(cs1)c1cc2NC(=O)COc2cc1)N1CCCCC1
5	-1.3	-0.9	-22.2	[C@H]1(Oc2c(O[C@H]1C)cccc2)C(=O)Nc1cc2NC(=O)[C@@H](Oc2cc1)C
6	-1.4	-1.2	-28.6	c12c([C@@H](CC(=O)N1)c1ccc(cc1)CC)cc1c(c2)OCCO1
7	0.4	-1.1	-27.8	S(=O)(=O)(c1cc2NC(=O)COc2cc1C)Nc1c2c(ccc1)CCCC2
8	-1.7	-1.3	-26.2	[C@@H]1([C@@H](C1)c1ccc(cc1)F)C(=O)Nc1ncccc1O
9	1.4	-1.1	-28.1	n1n(c(=O)ccc1c1ccccc1)CCNC(=O)[C@@H]1NC(=O)CNC1
10	-0.9	-0.9	-22.0	N1(C(=O)c2ccc(N(CCCC)C)cc2)c2c(NC(=O)C1)cccc2
11	-0.3	-1.0	-25.8	N1(C(=O)c2ccc(OC[C@@H]3OCCC3)cc2)c2c(NC(=O)C1)cccc2
12	-2.4	-0.8	-19.5	S(=O)(=O)(N1[C@@H](c2n(CC1)ccc2)C)c1cc2NC(=O)COc2cc1
13	2.6	-1.2	-32.0	S(=O)(=O)(N1[C@H](C(=O)Nc2c3c(nn2C)CCC3)CCC1)c1ccc(cc1)F
14	-0.3	-1.0	-17.2	c1(c(onc1C)C)CC(=O)Nc1nccc(c1)C

15	0.4	-1.1	-31.6	c1(c(n(nc1C)c1ccccc1)C)C(=O)C(=O)N1c2c(NC(=O)C1)cccc2
16	0.9	-1.1	-28.3	c1(c(ncc(c1)NC(=O)CC)N1CCC([NH+]2CCCCC2)CC1)C(=O)[O-]
17	0.4	-1.1	-22.0	S(=O)(=O)(c1sccc1)N(CC(=O)Nc1ncc(s1)C)C
18	-0.7	-1.6	-39.1	c1(n(c2ccc(cc2)F)ccn1)SCC(=O)Nc1c(cc(cc1)C)C
19	11.2	-1.2	-32.2	N1c2c(OCC1=O)cc(C(=O)NC[C@H]([N@@H+]1CC[C@@H](CC1)C)c1sccc1)cc2
20	-1.1	-1.3	-26.3	N1(C(=O)c2c(ccc(c2)Br)Cl)c2c(NC(=O)C1)cccc2
21	-1.7	-0.8	-18.8	[C@H]1(c2oc(cc2)CN(C(=O)C2=NNC(=O)CC2)C2CC2)C[C@@H]1C
22	-0.3	-1.1	-27.7	N1(C(=O)[C@H](N2[C@H](c3n(ccc3)C)CCC2)C)c2c(NC(=O)C1)cccc2
23	0.0	-0.9	-20.1	c1(C(=O)Nc2cc3NC(=O)[C@@H](Oc3cc2)C)c(cc(cc1)F)F
24	-0.3	-0.9	-23.2	S(=O)(=O)(c1c(c(c2oc(nn2)C2CC2)[nH]c1C)C)Nc1cc(Cl)ccc1
25	-0.5	-1.1	-27.0	c1(C(=O)N(CC(=O)Nc2nccc(c2)C)C)nc2c(nc1)cccc2
26	2.3	-1.0	-20.2	C(=O)(Nc1nccc(c1)C)c1cc(C[S@@](=O)C)ccc1
27	0.1	-1.0	-30.3	N1(c2c(cc(NC(=O)c3cc(NC(=O)c4occc4)c(cc3)C)cc2)CC1)C(=O)C
28	2.1	-1.3	-25.9	C\1(=C\c2cc(c(cc2)O)O)/C(=O)c2c(O1)cc(cc2)O
29	-0.1	-1.2	-28.6	N1(C(=O)[C@H](N2Cc3c(scc3)CC2)C)c2c(NC(=O)C1)cccc2
30	-0.3	-1.6	-35.7	c1(c2c(nn1C)CCC2)NC(=O)CSc1ccc(cc1)OC
31	-0.2	-1.1	-25.0	c1(sc(cc1)C(=O)C)C(=O)N1CC=C(CC1)c1ccccc1
32	-0.1	-1.0	-22.4	c1(nc(c(s1)C)C)NC(=O)CCCS(=O)(=O)c1ccc(cc1)C
33	1.5	-1.2	-27.5	c1(c(c2c(s1)CCC2)C(=O)N)NC(=O)[C@H](N1C[C@@H](OCC1)C)C
34	-1.4	-1.3	-25.5	[C@@]1(C(C1)(Cl)Cl)(C(=O)N1c2c(NC(=O)C1)cccc2)C
35	-0.8	-0.5	-15.5	N1(C(=O)C[C@@H](C(=O)Nc2cc3NC(=O)[C@@H](Oc3cc2)C)C1)Cc1ccc(cc1)C
36	-6.6	-1.4	-33.1	N1C(=O)[C@@H](Sc2c1cc(C(=O)N[C@H](C[NH+](C)C)CC(C)C)cc2)C
37	-0.3	-1.0	-23.0	c12c(NC(=O)C[C@H]1c1c(F)cccc1)cc1c(c2)OCCO1
38	-1.0	-1.3	-27.8	c12c(NC(=O)C[C@H]1c1ccc(cc1)F)cc1c(c2)CCC1
39	4.2	-1.1	-30.3	N1(C(=O)C=C([C@H]1O)NCCc1c2c([nH]c1)ccc(c2)Cl)c1ccc([N+](=O)[O-])cc1
40	-5.2	-1.1	-28.2	C(=O)(N(Cc1oc(cc1)C)CC[NH+](C)C)c1cc2NC(=O)COc2cc1
41	-0.1	-1.1	-28.4	N1(C(=O)CN(Cc2cc(c(cc2)OC)F)CC)c2c(NC(=O)C1)cccc2
42	-0.1	-0.9	-25.4	N1(C(=O)[C@@H](N(Cc2c(N3CCCC3)cccc2)C)C)c2c(NC(=O)C1)cccc2
43	2.5	-1.3	-33.6	N1(C(=O)CN2[C@@H](Cn3ncnc3)CCC2)c2c(NC(=O)C1)cccc2
44	-5.5	-0.9	-25.9	N1C(=O)[C@@H](Sc2c1cc(C(=O)N(CC(=O)Nc1c(F)cccc1F)CC)cc2)C
45	-1.6	-1.1	-27.3	c1(nc(cs1)CN1C[C@H](N(Cc2n(ccn2)C)CC1)C)NC(=O)C
46	-2.1	-0.7	-16.3	N1(C(=O)c2cc3NC(=O)COc3cc2)[C@@H](Cc2c1cccc2)C
47	-1.5	-1.1	-24.1	c1(C(=O)Nc2cc3NC(=O)[C@@H](Oc3cc2)C)c(c(Cl)ccc1)Cl
48	-5.3	-0.7	-17.1	S(=O)(=O)(c1cc2NC(=O)COc2cc1)N[C@@H]1CC[C@@H](C(F)(F)F)CC1
49	-2.8	-1.1	-28.0	S(=O)(=O)(c1cc2NC(=O)[C@H](Sc2cc1)C)Nc1ccc(cc1)C(C)C
50	-3.1	-1.2	-29.9	S(=O)(=O)(c1cc2NC(=O)[C@H](Sc2cc1)C)Nc1cc(c(cc1)OC)OC
51	-0.1	-0.9	-21.6	n1(c2c(OCC(=O)Nc3nccc(c3)C)ccc(c2)C)cnnc1
52	-1.8	-0.9	-22.2	N1c2c(OCC1=O)cc(C(=O)NCCc1cc3c(OCO3)cc1)cc2
53	-3.5	-0.6	-14.9	c1(nc(NC(=O)C)sc1)C(=O)N1C[C@H](c2ccc(cc2)F)OCC1
54	-1.7	-0.8	-19.4	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1C)NCc1ccc(cc1)C(C)C
55	-1.3	-0.9	-21.3	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1Br)N[C@@H](CCC(C)C)C
56	-1.0	-1.0	-26.5	N1(N=C(C(=O)Nc2ccc(F)cc2)CCC1=O)CC(=O)Nc1ccc(Cl)cc1

57	-1.5	-1.3	-28.4	c1(nc(NC(=O)C)sc1)C(=O)N[C@@H](C1CC1)c1ccccc1
58	-1.3	-1.0	-22.0	c1(C(=O)N([C@@H]2[C@H]3C[C@H]4C[C@@H]2C[C@@H](C3)C4)C)nc(NC(=O)C)sc1
59	-2.2	-1.4	-26.5	c1(nc(c(s1)C)C)NC(=O)[C@@H]1[C@H](C1)c1ccccc1
60	-0.2	-0.9	-21.1	S(=O)(=O)(N1Cc2c(CC1)ccc(NC(=O)c1oncc1)c2)CCC
61	-2.4	-0.9	-21.4	N1[C@@H](C(=O)NCCc2cc(c(cc2)OC)OC)CSCCC1=O
62	-2.7	-1.0	-22.6	N1c2cc(C(=O)COc3c(Cl)cccc3)ccc2OCC1=O
63	-1.1	-1.2	-22.9	N1(C(=O)c2sc(cc2)Br)c2c(NC(=O)C1)cccc2
64	-6.1	-1.4	-28.3	N1c2cc(C(=O)CN3CC[NH2+]CC3)ccc2OCC1=O
65	-3.6	-0.7	-18.0	N1C(=O)[C@@H](Sc2c1cc(C(=O)Nc1cc(c(cc1C)OC)OC)cc2)C
66	-1.7	-0.7	-18.5	N1(C(=O)COc2c1cccc2)CCC(=O)NC1(CC1)c1ccc(cc1)Br
67	1.4	-1.2	-25.4	N1C(=O)[C@H](Sc2c1cc(cc2)Cl)CC(=O)N[C@@H](COC)C
68	-0.6	-0.9	-23.6	N1(c2c(NC(=O)C1)cccc2)C(=O)CCCNC(=O)c1c(cc(cc1)F)F
69	-2.4	-0.8	-18.4	S(=O)(=O)(N1c2c(CC1)cccc2)c1cc2NC(=O)[C@H](Sc2cc1)C
70	-6.4	-0.9	-25.9	c1(c(ncc(NC(=O)c2sccc2)c1)N1CC[NH2+]CC1)C(=O)N(CCCC)C
71	2.6	-1.1	-26.5	c1(c(NC(=O)[C@@H](c2ccccc2)CC)c2c(o1)cccc2)C(=O)N
72	-0.5	-0.9	-17.9	N1c2c(OCC1=O)cc(C(=O)N[C@H]([C@@H]1OCCC1)C)cc2
73	-0.5	-1.1	-18.0	c1(NC(=O)[C@@H]2CNC(=O)CC2)ncc(s1)C
74	-0.4	-0.5	-14.1	N1(C(=O)COc2c1cccc2)CCC(=O)N(Cc1c(c(Cl)ccc1)Cl)C
75	1.1	-1.1	-23.6	N1(C(=O)CCC1)CC(=O)N(CC(=O)Nc1ccc(Cl)cc1)C
76	-1.3	-1.0	-22.6	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1C)N[C@H]1CC[C@@H](CC1)C
77	-1.4	-0.8	-23.1	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1C)CCC(=O)NCCc1ccccc1
78	-1.9	-1.0	-28.0	S(=O)(=O)(c1cn(c(=O)cc1)CC(=O)Nc1cc(c(cc1)F)F)N1CCCC1
79	-0.6	-1.0	-26.5	N1(c2c(NC(=O)C1)cccc2)C(=O)CSc1c2c(sc(c2)CC)ncn1
80	-3.9	-0.8	-18.4	N1C(=O)[C@@H](Sc2c1cc(C(=O)N1CC[C@@H](CCC1)C)cc2)C
81	-2.1	-0.9	-24.1	N1(C(=O)COc2c1cccc2)CCC(=O)NCc1cnc(OC(C)C)cc1
82	-1.1	-1.4	-24.5	c1(C(=O)N2[C@@H](COCC2)C)nc(NC(=O)C)sc1
83	-1.9	-0.8	-19.0	N1=C(CCC(=O)N1CCC(=O)NC1CCCCC1)c1ccccc1
84	-0.9	-0.8	-19.4	n1(nc(c(c1C)CNC(=O)[C@@H]1CNC(=O)CC1)C)c1ccccc1
85	-1.7	-1.1	-18.7	C(=O)([C@@H]1NC(=O)CCSC1)N[C@@H]1C(=O)SCC1
86	-6.4	-0.8	-22.5	S(=O)(=O)(c1cc2NC(=O)COc2cc1)[C@H](CC(=O)Nc1c(c(ccc1)C)C)C
87	-1.1	-1.3	-25.6	N1(C(=O)c2c(C)cccc2)c2c(NC(=O)C1)cccc2
88	1.6	-1.0	-29.2	N1C(=O)[C@H](Oc2c1cccc2)CC(=O)NCc1ccc(CN2CCOCC2)cc1
89	-0.2	-0.7	-18.4	N1(C(=O)COc2c1cccc2)CC(=O)N[C@H](c1ccc(cc1)Br)CC
90	-0.9	-0.9	-20.3	N1(C(=O)c2cc3c(NC(=O)CO3)cc2)[C@H](c2ccncc2)CCC1
91	-1.5	-0.3	-7.7	N1[C@H](C(=O)Nc2c1ccc(C(=O)N1CCN(CC1)C)c2)[C@H](CC)C
92	-1.7	-1.1	-25.0	C(=O)(N(C1CC1)C[C@@H]1COCC1)c1cc2c(NC(=O)CO2)cc1
93	-3.6	-0.9	-18.9	S(=O)(=O)(c1cc2NC(=O)COc2cc1)NCCSC(F)(F)F
94	-1.7	-0.9	-22.3	c1(nc(cs1)CN(Cc1c(N2CCCCC2)cccc1)C)NC(=O)C
95	3.0	-1.2	-28.5	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1Cl)N([C@H](COC)C)CC
96	1.2	-1.3	-27.8	C(=O)(c1ccc(cc1)Br)NCCC(=O)Nc1cnccc1
97	-1.7	-0.9	-21.6	N1(C(=O)COc2c1cccc2)CC(=O)NCCC1=CCCCC1

98	-6.3	-0.9	-23.9	S(=O)(=O)(c1cc2NC(=O)COc2cc1)CCC(=O)Nc1ccc(cc1)OCC
99	-2.5	-1.3	-22.8	N1C(=O)[C@@H](Sc2c1cc(C(=O)N(C)C)cc2)C
100	-2.2	-1.1	-22.9	C(=O)([C@@H]1CNC(=O)CC1)N[C@@H](Cc1c(C)cccc1)C
101	1.9	-1.0	-21.5	c1(=O)n(c2c(n1C)cccc2)CC(=O)Nc1cnccc1
102	-1.8	-1.0	-21.9	[C@H](c1sccc1)(N1CCOCC1)CNC(=O)[C@@H]1CNC(=O)CC1
103	-5.2	-0.8	-20.9	c1(sc(nn1)SCC(=O)Nc1ccc(OC(F)(F)F)cc1)NC(=O)C
104	-0.6	-0.9	-25.8	c1(c2c(nc(n1)CCC(=O)Nc1cc(cc(c1)C)C)onc2C)N1CCCCCC1
105	-1.3	-0.9	-20.1	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1C)NCc1sccc1
106	1.0	-1.3	-27.5	N1(C(=O)[C@H]2N(S(=O)(=O)C)CCC2)c2c(NC(=O)C1)cccc2
107	0.0	-1.1	-21.4	c1(=O)n(c2c(o1)cc(cc2)Cl)CCC(=O)N1CCC1
108	-3.7	-0.8	-22.5	S(=O)(=O)(N(c1cc(ccc1)C)Cc1ccccc1)c1cc2NC(=O)COc2cc1
109	-4.5	-1.0	-21.9	S(=O)(=O)(c1cc2NC(=O)[C@H](Sc2cc1)C)NC(CC)(C)C
110	-7.2	-1.0	-28.1	S(=O)(=O)(c1cc2NC(=O)COc2cc1)[C@H](CC(=O)Nc1cc(c(cc1)C)F)C
111	-5.7	-1.0	-24.6	S(=O)(=O)(c1cc2NC(=O)[C@H](Sc2cc1)C)CCC(=O)NCCCOC
112	-2.3	-1.0	-24.7	N1(C(=O)COc2c1cccc2)CCC(=O)N[C@H](c1c(oc(c1)C)C)C
113	-1.3	-0.9	-19.5	N1(C(=O)[C@@H]2CNC(=O)CC2)[C@H](c2cc(ccc2)C)CCC1
114	-1.1	-1.3	-30.5	N1(C(=O)CNc2cc3c(NC(=O)CO3)cc2Cl)C[C@H](CCC1)C
115	-1.9	-1.1	-21.4	S(=O)(=O)(c1cc2NC(=O)COc2cc1)N1CCCC1
116	4.2	-1.3	-24.7	N1=C(C(=O)N[C@@H]2CC[N@H+](CC2)CCC)CCC(=O)N1
117	-1.6	-1.1	-29.1	n1c(noc1CNc1cc2c(NC(=O)CO2)cc1Cl)c1c(C)cccc1
118	-0.5	-1.1	-24.6	N1c2cc(C(=O)COc3cc(ccc3Cl)Cl)ccc2OCC1=O
119	-0.1	-0.8	-17.1	N1(c2c(OCC1=O)ccc(c2)C)[C@@H](C(=O)N[C@H](CC)C)C
120	-4.3	-0.9	-22.5	S(=O)(=O)(c1cc2NC(=O)[C@H](Sc2cc1)C)NCc1ccc(Cl)cc1
121	-4.6	-1.0	-27.6	S(=O)(=O)(N1CCN(CC1)C1CCCCC1)c1cc2NC(=O)[C@H](Sc2cc1)C
122	-6.9	-1.0	-27.4	N1C(=O)[C@@H](Sc2c1cc(C(=O)NCCC(=O)NCc1cnccc1)cc2)C
123	-4.0	-0.7	-17.5	S(=O)(=O)(c1cc2NC(=O)COc2cc1)NCC1(CC1)c1ccccc1
124	-0.2	-0.7	-15.5	c1(NC(=O)[C@@H]2CNC(=O)CC2)nc(cs1)CN1CC[C@H](CC1)C
125	5.4	-1.4	-25.2	N1=C(C(=O)NC[C@@H]2[N@H+](CCC2)CC)CCC(=O)N1
126	-0.6	-1.1	-25.0	[C@@H]1(C(=O)N2CC[N@H+](CC2)C2CCCCC2)NC(=O)CCSC1
127	-0.3	-1.1	-27.8	S(=O)(=O)(c1cc(C(=O)N2c3c(NC(=O)C2)cccc3)c(cc1)Cl)N(C)C
128	-1.5	-1.0	-18.4	C(=O)(Nc1nccc(c1)C)Cc1c(cc(cc1)Cl)Cl
129	-1.2	-0.9	-22.3	C(=O)([C@@H]1CNC(=O)CC1)NCC1(c2ccc(cc2)OC)CCOCC1
130	4.4	-1.1	-30.2	c1(c(NC(=O)[C@H]2CN(C(=O)C2)c2ccc(cc2)C)c2c(o1)cccc2)C(=O)N
131	-2.0	-0.9	-21.1	c1(sc(nn1)SCC(=O)N1c2c(CCC1)cccc2)NC(=O)C
132	-1.5	-1.0	-18.5	c1(ncc(s1)Cc1c(cc(cc1)Cl)Cl)NC(=O)C
133	2.7	-1.1	-32.9	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1C)N(CC(=O)Nc1cc(C#N)ccc1)C
134	-3.3	-1.1	-26.6	c1(=O)[nH]c(=O)ccn1CC(=O)N[C@H](c1cc2NC(=O)COc2cc1)C
135	-1.1	-1.0	-21.3	N1=C(C(=O)N2CCN(Cc3cscc3)CC2)CCC(=O)N1
136	-0.4	-1.2	-23.2	n1c(NC(=O)C)scc1c1c(cc(cc1)OC)OC
137	8.8	-1.0	-23.9	N1([C@@H](C(=O)NC(C)C)C[C@H](C1)[NH3+])C(=O)CCN1C(=O)CCCC1
138	-0.9	-0.9	-19.2	c1(sc(nn1)SCc1ccc(C(F)(F)F)cc1)NC(=O)C

139	-0.4	-0.9	-19.6	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1Cl)N1CCCCCC1
140	-0.1	-0.9	-20.4	S(=O)(=O)(N1CCCC1)c1cc(C(=O)Nc2ncc(s2)C)ccc1
141	-1.5	-0.8	-17.6	C(=O)(Nc1cc(c(cc1OC)Cl)OC)c1cc(COC)ccc1
142	-1.3	-0.8	-22.1	c1(nc2c([nH]1)cccc2)[C@@H](NC(=O)C1=NNC(=O)CC1)Cc1ccccc1
143	-0.2	-0.7	-16.9	c1(nc(c(s1)C)c1ccc(cc1)OCC)NC(=O)c1nn(cc1)C
144	-5.6	-0.8	-21.6	S(=O)(=O)(c1cc2NC(=O)COc2cc1)CCC(=O)Nc1ccc(cc1)OC
145	-2.1	-1.0	-23.5	c1(nc(c(s1)C)c1cc2NC(=O)COc2cc1)NC(=O)C(C)(C)C
146	-4.1	-0.8	-21.6	S(=O)(=O)(c1cc2NC(=O)COc2cc1)[C@H](CC(=O)N1CCCCCC1)C
147	-0.3	-0.9	-27.1	N1C(=O)[C@@H](Nc2c1cc(c(c2)C)C)CC(=O)NCCc1cc(c(cc1)OC)OC
148	-1.2	-1.3	-30.6	c1(nc(NC(=O)C)sc1)C(=O)N1CC2(CCC1)CCCCCC2
149	11.5	-1.1	-26.3	N1(c2c(OCC1=O)ccc(c2)C)CC(=O)N1[C@@H](C(=O)NC)C[C@H](C1)[NH3+]
150	-0.4	-1.0	-25.0	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1Cl)CCC(=O)N(CCC)CCC
151	-0.1	-0.9	-23.2	N1(C(=O)c2oc3c(c2)cccc3OCC)c2c(NC(=O)C1)cccc2
152	-1.9	-0.9	-20.5	N1(N=C(CCC1=O)c1ccccc1)CC(=O)NC[C@@H]1OCCC1
153	-1.4	-1.0	-23.7	N1(C(=O)COc2c1cccc2)CCC(=O)NCc1ccccc1
154	-3.1	-1.0	-25.0	S(=O)(=O)(N(c1cc2c(cc1)cccc2)C)c1cc2NC(=O)COc2cc1
155	-5.0	-1.1	-18.4	c1(C(=O)Nc2cc(C(=O)C)ccc2)oncc1
156	2.3	-1.5	-27.9	n1nc2c(s1)ccc(C(=O)Nc1ccc(Br)cc1)c2
157	-3.6	-0.7	-19.9	c1(nc(oc1NCc1cnccc1)c1oc(cc1)COc1ccc(cc1)OC)C#N
158	-2.8	-0.7	-14.9	[C@@]12(C(=O)NCCn3c([nH+]cc3)C)C[C@H]3C[C@@H](C1)C[C@@H](C2)C3
159	-2.7	-0.9	-18.8	c12[nH]c(=O)cc(c1ccc(NC(=O)c1ccccc1)c2)CC
160	-3.0	-0.8	-21.7	n1c(C(=O)NC[C@@H](N2CCOCC2)c2ccc(cc2)OC)ccc(=O)[nH]1
161	-3.8	-1.0	-18.5	S(=O)(=O)(c1cc2[nH]c(=O)[nH]c2cc1)N[C@@H](CC)C
162	2.5	-1.3	-30.6	N1=C(c2cc(OC)ccc2)CS/C(=N/c2cc(OC)ccc2)/N1
163	-4.0	-0.9	-18.8	C(=O)(N1CCC(CC1)C)c1cc2NC(=O)CSc2cc1
164	-3.6	-0.8	-20.7	c1(=O)[nH]c2c([nH]1)ccc(NC(=O)c1cc(c(c(c1)OC)OC)/C=C/C)c2
165	4.0	-1.0	-20.2	S1(=O)(=O)C[C@@H](C(=O)Nc2c3c(ccc2)CCCC3)CC1
166	1.7	-1.4	-29.3	n1c(C(=O)Nc2c3c(ccc2)CCCC3)ccc(=O)n1C
167	12.0	-1.5	-33.4	c1(c(C(=O)N)ccs1)NC(=O)CC[N@@H+](Cc1c(ccs1)C)C
168	0.8	-1.5	-33.2	n1c(C(=O)NCc2cc(c(cc2)O)O)ccc2c1cccc2
169	-0.5	-1.4	-31.3	[C@@H]1(Oc2c(OC1)cccc2)C(=O)NCCc1cc(c(cc1)O)O
170	-4.3	-0.9	-20.7	c1(/c(=N/c2ccc(C(F)(F)F)cc2)/oc2c(c1)cccc2)C(=O)N
171	-3.2	-0.9	-19.3	c1(/c(=N/Cc2ccccc2)/oc2c(c1)cccc2)C(=O)N
172	1.7	-1.2	-25.4	[C@]12(C(=O)[C@@]3(CN([C@@H](N(C1)C3)c1cc(c(cc1)O)O)C2)C)C
173	-3.2	-1.2	-20.7	n12c(sc(n1)c1ccc(cc1)OCC)nnc2
174	-3.0	-1.1	-18.7	c1([nH]c(=O)cc(n1)C)Nc1c(ccc(c1)C)C
175	-2.8	-0.6	-14.4	S(=O)(=O)(Nc1c(ccc(c1)C)C)c1cc2NC(=O)C[C@@H](Sc2cc1)C
176	-3.0	-1.1	-22.7	n1(c2nc(C(=O)Nc3ccccc3)ccc2)cnnc1
177	1.0	-1.2	-28.8	S(=O)(=O)(c1cc2c3c(COc2cc1)cno3)NCc1ccccc1
178	-3.3	-1.2	-19.8	n1c(c2c[nH]c(=O)cc2)noc1c1cscc1
179	-2.7	-0.9	-23.4	c1(c2c([nH]c(=O)c1)cccc2)C(=O)NCc1[nH]c2c(c1)cc(cc2)OC

180	-5.7	-1.2	-23.6	c1(c2c([nH]c(=O)c1)cccc2)C(=O)NCCSCCC
181	-4.4	-0.8	-17.8	n1c(c[nH]c1)CCNC(=O)c1ccc(cc1)CCC(O)(C)C
182	-5.6	-1.0	-24.2	c1(c2c([nH]c(=O)c1)cccc2)C(=O)NCc1sc(nc1C)CCC
183	0.8	-1.3	-29.1	C(=O)(c1c(ccnc1)C)Nc1cc2c(oc(=O)cc2C)cc1C
184	-0.6	-1.1	-29.2	[N+](=O)(c1cc(NC(=O)CN([C@@H](c2cc(c(cc2)F)F)C)C)c(cc1)C)[O-]
185	3.2	-1.2	-28.5	n12c(nnc1CCCCC2)CCNC(=O)Nc1cc(c(cc1)C)Cl
186	2.0	-1.2	-23.0	c1(C(=O)Nc2c(c(C(=O)NC)ccc2)C)cocc1
187	1.2	-1.1	-33.0	c12n(nc(c1c(C(=O)Nc1c(c(C(=O)N)ccc1)C)cc(n2)C1CC1)C)C(C)(C)C
188	1.9	-1.2	-32.2	n12c(nnc1CCCCC2)CNC(=O)c1c(nc2c(c1)cc(cc2)C)C
189	-0.1	-1.1	-28.1	c1(nc(ncc1Cl)N1CCCC1)C(=O)Nc1c(cc(C(=O)N)cc1)C
190	1.7	-1.1	-29.4	n12c(nnc1CCCCC2)CNC(=O)c1cc(c(OC(C)C)cc1)OC
191	-0.3	-1.1	-25.6	[C@@H]1([C@@H](C1)c1cc(ccc1)C)C(=O)Nc1c(c(C(=O)N)ccc1)C
192	0.6	-1.1	-26.9	C(=O)(Nc1c(cc(cc1)OC)C)C(=O)NCc1c(nccc1)OCC
193	-0.1	-1.0	-20.4	C(=O)([C@H]1c2c(NC(=O)C1)cccc2)Nc1c(C)cccc1
194	2.9	-1.1	-27.4	c1(c(=O)[nH]c2c(c1)CCC2)C(=O)NCc1ncc(o1)c1ccccc1
195	1.3	-1.1	-25.7	n1c(noc1C)c1cc(c(NC(=O)c2ccc(cc2)OC)cc1)C
196	1.4	-1.1	-25.1	c1(nc(oc1SC)c1occc1)S(=O)(=O)c1ccc(cc1)Br
197	2.2	-1.2	-29.3	n1(c(nc2c(c1=O)SCC2)SCC(=O)Nc1c(ccc(c1)C)C)C
198	1.7	-1.0	-30.1	S(=O)(=O)(c1cc2c(N([C@H](C2)C)C(=O)C)cc1)NCCC(=O)Nc1c(C)cccc1
199	1.5	-1.1	-25.7	S(=O)(=O)(c1sc(c2oc(nc2)C2CC2)cc1)Nc1c(Cl)cccc1
200	1.0	-1.2	-29.6	c1(nc(no1)c1ccc(cc1)Cl)c1c(NC(=O)c2cocc2)ccs1
201	-0.1	-1.0	-29.7	c1(N2C[C@@H](CCC(=O)Nc3c(cc(cc3)OC)C)CCC2)cc(ncn1)NC1CC1
202	1.0	-1.2	-27.3	c12[C@H](c3c(cc(cc3)OC)C)N(CCc1nc[nH]2)CCCC
203	-0.2	-1.5	-31.9	c12[C@H](c3cc(c(c(c3)OCC)OCC)Cl)NCCc2nc[nH]1
204	9.2	-1.3	-27.6	C(=O)(c1cc(c(cc1)OC)OC)O[C@H]1C[C@@H]2[NH2+][C@H](C1)CC2
205	0.6	-1.8	-33.0	n1(c(nnc1)SCC(=O)Nc1ccc(Br)cc1)C
206	0.9	-1.1	-30.2	N1C(=O)[C@@H](Sc2c1cc(C(F)(F)F)cc2)CC(=O)Nc1c(cc(cc1)C)C
207	-0.1	-1.4	-25.6	o1c(ccc1C)CCC(=O)Nc1c(cc(cc1)C)C
208	1.4	-1.6	-29.8	n1(ncnc1)[C@H](CC(=O)Nc1c(cc(cc1)C)C)C
209	-0.3	-1.5	-27.8	n1(c(=O)scc1C)CC(=O)Nc1c(cc(cc1)C)C
210	1.1	-1.4	-34.7	c1(c(n(c(c1)C)CCc1sccc1)C)C(=O)CSc1n(c(nn1)C)C
211	0.0	-1.9	-37.7	N1=C(C(=O)NCCSc2ccccc2)CCC(=O)N1C
212	-1.8	-1.3	-29.6	c1(n(c(nn1)C)C)S[C@H](C(=O)Nc1ccc(N(C)C)cc1)C
213	-0.4	-1.7	-32.5	N1=C(C(=O)Nc2cc(cc(c2)C)C)CCC(=O)N1C
214	0.6	-1.5	-26.8	N1(C(=O)CSC1)CC(=O)Nc1c(cc(cc1)C)F
215	3.7	-1.3	-26.7	n1c(CC(=O)Nc2c(cc(cc2)C)F)c2c(o1)cccc2
216	0.1	-1.5	-27.4	c1(sc(nn1)NCC(C)C)S[C@H]1C(=O)CCCC1
217	1.9	-1.3	-26.4	[N+](=O)(c1c(c(NC(=O)[C@H]2CN(C(=O)C2)C)ccc1)C)[O-]
218	-0.7	-1.1	-30.3	N1([C@H](C(F)(F)F)CC(=O)Nc2c1cccc2)C(=O)CN(Cc1cn(nc1)C)C
219	0.2	-1.4	-31.8	c12n(nc(s1)NC[C@]1(N3CCOCC3)CCSC1)cc(n2)C
220	-0.1	-1.7	-37.6	S(=O)(=O)(c1ccc(CNC(=O)C2=NN(C(=O)CC2)C)cc1)N

221	13.5	-1.3	-35.9	C(=O)(Nc1c(ccc(c1)C)F)C(=O)NCc1cc(N2CC[NH+](CC2)C)ncc1
222	-1.6	-1.4	-33.8	c1(c(c(nn1C)C)CNCc1n(c(nn1)C)C)Oc1ccccc1
223	11.7	-1.6	-37.6	N1=C(C(=O)NC[C@H]2C[N@@H+](Cc3sccc3)CCC2)CCC(=O)N1C
224	-0.6	-1.4	-34.5	c1(n(c(nn1)C)C)CN1[C@H](c2nnc(o2)CC)Cc2c(C1)cccc2
225	0.4	-1.1	-26.3	c1(nnc(c2c1cccc2)C)N1CCN(c2c(OC)cccc2)CC1
226	2.1	-1.2	-30.3	N1=C(S[C@H](C(=O)Nc2c(cc(cc2)F)F)CC1=O)Nc1ccc(cc1)C
227	1.0	-1.3	-27.1	n1(c(=O)oc2c1cccc2)CC(=O)Nc1ccc(Br)cc1
228	2.1	-1.1	-24.8	c12n(ncc1C(=O)Nc1c(cc(cc1)C)C)c(cc(n2)C)N
229	0.8	-1.8	-28.2	c1(C(=O)Nc2ccc(Br)cc2)c(nns1)C
230	3.1	-1.3	-31.0	c12n([C@H](C(=O)N1)CC(=O)Nc1ccc(cc1)OCC)nc(n2)CC
231	8.9	-1.1	-30.4	c1(c(n(nc1)c1cc(F)ccc1)C1CC[NH2+]CC1)C(=O)NCc1cnccc1
232	2.4	-1.4	-35.8	S(=O)(=O)(c1cc2c(NC(=O)CO2)cc1C)NCCCc1c(onc1C)C
233	17.4	-1.5	-35.6	N1(C(=O)c2c(N(C(=O)C1)C)cccc2)CC(=O)N1CCC(CC1)[NH3+]
234	8.0	-1.5	-30.9	C(=O)(NCc1cc(c(cc1)OC)OCC)[C@H]1[NH2+]CCCC1
235	9.5	-1.3	-33.2	C1(C(=O)NCCc2ncccc2)(Oc2ccc(Cl)cc2)CC[NH2+]CC1
236	11.1	-1.0	-28.1	c1(C(=O)N2[C@@H](c3cnccc3)CCCC2)nnn(c1)CCN1CC[NH2+]CC1
237	3.3	-1.1	-26.9	c1(C(=O)N2CCc3c(=O)[nH][nH]c3CC2)c2c([nH]c(=O)c1)cccc2
238	2.0	-1.1	-38.4	c1(c(c2c(s1)CCCC2)C(=O)OCC)NC(=O)Cn1c(c2nnc(o2)CC)cc2c1cccc2
239	0.9	-1.3	-32.4	c1(c2nnc(o2)CC)cn(c2c1cccc2)CC(=O)N1CCOCC1
240	-1.8	-1.1	-24.4	N1(C(=O)COc2ccc(c3nnco3)cc2)C[C@H](C[C@H](C1)C)C
241	0.0	-1.1	-23.2	c12c(c(cc(=O)o1)CN1CC(=O)NCC1)ccc(c2C)C
242	-0.6	-1.1	-29.8	c1(oc(nn1)c1ccc(cc1)OC)[C@@H](Nc1ccc(NC(=O)C)cc1)C
243	-1.1	-1.3	-32.3	N1(C(=O)c2ncc(nc2)C)[C@H](c2cc3c(OCCCO3)cc2)CCC1
244	0.3	-1.4	-29.4	N(C(=O)c1ncc(nc1)C)[C@H](c1sccc1)C1CCCC1
245	-1.0	-1.1	-27.4	S(=O)(=O)(c1ccc(cc1)OCCOc1ccc(c2nnco2)cc1)N
246	-0.5	-1.0	-22.2	n1c(csc1COc1ccc(cc1)C)CN1CC(=O)NCC1
247	0.0	-1.1	-32.7	S(=O)(=O)(c1c2ncc(cc2ccc1)C)N1CCN(C(=O)c2ncc(nc2)C)CC1
248	-2.5	-1.2	-28.0	c1(C(=O)NCc2c(CN3C(=O)CCC3)cccc2)c(nccn1)N
249	5.7	-1.0	-20.3	S(=O)(=O)(CC(=O)N1CC(=O)NCC1)c1ccc(cc1)C
250	-0.5	-1.4	-28.8	N(C(=O)N)C(=O)CNc1c(CC(=O)N(C)C)cccc1
251	-0.4	-1.4	-35.2	N1(Cc2c(CNC(=O)c3ncc(nc3)C)cccc2)C[C@@H](O[C@@H](C1)C)C
252	-1.4	-1.3	-26.3	C(=O)(c1cc(ncc1)Cl)NCCCN(C(=O)C)C(C)C
253	0.1	-1.5	-28.1	n1(c(nnc1N)SCCCOc1c(C)cccc1)C
254	-1.2	-1.1	-26.3	c1(C(=O)NCc2cc(NC(=O)C3CCC3)ccc2)c(nccn1)N
255	-0.6	-1.4	-27.8	c1(C(=O)NCc2ccc(cc2)[C@@H](O)C)ncc(nc1)C
256	-1.5	-0.9	-23.9	N1([C@H](C(=O)NCCCN2CC(=O)NCC2)c2ccccc2)C(=O)CCCC1
257	-1.0	-1.3	-32.5	n1c(oc2c1nccc2)c1cc(NC(=O)c2c(nccc2)Cl)c(cc1)C
258	-0.7	-1.4	-23.9	c1(c(non1)c1ccc(cc1)Br)NC(=O)CC
259	-2.2	-1.3	-28.9	o1c(nnc1c1ccncc1)S[C@H](C(=O)NCCC(C)C)C
260	-1.5	-1.2	-29.5	n1(nc(c(c1C)CC(=O)NCc1ncc(nc1)C)C)c1ccccc1