

# Exploring Natural Product Activity and Species Source Candidates for Hunting ABCB1 Transporter Inhibitors: An *In Silico* Drug Discovery Study

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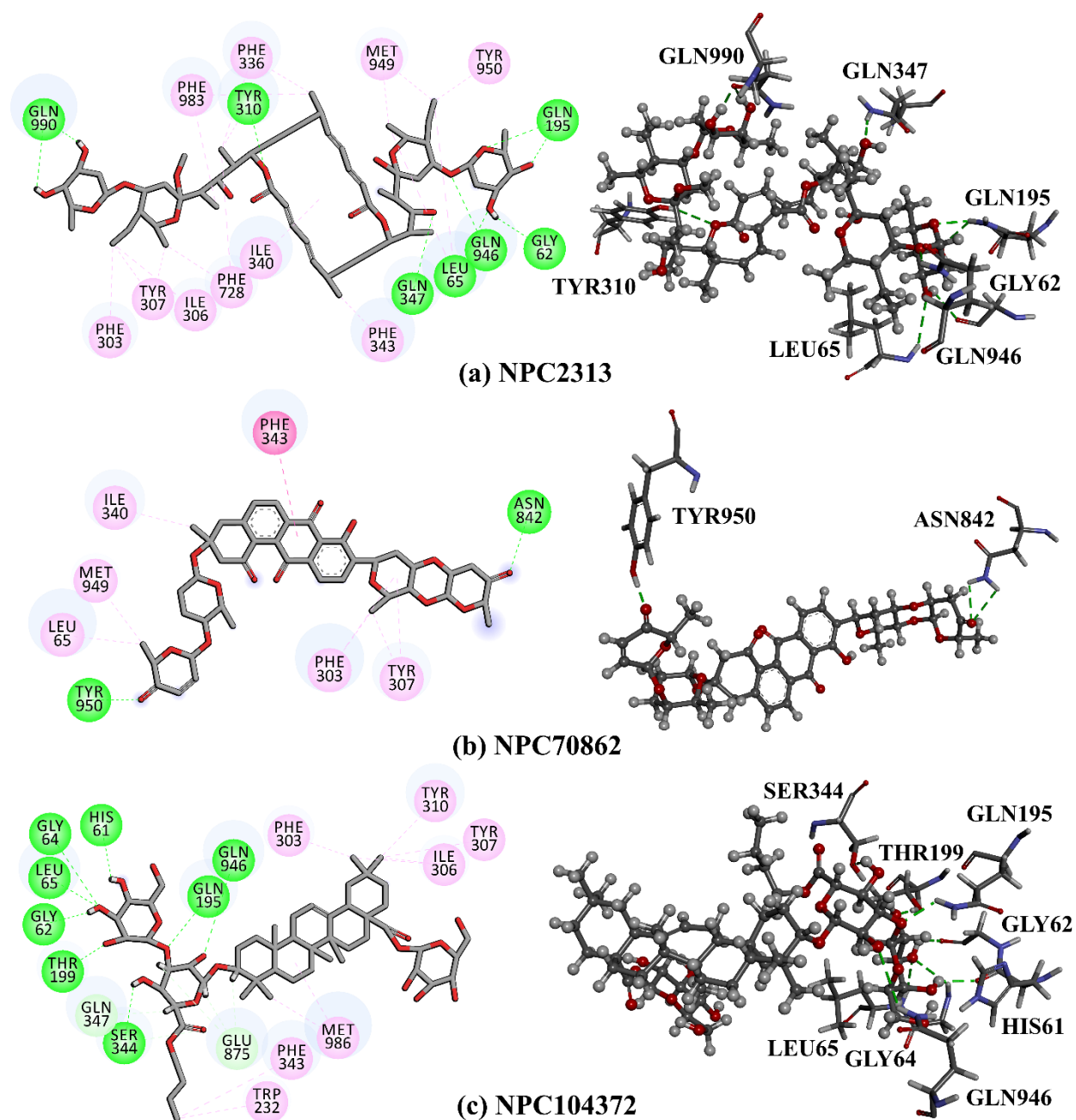
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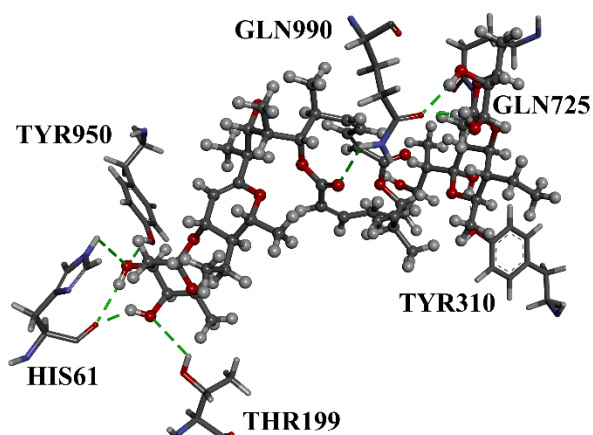
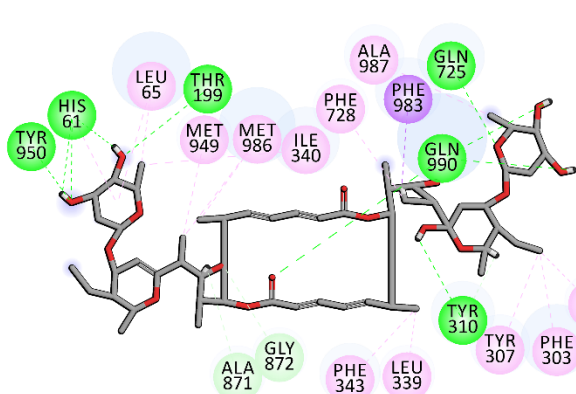
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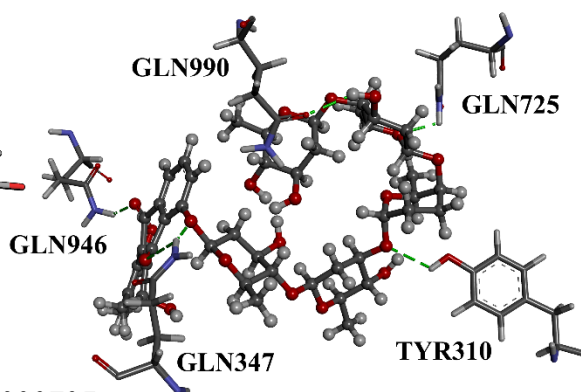
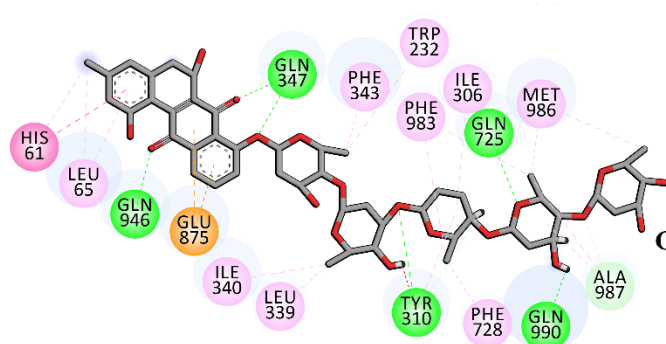
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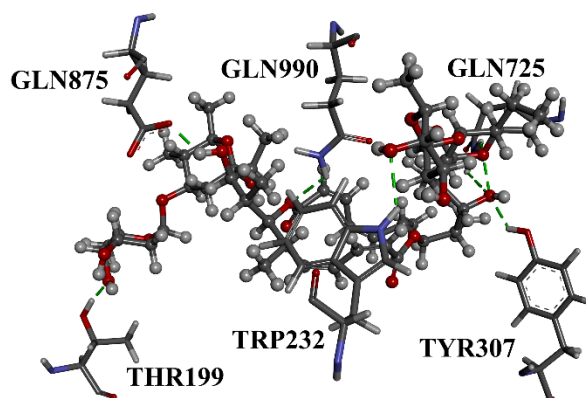
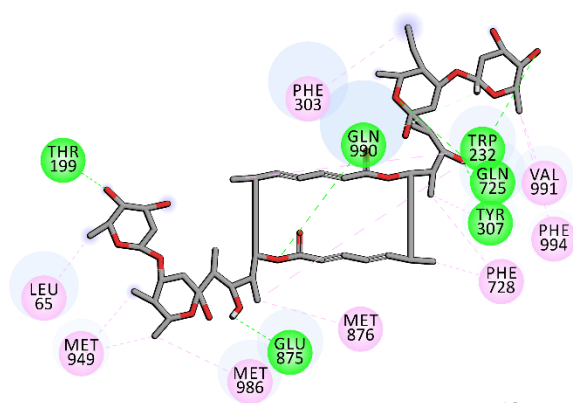
**Figure S1.** 3D and 2D representations of the binding modes of the nine potent molecules and taxol complexed with ABCB1 transporter.



(d) NPC197736

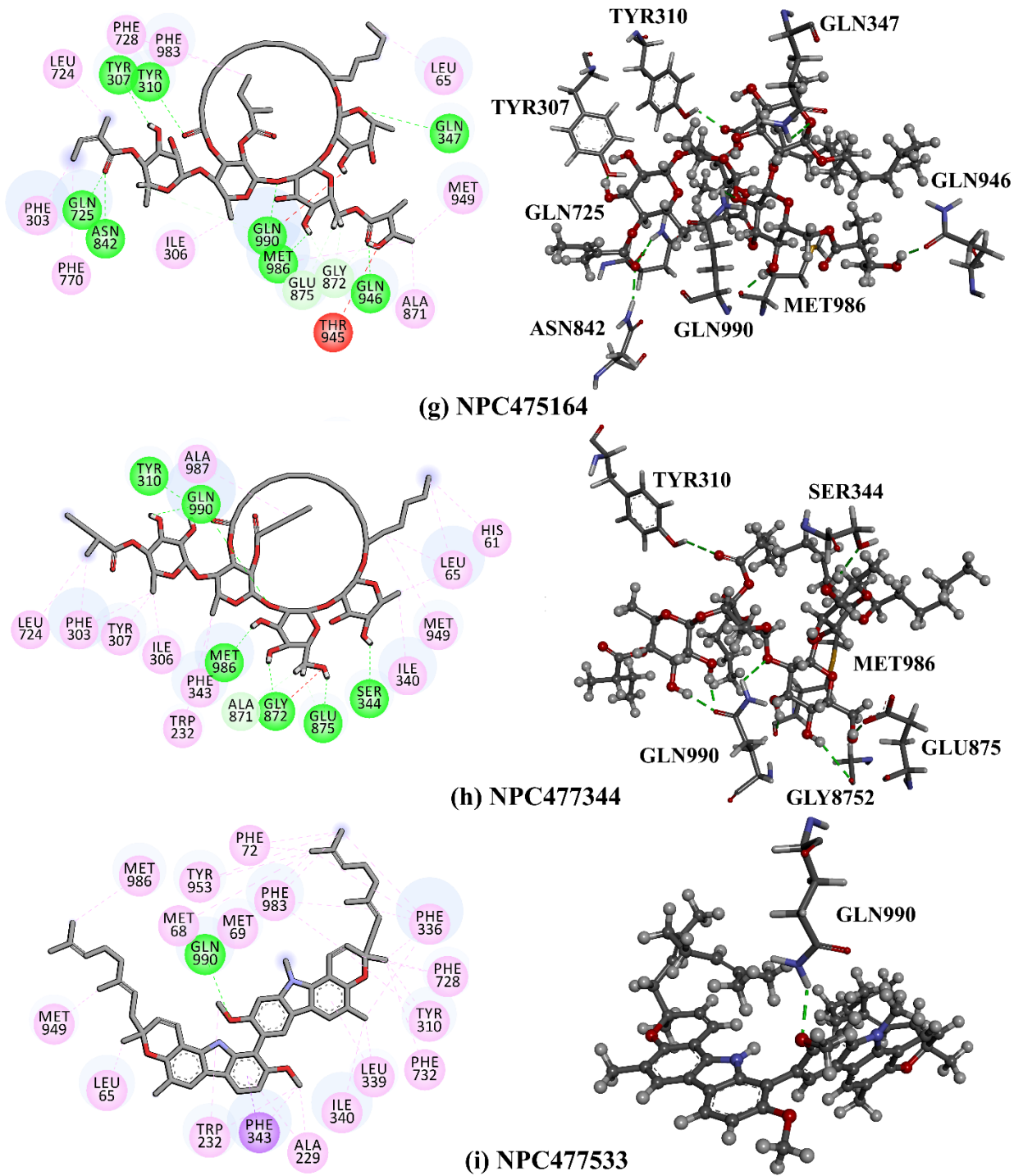


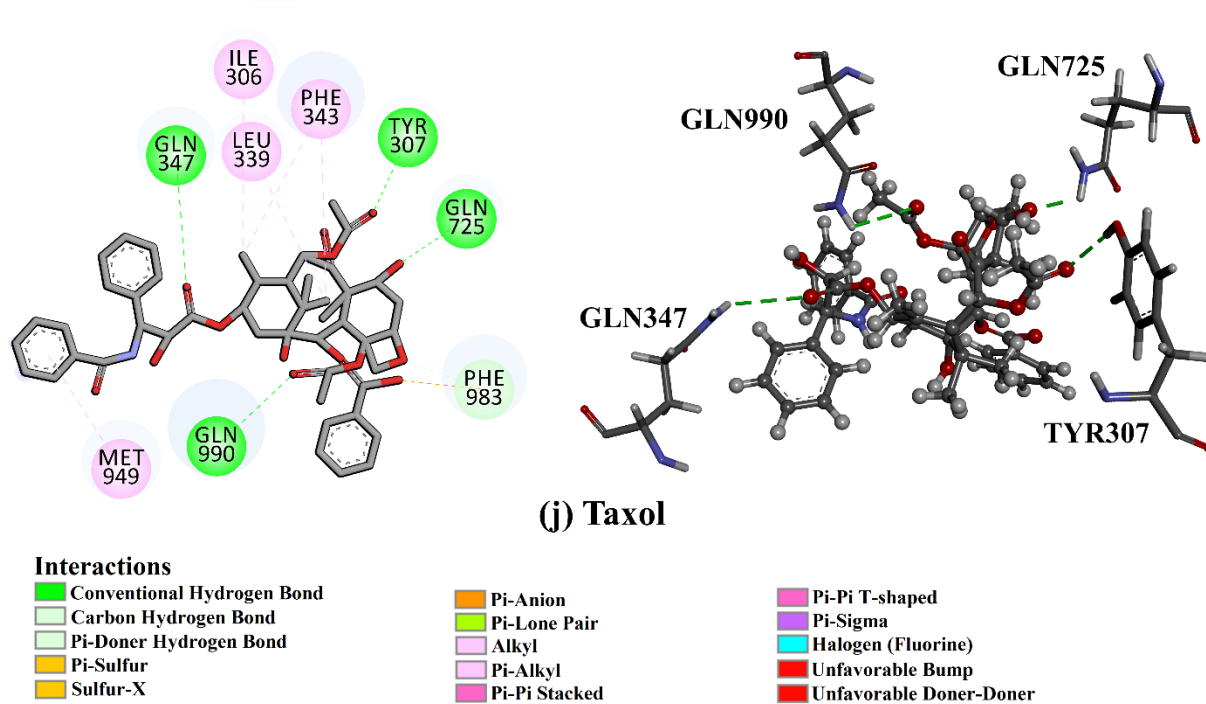
(e) NPC223735



(f) NPC471637

Figure S1. Continued.

**Figure S1.** *Continued.*

Figure S1. *Continued.*

**Table S1.** Estimated fast, moderate, and expensive docking scores for taxol and the top 866 potent NPASS compounds within the ABCB1 binding pocket.<sup>a</sup>

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Fast	Moderate	Expensive			Fast	Moderate	Expensive
	Taxol	-9.4	-8.0	-10.2	56	NPC472937	-10.3	-11.4	-12.1
1	NPC276231	-15.1	-15.9	-16.4	57	NPC469671	-10.3	-11.8	-12.1
2	NPC470601	-9.6	-13.0	-14.9	58	NPC475655	-9.6	-11.1	-12.1
3	NPC470602	-10.9	-13.0	-14.7	59	NPC473612	-11.7	-12.0	-12.0
4	NPC472437	-13.5	-12.9	-14.5	60	NPC329943	-11.4	-11.8	-12.0
5	NPC242269	-13.2	-14.1	-14.2	61	NPC36754	-12.0	-12.0	-12.0
6	NPC475493	-13.4	-13.7	-13.8	62	NPC127197	-12.0	-12.0	-12.0
7	NPC197736	-8.8	-10.9	-13.5	63	NPC270958	-10.2	-11.4	-12.0
8	NPC477533	-11.1	-12.6	-13.3	64	NPC81137	-8.8	-11.9	-12.0
9	NPC202104	-12.6	-13.5	-13.2	65	NPC472936	-10.6	-11.5	-12.0
10	NPC208258	-8.4	-12.1	-13.1	66	NPC143173	-12.0	-12.0	-12.0
11	NPC231271	-12.4	-12.6	-12.9	67	NPC2313	-9.7	-12.1	-12.0
12	NPC472395	-11.9	-12.1	-12.9	68	NPC477874	-11.7	-11.8	-12.0
13	NPC473507	-10.1	-11.5	-12.9	69	NPC471858	-11.5	-11.5	-11.9
14	NPC470426	-12.8	-12.8	-12.8	70	NPC471863	-12.1	-11.9	-11.9
15	NPC224528	-12.3	-12.6	-12.8	71	NPC96605	-8.5	-10.6	-11.9
16	NPC6702	-12.0	-12.5	-12.7	72	NPC473547	-11.9	-11.9	-11.9
17	NPC475258	-12.7	-12.7	-12.7	73	NPC472934	-10.7	-11.3	-11.9
18	NPC65118	-12.2	-12.7	-12.6	74	NPC473720	-11.8	-11.9	-11.9
19	NPC477207	-11.9	-12.5	-12.6	75	NPC474581	-10.6	-11.6	-11.9
20	NPC223735	-9.9	-11.4	-12.6	76	NPC477344	-10.2	-11.1	-11.9
21	NPC471850	-10.7	-12.0	-12.6	77	NPC78159	-11.3	-11.0	-11.9
22	NPC126676	-11.8	-11.6	-12.5	78	NPC475164	-9.3	-11.3	-11.9
23	NPC183736	-10.9	-12.3	-12.5	79	NPC47905	-10.8	-12.2	-11.9
24	NPC74086	-10.5	-10.8	-12.5	80	NPC202428	-11.2	-11.8	-11.9
25	NPC471860	-11.9	-12.1	-12.5	81	NPC475520	-11.9	-11.8	-11.9
26	NPC123859	-10.1	-12.1	-12.5	82	NPC475570	-11.7	-11.8	-11.8
27	NPC307205	-12.4	-12.4	-12.4	83	NPC94531	-11.0	-11.5	-11.8
28	NPC327962	-12.2	-12.7	-12.4	84	NPC471583	-11.8	-11.8	-11.8
29	NPC472236	-11.2	-12.4	-12.4	85	NPC322800	-11.2	-11.8	-11.8
30	NPC473403	-10.5	-12.3	-12.4	86	NPC9856	-11.8	-11.8	-11.8
31	NPC133209	-10.8	-11.5	-12.3	87	NPC245756	-11.7	-11.8	-11.8
32	NPC469447	-12.1	-12.4	-12.3	88	NPC471382	-11.8	-11.8	-11.8
33	NPC471859	-12.1	-12.3	-12.3	89	NPC471891	-11.8	-11.8	-11.8
34	NPC69383	-10.9	-11.5	-12.3	90	NPC321661	-11.2	-11.7	-11.8
35	NPC231712	-9.3	-12.1	-12.3	91	NPC475197	-10.4	-10.4	-11.8
36	NPC239990	-11.9	-12.3	-12.2	92	NPC119068	-9.6	-11.7	-11.8
37	NPC472939	-10.4	-11.9	-12.2	93	NPC229234	-10.6	-11.1	-11.8
38	NPC250835	-12.2	-12.2	-12.2	94	NPC476451	-11.8	-11.8	-11.8
39	NPC471637	-9.7	-11.4	-12.2	95	NPC284888	-11.7	-11.8	-11.8
40	NPC104372	-9.9	-11.0	-12.2	96	NPC471053	-9.5	-11.5	-11.8
41	NPC313179	-10.9	-10.4	-12.2	97	NPC476517	-11.3	-11.7	-11.7
42	NPC4638	-12.2	-11.5	-12.2	98	NPC279442	-9.3	-11.7	-11.7
43	NPC162440	-12.2	-12.2	-12.2	99	NPC273755	-9.7	-10.4	-11.7
44	NPC65034	-11.9	-12.1	-12.2	100	NPC477873	-11.2	-11.4	-11.7
45	NPC177362	-12.0	-12.1	-12.2	101	NPC48992	-11.4	-11.6	-11.7
46	NPC70862	-11.6	-11.8	-12.2	102	NPC57586	-8.7	-10.7	-11.7
47	NPC208011	-11.0	-10.9	-12.1	103	NPC301941	-11.8	-11.9	-11.7
48	NPC266545	-11.0	-10.9	-12.1	104	NPC63047	-11.7	-11.7	-11.7
49	NPC470582	-10.3	-10.5	-12.1	105	NPC172311	-10.2	-11.6	-11.7
50	NPC472371	-12.4	-12.6	-12.1	106	NPC286994	-11.6	-11.7	-11.7
51	NPC313421	-10.5	-12.1	-12.1	107	NPC472807	-10.9	-11.7	-11.7
52	NPC477531	-11.0	-12.1	-12.1	108	NPC473575	-9.5	-11.2	-11.7
53	NPC103250	-12.0	-12.1	-12.1	109	NPC168135	-10.3	-10.7	-11.7
54	NPC149962	-10.8	-10.8	-12.1	110	NPC24599	-11.7	-11.7	-11.7
55	NPC105942	-11.5	-12.0	-12.1	111	NPC123319	-11.1	-11.5	-11.7

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Fast	Moderate	Expensive			Fast	Moderate	Expensive
112	NPC34580	-10.9	-11.7	-11.7	171	NPC475544	-9.9	-10.9	-11.4
113	NPC473398	-11.6	-11.6	-11.7	172	NPC191863	-11.0	-11.4	-11.4
114	NPC475658	-11.7	-11.7	-11.7	173	NPC304307	-10.3	-10.5	-11.4
115	NPC477065	-11.5	-11.6	-11.7	174	NPC474181	-11.4	-11.4	-11.4
116	NPC252133	-10.7	-11.5	-11.6	175	NPC168188	-9.4	-11.4	-11.4
117	NPC292706	-8.9	-11.6	-11.6	176	NPC191193	-10.0	-10.8	-11.4
118	NPC325032	-10.1	-11.6	-11.6	177	NPC471861	-11.1	-11.5	-11.4
119	NPC472574	-9.2	-11.4	-11.6	178	NPC473469	-9.3	-10.8	-11.4
120	NPC472694	-9.8	-10.9	-11.6	179	NPC478124	-11.1	-11.4	-11.4
121	NPC40455	-11.0	-11.6	-11.6	180	NPC223242	-9.8	-11.4	-11.4
122	NPC469507	-11.5	-11.6	-11.6	181	NPC251226	-10.5	-11.4	-11.4
123	NPC471782	-11.5	-11.6	-11.6	182	NPC472803	-11.0	-11.3	-11.4
124	NPC472027	-11.6	-11.6	-11.6	183	NPC474585	-9.2	-11.4	-11.4
125	NPC24748	-11.6	-11.6	-11.6	184	NPC8369	-11.2	-11.4	-11.4
126	NPC249342	-11.6	-11.6	-11.6	185	NPC40496	-10.8	-11.2	-11.4
127	NPC475561	-11.5	-11.6	-11.6	186	NPC6576	-9.9	-10.7	-11.4
128	NPC229160	-11.0	-11.5	-11.6	187	NPC104910	-8.6	-11.3	-11.3
129	NPC290534	-11.7	-11.9	-11.6	188	NPC160415	-10.5	-11.3	-11.3
130	NPC475138	-10.4	-11.4	-11.6	189	NPC201244	-11.3	-11.4	-11.3
131	NPC53520	-11.1	-11.9	-11.6	190	NPC318282	-10.6	-11.2	-11.3
132	NPC157311	-11.0	-11.5	-11.6	191	NPC472235	-11.3	-11.3	-11.3
133	NPC25316	-11.4	-11.5	-11.6	192	NPC100390	-11.4	-11.4	-11.3
134	NPC475367	-11.3	-11.5	-11.6	193	NPC473881	-9.6	-10.7	-11.3
135	NPC280385	-8.7	-10.8	-11.5	194	NPC133775	-11.1	-10.6	-11.3
136	NPC43213	-11.4	-11.5	-11.5	195	NPC271607	-10.6	-11.2	-11.3
137	NPC197357	-8.7	-12.2	-11.5	196	NPC329833	-11.2	-11.2	-11.3
138	NPC209058	-11.5	-11.5	-11.5	197	NPC470765	-10.3	-11.2	-11.3
139	NPC469312	-11.4	-11.5	-11.5	198	NPC471506	-11.3	-11.3	-11.3
140	NPC475196	-9.8	-11.1	-11.5	199	NPC471654	-11.5	-11.2	-11.3
141	NPC89923	-11.2	-11.4	-11.5	200	NPC473490	-9.1	-10.4	-11.3
142	NPC41129	-10.0	-11.4	-11.5	201	NPC477209	-11.3	-11.3	-11.3
143	NPC320801	-11.2	-11.3	-11.5	202	NPC471856	-11.3	-11.3	-11.3
144	NPC477292	-10.3	-10.8	-11.5	203	NPC8761	-10.1	-11.3	-11.3
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146	NPC203486	-9.1	-11.3	-11.5	205	NPC157333	-10.3	-11.3	-11.3
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156	NPC187456	-11.3	-11.1	-11.5	215	NPC136922	-9.7	-10.8	-11.3
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158	NPC477959	-10.3	-11.3	-11.4	217	NPC27541	-9.5	-11.2	-11.3
159	NPC112274	-8.6	-12.4	-11.4	218	NPC314083	-8.4	-10.8	-11.3
160	NPC475288	-11.4	-11.4	-11.4	219	NPC51662	-9.8	-11.2	-11.3
161	NPC171148	-8.1	-11.3	-11.4	220	NPC8102	-11.0	-11.2	-11.3
162	NPC300183	-9.7	-11.4	-11.4	221	NPC79193	-11.4	-11.3	-11.2
163	NPC477208	-11.4	-11.4	-11.4	222	NPC473938	-11.1	-11.2	-11.2
164	NPC297617	-10.5	-11.4	-11.4	223	NPC81175	-11.2	-10.7	-11.2
165	NPC470753	-10.4	-10.4	-11.4	224	NPC131273	-10.5	-11.2	-11.2
166	NPC11266	-10.5	-10.6	-11.4	225	NPC42673	-11.1	-11.2	-11.2
167	NPC181298	-10.1	-11.4	-11.4	226	NPC112819	-10.8	-11.2	-11.2
168	NPC270498	-10.4	-11.0	-11.4	227	NPC264192	-11.2	-11.3	-11.2
169	NPC321496	-11.1	-11.4	-11.4	228	NPC329080	-8.0	-11.2	-11.2
170	NPC44805	-9.5	-11.4	-11.4	229	NPC121647	-10.6	-10.7	-11.2

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Fast	Moderate	Expensive			Fast	Moderate	Expensive
230	NPC195239	-11.2	-11.2	-11.2	289	NPC139774	-10.6	-11.0	-11.0
231	NPC471825	-11.0	-11.2	-11.2	290	NPC152850	-11.1	-11.0	-11.0
232	NPC69408	-11.0	-11.2	-11.2	291	NPC259350	-9.7	-11.0	-11.0
233	NPC86257	-11.1	-11.2	-11.2	292	NPC473565	-10.8	-10.9	-11.0
234	NPC17810	-11.0	-11.6	-11.2	293	NPC118086	-9.2	-11.1	-11.0
235	NPC197972	-8.8	-11.2	-11.2	294	NPC40574	-10.9	-11.0	-11.0
236	NPC247219	-10.9	-11.2	-11.2	295	NPC469561	-10.1	-10.7	-11.0
237	NPC469810	-10.5	-10.9	-11.2	296	NPC475248	-11.0	-11.0	-11.0
238	NPC470280	-11.2	-10.6	-11.2	297	NPC476565	-10.7	-10.9	-11.0
239	NPC327969	-10.2	-11.2	-11.2	298	NPC477219	-10.1	-11.0	-11.0
240	NPC474179	-11.1	-11.2	-11.2	299	NPC101991	-9.8	-10.7	-11.0
241	NPC475417	-11.1	-11.2	-11.2	300	NPC160527	-10.9	-11.0	-11.0
242	NPC477206	-10.6	-11.2	-11.2	301	NPC473666	-11.0	-11.0	-11.0
243	NPC147363	-10.3	-11.0	-11.2	302	NPC230276	-10.9	-11.0	-11.0
244	NPC15551	-11.1	-11.2	-11.2	303	NPC314358	-8.1	-10.4	-11.0
245	NPC254798	-8.5	-11.1	-11.2	304	NPC471153	-10.4	-10.8	-11.0
246	NPC290683	-10.7	-10.9	-11.2	305	NPC223187	-11.0	-11.0	-11.0
247	NPC42965	-11.3	-10.6	-11.2	306	NPC227132	-10.8	-10.9	-11.0
248	NPC132211	-11.1	-11.1	-11.1	307	NPC470273	-11.2	-10.9	-11.0
249	NPC250129	-11.1	-11.1	-11.1	308	NPC474736	-10.0	-11.0	-11.0
250	NPC27324	-10.8	-11.1	-11.1	309	NPC149873	-9.9	-10.9	-11.0
251	NPC312942	-10.3	-10.9	-11.1	310	NPC243893	-10.8	-10.9	-11.0
252	NPC477532	-10.3	-11.3	-11.1	311	NPC310621	-9.2	-11.0	-11.0
253	NPC909	-11.1	-11.1	-11.1	312	NPC473493	-9.2	-10.7	-11.0
254	NPC161060	-11.3	-11.3	-11.1	313	NPC102810	-10.1	-10.9	-11.0
255	NPC270268	-10.3	-10.9	-11.1	314	NPC158347	-11.0	-11.0	-11.0
256	NPC469996	-10.6	-11.3	-11.1	315	NPC235885	-9.7	-11.0	-11.0
257	NPC475373	-11.0	-11.1	-11.1	316	NPC257175	-10.6	-10.9	-11.0
258	NPC214550	-10.6	-10.9	-11.1	317	NPC157828	-11.0	-11.0	-11.0
259	NPC473177	-12.5	-11.1	-11.1	318	NPC471394	-11.0	-11.0	-11.0
260	NPC473757	-11.1	-11.1	-11.1	319	NPC471601	-9.3	-10.8	-11.0
261	NPC83331	-9.9	-10.9	-11.1	320	NPC473593	-10.9	-11.0	-11.0
262	NPC242446	-11.1	-11.1	-11.1	321	NPC474923	-11.0	-11.0	-11.0
263	NPC471396	-11.1	-11.1	-11.1	322	NPC475436	-10.9	-11.0	-11.0
264	NPC477066	-9.4	-11.1	-11.1	323	NPC476963	-9.9	-11.0	-11.0
265	NPC102088	-11.0	-11.1	-11.1	324	NPC119493	-10.3	-11.0	-11.0
266	NPC71933	-10.8	-11.0	-11.1	325	NPC329731	-9.6	-11.1	-11.0
267	NPC97388	-11.1	-11.1	-11.1	326	NPC89317	-10.7	-10.9	-11.0
268	NPC158020	-8.4	-11.1	-11.1	327	NPC98457	-8.4	-10.8	-11.0
269	NPC160413	-11.1	-11.1	-11.1	328	NPC207243	-9.8	-10.7	-10.9
270	NPC171619	-11.1	-11.1	-11.1	329	NPC109512	-10.9	-10.9	-10.9
271	NPC263485	-11.0	-11.2	-11.1	330	NPC127790	-10.9	-10.9	-10.9
272	NPC26881	-10.4	-11.1	-11.1	331	NPC12890	-10.9	-10.9	-10.9
273	NPC475420	-11.1	-11.1	-11.1	332	NPC153792	-10.9	-10.9	-10.9
274	NPC79107	-10.6	-11.1	-11.1	333	NPC473115	-9.3	-10.6	-10.9
275	NPC10064	-10.7	-11.0	-11.1	334	NPC475602	-10.9	-10.9	-10.9
276	NPC116701	-12.1	-12.3	-11.1	335	NPC102253	-10.8	-10.8	-10.9
277	NPC180605	-9.6	-11.0	-11.1	336	NPC131693	-10.4	-10.7	-10.9
278	NPC181845	-11.0	-11.1	-11.1	337	NPC220974	-10.8	-10.9	-10.9
279	NPC315525	-11.1	-11.1	-11.1	338	NPC477362	-10.8	-10.9	-10.9
280	NPC120351	-11.0	-11.1	-11.1	339	NPC126002	-10.8	-10.9	-10.9
281	NPC323198	-10.1	-11.1	-11.1	340	NPC141970	-9.8	-10.8	-10.9
282	NPC473441	-10.8	-11.1	-11.1	341	NPC183570	-10.1	-10.9	-10.9
283	NPC476817	-10.7	-11.1	-11.1	342	NPC20302	-10.7	-10.9	-10.9
284	NPC24370	-11.0	-11.1	-11.1	343	NPC470277	-11.6	-10.9	-10.9
285	NPC73929	-10.5	-10.8	-11.1	344	NPC476599	-9.7	-10.9	-10.9
286	NPC20388	-9.0	-11.1	-11.1	345	NPC241477	-10.9	-10.9	-10.9
287	NPC233727	-10.3	-10.9	-11.1	346	NPC477291	-10.2	-11.0	-10.9
288	NPC477067	-11.0	-11.0	-11.1	347	NPC62792	-10.3	-10.7	-10.9



Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Fast	Moderate	Expensive			Fast	Moderate	Expensive
348	NPC80650	-8.0	-10.9	-10.9	407	NPC474897	-10.8	-10.8	-10.8
349	NPC168319	-10.9	-10.9	-10.9	408	NPC81939	-8.8	-10.8	-10.8
350	NPC243594	-10.8	-10.9	-10.9	409	NPC114378	-10.1	-10.7	-10.8
351	NPC477391	-9.2	-10.5	-10.9	410	NPC188815	-9.6	-10.4	-10.8
352	NPC477901	-10.3	-10.9	-10.9	411	NPC195715	-10.7	-10.8	-10.8
353	NPC477914	-10.9	-10.9	-10.9	412	NPC256104	-10.5	-10.8	-10.8
354	NPC171007	-10.9	-10.9	-10.9	413	NPC470427	-10.8	-10.8	-10.8
355	NPC191382	-8.8	-10.7	-10.9	414	NPC476883	-10.4	-10.7	-10.8
356	NPC197447	-11.2	-10.9	-10.9	415	NPC476888	-10.6	-10.8	-10.8
357	NPC245055	-10.8	-10.9	-10.9	416	NPC126066	-10.8	-10.8	-10.8
358	NPC273467	-8.3	-10.9	-10.9	417	NPC166143	-10.8	-10.8	-10.8
359	NPC281134	-10.2	-10.8	-10.9	418	NPC298233	-10.8	-10.8	-10.8
360	NPC327095	-10.6	-10.8	-10.9	419	NPC309991	-10.2	-10.7	-10.8
361	NPC471403	-10.8	-10.9	-10.9	420	NPC319232	-10.7	-10.8	-10.8
362	NPC477903	-10.6	-10.5	-10.9	421	NPC470066	-10.7	-10.8	-10.8
363	NPC61411	-10.9	-10.9	-10.9	422	NPC155910	-9.5	-10.7	-10.8
364	NPC202866	-9.4	-11.0	-10.9	423	NPC180204	-10.5	-10.8	-10.8
365	NPC475369	-10.5	-10.9	-10.9	424	NPC6206	-10.0	-10.7	-10.8
366	NPC475605	-10.0	-10.8	-10.9	425	NPC12103	-9.8	-10.6	-10.8
367	NPC74969	-10.8	-10.9	-10.9	426	NPC202198	-10.2	-10.4	-10.8
368	NPC124358	-8.6	-10.5	-10.9	427	NPC227275	-8.9	-10.7	-10.8
369	NPC272549	-10.8	-10.9	-10.9	428	NPC29695	-10.3	-10.6	-10.8
370	NPC471541	-11.7	-10.7	-10.9	429	NPC4574	-10.0	-10.7	-10.8
371	NPC472361	-12.5	-11.7	-10.9	430	NPC470309	-9.9	-10.7	-10.8
372	NPC6215	-10.9	-10.9	-10.9	431	NPC470882	-10.8	-10.8	-10.8
373	NPC16657	-10.4	-10.7	-10.9	432	NPC473178	-11.5	-10.7	-10.8
374	NPC471617	-9.6	-10.8	-10.9	433	NPC474315	-10.6	-10.7	-10.8
375	NPC476257	-11.0	-10.7	-10.9	434	NPC476491	-10.2	-10.7	-10.8
376	NPC476890	-10.6	-10.8	-10.9	435	NPC132771	-10.4	-10.8	-10.7
377	NPC184933	-10.8	-11.0	-10.8	436	NPC138974	-9.9	-10.7	-10.7
378	NPC61382	-11.2	-11.0	-10.8	437	NPC224557	-10.2	-10.7	-10.7
379	NPC183580	-10.8	-10.8	-10.8	438	NPC253268	-10.6	-10.8	-10.7
380	NPC242728	-11.0	-10.3	-10.8	439	NPC266374	-8.9	-10.8	-10.7
381	NPC246904	-10.7	-10.8	-10.8	440	NPC277351	-10.8	-10.8	-10.7
382	NPC43353	-10.6	-10.8	-10.8	441	NPC292775	-10.7	-10.7	-10.7
383	NPC198893	-8.2	-11.9	-10.8	442	NPC292793	-10.6	-10.7	-10.7
384	NPC253456	-10.9	-10.8	-10.8	443	NPC474571	-10.8	-10.7	-10.7
385	NPC286528	-10.0	-10.8	-10.8	444	NPC476750	-9.6	-10.7	-10.7
386	NPC33064	-10.1	-10.8	-10.8	445	NPC476889	-10.5	-10.7	-10.7
387	NPC469722	-10.8	-10.8	-10.8	446	NPC291634	-10.3	-10.5	-10.7
388	NPC475654	-10.8	-10.8	-10.8	447	NPC3381	-10.2	-10.6	-10.7
389	NPC101067	-10.8	-10.8	-10.8	448	NPC470960	-10.7	-10.7	-10.7
390	NPC188239	-10.8	-10.8	-10.8	449	NPC471994	-10.7	-10.7	-10.7
391	NPC325740	-10.5	-11.0	-10.8	450	NPC478108	-9.7	-10.4	-10.7
392	NPC471432	-10.6	-10.7	-10.8	451	NPC191489	-9.9	-10.7	-10.7
393	NPC473851	-9.9	-10.4	-10.8	452	NPC204652	-10.2	-10.6	-10.7
394	NPC120994	-9.8	-10.7	-10.8	453	NPC22248	-10.7	-11.0	-10.7
395	NPC156298	-9.5	-12.2	-10.8	454	NPC271387	-10.0	-10.7	-10.7
396	NPC175477	-10.8	-10.8	-10.8	455	NPC280566	-11.4	-10.7	-10.7
397	NPC223236	-10.5	-10.8	-10.8	456	NPC96759	-10.7	-10.7	-10.7
398	NPC287063	-9.8	-10.8	-10.8	457	NPC233273	-10.1	-10.7	-10.7
399	NPC312536	-10.7	-10.8	-10.8	458	NPC320475	-10.5	-10.7	-10.7
400	NPC328287	-9.5	-10.8	-10.8	459	NPC324001	-11.0	-11.0	-10.7
401	NPC43747	-9.8	-10.5	-10.8	460	NPC476879	-9.4	-10.6	-10.7
402	NPC471135	-8.7	-10.8	-10.8	461	NPC476960	-9.7	-10.7	-10.7
403	NPC477392	-8.2	-10.5	-10.8	462	NPC132386	-10.7	-10.7	-10.7
404	NPC88326	-10.8	-11.3	-10.8	463	NPC290261	-9.0	-10.5	-10.7
405	NPC137657	-10.8	-10.8	-10.8	464	NPC315499	-10.9	-10.7	-10.7
406	NPC329761	-9.1	-10.7	-10.8	465	NPC317590	-10.3	-10.6	-10.7

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Fast	Moderate	Expensive			Fast	Moderate	Expensive
466	NPC96016	-9.3	-10.5	-10.7	525	NPC471963	-8.2	-10.4	-10.6
467	NPC157817	-10.7	-10.8	-10.7	526	NPC472206	-10.6	-10.6	-10.6
468	NPC211845	-10.7	-10.7	-10.7	527	NPC472238	-10.6	-10.6	-10.6
469	NPC241935	-10.7	-10.7	-10.7	528	NPC477101	-9.0	-10.6	-10.6
470	NPC2497	-10.7	-10.7	-10.7	529	NPC478060	-10.2	-10.6	-10.6
471	NPC289776	-9.1	-10.7	-10.7	530	NPC58052	-9.5	-10.6	-10.6
472	NPC298647	-10.4	-10.7	-10.7	531	NPC159338	-10.5	-10.6	-10.6
473	NPC322353	-10.5	-10.6	-10.7	532	NPC178025	-10.4	-10.6	-10.6
474	NPC478261	-10.7	-10.7	-10.7	533	NPC313867	-8.8	-10.5	-10.6
475	NPC79921	-9.2	-10.7	-10.7	534	NPC470750	-10.4	-10.6	-10.6
476	NPC85173	-10.7	-10.7	-10.7	535	NPC472231	-10.6	-10.6	-10.6
477	NPC144202	-10.3	-10.6	-10.7	536	NPC474190	-10.2	-10.9	-10.6
478	NPC199259	-10.7	-10.7	-10.7	537	NPC475244	-10.6	-10.6	-10.6
479	NPC254581	-10.7	-10.7	-10.7	538	NPC476077	-10.6	-11.2	-10.6
480	NPC322982	-10.2	-10.7	-10.7	539	NPC476126	-10.6	-10.6	-10.6
481	NPC469824	-9.2	-10.7	-10.7	540	NPC476878	-10.2	-10.6	-10.6
482	NPC476097	-10.7	-10.7	-10.7	541	NPC70155	-10.6	-10.6	-10.6
483	NPC57690	-10.6	-10.7	-10.7	542	NPC13494	-9.6	-10.4	-10.6
484	NPC227583	-9.0	-10.7	-10.7	543	NPC187255	-10.3	-10.5	-10.6
485	NPC241050	-9.6	-11.0	-10.7	544	NPC19013	-10.6	-10.6	-10.6
486	NPC268676	-10.5	-10.7	-10.7	545	NPC243065	-10.6	-10.6	-10.6
487	NPC469382	-10.2	-10.6	-10.7	546	NPC273199	-10.6	-10.6	-10.6
488	NPC470623	-9.7	-10.8	-10.7	547	NPC295676	-10.6	-10.6	-10.6
489	NPC472225	-10.7	-10.7	-10.7	548	NPC472863	-8.6	-10.5	-10.6
490	NPC124029	-9.1	-10.4	-10.7	549	NPC473535	-9.6	-10.6	-10.6
491	NPC267965	-10.7	-10.7	-10.7	550	NPC475230	-10.5	-10.6	-10.6
492	NPC284102	-10.7	-10.7	-10.7	551	NPC477494	-8.5	-10.6	-10.6
493	NPC289905	-10.5	-10.6	-10.7	552	NPC103782	-9.2	-10.6	-10.6
494	NPC473006	-10.0	-10.7	-10.7	553	NPC209174	-10.6	-10.6	-10.6
495	NPC475597	-10.7	-10.7	-10.7	554	NPC235557	-10.1	-10.5	-10.6
496	NPC91125	-8.4	-10.5	-10.7	555	NPC240042	-8.0	-10.5	-10.6
497	NPC141957	-10.0	-10.5	-10.7	556	NPC268530	-10.5	-10.6	-10.6
498	NPC147635	-10.1	-10.6	-10.7	557	NPC32064	-10.6	-10.6	-10.6
499	NPC252338	-10.2	-10.4	-10.7	558	NPC477899	-10.5	-11.4	-10.6
500	NPC270511	-10.2	-10.6	-10.7	559	NPC60150	-10.6	-10.6	-10.6
501	NPC312630	-10.6	-10.7	-10.7	560	NPC242774	-10.3	-10.6	-10.6
502	NPC323752	-10.5	-10.7	-10.7	561	NPC286786	-10.5	-10.6	-10.6
503	NPC37116	-10.6	-10.7	-10.7	562	NPC42670	-10.6	-10.6	-10.6
504	NPC477556	-10.4	-10.6	-10.7	563	NPC470418	-9.2	-10.6	-10.6
505	NPC51653	-9.1	-10.6	-10.7	564	NPC475988	-10.6	-10.6	-10.6
506	NPC58029	-10.7	-10.6	-10.7	565	NPC135043	-10.6	-10.6	-10.6
507	NPC262077	-9.1	-10.6	-10.6	566	NPC174122	-8.4	-10.5	-10.6
508	NPC45576	-10.6	-10.6	-10.6	567	NPC241636	-10.6	-10.6	-10.6
509	NPC470874	-10.7	-10.6	-10.6	568	NPC30222	-9.4	-10.5	-10.6
510	NPC472673	-9.1	-10.6	-10.6	569	NPC470274	-11.0	-10.5	-10.6
511	NPC105073	-10.3	-10.6	-10.6	570	NPC474106	-10.5	-10.6	-10.6
512	NPC118033	-10.2	-10.6	-10.6	571	NPC474107	-10.3	-10.6	-10.6
513	NPC23621	-10.6	-10.6	-10.6	572	NPC475718	-8.9	-10.6	-10.6
514	NPC74639	-10.7	-10.6	-10.6	573	NPC49911	-10.6	-10.6	-10.6
515	NPC78473	-10.4	-10.6	-10.6	574	NPC116742	-9.3	-10.6	-10.6
516	NPC96131	-11.3	-10.4	-10.6	575	NPC33949	-10.5	-10.5	-10.6
517	NPC15215	-10.6	-10.6	-10.6	576	NPC472926	-9.9	-10.4	-10.6
518	NPC155974	-10.4	-10.6	-10.6	577	NPC473279	-10.6	-10.6	-10.6
519	NPC176246	-8.6	-12.0	-10.6	578	NPC476216	-10.6	-10.5	-10.6
520	NPC202705	-10.4	-10.6	-10.6	579	NPC48305	-10.6	-10.6	-10.6
521	NPC27615	-10.6	-10.7	-10.6	580	NPC5292	-6.9	-10.5	-10.6
522	NPC283343	-10.6	-10.6	-10.6	581	NPC87393	-10.2	-10.5	-10.6
523	NPC300557	-10.3	-10.5	-10.6	582	NPC88668	-8.5	-10.4	-10.6
524	NPC41376	-9.9	-10.6	-10.6	583	NPC150977	-9.9	-10.5	-10.6

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Fast	Moderate	Expensive			Fast	Moderate	Expensive
584	NPC20734	-10.0	-10.5	-10.6	643	NPC472233	-10.5	-10.5	-10.5
585	NPC254146	-10.6	-10.6	-10.6	644	NPC475296	-8.1	-10.5	-10.5
586	NPC312660	-10.5	-10.6	-10.6	645	NPC93744	-10.4	-10.5	-10.5
587	NPC313921	-10.6	-10.6	-10.6	646	NPC190442	-10.5	-10.5	-10.5
588	NPC315848	-8.6	-10.4	-10.6	647	NPC225821	-10.4	-10.5	-10.5
589	NPC32017	-10.2	-10.6	-10.6	648	NPC240604	-10.5	-10.5	-10.5
590	NPC469452	-10.5	-10.7	-10.6	649	NPC266955	-10.1	-10.4	-10.5
591	NPC473467	-10.5	-10.6	-10.6	650	NPC4309	-10.3	-10.5	-10.5
592	NPC474790	-10.3	-10.5	-10.6	651	NPC470076	-10.3	-10.5	-10.5
593	NPC131405	-11.2	-11.8	-10.5	652	NPC472226	-10.5	-10.5	-10.5
594	NPC208994	-10.0	-10.3	-10.5	653	NPC473429	-10.2	-10.5	-10.5
595	NPC218301	-10.5	-10.5	-10.5	654	NPC475719	-10.4	-10.5	-10.5
596	NPC229976	-10.5	-10.5	-10.5	655	NPC477042	-10.5	-10.5	-10.5
597	NPC237182	-10.0	-10.5	-10.5	656	NPC477715	-9.9	-10.4	-10.5
598	NPC315974	-10.0	-10.5	-10.5	657	NPC477857	-9.5	-10.4	-10.5
599	NPC316930	-10.1	-10.4	-10.5	658	NPC282905	-10.5	-10.5	-10.5
600	NPC32715	-9.8	-10.4	-10.5	659	NPC40749	-8.3	-10.5	-10.5
601	NPC470873	-10.5	-10.5	-10.5	660	NPC470068	-10.3	-10.4	-10.5
602	NPC475548	-10.5	-10.5	-10.5	661	NPC477099	-9.4	-10.4	-10.5
603	NPC67569	-9.7	-10.5	-10.5	662	NPC477557	-10.5	-10.5	-10.5
604	NPC86346	-10.3	-10.5	-10.5	663	NPC51247	-10.3	-10.5	-10.5
605	NPC101886	-10.5	-10.5	-10.5	664	NPC90822	-10.3	-10.4	-10.5
606	NPC122056	-10.5	-10.5	-10.5	665	NPC163693	-10.4	-10.4	-10.5
607	NPC13743	-9.7	-10.5	-10.5	666	NPC176840	-10.4	-10.5	-10.5
608	NPC473573	-10.4	-10.5	-10.5	667	NPC18982	-10.4	-10.4	-10.5
609	NPC478036	-10.1	-10.5	-10.5	668	NPC247563	-10.3	-10.4	-10.5
610	NPC8374	-10.5	-10.5	-10.5	669	NPC255082	-10.2	-10.5	-10.5
611	NPC133506	-10.5	-10.5	-10.5	670	NPC255309	-10.4	-10.4	-10.5
612	NPC262083	-10.5	-10.5	-10.5	671	NPC27918	-10.5	-10.5	-10.5
613	NPC264875	-9.3	-10.6	-10.5	672	NPC298072	-10.0	-10.4	-10.5
614	NPC470419	-10.5	-10.5	-10.5	673	NPC310981	-10.6	-10.5	-10.5
615	NPC475027	-10.4	-10.5	-10.5	674	NPC34177	-10.5	-10.5	-10.5
616	NPC475151	-9.9	-10.5	-10.5	675	NPC470954	-10.5	-10.5	-10.5
617	NPC17274	-9.5	-10.5	-10.5	676	NPC185530	-10.4	-10.5	-10.5
618	NPC266513	-9.6	-11.6	-10.5	677	NPC234548	-12.0	-10.4	-10.5
619	NPC285184	-10.4	-10.5	-10.5	678	NPC471404	-10.3	-10.5	-10.5
620	NPC290746	-9.6	-10.6	-10.5	679	NPC473734	-8.6	-10.4	-10.5
621	NPC41318	-10.4	-10.5	-10.5	680	NPC475274	-10.3	-10.4	-10.5
622	NPC97078	-10.0	-10.5	-10.5	681	NPC476080	-8.8	-10.6	-10.5
623	NPC114441	-8.3	-10.3	-10.5	682	NPC477363	-10.3	-10.5	-10.5
624	NPC126128	-10.5	-10.5	-10.5	683	NPC153700	-9.5	-10.4	-10.4
625	NPC138775	-9.6	-10.4	-10.5	684	NPC174024	-10.1	-10.8	-10.4
626	NPC139783	-10.5	-10.5	-10.5	685	NPC245410	-10.4	-10.4	-10.4
627	NPC178541	-10.5	-10.5	-10.5	686	NPC267926	-10.4	-10.4	-10.4
628	NPC289383	-10.1	-11.6	-10.5	687	NPC27518	-10.3	-10.4	-10.4
629	NPC293038	-10.2	-10.5	-10.5	688	NPC307396	-10.4	-10.4	-10.4
630	NPC306799	-10.1	-10.4	-10.5	689	NPC40918	-10.4	-10.4	-10.4
631	NPC473173	-10.4	-10.5	-10.5	690	NPC471113	-10.4	-10.4	-10.4
632	NPC474370	-9.7	-10.5	-10.5	691	NPC478258	-10.5	-10.5	-10.4
633	NPC476091	-10.3	-10.5	-10.5	692	NPC49964	-10.2	-10.4	-10.4
634	NPC4910	-10.4	-10.4	-10.5	693	NPC99411	-9.7	-10.3	-10.4
635	NPC108476	-10.5	-10.5	-10.5	694	NPC151292	-8.1	-10.4	-10.4
636	NPC126815	-10.4	-10.5	-10.5	695	NPC278540	-10.3	-10.4	-10.4
637	NPC242068	-10.4	-10.5	-10.5	696	NPC39431	-10.4	-10.4	-10.4
638	NPC244606	-10.5	-10.5	-10.5	697	NPC469731	-10.4	-10.4	-10.4
639	NPC284162	-10.5	-10.5	-10.5	698	NPC470053	-9.4	-10.4	-10.4
640	NPC470126	-9.6	-10.5	-10.5	699	NPC475238	-10.4	-10.4	-10.4
641	NPC470223	-9.2	-10.5	-10.5	700	NPC56618	-9.7	-10.4	-10.4
642	NPC472229	-10.5	-10.5	-10.5	701	NPC93662	-10.4	-10.4	-10.4

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Fast	Moderate	Expensive			Fast	Moderate	Expensive
702	NPC117027	-10.4	-10.4	-10.4	761	NPC50615	-9.5	-11.4	-10.3
703	NPC177064	-10.4	-10.4	-10.4	762	NPC185665	-10.3	-10.3	-10.3
704	NPC198621	-9.0	-10.3	-10.4	763	NPC475253	-9.7	-10.4	-10.3
705	NPC209509	-10.1	-10.4	-10.4	764	NPC74727	-10.3	-10.4	-10.3
706	NPC273623	-10.3	-10.4	-10.4	765	NPC162033	-10.5	-11.1	-10.3
707	NPC293044	-10.4	-10.4	-10.4	766	NPC235364	-9.7	-10.3	-10.3
708	NPC470425	-10.4	-10.4	-10.4	767	NPC289086	-9.8	-10.4	-10.3
709	NPC471720	-10.4	-10.4	-10.4	768	NPC141053	-10.0	-10.4	-10.3
710	NPC473310	-10.2	-10.4	-10.4	769	NPC476830	-9.9	-10.7	-10.3
711	NPC474448	-10.5	-10.4	-10.4	770	NPC270586	-9.1	-10.4	-10.2
712	NPC93416	-10.5	-10.5	-10.4	771	NPC320026	-10.5	-10.7	-10.2
713	NPC110882	-10.2	-10.4	-10.4	772	NPC159526	-9.6	-10.4	-10.2
714	NPC194427	-10.3	-10.4	-10.4	773	NPC474564	-11.2	-12.0	-10.2
715	NPC206592	-10.4	-10.4	-10.4	774	NPC208189	-10.6	-10.8	-10.1
716	NPC209851	-8.6	-10.4	-10.4	775	NPC212768	-10.2	-10.5	-10.1
717	NPC251936	-10.4	-10.4	-10.4	776	NPC475540	-9.0	-10.6	-10.1
718	NPC305501	-10.2	-10.4	-10.4	777	NPC107674	-10.1	-10.3	-10.1
719	NPC34963	-10.4	-10.4	-10.4	778	NPC473085	-9.1	-10.4	-10.1
720	NPC472234	-10.4	-10.4	-10.4	779	NPC235824	-8.6	-10.5	-10.1
721	NPC472294	-8.9	-10.4	-10.4	780	NPC48599	-9.3	-10.5	-10.0
722	NPC473591	-10.0	-10.3	-10.4	781	NPC470312	-8.5	-10.6	-10.0
723	NPC477906	-9.0	-10.4	-10.4	782	NPC470892	-9.0	-10.4	-10.0
724	NPC120917	-10.3	-10.3	-10.4	783	NPC119481	-10.5	-11.2	-10.0
725	NPC151030	-8.2	-10.4	-10.4	784	NPC137414	-9.0	-10.4	-10.0
726	NPC168511	-10.4	-10.4	-10.4	785	NPC471049	-9.5	-10.5	-9.9
727	NPC274448	-10.2	-10.4	-10.4	786	NPC473220	-9.6	-10.9	-9.9
728	NPC310572	-9.8	-10.4	-10.4	787	NPC478127	-9.6	-10.7	-9.9
729	NPC43716	-8.7	-10.3	-10.4	788	NPC136948	-10.1	-10.4	-9.9
730	NPC469720	-10.4	-10.4	-10.4	789	NPC302392	-10.3	-10.3	-9.9
731	NPC472223	-10.4	-10.4	-10.4	790	NPC475651	-11.0	-11.5	-9.9
732	NPC474870	-10.4	-10.4	-10.4	791	NPC3952	-10.7	-10.7	-9.8
733	NPC48339	-9.5	-10.7	-10.4	792	NPC85316	-9.7	-11.5	-9.8
734	NPC153734	-10.4	-10.4	-10.4	793	NPC475249	-8.1	-10.9	-9.8
735	NPC190401	-9.8	-10.4	-10.4	794	NPC202898	-10.9	-12.2	-9.8
736	NPC472695	-8.8	-10.4	-10.4	795	NPC477468	-9.7	-10.6	-9.7
737	NPC108840	-10.4	-10.4	-10.4	796	NPC471777	-9.0	-11.2	-9.7
738	NPC255401	-10.4	-10.4	-10.4	797	NPC470275	-10.5	-10.8	-9.7
739	NPC275575	-9.8	-10.4	-10.4	798	NPC25736	-9.9	-10.6	-9.7
740	NPC312678	-9.8	-11.0	-10.4	799	NPC308262	-9.8	-11.1	-9.6
741	NPC469740	-10.5	-10.4	-10.4	800	NPC328928	-9.3	-10.9	-9.6
742	NPC65700	-10.8	-10.4	-10.4	801	NPC471582	-10.6	-11.0	-9.6
743	NPC289486	-10.3	-10.4	-10.4	802	NPC475536	-9.5	-10.8	-9.6
744	NPC41679	-10.4	-10.4	-10.4	803	NPC93685	-10.9	-11.1	-9.6
745	NPC469394	-10.0	-10.4	-10.4	804	NPC38350	-10.3	-10.4	-9.6
746	NPC470036	-10.3	-10.4	-10.4	805	NPC469317	-8.3	-10.5	-9.5
747	NPC472230	-10.4	-10.4	-10.4	806	NPC99088	-10.9	-11.4	-9.5
748	NPC473680	-10.2	-10.3	-10.4	807	NPC304322	-11.0	-11.6	-9.5
749	NPC475862	-10.4	-10.4	-10.4	808	NPC477902	-9.4	-10.5	-9.5
750	NPC18536	-10.3	-10.4	-10.4	809	NPC69273	-8.5	-10.9	-9.5
751	NPC204491	-8.3	-10.3	-10.4	810	NPC102843	-9.5	-12.1	-9.4
752	NPC292233	-9.3	-10.3	-10.4	811	NPC471980	-9.6	-11.2	-9.4
753	NPC35164	-10.3	-10.4	-10.4	812	NPC473749	-8.2	-10.8	-9.4
754	NPC470037	-10.3	-10.3	-10.4	813	NPC146563	-8.3	-10.5	-9.4
755	NPC57079	-10.1	-10.3	-10.4	814	NPC97884	-8.9	-10.8	-9.4
756	NPC104387	-10.4	-10.4	-10.3	815	NPC269095	-10.8	-10.8	-9.4
757	NPC249817	-10.2	-10.3	-10.3	816	NPC177834	-9.1	-10.7	-9.3
758	NPC6274	-10.3	-10.4	-10.3	817	NPC235841	-8.1	-10.4	-9.2
759	NPC472237	-10.3	-10.3	-10.3	818	NPC323074	-9.3	-10.7	-9.2
760	NPC47386	-10.1	-10.4	-10.3	819	NPC10005	-9.1	-10.4	-9.1

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Fast	Moderate	Expensive			Fast	Moderate	Expensive
820	NPC271494	-8.5	-10.6	-9.1	844	NPC473160	-10.4	-10.3	-6.6
821	NPC476784	-11.0	-10.4	-9.1	845	NPC473596	-9.5	-10.3	-6.6
822	NPC470504	-9.6	-10.4	-9.1	846	NPC474976	-10.3	-10.3	-6.6
823	NPC102725	-10.1	-10.4	-9.0	847	NPC475025	-10.2	-10.3	-6.6
824	NPC472215	-8.5	-10.5	-9.0	848	NPC477334	-9.3	-10.3	-6.6
825	NPC473890	-9.2	-10.7	-9.0	849	NPC63023	-9.9	-10.3	-6.6
826	NPC473020	-8.7	-10.4	-8.9	850	NPC11847	-9.9	-10.3	-6.6
827	NPC45943	-9.0	-10.9	-8.9	851	NPC122116	-10.3	-10.3	-6.6
828	NPC229962	-8.9	-10.4	-8.8	852	NPC133625	-8.3	-10.3	-6.5
829	NPC40716	-10.3	-10.3	-8.8	853	NPC16350	-8.2	-10.3	-6.5
830	NPC278272	-9.4	-11.3	-8.7	854	NPC473160	-10.4	-10.3	-6.5
831	NPC115601	-9.3	-11.1	-8.7	855	NPC473596	-9.5	-10.3	-6.5
832	NPC116024	-9.3	-10.6	-8.6	856	NPC474976	-10.3	-10.3	-6.5
833	NPC220293	-10.1	-10.8	-8.6	857	NPC475025	-10.2	-10.3	-6.5
834	NPC160084	-10.5	-11.5	-8.5	858	NPC477334	-9.3	-10.3	-6.5
835	NPC273798	-9.1	-10.5	-8.5	859	NPC63023	-9.9	-10.3	-6.4
836	NPC286809	-11.3	-12.1	-8.2	860	NPC11847	-9.9	-10.3	-6.4
837	NPC165234	-10.6	-12.3	-7.9	861	NPC122116	-10.3	-10.3	-6.4
838	NPC318581	-9.1	-10.8	-7.8	862	NPC133625	-8.3	-10.3	-6.4
839	NPC114287	-10.7	-11.1	-7.6	863	NPC16350	-10.3	-10.3	-6.4
840	NPC117478	-8.1	-10.4	-7.4	864	NPC190204	-8.2	-10.3	-6.4
841	NPC21691	-8.4	-11.6	-6.9	865	NPC200589	-9.1	-10.3	-6.4
842	NPC327699	-10.2	-11.3	-6.8	866	NPC201634	-10.3	-10.3	-6.4
843	NPC477074	-8.7	-10.6	-6.6					

<sup>a</sup>Data ranked based on the Expensive docking score.

**Table S2.** Estimated docking scores and MM-GBSA binding energies (in kcal/mol) over 1 ns implicit-solvent MD simulations for taxol and the top 86 NPs within the P-gp binding pocket.<sup>a</sup>

No.	Compound Name/Code	Docking Score (kcal/mol)			MM-GBSA Binding Energy (kcal/mol)
		Fast	Moderate	Expensive	
	Taxol	-9.4	-8.0	-10.2	-65.9
1	NPC197736	-8.8	-10.9	-13.5	-90.6
2	NPC475164	-9.3	-11.3	-11.9	-88.9
3	NPC2313	-9.7	-12.1	-12.0	-87.4
4	NPC104372	-9.9	-11.0	-12.2	-87.1
5	NPC471637	-9.7	-11.4	-12.2	-84.8
6	NPC70862	-11.6	-11.8	-12.2	-82.3
7	NPC477344	-10.2	-11.1	-11.9	-79.6
8	NPC477533	-11.1	-12.6	-13.3	-79.4
9	NPC223735	-9.9	-11.4	-12.6	-78.8
10	NPC472939	-10.4	-11.9	-12.2	-77.7
11	NPC475655	-9.6	-11.1	-12.1	-77.6
12	NPC472936	-10.6	-11.5	-12.0	-77.2
13	NPC329943	-11.4	-11.8	-12.0	-76.9
14	NPC208258	-8.4	-12.1	-13.1	-75.9
15	NPC470582	-10.3	-10.5	-12.1	-74.7
16	NPC276231	-15.1	-15.9	-16.4	-74.2
17	NPC313421	-10.5	-12.1	-12.1	-72.4
18	NPC123859	-10.1	-12.1	-12.5	-72.3
19	NPC471860	-11.9	-12.1	-12.5	-72.2
20	NPC149962	-10.8	-10.8	-12.1	-71.3
21	NPC471850	-10.7	-12.0	-12.6	-70.9
22	NPC474581	-10.6	-11.6	-11.9	-70.8
23	NPC472437	-13.5	-12.9	-14.5	-68.1
24	NPC231271	-12.4	-12.6	-12.9	-66.3
25	NPC472937	-10.3	-11.4	-12.1	-66.3
26	NPC74086	-10.5	-10.8	-12.5	-66.3
27	NPC471583	-11.8	-11.8	-11.8	-65.7
28	NPC471858	-11.5	-11.5	-11.9	-65.6
29	NPC177362	-12.0	-12.1	-12.2	-64.9
30	NPC202104	-12.6	-13.5	-13.2	-64.6
31	NPC470601	-9.6	-13.0	-14.9	-64.5
32	NPC65118	-12.2	-12.7	-12.6	-64.5
33	NPC471859	-12.1	-12.3	-12.3	-63.6
34	NPC472934	-10.7	-11.3	-11.9	-63.4
35	NPC327962	-12.2	-12.7	-12.4	-62.7
36	NPC477531	-11.0	-12.1	-12.1	-62.5
37	NPC322800	-11.2	-11.8	-11.8	-62.5
38	NPC313179	-10.9	-10.4	-12.2	-61.6
39	NPC78159	-11.3	-11.0	-11.9	-60.0
40	NPC473547	-11.9	-11.9	-11.9	-59.7
41	NPC47905	-10.8	-12.2	-11.9	-58.6
42	NPC69383	-10.9	-11.5	-12.3	-58.3
43	NPC239990	-11.9	-12.3	-12.2	-58.3
44	NPC231712	-9.3	-12.1	-12.3	-58.3
45	NPC81137	-8.8	-11.9	-12.0	-58.3
46	NPC242269	-13.2	-14.1	-14.2	-58.0
47	NPC469671	-10.3	-11.8	-12.1	-57.7
48	NPC65034	-11.9	-12.1	-12.2	-57.6
49	NPC4638	-12.2	-11.5	-12.2	-57.5
50	NPC477874	-11.7	-11.8	-12.0	-57.3
51	NPC470426	-12.8	-12.8	-12.8	-57.3
52	NPC202428	-11.2	-11.8	-11.9	-57.2
53	NPC162440	-12.2	-12.2	-12.2	-56.1
54	NPC126676	-11.8	-11.6	-12.5	-55.7
55	NPC133209	-10.8	-11.5	-12.3	-55.4

**Table S2. Continued.**

No.	Compound Name/Code	Docking Score (kcal/mol)			MM-GBSA Binding Energy (kcal/mol)
		Standard	Moderate	Expensive	
56	NPC266545	-11.0	-10.9	-12.1	-55.2
57	NPC473403	-10.5	-12.3	-12.4	-55.1
58	NPC475493	-13.4	-13.7	-13.8	-54.1
59	NPC469447	-12.1	-12.4	-12.3	-54.0
60	NPC96605	-8.5	-10.6	-11.9	-53.9
61	NPC224528	-12.3	-12.6	-12.8	-53.7
62	NPC105942	-11.5	-12.0	-12.1	-53.4
63	NPC472395	-11.9	-12.1	-12.9	-53.1
64	NPC471863	-12.1	-11.9	-11.9	-52.6
65	NPC472236	-11.2	-12.4	-12.4	-52.4
66	NPC183736	-10.9	-12.3	-12.5	-52.3
67	NPC472371	-12.4	-12.6	-12.1	-52.1
68	NPC473507	-10.1	-11.5	-12.9	-51.7
69	NPC270958	-10.2	-11.4	-12.0	-51.4
70	NPC475258	-12.7	-12.7	-12.7	-50.7
71	NPC475570	-11.7	-11.8	-11.8	-50.3
72	NPC103250	-12.0	-12.1	-12.1	-50.1
73	NPC307205	-12.4	-12.4	-12.4	-50.0
74	NPC473612	-11.7	-12.0	-12.0	-49.9
75	NPC36754	-12.0	-12.0	-12.0	-49.3
76	NPC473720	-11.8	-11.9	-11.9	-48.6
77	NPC143173	-12.0	-12.0	-12.0	-48.1
78	NPC250835	-12.2	-12.2	-12.2	-47.9
79	NPC6702	-12.0	-12.5	-12.7	-47.1
80	NPC94531	-11.0	-11.5	-11.8	-46.9
81	NPC475520	-11.9	-11.8	-11.9	-46.8
82	NPC477207	-11.9	-12.5	-12.6	-46.5
83	NPC208011	-11.0	-10.9	-12.1	-45.2
84	NPC127197	-12.0	-12.0	-12.0	-43.0
85	NPC9856	-11.8	-11.8	-11.8	-40.4
86	NPC470602	-10.9	-13.0	-14.7	-22.6

<sup>a</sup>Data ranked based on the MM-GBSA binding energy over the 1 ns implicit MD simulations.