

Supplementary Material

Discovery of selective inhibitor leads by targeting an allosteric site in Insulin-Regulated Aminopeptidase

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<div> <div>Rep.</div> <div>2D</div> <div>3D</div> <div>React.</div> <div>Standard</div> <div>Purch.</div> <div>In-Stock</div> <div>pH</div> <div>Ref Mid</div> <div>Charge</div> <div>-2 -1 0 +1 +2</div> <div></div> <div></div> </div>													
Molecular Weight (up to, Daltons)													
LogP (up to)		200	250	300	325	350	375	400	425	450	500	>500	Totals, by LogP
	-1	7,719	6,132	7,451	4,008	3,677	2,632	1,651	1,207	1,054	1,422	2,841	39,794
	0	29,273	21,724	33,586	21,166	21,547	13,000	6,809	4,249	2,871	2,853	2,805	159,883
	1	77,696	88,965	157,807	112,036	115,193	66,828	33,838	20,413	13,093	12,868	6,156	704,893
	2	100,929	187,772	396,402	319,413	231,293	231,825	126,158	82,640	58,856	52,909	16,812	1,805,009
	2.5	35,177	105,806	280,909	250,419	326,514	206,142	128,713	95,823	71,193	65,420	19,493	1,585,609
	3	20,249	84,355	262,517	248,186	377,939	282,752	181,246	141,630	111,534	110,991	35,445	1,856,844
	3.5	8,732	52,427	198,754	218,204	325,910	281,982	215,073	183,732	151,939	160,634	61,553	1,858,940
	4	2,609	24,056	117,310	139,596	234,162	240,875	255,592	216,924	181,436	208,383	96,290	1,717,233
	4.5	542	8,213	54,255	80,431	139,126	175,095	197,418	206,406	185,318	231,640	110,254	1,388,698
Totals, by Weight	5	93	2,271	20,547	35,136	68,741	103,831	120,103	150,108	158,689	228,537	170,303	1,058,359
	>5	27	750	8,702	18,028	43,936	84,740	119,766	180,013	222,032	478,712	848,071	2,004,777
													14M Protomers 8.2K Tranches

<div> <div>Rep.</div> <div>2D</div> <div>3D</div> <div>React.</div> <div>Anodyne</div> <div>Purch.</div> <div>In-Stock</div> <div>pH</div> <div>Ref</div> <div>Charge</div> <div>-2 -1 0 +1 +2</div> <div></div> <div></div> </div>													
Molecular Weight (up to, Daltons)													
LogP (up to)		200	250	300	325	350	375	400	425	450	500	>500	Totals, by LogP
	-1	5,811	4,565	5,585	2,895	2,687	1,947	1,196	817	610	872	1,560	15,732
	0	21,311	15,619	23,920	15,050	15,757	8,940	5,179	3,235	2,002	1,974	1,792	70,346
	1	58,640	61,897	110,983	79,182	82,677	49,658	29,497	15,351	9,938	8,825	4,142	334,739
	2	72,651	131,269	280,168	225,896	165,025	169,663	93,472	61,725	43,919	39,501	11,325	802,358
	2.5	25,171	75,496	199,503	178,925	235,035	149,771	94,225	70,224	51,985	47,917	12,813	688,959
	3	15,804	60,977	187,239	178,061	274,897	204,830	133,169	103,335	81,027	60,171	23,101	701,174
	3.5	6,787	38,433	141,659	158,058	241,061	204,940	157,607	133,892	110,285	115,848	40,814	0
	4	1,960	17,971	65,298	101,696	173,946	175,929	186,322	158,014	130,211	147,318	83,844	0
	4.5	398	5,688	38,665	58,416	103,295	129,648	143,846	149,535	131,741	160,887	80,267	0
Totals, by Weight	5	54	1,385	14,285	25,796	51,378	77,184	87,985	108,443	113,047	157,621	111,630	0
	>5	8	404	4,837	11,561	38,356	60,157	65,261	125,113	151,923	309,900	489,346	0
													2.6M Protomers 240 Tranches

Figure S1. Chemical space of ZINC15 in tranches of 3D protomers according to size (MW) and hydrophobicity (LogP), for a total of 14 million readily available compounds (in-stock with standard reactivity, upper) and the lead-like subset selected (lower). Screenshots were taken in March 2019.

Table S1. The top-ranked selection of compounds based on their estimated binding affinity for IRAP (given as VINA score in kcal/mol). The corresponding estimated affinity for ERAP1 and their difference to IRAP are also given as $\Delta\text{Delta} = \Delta(\Delta G_{\text{bind}}^{\text{(IRAP)}}) - \Delta G_{\text{bind}}^{\text{(ERAP1)}}$.

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	ΔDelta
1	ZINC000257220067	-11.7	-8.9	-2.8
2	ZINC000034895992	-11.6	-9.6	-2.0
3	ZINC000041548359	-11.6	-9.1	-2.5
4	ZINC000012550491	-11.6	-8.9	-2.7
5	ZINC000003617904	-11.6	-8.8	-2.8
6	ZINC000006117573	-11.5	-10.9	-0.6
7	ZINC000022241454	-11.5	-10.2	-1.3
8	ZINC000000489138	-11.5	-9.8	-1.7
9	ZINC000014689114	-11.5	-9.8	-1.7
10	ZINC000255187536	-11.5	-9.5	-2.0
11	ZINC000100191495	-11.5	-9.4	-2.1
12	ZINC000072807915	-11.5	-9.3	-2.2
13	ZINC000100193430	-11.5	-9.3	-2.2
14	ZINC000003947438	-11.4	-9.8	-1.6
15	ZINC000004722089	-11.4	-9.8	-1.6
16	ZINC000001810957	-11.4	-9.6	-1.8
17	ZINC000016543876	-11.4	-9.3	-2.1
18	ZINC000068269627	-11.4	-9.3	-2.1
19	ZINC000009318779	-11.4	-9.2	-2.2
20	ZINC000257310083	-11.4	-9.0	-2.4
21	ZINC000067263105	-11.3	-10.1	-1.2
22	ZINC000018053795	-11.3	-9.7	-1.6
23	ZINC000085879141	-11.3	-9.6	-1.7
24	ZINC000045070892	-11.3	-9.4	-1.9
25	ZINC000084686490	-11.3	-9.3	-2.0
26	ZINC000008848147	-11.3	-9.2	-2.1
27	ZINC000035398834	-11.3	-9.2	-2.1
28	ZINC000225746732	-11.3	-9.2	-2.1
29	ZINC000062639858	-11.3	-9.1	-2.2
30	ZINC000000187795	-11.3	-9.0	-2.3
31	ZINC000012557331	-11.3	-8.9	-2.4
32	ZINC000253433259	-11.3	-7.8	-3.5
33	ZINC000012323933	-11.2	-10.1	-1.1
34	ZINC000007030710	-11.2	-9.7	-1.5
35	ZINC000257206610	-11.2	-9.7	-1.5
36	ZINC000067643674	-11.2	-9.6	-1.6
37	ZINC000014689108	-11.2	-9.5	-1.7
38	ZINC000012557330	-11.2	-9.4	-1.8
39	ZINC000013278475	-11.2	-9.4	-1.8
40	ZINC000044908085	-11.2	-9.4	-1.8
41	ZINC000048249797	-11.2	-9.4	-1.8
42	ZINC000061067795	-11.2	-9.4	-1.8

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	<i>Delta</i>
43	ZINC000009338249	-11.2	-9.3	-1.9
44	ZINC000028790813	-11.2	-9.3	-1.9
45	ZINC000089857747	-11.2	-9.2	-2.0
46	ZINC000225752266	-11.2	-9.1	-2.1
47	ZINC000001431797	-11.2	-9.0	-2.2
48	ZINC000095951555	-11.2	-9.0	-2.2
49	ZINC000097413355	-11.2	-8.9	-2.3
50	ZINC000001620500	-11.2	-8.6	-2.6
51	ZINC000040386288	-11.2	-8.6	-2.6
52	ZINC000077522487	-11.2	-8.5	-2.7
53	ZINC000023995834	-11.2	-8.4	-2.8
54	ZINC000040473994	-11.2	-8.4	-2.8
55	ZINC000585093224	-11.2	-8.4	-2.8
56	ZINC000239762559	-11.2	-7.8	-3.4
57	ZINC000000136922	-11.1	-10.2	-0.9
58	ZINC000057563200	-11.1	-10.0	-1.1
59	ZINC000044874685	-11.1	-9.9	-1.2
60	ZINC000192753414	-11.1	-9.9	-1.2
61	ZINC000069775761	-11.1	-9.8	-1.3
62	ZINC000004003439	-11.1	-9.7	-1.4
63	ZINC000030875068	-11.1	-9.7	-1.4
64	ZINC000072437791	-11.1	-9.7	-1.4
65	ZINC000095393415	-11.1	-9.6	-1.5
66	ZINC000014791001	-11.1	-9.5	-1.6
67	ZINC000268943077	-11.1	-9.5	-1.6
68	ZINC000000082526	-11.1	-9.4	-1.7
69	ZINC000007030648	-11.1	-9.4	-1.7
70	ZINC000072300732	-11.1	-9.4	-1.7
71	ZINC000003617861	-11.1	-9.2	-1.9
72	ZINC000057771728	-11.1	-9.2	-1.9
73	ZINC000077503523	-11.1	-9.2	-1.9
74	ZINC000078914774	-11.1	-9.2	-1.9
75	ZINC000009318781	-11.1	-9.1	-2.0
76	ZINC000019327176	-11.1	-9.0	-2.1
77	ZINC000084563579	-11.1	-9.0	-2.1
78	ZINC000013562617	-11.1	-8.9	-2.2
79	ZINC000013691850	-11.1	-8.9	-2.2
80	ZINC000072290626	-11.1	-8.8	-2.3
81	ZINC000194368147	-11.1	-8.7	-2.4
82	ZINC000299785131	-11.1	-8.6	-2.5
83	ZINC000095415912	-11.1	-8.5	-2.6
84	ZINC000000065653	-11.1	-8.4	-2.7
85	ZINC000050857093	-11.1	-8.2	-2.9
86	ZINC000100756934	-11.1	-8.1	-3.0
87	ZINC000051467674	-11.1	-8.0	-3.1

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	<i>Delta</i>
88	ZINC000004807849	-11.0	-10.4	-0.6
89	ZINC000018177963	-11.0	-10.4	-0.6
90	ZINC000005426253	-11.0	-10.3	-0.7
91	ZINC000017888288	-11.0	-10.3	-0.7
92	ZINC000052955795	-11.0	-10.2	-0.8
93	ZINC000095469884	-11.0	-10.2	-0.8
94	ZINC000012323932	-11.0	-10.0	-1.0
95	ZINC000230113696	-11.0	-9.8	-1.2
96	ZINC000005893172	-11.0	-9.7	-1.3
97	ZINC000010256259	-11.0	-9.7	-1.3
98	ZINC000065167646	-11.0	-9.7	-1.3
99	ZINC000072896858	-11.0	-9.7	-1.3
100	ZINC000136345745	-11.0	-9.7	-1.3
101	ZINC000004100408	-11.0	-9.6	-1.4
102	ZINC000013973188	-11.0	-9.6	-1.4
103	ZINC000016228943	-11.0	-9.6	-1.4
104	ZINC000065925006	-11.0	-9.6	-1.4
105	ZINC000072896859	-11.0	-9.6	-1.4
106	ZINC000029134571	-11.0	-9.5	-1.5
107	ZINC000035671101	-11.0	-9.5	-1.5
108	ZINC000104346290	-11.0	-9.5	-1.5
109	ZINC000008771448	-11.0	-9.4	-1.6
110	ZINC000008776545	-11.0	-9.4	-1.6
111	ZINC000021835963	-11.0	-9.4	-1.6
112	ZINC000178511392	-11.0	-9.4	-1.6
113	ZINC000096122792	-11.0	-9.3	-1.7
114	ZINC000003313076	-11.0	-9.2	-1.8
115	ZINC000095387190	-11.0	-9.2	-1.8
116	ZINC000100193536	-11.0	-9.2	-1.8
117	ZINC000244816835	-11.0	-9.2	-1.8
118	ZINC000072290711	-11.0	-9.1	-1.9
119	ZINC000000088011	-11.0	-9.0	-2.0
120	ZINC000006086854	-11.0	-9.0	-2.0
121	ZINC000018181694	-11.0	-9.0	-2.0
122	ZINC000019973960	-11.0	-9.0	-2.0
123	ZINC000257211885	-11.0	-9.0	-2.0
124	ZINC000058202763	-11.0	-8.9	-2.1
125	ZINC000095447759	-11.0	-8.9	-2.1
126	ZINC000223692657	-11.0	-8.9	-2.1
127	ZINC000089827813	-11.0	-8.8	-2.2
128	ZINC000004722011	-11.0	-8.6	-2.4
129	ZINC000019796838	-11.0	-8.6	-2.4
130	ZINC000257257831	-11.0	-8.6	-2.4
131	ZINC000096238948	-11.0	-8.5	-2.5
132	ZINC000171342968	-11.0	-8.5	-2.5

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	<i>Delta</i>
133	ZINC000178206155	-11.0	-8.5	-2.5
134	ZINC000000439839	-11.0	-8.4	-2.6
135	ZINC000096837115	-10.9	-10.7	-0.2
136	ZINC000002465083	-10.9	-10.6	-0.3
137	ZINC000006117574	-10.9	-10.6	-0.3
138	ZINC000575617533	-10.9	-10.4	-0.5
139	ZINC000003852421	-10.9	-9.9	-1.0
140	ZINC000057511709	-10.9	-9.9	-1.0
141	ZINC000072290753	-10.9	-9.9	-1.0
142	ZINC000003875380	-10.9	-9.8	-1.1
143	ZINC000013691849	-10.9	-9.8	-1.1
144	ZINC000019973951	-10.9	-9.8	-1.1
145	ZINC000072277544	-10.9	-9.8	-1.1
146	ZINC000022549345	-10.9	-9.7	-1.2
147	ZINC000034407910	-10.9	-9.7	-1.2
148	ZINC000299793701	-10.9	-9.7	-1.2
149	ZINC000005360885	-10.9	-9.6	-1.3
150	ZINC000001758646	-10.9	-9.5	-1.4
151	ZINC000004003438	-10.9	-9.5	-1.4
152	ZINC000005088834	-10.9	-9.5	-1.4
153	ZINC000014240188	-10.9	-9.5	-1.4
154	ZINC000029134573	-10.9	-9.5	-1.4
155	ZINC000069778215	-10.9	-9.5	-1.4
156	ZINC000084598174	-10.9	-9.5	-1.4
157	ZINC000084598177	-10.9	-9.5	-1.4
158	ZINC000003438521	-10.9	-9.4	-1.5
159	ZINC000008316344	-10.9	-9.4	-1.5
160	ZINC000003245357	-10.9	-9.3	-1.6
161	ZINC000004998502	-10.9	-9.3	-1.6
162	ZINC000006556210	-10.9	-9.3	-1.6
163	ZINC000010218408	-10.9	-9.3	-1.6
164	ZINC000040266307	-10.9	-9.3	-1.6
165	ZINC000050859891	-10.9	-9.3	-1.6
166	ZINC000072432742	-10.9	-9.3	-1.6
167	ZINC000119429896	-10.9	-9.3	-1.6
168	ZINC000257206611	-10.9	-9.3	-1.6
169	ZINC000000390374	-10.9	-9.2	-1.7
170	ZINC000022191233	-10.9	-9.2	-1.7
171	ZINC000071915224	-10.9	-9.2	-1.7
172	ZINC000001711692	-10.9	-9.1	-1.8
173	ZINC000006576136	-10.9	-9.1	-1.8
174	ZINC000008738218	-10.9	-9.1	-1.8
175	ZINC000012875967	-10.9	-9.1	-1.8
176	ZINC000153353600	-10.9	-9.1	-1.8
177	ZINC000229224134	-10.9	-9.1	-1.8

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	<i>Delta</i>
178	ZINC000584897275	-10.9	-9.1	-1.8
179	ZINC000000333210	-10.9	-9.0	-1.9
180	ZINC0000002465084	-10.9	-9.0	-1.9
181	ZINC0000004535480	-10.9	-9.0	-1.9
182	ZINC00000047209496	-10.9	-9.0	-1.9
183	ZINC000000135810445	-10.9	-9.0	-1.9
184	ZINC000000253433605	-10.9	-9.0	-1.9
185	ZINC0000002646979	-10.9	-8.9	-2.0
186	ZINC00000011781217	-10.9	-8.9	-2.0
187	ZINC00000072300733	-10.9	-8.9	-2.0
188	ZINC00000075530760	-10.9	-8.9	-2.0
189	ZINC00000091943530	-10.9	-8.9	-2.0
190	ZINC00000020116324	-10.9	-8.8	-2.1
191	ZINC00000050857092	-10.9	-8.8	-2.1
192	ZINC00000069538683	-10.9	-8.8	-2.1
193	ZINC00000074014922	-10.9	-8.8	-2.1
194	ZINC000000284798034	-10.9	-8.8	-2.1
195	ZINC0000001465257	-10.9	-8.7	-2.2
196	ZINC0000002922856	-10.9	-8.7	-2.2
197	ZINC00000004732939	-10.9	-8.7	-2.2
198	ZINC00000005776998	-10.9	-8.7	-2.2
199	ZINC00000006887927	-10.9	-8.7	-2.2
200	ZINC000000040548686	-10.9	-8.7	-2.2
201	ZINC000000041546843	-10.9	-8.7	-2.2
202	ZINC00000043550595	-10.9	-8.7	-2.2
203	ZINC000000089827814	-10.9	-8.7	-2.2
204	ZINC000000177842371	-10.9	-8.7	-2.2
205	ZINC0000000585093122	-10.9	-8.7	-2.2
206	ZINC00000000390138	-10.9	-8.6	-2.3
207	ZINC000000003292603	-10.9	-8.6	-2.3
208	ZINC000000240454699	-10.9	-8.6	-2.3
209	ZINC0000000079035	-10.9	-8.5	-2.4
210	ZINC000000044919578	-10.9	-8.5	-2.4
211	ZINC000000069846908	-10.9	-8.5	-2.4
212	ZINC000000072096437	-10.9	-8.5	-2.4
213	ZINC000000091304527	-10.9	-8.5	-2.4
214	ZINC000000027755553	-10.9	-8.4	-2.5
215	ZINC00000008913866	-10.9	-8.3	-2.6
216	ZINC000000012867343	-10.9	-8.3	-2.6
217	ZINC000000077353582	-10.9	-8.3	-2.6
218	ZINC000000095415911	-10.9	-8.3	-2.6
219	ZINC000000097105546	-10.9	-8.3	-2.6
220	ZINC000000012508838	-10.9	-8.2	-2.7
221	ZINC0000000334003030	-10.9	-8.1	-2.8
222	ZINC00000000326909	-10.9	-7.9	-3.0

Table S2. Top-ranked selection of compounds based on their difference in the estimated binding affinity for IRAP versus ERAP1 ($\Delta\Delta G_{\text{bind}}^{(\text{IRAP})} - \Delta\Delta G_{\text{bind}}^{(\text{ERAP1})}$). Their ranking (#) is relative to the affinity for IRAP and follows that of **Table S1**. Entries marked in boldface indicate compounds that were finally selected for experimental screening.

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	$\Delta\Delta G_{\text{bind}}$
223	ZINC000008609997	-10.8	-8.3	-2.5
224	ZINC000097105494	-10.8	-8.3	-2.5
225	ZINC000013692677	-10.8	-8.2	-2.6
226	ZINC000023764785	-10.8	-8.2	-2.6
227	ZINC000003463362	-10.8	-8.1	-2.7
228	ZINC000257218603	-10.8	-7.9	-2.9
229	ZINC000091664087	-10.8	-7.4	-3.4
230	ZINC000000082954	-10.7	-8.2	-2.5
231	ZINC000002837442	-10.7	-8.2	-2.5
232	ZINC000005303591	-10.7	-8.2	-2.5
233	ZINC000025032259	-10.7	-8.1	-2.6
234	ZINC000100119126	-10.7	-8.0	-2.7
235	ZINC000012142779	-10.7	-7.9	-2.8
236	ZINC000012239509	-10.7	-7.9	-2.8
237	ZINC000065463577	-10.7	-7.9	-2.8
238	ZINC000050584912	-10.7	-7.6	-3.1
239	ZINC000040386093	-10.7	-7.5	-3.2
240	ZINC000092760184	-10.7	-7.5	-3.2
241	ZINC000252509448	-10.7	-7.4	-3.3
242	ZINC000004806959	-10.6	-8.1	-2.5
243	ZINC000008595944	-10.6	-8.1	-2.5
244	ZINC000040386114	-10.6	-8.1	-2.5
245	ZINC000215185750	-10.6	-8.1	-2.5
246	ZINC000253407066	-10.6	-8.1	-2.5
247	ZINC000575618196	-10.6	-8.1	-2.5
248	ZINC000096024249	-10.6	-8.0	-2.6
249	ZINC000021722970	-10.6	-7.9	-2.7
250	ZINC000067460397	-10.6	-7.9	-2.7
251	ZINC000096003964	-10.6	-7.9	-2.7
252	ZINC000306141880	-10.6	-7.4	-3.2
253	ZINC000100737122	-10.6	-7.1	-3.5
254	ZINC000095402766	-10.6	-6.9	-3.7
255	ZINC000014901170	-10.5	-8.0	-2.5
256	ZINC000084578820	-10.5	-8.0	-2.5
257	ZINC000274936458	-10.5	-8.0	-2.5
258	ZINC000096249561	-10.5	-7.9	-2.6
259	ZINC000001580185	-10.5	-7.7	-2.8
260	ZINC000004495846	-10.5	-7.6	-2.9
261	ZINC000257299555	-10.5	-7.6	-2.9
262	ZINC000012122382	-10.5	-7.5	-3.0

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	<i>Delta</i>
263	ZINC000075530913	-10.5	-7.3	-3.2
264	ZINC000040386098	-10.4	-7.9	-2.5
265	ZINC000069562405	-10.4	-7.9	-2.5
266	ZINC000079491038	-10.4	-7.8	-2.6
267	ZINC000006669352	-10.4	-7.7	-2.7
268	ZINC000012142783	-10.4	-7.7	-2.7
269	ZINC000238831563	-10.4	-7.7	-2.7
270	ZINC000253473237	-10.4	-7.7	-2.7
271	ZINC000257192562	-10.4	-7.7	-2.7
272	ZINC000238841632	-10.4	-7.6	-2.8
273	ZINC000257311417	-10.4	-7.6	-2.8
274	ZINC000095950700	-10.4	-7.5	-2.9
275	ZINC000306138347	-10.4	-7.5	-2.9
276	ZINC000081397352	-10.4	-7.4	-3.0
277	ZINC000096201851	-10.4	-7.4	-3.0
278	ZINC000278659999	-10.4	-7.4	-3.0
279	ZINC000092021781	-10.4	-7.3	-3.1
280	ZINC000091270544	-10.4	-7.1	-3.3
281	ZINC000005023816	-10.3	-7.8	-2.5
282	ZINC000012888207	-10.3	-7.8	-2.5
283	ZINC000014741626	-10.3	-7.8	-2.5
284	ZINC000061717590	-10.3	-7.8	-2.5
285	ZINC000069349055	-10.3	-7.8	-2.5
286	ZINC000170016387	-10.3	-7.8	-2.5
287	ZINC000584887110	-10.3	-7.8	-2.5
288	ZINC000002216953	-10.3	-7.7	-2.6
289	ZINC000006918427	-10.3	-7.7	-2.6
290	ZINC000065249112	-10.3	-7.7	-2.6
291	ZINC000065625052	-10.3	-7.7	-2.6
292	ZINC000075118384	-10.3	-7.7	-2.6
293	ZINC000119149039	-10.3	-7.7	-2.6
294	ZINC000065248686	-10.3	-7.6	-2.7
295	ZINC000065591272	-10.3	-7.6	-2.7
296	ZINC000005026046	-10.3	-7.5	-2.8
297	ZINC000058099587	-10.3	-7.3	-3.0
298	ZINC000154455008	-10.3	-7.3	-3.0
299	ZINC000091486946	-10.3	-7.2	-3.1
300	ZINC000170800517	-10.3	-7.1	-3.2
301	ZINC000000062112	-10.2	-7.7	-2.5
302	ZINC000005244779	-10.2	-7.7	-2.5
303	ZINC000006782318	-10.2	-7.7	-2.5
304	ZINC000018148904	-10.2	-7.7	-2.5
305	ZINC000069492530	-10.2	-7.7	-2.5
306	ZINC000079001413	-10.2	-7.7	-2.5
307	ZINC000000199600	-10.2	-7.6	-2.6

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	<i>Delta</i>
308	ZINC000003327891	-10.2	-7.6	-2.6
309	ZINC000004483817	-10.2	-7.6	-2.6
310	ZINC000042025678	-10.2	-7.6	-2.6
311	ZINC000057526383	-10.2	-7.6	-2.6
312	ZINC000065395709	-10.2	-7.6	-2.6
313	ZINC000096058349	-10.2	-7.6	-2.6
314	ZINC000257256038	-10.2	-7.6	-2.6
315	ZINC000006660103	-10.2	-7.5	-2.7
316	ZINC000057526528	-10.2	-7.5	-2.7
317	ZINC000091486133	-10.2	-7.5	-2.7
318	ZINC000097050589	-10.2	-7.5	-2.7
319	ZINC000330033487	-10.2	-7.5	-2.7
320	ZINC000095410774	-10.2	-7.4	-2.8
321	ZINC000096199614	-10.2	-7.4	-2.8
322	ZINC000000551535	-10.2	-7.2	-3.0
323	ZINC000096201858	-10.2	-6.9	-3.3
324	ZINC0000002390471	-10.1	-7.6	-2.5
325	ZINC000004511530	-10.1	-7.6	-2.5
326	ZINC000005348603	-10.1	-7.6	-2.5
327	ZINC000012407997	-10.1	-7.6	-2.5
328	ZINC000096010936	-10.1	-7.6	-2.5
329	ZINC000097086417	-10.1	-7.6	-2.5
330	ZINC000195547314	-10.1	-7.6	-2.5
331	ZINC000215185695	-10.1	-7.6	-2.5
332	ZINC000225489282	-10.1	-7.6	-2.5
333	ZINC000237955843	-10.1	-7.6	-2.5
334	ZINC000588229346	-10.1	-7.6	-2.5
335	ZINC000057526426	-10.1	-7.5	-2.6
336	ZINC000069740630	-10.1	-7.5	-2.6
337	ZINC000071282106	-10.1	-7.5	-2.6
338	ZINC000092078469	-10.1	-7.4	-2.7
339	ZINC000096158052	-10.1	-7.4	-2.7
340	ZINC000096251711	-10.1	-7.4	-2.7
341	ZINC000000106944	-10.1	-7.3	-2.8
342	ZINC000092022499	-10.1	-7.3	-2.8
343	ZINC000334160460	-10.1	-7.3	-2.8
344	ZINC000091321614	-10.1	-7.2	-2.9
345	ZINC000096069677	-10.1	-7.2	-2.9
346	ZINC000023642159	-10.1	-7.1	-3.0
347	ZINC000096240774	-10.1	-7.1	-3.0
348	ZINC000001648546	-10.1	-7.0	-3.1
349	ZINC000001381807	-10.0	-7.5	-2.5
350	ZINC000095375482	-10.0	-7.5	-2.5
351	ZINC000192929211	-10.0	-7.5	-2.5
352	ZINC000229623928	-10.0	-7.5	-2.5

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	<i>Delta</i>
353	ZINC000253433258	-10.0	-7.5	-2.5
354	ZINC000000201272	-10.0	-7.4	-2.6
355	ZINC000020729822	-10.0	-7.4	-2.6
356	ZINC000057526442	-10.0	-7.4	-2.6
357	ZINC000065507679	-10.0	-7.4	-2.6
358	ZINC000096038482	-10.0	-7.4	-2.6
359	ZINC000096069669	-10.0	-7.4	-2.6
360	ZINC000100756927	-10.0	-7.4	-2.6
361	ZINC000237699092	-10.0	-7.4	-2.6
362	ZINC000238121810	-10.0	-7.4	-2.6
363	ZINC000064871452	-10.0	-7.3	-2.7
364	ZINC000092065698	-10.0	-7.3	-2.7
365	ZINC000092077873	-10.0	-7.3	-2.7
366	ZINC000245171655	-10.0	-7.3	-2.7
367	ZINC000071497775	-10.0	-7.0	-3.0
368	ZINC000018240833	-9.9	-7.4	-2.5
369	ZINC000022067509	-9.9	-7.4	-2.5
370	ZINC000035869910	-9.9	-7.4	-2.5
371	ZINC000040385915	-9.9	-7.4	-2.5
372	ZINC000055418850	-9.9	-7.4	-2.5
373	ZINC000065170071	-9.9	-7.4	-2.5
374	ZINC000069895275	-9.9	-7.4	-2.5
375	ZINC000071746202	-9.9	-7.4	-2.5
376	ZINC000091270543	-9.9	-7.4	-2.5
377	ZINC000091487017	-9.9	-7.4	-2.5
378	ZINC000095503625	-9.9	-7.4	-2.5
379	ZINC000237740654	-9.9	-7.4	-2.5
380	ZINC000238886413	-9.9	-7.4	-2.5
381	ZINC000409428381	-9.9	-7.4	-2.5
382	ZINC000000353960	-9.9	-7.3	-2.6
383	ZINC000000389450	-9.9	-7.3	-2.6
384	ZINC000002630701	-9.9	-7.3	-2.6
385	ZINC000005202436	-9.9	-7.3	-2.6
386	ZINC000057731402	-9.9	-7.3	-2.6
387	ZINC000072235028	-9.9	-7.3	-2.6
388	ZINC000095989182	-9.9	-7.3	-2.6
389	ZINC000169680567	-9.9	-7.3	-2.6
390	ZINC000019328346	-9.9	-7.2	-2.7
391	ZINC000015078577	-9.9	-7.1	-2.8
392	ZINC000006490389	-9.9	-7.0	-2.9
393	ZINC000096251709	-9.9	-7.0	-2.9
394	ZINC000216315534	-9.9	-6.7	-3.2
395	ZINC000005202682	-9.8	-7.3	-2.5
396	ZINC000029054164	-9.8	-7.3	-2.5
397	ZINC000069595091	-9.8	-7.3	-2.5

#	ZINC ID	VINA score (kcal/mol)		
		IRAP	ERAP1	<i>Delta</i>
398	ZINC000072234903	-9.8	-7.3	-2.5
399	ZINC000075140034	-9.8	-7.3	-2.5
400	ZINC000091663451	-9.8	-7.3	-2.5
401	ZINC000096069697	-9.8	-7.3	-2.5
402	ZINC000107713021	-9.8	-7.3	-2.5
403	ZINC000092065700	-9.8	-7.2	-2.6
404	ZINC000096069207	-9.8	-7.2	-2.6
405	ZINC000096198984	-9.8	-7.2	-2.6
406	ZINC000257317306	-9.8	-7.2	-2.6
407	ZINC000328587242	-9.8	-7.2	-2.6
408	ZINC000069737923	-9.8	-7.1	-2.7
409	ZINC000238872716	-9.8	-7.1	-2.7
410	ZINC000003641308	-9.7	-7.2	-2.5
411	ZINC000040060202	-9.7	-7.2	-2.5
412	ZINC000040385901	-9.7	-7.2	-2.5
413	ZINC000096081777	-9.7	-7.2	-2.5
414	ZINC000585280336	-9.7	-7.2	-2.5
415	ZINC000002750765	-9.7	-7.1	-2.6
416	ZINC000096080454	-9.7	-7.1	-2.6
417	ZINC000096198954	-9.7	-7.1	-2.6
418	ZINC000097201269	-9.7	-7.1	-2.6
419	ZINC000121632943	-9.7	-7.0	-2.7
420	ZINC000257222272	-9.7	-7.0	-2.7
421	ZINC000071754931	-9.7	-6.9	-2.8
422	ZINC000091768990	-9.7	-6.9	-2.8
423	ZINC000257270100	-9.7	-6.8	-2.9

Table S3. Energy decomposition of the MM/PBSA results for the 305 compounds using the *PB-1* parameter set (for more details see the Methods section). All energy terms are given in kcal/mol and are sorted by the binding free energy (ΔG_{bind}), followed by the molecular mechanics van der Waals and electrostatic interactions terms (ΔE_{vdW} and ΔE_{el}), the polar contribution to the solvation free energy (ΔG_{pol}), the cavity formation and the van der Waals (dispersion) free energy terms that comprise the non-polar solvation free energy (ΔG_{np} and ΔG_{disp}). Compounds marked in boldface were finally selected for experimental screening.

#	ZINC ID	ΔG_{bind}	ΔE_{vdW}	ΔE_{el}	ΔG_{pol}	ΔG_{np}	ΔG_{disp}
1	ZINC000010256259	-15.7	-52.7	-41.4	55.5	-35.0	58.0
2	ZINC000035869910	-14.1	-54.6	-34.9	50.1	-36.8	62.1
3	ZINC000084578820	-13.9	-47.8	-35.2	44.3	-32.1	56.9
4	ZINC000257317306	-13.0	-50.1	-41.2	53.5	-36.6	61.4
5	ZINC000012888207	-11.0	-40.8	-27.0	35.4	-27.9	49.2
6	ZINC000015078577	-10.8	-49.4	-29.1	42.5	-34.7	59.9
7	ZINC000079491038	-10.5	-51.3	-27.7	45.5	-35.9	59.0
8	ZINC000084598177	-10.5	-49.0	-30.6	43.6	-32.1	57.6
9	ZINC000069562405	-9.8	-47.4	-25.3	37.8	-32.5	57.5
10	ZINC000005360885	-9.7	-48.1	-36.4	51.7	-31.8	55.0
11	ZINC000018148904	-9.5	-50.1	-32.7	50.6	-33.7	56.3
12	ZINC000022191233	-9.2	-53.6	-30.9	51.0	-36.6	61.0
13	ZINC000096199614	-9.1	-51.3	-27.5	46.5	-32.0	55.1
14	ZINC000004511530	-8.6	-49.2	-22.6	42.0	-33.4	54.6
15	ZINC000216315534	-8.3	-41.9	-27.2	37.8	-30.4	53.3
16	ZINC000000333210	-8.3	-50.6	-32.9	51.4	-33.1	56.9
17	ZINC000244816835	-8.1	-43.8	-34.1	47.4	-33.4	55.7
18	ZINC000044919578	-8.0	-43.0	-29.0	40.4	-29.6	53.2
19	ZINC000051467674	-8.0	-46.6	-40.6	55.1	-32.5	56.6
20	ZINC000091270543	-7.8	-53.6	-21.4	39.3	-36.1	64.0
21	ZINC000069737923	-7.7	-46.3	-29.6	42.9	-33.1	58.4
22	ZINC000223692657	-7.5	-50.8	-27.8	47.9	-33.1	56.3
23	ZINC000095410774	-7.4	-50.5	-22.8	42.7	-32.4	55.7
24	ZINC000003463362	-7.3	-50.0	-30.0	43.6	-34.3	63.4
25	ZINC000240454699	-7.0	-42.5	-24.0	35.5	-30.9	54.9
26	ZINC000096058349	-6.6	-54.1	-18.0	40.5	-34.1	59.2
27	ZINC000095415912	-6.5	-53.2	-29.2	50.0	-34.5	60.4
28	ZINC000067460397	-6.4	-50.1	-35.5	55.7	-31.9	55.4
29	ZINC000013973188	-6.2	-47.2	-29.6	47.3	-31.7	54.9
30	ZINC000014791001	-6.0	-47.0	-21.3	39.9	-32.3	54.6
31	ZINC000084686490	-5.9	-46.1	-33.1	50.5	-33.3	56.1
32	ZINC000334160460	-5.9	-49.1	-22.2	40.1	-33.4	58.7
33	ZINC000071915224	-5.8	-49.3	-26.0	43.6	-32.7	58.7
34	ZINC000074014922	-5.8	-47.0	-9.6	29.3	-31.1	52.6
35	ZINC000257299555	-5.7	-46.7	-36.0	51.2	-31.6	57.4
36	ZINC000091270544	-5.6	-52.4	-22.1	41.6	-35.4	62.7
37	ZINC000575618196	-5.6	-54.5	-27.7	50.3	-34.9	61.2

#	ZINC ID	ΔG_{bind}	ΔE_{vdW}	ΔE_{el}	ΔG_{pol}	ΔG_{np}	ΔG_{disp}
38	ZINC000154455008	-5.5	-44.9	-15.2	33.2	-32.7	54.2
39	ZINC000194368147	-5.4	-48.3	-30.0	49.2	-32.7	56.3
40	ZINC000071754931	-5.2	-40.8	-12.2	24.4	-29.3	52.7
41	ZINC000043550595	-5.1	-48.3	-29.1	46.5	-33.6	59.4
42	ZINC000008595944	-5.0	-53.1	-13.9	37.5	-34.0	58.4
43	ZINC000069778215	-5.0	-47.6	-42.2	60.1	-33.8	58.5
44	ZINC000100193430	-5.0	-47.9	-13.6	33.4	-30.3	53.4
45	ZINC000003438521	-4.9	-45.4	-22.7	39.2	-30.9	54.8
46	ZINC000075530913	-4.8	-49.2	-20.2	37.5	-34.1	61.2
47	ZINC000225746732	-4.8	-47.5	-20.8	38.7	-30.9	55.6
48	ZINC000003641308	-4.7	-45.0	-25.7	44.0	-31.2	53.1
49	ZINC000018053795	-4.7	-47.5	-22.6	42.2	-31.9	55.1
50	ZINC000008913866	-4.7	-50.7	-28.3	48.7	-33.7	59.4
51	ZINC000057563200	-4.5	-49.9	-17.6	37.5	-33.9	59.3
52	ZINC000044874685	-4.4	-44.2	-22.4	37.9	-32.2	56.5
53	ZINC000002216953	-4.4	-48.7	-24.8	43.1	-33.0	59.0
54	ZINC000095469884	-4.4	-40.0	-35.7	49.2	-28.5	50.7
55	ZINC000195547314	-4.3	-50.9	-13.5	34.8	-34.5	59.7
56	ZINC000100193536	-4.3	-48.7	-15.8	35.4	-31.6	56.4
57	ZINC000021835963	-4.3	-48.7	-26.2	46.3	-33.7	58.0
58	ZINC000092078469	-4.3	-45.0	-23.4	37.6	-31.0	57.5
59	ZINC000230113696	-4.3	-52.9	-22.8	44.8	-34.9	61.4
60	ZINC000057731402	-4.3	-51.2	-25.2	44.7	-34.1	61.5
61	ZINC000012142783	-4.2	-51.0	-21.5	41.3	-34.4	61.4
62	ZINC000091768990	-4.1	-52.4	-13.3	35.4	-33.6	59.9
63	ZINC000092065700	-4.0	-52.6	-19.8	39.9	-34.9	63.4
64	ZINC000006669352	-4.0	-47.6	-23.0	45.1	-33.4	54.9
65	ZINC000238121810	-4.0	-37.2	-88.8	99.9	-31.3	53.5
66	ZINC000016543876	-3.9	-46.0	-16.9	35.1	-31.4	55.3
67	ZINC000306141880	-3.9	-46.5	-29.1	45.9	-32.0	57.8
68	ZINC000004998502	-3.9	-53.5	-40.0	65.4	-35.7	59.9
69	ZINC000095950700	-3.9	-48.8	-19.4	37.5	-32.0	58.9
70	ZINC000096003964	-3.9	-49.1	-26.2	49.3	-32.8	55.0
71	ZINC000009338249	-3.8	-47.0	-27.4	46.6	-30.6	54.7
72	ZINC000585093122	-3.2	-45.2	-16.8	34.3	-30.8	55.2
73	ZINC000091943530	-3.1	-44.1	-16.2	33.7	-31.4	55.0
74	ZINC000092022499	-3.1	-53.4	-23.1	45.3	-35.3	63.3
75	ZINC000025032259	-3.0	-54.4	-21.9	48.0	-37.3	62.6
76	ZINC000064871452	-2.9	-49.9	-27.1	48.2	-34.0	59.9
77	ZINC000007030648	-2.9	-43.3	-20.2	37.0	-28.2	51.8
78	ZINC000012323932	-2.8	-42.7	-38.0	53.3	-30.6	55.2
79	ZINC000100119126	-2.7	-47.3	-19.9	41.2	-32.3	55.7
80	ZINC000008738218	-2.6	-41.0	-40.6	57.0	-30.3	52.3
81	ZINC000057526426	-2.6	-44.4	-27.1	44.7	-31.7	56.0
82	ZINC000095951555	-2.5	-42.9	-19.3	36.6	-29.4	52.4
83	ZINC000100191495	-2.4	-46.6	-14.2	35.4	-30.0	53.0

#	ZINC ID	ΔG_{bind}	ΔE_{vdW}	ΔE_{el}	ΔG_{pol}	ΔG_{np}	ΔG_{disp}
84	ZINC000257211885	-2.4	-50.3	-20.9	42.3	-32.5	59.1
85	ZINC000007030710	-2.4	-47.3	-24.4	43.8	-30.7	56.3
86	ZINC000003313076	-2.2	-41.7	-21.1	37.8	-28.0	50.8
87	ZINC000065248686	-2.2	-45.7	-14.1	33.4	-31.5	55.7
88	ZINC000077503523	-2.1	-45.1	-34.1	52.5	-30.9	55.5
89	ZINC000075140034	-2.1	-41.8	-19.3	35.3	-30.9	54.7
90	ZINC000002630701	-2.1	-49.0	-6.8	30.1	-31.6	55.0
91	ZINC000089827813	-2.1	-46.6	-28.8	49.3	-32.4	56.3
92	ZINC000001381807	-2.1	-37.1	-14.9	29.6	-26.7	47.1
93	ZINC000075118384	-2.0	-46.9	-33.8	55.2	-33.0	56.5
94	ZINC000257192562	-2.0	-45.9	-16.4	34.9	-32.6	58.1
95	ZINC000092760184	-1.9	-47.5	-20.1	39.5	-33.6	59.8
96	ZINC000040473994	-1.9	-49.6	-26.3	48.1	-32.8	58.7
97	ZINC000003292603	-1.8	-47.2	-19.3	38.6	-32.5	58.6
98	ZINC000011781217	-1.6	-52.0	-13.2	39.2	-35.2	59.6
99	ZINC000257206611	-1.5	-55.3	-11.4	39.7	-35.5	61.0
100	ZINC000100737122	-1.5	-52.3	-22.5	48.3	-34.3	59.3
101	ZINC000225489282	-1.5	-49.8	-16.6	40.0	-32.6	57.5
102	ZINC000004722089	-1.4	-48.1	-14.4	35.5	-30.2	55.8
103	ZINC000092021781	-1.4	-49.3	-20.5	42.5	-33.7	59.7
104	ZINC000067643674	-1.4	-44.8	-25.8	45.4	-30.2	54.0
105	ZINC000091486133	-1.3	-52.7	-25.9	47.8	-34.7	64.2
106	ZINC000008316344	-1.2	-51.0	-4.6	28.5	-33.0	58.9
107	ZINC000069846908	-1.2	-50.0	-33.8	58.0	-34.1	58.8
108	ZINC000019327176	-1.1	-40.2	-26.8	42.1	-27.8	51.5
109	ZINC000035398834	-1.1	-51.5	-9.7	35.6	-33.1	57.5
110	ZINC000095989182	-1.0	-43.2	-18.7	38.4	-28.9	51.4
111	ZINC000584887110	-1.0	-46.9	-14.2	35.2	-32.1	56.9
112	ZINC000097105546	-1.0	-44.7	-22.4	44.6	-30.0	51.5
113	ZINC000096251711	-0.9	-50.9	-15.0	39.6	-33.2	58.7
114	ZINC000229623928	-0.9	-50.6	-34.1	58.3	-33.9	59.4
115	ZINC000096238948	-0.9	-53.8	-13.0	38.8	-34.3	61.4
116	ZINC000171342968	-0.7	-48.4	-39.2	62.0	-33.5	58.5
117	ZINC000096024249	-0.7	-47.4	-18.1	41.7	-29.3	52.5
118	ZINC000050859891	-0.6	-48.4	-29.5	53.8	-31.1	54.4
119	ZINC000072234903	-0.6	-44.1	-12.5	34.2	-30.6	52.5
120	ZINC000257311417	-0.5	-40.7	-23.4	40.3	-29.5	52.8
121	ZINC000014240188	-0.5	-45.7	-17.2	39.1	-31.1	54.4
122	ZINC000278659999	-0.4	-47.8	-23.7	46.2	-33.0	57.9
123	ZINC000257218603	-0.4	-50.2	-24.7	45.8	-35.0	63.8
124	ZINC000022241454	-0.3	-39.1	-38.4	51.9	-26.7	51.9
125	ZINC000002465084	-0.3	-49.8	-23.7	49.9	-32.8	56.2
126	ZINC000095447759	-0.3	-46.9	-24.8	47.3	-30.8	54.9
127	ZINC000069492530	-0.1	-47.5	-19.0	43.1	-31.1	54.4
128	ZINC000119429896	-0.1	-49.5	-9.9	33.6	-33.8	59.6
129	ZINC000000326909	-0.1	-42.9	-17.0	37.1	-27.4	50.1

#	ZINC ID	ΔG_{bind}	ΔE_{vdW}	ΔE_{el}	ΔG_{pol}	ΔG_{np}	ΔG_{disp}
130	ZINC000257310083	0.0	-47.2	-16.6	37.1	-31.2	57.8
131	ZINC000096010936	0.0	-41.4	-26.7	45.4	-31.7	54.3
132	ZINC000010218408	0.0	-47.3	-19.2	42.9	-29.7	53.2
133	ZINC000077353582	0.0	-48.6	-15.4	40.5	-30.7	54.4
134	ZINC000091486946	0.1	-52.4	-21.3	44.0	-34.8	64.5
135	ZINC000002750765	0.1	-45.0	-24.4	44.7	-31.5	56.2
136	ZINC000135810445	0.1	-44.5	-31.9	52.9	-30.9	54.5
137	ZINC000069740630	0.1	-38.0	-20.4	36.1	-28.9	51.4
138	ZINC000177842371	0.1	-45.3	-26.9	48.9	-28.9	52.3
139	ZINC000096158052	0.2	-49.9	-20.8	43.2	-34.2	61.9
140	ZINC000040060202	0.2	-46.1	-17.7	39.3	-33.7	58.4
141	ZINC000253433259	0.3	-49.1	-19.7	44.2	-31.4	56.3
142	ZINC000023642159	0.3	-47.6	-27.3	48.4	-32.0	58.8
143	ZINC000095393415	0.4	-54.8	-14.5	42.4	-32.4	59.7
144	ZINC000257222272	0.5	-51.4	-7.3	33.9	-34.8	60.1
145	ZINC000328587242	0.5	-45.2	-23.7	42.3	-34.1	61.2
146	ZINC000002646979	0.5	-51.5	-22.3	47.4	-32.2	59.1
147	ZINC000238886413	0.5	-49.4	-11.6	37.1	-32.3	56.7
148	ZINC000097201269	0.7	-49.4	-16.9	41.4	-35.5	61.2
149	ZINC000065395709	0.7	-51.6	-22.3	50.7	-35.3	59.1
150	ZINC000006117573	0.8	-42.2	-28.0	47.0	-30.2	54.3
151	ZINC000016228943	0.8	-43.6	-26.3	45.9	-29.4	54.3
152	ZINC000040548686	0.9	-51.5	-23.2	49.8	-32.4	58.2
153	ZINC000042025678	1.0	-43.6	-12.3	33.3	-29.1	52.8
154	ZINC000192753414	1.1	-46.9	-32.1	56.3	-31.0	54.8
155	ZINC000069349055	1.1	-48.3	-24.2	47.9	-34.0	59.7
156	ZINC000058099587	1.2	-46.8	-18.8	42.1	-31.9	56.6
157	ZINC000004535480	1.2	-45.6	-15.4	38.6	-28.7	52.3
158	ZINC000005426253	1.2	-49.8	-11.6	36.2	-34.6	61.0
159	ZINC000050857093	1.2	-48.7	-25.4	51.1	-32.3	56.6
160	ZINC000178511392	1.3	-40.2	-33.5	52.3	-29.5	52.1
161	ZINC000005026046	1.3	-45.8	-14.0	35.2	-30.4	56.4
162	ZINC000095503625	1.4	-50.6	-24.3	51.5	-34.5	59.2
163	ZINC000035671101	1.4	-46.7	-8.2	30.9	-29.8	55.1
164	ZINC000069775761	1.5	-48.1	-21.8	45.0	-32.2	58.6
165	ZINC000097413355	1.6	-46.7	-27.5	47.9	-30.7	58.6
166	ZINC000013691850	1.6	-49.9	-15.3	42.3	-31.2	55.6
167	ZINC000585280336	1.6	-51.7	-30.1	57.6	-32.2	58.1
168	ZINC000050584912	1.6	-50.3	-6.3	32.9	-33.4	58.7
169	ZINC000069595091	1.8	-45.8	-22.4	46.0	-32.7	56.6
170	ZINC000022549345	1.8	-53.9	-18.2	47.5	-34.7	61.0
171	ZINC000409428381	1.8	-51.5	-12.2	39.2	-35.9	62.2
172	ZINC000072096437	1.8	-50.9	-18.3	45.9	-35.2	60.3
173	ZINC000065463577	1.8	-46.6	-32.2	55.7	-31.1	56.0
174	ZINC000072277544	1.8	-45.7	-15.0	37.7	-29.9	54.8
175	ZINC000072300733	1.9	-51.3	-12.8	40.6	-33.3	58.7

#	ZINC ID	ΔG_{bind}	ΔE_{vdW}	ΔE_{el}	ΔG_{pol}	ΔG_{np}	ΔG_{disp}
176	ZINC000052955795	2.0	-46.7	-27.1	49.1	-33.1	59.8
177	ZINC000012550491	2.2	-46.4	-23.5	47.0	-31.1	56.3
178	ZINC000003852421	2.2	-44.3	-12.3	35.0	-28.4	52.1
179	ZINC000001810957	2.2	-45.8	-17.2	41.9	-31.0	54.3
180	ZINC000091304527	2.2	-50.9	-14.0	40.6	-34.3	60.8
181	ZINC000040386093	2.3	-45.0	-13.8	38.2	-31.4	54.3
182	ZINC000072290753	2.3	-52.3	-26.0	53.7	-32.4	59.4
183	ZINC000057771728	2.3	-48.2	-24.0	49.7	-33.0	57.7
184	ZINC000005303591	2.5	-44.2	-20.2	42.9	-31.2	55.1
185	ZINC000034895992	2.5	-49.7	-29.9	56.3	-35.0	60.9
186	ZINC000072290711	2.5	-46.7	-16.6	39.1	-29.4	56.2
187	ZINC000040386098	2.6	-42.7	-13.8	36.9	-30.0	52.0
188	ZINC000014741626	2.6	-49.6	-6.8	33.0	-33.4	59.5
189	ZINC000306138347	2.7	-49.7	-17.2	44.5	-32.0	57.1
190	ZINC000257256038	2.7	-45.9	-24.2	47.3	-32.2	57.7
191	ZINC000013691849	2.8	-44.2	-33.9	56.2	-31.2	55.9
192	ZINC000079001413	2.8	-52.9	-9.1	38.0	-33.8	60.6
193	ZINC000002922856	2.8	-52.4	-15.5	46.1	-33.4	58.1
194	ZINC000023764785	2.8	-45.9	-15.6	40.0	-32.1	56.5
195	ZINC000013692677	3.2	-51.9	-30.8	59.8	-34.6	60.6
196	ZINC000029134571	3.2	-52.1	-19.6	50.3	-33.8	58.4
197	ZINC000040385901	3.2	-41.1	-13.0	36.0	-28.8	50.1
198	ZINC000096122792	3.3	-48.6	-9.2	37.6	-31.0	54.4
199	ZINC000008776545	3.3	-47.3	-15.4	40.4	-31.0	56.6
200	ZINC000072290626	3.3	-48.7	-19.4	45.1	-31.5	57.8
201	ZINC000096251709	3.4	-48.0	-18.9	44.7	-32.0	57.6
202	ZINC000028790813	3.4	-51.7	-24.1	52.5	-33.4	60.1
203	ZINC000096038482	3.4	-39.5	-24.6	43.4	-29.8	53.9
204	ZINC000044908085	3.4	-51.1	-21.0	48.6	-31.9	58.9
205	ZINC000170800517	3.5	-49.4	-18.5	44.9	-34.0	60.6
206	ZINC000091664087	3.6	-54.4	-7.8	39.1	-34.2	60.9
207	ZINC000085879141	3.6	-41.7	-10.6	32.2	-29.1	52.8
208	ZINC000257257831	3.7	-45.8	-12.3	38.3	-30.3	53.8
209	ZINC000072437791	3.8	-46.5	-12.5	38.1	-30.8	55.4
210	ZINC000095402766	3.9	-44.9	-16.8	40.7	-32.2	57.0
211	ZINC000096837115	3.9	-45.6	-27.4	50.7	-31.5	57.8
212	ZINC000003327891	4.0	-45.9	-11.8	36.6	-31.1	56.3
213	ZINC000019973951	4.1	-40.3	-29.4	48.2	-28.2	53.8
214	ZINC000006782318	4.1	-47.7	-18.1	43.9	-31.1	57.1
215	ZINC000096080454	4.2	-44.4	-19.6	44.1	-29.5	53.6
216	ZINC000005088834	4.3	-42.9	-7.6	31.3	-30.3	53.7
217	ZINC000245171655	4.3	-48.7	-10.2	39.1	-32.6	56.7
218	ZINC000097050589	4.4	-48.8	-13.2	42.6	-32.2	55.9
219	ZINC000012508838	4.4	-49.0	-24.8	54.5	-33.3	57.0
220	ZINC000065167646	4.4	-47.8	-21.8	49.2	-32.1	56.9
221	ZINC000253407066	4.5	-46.7	-13.8	41.2	-31.7	55.4

#	ZINC ID	ΔG_{bind}	ΔE_{vdW}	ΔE_{el}	ΔG_{pol}	ΔG_{np}	ΔG_{disp}
222	ZINC000071746202	4.6	-47.6	-15.1	39.6	-31.9	59.6
223	ZINC000257270100	4.6	-46.1	-10.6	37.3	-31.8	55.8
224	ZINC000071282106	4.7	-47.7	-15.4	40.9	-33.0	59.9
225	ZINC000008771448	4.7	-48.5	-23.5	51.6	-32.9	58.1
226	ZINC000000489138	4.8	-50.3	-20.6	51.6	-32.3	56.3
227	ZINC000153353600	4.9	-46.2	-8.9	35.1	-31.7	56.7
228	ZINC000003875380	4.9	-46.6	-15.5	39.6	-28.6	56.1
229	ZINC000065591272	5.3	-44.9	-9.7	35.0	-31.5	56.3
230	ZINC000019328346	5.4	-46.7	-22.0	48.9	-31.6	56.9
231	ZINC000072896859	5.4	-48.3	-6.8	34.3	-32.6	58.9
232	ZINC000057511709	5.4	-45.5	-22.5	49.1	-30.8	55.1
233	ZINC000034407910	5.5	-38.4	-15.1	36.8	-26.9	49.1
234	ZINC000062639858	5.6	-52.0	-3.0	33.8	-34.7	61.5
235	ZINC000299793701	5.8	-42.4	-24.9	47.1	-30.1	56.1
236	ZINC000091321614	5.9	-49.4	-18.7	47.5	-33.2	59.7
237	ZINC000030875068	6.0	-45.9	-10.0	37.4	-30.4	54.8
238	ZINC000071497775	6.0	-51.3	-25.4	56.4	-34.5	60.9
239	ZINC000072807915	6.0	-50.6	-7.2	36.8	-33.9	60.9
240	ZINC000012407997	6.3	-48.0	-11.5	40.0	-33.1	59.0
241	ZINC000006887927	6.3	-48.4	-23.8	52.3	-33.9	60.0
242	ZINC000584897275	6.4	-44.7	-36.7	60.9	-32.1	59.0
243	ZINC000253473237	6.5	-44.9	-8.3	35.6	-31.5	55.7
244	ZINC000096069207	6.6	-52.2	-20.5	51.6	-33.3	60.9
245	ZINC000027755553	6.7	-46.7	-15.5	44.1	-31.2	56.1
246	ZINC000048249797	6.7	-50.8	-10.3	42.1	-33.8	59.5
247	ZINC000330033487	6.8	-50.1	-15.9	47.2	-33.3	58.9
248	ZINC000002390471	6.8	-43.9	-12.4	37.7	-29.4	54.8
249	ZINC000084563579	6.9	-45.4	-20.3	49.7	-33.4	56.3
250	ZINC000047209496	6.9	-44.4	-13.3	40.4	-31.5	55.7
251	ZINC000255187536	6.9	-42.3	-21.3	46.6	-29.4	53.4
252	ZINC000072235028	7.0	-52.8	-12.4	45.9	-34.1	60.4
253	ZINC000004722011	7.2	-44.0	-7.1	33.8	-29.5	54.0
254	ZINC000096069697	7.7	-45.5	-9.3	36.2	-30.7	56.9
255	ZINC000005348603	7.8	-46.3	-8.7	39.0	-31.3	55.1
256	ZINC000239762559	8.1	-48.8	-21.2	52.5	-32.5	58.1
257	ZINC000022067509	8.1	-49.1	-30.2	62.4	-34.0	59.0
258	ZINC000018240833	8.1	-47.5	-37.8	67.0	-32.9	59.2
259	ZINC000192929211	8.4	-44.2	-24.0	52.8	-31.7	55.6
260	ZINC000040266307	8.7	-44.5	-22.2	50.7	-31.2	55.9
261	ZINC000077522487	8.8	-48.6	-28.5	58.3	-33.0	60.4
262	ZINC000017888288	9.0	-44.1	-16.9	45.5	-28.4	52.9
263	ZINC000170016387	9.1	-42.6	-20.3	47.9	-31.4	55.6
264	ZINC000068269627	9.3	-50.4	-27.6	60.1	-33.1	60.3
265	ZINC000004732939	9.3	-43.8	-12.5	42.8	-31.5	54.4
266	ZINC000006556210	9.3	-41.4	-11.3	39.4	-28.3	50.9
267	ZINC000136345745	9.4	-51.8	-19.5	55.0	-33.3	59.0

#	ZINC ID	ΔG_{bind}	ΔE_{vdW}	ΔE_{el}	ΔG_{pol}	ΔG_{np}	ΔG_{disp}
268	ZINC000000079035	9.6	-47.2	-19.1	50.2	-32.7	58.5
269	ZINC000091487017	9.7	-49.3	-11.4	43.6	-33.4	60.3
270	ZINC000238831563	9.8	-47.8	-11.4	45.2	-31.1	55.0
271	ZINC000002837442	9.8	-42.9	-16.1	43.4	-30.1	55.5
272	ZINC000237740654	10.0	-45.0	-3.6	32.9	-31.7	57.5
273	ZINC000000353960	10.1	-35.6	-38.0	65.4	-27.4	45.6
274	ZINC000253433605	10.1	-47.3	-14.5	47.9	-32.7	56.6
275	ZINC000008609997	10.1	-50.6	-13.5	48.4	-32.9	58.7
276	ZINC000000201272	10.3	-46.5	-7.2	39.9	-30.2	54.3
277	ZINC000061067795	10.6	-48.3	-13.8	47.4	-32.7	58.0
278	ZINC000004495846	10.7	-46.3	-26.6	56.9	-31.0	57.6
279	ZINC000107713021	11.0	-44.7	-2.8	32.5	-31.7	57.7
280	ZINC000019796838	11.1	-46.3	-11.2	42.9	-30.7	56.3
281	ZINC000089857747	11.1	-50.7	-7.6	44.1	-32.6	57.9
282	ZINC000001620500	11.5	-42.1	-26.7	56.1	-29.8	53.9
283	ZINC000009318781	11.6	-46.3	-25.9	60.2	-30.0	53.6
284	ZINC000268943077	11.6	-41.8	6.5	22.8	-29.3	53.4
285	ZINC000012557330	12.3	-43.0	-10.6	40.7	-27.7	52.8
286	ZINC000006918427	12.3	-45.0	-13.2	45.8	-30.0	54.7
287	ZINC000012142779	12.9	-50.2	-15.4	52.2	-34.2	60.5
288	ZINC000215185695	13.1	-47.4	-16.7	51.7	-34.3	59.9
289	ZINC000072432742	13.3	-49.1	1.8	35.2	-33.3	58.6
290	ZINC000005244779	13.5	-49.8	-9.7	47.4	-33.1	58.6
291	ZINC000284798034	13.6	-50.9	-22.8	62.0	-32.4	57.7
292	ZINC000012239509	13.9	-50.5	-7.5	45.9	-33.8	59.8
293	ZINC000012122382	14.2	-42.6	-9.7	40.2	-30.1	56.5
294	ZINC000013278475	14.4	-48.6	-19.5	59.8	-32.5	55.2
295	ZINC000575617533	14.4	-44.8	-10.3	42.4	-31.4	58.4
296	ZINC000004807849	14.7	-36.5	-47.4	74.5	-26.7	50.9
297	ZINC000237955843	16.3	-40.6	-42.8	73.6	-30.5	56.6
298	ZINC000018177963	16.7	-32.7	-55.9	82.0	-25.9	49.2
299	ZINC000006576136	17.2	-34.5	-6.9	37.6	-26.5	47.5
300	ZINC000069895275	18.4	-37.0	-10.2	43.9	-27.3	49.0
301	ZINC000004806959	18.7	-39.4	-29.2	63.2	-29.0	53.1
302	ZINC000237699092	21.8	-40.8	-8.7	45.0	-29.6	55.9
303	ZINC000008848147	21.9	-38.7	-0.8	39.0	-27.4	49.9
304	ZINC000003947438	22.2	-41.0	-21.6	59.8	-29.4	54.5
305	ZINC000096198984	24.0	-45.9	-8.9	52.1	-32.0	58.7

Table S4. Energy decomposition of the MM/PBSA results for the 305 compounds using the *PB-4* parameter set (for more details see the Methods section). All energy terms are given in kcal/mol with their standard deviation (*std*) and are sorted by the binding free energy (ΔG_{bind}) followed by the molecular mechanics van der Waals and electrostatic interactions terms (ΔE_{vdW} and ΔE_{el}) and the polar and non-polar contributions to the solvation free energy (ΔG_{pol} and ΔG_{np}). Compounds marked in boldface were finally selected for experimental screening.

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
1	ZINC000035869910	-38.7	4.4	-54.6	2.6	-35.5	5.1	57.7	3.7	-6.3	0.1
2	ZINC000003463362	-37.7	3.3	-50.0	2.8	-30.9	4.2	49.5	4.1	-6.3	0.2
3	ZINC000091270543	-36.9	3.4	-53.6	3.0	-23.0	3.8	46.0	3.0	-6.2	0.1
4	ZINC000084578820	-36.3	4.2	-47.8	2.6	-35.8	7.0	53.2	4.0	-5.8	0.1
5	ZINC000257317306	-36.2	4.5	-50.1	2.8	-41.5	3.3	62.1	4.2	-6.7	0.1
6	ZINC000084598177	-36.2	3.5	-49.0	2.5	-29.0	3.2	47.6	3.7	-5.8	0.1
7	ZINC000005360885	-36.0	4.2	-48.1	2.7	-36.1	4.9	53.9	2.7	-5.7	0.1
8	ZINC000095415912	-35.4	3.9	-53.2	2.7	-28.4	4.2	52.1	3.0	-6.0	0.1
9	ZINC000057563200	-35.4	4.4	-49.9	2.7	-17.6	4.6	38.4	3.2	-6.4	0.1
10	ZINC000022191233	-35.1	3.5	-53.6	2.9	-31.4	3.7	56.0	3.1	-6.1	0.1
11	ZINC000092065700	-34.4	3.7	-52.6	2.5	-19.7	2.9	44.5	3.6	-6.5	0.1
12	ZINC000079491038	-34.4	4.3	-51.3	2.7	-28.2	5.1	51.2	4.7	-6.1	0.2
13	ZINC000010256259	-34.3	3.8	-52.7	2.7	-42.1	3.7	66.5	3.7	-6.0	0.1
14	ZINC000069562405	-33.7	3.1	-47.4	2.6	-27.1	2.9	46.6	2.4	-5.8	0.1
15	ZINC000000333210	-33.6	3.2	-50.6	3.0	-32.6	3.7	55.3	3.0	-5.8	0.1
16	ZINC000084686490	-33.6	3.6	-46.1	2.4	-33.4	3.0	51.8	3.1	-6.0	0.1
17	ZINC000223692657	-33.5	3.3	-50.8	2.6	-28.2	3.9	51.2	2.7	-5.7	0.1
18	ZINC000018148904	-33.4	3.5	-50.1	2.6	-32.4	3.5	54.7	2.7	-5.7	0.1
19	ZINC000096199614	-33.3	3.7	-51.3	2.5	-28.0	3.7	51.5	2.7	-5.5	0.1
20	ZINC000069737923	-33.2	3.3	-46.3	2.3	-30.1	4.0	49.5	3.1	-6.3	0.1
21	ZINC000096058349	-33.1	3.8	-54.1	2.4	-18.0	2.3	44.9	2.7	-5.8	0.1
22	ZINC000043550595	-33.1	4.0	-48.3	2.5	-29.1	3.4	50.3	3.0	-6.1	0.1
23	ZINC000092078469	-33.0	3.9	-45.0	3.2	-24.1	3.6	42.2	3.6	-6.2	0.2
24	ZINC000092022499	-33.0	3.5	-53.4	2.6	-23.3	2.6	50.0	3.4	-6.3	0.1
25	ZINC000071915224	-32.9	3.7	-49.3	2.3	-26.5	3.5	48.7	3.4	-5.9	0.1
26	ZINC000095950700	-32.9	3.2	-48.8	2.7	-19.6	2.1	41.3	2.9	-5.8	0.1
27	ZINC000100193536	-32.8	3.6	-48.7	2.9	-15.8	2.9	37.6	2.7	-5.9	0.1
28	ZINC000091270544	-32.7	3.8	-52.4	2.7	-22.2	3.8	48.2	3.5	-6.3	0.1
29	ZINC000015078577	-32.6	3.8	-49.4	2.8	-29.5	4.6	52.5	4.6	-6.2	0.1
30	ZINC000051467674	-32.6	3.6	-46.6	2.7	-40.1	3.8	60.0	3.3	-5.9	0.1
31	ZINC000095410774	-32.5	3.2	-50.5	2.4	-24.2	3.1	47.7	2.7	-5.5	0.1
32	ZINC000240454699	-32.2	3.2	-42.5	2.5	-25.1	4.6	41.3	3.5	-5.9	0.1
33	ZINC000216315534	-32.1	2.7	-41.9	2.5	-28.6	4.7	44.1	3.7	-5.7	0.1
34	ZINC000089827813	-32.1	4.1	-46.6	3.2	-29.5	4.7	49.7	2.6	-5.6	0.1
35	ZINC000225746732	-32.0	2.6	-47.5	2.3	-21.3	2.3	42.2	2.3	-5.5	0.1
36	ZINC000004722089	-32.0	3.1	-48.1	2.5	-14.7	2.7	36.5	2.6	-5.7	0.1
37	ZINC000195547314	-31.9	3.2	-50.9	2.8	-14.0	3.2	39.2	2.7	-6.1	0.1
38	ZINC000334160460	-31.8	3.3	-49.1	2.5	-22.9	2.9	46.2	2.3	-5.9	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
39	ZINC000257299555	-31.5	3.6	-46.7	3.1	-38.1	4.3	58.9	3.7	-5.6	0.1
40	ZINC000075530913	-31.5	3.4	-49.2	2.3	-20.1	2.3	43.9	2.6	-6.1	0.1
41	ZINC000244816835	-31.5	3.3	-43.8	3.0	-34.4	3.6	52.7	2.9	-6.0	0.2
42	ZINC000057731402	-31.4	3.6	-51.2	2.6	-25.6	3.7	51.4	3.0	-6.1	0.1
43	ZINC000012888207	-31.4	2.6	-40.8	2.2	-27.7	3.4	42.3	2.8	-5.2	0.1
44	ZINC000091486946	-31.3	3.8	-52.4	2.6	-21.0	2.8	48.4	4.0	-6.3	0.1
45	ZINC000229623928	-31.2	4.0	-50.6	2.5	-33.6	3.7	59.2	3.9	-6.1	0.1
46	ZINC000025032259	-31.0	4.1	-54.4	2.7	-22.2	3.2	52.2	4.5	-6.7	0.1
47	ZINC000306141880	-31.0	3.2	-46.5	2.8	-29.4	4.2	50.8	2.9	-6.0	0.1
48	ZINC000021835963	-31.0	3.2	-48.7	2.2	-25.8	3.3	49.5	2.8	-6.0	0.1
49	ZINC000100191495	-31.0	3.6	-46.6	2.6	-14.5	2.6	35.6	2.8	-5.4	0.1
50	ZINC000002216953	-31.0	3.3	-48.7	2.4	-24.8	3.2	48.5	3.0	-6.0	0.1
51	ZINC000022241454	-31.0	3.6	-39.1	2.9	-39.2	6.6	52.9	6.4	-5.6	0.1
52	ZINC000100193430	-30.9	2.9	-47.9	2.4	-14.3	2.6	36.7	2.6	-5.4	0.1
53	ZINC000004998502	-30.8	4.8	-53.5	3.3	-39.4	4.2	68.1	4.5	-6.1	0.1
54	ZINC000154455008	-30.6	3.7	-44.9	2.8	-15.4	6.2	35.8	4.2	-6.0	0.1
55	ZINC000008316344	-30.5	3.9	-51.0	2.4	-5.6	2.6	32.0	4.0	-5.9	0.1
56	ZINC000095469884	-30.5	3.1	-40.0	2.8	-35.7	3.7	50.4	2.5	-5.2	0.1
57	ZINC000040473994	-30.5	3.1	-49.6	2.8	-26.5	4.0	51.3	2.7	-5.8	0.1
58	ZINC000044874685	-30.4	4.1	-44.2	2.8	-24.3	4.6	44.0	3.9	-5.9	0.1
59	ZINC000091486133	-30.3	3.5	-52.7	2.9	-25.7	3.2	54.4	3.2	-6.2	0.1
60	ZINC000194368147	-30.3	3.4	-48.3	2.8	-31.3	3.5	54.9	2.5	-5.6	0.1
61	ZINC000022549345	-30.2	3.5	-53.9	2.1	-16.6	3.8	46.7	5.3	-6.5	0.1
62	ZINC000096238948	-30.1	4.0	-53.8	2.7	-14.2	5.3	44.2	6.2	-6.3	0.1
63	ZINC000091768990	-30.1	3.7	-52.4	2.8	-14.9	2.6	43.1	2.6	-5.8	0.1
64	ZINC000069846908	-29.9	5.0	-50.0	3.0	-33.3	7.7	59.4	4.2	-6.0	0.1
65	ZINC000011781217	-29.8	3.6	-52.0	2.2	-13.7	2.4	42.4	3.6	-6.5	0.1
66	ZINC000257206611	-29.8	5.2	-55.3	3.1	-11.5	5.7	43.2	7.0	-6.2	0.1
67	ZINC000097201269	-29.7	5.8	-49.4	2.6	-17.3	4.2	43.5	5.6	-6.4	0.1
68	ZINC000230113696	-29.6	3.9	-52.9	2.8	-23.6	4.3	52.9	4.2	-6.1	0.1
69	ZINC000012142783	-29.6	5.4	-51.0	2.5	-22.0	5.0	49.8	5.8	-6.4	0.1
70	ZINC000575618196	-29.6	3.9	-54.5	2.7	-27.3	3.9	58.5	3.6	-6.2	0.1
71	ZINC000257222272	-29.5	3.1	-51.4	2.2	-7.4	2.0	35.6	2.8	-6.3	0.1
72	ZINC000044919578	-29.5	2.9	-43.0	2.1	-29.3	3.4	48.4	3.1	-5.6	0.1
73	ZINC000257211885	-29.4	5.5	-50.3	3.9	-20.9	3.8	47.7	4.0	-5.9	0.1
74	ZINC000014791001	-29.4	3.4	-47.0	2.3	-21.6	3.5	44.7	3.0	-5.5	0.1
75	ZINC000008913866	-29.3	4.4	-50.7	2.5	-29.7	6.1	56.9	5.2	-5.9	0.1
76	ZINC000034895992	-29.2	5.0	-49.7	2.7	-29.8	3.4	56.7	4.3	-6.4	0.1
77	ZINC000171342968	-29.2	4.9	-48.4	2.7	-40.1	3.9	65.5	3.9	-6.2	0.2
78	ZINC000008595944	-29.1	4.0	-53.1	2.3	-13.8	4.1	43.5	4.1	-5.9	0.1
79	ZINC000091943530	-29.0	3.9	-44.1	2.7	-17.5	4.4	38.7	3.3	-6.0	0.1
80	ZINC000071746202	-29.0	3.7	-47.6	2.6	-14.6	3.6	39.6	6.1	-6.3	0.1
81	ZINC000257310083	-28.9	3.3	-47.2	2.6	-17.0	2.4	41.0	2.4	-5.8	0.1
82	ZINC000328587242	-28.9	3.2	-45.2	2.7	-24.8	2.6	47.4	2.6	-6.4	0.1
83	ZINC000012323932	-28.9	5.3	-42.7	3.2	-38.4	7.2	57.7	3.8	-5.5	0.2
84	ZINC000075118384	-28.8	4.8	-46.9	2.9	-33.1	7.3	57.3	4.9	-6.1	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
85	ZINC000585280336	-28.8	5.1	-51.7	2.3	-29.6	5.8	58.2	4.5	-5.7	0.1
86	ZINC000096251711	-28.8	3.6	-50.9	3.0	-15.0	3.5	43.0	3.3	-5.9	0.1
87	ZINC000097413355	-28.8	2.9	-46.7	2.6	-27.2	3.2	50.9	3.4	-5.7	0.1
88	ZINC000257192562	-28.7	3.1	-45.9	2.2	-17.6	2.3	40.7	2.5	-5.9	0.1
89	ZINC000095951555	-28.7	2.9	-42.9	2.3	-19.4	3.3	38.9	2.7	-5.4	0.1
90	ZINC000007030648	-28.7	5.4	-43.3	2.9	-21.2	7.0	41.2	3.4	-5.3	0.1
91	ZINC000096003964	-28.7	4.9	-49.1	2.6	-26.9	4.8	52.8	3.3	-5.5	0.1
92	ZINC000004511530	-28.5	3.3	-49.2	2.1	-22.4	3.0	48.9	3.0	-5.7	0.1
93	ZINC000409428381	-28.4	3.8	-51.5	2.4	-12.1	4.9	41.9	4.8	-6.6	0.1
94	ZINC000096158052	-28.4	3.6	-49.9	2.5	-20.8	3.8	48.9	4.1	-6.6	0.1
95	ZINC000057526426	-28.3	3.0	-44.4	2.2	-28.2	3.1	50.3	3.0	-5.9	0.1
96	ZINC000014741626	-28.3	3.7	-49.6	2.2	-7.1	2.5	34.8	4.5	-6.3	0.1
97	ZINC000072290626	-28.2	4.5	-48.7	2.2	-18.8	5.2	45.2	5.8	-6.0	0.1
98	ZINC000067643674	-28.2	3.4	-44.8	2.5	-25.4	4.2	47.5	3.2	-5.6	0.1
99	ZINC000077503523	-28.2	3.7	-45.1	2.9	-34.1	6.6	56.3	4.6	-5.4	0.1
100	ZINC000100737122	-28.1	3.3	-52.3	2.5	-22.6	3.1	52.8	4.1	-6.0	0.1
101	ZINC000013973188	-28.1	4.1	-47.2	2.5	-29.0	3.6	53.8	3.7	-5.7	0.1
102	ZINC000069775761	-28.1	4.2	-48.1	2.6	-21.4	4.1	47.3	3.1	-6.0	0.2
103	ZINC000225489282	-28.0	3.7	-49.8	2.4	-17.0	4.8	44.6	4.4	-5.8	0.1
104	ZINC000008738218	-27.9	3.8	-41.0	2.9	-41.3	5.6	59.7	3.9	-5.3	0.1
105	ZINC000016228943	-27.9	3.1	-43.6	2.6	-26.4	3.3	47.8	3.1	-5.7	0.1
106	ZINC000035671101	-27.9	3.4	-46.7	2.0	-8.1	1.6	32.5	3.3	-5.7	0.1
107	ZINC000009338249	-27.6	4.9	-47.0	2.5	-27.3	4.7	52.1	4.0	-5.4	0.1
108	ZINC000069492530	-27.6	4.4	-47.5	2.6	-19.0	3.3	44.4	3.1	-5.6	0.1
109	ZINC000119429896	-27.6	3.6	-49.5	2.2	-11.7	2.9	39.9	3.3	-6.3	0.1
110	ZINC000585093122	-27.5	3.5	-45.2	2.6	-16.9	4.4	40.4	4.0	-5.8	0.1
111	ZINC000065248686	-27.5	3.3	-45.7	2.6	-14.8	2.7	38.6	2.3	-5.7	0.1
112	ZINC000003438521	-27.5	3.4	-45.4	2.3	-24.1	4.5	47.7	4.2	-5.7	0.1
113	ZINC000095393415	-27.4	4.4	-54.8	2.5	-14.4	3.2	47.4	5.0	-5.7	0.1
114	ZINC000079001413	-27.4	3.4	-52.9	2.5	-9.0	2.5	40.5	2.8	-6.0	0.1
115	ZINC000238121810	-27.4	5.9	-37.2	2.9	-110.9	10.4	126.7	8.2	-6.0	0.1
116	ZINC000007030710	-27.4	3.9	-47.3	2.7	-25.7	4.3	51.3	3.2	-5.6	0.1
117	ZINC000002750765	-27.3	3.6	-45.0	2.4	-24.2	2.9	47.7	3.7	-5.9	0.1
118	ZINC000100119126	-27.3	4.2	-47.3	2.8	-19.9	4.3	45.8	4.0	-5.8	0.1
119	ZINC000069778215	-27.2	3.7	-47.6	2.7	-41.7	4.2	68.1	3.8	-6.1	0.1
120	ZINC000092021781	-27.2	3.8	-49.3	2.9	-21.9	5.0	50.3	3.8	-6.2	0.1
121	ZINC000035398834	-27.2	3.3	-51.5	2.3	-8.9	2.5	38.9	3.3	-5.7	0.1
122	ZINC000013691850	-27.2	2.9	-49.9	2.5	-15.3	3.3	43.5	2.5	-5.4	0.1
123	ZINC000050859891	-27.2	4.1	-48.4	2.6	-28.7	4.7	55.6	5.3	-5.7	0.1
124	ZINC000003292603	-27.1	3.3	-47.2	2.4	-19.2	3.7	45.4	4.2	-6.1	0.1
125	ZINC000058099587	-27.1	4.3	-46.8	2.8	-18.8	3.4	44.6	4.2	-6.0	0.1
126	ZINC000050584912	-27.1	4.2	-50.3	2.8	-6.7	3.9	36.0	5.2	-6.2	0.1
127	ZINC000071754931	-26.9	3.2	-40.8	2.3	-12.7	3.3	32.0	3.0	-5.5	0.1
128	ZINC000075140034	-26.8	3.1	-41.8	2.4	-19.7	2.9	40.8	3.1	-6.1	0.1
129	ZINC000069349055	-26.8	5.7	-48.3	3.0	-24.4	8.4	52.3	6.0	-6.4	0.1
130	ZINC000064871452	-26.8	4.5	-49.9	2.5	-26.3	7.2	55.5	6.7	-6.1	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
131	ZINC000238886413	-26.8	4.6	-49.4	2.7	-11.3	3.3	39.7	3.1	-5.7	0.1
132	ZINC000040548686	-26.7	3.9	-51.5	2.2	-22.0	4.2	52.6	3.9	-5.8	0.1
133	ZINC000019973951	-26.7	4.1	-40.3	3.0	-29.7	6.5	49.1	5.4	-5.7	0.1
134	ZINC000002646979	-26.6	3.8	-51.5	2.3	-22.4	3.2	52.9	3.5	-5.7	0.1
135	ZINC000257218603	-26.6	4.1	-50.2	2.5	-24.7	5.1	54.9	4.9	-6.6	0.1
136	ZINC000044908085	-26.4	4.2	-51.1	2.7	-21.0	3.4	51.5	3.5	-5.9	0.1
137	ZINC000023642159	-26.4	3.8	-47.6	2.3	-27.5	4.0	54.8	4.0	-6.2	0.1
138	ZINC000092760184	-26.4	3.3	-47.5	2.4	-20.6	3.3	47.9	3.0	-6.3	0.1
139	ZINC000257256038	-26.3	3.6	-45.9	2.4	-25.3	3.1	50.7	3.0	-5.9	0.1
140	ZINC000074014922	-26.2	2.7	-47.0	2.1	-10.1	2.3	36.3	2.1	-5.5	0.1
141	ZINC000072234903	-26.2	3.2	-44.1	2.2	-12.2	3.9	35.8	5.0	-5.6	0.1
142	ZINC000050857093	-26.2	5.0	-48.7	2.5	-24.6	3.8	53.0	4.2	-5.9	0.1
143	ZINC000018240833	-26.2	4.3	-47.5	2.8	-36.3	5.3	63.8	4.2	-6.2	0.1
144	ZINC000095447759	-26.1	4.4	-46.9	2.9	-24.7	5.4	51.0	3.8	-5.5	0.1
145	ZINC000016543876	-26.1	4.1	-46.0	2.3	-18.4	3.8	44.0	2.6	-5.7	0.1
146	ZINC000010218408	-26.0	5.8	-47.3	2.8	-19.0	5.6	45.8	5.0	-5.5	0.1
147	ZINC000018053795	-25.9	4.5	-47.5	2.3	-23.2	3.7	50.7	4.3	-5.9	0.1
148	ZINC000072896859	-25.9	4.2	-48.3	2.6	-6.4	5.0	34.9	5.7	-6.1	0.1
149	ZINC000042025678	-25.9	3.6	-43.6	4.1	-13.2	5.4	36.9	3.6	-5.9	0.1
150	ZINC000040060202	-25.8	3.3	-46.1	2.8	-17.7	3.4	44.3	3.3	-6.3	0.1
151	ZINC000067460397	-25.7	3.3	-50.1	2.2	-34.7	3.6	64.7	3.6	-5.6	0.1
152	ZINC000584887110	-25.7	3.5	-46.9	2.2	-13.7	2.9	40.8	3.5	-5.9	0.1
153	ZINC000096837115	-25.6	5.0	-45.6	4.0	-26.8	7.8	53.1	8.2	-6.3	0.1
154	ZINC000071282106	-25.6	4.6	-47.7	2.6	-16.3	4.9	44.5	4.5	-6.1	0.1
155	ZINC000091304527	-25.6	3.8	-50.9	2.5	-14.3	4.5	45.8	5.0	-6.2	0.1
156	ZINC000003875380	-25.6	3.1	-46.6	1.9	-16.5	2.0	43.0	3.2	-5.5	0.1
157	ZINC000003313076	-25.5	3.5	-41.7	3.0	-21.4	4.5	42.7	2.9	-5.2	0.1
158	ZINC000052955795	-25.5	4.2	-46.7	2.6	-27.4	4.9	54.8	3.2	-6.1	0.1
159	ZINC000170800517	-25.5	3.2	-49.4	2.4	-18.6	2.4	48.8	3.0	-6.2	0.1
160	ZINC000178511392	-25.4	3.8	-40.2	2.5	-33.4	4.1	53.6	3.1	-5.4	0.1
161	ZINC000069595091	-25.3	4.1	-45.8	2.8	-22.3	3.9	49.0	6.2	-6.2	0.2
162	ZINC000096251709	-25.2	3.5	-48.0	2.1	-19.0	3.2	47.7	3.0	-5.9	0.1
163	ZINC000028790813	-25.2	5.4	-51.7	2.7	-23.6	5.6	56.4	5.4	-6.3	0.1
164	ZINC000153353600	-25.1	4.4	-46.2	2.7	-9.4	3.9	36.8	4.6	-6.2	0.2
165	ZINC000072096437	-25.1	4.0	-50.9	2.4	-18.7	4.2	50.8	4.1	-6.3	0.1
166	ZINC000002922856	-25.1	3.8	-52.4	2.7	-15.2	3.6	48.4	4.4	-5.9	0.1
167	ZINC000077353582	-25.1	4.3	-48.6	2.8	-15.7	3.0	44.8	2.7	-5.5	0.1
168	ZINC000072300733	-25.0	5.1	-51.3	2.7	-13.5	4.4	45.6	3.4	-5.9	0.1
169	ZINC000000326909	-25.0	3.5	-42.9	2.1	-16.5	3.4	39.7	2.6	-5.2	0.1
170	ZINC000002630701	-24.9	3.6	-49.0	2.0	-7.6	4.1	37.4	4.3	-5.7	0.1
171	ZINC000084563579	-24.8	4.1	-45.4	4.0	-21.3	15.9	48.1	12.0	-6.3	0.1
172	ZINC000177842371	-24.8	3.4	-45.3	2.0	-26.9	3.7	52.7	4.0	-5.3	0.1
173	ZINC000306138347	-24.8	3.3	-49.7	2.0	-17.4	3.2	48.0	3.1	-5.8	0.1
174	ZINC000095503625	-24.8	4.1	-50.6	2.6	-24.3	4.9	56.3	5.0	-6.2	0.1
175	ZINC000023764785	-24.7	5.5	-45.9	2.6	-14.8	4.5	42.0	4.4	-6.1	0.1
176	ZINC000005426253	-24.7	3.8	-49.8	2.4	-12.6	3.2	44.1	4.2	-6.3	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
177	ZINC000072290753	-24.6	4.2	-52.3	2.4	-25.4	4.1	58.9	3.8	-5.8	0.1
178	ZINC000095402766	-24.6	5.5	-44.9	2.5	-17.6	7.1	43.9	4.0	-6.0	0.1
179	ZINC000072290711	-24.6	3.7	-46.7	2.9	-17.3	3.3	44.9	4.1	-5.5	0.1
180	ZINC000069740630	-24.6	5.3	-38.0	2.6	-20.8	4.5	40.0	3.2	-5.8	0.1
181	ZINC000019327176	-24.5	4.7	-40.2	3.0	-26.9	5.7	48.2	6.1	-5.7	0.1
182	ZINC000008776545	-24.5	3.4	-47.3	2.4	-15.6	2.9	44.0	2.5	-5.6	0.1
183	ZINC000003641308	-24.5	4.5	-45.0	2.6	-25.1	7.2	51.3	8.7	-5.6	0.2
184	ZINC000096024249	-24.5	4.2	-47.4	2.4	-17.8	5.0	45.9	4.0	-5.2	0.1
185	ZINC000008771448	-24.4	4.8	-48.5	3.0	-22.3	5.8	52.5	6.8	-6.1	0.2
186	ZINC000065167646	-24.4	5.6	-47.8	2.7	-22.4	4.0	51.6	6.2	-5.8	0.1
187	ZINC000005026046	-24.4	3.6	-45.8	2.3	-14.0	2.7	41.3	4.9	-5.9	0.1
188	ZINC000072235028	-24.2	3.6	-52.8	2.4	-12.0	4.3	46.7	4.0	-6.1	0.1
189	ZINC000072277544	-24.2	3.9	-45.7	2.8	-14.8	5.4	42.2	5.1	-5.8	0.1
190	ZINC000192753414	-24.2	4.5	-46.9	2.7	-33.1	4.6	61.1	3.1	-5.4	0.1
191	ZINC000245171655	-24.2	3.1	-48.7	2.3	-10.2	2.7	40.7	2.6	-6.0	0.1
192	ZINC000065463577	-24.1	3.9	-46.6	2.7	-31.9	5.2	60.0	4.3	-5.5	0.1
193	ZINC000135810445	-24.1	4.5	-44.5	2.6	-33.4	5.4	59.2	5.0	-5.5	0.1
194	ZINC000096010936	-24.1	3.0	-41.4	2.8	-27.6	3.2	50.7	2.5	-5.8	0.1
195	ZINC000071497775	-24.0	4.2	-51.3	2.3	-25.4	6.6	58.9	5.6	-6.2	0.1
196	ZINC000040386093	-24.0	3.7	-45.0	2.7	-14.5	3.0	41.3	3.1	-5.7	0.1
197	ZINC000096122792	-24.0	3.4	-48.6	2.6	-9.0	2.7	39.2	3.4	-5.6	0.1
198	ZINC000278659999	-24.0	4.3	-47.8	2.4	-23.5	3.5	53.4	4.5	-6.1	0.1
199	ZINC000029134571	-24.0	3.3	-52.1	2.4	-19.8	3.2	53.9	3.3	-5.9	0.1
200	ZINC000096038482	-23.9	4.1	-39.5	2.9	-25.3	6.7	46.8	5.7	-5.9	0.1
201	ZINC000253433259	-23.9	3.2	-49.1	2.2	-19.7	2.8	50.4	2.6	-5.5	0.1
202	ZINC000097105546	-23.9	4.0	-44.7	2.6	-21.9	3.7	48.0	3.2	-5.4	0.1
203	ZINC000062639858	-23.9	4.0	-52.0	2.2	-3.7	3.5	38.2	4.7	-6.5	0.1
204	ZINC000013691849	-23.8	4.6	-44.2	3.0	-33.9	4.8	59.9	4.1	-5.5	0.1
205	ZINC000001381807	-23.7	2.7	-37.1	2.1	-15.1	2.3	33.5	2.9	-5.1	0.1
206	ZINC000006669352	-23.7	3.8	-47.6	2.2	-23.6	5.5	53.3	5.4	-5.8	0.1
207	ZINC000091664087	-23.3	4.4	-54.4	2.3	-8.4	3.4	45.5	3.8	-6.1	0.1
208	ZINC000014240188	-23.3	3.6	-45.7	2.8	-19.3	4.2	47.2	4.0	-5.6	0.1
209	ZINC000012550491	-23.3	3.2	-46.4	2.6	-24.3	3.5	53.3	2.9	-5.8	0.1
210	ZINC000095989182	-23.2	3.1	-43.2	2.2	-19.0	3.6	44.1	2.9	-5.2	0.1
211	ZINC000257311417	-23.2	3.3	-40.7	2.2	-22.2	4.6	45.6	4.8	-5.9	0.2
212	ZINC000013692677	-23.1	4.8	-51.9	3.1	-30.2	4.7	65.1	5.2	-6.2	0.1
213	ZINC000004535480	-23.1	4.3	-45.6	2.2	-15.5	4.7	43.2	5.4	-5.2	0.1
214	ZINC000002465084	-23.1	4.0	-49.8	2.5	-23.0	3.3	55.5	4.5	-5.8	0.1
215	ZINC000003327891	-23.1	3.1	-45.9	2.2	-11.5	2.2	40.1	3.2	-5.8	0.1
216	ZINC000006782318	-23.1	3.5	-47.7	2.3	-17.2	2.7	47.6	3.9	-5.8	0.1
217	ZINC000040386098	-23.0	3.6	-42.7	2.5	-14.7	3.4	39.9	3.3	-5.6	0.1
218	ZINC000085879141	-23.0	3.3	-41.7	2.4	-10.0	5.3	34.6	5.2	-5.9	0.1
219	ZINC000006117573	-22.9	3.4	-42.2	2.4	-29.4	2.9	54.6	3.4	-5.8	0.1
220	ZINC000005088834	-22.7	3.5	-42.9	3.6	-8.5	2.5	34.6	3.1	-5.9	0.1
221	ZINC000097050589	-22.7	4.8	-48.8	2.6	-13.0	4.7	45.0	5.3	-5.8	0.1
222	ZINC000065395709	-22.6	4.0	-51.6	2.4	-22.5	3.1	57.5	3.9	-6.0	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
223	ZINC000004495846	-22.6	5.1	-46.3	2.7	-25.8	4.2	55.3	4.7	-5.8	0.1
224	ZINC000072437791	-22.5	3.2	-46.5	2.2	-14.0	3.0	43.6	3.0	-5.6	0.1
225	ZINC000027755553	-22.5	3.4	-46.7	2.1	-15.9	3.0	46.1	3.3	-6.0	0.1
226	ZINC000096069207	-22.5	3.7	-52.2	2.8	-19.5	2.9	55.3	3.9	-6.1	0.1
227	ZINC000057771728	-22.4	4.4	-48.2	2.5	-23.3	5.5	55.2	5.7	-6.1	0.1
228	ZINC000239762559	-22.4	4.5	-48.8	2.5	-20.7	4.1	53.2	5.1	-6.0	0.1
229	ZINC000003852421	-22.3	3.2	-44.3	2.1	-12.6	2.6	39.9	2.8	-5.3	0.1
230	ZINC000091321614	-22.2	4.4	-49.4	2.4	-18.1	3.8	51.6	5.5	-6.2	0.1
231	ZINC000299793701	-22.0	4.2	-42.4	2.8	-25.9	5.0	51.8	3.9	-5.6	0.1
232	ZINC000012407997	-22.0	4.4	-48.0	2.8	-11.5	5.7	43.9	7.2	-6.3	0.1
233	ZINC000584897275	-21.8	5.0	-44.7	2.8	-36.2	4.3	65.5	6.0	-6.5	0.1
234	ZINC000096069697	-21.8	5.2	-45.5	2.3	-9.5	5.4	39.1	4.3	-5.8	0.1
235	ZINC000257257831	-21.8	3.7	-45.8	2.2	-13.1	4.8	42.6	4.5	-5.5	0.1
236	ZINC000253407066	-21.7	3.6	-46.7	2.4	-13.2	3.4	43.9	3.3	-5.8	0.1
237	ZINC000001810957	-21.6	4.4	-45.8	2.6	-17.6	3.6	47.5	4.6	-5.7	0.1
238	ZINC000000489138	-21.6	3.7	-50.3	2.3	-20.1	2.9	54.4	3.7	-5.7	0.1
239	ZINC000330033487	-21.5	4.2	-50.1	2.6	-15.4	4.4	50.2	3.6	-6.2	0.1
240	ZINC000057511709	-21.5	4.8	-45.5	2.0	-21.3	5.0	51.2	7.8	-5.9	0.1
241	ZINC000006887927	-21.1	5.0	-48.4	2.6	-23.5	3.7	57.1	5.3	-6.3	0.1
242	ZINC000096080454	-21.1	3.1	-44.4	2.3	-19.0	2.8	47.9	3.0	-5.6	0.1
243	ZINC000040385901	-21.0	3.8	-41.1	2.8	-13.7	2.9	39.3	3.2	-5.4	0.1
244	ZINC000237955843	-20.9	4.2	-40.6	2.6	-64.6	10.7	90.5	10.6	-6.3	0.2
245	ZINC000091487017	-20.8	4.0	-49.3	2.3	-11.6	3.0	46.2	3.6	-6.2	0.1
246	ZINC000004722011	-20.8	3.3	-44.0	2.2	-7.3	2.7	36.4	3.1	-5.9	0.1
247	ZINC000257270100	-20.8	5.7	-46.1	2.5	-11.5	2.9	42.6	4.7	-5.8	0.1
248	ZINC000009318781	-20.5	4.5	-46.3	2.8	-25.5	6.6	56.7	4.9	-5.5	0.1
249	ZINC000575617533	-20.5	3.9	-44.8	2.3	-10.6	3.0	41.3	4.7	-6.4	0.2
250	ZINC000065591272	-20.5	3.6	-44.9	2.2	-10.8	2.9	41.1	3.3	-5.9	0.1
251	ZINC000005303591	-20.5	3.9	-44.2	2.5	-20.1	3.9	49.7	4.2	-5.9	0.1
252	ZINC000077522487	-20.5	4.1	-48.6	2.2	-27.2	5.2	61.8	6.1	-6.5	0.1
253	ZINC000072807915	-20.4	4.7	-50.6	2.3	-8.1	3.6	44.8	5.8	-6.4	0.1
254	ZINC000019328346	-20.2	4.4	-46.7	4.6	-22.0	4.6	54.4	6.0	-5.9	0.1
255	ZINC000237740654	-20.2	4.5	-45.0	2.8	-28.0	10.4	59.0	11.9	-6.2	0.1
256	ZINC000048249797	-20.2	4.7	-50.8	2.7	-10.4	5.2	47.3	4.4	-6.3	0.1
257	ZINC000002390471	-20.1	3.3	-43.9	2.0	-12.0	2.3	41.8	3.1	-5.9	0.1
258	ZINC000030875068	-20.1	4.1	-45.9	2.2	-11.0	3.9	42.4	4.5	-5.7	0.1
259	ZINC000107713021	-19.9	4.2	-44.7	2.2	-3.4	2.9	34.5	3.7	-6.2	0.1
260	ZINC000068269627	-19.9	5.5	-50.4	2.4	-26.9	4.4	63.7	7.4	-6.2	0.1
261	ZINC000089857747	-19.7	3.7	-50.7	4.5	-7.1	5.1	43.9	9.7	-5.8	0.1
262	ZINC000000079035	-19.6	5.7	-47.2	2.3	-20.0	5.4	53.8	4.3	-6.2	0.1
263	ZINC000022067509	-19.6	8.1	-49.1	2.8	-56.9	11.1	92.3	9.7	-5.9	0.1
264	ZINC000001620500	-19.6	7.0	-42.1	2.8	-51.7	24.4	80.2	19.2	-6.0	0.1
265	ZINC000005244779	-19.6	4.5	-49.8	2.4	-9.1	2.7	45.4	4.4	-6.1	0.1
266	ZINC000040266307	-19.6	4.2	-44.5	2.5	-22.5	4.2	53.2	3.9	-5.8	0.1
267	ZINC000253473237	-19.5	3.4	-44.9	2.2	-8.2	2.9	39.7	3.1	-6.0	0.1
268	ZINC000017888288	-19.4	4.7	-44.1	2.3	-16.9	4.4	47.3	4.5	-5.6	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
269	ZINC000012122382	-19.2	6.0	-42.6	2.3	-9.5	4.8	38.9	6.5	-6.1	0.2
270	ZINC000002837442	-19.0	3.6	-42.9	2.8	-16.2	2.5	46.0	3.6	-5.9	0.2
271	ZINC000012239509	-19.0	5.3	-50.5	2.5	-8.0	5.0	45.8	3.9	-6.3	0.1
272	ZINC000004732939	-19.0	3.5	-43.8	2.2	-13.6	3.0	44.6	3.9	-6.1	0.1
273	ZINC000253433605	-19.0	5.1	-47.3	2.5	-14.9	7.6	49.1	5.6	-5.9	0.1
274	ZINC000006918427	-18.6	4.4	-45.0	2.5	-13.1	4.0	45.2	4.2	-5.7	0.1
275	ZINC000019796838	-18.4	4.6	-46.3	2.1	-10.9	3.4	44.4	3.9	-5.7	0.1
276	ZINC000008609997	-18.2	3.9	-50.6	2.4	-12.7	3.4	51.3	4.6	-6.2	0.1
277	ZINC000005348603	-18.1	4.3	-46.3	2.6	-9.9	4.8	43.7	5.3	-5.6	0.1
278	ZINC000047209496	-17.9	5.5	-44.4	2.4	-12.9	5.2	45.4	9.0	-5.9	0.1
279	ZINC000072432742	-17.9	5.0	-49.1	2.3	-23.0	9.9	60.3	10.1	-6.1	0.1
280	ZINC000192929211	-17.7	6.2	-44.2	2.7	-50.4	8.5	82.9	7.4	-5.9	0.1
281	ZINC000136345745	-17.6	4.7	-51.8	2.4	-18.5	4.8	58.7	4.6	-6.0	0.1
282	ZINC000215185695	-17.5	3.1	-47.4	2.1	-15.8	2.1	52.2	2.9	-6.5	0.1
283	ZINC000012508838	-17.1	4.7	-49.0	2.3	-24.7	4.2	62.5	5.2	-5.9	0.1
284	ZINC000006556210	-17.1	4.0	-41.4	2.6	-10.2	2.5	39.9	5.0	-5.4	0.1
285	ZINC000012142779	-16.9	5.8	-50.2	2.6	-15.4	9.7	55.2	7.6	-6.4	0.2
286	ZINC000034407910	-16.8	3.6	-38.4	2.1	-16.2	2.9	43.1	3.4	-5.2	0.1
287	ZINC000255187536	-16.7	3.9	-42.3	2.5	-21.5	3.7	52.6	3.7	-5.5	0.1
288	ZINC000268943077	-16.4	4.4	-41.8	2.6	-25.1	8.3	56.3	7.7	-5.9	0.1
289	ZINC000170016387	-16.3	3.7	-42.6	2.8	-20.5	5.3	53.0	5.0	-6.2	0.1
290	ZINC000012557330	-16.1	4.7	-43.0	2.5	-10.2	4.3	42.6	5.3	-5.6	0.1
291	ZINC000238831563	-15.8	4.7	-47.8	2.5	-11.5	4.4	49.2	4.0	-5.6	0.1
292	ZINC000004807849	-15.4	5.2	-36.5	3.5	-47.7	6.0	73.9	5.1	-5.1	0.1
293	ZINC000284798034	-15.2	4.4	-50.9	2.3	-22.1	4.5	63.5	5.1	-5.7	0.1
294	ZINC000013278475	-15.1	5.3	-48.6	2.9	-43.7	10.1	83.1	10.3	-5.9	0.2
295	ZINC000061067795	-15.1	4.2	-48.3	2.2	-15.0	3.9	54.2	5.0	-5.8	0.1
296	ZINC000018177963	-13.5	3.6	-32.7	3.1	-55.0	5.3	79.4	4.3	-5.2	0.1
297	ZINC000000201272	-13.1	4.7	-46.5	2.2	-6.7	5.2	45.6	4.2	-5.7	0.1
298	ZINC000006576136	-12.8	5.0	-34.5	2.6	-32.9	10.1	59.9	8.1	-5.3	0.1
299	ZINC000237699092	-11.6	6.4	-40.8	3.4	-32.2	15.3	67.7	15.9	-6.2	0.1
300	ZINC000000353960	-10.4	7.0	-35.6	2.7	-63.0	13.2	93.5	11.7	-5.3	0.1
301	ZINC000096198984	-10.0	5.0	-45.9	2.9	-8.7	3.7	51.0	5.6	-6.4	0.2
302	ZINC000004806959	-9.3	5.2	-39.4	2.6	-55.4	9.5	91.1	8.7	-5.5	0.1
303	ZINC000069895275	-9.0	4.8	-37.0	2.2	-35.4	13.7	68.8	12.0	-5.3	0.1
304	ZINC000003947438	-8.7	5.4	-41.0	2.4	-48.7	9.2	87.2	9.1	-6.1	0.1
305	ZINC000008848147	-5.4	4.9	-38.7	3.2	-26.7	14.3	65.4	12.0	-5.4	0.1

Table S5. Energy decomposition of the MM/GBSA results for the 305 compounds using the GB-1 parameter set (for more details see the Methods section). All energy terms are given in kcal/mol with their standard deviation (*std*) and are sorted by the binding free energy (ΔG_{bind}) followed by the molecular mechanics van der Waals and electrostatic interactions terms (ΔE_{vdW} and ΔE_{el}) and the polar and non-polar contributions to the solvation free energy (ΔG_{pol} and ΔG_{np}). Compounds marked in boldface were finally selected for experimental screening.

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
1	ZINC000257317306	-56.2	2.9	-50.1	2.8	-41.2	3.3	41.5	2.0	-6.5	0.2
2	ZINC000035869910	-55.5	3.3	-54.6	2.6	-34.9	5.2	40.7	2.8	-6.7	0.1
3	ZINC000010256259	-53.6	2.8	-52.7	2.7	-41.4	3.7	46.9	2.5	-6.4	0.1
4	ZINC000069778215	-53.5	3.0	-47.6	2.7	-42.2	4.2	42.6	2.2	-6.3	0.1
5	ZINC000091270543	-53.3	2.7	-53.6	3.0	-21.4	3.7	28.5	2.4	-6.7	0.1
6	ZINC000022191233	-53.1	2.7	-53.6	2.9	-30.9	3.7	38.1	2.5	-6.6	0.1
7	ZINC000004998502	-52.8	3.3	-53.5	3.3	-40.0	4.2	47.1	2.7	-6.3	0.2
8	ZINC000003463362	-52.6	2.8	-50.0	2.8	-30.0	4.2	33.8	2.8	-6.4	0.2
9	ZINC000095415912	-52.6	3.3	-53.2	2.7	-29.2	4.2	36.1	2.6	-6.3	0.1
10	ZINC000091486946	-52.2	2.6	-52.4	2.6	-21.3	2.8	28.1	2.3	-6.7	0.2
11	ZINC000092022499	-51.3	2.4	-53.4	2.6	-23.1	2.7	31.7	1.8	-6.6	0.1
12	ZINC000084578820	-51.1	3.2	-47.8	2.6	-35.2	7.0	37.8	3.8	-6.0	0.1
13	ZINC000091486133	-51.0	2.8	-52.7	2.9	-25.9	3.2	34.3	2.2	-6.6	0.2
14	ZINC000075530913	-50.9	2.2	-49.2	2.3	-20.2	2.3	24.7	1.5	-6.2	0.1
15	ZINC000096058349	-50.5	2.6	-54.1	2.4	-18.0	2.3	28.1	1.4	-6.5	0.1
16	ZINC000023642159	-50.5	2.9	-47.6	2.3	-27.3	4.0	30.2	2.0	-5.8	0.2
17	ZINC000091270544	-50.0	2.7	-52.4	2.7	-22.1	3.8	31.0	2.4	-6.5	0.2
18	ZINC000057563200	-50.0	3.1	-49.9	2.7	-17.6	4.6	23.4	2.1	-6.0	0.2
19	ZINC000000333210	-49.8	2.7	-50.6	3.0	-32.9	3.7	39.8	2.2	-6.1	0.1
20	ZINC000057731402	-49.7	2.9	-51.2	2.6	-25.2	3.7	33.0	2.1	-6.3	0.1
21	ZINC000092065700	-49.7	2.6	-52.6	2.5	-19.8	2.9	28.9	2.1	-6.1	0.2
22	ZINC000025032259	-49.1	2.9	-54.4	2.7	-21.9	3.2	33.6	2.3	-6.4	0.2
23	ZINC000008913866	-49.1	3.4	-50.7	2.5	-28.3	6.0	36.3	4.0	-6.4	0.1
24	ZINC000005360885	-49.0	3.3	-48.1	2.7	-36.4	4.9	41.1	2.4	-5.6	0.1
25	ZINC000002216953	-49.0	2.5	-48.7	2.4	-24.8	3.2	30.6	2.2	-6.2	0.1
26	ZINC000084598177	-49.0	2.5	-49.0	2.5	-30.6	3.3	36.3	2.4	-5.8	0.2
27	ZINC000015078577	-49.0	2.8	-49.4	2.8	-29.1	4.5	35.8	3.8	-6.3	0.2
28	ZINC000230113696	-48.9	2.8	-52.9	2.8	-22.8	4.3	33.0	3.3	-6.2	0.1
29	ZINC000334160460	-48.7	2.5	-49.1	2.5	-22.2	2.9	28.7	1.6	-6.1	0.1
30	ZINC000012142783	-48.6	3.1	-51.0	2.5	-21.5	5.1	30.1	4.3	-6.2	0.2
31	ZINC000051467674	-48.6	2.6	-46.6	2.7	-40.6	3.8	45.0	2.3	-6.4	0.1
32	ZINC000079491038	-48.5	2.9	-51.3	2.7	-27.7	5.0	37.0	3.8	-6.5	0.1
33	ZINC000257299555	-48.4	2.7	-46.7	3.1	-36.0	4.2	40.5	3.0	-6.2	0.1
34	ZINC000095950700	-48.4	2.4	-48.8	2.7	-19.4	2.1	25.9	1.8	-6.0	0.2
35	ZINC000096158052	-48.3	2.7	-49.9	2.5	-20.8	3.9	28.6	2.8	-6.2	0.2
36	ZINC000091768990	-48.2	2.6	-52.4	2.8	-13.3	2.6	23.8	2.0	-6.3	0.1
37	ZINC000018148904	-48.2	2.9	-50.1	2.6	-32.7	3.6	40.4	2.3	-5.8	0.1
38	ZINC000095410774	-48.2	2.5	-50.5	2.4	-22.8	3.0	31.3	2.2	-6.1	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
39	ZINC000575618196	-48.1	2.8	-54.5	2.7	-27.7	3.9	40.6	2.5	-6.4	0.1
40	ZINC000195547314	-47.9	2.8	-50.9	2.8	-13.5	3.3	22.8	2.0	-6.3	0.2
41	ZINC000072290753	-47.8	3.1	-52.3	2.4	-26.0	4.2	36.6	2.7	-6.1	0.1
42	ZINC000229623928	-47.7	2.5	-50.6	2.5	-34.1	3.8	43.3	3.0	-6.3	0.1
43	ZINC000065395709	-47.7	2.6	-51.6	2.4	-22.3	3.1	32.8	2.0	-6.6	0.1
44	ZINC000034895992	-47.2	3.0	-49.7	2.7	-29.9	3.5	38.7	2.4	-6.2	0.2
45	ZINC000002646979	-47.2	2.6	-51.5	2.3	-22.3	3.2	32.8	2.4	-6.3	0.1
46	ZINC000096199614	-47.0	2.9	-51.3	2.5	-27.5	3.7	37.5	2.2	-5.7	0.1
47	ZINC000100193430	-46.9	2.1	-47.9	2.4	-13.6	2.7	20.0	1.8	-5.3	0.1
48	ZINC000069562405	-46.8	2.5	-47.4	2.6	-25.3	2.9	31.8	2.0	-5.9	0.1
49	ZINC000069846908	-46.7	3.4	-50.0	3.0	-33.8	7.9	43.2	5.3	-6.1	0.2
50	ZINC000008595944	-46.7	2.6	-53.1	2.3	-13.9	4.1	26.2	3.0	-5.9	0.1
51	ZINC000100193536	-46.6	2.7	-48.7	2.9	-15.8	2.9	23.4	2.1	-5.5	0.2
52	ZINC000089827813	-46.6	3.3	-46.6	3.2	-28.8	4.7	34.5	2.5	-5.8	0.2
53	ZINC000064871452	-46.5	3.2	-49.9	2.5	-27.1	7.3	36.8	5.2	-6.2	0.2
54	ZINC000585280336	-46.5	3.8	-51.7	2.3	-30.1	5.9	41.7	3.5	-6.2	0.1
55	ZINC000075118384	-46.4	3.4	-46.9	2.9	-33.8	7.2	40.3	4.1	-5.9	0.2
56	ZINC000003641308	-46.3	5.2	-45.0	2.6	-25.7	7.4	30.1	4.1	-5.7	0.2
57	ZINC000257211885	-46.3	4.2	-50.3	3.9	-20.9	3.8	30.5	2.4	-5.6	0.2
58	ZINC000069737923	-46.2	2.8	-46.3	2.3	-29.6	4.0	35.8	2.5	-6.1	0.1
59	ZINC000257218603	-46.2	2.8	-50.2	2.5	-24.7	5.1	35.1	3.3	-6.4	0.1
60	ZINC000071915224	-46.2	2.6	-49.3	2.3	-26.0	3.5	35.1	2.6	-5.9	0.1
61	ZINC000223692657	-46.0	2.6	-50.8	2.6	-27.8	4.0	38.5	2.4	-6.0	0.1
62	ZINC000096238948	-46.0	3.0	-53.8	2.7	-13.0	5.3	27.1	4.4	-6.2	0.3
63	ZINC000007030710	-46.0	3.0	-47.3	2.7	-24.4	4.2	31.4	2.7	-5.6	0.1
64	ZINC000043550595	-45.9	2.7	-48.3	2.5	-29.1	3.5	37.7	2.0	-6.2	0.2
65	ZINC000096251711	-45.8	3.3	-50.9	3.0	-15.0	3.5	26.4	2.1	-6.2	0.2
66	ZINC000013692677	-45.8	3.8	-51.9	3.1	-30.8	4.7	43.5	3.3	-6.6	0.2
67	ZINC000257192562	-45.7	2.1	-45.9	2.2	-16.4	2.3	22.5	1.6	-5.9	0.2
68	ZINC000171342968	-45.7	3.2	-48.4	2.7	-39.2	3.9	48.3	2.8	-6.4	0.1
69	ZINC000194368147	-45.7	2.7	-48.3	2.8	-30.0	3.5	38.9	2.1	-6.4	0.1
70	ZINC000225746732	-45.7	2.2	-47.5	2.3	-20.8	2.3	28.0	1.9	-5.4	0.2
71	ZINC000100737122	-45.6	2.5	-52.3	2.5	-22.5	3.1	35.4	2.5	-6.2	0.1
72	ZINC000278659999	-45.5	2.5	-47.8	2.4	-23.7	3.5	31.9	2.0	-6.0	0.2
73	ZINC000225489282	-45.5	2.8	-49.8	2.4	-16.6	4.6	26.9	3.3	-6.1	0.1
74	ZINC000257206611	-45.4	2.9	-55.3	3.1	-11.4	5.7	27.7	4.5	-6.3	0.2
75	ZINC000095503625	-45.4	3.4	-50.6	2.6	-24.3	4.9	36.1	3.4	-6.6	0.2
76	ZINC000067460397	-45.4	2.3	-50.1	2.2	-35.5	3.5	46.1	2.6	-5.8	0.1
77	ZINC000004722089	-45.3	2.2	-48.1	2.5	-14.4	2.7	22.5	1.7	-5.3	0.1
78	ZINC000071282106	-45.3	3.2	-47.7	2.6	-15.4	4.9	24.0	3.0	-6.2	0.2
79	ZINC000097413355	-45.3	2.1	-46.7	2.6	-27.5	3.2	34.5	2.2	-5.7	0.1
80	ZINC000409428381	-45.3	3.1	-51.5	2.4	-12.2	4.9	25.0	3.4	-6.6	0.1
81	ZINC000092760184	-45.2	2.5	-47.5	2.4	-20.1	3.4	28.6	2.3	-6.2	0.2
82	ZINC000002922856	-45.2	3.1	-52.4	2.7	-15.5	3.6	29.0	2.6	-6.2	0.1
83	ZINC000004511530	-45.2	2.4	-49.2	2.1	-22.6	3.0	32.9	2.1	-6.3	0.1
84	ZINC000097201269	-45.1	3.3	-49.4	2.6	-16.9	4.3	27.7	2.7	-6.4	0.3

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
85	ZINC000005426253	-45.1	2.4	-49.8	2.4	-11.6	3.2	22.9	2.9	-6.5	0.1
86	ZINC000003292603	-45.1	2.6	-47.2	2.4	-19.3	3.6	27.5	2.6	-6.1	0.2
87	ZINC000014791001	-45.1	2.6	-47.0	2.3	-21.3	3.4	29.3	2.8	-6.1	0.1
88	ZINC000306141880	-45.0	2.6	-46.5	2.8	-29.1	4.2	36.6	3.0	-6.0	0.1
89	ZINC000096003964	-45.0	3.5	-49.1	2.6	-26.2	4.8	36.3	2.3	-5.9	0.1
90	ZINC000170800517	-44.9	2.3	-49.4	2.4	-18.5	2.4	29.5	1.8	-6.5	0.2
91	ZINC000009338249	-44.9	3.9	-47.0	2.5	-27.4	4.8	35.2	3.0	-5.6	0.1
92	ZINC000257310083	-44.8	2.5	-47.2	2.6	-16.6	2.4	24.4	1.6	-5.4	0.1
93	ZINC000000489138	-44.7	2.7	-50.3	2.3	-20.6	3.0	32.2	2.0	-6.1	0.1
94	ZINC000091664087	-44.7	2.9	-54.4	2.3	-7.8	3.5	23.9	2.3	-6.5	0.1
95	ZINC000095393415	-44.7	2.7	-54.8	2.5	-14.5	3.2	30.3	2.7	-5.8	0.1
96	ZINC000084686490	-44.7	2.4	-46.1	2.4	-33.1	3.1	40.6	2.0	-6.1	0.1
97	ZINC000019328346	-44.7	7.4	-46.7	4.6	-22.0	4.5	30.0	2.2	-5.9	0.2
98	ZINC000013973188	-44.7	2.5	-47.2	2.5	-29.6	3.6	38.1	2.5	-6.0	0.1
99	ZINC000040473994	-44.6	2.5	-49.6	2.8	-26.3	4.0	37.1	2.4	-5.9	0.1
100	ZINC000012323932	-44.6	3.3	-42.7	3.2	-38.0	7.3	41.7	4.2	-5.6	0.2
101	ZINC000079001413	-44.5	2.5	-52.9	2.5	-9.1	2.5	23.7	1.9	-6.2	0.2
102	ZINC000238886413	-44.3	3.1	-49.4	2.7	-11.6	3.3	22.6	1.5	-5.9	0.2
103	ZINC000240454699	-44.3	2.5	-42.5	2.5	-24.0	4.4	28.0	3.1	-5.8	0.1
104	ZINC000022549345	-44.3	2.1	-53.9	2.1	-18.2	3.8	33.7	3.6	-5.9	0.1
105	ZINC000238121810	-44.3	3.4	-37.2	2.9	-88.8	10.4	87.6	8.6	-6.0	0.2
106	ZINC000029134571	-44.3	2.4	-52.1	2.4	-19.6	3.3	33.5	2.6	-6.1	0.1
107	ZINC000069349055	-44.2	3.4	-48.3	3.0	-24.2	8.4	34.5	5.5	-6.2	0.2
108	ZINC000011781217	-44.2	2.6	-52.0	2.2	-13.2	2.4	27.3	2.0	-6.2	0.2
109	ZINC000100191495	-44.2	2.7	-46.6	2.6	-14.2	2.7	22.0	1.9	-5.4	0.1
110	ZINC000328587242	-44.2	2.4	-45.2	2.7	-23.7	2.6	30.9	1.8	-6.1	0.2
111	ZINC000071497775	-44.2	3.2	-51.3	2.3	-25.4	6.7	39.0	4.7	-6.4	0.2
112	ZINC000065248686	-44.1	2.5	-45.7	2.6	-14.1	2.7	21.5	1.5	-5.9	0.1
113	ZINC000069775761	-44.1	3.5	-48.1	2.6	-21.8	4.1	31.7	1.9	-5.9	0.1
114	ZINC000216315534	-44.1	2.4	-41.9	2.5	-27.2	4.7	30.6	3.3	-5.6	0.1
115	ZINC000096069207	-44.0	2.8	-52.2	2.8	-20.5	2.9	35.0	2.2	-6.4	0.2
116	ZINC000050584912	-44.0	3.3	-50.3	2.8	-6.3	3.9	18.6	3.7	-6.1	0.3
117	ZINC000002465084	-43.8	3.0	-49.8	2.5	-23.7	3.3	35.8	2.4	-6.1	0.1
118	ZINC000003438521	-43.8	2.5	-45.4	2.3	-22.7	4.5	29.9	2.8	-5.7	0.1
119	ZINC000021835963	-43.8	2.5	-48.7	2.2	-26.2	3.3	36.9	2.0	-5.8	0.1
120	ZINC000013691849	-43.6	3.3	-44.2	3.0	-33.9	4.8	40.2	2.7	-5.6	0.2
121	ZINC000072290711	-43.6	2.6	-46.7	2.9	-16.6	3.3	25.0	2.3	-5.3	0.2
122	ZINC000091304527	-43.6	2.8	-50.9	2.5	-14.0	4.5	27.5	3.3	-6.2	0.2
123	ZINC000077503523	-43.6	2.7	-45.1	2.9	-34.1	6.9	41.4	4.9	-5.7	0.2
124	ZINC000092078469	-43.5	3.7	-45.0	3.2	-23.4	3.5	30.3	2.7	-5.5	0.3
125	ZINC000096251709	-43.5	2.6	-48.0	2.1	-18.9	3.2	29.2	1.8	-5.8	0.2
126	ZINC000008316344	-43.5	2.5	-51.0	2.4	-4.6	2.6	18.0	2.0	-5.9	0.2
127	ZINC000244816835	-43.5	2.7	-43.8	3.0	-34.1	3.6	40.2	2.0	-5.8	0.1
128	ZINC000253433259	-43.4	2.3	-49.1	2.2	-19.7	2.9	31.2	2.3	-5.8	0.1
129	ZINC000072096437	-43.4	2.5	-50.9	2.4	-18.3	4.2	32.5	3.0	-6.7	0.1
130	ZINC000069492530	-43.4	2.9	-47.5	2.6	-19.0	3.3	28.6	1.9	-5.5	0.2

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
131	ZINC000257222272	-43.4	2.5	-51.4	2.2	-7.3	2.1	21.6	1.6	-6.3	0.1
132	ZINC000028790813	-43.4	3.4	-51.7	2.7	-24.1	5.5	38.4	3.6	-5.9	0.2
133	ZINC000065167646	-43.3	3.1	-47.8	2.7	-21.8	4.0	32.3	3.4	-6.0	0.1
134	ZINC000044908085	-43.3	3.2	-51.1	2.7	-21.0	3.5	34.5	2.7	-5.7	0.2
135	ZINC000044919578	-43.2	2.1	-43.0	2.1	-29.0	3.4	34.2	2.1	-5.5	0.1
136	ZINC000257256038	-43.2	2.3	-45.9	2.4	-24.2	3.1	33.2	1.8	-6.2	0.1
137	ZINC000072300733	-43.0	3.7	-51.3	2.7	-12.8	4.4	27.3	2.9	-6.2	0.2
138	ZINC000092021781	-43.0	2.9	-49.3	2.9	-20.5	5.0	33.0	3.5	-6.1	0.1
139	ZINC000006669352	-42.9	2.5	-47.6	2.2	-23.0	5.5	34.0	4.2	-6.3	0.1
140	ZINC000004495846	-42.9	2.7	-46.3	2.7	-26.6	4.2	35.6	3.5	-5.8	0.2
141	ZINC000584887110	-42.9	2.3	-46.9	2.2	-14.2	2.8	23.8	2.0	-5.7	0.1
142	ZINC000044874685	-42.8	2.9	-44.2	2.8	-22.4	4.6	29.5	3.6	-5.7	0.2
143	ZINC000052955795	-42.8	2.8	-46.7	2.6	-27.1	4.8	37.0	2.9	-6.0	0.1
144	ZINC000072437791	-42.7	2.1	-46.5	2.2	-12.5	3.0	22.2	2.0	-5.9	0.1
145	ZINC000012550491	-42.7	2.6	-46.4	2.6	-23.5	3.5	33.0	2.2	-5.7	0.1
146	ZINC000035398834	-42.5	2.3	-51.5	2.3	-9.7	2.6	24.6	2.1	-6.0	0.1
147	ZINC000135810445	-42.5	2.9	-44.5	2.6	-31.9	5.3	39.8	3.6	-5.9	0.2
148	ZINC000002750765	-42.5	2.4	-45.0	2.4	-24.4	3.0	32.8	2.3	-6.0	0.1
149	ZINC000065463577	-42.5	2.6	-46.6	2.7	-32.2	5.4	42.3	4.2	-5.9	0.1
150	ZINC000584897275	-42.3	2.6	-44.7	2.8	-36.7	4.3	44.8	3.0	-5.7	0.1
151	ZINC000057526426	-42.3	2.5	-44.4	2.2	-27.1	3.1	35.0	2.4	-5.7	0.1
152	ZINC000040548686	-42.2	2.5	-51.5	2.2	-23.2	4.2	38.5	2.7	-6.0	0.1
153	ZINC000072235028	-42.1	2.6	-52.8	2.4	-12.4	4.3	29.4	3.0	-6.3	0.1
154	ZINC000095469884	-42.1	2.6	-40.0	2.8	-35.7	3.7	38.6	1.9	-5.0	0.1
155	ZINC000100119126	-42.0	3.1	-47.3	2.8	-19.9	4.4	31.2	3.0	-6.0	0.2
156	ZINC000006887927	-42.0	2.5	-48.4	2.6	-23.8	3.7	36.4	2.4	-6.3	0.1
157	ZINC000072290626	-42.0	2.6	-48.7	2.2	-19.4	5.3	31.8	4.4	-5.7	0.1
158	ZINC000050857093	-42.0	3.6	-48.7	2.5	-25.4	3.8	38.4	2.7	-6.2	0.1
159	ZINC000119429896	-41.9	2.4	-49.5	2.2	-9.9	2.9	23.8	2.2	-6.3	0.2
160	ZINC000069595091	-41.9	2.9	-45.8	2.8	-22.4	3.9	32.2	3.1	-6.0	0.2
161	ZINC000096010936	-41.9	2.6	-41.4	2.8	-26.7	3.3	32.2	1.9	-5.9	0.1
162	ZINC000040060202	-41.8	2.6	-46.1	2.8	-17.7	3.4	27.9	2.4	-6.0	0.2
163	ZINC000095447759	-41.8	3.5	-46.9	2.9	-24.8	5.5	35.6	3.3	-5.8	0.1
164	ZINC000057771728	-41.8	3.3	-48.2	2.5	-24.0	5.5	36.6	3.4	-6.2	0.3
165	ZINC000068269627	-41.7	2.5	-50.4	2.4	-27.6	4.4	42.2	4.0	-5.9	0.2
166	ZINC000012888207	-41.7	2.1	-40.8	2.2	-27.0	3.4	31.2	2.2	-5.1	0.1
167	ZINC000050859891	-41.6	3.3	-48.4	2.6	-29.5	4.7	42.1	3.6	-5.9	0.2
168	ZINC000074014922	-41.6	2.2	-47.0	2.1	-9.6	2.2	20.6	1.9	-5.7	0.1
169	ZINC000040386093	-41.6	2.8	-45.0	2.7	-13.8	2.9	22.7	2.4	-5.4	0.2
170	ZINC000071746202	-41.5	2.8	-47.6	2.6	-15.1	3.6	27.3	2.6	-6.1	0.2
171	ZINC000012142779	-41.5	4.4	-50.2	2.6	-15.4	9.4	30.5	6.4	-6.4	0.2
172	ZINC000005244779	-41.4	2.4	-49.8	2.4	-9.7	2.7	24.1	2.4	-6.1	0.1
173	ZINC000096024249	-41.4	2.9	-47.4	2.4	-18.1	5.1	29.4	3.4	-5.3	0.2
174	ZINC000016228943	-41.4	2.5	-43.6	2.6	-26.3	3.4	33.9	2.1	-5.4	0.2
175	ZINC000245171655	-41.4	2.4	-48.7	2.3	-10.2	2.7	23.3	1.8	-5.8	0.2
176	ZINC000022241454	-41.4	3.2	-39.1	2.9	-38.4	6.7	41.0	5.3	-5.0	0.2

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
177	ZINC000062639858	-41.2	2.4	-52.0	2.2	-3.0	3.4	20.1	2.8	-6.4	0.2
178	ZINC000008771448	-41.2	4.1	-48.5	3.0	-23.5	6.0	36.6	4.8	-5.8	0.4
179	ZINC000009318781	-41.2	3.1	-46.3	2.8	-25.9	6.6	36.6	3.9	-5.5	0.1
180	ZINC000058099587	-41.2	2.8	-46.8	2.8	-18.8	3.4	29.8	2.4	-5.3	0.2
181	ZINC000178511392	-41.2	2.7	-40.2	2.5	-33.5	4.1	37.7	2.6	-5.2	0.1
182	ZINC000005303591	-41.1	2.3	-44.2	2.5	-20.2	3.9	28.9	2.4	-5.7	0.1
183	ZINC000010218408	-41.1	3.9	-47.3	2.8	-19.2	5.7	30.7	3.4	-5.3	0.2
184	ZINC000003875380	-41.1	2.1	-46.6	1.9	-15.5	2.0	25.9	1.7	-4.9	0.1
185	ZINC000072807915	-41.1	2.4	-50.6	2.3	-7.2	3.6	22.8	3.3	-6.1	0.2
186	ZINC000018053795	-41.0	2.9	-47.5	2.3	-22.6	3.8	34.8	2.6	-5.8	0.1
187	ZINC000014240188	-41.0	2.7	-45.7	2.8	-17.2	4.2	27.7	3.3	-5.8	0.1
188	ZINC000077353582	-41.0	3.2	-48.6	2.8	-15.4	3.1	28.6	2.1	-5.5	0.1
189	ZINC000239762559	-40.9	2.7	-48.8	2.5	-21.2	4.1	34.8	2.9	-5.7	0.2
190	ZINC000067643674	-40.9	2.4	-44.8	2.5	-25.8	4.2	35.1	2.3	-5.4	0.1
191	ZINC000089857747	-40.8	3.9	-50.7	4.5	-7.6	5.0	23.4	5.5	-5.9	0.3
192	ZINC000154455008	-40.7	3.4	-44.9	2.8	-15.2	6.0	25.2	2.8	-5.8	0.2
193	ZINC000306138347	-40.7	2.2	-49.7	2.0	-17.2	3.2	32.1	2.5	-5.9	0.2
194	ZINC000585093122	-40.6	2.4	-45.2	2.6	-16.8	4.4	27.0	2.8	-5.6	0.2
195	ZINC000008738218	-40.6	2.9	-41.0	2.9	-40.6	5.5	46.7	3.2	-5.6	0.1
196	ZINC000091487017	-40.6	2.4	-49.3	2.3	-11.4	3.0	26.4	2.4	-6.2	0.1
197	ZINC000007030648	-40.6	3.6	-43.3	2.9	-20.2	7.1	27.9	3.2	-5.0	0.3
198	ZINC000192753414	-40.5	3.1	-46.9	2.7	-32.1	4.6	44.2	2.3	-5.7	0.1
199	ZINC000096837115	-40.5	5.9	-45.6	4.0	-27.4	7.7	38.3	5.2	-5.7	0.3
200	ZINC000077522487	-40.5	2.5	-48.6	2.2	-28.5	5.2	42.4	4.0	-5.8	0.2
201	ZINC000018240833	-40.5	2.9	-47.5	2.8	-37.8	5.3	51.0	3.3	-6.2	0.2
202	ZINC000084563579	-40.4	3.1	-45.4	4.0	-20.3	15.5	31.0	12.0	-5.8	0.2
203	ZINC000095402766	-40.4	4.5	-44.9	2.5	-16.8	7.1	27.2	3.3	-5.9	0.1
204	ZINC000330033487	-40.4	3.0	-50.1	2.6	-15.9	4.3	31.8	2.5	-6.1	0.1
205	ZINC000136345745	-40.4	2.6	-51.8	2.4	-19.5	4.9	37.1	4.1	-6.2	0.2
206	ZINC000006117573	-40.3	2.4	-42.2	2.4	-28.0	2.9	35.4	2.1	-5.5	0.1
207	ZINC000040266307	-40.3	3.0	-44.5	2.5	-22.2	4.2	32.5	2.9	-6.1	0.2
208	ZINC000095989182	-40.2	2.5	-43.2	2.2	-18.7	3.6	27.1	2.2	-5.4	0.1
209	ZINC000000079035	-40.2	3.4	-47.2	2.3	-19.1	5.5	31.8	3.2	-5.7	0.1
210	ZINC000016543876	-40.2	3.2	-46.0	2.3	-16.9	3.7	28.5	2.2	-5.9	0.1
211	ZINC000071754931	-40.2	2.5	-40.8	2.3	-12.2	3.3	18.3	1.9	-5.5	0.1
212	ZINC000019327176	-40.2	3.2	-40.2	3.0	-26.8	5.7	31.9	3.4	-5.2	0.2
213	ZINC000177842371	-40.1	2.4	-45.3	2.0	-26.9	3.8	37.3	2.8	-5.3	0.1
214	ZINC000048249797	-40.1	2.6	-50.8	2.7	-10.3	5.2	27.1	3.5	-6.2	0.1
215	ZINC000012508838	-40.1	2.7	-49.0	2.3	-24.8	4.2	39.9	2.9	-6.2	0.1
216	ZINC000097105546	-40.1	2.5	-44.7	2.6	-22.4	3.8	32.6	3.4	-5.6	0.1
217	ZINC000013691850	-40.1	2.3	-49.9	2.5	-15.3	3.3	30.8	2.1	-5.7	0.1
218	ZINC000002630701	-40.1	2.4	-49.0	2.0	-6.8	4.2	21.4	3.4	-5.8	0.1
219	ZINC000096122792	-40.1	2.5	-48.6	2.6	-9.2	2.7	23.4	2.2	-5.7	0.1
220	ZINC000091321614	-39.9	2.8	-49.4	2.4	-18.7	3.8	34.3	3.4	-6.1	0.2
221	ZINC000075140034	-39.9	2.4	-41.8	2.4	-19.3	2.9	27.0	2.0	-5.7	0.2
222	ZINC000019973951	-39.9	3.8	-40.3	3.0	-29.4	6.4	34.9	3.3	-5.1	0.2

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
223	ZINC000014741626	-39.8	2.2	-49.6	2.2	-6.8	2.5	22.4	2.1	-5.8	0.2
224	ZINC000095951555	-39.8	2.4	-42.9	2.3	-19.3	3.3	27.8	1.8	-5.5	0.1
225	ZINC000096069697	-39.7	4.2	-45.5	2.3	-9.3	5.4	20.8	2.9	-5.7	0.2
226	ZINC000022067509	-39.7	3.0	-49.1	2.8	-30.2	10.7	45.7	8.9	-6.1	0.1
227	ZINC000023764785	-39.6	3.3	-45.9	2.6	-15.6	4.6	27.8	3.0	-5.9	0.2
228	ZINC000035671101	-39.6	2.1	-46.7	2.0	-8.2	1.6	20.4	1.5	-5.1	0.2
229	ZINC000097050589	-39.5	2.6	-48.8	2.6	-13.2	4.8	28.0	3.3	-5.6	0.1
230	ZINC000065591272	-39.4	2.3	-44.9	2.2	-9.7	2.8	21.1	1.9	-6.0	0.2
231	ZINC000284798034	-39.4	2.8	-50.9	2.3	-22.8	4.5	40.3	3.0	-6.1	0.2
232	ZINC000004535480	-39.4	2.5	-45.6	2.2	-15.4	4.8	26.7	3.9	-5.1	0.2
233	ZINC000006782318	-39.3	2.3	-47.7	2.3	-18.1	2.7	32.2	2.3	-5.7	0.2
234	ZINC000012407997	-39.2	3.4	-48.0	2.8	-11.5	5.8	26.3	4.7	-6.1	0.4
235	ZINC000005026046	-39.2	2.6	-45.8	2.3	-14.0	2.7	26.3	1.9	-5.7	0.2
236	ZINC000061067795	-39.2	2.3	-48.3	2.2	-13.8	3.9	29.1	3.0	-6.2	0.2
237	ZINC000040386098	-39.2	2.5	-42.7	2.5	-13.8	3.3	22.5	2.3	-5.2	0.2
238	ZINC000253407066	-39.1	2.5	-46.7	2.4	-13.8	3.4	27.6	2.6	-6.1	0.2
239	ZINC000299793701	-38.9	2.4	-42.4	2.8	-24.9	5.0	33.9	3.3	-5.5	0.1
240	ZINC000005348603	-38.9	2.6	-46.3	2.6	-8.7	4.7	22.0	3.6	-5.8	0.1
241	ZINC000091943530	-38.8	2.5	-44.1	2.7	-16.2	4.1	27.0	2.4	-5.5	0.2
242	ZINC000030875068	-38.8	2.4	-45.9	2.2	-10.0	4.0	22.8	2.5	-5.7	0.1
243	ZINC000003313076	-38.7	2.6	-41.7	3.0	-21.1	4.5	29.7	2.3	-5.5	0.1
244	ZINC000238831563	-38.6	3.2	-47.8	2.5	-11.4	4.4	26.7	2.5	-6.0	0.1
245	ZINC000153353600	-38.6	3.8	-46.2	2.7	-8.9	3.8	22.2	2.8	-5.7	0.2
246	ZINC000012239509	-38.6	2.9	-50.5	2.5	-7.5	4.9	25.5	3.2	-6.1	0.2
247	ZINC000096080454	-38.6	2.3	-44.4	2.3	-19.6	2.8	31.1	2.1	-5.7	0.1
248	ZINC000192929211	-38.5	2.7	-44.2	2.7	-24.0	8.6	35.6	7.1	-5.8	0.1
249	ZINC000072896859	-38.5	2.5	-48.3	2.6	-6.8	5.0	22.6	4.0	-6.0	0.2
250	ZINC000257270100	-38.5	3.4	-46.1	2.5	-10.6	2.9	24.0	2.5	-5.9	0.1
251	ZINC000257257831	-38.4	3.0	-45.8	2.2	-12.3	4.7	25.3	3.3	-5.7	0.2
252	ZINC000002837442	-38.3	2.8	-42.9	2.8	-16.1	2.5	26.4	1.6	-5.7	0.2
253	ZINC000008776545	-38.2	2.5	-47.3	2.4	-15.4	2.9	30.5	2.0	-6.0	0.1
254	ZINC000003327891	-38.1	2.3	-45.9	2.2	-11.8	2.2	25.3	1.8	-5.7	0.2
255	ZINC000001810957	-38.1	2.4	-45.8	2.6	-17.2	3.6	30.8	2.9	-5.9	0.2
256	ZINC000040385901	-38.0	2.9	-41.1	2.8	-13.0	2.9	21.0	2.2	-4.9	0.2
257	ZINC000008609997	-37.6	2.9	-50.6	2.4	-13.5	3.5	32.2	2.7	-5.7	0.2
258	ZINC000047209496	-37.3	3.1	-44.4	2.4	-13.3	5.2	26.2	5.1	-5.8	0.2
259	ZINC000253473237	-37.3	2.1	-44.9	2.2	-8.3	2.8	21.9	1.9	-5.9	0.2
260	ZINC000072277544	-37.2	3.7	-45.7	2.8	-15.0	5.4	29.2	3.9	-5.6	0.2
261	ZINC000215185695	-37.2	2.2	-47.4	2.1	-16.7	2.1	33.2	1.8	-6.3	0.2
262	ZINC000003852421	-37.0	2.0	-44.3	2.1	-12.3	2.6	24.8	2.0	-5.3	0.1
263	ZINC000057511709	-36.9	2.4	-45.5	2.0	-22.5	5.0	36.7	4.5	-5.5	0.2
264	ZINC000072234903	-36.8	2.7	-44.1	2.2	-12.5	3.9	25.6	3.2	-5.8	0.1
265	ZINC000027755553	-36.8	2.5	-46.7	2.1	-15.5	3.0	31.1	2.3	-5.5	0.1
266	ZINC000072432742	-36.6	2.5	-49.1	2.3	1.8	9.9	17.0	9.4	-6.3	0.1
267	ZINC000253433605	-36.5	3.4	-47.3	2.5	-14.5	7.6	31.1	5.9	-5.8	0.2
268	ZINC000107713021	-36.4	2.5	-44.7	2.2	-2.8	2.9	16.8	2.6	-5.7	0.2

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
269	ZINC000042025678	-36.4	2.7	-43.6	4.1	-12.3	5.3	24.6	2.6	-5.1	0.2
270	ZINC000000326909	-36.3	2.7	-42.9	2.1	-17.0	3.4	28.3	1.9	-4.7	0.2
271	ZINC000004807849	-36.3	2.6	-36.5	3.5	-47.4	6.0	52.9	4.0	-5.3	0.2
272	ZINC000019796838	-36.1	2.6	-46.3	2.1	-11.2	3.5	26.7	2.6	-5.4	0.2
273	ZINC000575617533	-36.1	2.3	-44.8	2.3	-10.3	2.9	24.7	2.8	-5.7	0.2
274	ZINC000096038482	-36.0	3.0	-39.5	2.9	-24.6	6.7	33.4	4.4	-5.3	0.2
275	ZINC000013278475	-36.0	3.3	-48.6	2.9	-19.5	10.1	38.2	9.3	-6.0	0.2
276	ZINC000170016387	-35.9	2.4	-42.6	2.8	-20.3	5.4	32.8	4.0	-5.7	0.2
277	ZINC000257311417	-35.5	2.5	-40.7	2.2	-23.4	4.5	34.1	3.5	-5.5	0.2
278	ZINC000069740630	-35.5	5.0	-38.0	2.6	-20.4	4.3	28.2	2.2	-5.3	0.3
279	ZINC000018177963	-35.3	2.2	-32.7	3.1	-55.9	5.3	58.4	3.2	-5.1	0.1
280	ZINC000017888288	-35.1	2.7	-44.1	2.3	-16.9	4.5	31.0	3.1	-5.1	0.2
281	ZINC000002390471	-35.1	2.1	-43.9	2.0	-12.4	2.2	26.7	1.9	-5.5	0.2
282	ZINC000004722011	-35.0	2.5	-44.0	2.2	-7.1	2.8	21.3	2.2	-5.2	0.2
283	ZINC000005088834	-35.0	3.2	-42.9	3.6	-7.6	2.4	21.1	1.8	-5.5	0.2
284	ZINC000004732939	-34.8	2.6	-43.8	2.2	-12.5	3.0	27.0	2.4	-5.5	0.1
285	ZINC000012122382	-34.7	2.7	-42.6	2.3	-9.7	4.8	23.0	3.5	-5.4	0.2
286	ZINC000237740654	-34.7	3.1	-45.0	2.8	-3.6	10.2	19.7	10.0	-5.8	0.3
287	ZINC000001381807	-34.6	2.0	-37.1	2.1	-14.9	2.3	22.4	1.5	-5.0	0.1
288	ZINC000000201272	-34.5	3.0	-46.5	2.2	-7.2	5.3	24.9	3.8	-5.8	0.1
289	ZINC000085879141	-34.0	2.4	-41.7	2.4	-10.6	5.3	23.3	3.5	-5.1	0.1
290	ZINC000001620500	-33.9	6.5	-42.1	2.8	-26.7	24.3	40.3	18.3	-5.4	0.2
291	ZINC000237955843	-33.8	3.9	-40.6	2.6	-42.8	10.6	55.2	9.6	-5.6	0.2
292	ZINC000255187536	-33.7	2.4	-42.3	2.5	-21.3	3.7	35.5	2.6	-5.6	0.2
293	ZINC000012557330	-33.7	2.4	-43.0	2.5	-10.6	4.3	25.1	3.4	-5.2	0.2
294	ZINC000006918427	-33.6	3.2	-45.0	2.5	-13.2	4.0	30.2	2.8	-5.6	0.2
295	ZINC000034407910	-33.3	1.9	-38.4	2.1	-15.1	2.8	25.1	1.9	-4.9	0.1
296	ZINC000006556210	-33.2	2.5	-41.4	2.6	-11.3	2.5	24.8	2.5	-5.2	0.2
297	ZINC000268943077	-32.5	2.7	-41.8	2.6	6.5	8.3	8.2	7.7	-5.4	0.2
298	ZINC000004806959	-32.3	2.7	-39.4	2.6	-29.2	9.6	42.0	8.3	-5.7	0.1
299	ZINC000096198984	-32.0	2.9	-45.9	2.9	-8.9	3.7	28.7	3.4	-5.9	0.3
300	ZINC000003947438	-30.6	2.7	-41.0	2.4	-21.6	9.2	37.3	7.9	-5.3	0.2
301	ZINC000000353960	-30.5	3.7	-35.6	2.7	-38.0	13.3	48.0	10.7	-4.9	0.2
302	ZINC000237699092	-28.0	3.5	-40.8	3.4	-8.7	15.4	26.6	14.8	-5.1	0.3
303	ZINC000069895275	-25.4	3.5	-37.0	2.2	-10.2	13.6	26.9	11.3	-5.0	0.2
304	ZINC000006576136	-22.8	2.3	-34.5	2.6	-6.9	10.0	23.3	8.6	-4.7	0.1
305	ZINC000008848147	-22.4	2.6	-38.7	3.2	-0.8	14.1	22.1	12.5	-5.0	0.1

Table S6. Energy decomposition of the MM/GBSA results for the 305 compounds using the GB-5 parameter set (for more details see the Methods section). All energy terms are given in kcal/mol with their standard deviation (*std*) and are sorted by the binding free energy (ΔG_{bind}) followed by the molecular mechanics van der Waals and electrostatic interactions terms (ΔE_{vdW} and ΔE_{el}) and the polar and non-polar contributions to the solvation free energy (ΔG_{pol} and ΔG_{np}). Compounds marked in boldface were finally selected for experimental screening.

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
1	ZINC000257317306	-61.7	3.4	-50.1	2.8	-41.5	3.3	34.4	2.5	-4.5	0.1
2	ZINC000035869910	-59.9	3.9	-54.6	2.6	-35.5	5.1	34.9	2.9	-4.7	0.1
3	ZINC000069778215	-56.4	3.8	-47.6	2.7	-41.7	4.2	37.2	2.8	-4.4	0.1
4	ZINC000023642159	-56.4	3.4	-47.6	2.3	-27.5	4.0	22.8	2.5	-4.0	0.1
5	ZINC000096058349	-55.7	3.2	-54.1	2.4	-18.0	2.3	20.9	2.2	-4.5	0.1
6	ZINC000096158052	-55.4	3.3	-49.9	2.5	-20.8	3.8	19.6	3.0	-4.3	0.1
7	ZINC000091270543	-53.9	3.0	-53.6	3.0	-23.0	3.8	27.5	2.3	-4.7	0.1
8	ZINC000257211885	-53.7	5.5	-50.3	3.9	-20.9	3.8	21.5	3.1	-3.9	0.1
9	ZINC000278659999	-52.4	3.4	-47.8	2.4	-23.5	3.5	23.1	2.4	-4.2	0.1
10	ZINC000008595944	-52.4	3.2	-53.1	2.3	-13.8	4.1	18.6	3.6	-4.1	0.1
11	ZINC000096251709	-52.2	3.5	-48.0	2.1	-19.0	3.2	18.8	2.2	-4.0	0.1
12	ZINC000091486946	-52.0	2.8	-52.4	2.6	-21.0	2.8	26.0	2.7	-4.6	0.1
13	ZINC000409428381	-51.9	3.8	-51.5	2.4	-12.1	4.9	16.4	3.1	-4.6	0.1
14	ZINC000065395709	-51.5	3.0	-51.6	2.4	-22.5	3.1	27.1	2.0	-4.6	0.1
15	ZINC000003463362	-51.5	3.4	-50.0	2.8	-30.9	4.2	33.8	2.5	-4.4	0.1
16	ZINC000075530913	-51.0	2.5	-49.2	2.3	-20.1	2.3	22.5	1.8	-4.3	0.1
17	ZINC000091486133	-50.6	3.1	-52.7	2.9	-25.7	3.2	32.4	2.2	-4.6	0.1
18	ZINC000257218603	-50.6	3.4	-50.2	2.5	-24.7	5.1	28.8	3.5	-4.5	0.1
19	ZINC000008913866	-50.6	3.5	-50.7	2.5	-29.7	6.1	34.2	4.4	-4.4	0.1
20	ZINC000003641308	-50.2	6.8	-45.0	2.6	-25.1	7.2	23.9	3.5	-4.0	0.1
21	ZINC000057731402	-50.0	3.3	-51.2	2.6	-25.6	3.7	31.1	2.1	-4.4	0.1
22	ZINC000096251711	-49.9	4.0	-50.9	3.0	-15.0	3.5	20.4	2.4	-4.3	0.1
23	ZINC000092022499	-49.8	2.6	-53.4	2.6	-23.3	2.6	31.4	2.0	-4.6	0.1
24	ZINC000022191233	-49.4	3.0	-53.6	2.9	-31.4	3.7	40.2	2.8	-4.6	0.1
25	ZINC000170800517	-49.3	2.8	-49.4	2.4	-18.6	2.4	23.3	2.1	-4.5	0.1
26	ZINC000007030710	-48.9	3.7	-47.3	2.7	-25.7	4.3	28.0	3.1	-3.9	0.1
27	ZINC000091270544	-48.9	3.0	-52.4	2.7	-22.2	3.8	30.3	2.6	-4.5	0.1
28	ZINC000084578820	-48.8	3.6	-47.8	2.6	-35.8	7.0	39.0	3.7	-4.1	0.1
29	ZINC000072290753	-48.8	4.0	-52.3	2.4	-25.4	4.1	33.2	3.3	-4.2	0.1
30	ZINC000015078577	-48.7	3.4	-49.4	2.8	-29.5	4.6	34.7	3.2	-4.4	0.1
31	ZINC000010256259	-48.6	3.3	-52.7	2.7	-42.1	3.7	50.7	3.1	-4.5	0.1
32	ZINC000077503523	-48.4	3.3	-45.1	2.9	-34.1	6.6	34.7	4.8	-4.0	0.1
33	ZINC000019328346	-48.3	8.8	-46.7	4.6	-22.0	4.6	24.5	3.0	-4.1	0.1
34	ZINC000003875380	-48.2	2.6	-46.6	1.9	-16.5	2.0	18.2	2.2	-3.4	0.1
35	ZINC000095415912	-48.2	3.5	-53.2	2.7	-28.4	4.2	37.7	2.7	-4.4	0.1
36	ZINC000092065700	-48.1	2.9	-52.6	2.5	-19.7	2.9	28.5	2.3	-4.3	0.1
37	ZINC000095950700	-48.0	2.7	-48.8	2.7	-19.6	2.1	24.7	2.2	-4.2	0.1
38	ZINC000257222272	-47.9	3.1	-51.4	2.2	-7.4	2.0	15.2	2.1	-4.4	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
39	ZINC000096238948	-47.8	4.3	-53.8	2.7	-14.2	5.3	24.6	3.2	-4.3	0.2
40	ZINC000095410774	-47.5	2.9	-50.5	2.4	-24.2	3.1	31.4	2.6	-4.2	0.1
41	ZINC000100737122	-47.4	3.0	-52.3	2.5	-22.6	3.1	31.8	2.9	-4.3	0.1
42	ZINC000257299555	-47.4	2.9	-46.7	3.1	-38.1	4.3	41.7	3.4	-4.3	0.1
43	ZINC000002465084	-47.0	4.2	-49.8	2.5	-23.0	3.3	30.1	2.9	-4.2	0.1
44	ZINC000004998502	-47.0	3.4	-53.5	3.3	-39.4	4.2	50.3	3.0	-4.4	0.1
45	ZINC000000333210	-46.9	3.0	-50.6	3.0	-32.6	3.7	40.5	2.5	-4.3	0.1
46	ZINC000091768990	-46.8	2.7	-52.4	2.8	-14.9	2.6	24.8	2.2	-4.4	0.1
47	ZINC000229623928	-46.8	2.9	-50.6	2.5	-33.6	3.7	41.9	3.2	-4.4	0.1
48	ZINC000057563200	-46.8	3.4	-49.9	2.7	-17.6	4.6	24.9	2.4	-4.1	0.1
49	ZINC000002216953	-46.7	2.8	-48.7	2.4	-24.8	3.2	31.0	2.7	-4.3	0.1
50	ZINC000034895992	-46.7	3.5	-49.7	2.7	-29.8	3.4	37.1	3.0	-4.3	0.1
51	ZINC000334160460	-46.7	2.9	-49.1	2.5	-22.9	2.9	29.6	2.1	-4.2	0.1
52	ZINC000097201269	-46.5	3.7	-49.4	2.6	-17.3	4.2	24.7	3.0	-4.4	0.2
53	ZINC000091304527	-46.3	3.2	-50.9	2.5	-14.3	4.5	23.2	3.0	-4.3	0.2
54	ZINC000009338249	-46.3	3.9	-47.0	2.5	-27.3	4.7	31.9	2.9	-3.9	0.1
55	ZINC000071746202	-46.2	3.7	-47.6	2.6	-14.6	3.6	20.3	2.9	-4.2	0.1
56	ZINC000194368147	-46.1	3.2	-48.3	2.8	-31.3	3.5	37.9	2.4	-4.4	0.1
57	ZINC000097413355	-45.9	2.4	-46.7	2.6	-27.2	3.2	31.9	2.6	-3.9	0.1
58	ZINC000084598177	-45.9	2.8	-49.0	2.5	-29.0	3.2	36.1	2.6	-4.0	0.1
59	ZINC000012323932	-45.8	4.1	-42.7	3.2	-38.4	7.2	39.1	3.4	-3.9	0.1
60	ZINC000096199614	-45.8	3.2	-51.3	2.5	-28.0	3.7	37.5	2.3	-3.9	0.1
61	ZINC000225746732	-45.7	2.4	-47.5	2.3	-21.3	2.3	26.9	2.2	-3.8	0.1
62	ZINC000257310083	-45.7	3.3	-47.2	2.6	-17.0	2.4	22.2	2.0	-3.7	0.1
63	ZINC000025032259	-45.7	3.2	-54.4	2.7	-22.2	3.2	35.4	2.6	-4.5	0.1
64	ZINC000069562405	-45.0	2.8	-47.4	2.6	-27.1	2.9	33.5	2.4	-4.1	0.1
65	ZINC000306141880	-45.0	2.8	-46.5	2.8	-29.4	4.2	35.0	2.7	-4.2	0.1
66	ZINC000096069207	-45.0	3.5	-52.2	2.8	-19.5	2.9	31.1	2.5	-4.5	0.1
67	ZINC000051467674	-44.9	3.0	-46.6	2.7	-40.1	3.8	46.2	2.6	-4.4	0.1
68	ZINC000575618196	-44.9	3.2	-54.5	2.7	-27.3	3.9	41.4	2.7	-4.5	0.1
69	ZINC000012142783	-44.9	4.2	-51.0	2.5	-22.0	5.0	32.4	5.1	-4.3	0.1
70	ZINC000257206611	-44.6	3.1	-55.3	3.1	-11.5	5.7	26.6	3.9	-4.4	0.1
71	ZINC000013692677	-44.5	3.9	-51.9	3.1	-30.2	4.7	42.1	3.3	-4.6	0.1
72	ZINC000040473994	-44.5	2.8	-49.6	2.8	-26.5	4.0	35.6	2.4	-4.1	0.1
73	ZINC000238121810	-44.4	4.5	-37.2	2.9	-110.9	10.4	107.9	8.3	-4.1	0.1
74	ZINC000257192562	-44.4	2.3	-45.9	2.2	-17.6	2.3	23.3	2.0	-4.1	0.1
75	ZINC000065248686	-44.2	2.7	-45.7	2.6	-14.8	2.7	20.4	1.9	-4.1	0.1
76	ZINC000092078469	-43.7	4.6	-45.0	3.2	-24.1	3.6	29.1	3.5	-3.8	0.2
77	ZINC000079491038	-43.5	3.3	-51.3	2.7	-28.2	5.1	40.5	4.0	-4.5	0.1
78	ZINC000089827813	-43.5	3.4	-46.6	3.2	-29.5	4.7	36.6	2.9	-4.0	0.1
79	ZINC000225489282	-43.4	2.9	-49.8	2.4	-17.0	4.8	27.6	3.9	-4.2	0.1
80	ZINC000330033487	-43.4	4.3	-50.1	2.6	-15.4	4.4	26.4	2.8	-4.3	0.1
81	ZINC000195547314	-43.2	3.1	-50.9	2.8	-14.0	3.2	26.1	2.1	-4.3	0.1
82	ZINC000328587242	-43.1	2.5	-45.2	2.7	-24.8	2.6	31.1	2.0	-4.2	0.1
83	ZINC000000489138	-43.0	3.1	-50.3	2.3	-20.1	2.9	31.6	2.0	-4.2	0.1
84	ZINC000092760184	-42.9	2.8	-47.5	2.4	-20.6	3.3	29.5	2.6	-4.3	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
85	ZINC000257256038	-42.9	2.7	-45.9	2.4	-25.3	3.1	32.6	1.9	-4.3	0.1
86	ZINC000100193536	-42.9	2.8	-48.7	2.9	-15.8	2.9	25.5	2.2	-3.8	0.1
87	ZINC000071915224	-42.8	2.7	-49.3	2.3	-26.5	3.5	37.1	2.8	-4.1	0.1
88	ZINC000230113696	-42.7	3.0	-52.9	2.8	-23.6	4.3	38.1	3.8	-4.3	0.1
89	ZINC000072300733	-42.7	4.6	-51.3	2.7	-13.5	4.4	26.4	3.2	-4.3	0.1
90	ZINC000071282106	-42.6	4.0	-47.7	2.6	-16.3	4.9	25.7	2.4	-4.3	0.1
91	ZINC000005360885	-42.6	3.7	-48.1	2.7	-36.1	4.9	45.4	2.3	-3.9	0.1
92	ZINC000100193430	-42.6	2.3	-47.9	2.4	-14.3	2.6	23.3	1.9	-3.7	0.1
93	ZINC000012550491	-42.6	2.9	-46.4	2.6	-24.3	3.5	32.1	2.5	-4.0	0.1
94	ZINC000072096437	-42.6	2.8	-50.9	2.4	-18.7	4.2	31.6	2.7	-4.6	0.1
95	ZINC000244816835	-42.6	3.1	-43.8	3.0	-34.4	3.6	39.7	2.1	-4.1	0.1
96	ZINC000065463577	-42.5	2.8	-46.6	2.7	-31.9	5.2	40.2	4.8	-4.1	0.1
97	ZINC000002750765	-42.5	2.8	-45.0	2.4	-24.2	2.9	30.9	2.7	-4.2	0.1
98	ZINC000075118384	-42.3	3.9	-46.9	2.9	-33.1	7.3	41.8	4.1	-4.1	0.1
99	ZINC000223692657	-42.2	2.9	-50.8	2.6	-28.2	3.9	40.9	2.7	-4.2	0.1
100	ZINC000069846908	-42.2	3.8	-50.0	3.0	-33.3	7.7	45.3	5.0	-4.2	0.1
101	ZINC000069737923	-42.1	3.1	-46.3	2.3	-30.1	4.0	38.6	2.8	-4.3	0.1
102	ZINC000018148904	-42.1	2.9	-50.1	2.6	-32.4	3.5	44.5	2.6	-4.1	0.1
103	ZINC000013691850	-42.0	2.6	-49.9	2.5	-15.3	3.3	27.2	2.0	-3.9	0.1
104	ZINC000095393415	-41.9	2.9	-54.8	2.5	-14.4	3.2	31.2	2.8	-4.0	0.1
105	ZINC000011781217	-41.8	3.2	-52.0	2.2	-13.7	2.4	28.3	2.1	-4.3	0.1
106	ZINC000091664087	-41.7	3.2	-54.4	2.3	-8.4	3.4	25.6	2.4	-4.5	0.1
107	ZINC000003292603	-41.7	3.5	-47.2	2.4	-19.2	3.7	28.9	3.0	-4.2	0.1
108	ZINC000013691849	-41.6	4.0	-44.2	3.0	-33.9	4.8	40.5	2.7	-3.9	0.1
109	ZINC000003438521	-41.6	2.7	-45.4	2.3	-24.1	4.5	31.8	2.9	-3.9	0.1
110	ZINC000096024249	-41.5	3.4	-47.4	2.4	-17.8	5.0	27.4	3.4	-3.7	0.1
111	ZINC000022067509	-41.5	4.6	-49.1	2.8	-56.9	11.1	68.7	8.5	-4.2	0.1
112	ZINC000216315534	-41.4	2.9	-41.9	2.5	-28.6	4.7	32.9	4.0	-3.9	0.1
113	ZINC000238886413	-41.3	4.0	-49.4	2.7	-11.3	3.3	23.5	2.3	-4.1	0.1
114	ZINC000096003964	-41.3	4.1	-49.1	2.6	-26.9	4.8	38.8	2.6	-4.1	0.1
115	ZINC000040060202	-41.3	3.5	-46.1	2.8	-17.7	3.4	26.6	2.0	-4.1	0.1
116	ZINC000095503625	-41.1	3.5	-50.6	2.6	-24.3	4.9	38.3	3.3	-4.6	0.1
117	ZINC000092021781	-41.1	3.4	-49.3	2.9	-21.9	5.0	34.4	2.9	-4.2	0.1
118	ZINC000043550595	-41.1	2.9	-48.3	2.5	-29.1	3.4	40.5	2.0	-4.3	0.1
119	ZINC000107713021	-41.0	3.0	-44.7	2.2	-3.4	2.9	11.1	3.1	-4.0	0.1
120	ZINC000257270100	-41.0	4.5	-46.1	2.5	-11.5	2.9	20.6	3.4	-4.1	0.1
121	ZINC000005426253	-40.9	2.9	-49.8	2.4	-12.6	3.2	26.1	3.7	-4.5	0.1
122	ZINC000044874685	-40.9	3.1	-44.2	2.8	-24.3	4.6	31.6	3.6	-4.0	0.1
123	ZINC000004722089	-40.7	2.3	-48.1	2.5	-14.7	2.7	25.8	1.8	-3.7	0.1
124	ZINC000014741626	-40.6	2.6	-49.6	2.2	-7.1	2.5	20.1	2.5	-4.0	0.1
125	ZINC000069595091	-40.6	3.4	-45.8	2.8	-22.3	3.9	31.6	3.0	-4.2	0.1
126	ZINC000003327891	-40.5	2.6	-45.9	2.2	-11.5	2.2	20.8	2.0	-4.0	0.1
127	ZINC000100119126	-40.5	3.4	-47.3	2.8	-19.9	4.3	30.9	3.4	-4.2	0.1
128	ZINC000071754931	-40.4	2.8	-40.8	2.3	-12.7	3.3	16.9	2.0	-3.8	0.1
129	ZINC000069349055	-40.4	3.5	-48.3	3.0	-24.4	8.4	36.7	5.7	-4.3	0.1
130	ZINC000096010936	-40.4	3.1	-41.4	2.8	-27.6	3.2	32.7	2.3	-4.1	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
131	ZINC000014791001	-40.3	2.9	-47.0	2.3	-21.6	3.5	32.5	3.1	-4.3	0.1
132	ZINC000100191495	-40.3	2.8	-46.6	2.6	-14.5	2.6	24.6	2.0	-3.7	0.1
133	ZINC000004511530	-40.3	2.6	-49.2	2.1	-22.4	3.0	35.7	2.3	-4.3	0.1
134	ZINC000002646979	-40.2	2.7	-51.5	2.3	-22.4	3.2	38.0	2.7	-4.3	0.1
135	ZINC000071497775	-40.2	3.3	-51.3	2.3	-25.4	6.6	41.0	5.0	-4.5	0.1
136	ZINC000022549345	-40.2	2.2	-53.9	2.1	-16.6	3.8	34.3	3.8	-4.1	0.1
137	ZINC000585280336	-40.1	4.5	-51.7	2.3	-29.6	5.8	45.5	3.3	-4.3	0.1
138	ZINC000005026046	-40.1	3.3	-45.8	2.3	-14.0	2.7	23.6	2.1	-3.9	0.1
139	ZINC000035398834	-40.1	2.4	-51.5	2.3	-8.9	2.5	24.5	2.1	-4.1	0.1
140	ZINC000072896859	-40.0	3.2	-48.3	2.6	-6.4	5.0	18.8	5.1	-4.2	0.1
141	ZINC000072290711	-39.9	2.6	-46.7	2.9	-17.3	3.3	27.8	2.4	-3.7	0.1
142	ZINC000064871452	-39.9	3.4	-49.9	2.5	-26.3	7.2	40.5	5.2	-4.3	0.1
143	ZINC000050584912	-39.8	3.3	-50.3	2.8	-6.7	3.9	21.3	3.7	-4.2	0.2
144	ZINC000067460397	-39.8	2.7	-50.1	2.2	-34.7	3.6	49.0	2.8	-4.0	0.1
145	ZINC000040386093	-39.8	3.1	-45.0	2.7	-14.5	3.0	23.6	2.9	-3.8	0.1
146	ZINC000067643674	-39.7	2.7	-44.8	2.5	-25.4	4.2	34.2	2.4	-3.7	0.1
147	ZINC000065167646	-39.6	3.6	-47.8	2.7	-22.4	4.0	34.7	3.9	-4.1	0.1
148	ZINC000008738218	-39.6	3.3	-41.0	2.9	-41.3	5.6	46.7	3.1	-3.9	0.1
149	ZINC000079001413	-39.4	2.6	-52.9	2.5	-9.0	2.5	26.8	2.1	-4.3	0.1
150	ZINC000044919578	-39.4	2.5	-43.0	2.1	-29.3	3.4	36.7	2.1	-3.8	0.1
151	ZINC000013973188	-39.3	2.7	-47.2	2.5	-29.0	3.6	41.1	2.8	-4.2	0.1
152	ZINC000007030648	-39.3	4.1	-43.3	2.9	-21.2	7.0	28.7	3.2	-3.5	0.2
153	ZINC000135810445	-39.1	3.3	-44.5	2.6	-33.4	5.4	42.9	3.5	-4.1	0.1
154	ZINC000002922856	-39.1	3.2	-52.4	2.7	-15.2	3.6	32.8	2.9	-4.3	0.1
155	ZINC000096080454	-39.1	2.8	-44.4	2.3	-19.0	2.8	28.2	2.4	-3.9	0.1
156	ZINC000240454699	-39.0	2.7	-42.5	2.5	-25.1	4.6	32.7	3.4	-4.0	0.1
157	ZINC000095402766	-39.0	4.6	-44.9	2.5	-17.6	7.1	27.6	3.4	-4.1	0.1
158	ZINC000008316344	-39.0	2.5	-51.0	2.4	-5.6	2.6	21.7	2.4	-4.1	0.1
159	ZINC000084686490	-38.9	2.6	-46.1	2.4	-33.4	3.0	44.8	2.2	-4.2	0.1
160	ZINC000253433259	-38.9	2.7	-49.1	2.2	-19.7	2.8	33.9	2.6	-4.0	0.1
161	ZINC000584887110	-38.9	2.5	-46.9	2.2	-13.7	2.9	25.7	2.4	-4.0	0.1
162	ZINC000012888207	-38.8	2.3	-40.8	2.2	-27.7	3.4	33.2	2.3	-3.5	0.1
163	ZINC000014240188	-38.8	2.8	-45.7	2.8	-19.3	4.2	30.2	3.5	-4.0	0.1
164	ZINC000069775761	-38.7	4.1	-48.1	2.6	-21.4	4.1	34.9	2.2	-4.1	0.1
165	ZINC000096069697	-38.7	4.5	-45.5	2.3	-9.5	5.4	20.3	3.0	-3.9	0.2
166	ZINC000154455008	-38.7	4.0	-44.9	2.8	-15.4	6.2	25.7	2.7	-4.0	0.1
167	ZINC000010218408	-38.6	4.3	-47.3	2.8	-19.0	5.6	31.4	3.8	-3.7	0.2
168	ZINC000050859891	-38.6	3.6	-48.4	2.6	-28.7	4.7	42.6	3.9	-4.1	0.1
169	ZINC000072290626	-38.6	2.9	-48.7	2.2	-18.8	5.2	32.8	4.7	-4.0	0.1
170	ZINC000069492530	-38.5	3.0	-47.5	2.6	-19.0	3.3	31.8	2.1	-3.8	0.1
171	ZINC000005348603	-38.5	3.1	-46.3	2.6	-9.9	4.8	21.7	3.3	-4.1	0.1
172	ZINC000052955795	-38.5	3.6	-46.7	2.6	-27.4	4.9	39.8	2.6	-4.2	0.1
173	ZINC000171342968	-38.5	3.4	-48.4	2.7	-40.1	3.9	54.5	3.1	-4.4	0.1
174	ZINC000006887927	-38.2	2.7	-48.4	2.6	-23.5	3.7	38.1	2.7	-4.4	0.1
175	ZINC000013278475	-38.2	4.3	-48.6	2.9	-43.7	10.1	58.3	8.8	-4.2	0.1
176	ZINC000018053795	-38.2	3.6	-47.5	2.3	-23.2	3.7	36.5	3.0	-4.0	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
177	ZINC000044908085	-38.2	3.4	-51.1	2.7	-21.0	3.4	37.9	2.8	-4.0	0.1
178	ZINC000022241454	-38.1	3.8	-39.1	2.9	-39.2	6.6	43.6	5.3	-3.4	0.1
179	ZINC000253407066	-38.1	3.1	-46.7	2.4	-13.2	3.4	26.0	2.6	-4.2	0.1
180	ZINC000057526426	-38.1	2.9	-44.4	2.2	-28.2	3.1	38.5	2.8	-4.0	0.1
181	ZINC000009318781	-38.1	3.9	-46.3	2.8	-25.5	6.6	37.5	4.4	-3.9	0.1
182	ZINC000040548686	-38.0	2.7	-51.5	2.2	-22.0	4.2	39.7	2.8	-4.2	0.1
183	ZINC000072235028	-38.0	2.8	-52.8	2.4	-12.0	4.3	31.2	3.0	-4.4	0.1
184	ZINC000096122792	-38.0	2.8	-48.6	2.6	-9.0	2.7	23.6	2.8	-3.9	0.1
185	ZINC000028790813	-37.9	3.7	-51.7	2.7	-23.6	5.6	41.5	3.9	-4.1	0.1
186	ZINC000239762559	-37.8	3.4	-48.8	2.5	-20.7	4.1	35.7	3.2	-4.0	0.1
187	ZINC000029134571	-37.7	2.6	-52.1	2.4	-19.8	3.2	38.5	3.1	-4.3	0.1
188	ZINC000089857747	-37.7	3.2	-50.7	4.5	-7.1	5.1	24.3	6.6	-4.1	0.2
189	ZINC000048249797	-37.7	3.1	-50.8	2.7	-10.4	5.2	27.8	2.9	-4.3	0.1
190	ZINC000002630701	-37.7	2.6	-49.0	2.0	-7.6	4.1	23.0	3.7	-4.0	0.1
191	ZINC000091487017	-37.6	2.6	-49.3	2.3	-11.6	3.0	27.6	2.5	-4.3	0.1
192	ZINC000021835963	-37.6	2.8	-48.7	2.2	-25.8	3.3	40.9	2.2	-4.0	0.1
193	ZINC000153353600	-37.6	4.2	-46.2	2.7	-9.4	3.9	22.0	2.4	-3.9	0.1
194	ZINC000019327176	-37.6	3.8	-40.2	3.0	-26.9	5.7	33.0	3.6	-3.6	0.1
195	ZINC000005303591	-37.6	2.9	-44.2	2.5	-20.1	3.9	30.6	2.1	-3.9	0.1
196	ZINC000245171655	-37.5	2.7	-48.7	2.3	-10.2	2.7	25.4	2.0	-4.0	0.1
197	ZINC000050857093	-37.5	4.3	-48.7	2.5	-24.6	3.8	40.1	3.2	-4.3	0.1
198	ZINC000004495846	-37.5	2.8	-46.3	2.7	-25.8	4.2	38.6	4.0	-4.0	0.1
199	ZINC000068269627	-37.5	2.8	-50.4	2.4	-26.9	4.4	44.0	3.8	-4.1	0.1
200	ZINC000074014922	-37.5	2.4	-47.0	2.1	-10.1	2.3	23.5	2.4	-4.0	0.1
201	ZINC000058099587	-37.3	3.1	-46.8	2.8	-18.8	3.4	32.1	2.5	-3.7	0.1
202	ZINC000091321614	-37.3	3.1	-49.4	2.4	-18.1	3.8	34.5	3.7	-4.2	0.1
203	ZINC000095447759	-37.2	3.5	-46.9	2.9	-24.7	5.4	38.4	3.8	-4.0	0.1
204	ZINC000072437791	-37.1	2.2	-46.5	2.2	-14.0	3.0	27.5	2.1	-4.1	0.1
205	ZINC000238831563	-37.1	4.0	-47.8	2.5	-11.5	4.4	26.4	2.4	-4.2	0.1
206	ZINC000584897275	-37.0	2.9	-44.7	2.8	-36.2	4.3	47.8	3.2	-4.0	0.1
207	ZINC000077353582	-36.9	3.9	-48.6	2.8	-15.7	3.0	31.2	2.1	-3.9	0.1
208	ZINC000004807849	-36.9	3.1	-36.5	3.5	-47.7	6.0	50.9	3.7	-3.7	0.2
209	ZINC000284798034	-36.9	3.4	-50.9	2.3	-22.1	4.5	40.3	3.1	-4.2	0.1
210	ZINC000062639858	-36.8	2.5	-52.0	2.2	-3.7	3.5	23.3	3.2	-4.4	0.2
211	ZINC000012142779	-36.8	4.7	-50.2	2.6	-15.4	9.7	33.2	6.6	-4.4	0.1
212	ZINC000192929211	-36.7	3.4	-44.2	2.7	-50.4	8.5	62.0	6.9	-4.0	0.1
213	ZINC000097105546	-36.7	2.8	-44.7	2.6	-21.9	3.7	33.7	3.6	-3.9	0.1
214	ZINC000136345745	-36.7	2.8	-51.8	2.4	-18.5	4.8	38.0	4.4	-4.3	0.1
215	ZINC000097050589	-36.7	3.3	-48.8	2.6	-13.0	4.7	29.0	3.5	-3.9	0.1
216	ZINC000040386098	-36.6	2.9	-42.7	2.5	-14.7	3.4	24.4	2.7	-3.6	0.1
217	ZINC000299793701	-36.6	2.9	-42.4	2.8	-25.9	5.0	35.5	3.4	-3.8	0.1
218	ZINC000119429896	-36.5	2.6	-49.5	2.2	-11.7	2.9	29.0	2.4	-4.4	0.1
219	ZINC000035671101	-36.5	2.2	-46.7	2.0	-8.1	1.6	21.8	1.7	-3.6	0.1
220	ZINC000018240833	-36.5	3.4	-47.5	2.8	-36.3	5.3	51.6	3.3	-4.3	0.1
221	ZINC000306138347	-36.3	2.3	-49.7	2.0	-17.4	3.2	34.8	2.9	-4.1	0.1
222	ZINC000061067795	-36.3	2.6	-48.3	2.2	-15.0	3.9	31.4	2.8	-4.3	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
223	ZINC000095469884	-36.2	2.9	-40.0	2.8	-35.7	3.7	42.9	1.9	-3.4	0.1
224	ZINC000004535480	-36.1	2.7	-45.6	2.2	-15.5	4.7	28.5	4.2	-3.5	0.1
225	ZINC000096837115	-36.1	6.1	-45.6	4.0	-26.8	7.8	40.3	5.2	-4.0	0.2
226	ZINC000008771448	-36.0	3.9	-48.5	3.0	-22.3	5.8	38.9	4.9	-4.1	0.3
227	ZINC000040385901	-36.0	3.2	-41.1	2.8	-13.7	2.9	22.3	2.4	-3.4	0.1
228	ZINC000008776545	-35.8	2.6	-47.3	2.4	-15.6	2.9	31.3	2.2	-4.1	0.1
229	ZINC000023764785	-35.7	3.3	-45.9	2.6	-14.8	4.5	29.0	3.2	-4.1	0.1
230	ZINC000003947438	-35.7	3.4	-41.0	2.4	-48.7	9.2	57.7	7.8	-3.7	0.1
231	ZINC000192753414	-35.6	3.6	-46.9	2.7	-33.1	4.6	48.2	2.4	-3.9	0.1
232	ZINC000095989182	-35.6	2.8	-43.2	2.2	-19.0	3.6	30.3	2.6	-3.8	0.1
233	ZINC000006669352	-35.5	2.7	-47.6	2.2	-23.6	5.5	40.1	4.7	-4.4	0.1
234	ZINC000253473237	-35.5	2.4	-44.9	2.2	-8.2	2.9	21.8	1.7	-4.1	0.1
235	ZINC000072807915	-35.5	2.7	-50.6	2.3	-8.1	3.6	27.4	3.4	-4.2	0.1
236	ZINC000016228943	-35.5	2.6	-43.6	2.6	-26.4	3.3	38.3	2.4	-3.7	0.1
237	ZINC000077522487	-35.4	2.6	-48.6	2.2	-27.2	5.2	44.4	4.5	-4.1	0.1
238	ZINC000177842371	-35.3	2.6	-45.3	2.0	-26.9	3.7	40.5	3.0	-3.7	0.1
239	ZINC000178511392	-35.2	2.8	-40.2	2.5	-33.4	4.1	42.1	2.6	-3.6	0.1
240	ZINC000005244779	-35.1	2.5	-49.8	2.4	-9.1	2.7	28.0	2.5	-4.2	0.1
241	ZINC000006782318	-35.1	2.6	-47.7	2.3	-17.2	2.7	33.7	2.4	-4.0	0.1
242	ZINC000042025678	-35.1	3.0	-43.6	4.1	-13.2	5.4	25.4	2.3	-3.6	0.2
243	ZINC000012239509	-35.0	3.7	-50.5	2.5	-8.0	5.0	27.7	2.6	-4.2	0.1
244	ZINC000057771728	-34.9	3.3	-48.2	2.5	-23.3	5.5	40.9	3.6	-4.3	0.2
245	ZINC000000079035	-34.8	3.6	-47.2	2.3	-20.0	5.4	36.4	3.4	-4.0	0.1
246	ZINC000075140034	-34.7	2.6	-41.8	2.4	-19.7	2.9	30.9	2.3	-4.0	0.1
247	ZINC000095951555	-34.6	2.8	-42.9	2.3	-19.4	3.3	31.4	2.2	-3.8	0.1
248	ZINC000065591272	-34.4	2.4	-44.9	2.2	-10.8	2.9	25.4	2.1	-4.2	0.1
249	ZINC000257257831	-34.4	3.2	-45.8	2.2	-13.1	4.8	28.4	3.7	-3.9	0.1
250	ZINC000091943530	-34.4	2.9	-44.1	2.7	-17.5	4.4	31.0	2.9	-3.8	0.1
251	ZINC000016543876	-34.4	3.4	-46.0	2.3	-18.4	3.8	34.1	2.4	-4.1	0.1
252	ZINC000030875068	-34.3	2.6	-45.9	2.2	-11.0	3.9	26.5	2.7	-3.9	0.1
253	ZINC000096038482	-34.2	3.7	-39.5	2.9	-25.3	6.7	34.3	4.0	-3.7	0.1
254	ZINC000040266307	-34.2	3.1	-44.5	2.5	-22.5	4.2	37.0	2.6	-4.2	0.1
255	ZINC000084563579	-34.0	3.5	-45.4	4.0	-21.3	15.9	36.6	13.5	-4.0	0.1
256	ZINC000253433605	-34.0	3.8	-47.3	2.5	-14.9	7.6	32.2	5.8	-4.1	0.1
257	ZINC000585093122	-33.9	2.5	-45.2	2.6	-16.9	4.4	32.1	3.1	-3.9	0.1
258	ZINC000019796838	-33.9	3.3	-46.3	2.1	-10.9	3.4	27.0	2.8	-3.8	0.1
259	ZINC000008609997	-33.9	3.3	-50.6	2.4	-12.7	3.4	33.3	2.7	-3.9	0.1
260	ZINC000257311417	-33.7	2.9	-40.7	2.2	-22.2	4.6	33.0	3.5	-3.8	0.1
261	ZINC000255187536	-33.6	2.8	-42.3	2.5	-21.5	3.7	34.1	2.4	-3.9	0.1
262	ZINC000237955843	-33.5	4.0	-40.6	2.6	-64.6	10.7	75.6	9.4	-3.9	0.2
263	ZINC000000326909	-33.4	2.7	-42.9	2.1	-16.5	3.4	29.3	2.1	-3.3	0.1
264	ZINC000034407910	-33.4	2.1	-38.4	2.1	-16.2	2.9	24.7	2.0	-3.4	0.1
265	ZINC000003313076	-33.4	2.9	-41.7	3.0	-21.4	4.5	33.6	2.2	-3.8	0.1
266	ZINC000001381807	-33.2	2.1	-37.1	2.1	-15.1	2.3	22.5	1.8	-3.5	0.1
267	ZINC000006117573	-33.1	2.5	-42.2	2.4	-29.4	2.9	42.3	2.3	-3.8	0.1
268	ZINC000057511709	-33.0	2.8	-45.5	2.0	-21.3	5.0	37.6	4.6	-3.8	0.1

#	ZINC ID	ΔG_{bind}	<i>std</i>	ΔE_{vdW}	<i>std</i>	ΔE_{el}	<i>std</i>	ΔG_{pol}	<i>std</i>	ΔG_{np}	<i>std</i>
269	ZINC000072432742	-33.0	2.9	-49.1	2.3	-23.0	9.9	43.4	9.5	-4.3	0.1
270	ZINC000018177963	-33.0	2.7	-32.7	3.1	-55.0	5.3	58.3	3.2	-3.6	0.1
271	ZINC000072234903	-32.5	3.0	-44.1	2.2	-12.2	3.9	27.9	3.9	-4.0	0.1
272	ZINC000001810957	-32.5	2.5	-45.8	2.6	-17.6	3.6	35.0	2.9	-4.1	0.1
273	ZINC000215185695	-32.3	2.4	-47.4	2.1	-15.8	2.1	35.3	1.9	-4.4	0.1
274	ZINC000047209496	-32.2	3.4	-44.4	2.4	-12.9	5.2	29.2	6.0	-4.0	0.1
275	ZINC000002390471	-32.2	2.3	-43.9	2.0	-12.0	2.3	27.6	2.1	-3.8	0.1
276	ZINC000268943077	-32.1	2.7	-41.8	2.6	-25.1	8.3	38.5	8.3	-3.7	0.1
277	ZINC000019973951	-32.0	4.5	-40.3	3.0	-29.7	6.5	41.6	3.2	-3.5	0.2
278	ZINC000002837442	-31.8	2.9	-42.9	2.8	-16.2	2.5	31.4	1.7	-4.0	0.1
279	ZINC000012407997	-31.8	3.3	-48.0	2.8	-11.5	5.7	32.0	4.9	-4.2	0.2
280	ZINC000012508838	-31.7	3.0	-49.0	2.3	-24.7	4.2	46.3	3.3	-4.3	0.1
281	ZINC000004806959	-31.7	2.8	-39.4	2.6	-55.4	9.5	67.1	8.3	-4.0	0.1
282	ZINC000575617533	-31.6	2.4	-44.8	2.3	-10.6	3.0	27.7	3.2	-3.9	0.2
283	ZINC000072277544	-31.6	3.8	-45.7	2.8	-14.8	5.4	32.9	4.0	-3.9	0.1
284	ZINC000237740654	-31.6	3.2	-45.0	2.8	-28.0	10.4	45.5	10.2	-4.0	0.2
285	ZINC000012122382	-31.4	2.8	-42.6	2.3	-9.5	4.8	24.4	3.2	-3.8	0.2
286	ZINC000001620500	-31.1	6.8	-42.1	2.8	-51.7	24.4	66.5	18.4	-3.8	0.1
287	ZINC000069740630	-30.6	4.8	-38.0	2.6	-20.8	4.5	31.8	2.5	-3.7	0.2
288	ZINC000004722011	-30.6	2.6	-44.0	2.2	-7.3	2.7	24.4	2.4	-3.6	0.1
289	ZINC000005088834	-30.3	3.1	-42.9	3.6	-8.5	2.5	25.0	2.0	-3.8	0.1
290	ZINC000027755553	-30.2	2.7	-46.7	2.1	-15.9	3.0	36.2	2.4	-3.8	0.1
291	ZINC000170016387	-29.8	2.7	-42.6	2.8	-20.5	5.3	37.3	4.4	-4.0	0.1
292	ZINC000012557330	-29.6	2.7	-43.0	2.5	-10.2	4.3	27.1	3.4	-3.6	0.2
293	ZINC000004732939	-29.5	3.0	-43.8	2.2	-13.6	3.0	31.7	2.8	-3.8	0.1
294	ZINC000006556210	-29.3	2.5	-41.4	2.6	-10.2	2.5	25.9	3.2	-3.6	0.1
295	ZINC000003852421	-29.3	2.1	-44.3	2.1	-12.6	2.6	31.2	2.2	-3.7	0.1
296	ZINC000017888288	-29.3	3.1	-44.1	2.3	-16.9	4.4	35.3	3.0	-3.6	0.1
297	ZINC000096198984	-28.3	3.3	-45.9	2.9	-8.7	3.7	30.4	3.7	-4.1	0.2
298	ZINC000085879141	-28.3	2.5	-41.7	2.4	-10.0	5.3	27.0	3.8	-3.5	0.1
299	ZINC000006918427	-28.1	3.6	-45.0	2.5	-13.1	4.0	33.9	2.8	-3.9	0.2
300	ZINC000000353960	-27.6	4.1	-35.6	2.7	-63.0	13.2	74.4	10.6	-3.4	0.2
301	ZINC000000201272	-26.5	3.2	-46.5	2.2	-6.7	5.2	30.6	4.1	-4.0	0.1
302	ZINC000237699092	-26.3	3.7	-40.8	3.4	-32.2	15.3	50.2	14.6	-3.6	0.2
303	ZINC000069895275	-24.7	3.8	-37.0	2.2	-35.4	13.7	51.2	11.2	-3.5	0.1
304	ZINC000006576136	-24.3	3.1	-34.5	2.6	-32.9	10.1	46.4	7.8	-3.2	0.1
305	ZINC000008848147	-21.5	3.5	-38.7	3.2	-26.7	14.3	47.4	11.6	-3.5	0.1

Table S7. Summary of docking and free energy results obtained for the selected 33 compounds, indicated by compound ID (**Figure S2**), ZINC ID(s) and MolPort ID. The first ZINC ID (*) in multiple sets indicate the enantiomer or diastereomer identified through the virtual screening procedure, whereas the compounds obtained from MolPort were mixtures of the corresponding stereoisomers. The free energy results from MM/PBSA and MM/GBSA calculations are reported for 2 parameter sets employed in the PBSA and GBSA methods. Ranking in boldface (#) indicates highly ranked compound in each parameter set.

ID	ZINC ID	MolPort ID	VINA score (kcal/mol)		MM/PB(GB)SA ΔG_{bind} (kcal/mol)			
			<i>IRAP</i>	<i>ERAP1</i>	<i>PB-1</i> (rank)	<i>PB-4</i> (rank)	<i>GB-1</i> (rank)	<i>GB-5</i> (rank)
1	000091486133* 000091486131	MolPort-027- 863-667	-10.2	-7.5	-1.3 (#105)	-30.3 (#59)	-51.0 (#13)	-50.6 (#17)
2	000244816835	MolPort-039- 039-060	-11.0	-9.2	-8.1 (#17)	-31.5 (#41)	-43.5 (#127)	-42.6 (#95)
3	000015078577* 000015078575	MolPort-005- 163-536	-9.9	-7.1	-10.8 (#6)	-32.6 (#29)	-49.0 (#27)	-48.7 (#30)
4	000091270543* 000091270544	MolPort-027- 857-260	-9.9	-7.4	-7.8 (#20)	-36.9 (#3)	-53.3 (#5)	-53.9 (#7)
5	000223692657* 000223692703	MolPort-038- 425-524	-11.0	-8.9	-7.5 (#22)	-33.5 (#17)	-46.0 (#61)	-42.2 (#99)
6	000035869910* 000035869911 000169680566 000169680567	MolPort-006- 484-933	-9.9	-7.4	-14.1 (#2)	-38.7 (#1)	-55.5 (#2)	-59.9 (#2)
7	000008595944	MolPort-007- 773-311	-10.6	-8.1	-5.0 (#42)	-29.1 (#78)	-46.7 (#50)	-52.4 (#10)
8	000095410774* 000095410775 000095410776 000095410777	MolPort-027- 906-298	-10.2	-7.4	-7.4 (#23)	-32.5 (#31)	-48.2 (#38)	-47.5 (#40)
9	000057563200	MolPort-035- 834-132	-11.1	-10.0	-4.5 (#51)	-35.4 (#9)	-50.0 (#18)	-46.8 (#48)
10	000069562405* 000069562406 000069562399 000069562402	MolPort-020- 152-989	-10.4	-7.9	-9.8 (#9)	-33.7 (#14)	-46.8 (#48)	-45.0 (#64)
11	000051467674* 000051467673	MolPort-019- 674-325	-11.1	-8.0	-8.0 (#19)	-32.6 (#30)	-48.6 (#31)	-44.9 (#67)
12	000069778215	MolPort-020- 162-189	-10.9	-9.5	-5.0 (#43)	-27.2 (#119)	-53.5 (#4)	-56.4 (#3)
13	000095415912* 000095415911 000095415910 000095415909	MolPort-028- 771-825	-11.1	-8.5	-6.5 (#27)	-35.4 (#8)	-52.6 (#9)	-48.2 (#35)
14	000044919578* 000044919582	MolPort-009- 543-745	-10.9	-8.5	-8.0 (#18)	-29.5 (#72)	-43.2 (#135)	-39.4 (#150)

ID	ZINC ID	MolPort ID	VINA score (kcal/mol)		MM/PB(GB)SA ΔG_{bind} (kcal/mol)			
			<i>IRAP</i>	<i>ERAP1</i>	<i>PB-1</i> (rank)	<i>PB-4</i> (rank)	<i>GB-1</i> (rank)	<i>GB-5</i> (rank)
15	000023642159* 000023642157	MolPort-004-188-947	-10.1	-7.1	0.3 (#142)	-26.4 (#137)	-50.5 (#16)	-56.4 (#4)
16	000084598177* 000084598174	MolPort-027-679-372	-10.9	-9.5	-10.5 (#8)	-36.2 (#6)	-49.0 (#26)	-45.9 (#58)
17	000005360885* 000005360891	MolPort-005-610-771	-10.9	-9.6	-9.7 (#10)	-36.0 (#7)	-49.0 (#24)	-42.6 (#91)
18	000043550595	MolPort-009-519-757	-10.9	-8.7	-5.1 (#41)	-33.1 (#22)	-45.9 (#64)	-41.1 (#118)
19	000240454699* 000240454698	MolPort-039-259-003	-10.9	-8.6	-7.0 (#25)	-32.2 (#32)	-44.3 (#103)	-39.0 (#156)
20	000022191233	MolPort-009-450-517	-10.9	-9.2	-9.2 (#12)	-35.1 (#10)	-53.1 (#6)	-49.4 (#24)
21	000003463362* 000003463364 000003463365	MolPort-004-164-037	-10.8	-8.1	-7.3 (#24)	-37.7 (#2)	-52.6 (#8)	-51.5 (#15)
22	000084578820* 000084578821 000084578815 000084578818	MolPort-027-704-758	-10.5	-8.0	-13.9 (#3)	-36.3 (#4)	-51.1 (#12)	-48.8 (#28)
23	000071915224* 000071915223	MolPort-020-057-841	-10.9	-9.2	-5.8 (#33)	-32.9 (#25)	-46.2 (#60)	-42.8 (#87)
24	000025032259* 000025032263	MolPort-009-027-892	-10.7	-8.1	-3.0 (#75)	-31.0 (#46)	-49.1 (#22)	-45.7 (#63)
25	000069737923* 000069737924	MolPort-020-053-566	-9.8	-7.1	-7.7 (#21)	-33.2 (#20)	-46.2 (#58)	-42.1 (#101)
26	000010256259* 000010256257	MolPort-003-173-337	-11.0	-9.7	-15.7 (#1)	-34.3 (#13)	-53.6 (#3)	-48.6 (#31)
27	000000333210* 000000333211	MolPort-003-801-767	-10.9	-9.0	-8.3 (#16)	-33.6 (#15)	-49.8 (#19)	-46.9 (#45)
28	000004998502* 000004998501	MolPort-000-832-181	-10.9	-9.3	-3.9 (#68)	-30.8 (#53)	-52.8 (#7)	-47.0 (#44)
29	000008913866* 000008913865	MolPort-000-828-576	-10.9	-8.3	-4.7 (#50)	-29.3 (#75)	-49.1 (#23)	-50.6 (#19)
30	000018148904* 000100900762	MolPort-000-694-123	-10.2	-7.7	-9.5 (#11)	-33.4 (#18)	-48.2 (#37)	-42.1 (#102)
31	000079491038	MolPort-023-297-297	-10.4	-7.8	-10.5 (#7)	-34.4 (#12)	-48.5 (#32)	-43.5 (#77)
32	000004511530	MolPort-000-407-697	-10.1	-7.6	-8.6 (#14)	-28.5 (#92)	-45.2 (#83)	-40.3 (#133)
33	000002216953	MolPort-001-905-390	-10.3	-7.7	-4.4 (#53)	-31.0 (#50)	-49.0 (#25)	-46.7 (#49)

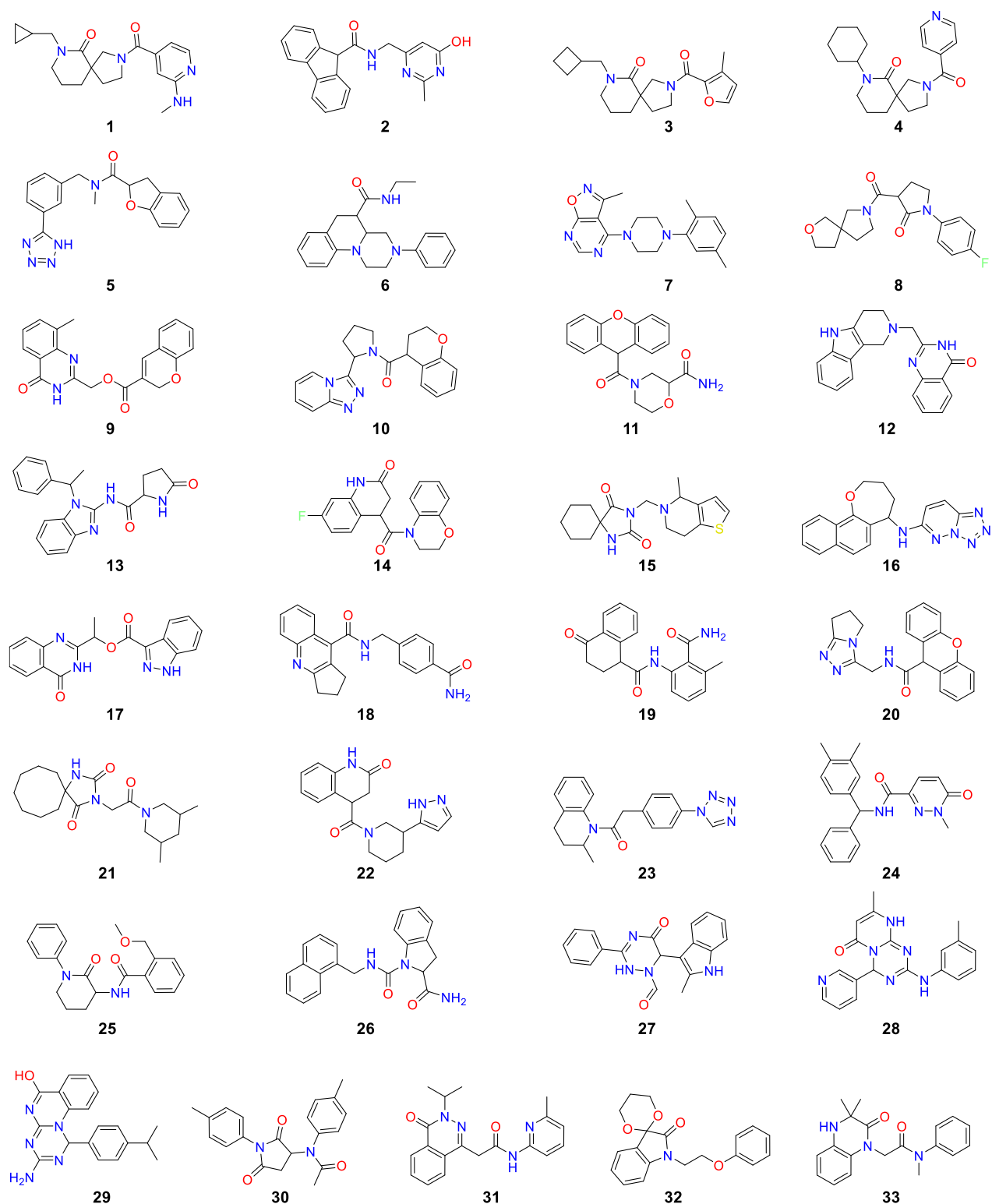


Figure S2. Structures of the 33 compounds selected for evaluation as inhibitors of IRAP. Where applicable, stereochemistry is not defined to indicate that mixture of enantiomers or diastereomers was obtained from MolPort and was used without further purification.

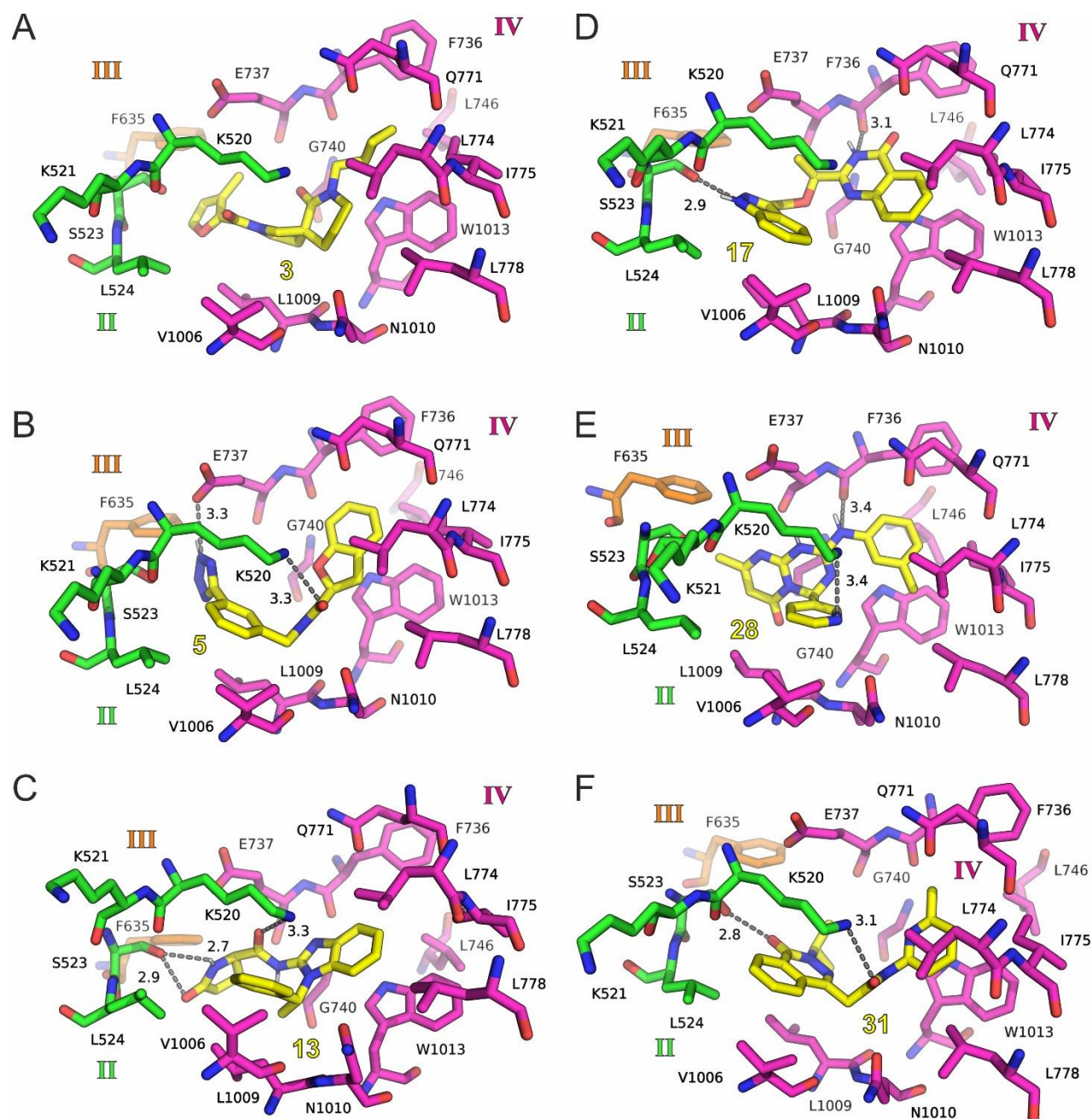
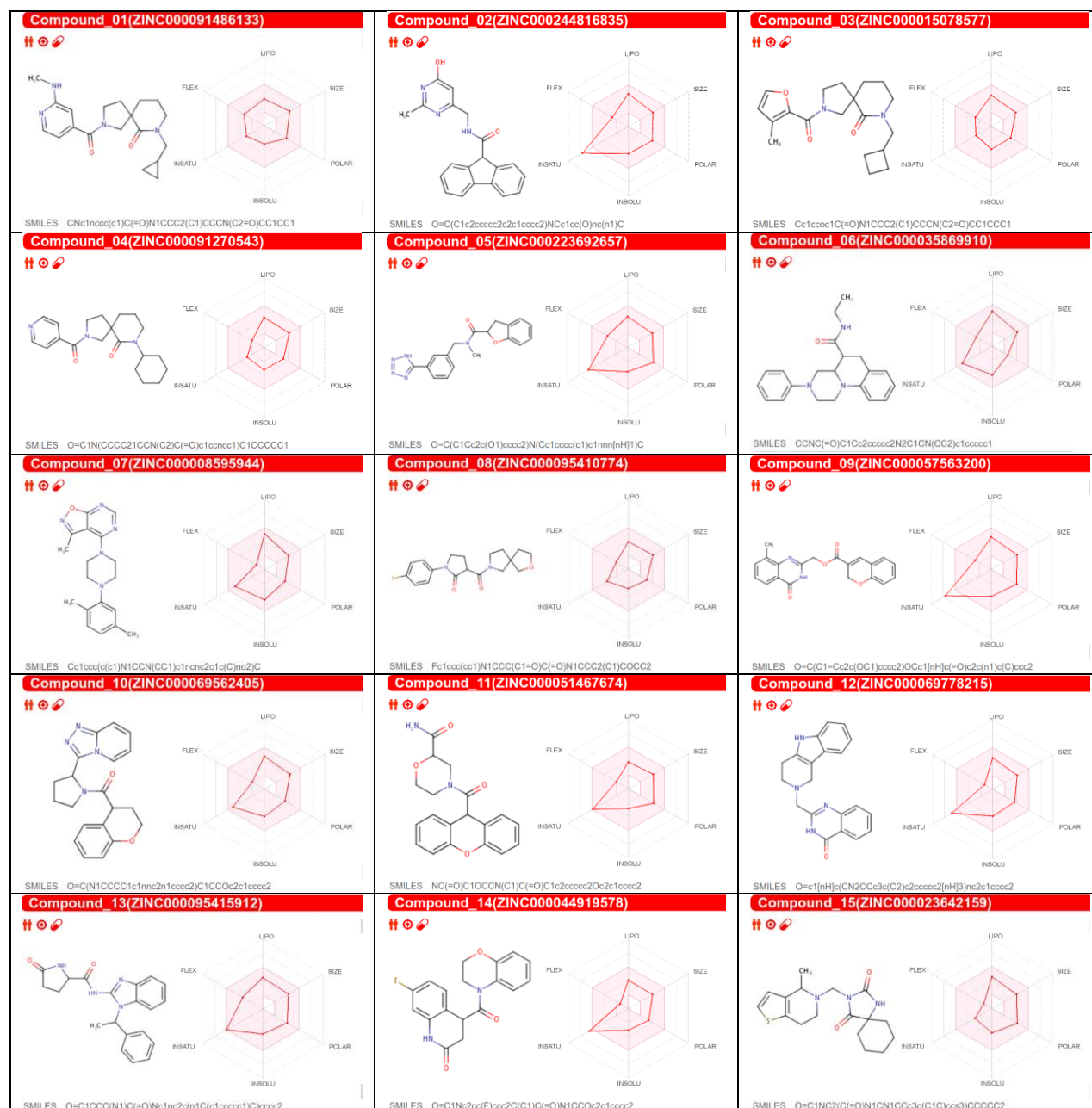


Figure S3. Bound conformations of the active compounds **3**, **5**, **13**, **17**, **28** and **31** inside the targeted pocket of IRAP. Surrounding residues are color-coded according to IRAP domain (II, III or IV) as indicated. Potential hydrogen-bonding interactions are shown with dashed lines and the corresponding heavy-atom distances (Å).

Figure S4. Computed physiochemical descriptors and radar plots as obtained using SwissADME server for compounds 1–33 (including ZINC ID). The colored zone in the radar plots indicates favorable physiochemical space for oral bioavailability, using the following descriptors: Lipophilicity ($-0.7 < \text{xLogP}_3 < 5.0$); Size ($150 < \text{MW} < 500$, g/mol); Polarity ($20 < \text{TPSA} < 130$, Å²); Insolubility ($0 < \text{LogS}_{\text{ESOL}} < 6$); Insaturation ($0.25 < \text{Fsp}_3 < 1$); Flexibility ($0 < \text{rotatable torsions} < 9$). Detailed information about the descriptors can be found in reference [1] given below.



¹ Daina, A., Michielin, O. & Zoete, V. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Sci Rep 7, 42717 (2017).

ID	1	2	3	4	5	6	7
ZINC ID	ZINC000091486133	ZINC000244816835	ZINC000015078577	ZINC000091270543	ZINC000223692657	ZINC000035869910	ZINC000008595944
Formula	C19H26N4O2	C20H17N3O2	C19H26N2O3	C20H27N3O2	C18H17N5O2	C21H25N3O	C18H21N5O
MW	342.4	331.4	330.4	341.5	335.4	335.4	323.4
#Heavy atoms	25	25	24	25	25	25	24
#Aromatic heavy atoms	6	18	5	6	17	12	15
Fraction Csp3	0.63	0.15	0.68	0.65	0.22	0.38	0.39
#Rotatable bonds	5	4	4	3	5	4	2
#H-bond acceptors	3	4	3	3	5	1	4
#H-bond donors	1	2	0	0	1	1	0
MR	103.83	94.57	98.77	104.14	90.96	108.02	100.99
TPSA	65.54	75.11	53.76	53.51	84	35.58	58.29
iLOGP	2.85	2.38	3.45	2.96	2.34	2.71	3.2
XLOGP3	1.28	2.72	2.34	2.03	2.27	3.39	3.5
ESOL Class	Soluble	Soluble	Soluble	Soluble	Soluble	Moderately soluble	Moderately soluble
GI absorption	High	High	High	High	High	High	High
BBB permeant	No	Yes	Yes	Yes	No	Yes	Yes
Pgp substrate	Yes	Yes	Yes	Yes	No	Yes	No
CYP1A2 inhibitor	No	No	No	No	No	No	Yes
CYP2C19 inhibitor	No	Yes	No	No	Yes	Yes	No
CYP2C9 inhibitor	No	Yes	Yes	Yes	Yes	No	Yes
CYP2D6 inhibitor	Yes	Yes	Yes	Yes	No	Yes	Yes
CYP3A4 inhibitor	No	Yes	Yes	Yes	Yes	Yes	Yes
log Kp (cm/s)	-7.48	-6.39	-6.65	-6.94	-6.73	-5.94	-5.79
Lipinski #violations	0	0	0	0	0	0	0
Ghose #violations	0	0	0	0	0	0	0
Veber #violations	0	0	0	0	0	0	0
Egan #violations	0	0	0	0	0	0	0
Muegge #violations	0	0	0	0	0	0	0
Bioavailability Score	0.55	0.55	0.55	0.55	0.56	0.55	0.55
PAINS #alerts	0	0	0	0	0	0	0
Brenk #alerts	0	0	0	0	0	0	0
Leadlikeness #violations	0	0	0	0	0	0	0
Synthetic Accessibility	3.69	3.22	3.97	3.43	3.13	3.43	3.23

ID	8	9	10	11	12	13	14
ZINC ID	ZINC000095410774	ZINC000057563200	ZINC000069562405	ZINC000051467674	ZINC000069778215	ZINC000095415912	ZINC000044919578
Formula	C18H21FN2O3	C20H16N2O4	C20H20N4O2	C19H18N2O4	C20H18N4O	C20H20N4O2	C18H15FN2O3
MW	332.4	348.4	348.4	338.4	330.4	348.4	326.3
#Heavy atoms	24	26	26	25	25	26	24
#Aromatic heavy atoms	6	16	15	12	19	15	12
Fraction Csp3	0.56	0.15	0.35	0.26	0.2	0.25	0.22
#Rotatable bonds	3	4	3	3	2	5	2
#H-bond acceptors	4	5	4	4	3	3	4
#H-bond donors	0	1	0	1	2	2	1
MR	93.31	97.18	100.56	93.7	102.95	103.83	92.55
TPSA	49.85	81.28	59.73	81.86	64.78	76.02	58.64
iLOGP	2.75	3.07	2.96	2.19	2.15	1.58	2.42
XLOGP3	1.41	2.69	2.76	1.23	2.45	2.39	1.64
ESOL Class	Soluble	Soluble	Soluble	Soluble	Soluble	Soluble	Soluble
GI absorption	High	High	High	High	High	High	High
BBB permeant	Yes	No	Yes	No	Yes	Yes	Yes
Pgp substrate	Yes	No	No	Yes	Yes	Yes	Yes
CYP1A2 inhibitor	No	Yes	No	No	Yes	No	No
CYP2C19 inhibitor	No	Yes	Yes	No	No	Yes	Yes
CYP2C9 inhibitor	No	Yes	Yes	No	No	No	No
CYP2D6 inhibitor	Yes	No	Yes	Yes	Yes	Yes	Yes
CYP3A4 inhibitor	Yes	Yes	Yes	No	Yes	Yes	Yes
log Kp (cm/s)	-7.33	-6.52	-6.47	-7.49	-6.58	-6.73	-7.13
Lipinski #violations	0	0	0	0	0	0	0
Ghose #violations	0	0	0	0	0	0	0
Veber #violations	0	0	0	0	0	0	0
Egan #violations	0	0	0	0	0	0	0
Muegge #violations	0	0	0	0	0	0	0
Bioavailability Score	0.55	0.55	0.55	0.55	0.55	0.55	0.55
PAINS #alerts	0	0	0	0	1	0	0
Brenk #alerts	1	0	0	0	0	0	0
Leadlikeness #violations	0	0	0	0	0	0	0
Synthetic Accessibility	3.64	3.31	3.77	3.7	2.67	3.32	3.16

ID	15	16	17	18	19	20	21
ZINC ID	ZINC000023642159	ZINC000084598177	ZINC000005360885	ZINC000043550595	ZINC000240454699	ZINC000022191233	ZINC000003463362
Formula	C17H23N3O2S	C18H16N6O	C18H14N4O3	C21H19N3O2	C19H18N2O3	C20H18N4O2	C19H31N3O3
MW	333.5	332.4	334.3	345.4	322.4	346.4	349.5
#Heavy atoms	23	25	25	26	24	26	25
#Aromatic heavy atoms	5	19	19	16	12	17	0
Fraction Csp3	0.65	0.22	0.11	0.19	0.21	0.25	0.84
#Rotatable bonds	2	2	4	5	4	4	3
#H-bond acceptors	3	5	5	3	3	4	3
#H-bond donors	1	1	2	2	2	1	1
MR	101.95	93.87	92.59	99.95	91.19	95.57	108.47
TPSA	80.89	77.23	100.73	85.08	89.26	69.04	69.72
iLOGP	2.97	2.77	1.59	2.34	1.78	2.62	3.37
XLOGP3	2.52	3.43	2.64	2.52	2.36	1.83	3.07
ESOL Class	Soluble	Moderately soluble	Soluble	Soluble	Soluble	Soluble	Soluble
GI absorption	High	High	High	High	High	High	High
BBB permeant	No	Yes	No	No	No	Yes	Yes
Pgp substrate	Yes	No	No	Yes	Yes	Yes	Yes
CYP1A2 inhibitor	No	Yes	No	Yes	No	Yes	No
CYP2C19 inhibitor	Yes	Yes	Yes	No	No	Yes	No
CYP2C9 inhibitor	Yes	No	No	Yes	No	No	No
CYP2D6 inhibitor	Yes	No	No	Yes	No	Yes	No
CYP3A4 inhibitor	Yes	No	No	Yes	Yes	Yes	No
log Kp (cm/s)	-6.54	-5.89	-6.47	-6.62	-6.59	-7.11	-6.25
Lipinski #violations	0	0	0	0	0	0	0
Ghose #violations	0	0	0	0	0	0	0
Veber #violations	0	0	0	0	0	0	0
Egan #violations	0	0	0	0	0	0	0
Muegge #violations	0	0	0	0	0	0	0
Bioavailability Score	0.55	0.55	0.55	0.55	0.55	0.55	0.55
PAINS #alerts	0	0	0	0	0	0	0
Brenk #alerts	1	0	0	0	0	0	1
Leadlikeness #violations	0	0	0	0	0	0	0
Synthetic Accessibility	4.17	3.59	3.16	2.61	3.05	3.65	4.19

ID	22	23	24	25	26	27
ZINC ID	ZINC000084578820	ZINC000071915224	ZINC000025032259	ZINC000069737923	ZINC000010256259	ZINC000000333210
Formula	C18H20N4O2	C19H19N5O	C21H21N3O2	C20H22N2O3	C21H19N3O2	C19H16N4O2
MW	324.4	333.4	347.4	338.4	345.4	332.4
#Heavy atoms	24	25	26	25	26	25
#Aromatic heavy atoms	11	17	18	12	16	15
Fraction Csp3	0.39	0.26	0.19	0.3	0.14	0.11
#Rotatable bonds	3	4	5	6	5	3
#H-bond acceptors	3	4	3	3	2	3
#H-bond donors	2	0	1	1	2	2
MR	96.91	98.26	101.66	99.47	104.34	106.35
TPSA	78.09	63.91	63.99	58.64	75.43	77.56
iLOGP	1.77	2.94	3.02	2.87	2.34	1.81
XLOGP3	0.8	3	3.09	2.46	2.87	2.79
ESOL Class	Soluble	Moderately soluble	Moderately soluble	Soluble	Soluble	Soluble
GI absorption	High	High	High	High	High	High
BBB permeant	No	Yes	Yes	Yes	Yes	No
Pgp substrate	Yes	No	No	Yes	Yes	No
CYP1A2 inhibitor	No	No	No	No	No	No
CYP2C19 inhibitor	No	Yes	Yes	Yes	Yes	Yes
CYP2C9 inhibitor	No	Yes	Yes	Yes	Yes	Yes
CYP2D6 inhibitor	Yes	No	No	Yes	Yes	No
CYP3A4 inhibitor	No	No	Yes	Yes	Yes	No
log Kp (cm/s)	-7.71	-6.2	-6.23	-6.62	-6.37	-6.35
Lipinski #violations	0	0	0	0	0	0
Ghose #violations	0	0	0	0	0	0
Veber #violations	0	0	0	0	0	0
Egan #violations	0	0	0	0	0	0
Muegge #violations	0	0	0	0	0	0
Bioavailability Score	0.55	0.55	0.55	0.55	0.55	0.55
PAINS #alerts	0	0	0	0	0	1
Brenk #alerts	0	0	0	0	0	1
Leadlikeness #violations	0	0	0	0	0	0
Synthetic Accessibility	3.4	3	3.13	2.78	3.12	3.79

ID	28	29	30	31	32	33
ZINC ID	ZINC000004998502	ZINC000008913866	ZINC000018148904	ZINC000079491038	ZINC000004511530	ZINC000002216953
Formula	C19H18N6O	C19H19N5O	C20H20N2O3	C19H20N4O2	C19H19NO4	C19H21N3O2
MW	346.4	333.4	336.4	336.4	325.4	323.4
#Heavy atoms	26	25	25	25	24	24
#Aromatic heavy atoms	18	16	12	16	12	12
Fraction Csp3	0.16	0.21	0.25	0.26	0.32	0.26
#Rotatable bonds	3	2	4	5	4	4
#H-bond acceptors	4	4	3	4	4	2
#H-bond donors	2	2	0	1	0	1
MR	107.01	104.44	100.15	98.44	91.82	102.3
TPSA	87.43	88.79	57.69	76.88	48	52.65
iLOGP	2.82	2.72	2.95	2.91	3.47	3.06
XLOGP3	1.6	2.84	2.62	2.67	2.51	2.75
ESOL Class	Soluble	Moderately soluble	Soluble	Soluble	Soluble	Soluble
GI absorption	High	High	High	High	High	High
BBB permeant	No	No	Yes	Yes	Yes	Yes
Pgp substrate	No	No	No	No	Yes	No
CYP1A2 inhibitor	No	No	No	No	Yes	Yes
CYP2C19 inhibitor	Yes	No	Yes	Yes	No	Yes
CYP2C9 inhibitor	No	Yes	Yes	Yes	Yes	Yes
CYP2D6 inhibitor	No	No	No	No	Yes	Yes
CYP3A4 inhibitor	Yes	No	Yes	No	Yes	Yes
log Kp (cm/s)	-7.28	-6.32	-6.49	-6.46	-6.5	-6.32
Lipinski #violations	0	0	0	0	0	0
Ghose #violations	0	0	0	0	0	0
Veber #violations	0	0	0	0	0	0
Egan #violations	0	0	0	0	0	0
Muegge #violations	0	0	0	0	0	0
Bioavailability Score	0.55	0.55	0.55	0.55	0.55	0.55
PAINS #alerts	0	0	0	0	0	0
Brenk #alerts	0	0	1	0	0	0
Leadlikeness #violations	0	0	0	0	0	0
Synthetic Accessibility	4.34	4.15	2.75	2.81	3.21	2.55

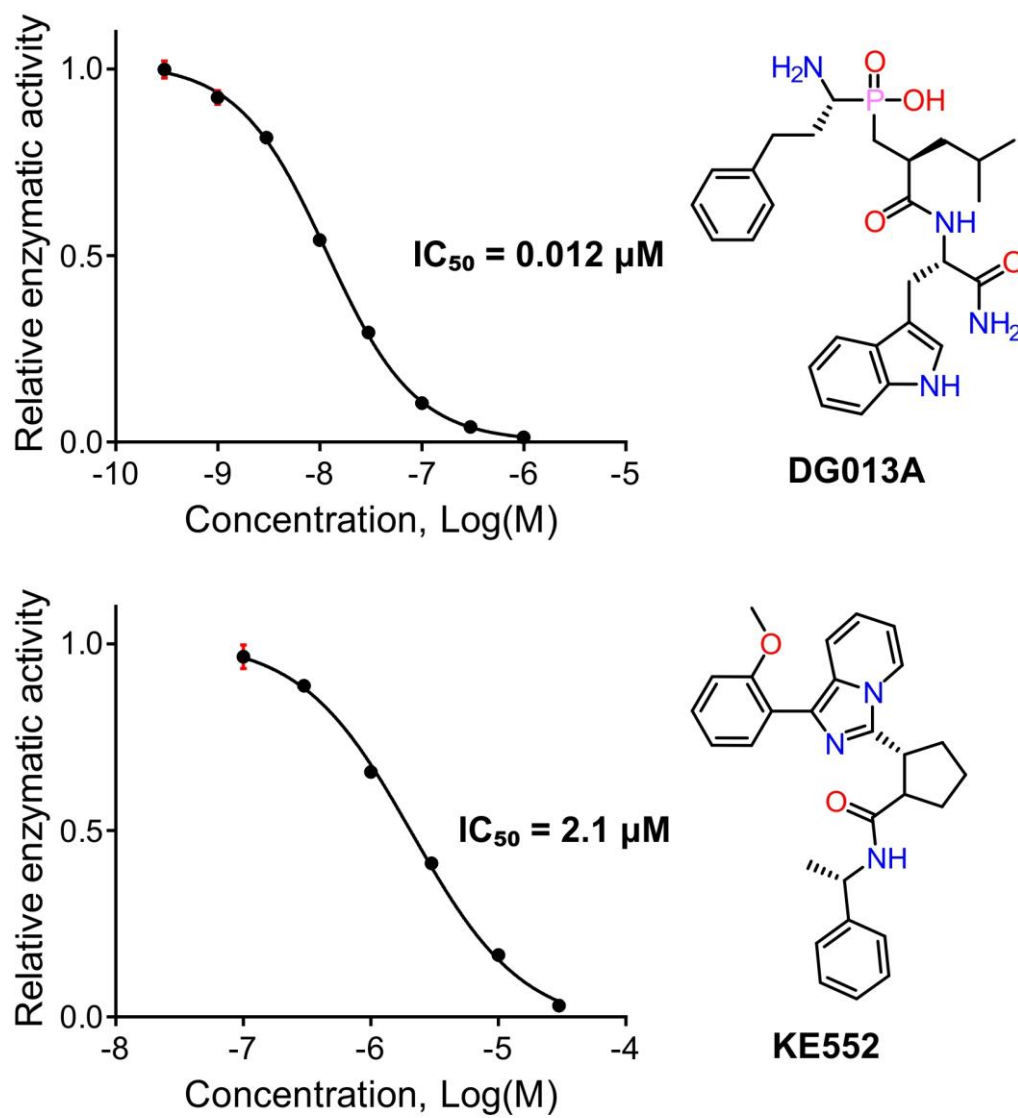


Figure S5. Validation of the effect of the known inhibitors **DG013A** and **KE552** on hydrolysis of the small fluorogenic substrate Leu-AMC by IRAP. Error bars indicate standard deviation and are shown only if they are significantly larger than the size of data points.

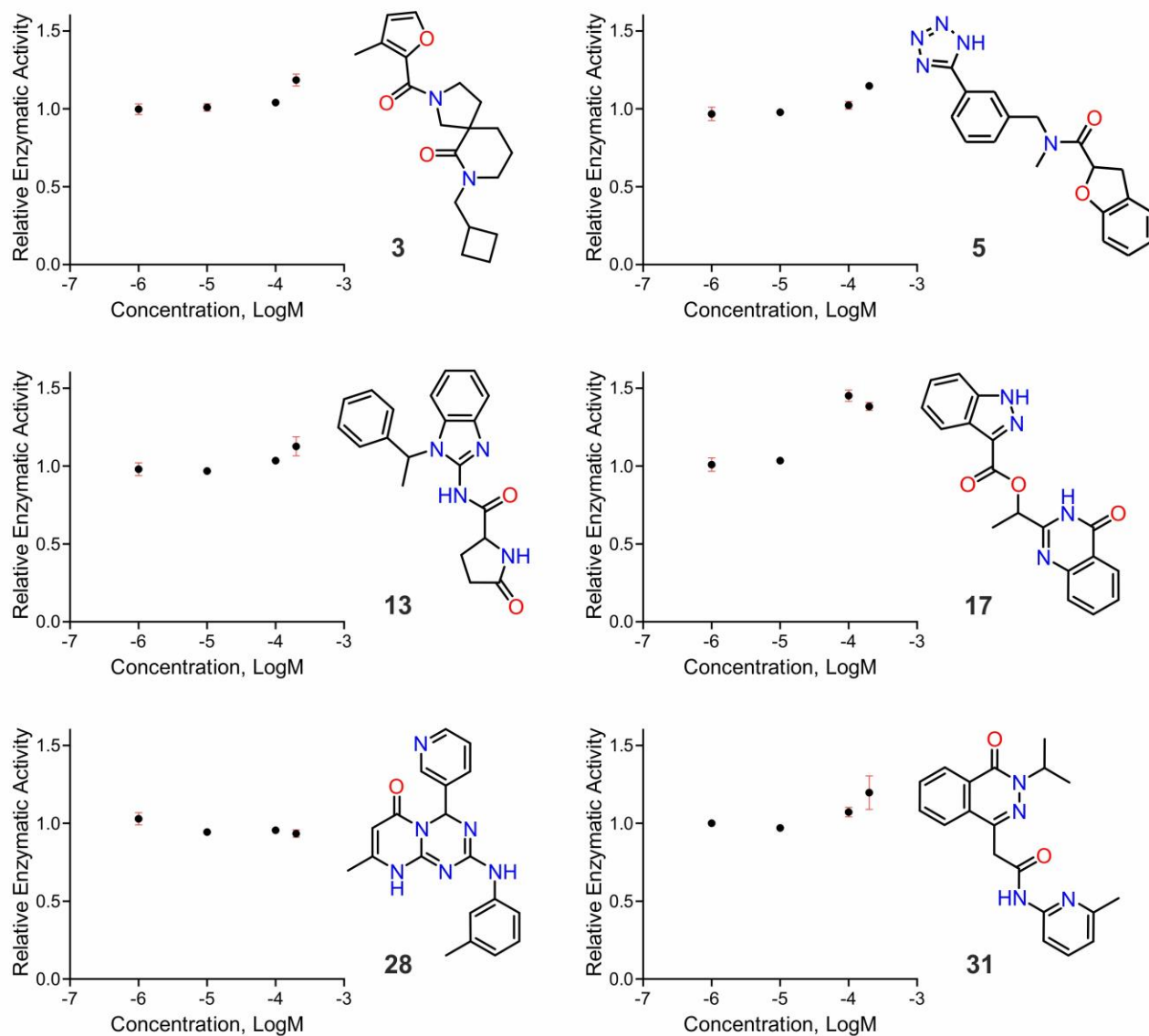


Figure S6. Effect of the hit compounds (**3**, **5**, **13**, **17**, **28** and **31**) on hydrolysis of the small fluorogenic substrate Leu-AMC by the homologous ER aminopeptidase ERAP1. Error bars indicate standard deviation and are shown only if they are significantly larger than the size of data points.

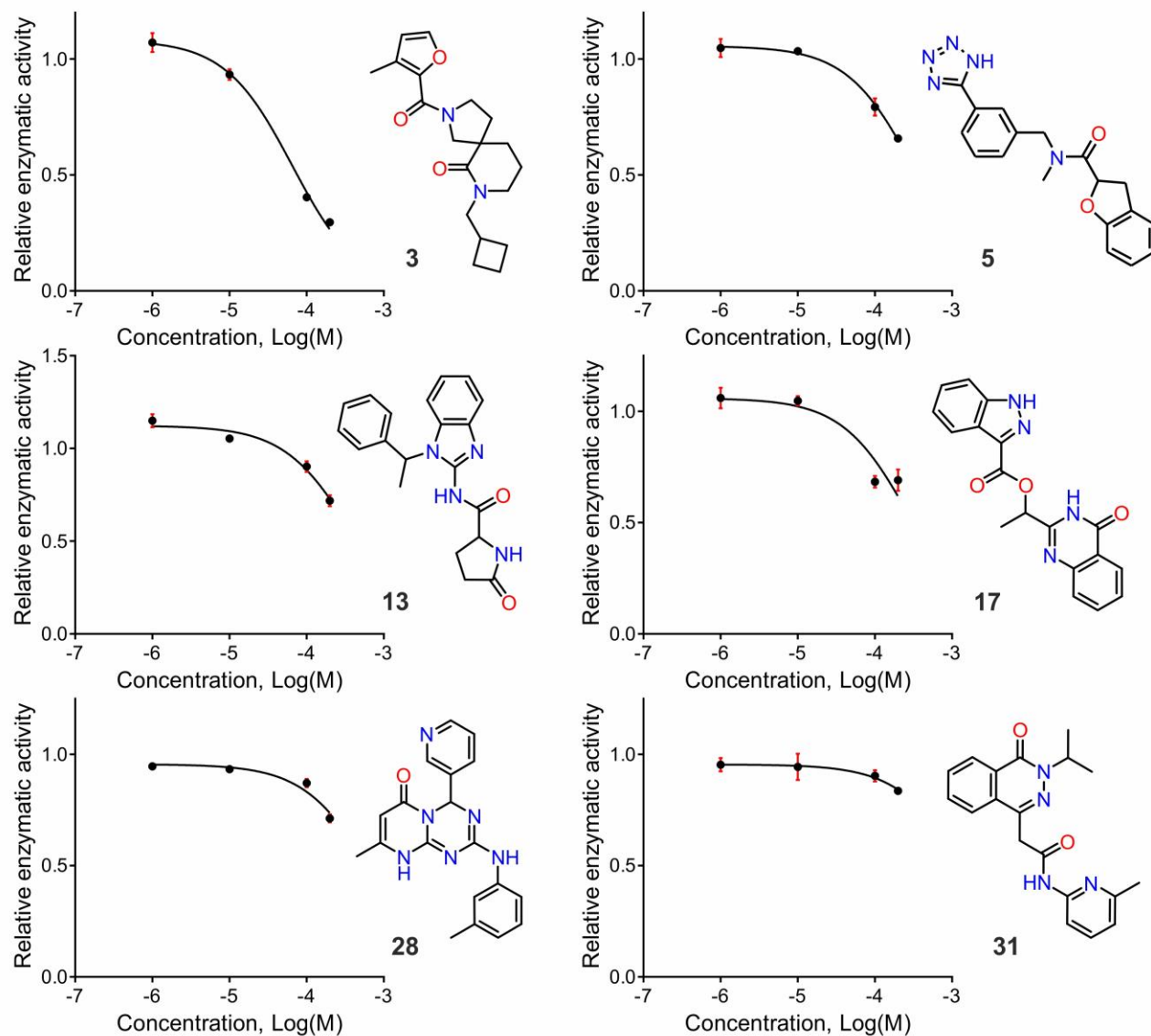


Figure S7. Effect of the hit compounds (**3**, **5**, **13**, **17**, **28** and **31**) on hydrolysis of the small fluorogenic substrate Arg-AMC by the homologous ER aminopeptidase ERAP2. Error bars indicate standard deviation and are shown only if they are significantly larger than the size of data points.

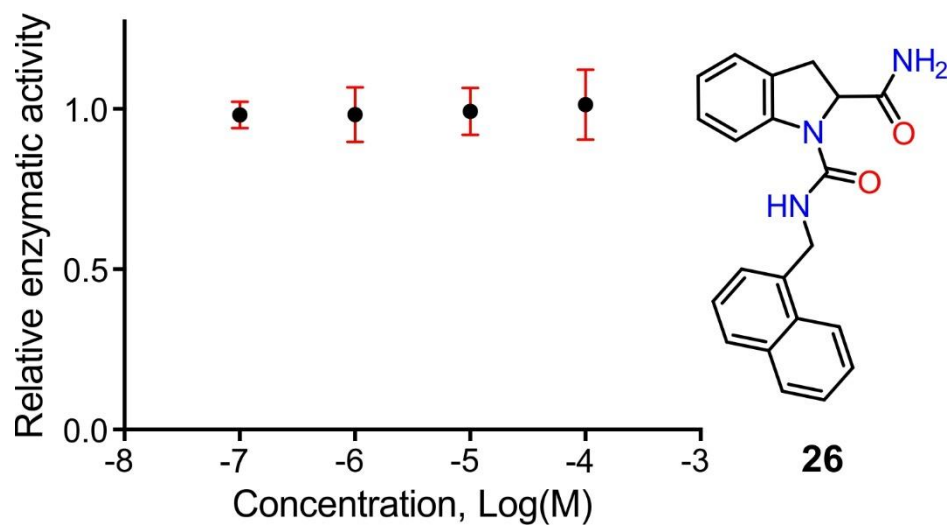


Figure S8. The effect of **26** on hydrolysis of the small fluorogenic substrate Leu-AMC, here at a concentration of 5 μ M, by IRAP. Error bars indicate standard deviation.