

Table S1. Evaluated standard docking scores (in kcal/mol) for the investigated compounds with docking scores less than -7.0 kcal/mol against the BRD4-BD1 (Exhaustiveness number = 50).

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
	R6S	-9.9	48	SD003836	-9.1	96	SD000605	-8.9
1	SD003509	-10.1	49	SD006034	-9.1	97	SD000929	-8.8
2	SD003873	-10.1	50	SD000645	-9.1	98	SD000896	-8.8
3	SD006001	-9.9	51	SD000946	-9.0	99	SD000863	-8.8
4	SD003842	-9.8	52	SD001084	-9.0	100	SD001074	-8.8
5	SD000497	-9.8	53	SD003217	-9.0	101	SD001051	-8.8
6	SD001949	-9.7	54	SD001678	-9.0	102	SD001271	-8.8
7	SD003490	-9.7	55	SD000012	-9.0	103	SD001279	-8.8
8	SD000062	-9.7	56	SD001987	-9.0	104	SD001274	-8.8
9	SD000944	-9.6	57	SD002471	-9.0	105	SD000140	-8.8
10	SD001524	-9.6	58	SD000265	-9.0	106	SD000146	-8.8
11	SD002150	-9.6	59	SD000306	-9.0	107	SD001638	-8.8
12	SD002280	-9.6	60	SD000330	-9.0	108	SD001367	-8.8
13	SD003376	-9.6	61	SD002620	-9.0	109	SD001865	-8.8
14	SD003145	-9.6	62	SD003573	-9.0	110	SD001599	-8.8
15	SD003291	-9.5	63	SD003749	-9.0	111	SD002051	-8.8
16	SD002790	-9.5	64	SD003802	-9.0	112	SD002114	-8.8
17	SD000943	-9.4	65	SD003939	-9.0	113	SD002115	-8.8
18	SD001942	-9.4	66	SD000412	-9.0	114	SD002322	-8.8
19	SD002303	-9.4	67	SD000414	-9.0	115	SD002506	-8.8
20	SD002172	-9.4	68	SD000719	-9.0	116	SD002417	-8.8
21	SD002496	-9.4	69	SD000709	-9.0	117	SD002582	-8.8
22	SD000686	-9.4	70	SD000839	-9.0	118	SD002800	-8.8
23	SD000883	-9.3	71	SD000858	-8.9	119	SD003415	-8.8
24	SD003224	-9.3	72	SD001004	-8.9	120	SD003151	-8.8
25	SD003820	-9.3	73	SD001347	-8.9	121	SD003543	-8.8
26	SD003943	-9.3	74	SD001419	-8.9	122	SD003714	-8.8
27	SD006014	-9.3	75	SD001471	-8.9	123	SD003791	-8.8
28	SD001640	-9.2	76	SD001406	-8.9	124	SD003876	-8.8
29	SD003076	-9.2	77	SD001705	-8.9	125	SD003905	-8.8
30	SD002297	-9.2	78	SD001634	-8.9	126	SD003930	-8.8
31	SD003363	-9.2	79	SD000168	-8.9	127	SD000575	-8.8
32	SD002572	-9.2	80	SD001727	-8.9	128	SD000691	-8.8
33	SD003570	-9.2	81	SD001623	-8.9	129	SD000671	-8.8
34	SD003940	-9.2	82	SD001776	-8.9	130	SD000735	-8.8
35	SD000554	-9.2	83	SD000199	-8.9	131	SD000895	-8.7
36	SD000846	-9.2	84	SD002006	-8.9	132	SD000949	-8.7
37	SD001057	-9.1	85	SD003341	-8.9	133	SD001025	-8.7
38	SD001459	-9.1	86	SD002373	-8.9	134	SD001468	-8.7
39	SD001505	-9.1	87	SD002633	-8.9	135	SD001854	-8.7
40	SD001644	-9.1	88	SD002712	-8.9	136	SD001910	-8.7
41	SD001676	-9.1	89	SD002713	-8.9	137	SD002027	-8.7
42	SD001713	-9.1	90	SD003034	-8.9	138	SD002123	-8.7
43	SD001824	-9.1	91	SD003738	-8.9	139	SD002218	-8.7
44	SD002018	-9.1	92	SD003901	-8.9	140	SD002702	-8.7
45	SD003347	-9.1	93	SD003895	-8.9	141	SD003385	-8.7
46	SD002327	-9.1	94	SD006006	-8.9	142	SD003400	-8.7
47	SD003350	-9.1	95	SD006007	-8.9	143	SD003127	-8.7

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
144	SD003706	-8.7	192	SD001104	-8.5	240	SD000188	-8.4
145	SD003764	-8.7	193	SD001160	-8.5	241	SD001915	-8.4
146	SD003908	-8.7	194	SD001156	-8.5	242	SD001954	-8.4
147	SD006052	-8.7	195	SD001534	-8.5	243	SD001982	-8.4
148	SD003937	-8.7	196	SD001481	-8.5	244	SD002024	-8.4
149	SD000438	-8.7	197	SD001564	-8.5	245	SD001969	-8.4
150	SD000495	-8.7	198	SD001602	-8.5	246	SD002106	-8.4
151	SD000606	-8.7	199	SD001688	-8.5	247	SD002007	-8.4
152	SD000674	-8.7	200	SD001617	-8.5	248	SD000206	-8.4
153	SD000725	-8.7	201	SD001858	-8.5	249	SD003306	-8.4
154	SD000928	-8.6	202	SD000192	-8.5	250	SD002182	-8.4
155	SD000952	-8.6	203	SD002098	-8.5	251	SD002207	-8.4
156	SD001048	-8.6	204	SD002133	-8.5	252	SD002145	-8.4
157	SD001107	-8.6	205	SD002120	-8.5	253	SD000222	-8.4
158	SD000145	-8.6	206	SD002129	-8.5	254	SD002277	-8.4
159	SD001575	-8.6	207	SD002200	-8.5	255	SD002287	-8.4
160	SD001551	-8.6	208	SD002255	-8.5	256	SD003353	-8.4
161	SD000176	-8.6	209	SD003337	-8.5	257	SD002559	-8.4
162	SD001849	-8.6	210	SD002345	-8.5	258	SD002593	-8.4
163	SD003273	-8.6	211	SD002441	-8.5	259	SD002740	-8.4
164	SD002045	-8.6	212	SD002510	-8.5	260	SD003407	-8.4
165	SD002108	-8.6	213	SD000261	-8.5	261	SD002708	-8.4
166	SD002192	-8.6	214	SD002760	-8.5	262	SD002534	-8.4
167	SD002225	-8.6	215	SD003417	-8.5	263	SD003413	-8.4
168	SD000225	-8.6	216	SD003044	-8.5	264	SD003439	-8.4
169	SD002323	-8.6	217	SD003545	-8.5	265	SD003093	-8.4
170	SD002845	-8.6	218	SD003515	-8.5	266	SD000308	-8.4
171	SD003412	-8.6	219	SD000351	-8.5	267	SD000315	-8.4
172	SD003052	-8.6	220	SD003778	-8.5	268	SD003531	-8.4
173	SD003103	-8.6	221	SD003857	-8.5	269	SD003596	-8.4
174	SD003487	-8.6	222	SD003878	-8.5	270	SD003622	-8.4
175	SD003497	-8.6	223	SD006047	-8.5	271	SD003624	-8.4
176	SD003643	-8.6	224	SD003711	-8.5	272	SD003716	-8.4
177	SD003818	-8.6	225	SD000574	-8.5	273	SD003774	-8.4
178	SD003828	-8.6	226	SD000724	-8.5	274	SD003813	-8.4
179	SD003854	-8.6	227	SD000968	-8.4	275	SD003767	-8.4
180	SD006050	-8.6	228	SD003175	-8.4	276	SD003941	-8.4
181	SD000447	-8.6	229	SD000983	-8.4	277	SD006036	-8.4
182	SD000660	-8.6	230	SD001068	-8.4	278	SD000057	-8.4
183	SD000700	-8.6	231	SD001095	-8.4	280	SD006013	-8.4
184	SD000726	-8.6	232	SD000119	-8.4	281	SD000404	-8.4
185	SD000874	-8.5	233	SD001313	-8.4	282	SD000407	-8.4
186	SD000855	-8.5	234	SD001489	-8.4	283	SD000448	-8.4
187	SD000856	-8.5	235	SD003242	-8.4	279	SD000702	-8.4
188	SD001002	-8.5	236	SD000158	-8.4	284	SD000699	-8.4
189	SD001015	-8.5	237	SD003264	-8.4	285	SD000816	-8.4
190	SD001033	-8.5	238	SD001683	-8.4	286	SD000782	-8.4
191	SD000105	-8.5	239	SD001802	-8.4	287	SD000787	-8.4

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
288	SD000867	-8.3	336	SD006011	-8.3	384	SD002179	-8.2
289	SD000966	-8.3	337	SD000076	-8.3	385	SD001668	-8.2
290	SD000994	-8.3	338	SD000410	-8.3	386	SD002188	-8.2
291	SD001052	-8.3	339	SD000413	-8.3	387	SD002269	-8.2
292	SD003180	-8.3	340	SD000564	-8.3	388	SD002190	-8.2
293	SD001001	-8.3	341	SD000567	-8.3	389	SD002305	-8.2
294	SD001158	-8.3	342	SD000662	-8.3	390	SD003362	-8.2
295	SD001228	-8.3	343	SD000703	-8.3	391	SD002460	-8.2
296	SD001153	-8.3	344	SD000783	-8.3	392	SD002448	-8.2
297	SD001157	-8.3	345	SD000790	-8.3	393	SD002470	-8.2
298	SD001445	-8.3	346	SD000848	-8.2	394	SD002575	-8.2
299	SD001467	-8.3	347	SD000097	-8.2	395	SD002561	-8.2
300	SD003226	-8.3	348	SD001100	-8.2	396	SD003382	-8.2
301	SD001578	-8.3	349	SD000091	-8.2	397	SD002733	-8.2
302	SD001580	-8.3	350	SD001161	-8.2	398	SD003405	-8.2
303	SD001571	-8.3	351	SD001154	-8.2	399	SD002795	-8.2
304	SD003262	-8.3	352	SD001236	-8.2	400	SD002773	-8.2
305	SD001807	-8.3	353	SD001319	-8.2	401	SD002782	-8.2
306	SD001852	-8.3	354	SD000127	-8.2	402	SD002895	-8.2
307	SD001818	-8.3	355	SD001409	-8.2	403	SD002932	-8.2
308	SD001885	-8.3	356	SD001412	-8.2	404	SD003419	-8.2
309	SD001893	-8.3	357	SD001374	-8.2	405	SD003016	-8.2
310	SD001939	-8.3	358	SD001416	-8.2	406	SD003438	-8.2
311	SD002088	-8.3	359	SD001447	-8.2	407	SD003132	-8.2
312	SD002105	-8.3	360	SD001278	-8.2	408	SD000312	-8.2
313	SD002186	-8.3	361	SD001515	-8.2	409	SD003505	-8.2
314	SD000214	-8.3	362	SD001604	-8.2	410	SD003488	-8.2
315	SD002189	-8.3	363	SD001675	-8.2	411	SD000328	-8.2
316	SD002170	-8.3	364	SD001711	-8.2	412	SD003615	-8.2
317	SD002459	-8.3	365	SD001658	-8.2	413	SD003701	-8.2
318	SD002436	-8.3	366	SD001635	-8.2	414	SD003688	-8.2
319	SD002524	-8.3	367	SD001762	-8.2	415	SD003776	-8.2
320	SD000249	-8.3	368	SD001111	-8.2	416	SD000361	-8.2
321	SD002734	-8.3	369	SD001763	-8.2	417	SD003832	-8.2
322	SD002850	-8.3	370	SD001820	-8.2	418	SD003883	-8.2
323	SD003020	-8.3	371	SD001859	-8.2	419	SD003945	-8.2
324	SD002963	-8.3	372	SD001889	-8.2	420	SD000068	-8.2
325	SD000320	-8.3	373	SD001909	-8.2	421	SD000386	-8.2
326	SD000326	-8.3	374	SD001933	-8.2	422	SD000582	-8.2
327	SD003547	-8.3	375	SD001965	-8.2	423	SD000609	-8.2
328	SD003549	-8.3	376	SD002014	-8.2	424	SD000652	-8.2
329	SD003703	-8.3	377	SD003303	-8.2	425	SD000781	-8.2
330	SD000358	-8.3	378	SD003301	-8.2	426	SD000840	-8.2
331	SD003814	-8.3	379	SD002082	-8.2	427	SD000796	-8.2
332	SD003796	-8.3	380	SD000208	-8.2	428	SD000945	-8.1
333	SD003835	-8.3	381	SD002157	-8.2	429	SD000989	-8.1
334	SD003900	-8.3	382	SD002116	-8.2	430	SD001044	-8.1
335	SD003769	-8.3	383	SD003320	-8.2	431	SD001054	-8.1

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
432	SD001090	-8.1	480	SD000273	-8.1	528	SD000151	-8.0
433	SD001159	-8.1	481	SD002826	-8.1	529	SD001366	-8.0
434	SD000942	-8.1	482	SD002779	-8.1	530	SD001680	-8.0
435	SD001170	-8.1	483	SD003434	-8.1	531	SD001689	-8.0
436	SD003184	-8.1	484	SD000307	-8.1	532	SD001682	-8.0
437	SD001200	-8.1	485	SD000310	-8.1	533	SD001712	-8.0
438	SD001260	-8.1	486	SD003387	-8.1	534	SD001756	-8.0
439	SD001335	-8.1	487	SD003581	-8.1	535	SD001783	-8.0
440	SD001395	-8.1	488	SD003631	-8.1	536	SD001751	-8.0
441	SD001420	-8.1	489	SD003626	-8.1	537	SD001822	-8.0
442	SD001512	-8.1	490	SD000352	-8.1	538	SD001946	-8.0
443	SD001516	-8.1	491	SD003772	-8.1	539	SD001955	-8.0
444	SD001584	-8.1	492	SD003719	-8.1	540	SD001872	-8.0
445	SD003243	-8.1	493	SD003720	-8.1	541	SD003289	-8.0
446	SD001179	-8.1	494	SD003794	-8.1	542	SD002022	-8.0
447	SD001706	-8.1	495	SD000359	-8.1	543	SD003309	-8.0
448	SD001754	-8.1	496	SD003862	-8.1	544	SD002009	-8.0
449	SD000178	-8.1	497	SD006027	-8.1	545	SD002084	-8.0
450	SD001801	-8.1	498	SD003931	-8.1	546	SD002117	-8.0
451	SD003270	-8.1	499	SD006051	-8.1	547	SD003325	-8.0
452	SD000190	-8.1	500	SD000546	-8.1	548	SD002208	-8.0
453	SD001766	-8.1	501	SD000623	-8.1	549	SD002274	-8.0
454	SD001937	-8.1	502	SD000470	-8.1	550	SD002254	-8.0
455	SD001961	-8.1	503	SD000471	-8.1	551	SD003346	-8.0
456	SD002010	-8.1	504	SD000710	-8.1	552	SD002278	-8.0
457	SD002019	-8.1	505	SD000770	-8.1	553	SD000226	-8.0
458	SD002015	-8.1	506	SD000870	-8.0	554	SD002298	-8.0
459	SD002053	-8.1	507	SD000865	-8.0	555	SD003329	-8.0
460	SD002058	-8.1	508	SD000991	-8.0	556	SD002421	-8.0
461	SD001831	-8.1	509	SD000996	-8.0	557	SD002476	-8.0
462	SD000210	-8.1	510	SD001036	-8.0	558	SD003355	-8.0
463	SD002195	-8.1	511	SD001043	-8.0	559	SD002681	-8.0
464	SD002271	-8.1	512	SD001046	-8.0	560	SD002586	-8.0
465	SD003345	-8.1	513	SD000948	-8.0	561	SD002690	-8.0
466	SD002289	-8.1	514	SD001080	-8.0	562	SD002718	-8.0
467	SD002339	-8.1	515	SD001102	-8.0	563	SD002698	-8.0
468	SD002388	-8.1	516	SD001143	-8.0	564	SD002699	-8.0
469	SD003354	-8.1	517	SD003191	-8.0	565	SD002759	-8.0
470	SD002438	-8.1	518	SD001162	-8.0	566	SD002859	-8.0
471	SD002440	-8.1	519	SD000112	-8.0	567	SD000278	-8.0
472	SD000241	-8.1	520	SD001155	-8.0	568	SD002875	-8.0
473	SD002560	-8.1	521	SD001235	-8.0	569	SD003026	-8.0
474	SD002570	-8.1	522	SD001263	-8.0	570	SD000294	-8.0
475	SD000248	-8.1	523	SD000125	-8.0	571	SD003436	-8.0
476	SD003049	-8.1	524	SD001387	-8.0	572	SD003040	-8.0
477	SD002626	-8.1	525	SD001421	-8.0	573	SD003032	-8.0
478	SD002696	-8.1	526	SD001474	-8.0	574	SD003481	-8.0
479	SD002700	-8.1	527	SD001476	-8.0	575	SD003575	-8.0

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
576	SD003712	-8.0	624	SD001899	-7.9	672	SD003734	-7.9
577	SD000362	-8.0	625	SD001773	-7.9	673	SD003754	-7.9
578	SD003834	-8.0	626	SD001936	-7.9	674	SD003830	-7.9
579	SD003866	-8.0	627	SD001884	-7.9	675	SD003833	-7.9
580	SD006017	-8.0	628	SD001775	-7.9	676	SD003847	-7.9
581	SD003947	-8.0	629	SD001948	-7.9	677	SD003879	-7.9
582	SD006053	-8.0	630	SD001994	-7.9	678	SD000367	-7.9
583	SD000385	-8.0	631	SD002028	-7.9	679	SD003924	-7.9
584	SD000408	-8.0	632	SD002004	-7.9	680	SD003928	-7.9
585	SD000423	-8.0	633	SD003075	-7.9	681	SD000034	-7.9
586	SD000544	-8.0	634	SD002109	-7.9	682	SD000523	-7.9
587	SD000646	-8.0	635	SD002125	-7.9	683	SD000591	-7.9
588	SD000774	-8.0	636	SD002128	-7.9	684	SD000628	-7.9
589	SD000701	-8.0	637	SD002292	-7.9	685	SD000618	-7.9
590	SD000813	-8.0	638	SD002283	-7.9	686	SD000624	-7.9
591	SD000789	-8.0	639	SD002279	-7.9	687	SD000647	-7.9
592	SD000687	-8.0	640	SD002383	-7.9	688	SD000572	-7.9
593	SD000884	-7.9	641	SD002406	-7.9	689	SD000844	-7.9
594	SD000885	-7.9	642	SD002369	-7.9	690	SD000845	-7.9
595	SD000913	-7.9	643	SD002428	-7.9	691	SD000785	-7.9
596	SD000860	-7.9	644	SD002371	-7.9	692	SD000737	-7.9
597	SD000004	-7.9	645	SD002462	-7.9	693	SD000815	-7.9
598	SD000879	-7.9	646	SD002477	-7.9	694	SD000688	-7.9
599	SD000977	-7.9	647	SD000020	-7.9	695	SD000894	-7.8
600	SD000993	-7.9	648	SD000256	-7.9	696	SD000005	-7.8
601	SD001061	-7.9	649	SD000257	-7.9	697	SD000975	-7.8
602	SD003179	-7.9	650	SD000260	-7.9	698	SD001039	-7.8
603	SD001077	-7.9	651	SD003398	-7.9	699	SD001041	-7.8
604	SD001085	-7.9	652	SD002723	-7.9	700	SD001022	-7.8
605	SD001079	-7.9	653	SD002533	-7.9	701	SD001093	-7.8
606	SD001067	-7.9	654	SD002817	-7.9	702	SD001075	-7.8
607	SD000926	-7.9	655	SD002846	-7.9	703	SD001047	-7.8
608	SD001196	-7.9	656	SD002786	-7.9	704	SD001126	-7.8
609	SD001353	-7.9	657	SD000280	-7.9	705	SD003171	-7.8
610	SD001345	-7.9	658	SD002872	-7.9	706	SD001149	-7.8
611	SD001413	-7.9	659	SD003422	-7.9	707	SD001244	-7.8
612	SD001434	-7.9	660	SD002948	-7.9	708	SD001262	-7.8
613	SD001422	-7.9	661	SD003425	-7.9	709	SD001322	-7.8
614	SD001510	-7.9	662	SD002537	-7.9	710	SD003064	-7.8
615	SD001568	-7.9	663	SD003031	-7.9	711	SD001381	-7.8
616	SD001453	-7.9	664	SD003449	-7.9	712	SD001392	-7.8
617	SD001655	-7.9	665	SD003149	-7.9	713	SD001411	-7.8
618	SD001686	-7.9	666	SD000025	-7.9	714	SD001426	-7.8
619	SD001690	-7.9	667	SD003559	-7.9	715	SD001446	-7.8
620	SD001757	-7.9	668	SD003582	-7.9	716	SD001415	-7.8
621	SD001110	-7.9	669	SD003585	-7.9	717	SD001424	-7.8
622	SD000184	-7.9	670	SD003654	-7.9	718	SD001450	-7.8
623	SD000189	-7.9	671	SD003537	-7.9	719	SD001469	-7.8

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
720	SD001533	-7.8	768	SD002939	-7.8	816	SD001150	-7.7
721	SD001536	-7.8	769	SD002999	-7.8	817	SD001089	-7.7
722	SD001539	-7.8	770	SD003429	-7.8	818	SD001227	-7.7
723	SD001596	-7.8	771	SD002964	-7.8	819	SD001253	-7.7
724	SD001628	-7.8	772	SD003039	-7.8	820	SD001251	-7.7
725	SD001572	-7.8	773	SD003143	-7.8	821	SD001272	-7.7
726	SD001685	-7.8	774	SD003125	-7.8	822	SD000126	-7.7
727	SD001677	-7.8	775	SD000317	-7.8	823	SD003210	-7.7
728	SD001720	-7.8	776	SD003571	-7.8	824	SD001308	-7.7
729	SD001753	-7.8	777	SD000349	-7.8	825	SD001451	-7.7
730	SD001755	-7.8	778	SD003658	-7.8	826	SD001276	-7.7
731	SD001803	-7.8	779	SD003534	-7.8	827	SD003239	-7.7
732	SD001796	-7.8	780	SD003740	-7.8	828	SD000147	-7.7
733	SD001797	-7.8	781	SD003729	-7.8	829	SD001543	-7.7
734	SD001800	-7.8	782	SD003869	-7.8	830	SD001569	-7.7
735	SD001888	-7.8	783	SD003874	-7.8	831	SD001611	-7.7
736	SD001938	-7.8	784	SD003858	-7.8	832	SD001694	-7.7
737	SD001873	-7.8	785	SD003888	-7.8	833	SD001726	-7.7
738	SD003300	-7.8	786	SD003942	-7.8	834	SD000932	-7.7
739	SD002020	-7.8	787	SD003916	-7.8	835	SD003260	-7.7
740	SD003308	-7.8	788	SD006048	-7.8	836	SD001709	-7.7
741	SD002016	-7.8	789	SD000396	-7.8	837	SD000174	-7.7
742	SD000205	-7.8	790	SD000379	-7.8	838	SD001778	-7.7
743	SD002165	-7.8	791	SD000406	-7.8	839	SD003265	-7.7
744	SD001833	-7.8	792	SD000532	-7.8	840	SD000177	-7.7
745	SD001666	-7.8	793	SD000562	-7.8	841	SD001782	-7.7
746	SD002201	-7.8	794	SD000576	-7.8	842	SD003277	-7.7
747	SD000221	-7.8	795	SD000633	-7.8	843	SD001825	-7.7
748	SD002203	-7.8	796	SD000635	-7.8	844	SD001847	-7.7
749	SD002346	-7.8	797	SD000651	-7.8	845	SD003193	-7.7
750	SD002387	-7.8	798	SD000657	-7.8	846	SD001867	-7.7
751	SD002324	-7.8	799	SD000723	-7.8	847	SD001901	-7.7
752	SD002370	-7.8	800	SD000508	-7.8	848	SD001883	-7.7
753	SD002447	-7.8	801	SD000914	-7.7	849	SD001931	-7.7
754	SD002492	-7.8	802	SD000974	-7.7	850	SD003295	-7.7
755	SD002522	-7.8	803	SD000985	-7.7	851	SD001894	-7.7
756	SD003360	-7.8	804	SD003177	-7.7	852	SD001977	-7.7
757	SD002504	-7.8	805	SD001042	-7.7	853	SD002011	-7.7
758	SD002630	-7.8	806	SD001070	-7.7	854	SD002013	-7.7
759	SD000024	-7.8	807	SD001021	-7.7	855	SD001600	-7.7
760	SD002636	-7.8	808	SD001092	-7.7	856	SD003307	-7.7
761	SD002695	-7.8	809	SD001072	-7.7	857	SD000204	-7.7
762	SD003364	-7.8	810	SD000924	-7.7	858	SD000198	-7.7
763	SD002714	-7.8	811	SD000090	-7.7	859	SD002044	-7.7
764	SD003401	-7.8	812	SD001066	-7.7	860	SD002075	-7.7
765	SD002918	-7.8	813	SD001119	-7.7	861	SD002110	-7.7
766	SD002883	-7.8	814	SD001049	-7.7	862	SD002119	-7.7
767	SD000287	-7.8	815	SD001121	-7.7	863	SD002134	-7.7

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
864	SD002191	-7.7	912	SD003781	-7.7	960	SD001549	-7.6
865	SD002136	-7.7	913	SD003870	-7.7	961	SD001483	-7.6
866	SD002217	-7.7	914	SD003863	-7.7	962	SD001645	-7.6
867	SD003340	-7.7	915	SD003889	-7.7	963	SD000161	-7.6
868	SD002313	-7.7	916	SD003917	-7.7	964	SD001719	-7.6
869	SD003358	-7.7	917	SD003946	-7.7	965	SD000171	-7.6
870	SD002307	-7.7	918	SD006022	-7.7	966	SD001760	-7.6
871	SD002411	-7.7	919	SD000036	-7.7	967	SD001112	-7.6
872	SD002439	-7.7	920	SD000390	-7.7	968	SD000179	-7.6
873	SD002457	-7.7	921	SD000397	-7.7	969	SD001750	-7.6
874	SD002488	-7.7	922	SD000402	-7.7	970	SD000186	-7.6
875	SD002486	-7.7	923	SD000518	-7.7	971	SD000182	-7.6
876	SD002501	-7.7	924	SD000599	-7.7	972	SD001921	-7.6
877	SD003378	-7.7	925	SD000626	-7.7	973	SD001767	-7.6
878	SD002531	-7.7	926	SD000629	-7.7	974	SD001844	-7.6
879	SD002562	-7.7	927	SD000617	-7.7	975	SD001957	-7.6
880	SD003384	-7.7	928	SD000480	-7.7	976	SD001993	-7.6
881	SD000262	-7.7	929	SD000675	-7.7	977	SD001981	-7.6
882	SD002707	-7.7	930	SD000706	-7.7	978	SD002021	-7.6
883	SD000266	-7.7	931	SD000803	-7.7	979	SD001988	-7.6
884	SD002756	-7.7	932	SD000820	-7.7	980	SD002029	-7.6
885	SD002758	-7.7	933	SD000794	-7.7	981	SD002012	-7.6
886	SD002749	-7.7	934	SD000791	-7.7	982	SD001975	-7.6
887	SD002763	-7.7	935	SD000087	-7.6	983	SD002080	-7.6
888	SD002767	-7.7	936	SD000893	-7.6	984	SD002089	-7.6
889	SD002772	-7.7	937	SD000877	-7.6	985	SD002141	-7.6
890	SD002796	-7.7	938	SD000083	-7.6	986	SD001667	-7.6
891	SD002755	-7.7	939	SD000922	-7.6	987	SD002253	-7.6
892	SD002834	-7.7	940	SD001006	-7.6	988	SD002357	-7.6
893	SD002829	-7.7	941	SD001029	-7.6	989	SD002341	-7.6
894	SD002802	-7.7	942	SD000102	-7.6	990	SD002473	-7.6
895	SD002866	-7.7	943	SD001078	-7.6	991	SD002505	-7.6
896	SD003420	-7.7	944	SD001108	-7.6	992	SD002425	-7.6
897	SD002959	-7.7	945	SD000941	-7.6	993	SD002547	-7.6
898	SD003414	-7.7	946	SD001205	-7.6	994	SD002517	-7.6
899	SD003041	-7.7	947	SD001233	-7.6	995	SD000245	-7.6
900	SD003051	-7.7	948	SD001217	-7.6	996	SD002567	-7.6
901	SD000314	-7.7	949	SD001234	-7.6	997	SD002530	-7.6
902	SD000316	-7.7	950	SD001219	-7.6	998	SD000254	-7.6
903	SD000319	-7.7	951	SD001328	-7.6	999	SD000021	-7.6
904	SD000331	-7.7	952	SD003067	-7.6	1000	SD002638	-7.6
905	SD000343	-7.7	953	SD001350	-7.6	1001	SD000264	-7.6
906	SD003601	-7.7	954	SD001418	-7.6	1002	SD002721	-7.6
907	SD003630	-7.7	955	SD001432	-7.6	1003	SD002705	-7.6
908	SD003665	-7.7	956	SD000144	-7.6	1004	SD002757	-7.6
909	SD003647	-7.7	957	SD001360	-7.6	1005	SD002741	-7.6
910	SD003726	-7.7	958	SD001506	-7.6	1006	SD002742	-7.6
911	SD003731	-7.7	959	SD001525	-7.6	1007	SD003402	-7.6

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
1008	SD002805	-7.6	1056	SD000670	-7.6	1104	SD003299	-7.5
1009	SD002898	-7.6	1057	SD000817	-7.6	1105	SD001966	-7.5
1010	SD002878	-7.6	1058	SD000809	-7.6	1106	SD002043	-7.5
1011	SD002865	-7.6	1059	SD000722	-7.6	1107	SD000197	-7.5
1012	SD002884	-7.6	1060	SD000889	-7.5	1108	SD002001	-7.5
1013	SD002991	-7.6	1061	SD000909	-7.5	1109	SD001997	-7.5
1014	SD002994	-7.6	1062	SD000872	-7.5	1110	SD003324	-7.5
1015	SD002962	-7.6	1063	SD000976	-7.5	1111	SD002196	-7.5
1016	SD003004	-7.6	1064	SD001030	-7.5	1112	SD002276	-7.5
1017	SD003029	-7.6	1065	SD000100	-7.5	1113	SD002295	-7.5
1018	SD003104	-7.6	1066	SD003182	-7.5	1114	SD002232	-7.5
1019	SD003134	-7.6	1067	SD001076	-7.5	1115	SD002352	-7.5
1020	SD000311	-7.6	1068	SD001026	-7.5	1116	SD002348	-7.5
1021	SD000321	-7.6	1069	SD000104	-7.5	1117	SD000231	-7.5
1022	SD003495	-7.6	1070	SD003178	-7.5	1118	SD002456	-7.5
1023	SD003510	-7.6	1071	SD001050	-7.5	1119	SD002223	-7.5
1024	SD003540	-7.6	1072	SD001125	-7.5	1120	SD002472	-7.5
1025	SD003603	-7.6	1073	SD001208	-7.5	1121	SD002475	-7.5
1026	SD003577	-7.6	1074	SD001226	-7.5	1122	SD002424	-7.5
1027	SD003704	-7.6	1075	SD001198	-7.5	1123	SD003366	-7.5
1028	SD003705	-7.6	1076	SD001339	-7.5	1124	SD000243	-7.5
1029	SD003724	-7.6	1077	SD001266	-7.5	1125	SD002502	-7.5
1030	SD003718	-7.6	1078	SD001370	-7.5	1126	SD002541	-7.5
1031	SD003744	-7.6	1079	SD001281	-7.5	1127	SD002684	-7.5
1032	SD003745	-7.6	1080	SD001282	-7.5	1128	SD002783	-7.5
1033	SD003739	-7.6	1081	SD001414	-7.5	1129	SD002753	-7.5
1034	SD003795	-7.6	1082	SD001464	-7.5	1130	SD002554	-7.5
1035	SD003821	-7.6	1083	SD003225	-7.5	1131	SD002798	-7.5
1036	SD003850	-7.6	1084	SD001503	-7.5	1132	SD000275	-7.5
1037	SD003829	-7.6	1085	SD000153	-7.5	1133	SD002780	-7.5
1038	SD003899	-7.6	1086	SD001570	-7.5	1134	SD002858	-7.5
1039	SD003865	-7.6	1087	SD001595	-7.5	1135	SD002860	-7.5
1040	SD003949	-7.6	1088	SD001679	-7.5	1136	SD003409	-7.5
1041	SD003904	-7.6	1089	SD001702	-7.5	1137	SD002903	-7.5
1042	SD006004	-7.6	1090	SD001181	-7.5	1138	SD002956	-7.5
1043	SD006030	-7.6	1091	SD001615	-7.5	1139	SD002960	-7.5
1044	SD006032	-7.6	1092	SD001805	-7.5	1140	SD000289	-7.5
1045	SD006015	-7.6	1093	SD001781	-7.5	1141	SD002990	-7.5
1046	SD000436	-7.6	1094	SD001813	-7.5	1142	SD003440	-7.5
1047	SD000550	-7.6	1095	SD001848	-7.5	1143	SD003142	-7.5
1048	SD000551	-7.6	1096	SD001868	-7.5	1144	SD003472	-7.5
1049	SD000555	-7.6	1097	SD001905	-7.5	1145	SD000327	-7.5
1050	SD000563	-7.6	1098	SD001923	-7.5	1146	SD003572	-7.5
1051	SD000580	-7.6	1099	SD001956	-7.5	1147	SD003602	-7.5
1052	SD000521	-7.6	1100	SD003282	-7.5	1148	SD003632	-7.5
1053	SD000620	-7.6	1101	SD001777	-7.5	1149	SD003514	-7.5
1054	SD000642	-7.6	1102	SD001962	-7.5	1150	SD003698	-7.5
1055	SD000615	-7.6	1103	SD001978	-7.5	1151	SD003687	-7.5

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
1152	SD003823	-7.5	1200	SD000169	-7.4	1248	SD003380	-7.4
1153	SD003826	-7.5	1201	SD001738	-7.4	1249	SD000267	-7.4
1154	SD003875	-7.5	1202	SD001779	-7.4	1250	SD002777	-7.4
1155	SD003766	-7.5	1203	SD000165	-7.4	1251	SD003411	-7.4
1156	SD003890	-7.5	1204	SD001823	-7.4	1252	SD000276	-7.4
1157	SD003907	-7.5	1205	SD001817	-7.4	1253	SD002801	-7.4
1158	SD000446	-7.5	1206	SD001841	-7.4	1254	SD002887	-7.4
1159	SD000589	-7.5	1207	SD001891	-7.4	1255	SD000281	-7.4
1160	SD000594	-7.5	1208	SD001929	-7.4	1256	SD002864	-7.4
1161	SD000704	-7.5	1209	SD001918	-7.4	1257	SD000284	-7.4
1162	SD000713	-7.5	1210	SD001843	-7.4	1258	SD002974	-7.4
1163	SD000714	-7.5	1211	SD002035	-7.4	1259	SD002993	-7.4
1164	SD000753	-7.5	1212	SD000193	-7.4	1260	SD003007	-7.4
1165	SD000658	-7.5	1213	SD002057	-7.4	1261	SD003091	-7.4
1166	SD000755	-7.5	1214	SD002063	-7.4	1262	SD003129	-7.4
1167	SD000717	-7.5	1215	SD003317	-7.4	1263	SD003057	-7.4
1168	SD000804	-7.5	1216	SD002130	-7.4	1264	SD003119	-7.4
1169	SD000509	-7.5	1217	SD002151	-7.4	1265	SD003121	-7.4
1170	SD000919	-7.4	1218	SD002118	-7.4	1266	SD003486	-7.4
1171	SD000859	-7.4	1219	SD002167	-7.4	1267	SD003482	-7.4
1172	SD000849	-7.4	1220	SD002168	-7.4	1268	SD000334	-7.4
1173	SD000905	-7.4	1221	SD002202	-7.4	1269	SD003530	-7.4
1174	SD000862	-7.4	1222	SD002312	-7.4	1270	SD000345	-7.4
1175	SD000961	-7.4	1223	SD002206	-7.4	1271	SD003595	-7.4
1176	SD001031	-7.4	1224	SD002336	-7.4	1272	SD003695	-7.4
1177	SD001032	-7.4	1225	SD002354	-7.4	1273	SD003809	-7.4
1178	SD001016	-7.4	1226	SD002304	-7.4	1274	SD003827	-7.4
1179	SD001059	-7.4	1227	SD002338	-7.4	1275	SD003885	-7.4
1180	SD000940	-7.4	1228	SD002318	-7.4	1276	SD006016	-7.4
1181	SD001225	-7.4	1229	SD002404	-7.4	1277	SD003927	-7.4
1182	SD001187	-7.4	1230	SD002325	-7.4	1278	SD006005	-7.4
1183	SD001222	-7.4	1231	SD000237	-7.4	1279	SD000054	-7.4
1184	SD001320	-7.4	1232	SD002458	-7.4	1280	SD000058	-7.4
1185	SD001352	-7.4	1233	SD002434	-7.4	1281	SD000070	-7.4
1186	SD001399	-7.4	1234	SD002490	-7.4	1282	SD000072	-7.4
1187	SD001425	-7.4	1235	SD002443	-7.4	1283	SD000049	-7.4
1188	SD001429	-7.4	1236	SD002381	-7.4	1284	SD000066	-7.4
1189	SD001431	-7.4	1237	SD002487	-7.4	1285	SD000400	-7.4
1190	SD003229	-7.4	1238	SD003367	-7.4	1286	SD000444	-7.4
1191	SD001531	-7.4	1239	SD002591	-7.4	1287	SD000477	-7.4
1192	SD001518	-7.4	1240	SD000251	-7.4	1288	SD000590	-7.4
1193	SD001508	-7.4	1241	SD002454	-7.4	1289	SD000603	-7.4
1194	SD001583	-7.4	1242	SD000255	-7.4	1290	SD000712	-7.4
1195	SD001597	-7.4	1243	SD002631	-7.4	1291	SD000672	-7.4
1196	SD001660	-7.4	1244	SD002585	-7.4	1292	SD000472	-7.4
1197	SD001699	-7.4	1245	SD003390	-7.4	1293	SD000752	-7.4
1198	SD001659	-7.4	1246	SD002419	-7.4	1294	SD000741	-7.4
1199	SD001710	-7.4	1247	SD002694	-7.4	1295	SD000802	-7.4

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
1296	SD000826	-7.4	1344	SD002103	-7.3	1392	SD003597	-7.3
1297	SD000797	-7.4	1345	SD002166	-7.3	1393	SD003621	-7.3
1298	SD000954	-7.3	1346	SD002146	-7.3	1394	SD003648	-7.3
1299	SD003059	-7.3	1347	SD002152	-7.3	1395	SD003568	-7.3
1300	SD000098	-7.3	1348	SD002242	-7.3	1396	SD003725	-7.3
1301	SD000997	-7.3	1349	SD002272	-7.3	1397	SD003690	-7.3
1302	SD000923	-7.3	1350	SD002197	-7.3	1398	SD003815	-7.3
1303	SD001018	-7.3	1351	SD002249	-7.3	1399	SD000373	-7.3
1304	SD001064	-7.3	1352	SD002286	-7.3	1400	SD006020	-7.3
1305	SD001055	-7.3	1353	SD000216	-7.3	1401	SD000044	-7.3
1306	SD001024	-7.3	1354	SD002363	-7.3	1402	SD000073	-7.3
1307	SD000950	-7.3	1355	SD002342	-7.3	1403	SD003936	-7.3
1308	SD001082	-7.3	1356	SD002365	-7.3	1404	SD000417	-7.3
1309	SD001083	-7.3	1357	SD002420	-7.3	1405	SD000437	-7.3
1310	SD001087	-7.3	1358	SD002429	-7.3	1406	SD000452	-7.3
1311	SD000111	-7.3	1359	SD002464	-7.3	1407	SD000476	-7.3
1312	SD001194	-7.3	1360	SD003079	-7.3	1408	SD000573	-7.3
1313	SD001105	-7.3	1361	SD002483	-7.3	1409	SD000720	-7.3
1314	SD003202	-7.3	1362	SD002565	-7.3	1410	SD000744	-7.3
1315	SD001218	-7.3	1363	SD002566	-7.3	1411	SD000747	-7.3
1316	SD003206	-7.3	1364	SD002574	-7.3	1412	SD000805	-7.3
1317	SD001214	-7.3	1365	SD002640	-7.3	1413	SD000847	-7.3
1318	SD003205	-7.3	1366	SD002643	-7.3	1414	SD000829	-7.3
1319	SD001391	-7.3	1367	SD000259	-7.3	1415	SD000811	-7.3
1320	SD001270	-7.3	1368	SD002682	-7.3	1416	SD000901	-7.2
1321	SD001372	-7.3	1369	SD002687	-7.3	1417	SD000921	-7.2
1322	SD001402	-7.3	1370	SD002628	-7.3	1418	SD000986	-7.2
1323	SD001472	-7.3	1371	SD002670	-7.3	1419	SD000987	-7.2
1324	SD001576	-7.3	1372	SD002808	-7.3	1420	SD001005	-7.2
1325	SD001619	-7.3	1373	SD003406	-7.3	1421	SD000095	-7.2
1326	SD001629	-7.3	1374	SD002934	-7.3	1422	SD000992	-7.2
1327	SD001647	-7.3	1375	SD002938	-7.3	1423	SD001040	-7.2
1328	SD001649	-7.3	1376	SD000288	-7.3	1424	SD001053	-7.2
1329	SD001703	-7.3	1377	SD002941	-7.3	1425	SD001065	-7.2
1330	SD001708	-7.3	1378	SD002949	-7.3	1426	SD001135	-7.2
1331	SD003259	-7.3	1379	SD003042	-7.3	1427	SD001088	-7.2
1332	SD000173	-7.3	1380	SD003133	-7.3	1428	SD000951	-7.2
1333	SD001739	-7.3	1381	SD000295	-7.3	1429	SD003194	-7.2
1334	SD003072	-7.3	1382	SD003379	-7.3	1430	SD001099	-7.2
1335	SD001788	-7.3	1383	SD003148	-7.3	1431	SD001183	-7.2
1336	SD001789	-7.3	1384	SD000305	-7.3	1432	SD001176	-7.2
1337	SD001862	-7.3	1385	SD003126	-7.3	1433	SD000124	-7.2
1338	SD001922	-7.3	1386	SD003479	-7.3	1434	SD001337	-7.2
1339	SD001925	-7.3	1387	SD003483	-7.3	1435	SD001371	-7.2
1340	SD002040	-7.3	1388	SD000322	-7.3	1436	SD001307	-7.2
1341	SD003272	-7.3	1389	SD000027	-7.3	1437	SD001437	-7.2
1342	SD003196	-7.3	1390	SD003592	-7.3	1438	SD001364	-7.2
1343	SD002008	-7.3	1391	SD003611	-7.3	1439	SD001277	-7.2

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
1440	SD001523	-7.2	1488	SD002920	-7.2	1536	SD000972	-7.1
1441	SD003238	-7.2	1489	SD002823	-7.2	1537	SD000864	-7.1
1442	SD001493	-7.2	1490	SD002971	-7.2	1538	SD001011	-7.1
1443	SD000155	-7.2	1491	SD002984	-7.2	1539	SD000984	-7.1
1444	SD001632	-7.2	1492	SD000293	-7.2	1540	SD000086	-7.1
1445	SD003245	-7.2	1493	SD003038	-7.2	1541	SD001037	-7.1
1446	SD001654	-7.2	1494	SD003046	-7.2	1542	SD000099	-7.1
1447	SD001669	-7.2	1495	SD000323	-7.2	1543	SD003176	-7.1
1448	SD001656	-7.2	1496	SD000030	-7.2	1544	SD001081	-7.1
1449	SD003256	-7.2	1497	SD003502	-7.2	1545	SD001123	-7.1
1450	SD001707	-7.2	1498	SD003562	-7.2	1546	SD003190	-7.1
1451	SD000164	-7.2	1499	SD003513	-7.2	1547	SD001171	-7.1
1452	SD001731	-7.2	1500	SD003583	-7.2	1548	SD001199	-7.1
1453	SD001748	-7.2	1501	SD000346	-7.2	1549	SD001188	-7.1
1454	SD001882	-7.2	1502	SD003590	-7.2	1550	SD001252	-7.1
1455	SD003074	-7.2	1503	SD003619	-7.2	1551	SD001250	-7.1
1456	SD001944	-7.2	1504	SD003676	-7.2	1552	SD001211	-7.1
1457	SD001952	-7.2	1505	SD003681	-7.2	1553	SD001362	-7.1
1458	SD003290	-7.2	1506	SD003732	-7.2	1554	SD001265	-7.1
1459	SD002081	-7.2	1507	SD003708	-7.2	1555	SD001348	-7.1
1460	SD002099	-7.2	1508	SD003535	-7.2	1556	SD001306	-7.1
1461	SD002124	-7.2	1509	SD003867	-7.2	1557	SD001309	-7.1
1462	SD002177	-7.2	1510	SD003838	-7.2	1558	SD001430	-7.1
1463	SD002113	-7.2	1511	SD003673	-7.2	1559	SD001435	-7.1
1464	SD002140	-7.2	1512	SD003768	-7.2	1560	SD001462	-7.1
1465	SD003304	-7.2	1513	SD006008	-7.2	1561	SD001443	-7.1
1466	SD002180	-7.2	1514	SD003909	-7.2	1562	SD001492	-7.1
1467	SD002154	-7.2	1515	SD000050	-7.2	1563	SD001557	-7.1
1468	SD002259	-7.2	1516	SD000061	-7.2	1564	SD001480	-7.1
1469	SD002335	-7.2	1517	SD000399	-7.2	1565	SD000152	-7.1
1470	SD002291	-7.2	1518	SD000405	-7.2	1566	SD001542	-7.1
1471	SD002407	-7.2	1519	SD000421	-7.2	1567	SD001639	-7.1
1472	SD002161	-7.2	1520	SD000549	-7.2	1568	SD001633	-7.1
1473	SD002433	-7.2	1521	SD000487	-7.2	1569	SD001695	-7.1
1474	SD002413	-7.2	1522	SD000595	-7.2	1570	SD001180	-7.1
1475	SD002538	-7.2	1523	SD000602	-7.2	1571	SD001722	-7.1
1476	SD000252	-7.2	1524	SD000636	-7.2	1572	SD001723	-7.1
1477	SD000258	-7.2	1525	SD000640	-7.2	1573	SD001681	-7.1
1478	SD002583	-7.2	1526	SD000762	-7.2	1574	SD000013	-7.1
1479	SD002693	-7.2	1527	SD000763	-7.2	1575	SD001749	-7.1
1480	SD002587	-7.2	1528	SD000768	-7.2	1576	SD001857	-7.1
1481	SD002724	-7.2	1529	SD000801	-7.2	1577	SD001765	-7.1
1482	SD002735	-7.2	1530	SD000837	-7.2	1578	SD001906	-7.1
1483	SD000268	-7.2	1531	SD000818	-7.2	1579	SD001916	-7.1
1484	SD002750	-7.2	1532	SD000842	-7.2	1580	SD001895	-7.1
1485	SD003408	-7.2	1533	SD000507	-7.2	1581	SD003297	-7.1
1486	SD002811	-7.2	1534	SD000002	-7.1	1582	SD003288	-7.1
1487	SD002788	-7.2	1535	SD000904	-7.1	1583	SD001986	-7.1

Table S1. Continued.

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
1584	SD003298	-7.1	1632	SD003773	-7.1	1680	SD001718	-7.0
1585	SD001984	-7.1	1633	SD003849	-7.1	1681	SD001730	-7.0
1586	SD002030	-7.1	1634	SD000376	-7.1	1682	SD001734	-7.0
1587	SD002042	-7.1	1635	SD003846	-7.1	1683	SD001809	-7.0
1588	SD001970	-7.1	1636	SD000067	-7.1	1684	SD002052	-7.0
1589	SD002156	-7.1	1637	SD000074	-7.1	1685	SD002055	-7.0
1590	SD000212	-7.1	1638	SD000392	-7.1	1686	SD002073	-7.0
1591	SD002226	-7.1	1639	SD000415	-7.1	1687	SD002095	-7.0
1592	SD002228	-7.1	1640	SD000552	-7.1	1688	SD002062	-7.0
1593	SD000219	-7.1	1641	SD000579	-7.1	1689	SD002096	-7.0
1594	SD002266	-7.1	1642	SD000637	-7.1	1690	SD002091	-7.0
1595	SD002245	-7.1	1643	SD000665	-7.1	1691	SD003314	-7.0
1596	SD002261	-7.1	1644	SD000571	-7.1	1692	SD002111	-7.0
1597	SD002246	-7.1	1645	SD000695	-7.1	1693	SD002181	-7.0
1598	SD002275	-7.1	1646	SD000656	-7.1	1694	SD000217	-7.0
1599	SD000228	-7.1	1647	SD000800	-7.1	1695	SD002268	-7.0
1600	SD002309	-7.1	1648	SD000771	-7.1	1696	SD002237	-7.0
1601	SD002224	-7.1	1649	SD000810	-7.1	1697	SD002284	-7.0
1602	SD002430	-7.1	1650	SD000886	-7.0	1698	SD002385	-7.0
1603	SD003359	-7.1	1651	SD000912	-7.0	1699	SD002347	-7.0
1604	SD002466	-7.1	1652	SD000903	-7.0	1700	SD003356	-7.0
1605	SD002445	-7.1	1653	SD000850	-7.0	1701	SD002455	-7.0
1606	SD002579	-7.1	1654	SD000888	-7.0	1702	SD002412	-7.0
1607	SD002452	-7.1	1655	SD003167	-7.0	1703	SD002427	-7.0
1608	SD002569	-7.1	1656	SD000907	-7.0	1704	SD002556	-7.0
1609	SD002540	-7.1	1657	SD000953	-7.0	1705	SD002539	-7.0
1610	SD003383	-7.1	1658	SD003161	-7.0	1706	SD002568	-7.0
1611	SD002551	-7.1	1659	SD000955	-7.0	1707	SD002521	-7.0
1612	SD002747	-7.1	1660	SD001101	-7.0	1708	SD002577	-7.0
1613	SD002748	-7.1	1661	SD001091	-7.0	1709	SD002507	-7.0
1614	SD000271	-7.1	1662	SD001191	-7.0	1710	SD002580	-7.0
1615	SD002809	-7.1	1663	SD001130	-7.0	1711	SD002689	-7.0
1616	SD002848	-7.1	1664	SD001184	-7.0	1712	SD002784	-7.0
1617	SD002815	-7.1	1665	SD001201	-7.0	1713	SD002746	-7.0
1618	SD002807	-7.1	1666	SD001273	-7.0	1714	SD002709	-7.0
1619	SD002912	-7.1	1667	SD001336	-7.0	1715	SD002825	-7.0
1620	SD002904	-7.1	1668	SD001355	-7.0	1716	SD002876	-7.0
1621	SD002957	-7.1	1669	SD000136	-7.0	1717	SD002901	-7.0
1622	SD002958	-7.1	1670	SD001403	-7.0	1718	SD000283	-7.0
1623	SD002946	-7.1	1671	SD003214	-7.0	1719	SD002954	-7.0
1624	SD003426	-7.1	1672	SD001275	-7.0	1720	SD003427	-7.0
1625	SD003437	-7.1	1673	SD001405	-7.0	1721	SD002923	-7.0
1626	SD003099	-7.1	1674	SD001502	-7.0	1722	SD003000	-7.0
1627	SD000298	-7.1	1675	SD001504	-7.0	1723	SD002988	-7.0
1628	SD002619	-7.1	1676	SD001520	-7.0	1724	SD003110	-7.0
1629	SD003651	-7.1	1677	SD001470	-7.0	1725	SD003159	-7.0
1630	SD000353	-7.1	1678	SD000159	-7.0	1726	SD003152	-7.0
1631	SD003743	-7.1	1679	SD001662	-7.0	1727	SD000296	-7.0

Table S1. *Continued.*

No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)	No.	SuperDRUG2 Code	Standard Docking Score (kcal/mol)
1728	SD003157	-7.0	1740	SD003839	-7.0	1751	SD000450	-7.0
1729	SD000309	-7.0	1741	SD003860	-7.0	1752	SD000541	-7.0
1730	SD003484	-7.0	1742	SD003919	-7.0	1753	SD000456	-7.0
1731	SD003507	-7.0	1743	SD003898	-7.0	1754	SD000556	-7.0
1732	SD003499	-7.0	1744	SD003856	-7.0	1755	SD000613	-7.0
1733	SD003528	-7.0	1745	SD003770	-7.0	1756	SD000680	-7.0
1734	SD000340	-7.0	1746	SD006033	-7.0	1757	SD000766	-7.0
1735	SD003517	-7.0	1747	SD000053	-7.0	1758	SD000729	-7.0
1736	SD003520	-7.0	1748	SD006012	-7.0	1759	SD000736	-7.0
1737	SD003782	-7.0	1749	SD000047	-7.0	1760	SD000814	-7.0
1738	SD003787	-7.0	1750	SD000424	-7.0	1761	SD000739	-7.0
1739	SD003790	-7.0						