

Non- β -Lactam Allosteric Inhibitors Target Methicillin-Resistant *Staphylococcus aureus*: An *In Silico* Drug Discovery Study

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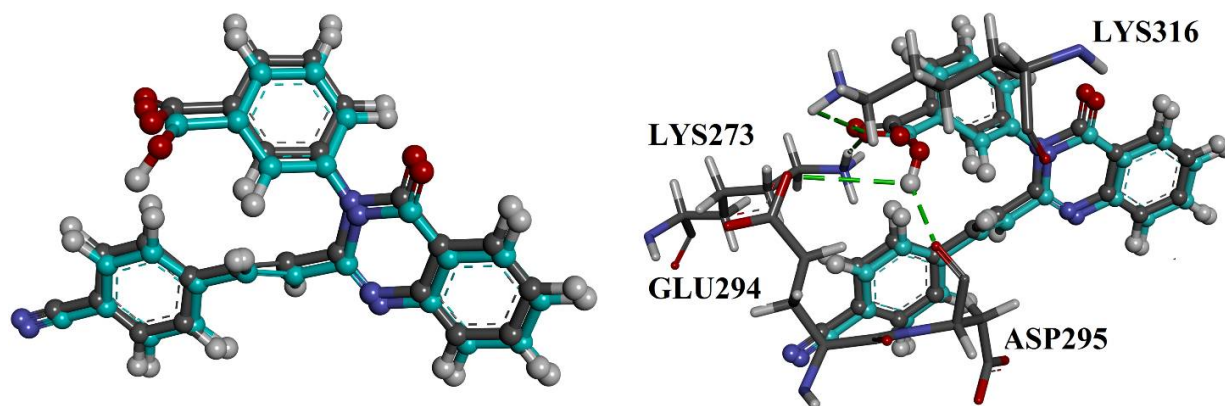


Figure S1. 3D representations of the predicted binding modes of ionized (in gray) and unionized (in cyan) QNZ complexed with the PBP2a inside the allosteric site.

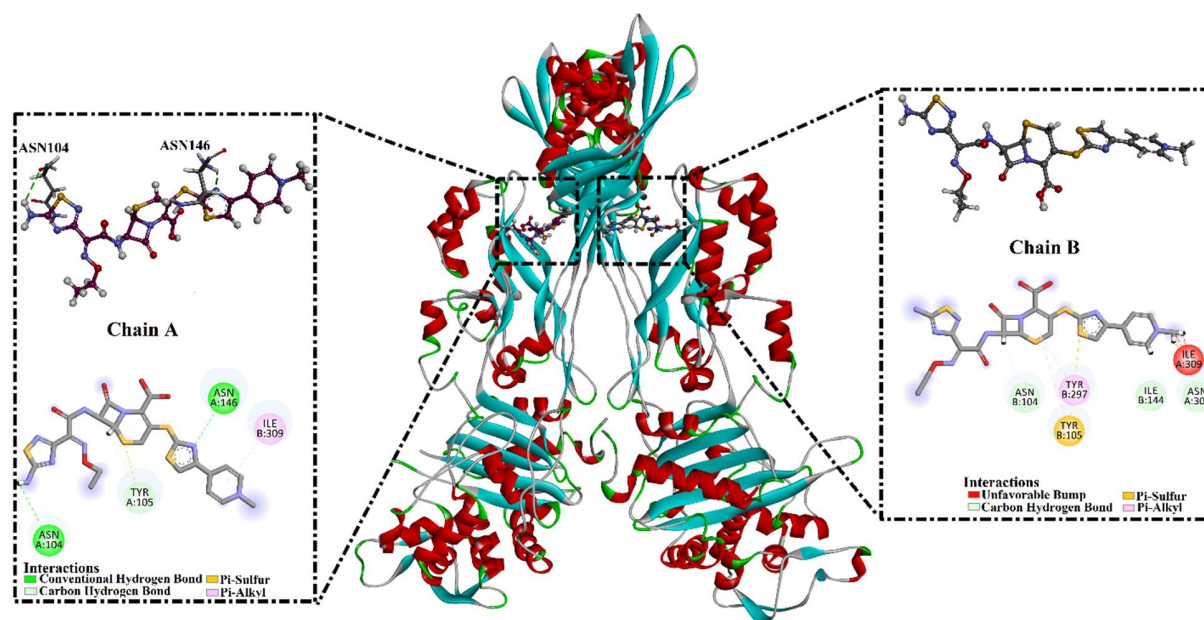


Figure S2. 3D and 2D representations of the experimental binding modes of CFT complexed with the PBP2a inside the allosteric site of chains A and B (PDB code: 3ZG0).

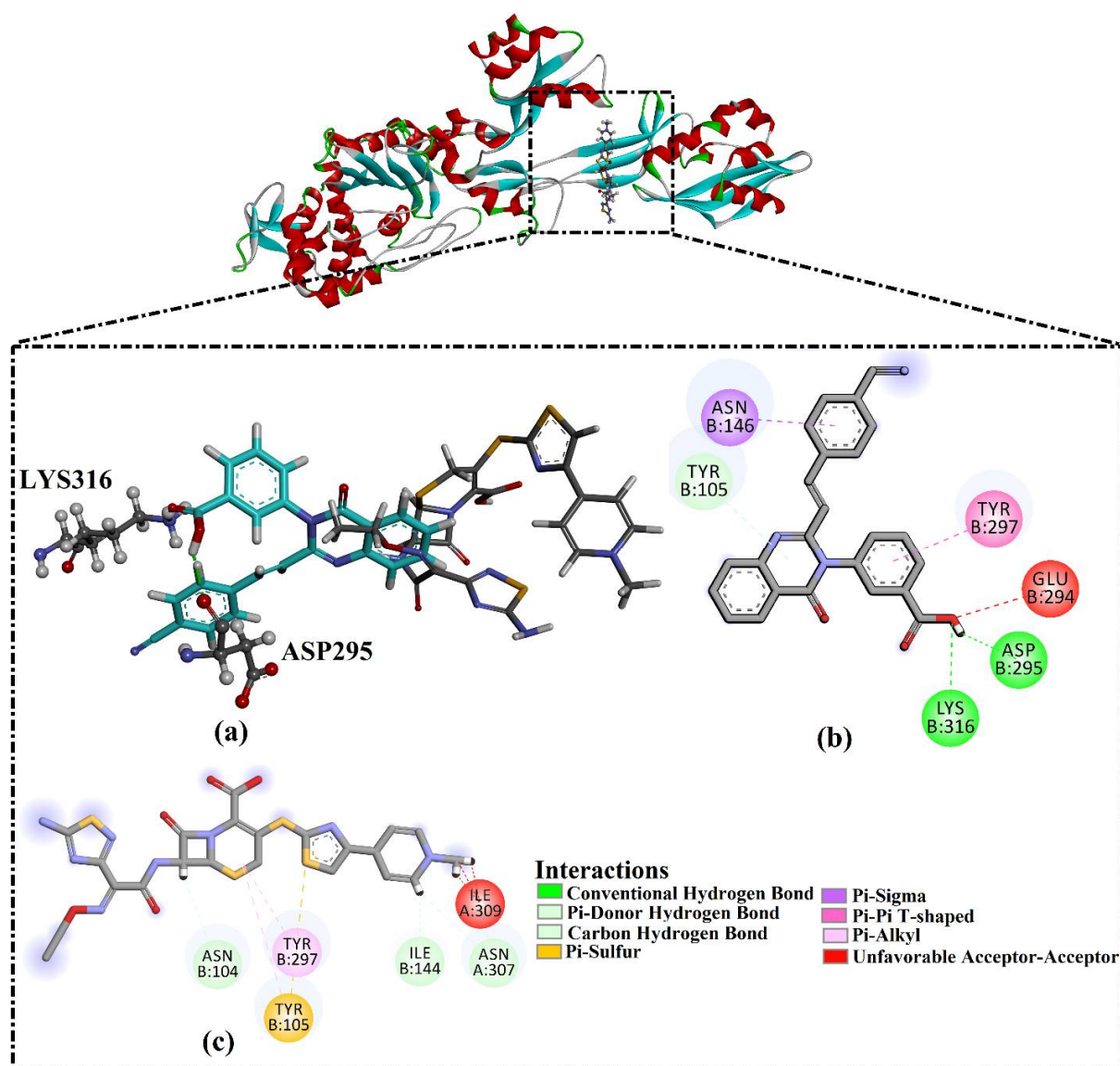


Figure S3: (a) 3D representations of the docked structures of QNZ (in cyan) and CFT (in gray) and 2D representations of the predicted binding modes of (b) QNZ and (c) CFT complexed with the PBP2a inside the allosteric site in acidic medium.

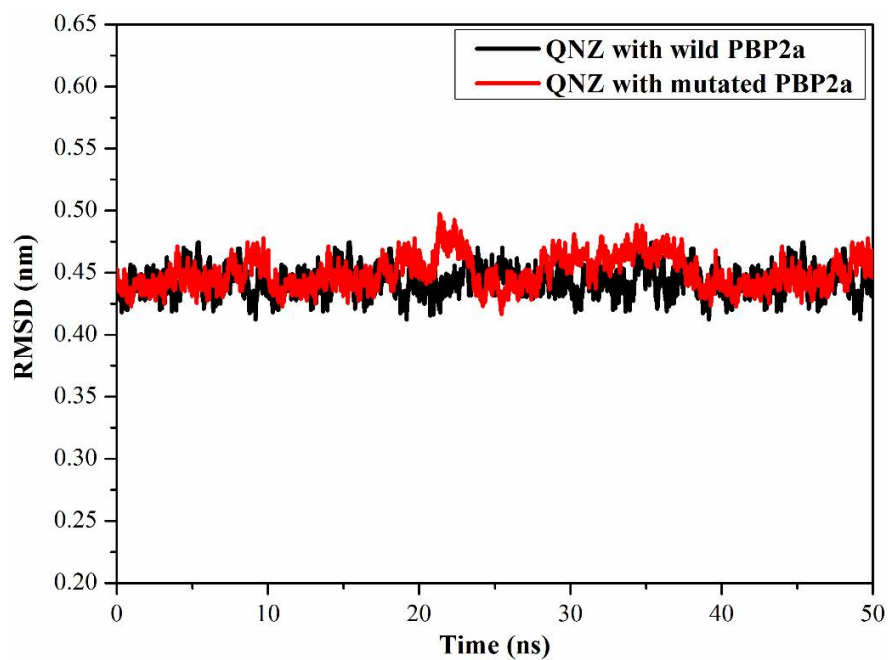


Figure S4. Root-mean-square deviation (RMSD) of the backbone atoms from the initial structure of QNZ with wild (in black), and double mutated PBP2a allosteric site (in red) in acidic medium throughout the 50 ns MD simulations.

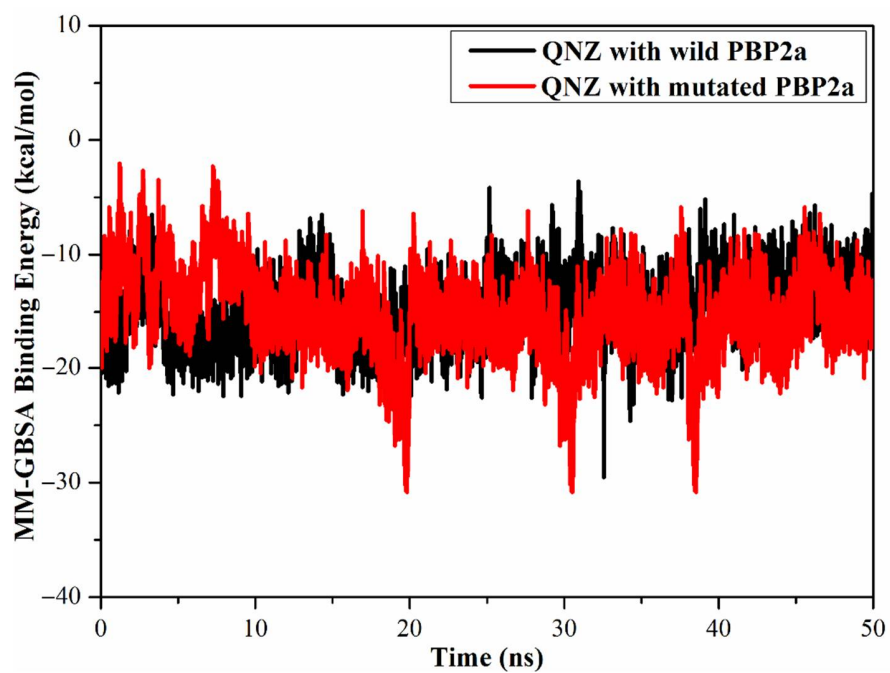


Figure S5. Estimated MM-GBSA binding energy per frame for QNZ with wild (in black) and mutated PBP2a allosteric site (in red) in acidic medium throughout the 50 ns MD simulations.

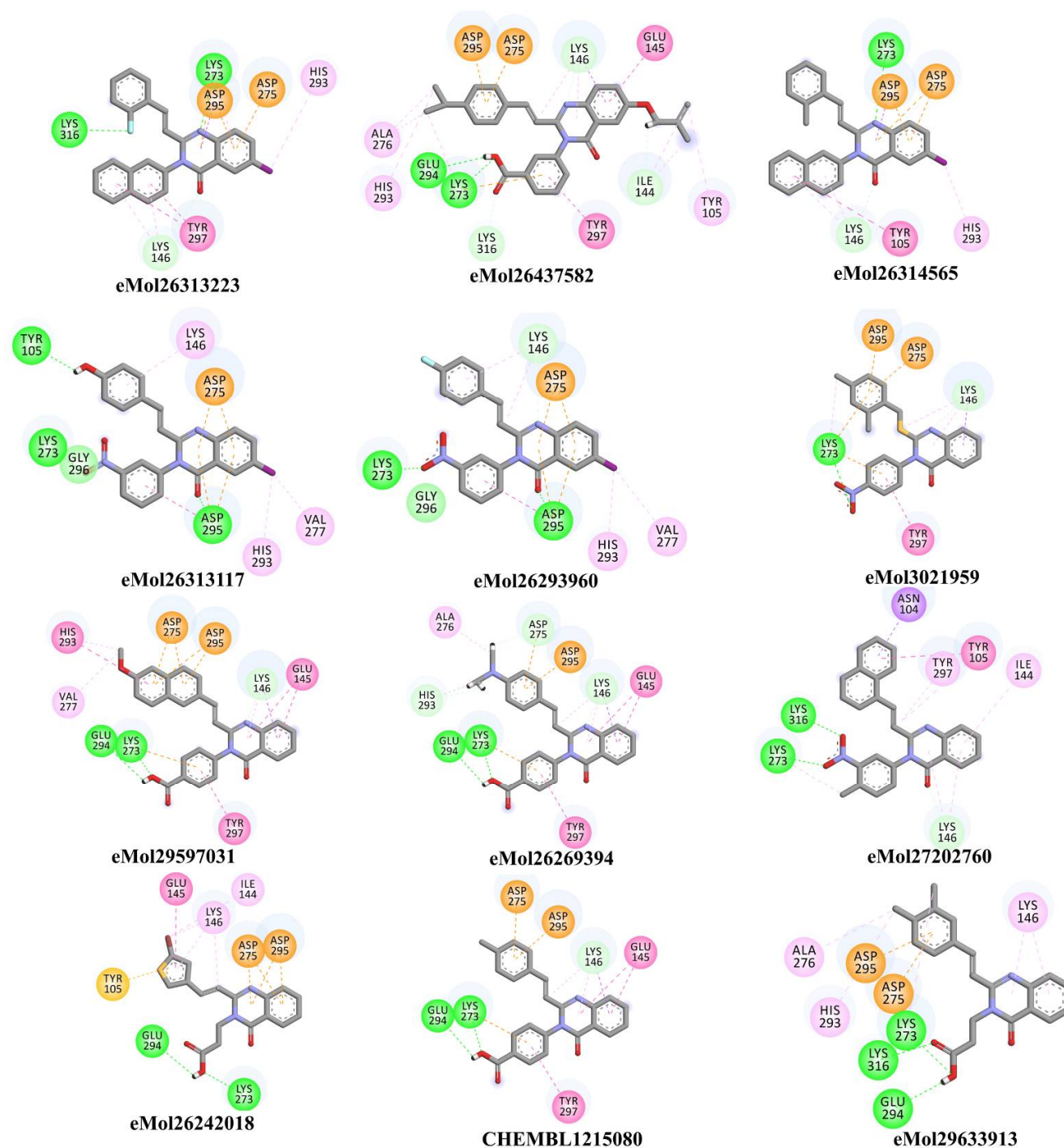


Figure S6. 2D representations of the predicted docked binding modes of the top 35 potent inhibitors in complex with mutated PBP2a allosteric site in acidic medium.

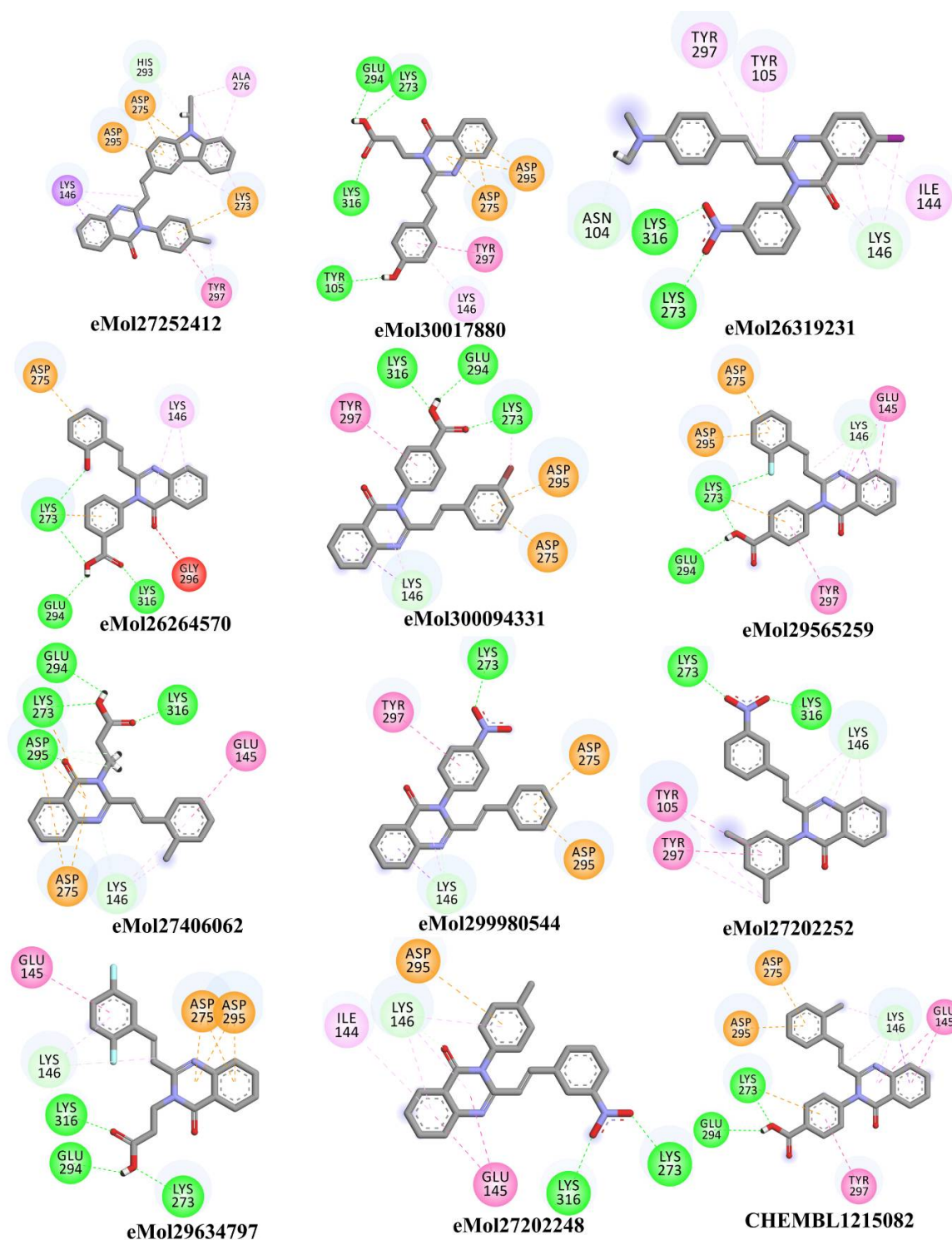


Figure S6. Continued.

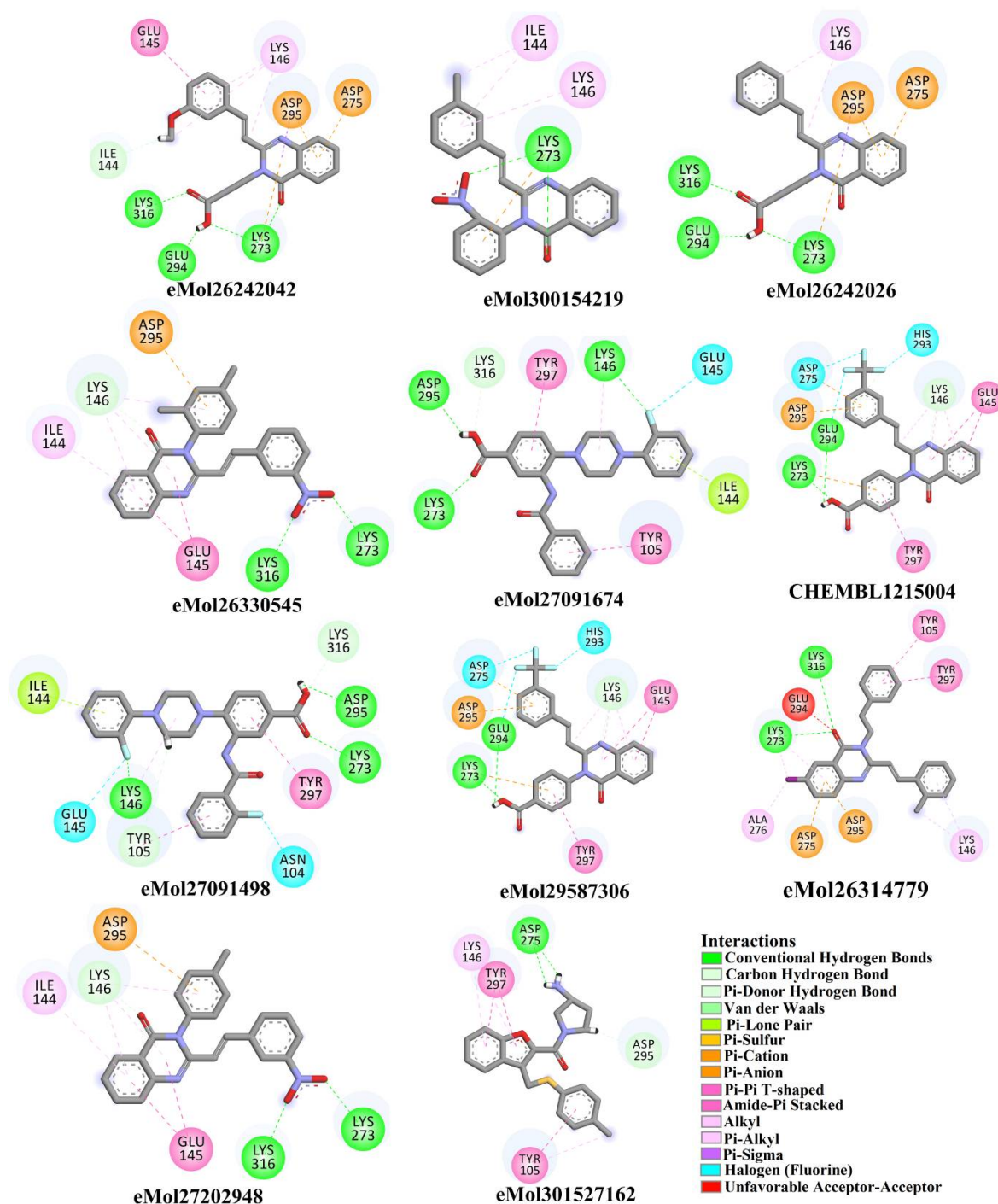


Figure S6. Continued.

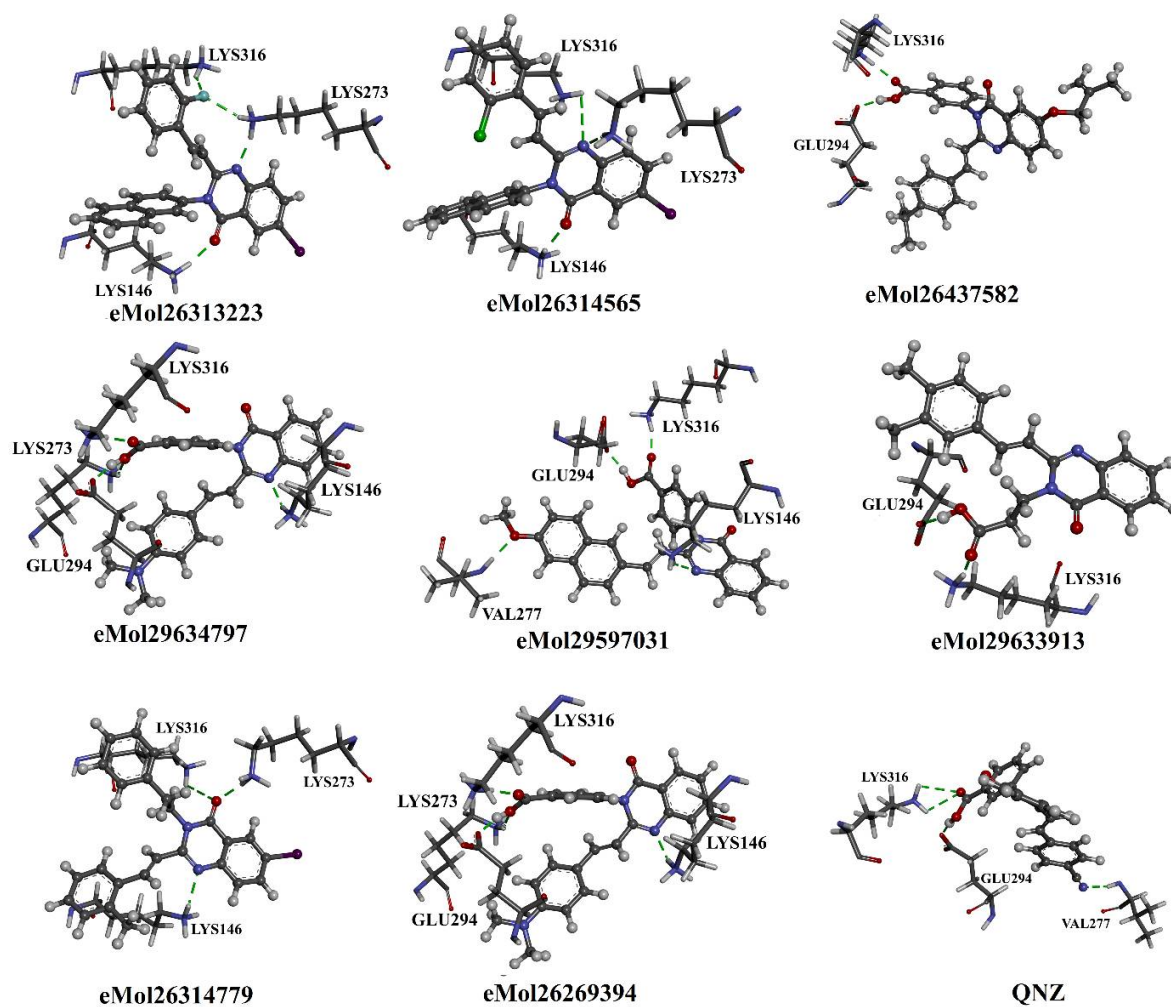


Figure S7. 3D representations of AMBER-based minimized structures of the eight potent molecules and QNZ in complex with the mutated PBP2a in acidic medium.

Table S1. Calculated conventional docking scores (in kcal/mol) for QNZ and the top 5000 potent allosteric inhibitors against mutated PBP2a allosteric site in acidic medium.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
	QNZ	-6.9	49	eMol23246696	-8.5	98	eMol45585832	-8.2
1	eMol30323345	-9.8	50	eMol23157132	-8.4	99	eMol956623	-8.2
2	CHEMBL1214717	-9.4	51	CHEMBL3818377	-8.4	100	CHEMBL3818775	-8.2
3	eMol29587310	-9.4	52	eMol31786896	-8.4	101	eMol46480173	-8.2
4	eMol45585846	-9.4	53	eMol19076714	-8.4	102	eMol24530483	-8.2
5	eMol23239806	-9.3	54	eMol579568	-8.4	103	eMol26437582	-8.2
6	CHEMBL1214718	-9.2	55	eMol300994534	-8.4	104	eMol6263471	-8.2
7	eMol29597031	-9.2	56	eMol48938145	-8.4	105	eMol681936	-8.2
8	eMol45585848	-9.2	57	eMol18962382	-8.4	106	CHEMBL1558437	-8.2
9	eMol23186178	-9.1	58	eMol24519844	-8.4	107	eMol26809774	-8.2
10	eMol18542844	-9.1	59	eMol27202240	-8.4	108	eMol26330545	-8.2
11	eMol30323633	-9.0	60	eMol27202248	-8.4	109	CHEMBL3818929	-8.2
12	CHEMBL1534883	-9.0	61	CHEMBL1215080	-8.4	110	eMol1088331	-8.2
13	eMol1344114	-9.0	62	eMol43906059	-8.4	111	eMol26314565	-8.2
14	eMol24519694	-9.0	63	CHEMBL4103504	-8.3	112	eMol26319231	-8.2
15	eMol19076718	-8.9	64	eMol27202910	-8.3	113	eMol46480165	-8.2
16	eMol26313117	-8.9	65	eMol31532412	-8.3	114	eMol20347873	-8.2
17	eMol19076712	-8.9	66	CHEMBL395193	-8.3	115	eMol206926236	-8.2
18	CHEMBL1214794	-8.9	67	eMol23239141	-8.3	116	eMol300094331	-8.2
19	eMol26196290	-8.9	68	eMol26313223	-8.3	117	eMol23178762	-8.1
20	eMol45585824	-8.9	69	CHEMBL3805924	-8.3	118	eMol4518648	-8.1
21	CHEMBL1214720	-8.8	70	eMol23181799	-8.3	119	CHEMBL1214935	-8.1
22	eMol30341049	-8.8	71	eMol23175530	-8.3	120	eMol18550846	-8.1
23	eMol43906045	-8.8	72	CHEMBL3818584	-8.3	121	eMol43906051	-8.1
24	eMol20379909	-8.8	73	eMol18542848	-8.3	122	eMol566574	-8.1
25	eMol18542846	-8.8	74	eMol27202258	-8.3	123	CHEMBL3819445	-8.1
26	eMol20337486	-8.8	75	eMol679826	-8.3	124	eMol20368046	-8.1
27	eMol20378769	-8.7	76	eMol25810071	-8.3	125	eMol27252412	-8.1
28	eMol31781482	-8.7	77	eMol25810075	-8.3	126	CHEMBL1214647	-8.1
29	eMol2403964	-8.7	78	eMol25810083	-8.3	127	CHEMBL508966	-8.1
30	eMol1166007	-8.7	79	eMol26242044	-8.3	128	eMol2992482	-8.1
31	CHEMBL1214938	-8.7	80	eMol193446288	-8.3	129	eMol46490873	-8.1
32	eMol20375178	-8.7	81	eMol25819217	-8.3	130	CHEMBL3817888	-8.1
33	CHEMBL1214941	-8.6	82	CHEMBL1215003	-8.2	131	eMol26314779	-8.1
34	eMol19076754	-8.6	83	CHEMBL518358	-8.2	132	eMol27202956	-8.1
35	eMol19076742	-8.6	84	eMol29653471	-8.2	133	eMol566488	-8.1
36	eMol23241028	-8.6	85	eMol43906053	-8.2	134	eMol20361212	-8.1
37	eMol30323569	-8.6	86	eMol45622745	-8.2	135	eMol27202348	-8.1
38	CHEMBL1215648	-8.6	87	eMol587826	-8.2	136	eMol2992792	-8.1
39	eMol26196326	-8.6	88	eMol588192	-8.2	137	eMol26264570	-8.1
40	eMol45585842	-8.6	89	CHEMBL1214713	-8.2	138	eMol26293960	-8.1
41	eMol565168	-8.6	90	CHEMBL1384683	-8.2	139	eMol565798	-8.1
42	CHEMBL1215650	-8.5	91	eMol23243407	-8.2	140	eMol11920256	-8.1
43	CHEMBL1579061	-8.5	92	eMol26270654	-8.2	141	eMol4562556	-8.1
44	eMol26269394	-8.5	93	eMol46365626	-8.2	142	eMol16797514	-8.1
45	CHEMBL1215649	-8.5	94	CHEMBL1214936	-8.2	143	eMol26242050	-8.1
46	eMol22447774	-8.5	95	eMol26196312	-8.2	144	eMol23147497	-8.1
47	eMol26196316	-8.5	96	eMol26242034	-8.2	145	CHEMBL1443074	-8.0
48	CHEMBL3818129	-8.5	97	eMol299980544	-8.2	146	eMol18940433	-8.0

Table S1. *Continued.*

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
147	eMol26242018	-8.0	196	eMol1035565	-7.9	245	eMol4552457	-7.8
148	eMol27202760	-8.0	197	eMol26242038	-7.9	246	eMol679554	-7.8
149	eMol30248263	-8.0	198	eMol31297102	-7.9	247	CHEMBL1212961	-7.8
150	eMol43731200	-8.0	199	eMol4381378	-7.9	248	eMol18550688	-7.8
151	eMol679556	-8.0	200	eMol679552	-7.9	249	eMol24313582	-7.8
152	eMol679822	-8.0	201	eMol19266609	-7.9	250	eMol27406062	-7.8
153	CHEMBL1215797	-8.0	202	eMol23190351	-7.9	251	eMol300136046	-7.8
154	eMol20377597	-8.0	203	eMol26242032	-7.9	252	eMol314064301	-7.8
155	eMol27091498	-8.0	204	eMol30671942	-7.9	253	eMol46480212	-7.8
156	eMol4397966	-8.0	205	eMol33366267	-7.9	254	eMol566288	-7.8
157	eMol4577396	-8.0	206	eMol36912832	-7.9	255	eMol26315830	-7.8
158	CHEMBL1214648	-8.0	207	eMol46363574	-7.9	256	eMol4579154	-7.8
159	CHEMBL3818572	-8.0	208	eMol75958504	-7.9	257	eMol46367311	-7.8
160	eMol13856171	-8.0	209	eMol587628	-7.9	258	CHEMBL3819597	-7.8
161	eMol27091674	-8.0	210	eMol1035521	-7.9	259	eMol206970196	-7.8
162	eMol43906055	-8.0	211	eMol20342278	-7.9	260	eMol29633913	-7.8
163	eMol4558540	-8.0	212	eMol20378767	-7.9	261	eMol4555647	-7.8
164	CHEMBL1601398	-8.0	213	eMol25908513	-7.9	262	eMol45622743	-7.8
165	eMol2507718	-8.0	214	eMol26309353	-7.9	263	eMol4581546	-7.8
166	eMol26242046	-8.0	215	CHEMBL2259943	-7.9	264	CHEMBL2403015	-7.8
167	eMol36912834	-8.0	216	CHEMBL3818035	-7.9	265	eMol20342220	-7.8
168	eMol580072	-8.0	217	eMol27091442	-7.9	266	eMol24520354	-7.8
169	eMol28321864	-8.0	218	eMol56752349	-7.9	267	eMol27202992	-7.8
170	eMol579718	-8.0	219	CHEMBL3819481	-7.9	268	eMol29638777	-7.8
171	CHEMBL1215578	-8.0	220	CHEMBL462179	-7.9	269	eMol45622749	-7.8
172	eMol1755402	-8.0	221	eMol179164959	-7.9	270	CHEMBL1214861	-7.8
173	eMol18551342	-8.0	222	eMol206910852	-7.9	271	eMol25813417	-7.8
174	CHEMBL3818732	-8.0	223	eMol25810001	-7.9	272	eMol208103615	-7.8
175	eMol206992517	-8.0	224	eMol25810077	-7.9	273	eMol29565259	-7.8
176	eMol256911679	-8.0	225	eMol27202994	-7.9	274	eMol45585838	-7.8
177	eMol27202252	-8.0	226	eMol43906047	-7.9	275	eMol561887	-7.8
178	eMol301527162	-8.0	227	eMol43906063	-7.9	276	eMol23202652	-7.8
179	eMol579756	-8.0	228	eMol679550	-7.9	277	eMol26242026	-7.8
180	eMol679664	-8.0	229	CHEMBL3582080	-7.9	278	eMol26242040	-7.8
181	CHEMBL2259944	-8.0	230	eMol177199339	-7.9	280	eMol4555657	-7.8
182	CHEMBL485839	-8.0	231	eMol20342262	-7.9	281	eMol4572924	-7.8
183	eMol27202242	-8.0	232	eMol206911267	-7.9	282	CHEMBL3819187	-7.8
184	eMol4552519	-8.0	233	eMol300994251	-7.9	283	eMol4389171	-7.8
185	eMol25810089	-8.0	234	eMol46480254	-7.9	279	eMol4740224	-7.8
186	eMol4581322	-8.0	235	eMol48768479	-7.9	284	eMol30646140	-7.7
187	eMol679670	-8.0	236	eMol566380	-7.9	285	eMol4580802	-7.7
188	eMol679824	-8.0	237	eMol581308	-7.9	286	eMol58034831	-7.7
189	CHEMBL1215081	-7.9	238	eMol681814	-7.9	287	eMol72993476	-7.7
190	eMol24389393	-7.9	239	CHEMBL2259942	-7.8	288	eMol1748795	-7.7
191	eMol25966646	-7.9	240	CHEMBL3819186	-7.8	289	eMol179165002	-7.7
192	eMol26196328	-7.9	241	eMol179164947	-7.8	290	eMol206985996	-7.7
193	eMol26242022	-7.9	242	eMol19267414	-7.8	291	eMol26310961	-7.7
194	eMol45585844	-7.9	243	eMol26251042	-7.8	292	eMol27202264	-7.7
195	eMol4566756	-7.9	244	eMol27380659	-7.8	293	eMol4446697	-7.7

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
294	eMol4579587	-7.7	346	eMol25810163	-7.6	398	eMol26312078	-7.5
295	eMol25909178	-7.7	347	eMol27202262	-7.6	399	eMol26405201	-7.5
296	eMol26311238	-7.7	348	eMol27202268	-7.6	400	eMol45935562	-7.5
297	eMol300445092	-7.7	349	eMol7635480	-7.6	401	eMol46400681	-7.5
298	eMol30665797	-7.7	350	eMol935864	-7.6	402	eMol24116475	-7.5
299	CHEMBL1215004	-7.7	351	CHEMBL3819338	-7.6	403	eMol25896479	-7.5
300	CHEMBL3817850	-7.7	352	CHEMBL1215803	-7.6	404	eMol4587779	-7.5
301	eMol179165014	-7.7	353	CHEMBL485838	-7.6	405	eMol679668	-7.5
302	eMol19076364	-7.7	354	eMol26327269	-7.6	406	CHEMBL1584455	-7.5
303	eMol25965034	-7.7	355	eMol588102	-7.6	407	eMol26314331	-7.5
304	eMol29587306	-7.7	356	eMol8267101	-7.6	408	eMol4386746	-7.5
305	eMol4116278	-7.7	357	eMol26242048	-7.6	409	eMol4480890	-7.5
306	eMol43731202	-7.7	358	eMol3060078	-7.6	410	eMol45935466	-7.5
307	eMol45585836	-7.7	359	eMol46480052	-7.6	411	eMol19266607	-7.5
308	eMol46480194	-7.7	360	eMol956409	-7.6	412	eMol206908008	-7.5
309	eMol679666	-7.7	361	eMol29634797	-7.6	413	eMol26255667	-7.5
310	eMol681860	-7.7	362	eMol4574833	-7.6	414	eMol300014864	-7.5
311	CHEMBL1371074	-7.7	363	eMol46210804	-7.6	415	eMol316351191	-7.5
312	eMol24511821	-7.7	364	eMol46365712	-7.6	416	eMol565754	-7.5
313	eMol26242024	-7.7	365	eMol1675430	-7.6	417	eMol587646	-7.5
314	eMol27202958	-7.7	366	eMol25784115	-7.6	418	CHEMBL38193326	-7.5
315	eMol20342268	-7.7	367	eMol2992488	-7.6	419	CHEMBL602627	-7.5
316	eMol233046940	-7.7	368	eMol46509917	-7.6	420	eMol18940061	-7.5
317	CHEMBL1528362	-7.7	369	eMol944638	-7.6	421	eMol26313085	-7.5
318	eMol19076348	-7.7	370	CHEMBL1214868	-7.6	422	eMol28321866	-7.5
319	eMol24525196	-7.7	371	eMol1764376	-7.6	423	eMol43745241	-7.5
320	eMol26141700	-7.7	372	eMol18958642	-7.6	424	eMol4567258	-7.5
321	eMol26311024	-7.7	373	eMol20377433	-7.6	425	eMol4580053	-7.5
322	eMol27202742	-7.7	374	eMol26683947	-7.6	426	eMol46528447	-7.5
323	eMol4413761	-7.7	375	eMol3318312	-7.6	427	eMol49384601	-7.5
324	CHEMBL517897	-7.7	376	eMol4577787	-7.6	428	eMol50556474	-7.5
325	eMol20342205	-7.7	377	eMol5779489	-7.6	429	eMol566256	-7.5
326	eMol23249723	-7.7	378	CHEMBL520033	-7.5	430	eMol1040103	-7.5
327	eMol43744848	-7.7	379	eMol17203477	-7.5	431	eMol20337444	-7.5
328	eMol48982653	-7.7	380	eMol18860491	-7.5	432	eMol206985560	-7.5
329	CHEMBL3805841	-7.7	381	eMol193447787	-7.5	433	eMol25816251	-7.5
330	CHEMBL3817906	-7.7	382	CHEMBL3817957	-7.5	434	eMol27187406	-7.5
331	eMol25955419	-7.7	383	CHEMBL3818012	-7.5	435	eMol3535618	-7.5
332	eMol562493	-7.7	384	eMol16374637	-7.5	436	eMol4551561	-7.5
333	eMol588242	-7.7	385	eMol24029848	-7.5	437	eMol46479990	-7.5
334	eMol7667302	-7.7	386	eMol3427847	-7.5	438	eMol566118	-7.5
335	eMol26242042	-7.6	387	eMol43906067	-7.5	439	eMol588256	-7.5
336	eMol43731476	-7.6	388	eMol4448933	-7.5	440	eMol6753441	-7.5
337	eMol588388	-7.6	389	eMol51435800	-7.5	441	CHEMBL114364	-7.5
338	CHEMBL323866	-7.6	390	eMol11690694	-7.5	442	CHEMBL250917	-7.5
339	eMol2992508	-7.6	391	eMol16683412	-7.5	443	CHEMBL3818515	-7.5
340	eMol43757885	-7.6	392	eMol27202960	-7.5	444	eMol1429358	-7.5
341	eMol7265152	-7.6	393	eMol45944068	-7.5	445	eMol1679768	-7.5
342	CHEMBL3819140	-7.6	394	eMol935130	-7.5	446	eMol2208925	-7.5
343	eMol3103759	-7.6	395	eMol1751766	-7.5	447	eMol23250559	-7.5
344	eMol32369766	-7.6	396	eMol206987969	-7.5	448	CHEMBL114364	-7.5
345	eMol4726858	-7.6	397	eMol233088901	-7.5	449	CHEMBL250917	-7.5

Table S1. *Continued.*

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
448	eMol25810127	-7.5	500	eMol26242054	-7.4	552	eMol25901925	-7.3
449	eMol27202290	-7.5	501	eMol26316348	-7.4	553	eMol26245604	-7.3
450	eMol45701494	-7.5	502	eMol27202980	-7.4	554	eMol26259383	-7.3
451	eMol23247039	-7.4	503	eMol43906057	-7.4	555	eMol26324339	-7.3
452	eMol24493983	-7.4	504	eMol46479912	-7.4	556	eMol299991997	-7.3
453	eMol24520756	-7.4	505	eMol46479980	-7.4	557	eMol4075283	-7.3
454	eMol25965334	-7.4	506	CHEMBL3818704	-7.4	558	eMol44673597	-7.3
455	eMol26320021	-7.4	507	eMol26242036	-7.4	559	eMol4485131	-7.3
456	eMol37002179	-7.4	508	eMol565478	-7.4	560	eMol4708971	-7.3
457	eMol4388132	-7.4	509	CHEMBL1402619	-7.4	561	eMol561655	-7.3
458	eMol46480026	-7.4	510	CHEMBL3805023	-7.4	562	eMol956477	-7.3
459	eMol579044	-7.4	511	eMol1025907	-7.4	563	CHEMBL3818910	-7.3
460	eMol587808	-7.4	512	eMol16351683	-7.4	564	eMol207355370	-7.3
461	eMol588272	-7.4	513	eMol206875270	-7.4	565	eMol24520050	-7.3
462	CHEMBL117642	-7.4	514	eMol25810171	-7.4	566	eMol25918241	-7.3
463	CHEMBL1994876	-7.4	515	eMol25937897	-7.4	567	eMol26242052	-7.3
464	eMol27202402	-7.4	516	eMol26311934	-7.4	568	eMol26300049	-7.3
465	eMol3018072	-7.4	517	eMol26936203	-7.4	569	eMol4578697	-7.3
466	eMol46210806	-7.4	518	eMol27202936	-7.4	570	eMol4715267	-7.3
467	eMol75932399	-7.4	519	eMol27202948	-7.4	571	CHEMBL455639	-7.3
468	CHEMBL1499977	-7.4	520	eMol299962831	-7.4	572	eMol1040791	-7.3
469	eMol20354197	-7.4	521	eMol566142	-7.4	573	eMol1678605	-7.3
470	eMol20378545	-7.4	522	CHEMBL1360793	-7.4	574	eMol27091590	-7.3
471	eMol24427880	-7.4	523	CHEMBL1988177	-7.4	575	eMol27115486	-7.3
472	eMol24428326	-7.4	524	CHEMBL3805378	-7.4	576	eMol316344188	-7.3
473	eMol26356948	-7.4	525	CHEMBL511010	-7.4	577	CHEMBL3582082	-7.3
474	eMol27202250	-7.4	526	eMol20356176	-7.4	578	eMol1149947	-7.3
475	eMol27203000	-7.4	527	eMol30017880	-7.4	579	eMol179165005	-7.3
476	eMol2993022	-7.4	528	eMol4934666	-7.4	580	eMol180102976	-7.3
477	eMol46479157	-7.4	529	eMol16352353	-7.4	581	eMol20375154	-7.3
478	eMol24058094	-7.4	530	eMol179177638	-7.4	582	eMol26262902	-7.3
479	eMol24524408	-7.4	531	eMol19076404	-7.4	583	eMol26314721	-7.3
480	eMol26189153	-7.4	532	eMol25902329	-7.4	584	eMol46370139	-7.3
481	eMol27202902	-7.4	533	eMol45928112	-7.4	585	eMol565838	-7.3
482	eMol27338418	-7.4	534	eMol4698359	-7.4	586	CHEMBL116634	-7.3
483	eMol44127206	-7.4	535	eMol4739467	-7.4	587	eMol19076688	-7.3
484	eMol4521223	-7.4	536	CHEMBL1214645	-7.3	588	eMol206964256	-7.3
485	eMol181128729	-7.4	537	CHEMBL1215006	-7.3	589	eMol23191317	-7.3
486	eMol26246365	-7.4	538	eMol1683032	-7.3	590	eMol25902283	-7.3
487	eMol26327656	-7.4	539	eMol24538139	-7.3	591	eMol26230266	-7.3
488	eMol32812942	-7.4	540	eMol26250892	-7.3	592	eMol26315986	-7.3
489	eMol46411087	-7.4	541	eMol276247952	-7.3	593	eMol276247970	-7.3
490	eMol4725672	-7.4	542	eMol299966748	-7.3	594	eMol300990951	-7.3
491	eMol581076	-7.4	543	eMol300978663	-7.3	595	eMol31358919	-7.3
492	eMol956403	-7.4	544	eMol4090808	-7.3	596	eMol43745829	-7.3
493	eMol9919488	-7.4	545	eMol4566508	-7.3	597	eMol1764190	-7.3
494	CHEMBL1215082	-7.4	546	eMol4713633	-7.3	598	eMol207259512	-7.3
495	CHEMBL3819363	-7.4	547	eMol4732807	-7.3	599	eMol23206884	-7.3
496	CHEMBL3819532	-7.4	548	CHEMBL397391	-7.3	600	eMol23242679	-7.3
497	CHEMBL82690	-7.4	549	eMol1324430	-7.3	601	eMol2385157	-7.3
498	eMol25903079	-7.4	550	eMol206850549	-7.3	602	eMol24520802	-7.3
499	eMol25903125	-7.4	551	eMol24526444	-7.3	603	eMol24532024	-7.3

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
604	eMol25797977	-7.3	654	eMol316831112	-7.2	704	CHEMBL3806097	-7.2
605	eMol27202984	-7.3	655	eMol35699388	-7.2	705	CHEMBL577676	-7.2
606	eMol27202996	-7.3	656	eMol43730464	-7.2	706	CHEMBL585981	-7.2
607	eMol27252901	-7.3	657	eMol46479958	-7.2	707	eMol18516265	-7.2
608	eMol35717814	-7.3	658	eMol935636	-7.2	708	eMol18550720	-7.2
609	eMol43745056	-7.3	659	CHEMBL296691	-7.2	709	eMol20337448	-7.2
610	eMol4549830	-7.3	660	eMol179164953	-7.2	710	eMol2409922	-7.2
611	eMol588158	-7.3	661	eMol23208796	-7.2	711	eMol24521662	-7.2
612	eMol684240	-7.3	662	eMol23241510	-7.2	712	eMol25825125	-7.2
613	eMol956435	-7.3	663	eMol24521330	-7.2	713	eMol27202756	-7.2
614	CHEMBL115809	-7.3	664	eMol25770408	-7.2	714	eMol32813234	-7.2
615	eMol1429356	-7.3	665	eMol25902291	-7.2	715	eMol4433627	-7.2
616	eMol19076598	-7.3	666	eMol25968613	-7.2	716	eMol936632	-7.2
617	eMol19076750	-7.3	667	eMol26219237	-7.2	717	eMol2231344	-7.2
618	eMol206907968	-7.3	668	eMol4726520	-7.2	718	eMol23201309	-7.2
619	eMol25907499	-7.3	669	eMol5847921	-7.2	719	eMol26300005	-7.2
620	eMol25913211	-7.3	670	eMol588228	-7.2	720	eMol27202506	-7.2
621	eMol25936279	-7.3	671	eMol935898	-7.2	721	eMol27202920	-7.2
622	eMol27202388	-7.3	672	CHEMBL3817866	-7.2	722	eMol31760166	-7.2
623	eMol300154219	-7.3	673	CHEMBL4099863	-7.2	723	eMol43746869	-7.2
624	eMol4477952	-7.3	674	CHEMBL47157	-7.2	724	eMol4408548	-7.2
625	eMol579714	-7.3	675	CHEMBL579620	-7.2	725	eMol4706083	-7.2
626	eMol581304	-7.3	676	eMol16056893	-7.2	726	eMol565918	-7.2
627	CHEMBL116408	-7.3	677	eMol17192354	-7.2	727	CHEMBL3806178	-7.2
628	eMol2330950	-7.3	678	eMol180102764	-7.2	728	eMol18551352	-7.2
629	eMol25895023	-7.3	679	eMol19076602	-7.2	729	eMol2130046	-7.2
630	eMol25966304	-7.3	680	eMol26285666	-7.2	730	eMol23170772	-7.2
631	eMol26285150	-7.3	681	eMol26289047	-7.2	731	eMol24518463	-7.2
632	eMol26326968	-7.3	682	eMol26314361	-7.2	732	eMol25958221	-7.2
633	eMol27202912	-7.3	683	eMol26569999	-7.2	733	eMol26277244	-7.2
634	eMol27202970	-7.3	684	eMol26936207	-7.2	734	eMol26292416	-7.2
635	eMol2880336	-7.3	685	eMol27202540	-7.2	735	eMol26310907	-7.2
636	eMol30744925	-7.3	686	eMol2768990	-7.2	736	eMol26316052	-7.2
637	eMol43731530	-7.3	687	eMol4606566	-7.2	737	eMol26328784	-7.2
638	eMol46400679	-7.3	688	eMol46370137	-7.2	738	eMol27202410	-7.2
639	eMol4728946	-7.3	689	eMol46400677	-7.2	739	eMol27202762	-7.2
640	eMol8238281	-7.3	690	eMol46491554	-7.2	740	eMol32813226	-7.2
641	CHEMBL3818933	-7.3	691	eMol4713307	-7.2	741	eMol33346435	-7.2
642	eMol11071566	-7.3	692	CHEMBL117438	-7.2	742	eMol4490859	-7.2
643	eMol24521048	-7.3	693	CHEMBL3818229	-7.2	743	eMol46445765	-7.2
644	eMol25771182	-7.3	694	eMol22370884	-7.2	744	eMol46479996	-7.2
645	eMol29649914	-7.3	695	eMol27045407	-7.2	745	CHEMBL326628	-7.2
646	eMol45622753	-7.3	696	eMol27202398	-7.2	746	CHEMBL4079984	-7.2
647	eMol588168	-7.3	697	eMol27202754	-7.2	747	eMol1120546	-7.2
648	CHEMBL116817	-7.2	698	eMol27202914	-7.2	748	eMol181109768	-7.2
649	CHEMBL1632342	-7.2	699	eMol27202918	-7.2	749	eMol27202350	-7.2
650	eMol179164956	-7.2	700	eMol32246523	-7.2	750	eMol43731774	-7.2
651	eMol24419686	-7.2	701	eMol4709495	-7.2	751	eMol45133343	-7.2
652	eMol26285928	-7.2	702	eMol4718679	-7.2	752	eMol46400687	-7.2
653	eMol27202916	-7.2	703	eMol5444969	-7.2	753	eMol566406	-7.2

Table S1. *Continued.*

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
754	eMol679820	-7.2	806	eMol587916	-7.1	858	eMol27187414	-7.1
755	CHEMBL3805042	-7.2	807	CHEMBL34185	-7.1	859	eMol27202282	-7.1
756	CHEMBL3819311	-7.2	808	CHEMBL3804857	-7.1	860	eMol30104228	-7.1
757	eMol206921779	-7.2	809	CHEMBL3818747	-7.1	861	eMol5444645	-7.1
758	eMol2141753	-7.2	810	CHEMBL38330	-7.1	862	eMol5444883	-7.1
759	eMol23246986	-7.2	811	eMol20337442	-7.1	863	eMol588078	-7.1
760	eMol24113359	-7.2	812	eMol20380394	-7.1	864	CHEMBL3818856	-7.1
761	eMol24428240	-7.2	813	eMol23185851	-7.1	865	eMol18542840	-7.1
762	eMol24520240	-7.2	814	eMol25770418	-7.1	866	eMol24428006	-7.1
763	eMol25810099	-7.2	815	eMol25902049	-7.1	867	eMol2517109	-7.1
764	eMol25829045	-7.2	816	eMol26319543	-7.1	868	eMol25819233	-7.1
765	eMol27045405	-7.2	817	eMol26936201	-7.1	869	eMol25903659	-7.1
766	eMol27045521	-7.2	818	eMol3033983	-7.1	870	eMol25945602	-7.1
767	eMol30322739	-7.2	819	eMol6263477	-7.1	871	eMol25966294	-7.1
768	eMol44548966	-7.2	820	CHEMBL114005	-7.1	872	eMol26189151	-7.1
769	eMol45708568	-7.2	821	CHEMBL3805407	-7.1	873	eMol26312838	-7.1
770	eMol4738130	-7.2	822	eMol16351675	-7.1	874	eMol26314117	-7.1
771	eMol50301465	-7.2	823	eMol24521248	-7.1	875	eMol27202280	-7.1
772	eMol1156520	-7.2	824	eMol26264151	-7.1	876	eMol27202380	-7.1
773	eMol18550714	-7.2	825	eMol26276502	-7.1	877	eMol29665906	-7.1
774	eMol18961180	-7.2	826	eMol26313449	-7.1	878	eMol32812998	-7.1
775	eMol23241342	-7.2	827	eMol26331720	-7.1	879	eMol33339294	-7.1
776	eMol24519079	-7.2	828	eMol27202362	-7.1	880	eMol4572232	-7.1
777	eMol25963663	-7.2	829	eMol33346433	-7.1	881	eMol46545587	-7.1
778	eMol26289870	-7.2	830	eMol43731198	-7.1	882	eMol48597407	-7.1
779	eMol26330383	-7.2	831	eMol45935468	-7.1	883	eMol579510	-7.1
780	eMol27202358	-7.2	832	eMol46509913	-7.1	884	eMol588368	-7.1
781	eMol3317346	-7.2	833	eMol4732869	-7.1	885	CHEMBL1215796	-7.1
782	CHEMBL1302012	-7.1	834	CHEMBL113923	-7.1	886	CHEMBL1591720	-7.1
783	CHEMBL3806218	-7.1	835	CHEMBL1383006	-7.1	887	CHEMBL3818171	-7.1
784	CHEMBL3818209	-7.1	836	CHEMBL1559857	-7.1	888	CHEMBL395117	-7.1
785	CHEMBL3818582	-7.1	837	CHEMBL3805665	-7.1	889	eMol1165997	-7.1
786	eMol18550716	-7.1	838	eMol16351673	-7.1	890	eMol20310561	-7.1
787	eMol206980481	-7.1	839	eMol19076826	-7.1	891	eMol20378615	-7.1
788	eMol26250339	-7.1	840	eMol20380392	-7.1	892	eMol206920578	-7.1
789	eMol26310839	-7.1	841	eMol25810081	-7.1	893	eMol206965980	-7.1
790	eMol43731776	-7.1	842	eMol26251302	-7.1	894	eMol2194316	-7.1
791	eMol46534208	-7.1	843	eMol26270766	-7.1	895	eMol2408165	-7.1
792	eMol5672543	-7.1	844	eMol26276632	-7.1	896	eMol24520553	-7.1
793	CHEMBL1414265	-7.1	845	eMol26314895	-7.1	897	eMol25790309	-7.1
794	CHEMBL247353	-7.1	846	eMol26936209	-7.1	898	eMol25913057	-7.1
795	eMol16351883	-7.1	847	eMol27187400	-7.1	899	eMol26314359	-7.1
796	eMol16375743	-7.1	848	eMol4146706	-7.1	900	eMol26315688	-7.1
797	eMol17202599	-7.1	849	eMol45932769	-7.1	901	eMol27202336	-7.1
798	eMol18866942	-7.1	850	eMol936420	-7.1	902	eMol27202496	-7.1
799	eMol20344945	-7.1	851	CHEMBL1551922	-7.1	903	eMol27202778	-7.1
800	eMol206964558	-7.1	852	CHEMBL3818977	-7.1	904	eMol300089978	-7.1
801	eMol2115166	-7.1	853	eMol206990555	-7.1	905	eMol3181655	-7.1
802	eMol23242609	-7.1	854	eMol2166708	-7.1	906	eMol579926	-7.1
803	eMol26292060	-7.1	855	eMol24524699	-7.1	907	CHEMBL1439596	-7.1
804	eMol36016142	-7.1	856	eMol25771206	-7.1	908	CHEMBL1562035	-7.1
805	eMol560303	-7.1	857	eMol26286396	-7.1	909	CHEMBL3818499	-7.1

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
910	CHEMBL3819196	-7.1	961	eMol2308510	-7.0	1012	CHEMBL3818158	-7.0
911	CHEMBL550397	-7.1	962	eMol25901881	-7.0	1013	eMol18550710	-7.0
912	eMol1035551	-7.1	963	eMol26263266	-7.0	1014	eMol24430685	-7.0
913	eMol18550722	-7.1	964	eMol26315041	-7.0	1015	eMol2513652	-7.0
914	eMol206849669	-7.1	965	eMol26524217	-7.0	1016	eMol25770414	-7.0
915	eMol24430231	-7.1	966	eMol46400683	-7.0	1017	eMol25931375	-7.0
916	eMol24531722	-7.1	967	eMol4709315	-7.0	1018	eMol26141682	-7.0
917	eMol24531798	-7.1	968	eMol72578631	-7.0	1019	eMol26309887	-7.0
918	eMol25912447	-7.1	969	CHEMBL2297150	-7.0	1020	eMol26313748	-7.0
919	eMol26288955	-7.1	970	CHEMBL3818347	-7.0	1021	eMol26762439	-7.0
920	eMol26326313	-7.1	971	CHEMBL3818366	-7.0	1022	eMol27202208	-7.0
921	eMol26350850	-7.1	972	eMol16379841	-7.0	1023	eMol36015268	-7.0
922	eMol27187440	-7.1	973	eMol19076734	-7.0	1024	eMol566554	-7.0
923	eMol299994300	-7.1	974	eMol19076828	-7.0	1025	ChEBI114797	-7.0
924	eMol3021959	-7.1	975	eMol20356657	-7.0	1026	CHEMBL1452417	-7.0
925	eMol31278496	-7.1	976	eMol23152351	-7.0	1027	CHEMBL1967636	-7.0
926	eMol36016132	-7.1	977	eMol25816255	-7.0	1028	CHEMBL3627816	-7.0
927	eMol4491662	-7.1	978	eMol25895009	-7.0	1029	CHEMBL38232	-7.0
928	eMol956263	-7.1	979	eMol26310653	-7.0	1030	CHEMBL90574	-7.0
929	CHEMBL1423402	-7.1	980	eMol26314551	-7.0	1031	eMol16351609	-7.0
930	CHEMBL1552848	-7.1	981	eMol27202320	-7.0	1032	eMol206978896	-7.0
931	CHEMBL299107	-7.1	982	eMol29987858	-7.0	1033	eMol206996167	-7.0
932	CHEMBL3804866	-7.1	983	eMol3775722	-7.0	1034	eMol2232474	-7.0
933	eMol106491702	-7.1	984	eMol4565043	-7.0	1035	eMol23237618	-7.0
934	eMol16351677	-7.1	985	eMol565850	-7.0	1036	eMol24520280	-7.0
935	eMol206909136	-7.1	986	eMol6157528	-7.0	1037	eMol25827835	-7.0
936	eMol23244410	-7.1	987	CHEMBL1214934	-7.0	1038	eMol25896473	-7.0
937	eMol24520023	-7.1	988	CHEMBL1900041	-7.0	1039	eMol26262940	-7.0
938	eMol24526765	-7.1	989	CHEMBL2297667	-7.0	1040	eMol26349365	-7.0
939	eMol25784531	-7.1	990	CHEMBL3818626	-7.0	1041	eMol26355834	-7.0
940	eMol25913175	-7.1	991	eMol15983174	-7.0	1042	eMol26581878	-7.0
941	eMol25924517	-7.1	992	eMol19076732	-7.0	1043	eMol44057517	-7.0
942	eMol26293580	-7.1	993	eMol206965358	-7.0	1044	eMol4719207	-7.0
943	eMol26570001	-7.1	994	eMol206987841	-7.0	1045	eMol48554523	-7.0
944	eMol27202232	-7.1	995	eMol24427986	-7.0	1046	eMol560313	-7.0
945	eMol27202422	-7.1	996	eMol24519100	-7.0	1047	eMol566074	-7.0
946	eMol316862506	-7.1	997	eMol25895011	-7.0	1048	eMol784256	-7.0
947	eMol36904288	-7.1	998	eMol26262168	-7.0	1049	CHEMBL1357492	-7.0
948	eMol43744846	-7.1	999	eMol26299531	-7.0	1050	eMol1324432	-7.0
949	eMol679754	-7.1	1000	eMol26324447	-7.0	1051	eMol206979384	-7.0
950	CHEMBL1373990	-7.0	1001	eMol27202224	-7.0	1052	eMol2194269	-7.0
951	CHEMBL1394809	-7.0	1002	eMol27202288	-7.0	1053	eMol24548037	-7.0
952	CHEMBL3804880	-7.0	1003	eMol27202520	-7.0	1054	eMol25903928	-7.0
953	CHEMBL3819459	-7.0	1004	eMol276260499	-7.0	1055	eMol25964562	-7.0
954	eMol1149869	-7.0	1005	eMol29262171	-7.0	1056	eMol2597848	-7.0
955	eMol16352193	-7.0	1006	eMol36016032	-7.0	1057	eMol26237970	-7.0
956	eMol17203597	-7.0	1007	eMol4708889	-7.0	1058	eMol26317983	-7.0
957	eMol1752196	-7.0	1008	eMol5779704	-7.0	1059	eMol26775365	-7.0
958	eMol19076370	-7.0	1009	CHEMBL1553991	-7.0	1060	eMol27187482	-7.0
959	eMol206843436	-7.0	1010	CHEMBL1882658	-7.0	1061	eMol30132606	-7.0
960	eMol206964210	-7.0	1011	CHEMBL3805512	-7.0	1062	eMol3138656	-7.0

Table S1. Continued.

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1063:	eMol36015282	-7.0	1114:	eMol206904349	-7.0	1165:	eMol300979175	-6.9
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1065:	eMol46525150	-7.0	1116:	eMol25927095	-7.0	1167:	eMol36015494	-6.9
1066:	eMol4744993	-7.0	1117:	eMol27045527	-7.0	1168:	eMol43678312	-6.9
1067:	eMol49849265	-7.0	1118:	eMol27202360	-7.0	1169:	eMol46544815	-6.9
1068:	eMol685328	-7.0	1119:	eMol27202532	-7.0	1170:	eMol11867096	-6.9
1069:	CHEMBL3804836	-7.0	1120:	eMol27202896	-7.0	1171:	eMol17203549	-6.9
1070:	CHEMBL3818974	-7.0	1121:	eMol27435660	-7.0	1172:	eMol206964418	-6.9
1071:	CHEMBL3819285	-7.0	1122:	eMol43749117	-7.0	1173:	eMol206969744	-6.9
1072:	CHEMBL46581	-7.0	1123:	eMol4475588	-7.0	1174:	eMol206972648	-6.9
1073:	eMol18542077	-7.0	1124:	eMol45621707	-7.0	1175:	eMol206987102	-6.9
1074:	eMol19031814	-7.0	1125:	eMol4712268	-7.0	1176:	eMol22299802	-6.9
1075:	eMol24430273	-7.0	1126:	eMol4745700	-7.0	1177:	eMol24519081	-6.9
1076:	eMol25902841	-7.0	1127:	CHEMBL1451971	-7.0	1178:	eMol24546968	-6.9
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1078:	eMol27202894	-7.0	1129:	CHEMBL3805136	-7.0	1180:	eMol25813419	-6.9
1079:	eMol30104216	-7.0	1130:	CHEMBL3819605	-7.0	1181:	eMol25913361	-6.9
1080:	eMol3091619	-7.0	1131:	eMol14069413	-7.0	1182:	eMol26141662	-6.9
1081:	eMol5538242	-7.0	1132:	eMol20352703	-7.0	1183:	eMol26249494	-6.9
1082:	eMol565910	-7.0	1133:	eMol23239776	-7.0	1184:	eMol26256475	-6.9
1083:	eMol935992	-7.0	1134:	eMol25896475	-7.0	1185:	eMol26264167	-6.9
1084:	eMol9989242	-7.0	1135:	eMol25902133	-7.0	1186:	eMol26300497	-6.9
1085:	CHEMBL1303106	-7.0	1136:	eMol25929538	-7.0	1187:	eMol26310555	-6.9
1086:	eMol1170739	-7.0	1137:	eMol25963073	-7.0	1188:	eMol27202884	-6.9
1087:	eMol19076366	-7.0	1138:	eMol25968661	-7.0	1189:	eMol276247954	-6.9
1088:	eMol206875356	-7.0	1139:	eMol26141678	-7.0	1190:	eMol300978919	-6.9
1089:	eMol24008012	-7.0	1140:	eMol26189265	-7.0	1191:	eMol35693189	-6.9
1090:	eMol25954676	-7.0	1141:	eMol26295757	-7.0	1192:	eMol36898082	-6.9
1091:	eMol25961619	-7.0	1142:	eMol26313219	-7.0	1193:	eMol679750	-6.9
1092:	eMol26245266	-7.0	1143:	eMol26327169	-7.0	1194:	eMol72964183	-6.9
1093:	eMol26290986	-7.0	1144:	eMol27202900	-7.0	1195:	eMol935934	-6.9
1094:	eMol26312834	-7.0	1145:	eMol276247964	-7.0	1196:	CHEMBL1867264	-6.9
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1097:	eMol27202758	-7.0	1148:	eMol30083452	-7.0	1199:	eMol16374969	-6.9
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1099:	eMol300273851	-7.0	1150:	eMol560309	-7.0	1201:	eMol207355368	-6.9
1100:	eMol36015642	-7.0	1151:	eMol15924858	-6.9	1202:	eMol23246252	-6.9
1101:	eMol45787893	-7.0	1152:	eMol1683469	-6.9	1203:	eMol25902478	-6.9
1102:	eMol4735810	-7.0	1153:	eMol18551390	-6.9	1204:	eMol27202274	-6.9
1103:	eMol561781	-7.0	1154:	eMol19076694	-6.9	1205:	eMol27202906	-6.9
1104:	eMol561985	-7.0	1155:	eMol20368452	-6.9	1206:	eMol277677808	-6.9
1105:	eMol6777617	-7.0	1156:	eMol206910454	-6.9	1207:	eMol2981967	-6.9
1106:	CHEMBL1554351	-7.0	1157:	eMol26262090	-6.9	1208:	eMol4713349	-6.9
1107:	CHEMBL3806234	-7.0	1158:	eMol26310743	-6.9	1209:	CHEMBL1405217	-6.9
1108:	CHEMBL3819289	-7.0	1159:	eMol26313445	-6.9	1210:	CHEMBL1437240	-6.9
1109:	CHEMBL4091026	-7.0	1160:	eMol27045535	-6.9	1211:	CHEMBL3818631	-6.9
1110:	eMol15983252	-7.0	1161:	eMol27202324	-6.9	1212:	eMol17205607	-6.9
1111:	eMol16390197	-7.0	1162:	eMol27202744	-6.9	1213:	eMol20379434	-6.9
1112:	eMol18588453	-7.0	1163:	eMol276247956	-6.9	1214:	eMol206846147	-6.9
1113:	eMol19076492	-7.0	1164:	eMol2987076	-6.9	1215:	eMol206907645	-6.9

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
1216:	eMol23166688	-6.9	1267	eMol25962247	-6.9	1323	eMol2124007	-6.9
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1218:	eMol24518467	-6.9	1269	eMol27202334	-6.9	1325	eMol24100760	-6.9
1219:	eMol24520575	-6.9	1270	eMol27202782	-6.9	1326	eMol25813397	-6.9
1220:	eMol25770140	-6.9	1271	eMol36015106	-6.9	1327	eMol25813443	-6.9
1221:	eMol25795727	-6.9	1272	eMol681896	-6.9	1328	eMol25938613	-6.9
1222:	eMol2588283	-6.9	1273	CHEMBL1380757	-6.9	1329	eMol26272160	-6.9
1223:	eMol26242020	-6.9	1274	CHEMBL1521258	-6.9	1330	eMol27187248	-6.9
1224:	eMol26262644	-6.9	1275	CHEMBL1597816	-6.9	1331	eMol27202392	-6.9
1225:	eMol26316338	-6.9	1276	eMol1454668	-6.9	1332	eMol27202394	-6.9
1226:	eMol26323441	-6.9	1277	eMol20333678	-6.9	1333	eMol27202400	-6.9
1227:	eMol26339205	-6.9	1278	eMol206964698	-6.9	1334	eMol27202794	-6.9
1228:	eMol27202226	-6.9	1279	eMol23198915	-6.9	1335	eMol27202904	-6.9
1229:	eMol3005040	-6.9	1280	eMol24507755	-6.9	1336	eMol27670260	-6.9
1230:	eMol32813186	-6.9	1281	eMol24525232	-6.9	1337	eMol2768992	-6.9
1231:	eMol36015820	-6.9	1282	eMol25810165	-6.9	1338	eMol31399220	-6.9
1232:	eMol44059508	-6.9	1283	eMol25896463	-6.9	1339	eMol46445438	-6.9
1233:	eMol4475278	-6.9	1284	eMol25903653	-6.9	1340	CHEMBL1573403	-6.9
1234:	eMol4482176	-6.9	1285	eMol26141674	-6.9	1341	CHEMBL1708737	-6.9
1235:	eMol46509915	-6.9	1286	eMol26285794	-6.9	1342	CHEMBL3804897	-6.9
1236:	eMol4708095	-6.9	1287	eMol26322685	-6.9	1343	CHEMBL3818915	-6.9
1237:	CHEMBL1376830	-6.9	1288	eMol314783893	-6.9	1344	eMol1751356	-6.9
1238:	CHEMBL1642185	-6.9	1289	eMol316838531	-6.9	1345	eMol20369159	-6.9
1239:	CHEMBL3804835	-6.9	1290	eMol3458659	-6.9	1346	eMol206906676	-6.9
1240:	eMol177234561	-6.9	1291	eMol4095805	-6.9	1347	eMol206962769	-6.9
1241:	eMol18614804	-6.9	1292	eMol43745140	-6.9	1348	eMol24535222	-6.9
1242:	eMol18939007	-6.9	1293	eMol45560661	-6.9	1349	eMol2454468	-6.9
1243:	eMol19076402	-6.9	1294	eMol46509911	-6.9	1350	eMol25770138	-6.9
1244:	eMol206843418	-6.9	1295	eMol4702761	-6.9	1351	eMol25816249	-6.9
1245:	eMol24537876	-6.9	1296	eMol4729332	-6.9	1352	eMol25881264	-6.9
1246:	eMol25829407	-6.9	1297	CHEMBL1215800	-6.9	1353	eMol26249794	-6.9
1247:	eMol26141694	-6.9	1298	CHEMBL3818900	-6.9	1354	eMol27202342	-6.9
1248:	eMol26288755	-6.9	1299	eMol1170743	-6.9	1355	eMol2992544	-6.9
1249:	eMol26296745	-6.9	1300	eMol20344947	-6.9	1356	eMol36015274	-6.9
1250:	eMol27009455	-6.9	1301	eMol206843458	-6.9	1357	eMol36015492	-6.9
1251:	eMol27187452	-6.9	1302	eMol24518839	-6.9	1358	eMol43772496	-6.9
1252:	eMol27202270	-6.9	1303	eMol25797913	-6.9	1359	eMol935732	-6.9
1253:	eMol300120324	-6.9	1304	eMol26276724	-6.9	1360	CHEMBL1215718	-6.8
1254:	eMol36016024	-6.9	1305	eMol26312476	-6.9	1361	CHEMBL1473864	-6.8
1255:	eMol4729129	-6.9	1306	eMol26336500	-6.9	1362	CHEMBL3805000	-6.8
1256:	eMol588436	-6.9	1307	eMol27202204	-6.9	1363	CHEMBL3805183	-6.8
1257:	eMol6152648	-6.9	1308	eMol27202490	-6.9	1364	eMol16352261	-6.8
1258:	CHEMBL1423559	-6.9	1314	eMol936008	-6.9	1365	eMol1753924	-6.8
1259:	CHEMBL1551465	-6.9	1315	eMol97777935	-6.9	1366	eMol19076612	-6.8
1260:	CHEMBL3806000	-6.9	1316	CHEMBL1365625	-6.9	1367	eMol206843434	-6.8
1261:	CHEMBL3818963	-6.9	1317	CHEMBL1563292	-6.9	1368	eMol206907719	-6.8
1262:	CHEMBL3819529	-6.9	1318	CHEMBL3805374	-6.9	1369	eMol2390664	-6.8
1263:	eMol16352167	-6.9	1319	CHEMBL3819159	-6.9	1370	eMol25881326	-6.8
1264:	eMol19031727	-6.9	1320	CHEMBL46934	-6.9	1371	eMol26196310	-6.8
1265:	eMol20368839	-6.9	1321	eMol16352175	-6.9	1372	eMol26313588	-6.8
1266:	eMol2087020	-6.9	1322	eMol206843438	-6.9	1373	eMol26353495	-6.8

Table S1. *Continued.*

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
1374:	eMol26773948	-6.8	1425:	eMol25915192	-6.8	1476:	eMol27186978	-6.8
1375:	eMol27187362	-6.8	1426:	eMol26132228	-6.8	1477:	eMol27202214	-6.8
1376:	eMol27202216	-6.8	1427:	eMol26275086	-6.8	1478:	eMol27202316	-6.8
1377:	eMol27202470	-6.8	1428:	eMol26312734	-6.8	1479:	eMol27202498	-6.8
1378:	eMol300151404	-6.8	1429:	eMol26313903	-6.8	1480:	eMol27202516	-6.8
1379:	eMol32246513	-6.8	1430:	eMol27202302	-6.8	1481:	eMol27203792	-6.8
1380:	eMol36015640	-6.8	1431:	eMol27202420	-6.8	1482:	eMol28321868	-6.8
1381:	eMol36016150	-6.8	1432:	eMol27202512	-6.8	1483:	eMol29955345	-6.8
1382:	eMol43745867	-6.8	1433:	eMol27202522	-6.8	1484:	eMol3416565	-6.8
1383:	eMol45585830	-6.8	1434:	eMol27202796	-6.8	1485:	eMol45560665	-6.8
1384:	eMol45948876	-6.8	1435:	eMol27202810	-6.8	1486:	eMol4559848	-6.8
1385:	eMol48957687	-6.8	1436:	eMol276221097	-6.8	1487:	eMol5444783	-6.8
1386:	CHEMBL1574680	-6.8	1437:	eMol303143674	-6.8	1488:	eMol579900	-6.8
1387:	CHEMBL2263322	-6.8	1438:	eMol3052109	-6.8	1489:	eMol681904	-6.8
1388:	CHEMBL2297666	-6.8	1439:	eMol4472622	-6.8	1490:	eMol99063354	-6.8
1389:	CHEMBL3805091	-6.8	1440:	eMol4701187	-6.8	1491:	CHEMBL1983712	-6.8
1390:	CHEMBL3805234	-6.8	1441:	eMol565950	-6.8	1492:	eMol16351695	-6.8
1391:	CHEMBL3806297	-6.8	1442:	CHEMBL295884	-6.8	1493:	eMol1755604	-6.8
1392:	eMol16351581	-6.8	1443:	CHEMBL3819359	-6.8	1494:	eMol206843432	-6.8
1393:	eMol16351857	-6.8	1444:	eMol18809799	-6.8	1495:	eMol206907070	-6.8
1394:	eMol20379714	-6.8	1445:	eMol19076600	-6.8	1496:	eMol24537526	-6.8
1395:	eMol25902666	-6.8	1446:	eMol207161823	-6.8	1497:	eMol2464575	-6.8
1396:	eMol26262986	-6.8	1447:	eMol24518650	-6.8	1498:	eMol25775761	-6.8
1397:	eMol26299003	-6.8	1448:	eMol24529894	-6.8	1499:	eMol25810093	-6.8
1398:	eMol26311192	-6.8	1449:	eMol24530962	-6.8	1500:	eMol25813423	-6.8
1399:	eMol26344402	-6.8	1450:	eMol25828609	-6.8	1501:	eMol26300679	-6.8
1400:	eMol27045529	-6.8	1451:	eMol25881336	-6.8	1502:	eMol27045531	-6.8
1401:	eMol27202284	-6.8	1452:	eMol26270390	-6.8	1503:	eMol27202354	-6.8
1402:	eMol27202390	-6.8	1453:	eMol27187286	-6.8	1504:	eMol27202508	-6.8
1403:	eMol27202472	-6.8	1454:	eMol27187438	-6.8	1505:	eMol27202526	-6.8
1404:	eMol27202488	-6.8	1455:	eMol27202298	-6.8	1506:	eMol27202774	-6.8
1405:	eMol27202518	-6.8	1456:	eMol27202344	-6.8	1507:	eMol43704541	-6.8
1406:	eMol43789923	-6.8	1457:	eMol27203752	-6.8	1508:	eMol4698777	-6.8
1407:	eMol4740690	-6.8	1458:	eMol300132718	-6.8	1509:	eMol5445037	-6.8
1408:	eMol5444735	-6.8	1459:	eMol43474659	-6.8	1510:	eMol579240	-6.8
1409:	eMol588270	-6.8	1460:	CHEMBL1472653	-6.8	1511:	CHEMBL1317703	-6.8
1410:	CHEMBL1214866	-6.8	1461:	CHEMBL1474371	-6.8	1512:	CHEMBL1376406	-6.8
1411:	CHEMBL1510504	-6.8	1462:	CHEMBL1902190	-6.8	1513:	CHEMBL1501960	-6.8
1412:	CHEMBL1716475	-6.8	1463:	CHEMBL3417627	-6.8	1514:	CHEMBL1502049	-6.8
1413:	CHEMBL43701	-6.8	1464:	eMol13526748	-6.8	1515:	eMol12904258	-6.8
1414:	CHEMBL594345	-6.8	1465:	eMol17186560	-6.8	1516:	eMol1745976	-6.8
1415:	eMol1120278	-6.8	1466:	eMol18551298	-6.8	1517:	eMol20347819	-6.8
1416:	eMol11749194	-6.8	1467:	eMol19076670	-6.8	1518:	eMol20348534	-6.8
1417:	eMol11764832	-6.8	1468:	eMol206977589	-6.8	1519:	eMol20382776	-6.8
1418:	eMol20333666	-6.8	1469:	eMol206985300	-6.8	1520:	eMol206904385	-6.8
1419:	eMol20354854	-6.8	1470:	eMol2236870	-6.8	1521:	eMol206906244	-6.8
1420:	eMol206910858	-6.8	1471:	eMol23158354	-6.8	1522:	eMol24526415	-6.8
1421:	eMol23247689	-6.8	1472:	eMol24100006	-6.8	1523:	eMol24545861	-6.8
1422:	eMol24519266	-6.8	1473:	eMol24518499	-6.8	1524:	eMol25875519	-6.8
1423:	eMol24540588	-6.8	1474:	eMol26264896	-6.8	1525:	eMol26244563	-6.8
1424:	eMol24641150	-6.8	1475:	eMol27115464	-6.8	1526:	eMol26259033	-6.8

Table S1. Continued.

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1528:	eMol26338914	-6.8	1579:	CHEMBL4060648	-6.8	1630:	eMol4535449	-6.7
1529:	eMol27490297	-6.8	1580:	eMol16407928	-6.8	1631:	eMol49205494	-6.7
1530:	eMol36015298	-6.8	1581:	eMol18536845	-6.8	1632:	eMol5509851	-6.7
1531:	eMol43731438	-6.8	1582:	eMol19764608	-6.8	1633:	CHEMBL1357400	-6.7
1532:	eMol5445003	-6.8	1583:	eMol232769854	-6.8	1634:	CHEMBL1414779	-6.7
1533:	eMol561553	-6.8	1584:	eMol23983178	-6.8	1635:	CHEMBL3806144	-6.7
1534:	eMol561867	-6.8	1585:	eMol24432101	-6.8	1636:	eMol1035523	-6.7
1535:	eMol7261106	-6.8	1586:	eMol25153702	-6.8	1637:	eMol16379399	-6.7
1536:	eMol7274676	-6.8	1587:	eMol25816253	-6.8	1638:	eMol16390191	-6.7
1537:	eMol936252	-6.8	1588:	eMol25819229	-6.8	1639:	eMol16856	-6.7
1538:	CHEMBL1399555	-6.8	1589:	eMol27045413	-6.8	1640:	eMol18532109	-6.7
1539:	eMol16379069	-6.8	1590:	eMol27045585	-6.8	1641:	eMol19076832	-6.7
1540:	eMol16379735	-6.8	1591:	eMol27202196	-6.8	1642:	eMol20354735	-6.7
1541:	eMol1676253	-6.8	1592:	eMol27202326	-6.8	1643:	eMol206843416	-6.7
1542:	eMol1751618	-6.8	1593:	eMol27202514	-6.8	1644:	eMol206847221	-6.7
1543:	eMol20382225	-6.8	1594:	eMol27202740	-6.8	1645:	eMol206992993	-6.7
1544:	eMol206977831	-6.8	1595:	eMol31340346	-6.8	1646:	eMol20732599	-6.7
1545:	eMol24427974	-6.8	1596:	eMol4418979	-6.8	1647:	eMol25782835	-6.7
1546:	eMol24530395	-6.8	1597:	eMol46526926	-6.8	1648:	eMol25784119	-6.7
1547:	eMol2480990	-6.8	1598:	CHEMBL1214798	-6.7	1649:	eMol25817109	-6.7
1548:	eMol25813405	-6.8	1599:	CHEMBL416260	-6.7	1650:	eMol26052954	-6.7
1549:	eMol25903601	-6.8	1600:	eMol20376367	-6.7	1651:	eMol26141632	-6.7
1550:	eMol26295370	-6.8	1601:	eMol20381008	-6.7	1652:	eMol26267262	-6.7
1551:	eMol26308952	-6.8	1602:	eMol24453856	-6.7	1653:	eMol26298841	-6.7
1552:	eMol27045571	-6.8	1603:	eMol25810169	-6.7	1654:	eMol27202908	-6.7
1553:	eMol27187238	-6.8	1604:	eMol25902941	-6.7	1655:	eMol300135787	-6.7
1554:	eMol27187318	-6.8	1605:	eMol25937625	-6.7	1656:	eMol3460427	-6.7
1555:	eMol27187472	-6.8	1606:	eMol27202266	-6.7	1657:	eMol36015846	-6.7
1556:	eMol27202764	-6.8	1607:	eMol27202510	-6.7	1658:	eMol36016030	-6.7
1557:	eMol27490289	-6.8	1608:	eMol27202780	-6.7	1659:	eMol3651760	-6.7
1558:	eMol30104226	-6.8	1609:	eMol300397022	-6.7	1660:	eMol42849976	-6.7
1559:	eMol33332787	-6.8	1610:	eMol317731902	-6.7	1661:	eMol4709725	-6.7
1560:	eMol36015124	-6.8	1611:	eMol36015372	-6.7	1662:	CHEMBL1413460	-6.7
1561:	eMol36015848	-6.8	1612:	eMol36015814	-6.7	1663:	CHEMBL1440095	-6.7
1562:	eMol36734201	-6.8	1613:	eMol42925165	-6.7	1664:	CHEMBL1595228	-6.7
1563:	eMol46210808	-6.8	1614:	eMol4717060	-6.7	1665:	CHEMBL4068913	-6.7
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1565:	eMol935668	-6.8	1616:	eMol560055	-6.7	1667:	eMol16352169	-6.7
1566:	CHEMBL1492662	-6.8	1617:	eMol561535	-6.7	1668:	eMol1681902	-6.7
1567:	CHEMBL1516504	-6.8	1618:	eMol562333	-6.7	1669:	eMol18588437	-6.7
1568:	eMol1125990	-6.8	1619:	CHEMBL1215798	-6.7	1670:	eMol18954506	-6.7
1569:	eMol1681774	-6.8	1620:	CHEMBL1237285	-6.7	1671:	eMol193764290	-6.7
1570:	eMol206964622	-6.8	1621:	CHEMBL1601068	-6.7	1672:	eMol20358311	-6.7
1571:	eMol206980093	-6.8	1622:	CHEMBL3818685	-6.7	1673:	eMol208112836	-6.7
1572:	eMol24541186	-6.8	1623:	eMol1749678	-6.7	1674:	eMol23154795	-6.7
1573:	eMol25813421	-6.8	1624:	eMol19076368	-6.7	1675:	eMol25784517	-6.7
1574:	eMol25959987	-6.8	1625:	eMol20358115	-6.7	1676:	eMol25963297	-6.7
1575:	eMol27202278	-6.8	1626:	eMol25810017	-6.7	1677:	eMol26314205	-6.7
1576:	eMol27202356	-6.8	1627:	eMol27187280	-6.7	1678:	eMol27485970	-6.7
1577:	eMol3581771	-6.8	1628:	eMol27202414	-6.7	1679:	eMol36015368	-6.7
1548:	eMol25813405	-6.8	1599:	CHEMBL416260	-6.7	1650:	eMol26052954	-6.7

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
1680	eMol36015832	-6.7	1731	eMol36015102	-6.7	1782	eMol300252505	-6.7
1681	eMol4730653	-6.7	1732	eMol36015520	-6.7	1783	eMol3494756	-6.7
1682	eMol5444865	-6.7	1733	eMol36016040	-6.7	1784	eMol36913016	-6.7
1683	eMol561447	-6.7	1734	eMol36734203	-6.7	1785	eMol43743366	-6.7
1684	eMol624281	-6.7	1735	eMol45932361	-6.7	1786	eMol4710992	-6.7
1685	eMol679752	-6.7	1736	eMol560185	-6.7	1787	eMol4737014	-6.7
1686	CHEMBL1214790	-6.7	1737	eMol935816	-6.7	1788	eMol53754573	-6.7
1687	CHEMBL1476683	-6.7	1738	CHEMBL1214797	-6.7	1789	eMol54826500	-6.7
1688	CHEMBL1866012	-6.7	1739	CHEMBL1427466	-6.7	1790	eMol565990	-6.7
1689	CHEMBL1872793	-6.7	1740	CHEMBL2134755	-6.7	1791	CHEMBL1593176	-6.7
1690	CHEMBL3819643	-6.7	1741	CHEMBL301308	-6.7	1792	CHEMBL1870195	-6.7
1691	CHEMBL4085469	-6.7	1742	eMol1415360	-6.7	1793	CHEMBL37653	-6.7
1692	eMol1444423	-6.7	1743	eMol16352263	-6.7	1794	CHEMBL38176	-6.7
1693	eMol16351865	-6.7	1744	eMol16390485	-6.7	1795	eMol1119962	-6.7
1694	eMol16351871	-6.7	1745	eMol16805743	-6.7	1796	eMol11970394	-6.7
1695	eMol16370299	-6.7	1746	eMol18551296	-6.7	1797	eMol1266025	-6.7
1696	eMol18550690	-6.7	1747	eMol18879479	-6.7	1798	eMol16351573	-6.7
1697	eMol18780688	-6.7	1748	eMol20337454	-6.7	1799	eMol16758472	-6.7
1698	eMol206924376	-6.7	1749	eMol20382098	-6.7	1800	eMol206910448	-6.7
1699	eMol2180510	-6.7	1750	eMol23238997	-6.7	1801	eMol25813407	-6.7
1700	eMol24555667	-6.7	1751	eMol25901997	-6.7	1802	eMol25896465	-6.7
1701	eMol25815831	-6.7	1752	eMol26281046	-6.7	1803	eMol25942258	-6.7
1702	eMol25902460	-6.7	1753	eMol26337174	-6.7	1804	eMol26141624	-6.7
1703	eMol26141660	-6.7	1754	eMol27187474	-6.7	1805	eMol27187228	-6.7
1704	eMol26293000	-6.7	1755	eMol27202202	-6.7	1806	eMol27202330	-6.7
1705	eMol26310199	-6.7	1756	eMol27202456	-6.7	1807	eMol27202746	-6.7
1706	eMol26319897	-6.7	1757	eMol27202492	-6.7	1808	eMol27202962	-6.7
1707	eMol26344183	-6.7	1758	eMol30341805	-6.7	1809	eMol300229303	-6.7
1708	eMol27115470	-6.7	1759	eMol33346437	-6.7	1810	eMol3004720	-6.7
1709	eMol27202440	-6.7	1760	eMol36734043	-6.7	1811	eMol3381941	-6.7
1710	eMol27202800	-6.7	1761	eMol579396	-6.7	1812	eMol3457653	-6.7
1711	eMol27202922	-6.7	1762	eMol7294872	-6.7	1813	eMol43751233	-6.7
1712	eMol300145258	-6.7	1763	eMol98023415	-6.7	1814	eMol4696216	-6.7
1713	eMol32246803	-6.7	1764	CHEMBL1214791	-6.7	1815	eMol560307	-6.7
1714	eMol36016026	-6.7	1765	CHEMBL3805351	-6.7	1816	eMol7635460	-6.7
1715	eMol7271648	-6.7	1766	CHEMBL4075913	-6.7	1817	CHEMBL3805445	-6.7
1716	eMol956529	-6.7	1767	eMol16352273	-6.7	1818	eMol14855102	-6.7
1717	CHEMBL1449683	-6.7	1768	eMol19076340	-6.7	1819	eMol15245309	-6.7
1718	CHEMBL301330	-6.7	1769	eMol20364228	-6.7	1820	eMol18808193	-6.7
1719	CHEMBL3819609	-6.7	1770	eMol20374086	-6.7	1821	eMol206977399	-6.7
1720	eMol1458294	-6.7	1771	eMol20382812	-6.7	1822	eMol207368461	-6.7
1721	eMol19076334	-6.7	1772	eMol23155886	-6.7	1823	eMol2213417	-6.7
1722	eMol206843414	-6.7	1773	eMol23244991	-6.7	1824	eMol24531994	-6.7
1723	eMol26141650	-6.7	1774	eMol24427994	-6.7	1825	eMol25910177	-6.7
1724	eMol26326538	-6.7	1775	eMol25881344	-6.7	1826	eMol26264081	-6.7
1725	eMol27187404	-6.7	1776	eMol26141340	-6.7	1827	eMol26284998	-6.7
1726	eMol27202292	-6.7	1777	eMol26141622	-6.7	1828	eMol26309549	-6.7
1727	eMol27202364	-6.7	1778	eMol26248577	-6.7	1829	eMol26312290	-6.7
1728	eMol27202408	-6.7	1779	eMol27187214	-6.7	1830	eMol26325538	-6.7
1729	eMol32392848	-6.7	1780	eMol27202308	-6.7	1831	eMol26779126	-6.7
1730	eMol3401751	-6.7	1781	eMol276247938	-6.7	1832	eMol27187346	-6.7
1701	eMol25815831	-6.7	1752	eMol26281046	-6.7	1803	eMol25942258	-6.7

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
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1834:	eMol43754815	-6.7	1885	eMol7261256	-6.6	1936	eMol96989666	-6.6
1835:	eMol4557017	-6.7	1886	CHEMBL1581170	-6.6	1937	CHEMBL1547176	-6.6
1836:	eMol46541996	-6.7	1887	CHEMBL1984743	-6.6	1938	CHEMBL1889180	-6.6
1837:	eMol562393	-6.7	1888	CHEMBL3818386	-6.6	1939	CHEMBL2355688	-6.6
1838:	eMol6157526	-6.7	1889	eMol11879378	-6.6	1940	CHEMBL3805622	-6.6
1839:	eMol7268112	-6.7	1890	eMol16352159	-6.6	1941	CHEMBL3819491	-6.6
1840:	eMol956427	-6.7	1891	eMol16352189	-6.6	1942	eMol11663659	-6.6
1841:	CHEMBL1516226	-6.6	1892	eMol19031808	-6.6	1943	eMol20360019	-6.6
1842:	CHEMBL1601841	-6.6	1893	eMol19076342	-6.6	1944	eMol20360818	-6.6
1843:	CHEMBL1903920	-6.6	1894	eMol19764926	-6.6	1945	eMol206962178	-6.6
1844:	CHEMBL3818857	-6.6	1895	eMol20382919	-6.6	1946	eMol206978287	-6.6
1845:	eMol16351859	-6.6	1896	eMol24107121	-6.6	1947	eMol206987243	-6.6
1846:	eMol16351867	-6.6	1897	eMol24547204	-6.6	1948	eMol2409707	-6.6
1847:	eMol2423428	-6.6	1898	eMol2488724	-6.6	1949	eMol25961959	-6.6
1848:	eMol24545576	-6.6	1899	eMol25963261	-6.6	1950	eMol27202412	-6.6
1849:	eMol25775755	-6.6	1900	eMol27202314	-6.6	1951	eMol27202484	-6.6
1850:	eMol25810167	-6.6	1901	eMol27202500	-6.6	1952	eMol27202814	-6.6
1851:	eMol25813411	-6.6	1902	eMol27202528	-6.6	1953	eMol27202844	-6.6
1852:	eMol25967144	-6.6	1903	eMol27202892	-6.6	1954	eMol29565470	-6.6
1853:	eMol27045525	-6.6	1904	eMol3443403	-6.6	1955	eMol5509853	-6.6
1854:	eMol27187442	-6.6	1905	eMol36898008	-6.6	1956	eMol5538254	-6.6
1855:	eMol27202206	-6.6	1906	eMol565896	-6.6	1957	eMol560071	-6.6
1856:	eMol27202340	-6.6	1907	eMol7701728	-6.6	1958	eMol581330	-6.6
1857:	eMol27202770	-6.6	1908	CHEMBL1214867	-6.6	1959	eMol7260196	-6.6
1858:	eMol30104210	-6.6	1909	CHEMBL1418314	-6.6	1960	eMol936014	-6.6
1859:	eMol43771200	-6.6	1910	CHEMBL1516180	-6.6	1961	eMol98980408	-6.6
1860:	eMol45951607	-6.6	1911	eMol11687945	-6.6	1962	eMol99520559	-6.6
1861:	eMol50575071	-6.6	1912	eMol16351575	-6.6	1963	CHEMBL1490844	-6.6
1862:	eMol565972	-6.6	1913	eMol16407954	-6.6	1964	CHEMBL1880647	-6.6
1863:	eMol579916	-6.6	1914	eMol206843424	-6.6	1965	eMol16390181	-6.6
1864:	CHEMBL1402158	-6.6	1915	eMol206978315	-6.6	1966	eMol17193486	-6.6
1865:	CHEMBL1903268	-6.6	1916	eMol206993297	-6.6	1967	eMol18900038	-6.6
1866:	CHEMBL297579	-6.6	1917	eMol24520907	-6.6	1968	eMol206904367	-6.6
1867:	eMol13734651	-6.6	1918	eMol24526901	-6.6	1969	eMol25782831	-6.6
1868:	eMol16379439	-6.6	1919	eMol25797961	-6.6	1970	eMol25829419	-6.6
1869:	eMol20381366	-6.6	1920	eMol25908587	-6.6	1971	eMol25962071	-6.6
1870:	eMol20383035	-6.6	1921	eMol27202386	-6.6	1972	eMol26260063	-6.6
1871:	eMol206843410	-6.6	1922	eMol27202566	-6.6	1973	eMol26340085	-6.6
1872:	eMol206970436	-6.6	1923	eMol27202788	-6.6	1974	eMol26594563	-6.6
1873:	eMol24427888	-6.6	1924	eMol27202798	-6.6	1975	eMol27045277	-6.6
1874:	eMol25771176	-6.6	1925	eMol27490345	-6.6	1976	eMol27187316	-6.6
1875:	eMol25926749	-6.6	1926	eMol3315989	-6.6	1977	eMol27202966	-6.6
1876:	eMol26243624	-6.6	1927	eMol36015342	-6.6	1978	eMol3455505	-6.6
1877:	eMol26288251	-6.6	1928	eMol43744872	-6.6	1979	eMol43732496	-6.6
1878:	eMol27202352	-6.6	1929	eMol45705372	-6.6	1980	CHEMBL1473628	-6.6
1879:	eMol27202802	-6.6	1930	eMol46210816	-6.6	1981	CHEMBL3818892	-6.6
1880:	eMol2992494	-6.6	1931	eMol46370141	-6.6	1982	CHEMBL3914501	-6.6
1881:	eMol3252720	-6.6	1932	eMol4703775	-6.6	1983	eMol16351607	-6.6
1882:	eMol3670123	-6.6	1933	eMol4718173	-6.6	1984	eMol16352163	-6.6
1883:	eMol5444963	-6.6	1934	eMol6263469	-6.6	1985	eMol16786052	-6.6
1854:	eMol27187442	-6.6	1905	eMol36898008	-6.6	1956	eMol5538254	-6.6

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
1986:	eMol19076700	-6.6	2016	eMol27202426	-6.6	2067	eMol1237695	-6.5
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1988:	eMol2386034	-6.6	2018	eMol30104206	-6.6	2069	eMol19076362	-6.5
1989:	eMol24519974	-6.6	2019	eMol36016676	-6.6	2070	eMol20380980	-6.5
1990:	eMol26339810	-6.6	2020	eMol45645578	-6.6	2071	eMol23982014	-6.5
1991:	eMol27202210	-6.6	2021	eMol4567983	-6.6	2072	eMol2513700	-6.5
1992:	eMol27202978	-6.6	2022	eMol46210768	-6.6	2073	eMol2519315	-6.5
1993:	eMol2889094	-6.6	2023	eMol4727438	-6.6	2074	eMol25813413	-6.5
1994:	eMol289941482	-6.6	2024	eMol6467547	-6.6	2075	eMol25881262	-6.5
1995:	eMol2993559	-6.6	2025	eMol7259996	-6.6	2076	eMol26350874	-6.5
1996:	eMol3459687	-6.6	2026	eMol7266104	-6.6	2077	eMol27045523	-6.5
1997:	eMol36015734	-6.6	2027	CHEMBL1475827	-6.6	2078	eMol27187266	-6.5
1998:	eMol36016022	-6.6	2028	CHEMBL249301	-6.6	2079	eMol27202200	-6.5
1999:	eMol44057501	-6.6	2029	CHEMBL297442	-6.6	2080	eMol27202530	-6.5
2000:	eMol561659	-6.6	2030	eMol16352161	-6.6	2081	eMol36015714	-6.5
2001:	CHEMBL1513163	-6.6	2031	eMol1834904	-6.6	2082	eMol36015812	-6.5
2002:	CHEMBL1610757	-6.6	2032	eMol18551350	-6.6	2083	eMol36016036	-6.5
2003:	CHEMBL3805404	-6.6	2033	eMol206904341	-6.6	2084	eMol36016052	-6.5
2004:	eMol1032463	-6.6	2034	eMol206906698	-6.6	2085	eMol36733911	-6.5
2005:	eMol16351585	-6.6	2035	eMol206992362	-6.6	2086	eMol36898044	-6.5
2006:	eMol16351605	-6.6	2036	eMol25825123	-6.6	2087	eMol45803170	-6.5
2007:	eMol206961858	-6.6	2037	eMol25966292	-6.6	2088	eMol561977	-6.5
2008:	eMol206985304	-6.6	2038	eMol26263883	-6.6	2089	eMol566052	-6.5
2009:	eMol207355363	-6.6	2039	eMol26337698	-6.6	2090	eMol956197	-6.5
2010:	eMol25784123	-6.6	2040	eMol317395728	-6.6	2091	CHEMBL111006	-6.5
2011:	eMol25813409	-6.6	2041	eMol33346431	-6.6	2092	CHEMBL118001	-6.5
2012:	eMol25813427	-6.6	2042	eMol44218497	-6.6	2093	CHEMBL1895705	-6.5
2013:	eMol26195582	-6.6	2043	eMol4727713	-6.6	2094	CHEMBL3935405	-6.5
2014:	eMol27187274	-6.6	2044	eMol4730084	-6.6	2095	CHEMBL561127	-6.5
1994:	eMol289941482	-6.6	2045	eMol587920	-6.6	2096	eMol16352191	-6.5
1995:	eMol2993559	-6.6	2046	eMol956475	-6.6	2097	eMol16759756	-6.5
1996:	eMol3459687	-6.6	2047	CHEMBL3818297	-6.6	2098	eMol19031731	-6.5
1997:	eMol36015734	-6.6	2048	eMol19351378	-6.6	2099	eMol206910196	-6.5
1998:	eMol36016022	-6.6	2049	eMol206962232	-6.6	2100	eMol206969636	-6.5
1999:	eMol44057501	-6.6	2050	eMol27038267	-6.6	2101	eMol207116159	-6.5
2000:	eMol561659	-6.6	2051	eMol27045559	-6.6	2102	eMol23245699	-6.5
2001:	CHEMBL1513163	-6.6	2052	eMol27202286	-6.6	2103	eMol25896431	-6.5
2002:	CHEMBL1610757	-6.6	2053	eMol27202462	-6.6	2104	eMol26195584	-6.5
2003:	CHEMBL3805404	-6.6	2054	eMol29642547	-6.6	2105	eMol27187386	-6.5
2004:	eMol1032463	-6.6	2055	eMol3172250	-6.6	2106	eMol27187470	-6.5
2005:	eMol16351585	-6.6	2056	eMol36010133	-6.6	2107	eMol27509217	-6.5
2006:	eMol16351605	-6.6	2057	eMol36016622	-6.6	2108	eMol2881132	-6.5
2007:	eMol206961858	-6.6	2058	eMol43772416	-6.6	2109	eMol300020871	-6.5
2008:	eMol206985304	-6.6	2059	eMol46210820	-6.6	2110	eMol43743380	-6.5
2009:	eMol207355363	-6.6	2060	eMol561519	-6.6	2111	eMol43995461	-6.5
2010:	eMol25784123	-6.6	2061	CHEMBL1475371	-6.5	2112	eMol4706823	-6.5
2011:	eMol25813409	-6.6	2062	CHEMBL245490	-6.5	2113	eMol4716299	-6.5
2012:	eMol25813427	-6.6	2063	CHEMBL3417654	-6.5	2114	eMol4728654	-6.5
2013:	eMol26195582	-6.6	2064	CHEMBL53995	-6.5	2115	eMol560189	-6.5
2014:	eMol27187274	-6.6	2065	CHEMBL565080	-6.5	2116	eMol581246	-6.5
2015:	eMol27202328	-6.6	2066	eMol1165995	-6.5	2117	eMol639662	-6.5
2007:	eMol206961858	-6.6	2037	eMol25966292	-6.6	2088	eMol561977	-6.5

Table S1. *Continued.*

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
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2120:	CHEMBL314385	-6.5	2171:	CHEMBL4076110	-6.5	2222:	CHEMBL1310211	-6.5
2121:	eMol11758466	-6.5	2172:	eMol1120544	-6.5	2223:	CHEMBL1434827	-6.5
2122:	eMol16351577	-6.5	2173:	eMol1386911	-6.5	2224:	CHEMBL1592831	-6.5
2123:	eMol177539683	-6.5	2174:	eMol16352171	-6.5	2225:	CHEMBL298576	-6.5
2124:	eMol206843485	-6.5	2175:	eMol24520475	-6.5	2226:	CHEMBL3817977	-6.5
2125:	eMol22370932	-6.5	2176:	eMol25813401	-6.5	2227:	eMol11371397	-6.5
2126:	eMol23236781	-6.5	2177:	eMol25813415	-6.5	2228:	eMol13502306	-6.5
2127:	eMol24152474	-6.5	2178:	eMol25813435	-6.5	2229:	eMol16352257	-6.5
2128:	eMol24524791	-6.5	2179:	eMol25881328	-6.5	2230:	eMol18823378	-6.5
2129:	eMol25813431	-6.5	2180:	eMol26286432	-6.5	2231:	eMol20375967	-6.5
2130:	eMol25881340	-6.5	2181:	eMol27187342	-6.5	2232:	eMol206906624	-6.5
2131:	eMol25962331	-6.5	2182:	eMol27341385	-6.5	2233:	eMol206977577	-6.5
2132:	eMol26184916	-6.5	2183:	eMol30185530	-6.5	2234:	eMol206994514	-6.5
2133:	eMol27202430	-6.5	2184:	eMol3063037	-6.5	2235:	eMol25807807	-6.5
2134:	eMol3204435	-6.5	2185:	eMol3501366	-6.5	2236:	eMol25810159	-6.5
2135:	eMol36733941	-6.5	2186:	eMol36015620	-6.5	2237:	eMol27187032	-6.5
2136:	eMol36734171	-6.5	2187:	eMol36733903	-6.5	2238:	eMol3206345	-6.5
2137:	eMol5444999	-6.5	2188:	eMol44519141	-6.5	2239:	eMol36013033	-6.5
2138:	CHEMBL1415081	-6.5	2189:	eMol4726940	-6.5	2240:	eMol36015822	-6.5
2139:	CHEMBL1514215	-6.5	2190:	eMol5538220	-6.5	2241:	eMol42762132	-6.5
2140:	CHEMBL1903537	-6.5	2191:	eMol5538898	-6.5	2242:	eMol5444995	-6.5
2141:	CHEMBL563538	-6.5	2192:	eMol6869460	-6.5	2243:	CHEMBL301313	-6.5
2142:	eMol11903726	-6.5	2193:	eMol98690075	-6.5	2244:	eMol1035485	-6.5
2143:	eMol16373087	-6.5	2194:	CHEMBL113883	-6.5	2245:	eMol18879511	-6.5
2144:	eMol16390221	-6.5	2195:	CHEMBL1443220	-6.5	2246:	eMol206843430	-6.5
2145:	eMol16407934	-6.5	2196:	CHEMBL1497333	-6.5	2247:	eMol206924378	-6.5
2146:	eMol1679112	-6.5	2197:	CHEMBL260456	-6.5	2248:	eMol206969606	-6.5
2147:	eMol19382530	-6.5	2198:	CHEMBL51165	-6.5	2249:	eMol22375727	-6.5
2148:	eMol2001733	-6.5	2199:	CHEMBL53479	-6.5	2250:	eMol26141688	-6.5
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2150:	eMol206978824	-6.5	2201:	eMol1673994	-6.5	2252:	eMol27187466	-6.5
2151:	eMol23982214	-6.5	2202:	eMol20382826	-6.5	2253:	eMol300261713	-6.5
2152:	eMol24427912	-6.5	2203:	eMol206843412	-6.5	2254:	eMol3327781	-6.5
2153:	eMol25844601	-6.5	2204:	eMol25810097	-6.5	2255:	eMol3485283	-6.5
2154:	eMol26242028	-6.5	2205:	eMol25813425	-6.5	2256:	eMol3517784	-6.5
2155:	eMol26248549	-6.5	2206:	eMol25817107	-6.5	2257:	eMol44603525	-6.5
2156:	eMol27045467	-6.5	2207:	eMol25957029	-6.5	2258:	eMol45787891	-6.5
2157:	eMol27187234	-6.5	2208:	eMol26254010	-6.5	2259:	eMol4727426	-6.5
2158:	eMol27202310	-6.5	2209:	eMol26291793	-6.5	2260:	CHEMBL185809	-6.5
2159:	eMol3087147	-6.5	2210:	eMol27045479	-6.5	2261:	CHEMBL3805880	-6.5
2160:	eMol36636763	-6.5	2211:	eMol27045553	-6.5	2262:	eMol11070727	-6.5
2161:	eMol4538051	-6.5	2212:	eMol27045583	-6.5	2263:	eMol1149891	-6.5
2162:	eMol45930049	-6.5	2213:	eMol27202416	-6.5	2264:	eMol11816884	-6.5
2163:	eMol5444633	-6.5	2214:	eMol2991923	-6.5	2265:	eMol16351681	-6.5
2164:	eMol566608	-6.5	2215:	eMol36734029	-6.5	2266:	eMol18931802	-6.5
2165:	eMol581404	-6.5	2216:	eMol42927497	-6.5	2267:	eMol206963325	-6.5
2166:	eMol6514347	-6.5	2217:	eMol45904698	-6.5	2268:	eMol26349730	-6.5
2167:	eMol7291156	-6.5	2218:	eMol4718135	-6.5	2269:	eMol27187320	-6.5
2168:	CHEMBL1323375	-6.5	2219:	eMol4727659	-6.5	2270:	eMol27202424	-6.5
2139:	CHEMBL1514215	-6.5	2190:	eMol5538220	-6.5	2241:	eMol42762132	-6.5

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
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2272:	eMol27202486	-6.5	2323	eMol1679964	-6.4	2374	eMol32661616	-6.4
2273:	eMol27202536	-6.5	2324	eMol206962711	-6.4	2375	eMol43995617	-6.4
2274:	eMol29968406	-6.5	2325	eMol24306794	-6.4	2376	eMol46210770	-6.4
2275:	eMol300149359	-6.5	2326	eMol25810105	-6.4	2377	eMol7266174	-6.4
2276:	eMol33338072	-6.5	2327	eMol26299887	-6.4	2378	eMol9815169	-6.4
2277:	eMol35387961	-6.5	2328	eMol27187282	-6.4	2379	CHEMBL3417641	-6.4
2278:	eMol36010145	-6.5	2329	eMol27202230	-6.4	2380	eMol16374771	-6.4
2279:	eMol36015328	-6.5	2330	eMol27202786	-6.4	2381	eMol193274586	-6.4
2280:	eMol36015854	-6.5	2331	eMol316926407	-6.4	2382	eMol20377949	-6.4
2281:	eMol36016050	-6.5	2332	eMol32246985	-6.4	2383	eMol24525072	-6.4
2282:	eMol36898026	-6.5	2333	eMol3407217	-6.4	2384	eMol26291212	-6.4
2283:	eMol43746855	-6.5	2334	eMol3501354	-6.4	2385	eMol26343081	-6.4
2284:	eMol566444	-6.5	2335	eMol36898002	-6.4	2386	eMol27202212	-6.4
2285:	CHEMBL189170	-6.5	2336	eMol4467282	-6.4	2387	eMol27202404	-6.4
2286:	CHEMBL3804860	-6.5	2337	eMol561361	-6.4	2388	eMol27202418	-6.4
2287:	CHEMBL3818548	-6.5	2338	eMol679600	-6.4	2389	eMol27202468	-6.4
2288:	eMol16373089	-6.5	2339	CHEMBL1214865	-6.4	2390	eMol27349409	-6.4
2289:	eMol16385710	-6.5	2340	CHEMBL3806281	-6.4	2391	eMol29623495	-6.4
2290:	eMol1679132	-6.5	2341	eMol1131454	-6.4	2392	eMol3245568	-6.4
2291:	eMol18550756	-6.5	2342	eMol16379821	-6.4	2393	eMol34103610	-6.4
2292:	eMol2166967	-6.5	2343	eMol16385692	-6.4	2394	eMol36015842	-6.4
2293:	eMol25810173	-6.5	2344	eMol1682570	-6.4	2395	eMol3663282	-6.4
2294:	eMol27202194	-6.5	2345	eMol23180310	-6.4	2396	eMol5444549	-6.4
2295:	eMol27202370	-6.5	2346	eMol23254399	-6.4	2397	CHEMBL1321779	-6.4
2296:	eMol27202976	-6.5	2347	eMol26131908	-6.4	2398	CHEMBL1577901	-6.4
2297:	eMol3518572	-6.5	2348	eMol27182628	-6.4	2399	CHEMBL294968	-6.4
2298:	eMol36015838	-6.5	2349	eMol3055183	-6.4	2400	CHEMBL3417643	-6.4
2299:	eMol44017453	-6.5	2350	eMol3316007	-6.4	2401	CHEMBL3818714	-6.4
2300:	eMol46210810	-6.5	2351	eMol3707946	-6.4	2402	eMol1448891	-6.4
2301:	eMol5444547	-6.5	2352	eMol5445035	-6.4	2403	eMol19248288	-6.4
2302:	eMol5779863	-6.5	2353	eMol7270136	-6.4	2404	eMol26288149	-6.4
2303:	eMol6806127	-6.5	2354	CHEMBL1396361	-6.4	2405	eMol27186996	-6.4
2304:	eMol206985650	-6.4	2355	CHEMBL1593196	-6.4	2406	eMol27202294	-6.4
2305:	eMol26141664	-6.4	2356	CHEMBL184749	-6.4	2407	eMol27202538	-6.4
2306:	eMol26236636	-6.4	2357	CHEMBL3417618	-6.4	2408	eMol27202806	-6.4
2307:	eMol27202220	-6.4	2358	CHEMBL3818360	-6.4	2409	eMol27202890	-6.4
2308:	eMol27202276	-6.4	2359	eMol11905854	-6.4	2410	eMol2871294	-6.4
2309:	eMol27490285	-6.4	2360	eMol16407926	-6.4	2411	eMol2992552	-6.4
2310:	eMol2768996	-6.4	2361	eMol16408016	-6.4	2412	eMol300250258	-6.4
2311:	eMol3376801	-6.4	2362	eMol16408020	-6.4	2413	eMol316452059	-6.4
2312:	eMol36015840	-6.4	2363	eMol17163712	-6.4	2414	eMol3443675	-6.4
2313:	eMol36015962	-6.4	2364	eMol25816257	-6.4	2415	eMol3494000	-6.4
2314:	eMol45705672	-6.4	2365	eMol25966290	-6.4	2416	eMol36015116	-6.4
2315:	eMol4759218	-6.4	2366	eMol26289584	-6.4	2417	eMol36733933	-6.4
2316:	eMol5445013	-6.4	2367	eMol27187034	-6.4	2418	eMol43731752	-6.4
2317:	CHEMBL1391688	-6.4	2368	eMol27202748	-6.4	2419	eMol43743368	-6.4
2318:	CHEMBL1553786	-6.4	2369	eMol30104222	-6.4	2420	eMol46210772	-6.4
2319:	CHEMBL3804979	-6.4	2370	eMol316975064	-6.4	2421	eMol4694025	-6.4
2320:	CHEMBL51620	-6.4	2371	eMol31780057	-6.4	2422	eMol561611	-6.4
2321:	eMol13491303	-6.4	2372	eMol3220074	-6.4	2423	CHEMBL1215651	-6.4
2292:	eMol2166967	-6.5	2343	eMol16385692	-6.4	2394	eMol36015842	-6.4

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
2424	eMol16056917	-6.4	2475	eMol16379145	-6.4	2526	eMol11671108	-6.3
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2426	eMol18536843	-6.4	2477	eMol16390077	-6.4	2528	eMol206843422	-6.3
2427	eMol24021853	-6.4	2478	eMol23254331	-6.4	2529	eMol24302059	-6.3
2428	eMol26196308	-6.4	2479	eMol26347234	-6.4	2530	eMol24534942	-6.3
2429	eMol26349111	-6.4	2480	eMol27045491	-6.4	2531	eMol26315552	-6.3
2430	eMol27202228	-6.4	2481	eMol27202428	-6.4	2532	eMol27202964	-6.3
2431	eMol27202812	-6.4	2482	eMol27202816	-6.4	2533	eMol34181785	-6.3
2432	eMol29585788	-6.4	2483	eMol29633215	-6.4	2534	eMol36010131	-6.3
2433	eMol36015522	-6.4	2484	eMol30104214	-6.4	2535	eMol36015330	-6.3
2434	eMol45585828	-6.4	2485	eMol35700126	-6.4	2536	eMol36016278	-6.3
2435	eMol4700479	-6.4	2486	eMol36015614	-6.4	2537	eMol36016614	-6.3
2436	eMol50159532	-6.4	2487	eMol43745108	-6.4	2538	eMol43747047	-6.3
2437	eMol581334	-6.4	2488	eMol44123579	-6.4	2539	eMol46346846	-6.3
2438	CHEMBL1366795	-6.4	2489	eMol45951547	-6.4	2540	eMol4702936	-6.3
2439	CHEMBL1608564	-6.4	2490	eMol5444515	-6.4	2541	eMol52129783	-6.3
2440	CHEMBL3959539	-6.4	2491	eMol5444959	-6.4	2542	eMol5538570	-6.3
2441	CHEMBL47230	-6.4	2492	eMol6523821	-6.4	2543	eMol7289730	-6.3
2442	eMol11893182	-6.4	2493	CHEMBL1345911	-6.4	2544	CHEMBL1169938	-6.3
2443	eMol19250818	-6.4	2494	CHEMBL299336	-6.4	2545	CHEMBL1394032	-6.3
2444	eMol20350994	-6.4	2495	CHEMBL50538	-6.4	2546	CHEMBL341356	-6.3
2445	eMol23246486	-6.4	2496	eMol11915751	-6.4	2547	CHEMBL49924	-6.3
2446	eMol23248155	-6.4	2497	eMol16352259	-6.4	2548	eMol100292265	-6.3
2447	eMol24473893	-6.4	2498	eMol20333676	-6.4	2549	eMol1748351	-6.3
2448	eMol25797965	-6.4	2499	eMol20351269	-6.4	2550	eMol18550708	-6.3
2449	eMol27202368	-6.4	2500	eMol206907679	-6.4	2551	eMol26141690	-6.3
2450	eMol276247966	-6.4	2501	eMol22050213	-6.4	2552	eMol26249989	-6.3
2451	eMol300994278	-6.4	2502	eMol24423650	-6.4	2553	eMol27182514	-6.3
2452	eMol32246425	-6.4	2503	eMol24539609	-6.4	2554	eMol27187000	-6.3
2453	eMol36010141	-6.4	2504	eMol26141636	-6.4	2555	eMol27187420	-6.3
2454	eMol36015364	-6.4	2505	eMol26263630	-6.4	2556	eMol27202222	-6.3
2455	eMol36015864	-6.4	2506	eMol26297652	-6.4	2557	eMol27202366	-6.3
2456	eMol36016154	-6.4	2507	eMol27187354	-6.4	2558	eMol29456700	-6.3
2457	eMol3666911	-6.4	2508	eMol27187408	-6.4	2559	eMol2997342	-6.3
2458	eMol4388249	-6.4	2509	eMol27202374	-6.4	2560	eMol3131192	-6.3
2459	eMol4515790	-6.4	2510	eMol27202448	-6.4	2561	eMol32170345	-6.3
2460	eMol5444429	-6.4	2511	eMol27490301	-6.4	2562	eMol3464492	-6.3
2461	eMol5444627	-6.4	2512	eMol32246825	-6.4	2563	eMol3523182	-6.3
2462	eMol5444961	-6.4	2513	eMol3352043	-6.4	2564	eMol36015110	-6.3
2463	eMol581222	-6.4	2514	eMol3380583	-6.4	2565	eMol36015528	-6.3
2464	eMol7259360	-6.4	2515	eMol36015340	-6.4	2566	eMol43716283	-6.3
2465	eMol7281766	-6.4	2516	eMol36379003	-6.4	2567	eMol43757857	-6.3
2466	ChEBI94303	-6.4	2517	eMol36733939	-6.4	2568	eMol679698	-6.3
2467	CHEMBL1567670	-6.4	2518	eMol42849980	-6.4	2569	eMol7272218	-6.3
2468	CHEMBL422227	-6.4	2519	eMol565722	-6.4	2570	eMol7282414	-6.3
2469	CHEMBL50824	-6.4	2520	eMol7274760	-6.4	2571	eMol7284218	-6.3
2470	eMol129040	-6.4	2521	eMol7282976	-6.4	2572	CHEMBL110431	-6.3
2471	eMol1319929	-6.4	2522	CHEMBL1358305	-6.3	2573	CHEMBL1214796	-6.3
2472	eMol1386917	-6.4	2523	CHEMBL1555962	-6.3	2574	CHEMBL1877088	-6.3
2473	eMol1518824	-6.4	2524	CHEMBL3397268	-6.3	2575	eMol1444337	-6.3
2474	eMol16056959	-6.4	2525	CHEMBL418632	-6.3	2576	eMol16379079	-6.3
2445	eMol23246486	-6.4	2496	eMol11915751	-6.4	2547	CHEMBL49924	-6.3

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
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2578:	eMol18899052	-6.3	2629	eMol24423574	-6.3	2680	eMol26245163	-6.3
2579:	eMol23255741	-6.3	2630	eMol25775765	-6.3	2681	eMol26249746	-6.3
2580:	eMol24113467	-6.3	2631	eMol25896467	-6.3	2682	eMol27202296	-6.3
2581:	eMol25813433	-6.3	2632	eMol26141634	-6.3	2683	eMol27490295	-6.3
2582:	eMol26283738	-6.3	2633	eMol27187480	-6.3	2684	eMol27490303	-6.3
2583:	eMol27182880	-6.3	2634	eMol27202494	-6.3	2685	eMol27490307	-6.3
2584:	eMol27202478	-6.3	2635	eMol277684393	-6.3	2686	eMol3393385	-6.3
2585:	eMol31857901	-6.3	2636	eMol3017868	-6.3	2687	eMol35672400	-6.3
2586:	eMol31950403	-6.3	2637	eMol36015338	-6.3	2688	eMol36016046	-6.3
2587:	eMol3302941	-6.3	2638	eMol42713805	-6.3	2689	eMol36016282	-6.3
2588:	eMol36016020	-6.3	2639	eMol784260	-6.3	2690	eMol43749119	-6.3
2589:	eMol43995169	-6.3	2640	CHEMBL1898021	-6.3	2691	eMol4727272	-6.3
2590:	eMol45904696	-6.3	2641	CHEMBL3397270	-6.3	2692	CHEMBL1700745	-6.3
2591:	eMol48213031	-6.3	2642	CHEMBL3417621	-6.3	2693	CHEMBL1892332	-6.3
2592:	eMol51984479	-6.3	2643	CHEMBL50207	-6.3	2694	CHEMBL298073	-6.3
2593:	eMol5444431	-6.3	2644	eMol11069169	-6.3	2695	CHEMBL3627817	-6.3
2594:	eMol5476297	-6.3	2645	eMol16379789	-6.3	2696	CHEMBL54233	-6.3
2595:	eMol5660295	-6.3	2646	eMol16867315	-6.3	2697	eMol11990345	-6.3
2596:	eMol6491039	-6.3	2647	eMol1749410	-6.3	2698	eMol1456432	-6.3
2597:	CHEMBL1902987	-6.3	2648	eMol2169306	-6.3	2699	eMol16375739	-6.3
2598:	CHEMBL2296351	-6.3	2649	eMol24113595	-6.3	2700	eMol16379719	-6.3
2599:	CHEMBL597034	-6.3	2650	eMol26141520	-6.3	2701	eMol206921739	-6.3
2600:	eMol11319931	-6.3	2651	eMol26313303	-6.3	2702	eMol206965396	-6.3
2601:	eMol16373093	-6.3	2652	eMol26351308	-6.3	2703	eMol24104760	-6.3
2602:	eMol1763812	-6.3	2653	eMol27187510	-6.3	2704	eMol27202804	-6.3
2603:	eMol2308402	-6.3	2654	eMol27202346	-6.3	2705	eMol31991509	-6.3
2604:	eMol24112863	-6.3	2655	eMol29577066	-6.3	2706	eMol34103848	-6.3
2605:	eMol24507725	-6.3	2656	eMol30308339	-6.3	2707	eMol34206757	-6.3
2606:	eMol24659821	-6.3	2657	eMol316473463	-6.3	2708	eMol36015788	-6.3
2607:	eMol2482511	-6.3	2658	eMol36010125	-6.3	2709	eMol36016044	-6.3
2608:	eMol26141620	-6.3	2659	eMol36015672	-6.3	2710	eMol36016122	-6.3
2609:	eMol26570013	-6.3	2660	eMol43686162	-6.3	2711	eMol36016422	-6.3
2610:	eMol27187014	-6.3	2661	eMol43749045	-6.3	2712	eMol36016572	-6.3
2611:	eMol27202458	-6.3	2662	eMol43771176	-6.3	2713	eMol43777076	-6.3
2612:	eMol27202838	-6.3	2663	eMol45932359	-6.3	2714	eMol4694984	-6.3
2613:	eMol29959342	-6.3	2664	eMol4896150	-6.3	2715	eMol5785536	-6.3
2614:	eMol32014364	-6.3	2665	eMol5839003	-6.3	2716	eMol7267392	-6.3
2615:	eMol36015646	-6.3	2666	eMol7259022	-6.3	2717	CHEMBL1214792	-6.3
2616:	eMol45787959	-6.3	2667	CHEMBL1442224	-6.3	2718	CHEMBL1887151	-6.3
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2618:	CHEMBL1971499	-6.3	2669	CHEMBL1999721	-6.3	2720	CHEMBL3417650	-6.3
2619:	CHEMBL3759501	-6.3	2670	CHEMBL51005	-6.3	2721	eMol13522798	-6.3
2620:	CHEMBL3955772	-6.3	2671	eMol101721906	-6.3	2722	eMol16760834	-6.3
2621:	CHEMBL400335	-6.3	2672	eMol16374577	-6.3	2723	eMol16768525	-6.3
2622:	CHEMBL50895	-6.3	2673	eMol16407950	-6.3	2724	eMol179424331	-6.3
2623:	eMol13396564	-6.3	2674	eMol18551172	-6.3	2725	eMol19248286	-6.3
2624:	eMol1438752	-6.3	2675	eMol25909136	-6.3	2726	eMol206843460	-6.3
2625:	eMol16379783	-6.3	2676	eMol26141642	-6.3	2727	eMol206911215	-6.3
2626:	eMol18961318	-6.3	2677	eMol26141692	-6.3	2728	eMol25813403	-6.3
2627:	eMol206910400	-6.3	2678	eMol26141696	-6.3	2729	eMol25889438	-6.3
2598:	CHEMBL2296351	-6.3	2649	eMol24113595	-6.3	2700	eMol16379719	-6.3

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
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2732:	eMol35670816	-6.3	2783	eMol29272190	-6.2	2834	eMol25797959	-6.2
2733:	eMol3792963	-6.3	2784	eMol31758474	-6.2	2835	eMol27202474	-6.2
2734:	eMol43943011	-6.3	2785	eMol32245085	-6.2	2836	eMol33346439	-6.2
2735:	eMol4505656	-6.3	2786	eMol36015358	-6.2	2837	eMol3518574	-6.2
2736:	eMol4736890	-6.3	2787	eMol36015498	-6.2	2838	eMol3651674	-6.2
2737:	eMol4839170	-6.3	2788	eMol36016042	-6.2	2839	eMol43780682	-6.2
2738:	eMol565320	-6.3	2789	eMol36016160	-6.2	2840	eMol4461665	-6.2
2739:	CHEMBL1325661	-6.3	2790	eMol43731196	-6.2	2841	eMol4540512	-6.2
2740:	CHEMBL1545153	-6.3	2791	eMol46572914	-6.2	2842	eMol579696	-6.2
2741:	CHEMBL1600359	-6.3	2792	eMol4887803	-6.2	2843	eMol587574	-6.2
2742:	CHEMBL1882595	-6.3	2793	eMol624287	-6.2	2844	CHEMBL1560726	-6.2
2743:	CHEMBL1901940	-6.3	2794	eMol7276794	-6.2	2845	CHEMBL3644258	-6.2
2744:	CHEMBL3099881	-6.3	2795	eMol9989330	-6.2	2846	CHEMBL3819208	-6.2
2745:	CHEMBL48826	-6.3	2796:	CHEMBL3417652	-6.2	2847	eMol11696283	-6.2
2746:	eMol1201946	-6.3	2797	eMol17485893	-6.2	2848	eMol13542778	-6.2
2747:	eMol13550711	-6.3	2798	eMol25816263	-6.2	2849	eMol16374765	-6.2
2748:	eMol16351583	-6.3	2799	eMol25963003	-6.2	2850	eMol16379793	-6.2
2749:	eMol16374759	-6.3	2800	eMol29639001	-6.2	2851	eMol16379835	-6.2
2750:	eMol16407932	-6.3	2801	eMol3155052	-6.2	2852	eMol1746769	-6.2
2751:	eMol1682098	-6.3	2802	eMol3244958	-6.2	2853	eMol206985138	-6.2
2752:	eMol19031739	-6.3	2803	eMol34147565	-6.2	2854	eMol25909732	-6.2
2753:	eMol20382915	-6.3	2804	eMol42849978	-6.2	2855	eMol26243041	-6.2
2754:	eMol27045537	-6.3	2805	eMol43678568	-6.2	2856	eMol26348427	-6.2
2755:	eMol27202974	-6.3	2806	eMol43685794	-6.2	2857	eMol27182890	-6.2
2756:	eMol3024862	-6.3	2807	eMol43757813	-6.2	2858	eMol27202332	-6.2
2757:	eMol33332789	-6.3	2808	eMol44074398	-6.2	2859	eMol3050679	-6.2
2758:	eMol3517993	-6.3	2809	eMol46210814	-6.2	2860	eMol3165810	-6.2
2759:	eMol35670712	-6.3	2810	eMol4935136	-6.2	2861	eMol34126656	-6.2
2760:	eMol35670806	-6.3	2811	eMol5445011	-6.2	2862	eMol3516732	-6.2
2761:	eMol36016412	-6.3	2812	eMol7289098	-6.2	2863	eMol36015356	-6.2
2762:	eMol36016546	-6.3	2813	eMol7293496	-6.2	2864	eMol36734199	-6.2
2763:	eMol4718351	-6.3	2814:	CHEMBL1499094	-6.2	2865	eMol44000007	-6.2
2764:	eMol5444399	-6.3	2815	eMol11939519	-6.2	2866	eMol5444827	-6.2
2765:	eMol5444655	-6.3	2816	eMol14273668	-6.2	2867	eMol5445017	-6.2
2766:	eMol8066589	-6.3	2817	eMol193281590	-6.2	2868	eMol7266492	-6.2
2767:	CHEMBL1301253	-6.2	2818	eMol1995647	-6.2	2869	CHEMBL1478140	-6.2
2768:	CHEMBL1305555	-6.2	2819	eMol206843420	-6.2	2870	CHEMBL1514702	-6.2
2769:	CHEMBL1443325	-6.2	2820	eMol25938966	-6.2	2871	CHEMBL296038	-6.2
2770:	CHEMBL364326	-6.2	2821	eMol26230180	-6.2	2872	CHEMBL3804951	-6.2
2771:	CHEMBL49199	-6.2	2822	eMol26288616	-6.2	2873	eMol2123648	-6.2
2772:	eMol11054214	-6.2	2823	eMol27202952	-6.2	2874	eMol2210792	-6.2
2773:	eMol16373091	-6.2	2824	eMol30078849	-6.2	2875	eMol2388346	-6.2
2774:	eMol16379797	-6.2	2825	eMol36015866	-6.2	2876	eMol24093211	-6.2
2775:	eMol18897534	-6.2	2826	eMol36510871	-6.2	2877	eMol24113477	-6.2
2776:	eMol18940279	-6.2	2827	eMol43782296	-6.2	2878	eMol24505508	-6.2
2777:	eMol206907052	-6.2	2828	eMol4486344	-6.2	2879	eMol26264906	-6.2
2778:	eMol25902692	-6.2	2829	eMol45706150	-6.2	2880	eMol27202198	-6.2
2779:	eMol26250756	-6.2	2830	eMol7260242	-6.2	2881	eMol27202406	-6.2
2780:	eMol27186994	-6.2	2831:	CHEMBL3923521	-6.2	2882	eMol32163535	-6.2
2751:	eMol1682098	-6.3	2802	eMol3244958	-6.2	2853	eMol206985138	-6.2

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
2883:	eMol36733919	-6.2	2934	eMol11921274	-6.2	2985	eMol32661622	-6.1
2884:	eMol43743426	-6.2	2935	eMol13485875	-6.2	2986	eMol3518576	-6.1
2885:	eMol43774431	-6.2	2936	eMol16351807	-6.2	2987	eMol36010129	-6.1
2886:	eMol45922019	-6.2	2937	eMol17219415	-6.2	2988	eMol36888157	-6.1
2887:	eMol5538224	-6.2	2938	eMol20382754	-6.2	2989	eMol42616136	-6.1
2888:	CHEMBL281172	-6.2	2939	eMol2362615	-6.2	2990	eMol7297106	-6.1
2889:	CHEMBL298152	-6.2	2940	eMol25784537	-6.2	2991	eMol935440	-6.1
2890:	CHEMBL3936506	-6.2	2941	eMol25784541	-6.2	2992	eMol9814195	-6.1
2891:	CHEMBL42991	-6.2	2942	eMol27202452	-6.2	2993	CHEMBL1473299	-6.1
2892:	CHEMBL50206	-6.2	2943	eMol32661606	-6.2	2994	CHEMBL344096	-6.1
2893:	eMol11874754	-6.2	2944	eMol3374251	-6.2	2995	CHEMBL3805207	-6.1
2894:	eMol16379617	-6.2	2945	eMol34147303	-6.2	2996	eMol1118798	-6.1
2895:	eMol1673934	-6.2	2946	eMol36010157	-6.2	2997	eMol1266015	-6.1
2896:	eMol2025066	-6.2	2947	eMol36015756	-6.2	2998	eMol17485895	-6.1
2897:	eMol20341799	-6.2	2948	eMol36015934	-6.2	2999	eMol179180654	-6.1
2898:	eMol32247725	-6.2	2949	eMol36015942	-6.2	3000	eMol19031804	-6.1
2899:	eMol34207047	-6.2	2950	eMol3988552	-6.2	3001	eMol25814743	-6.1
2900:	eMol36010087	-6.2	2951	eMol4695032	-6.2	3002	eMol25819227	-6.1
2901:	eMol36015844	-6.2	2952	eMol4714641	-6.2	3003	eMol25825139	-6.1
2902:	eMol36016018	-6.2	2953	eMol50288672	-6.2	3004	eMol26236634	-6.1
2903:	eMol43416567	-6.2	2954	eMol5444631	-6.2	3005	eMol27045475	-6.1
2904:	eMol43704543	-6.2	2955	eMol5444939	-6.2	3006	eMol27202772	-6.1
2905:	eMol43777016	-6.2	2956	eMol7267352	-6.2	3007	eMol27202950	-6.1
2906:	eMol5444507	-6.2	2957	CHEMBL1214795	-6.2	3008	eMol31832997	-6.1
2907:	eMol82729703	-6.2	2958	CHEMBL260470	-6.2	3009	eMol33657715	-6.1
2908:	CHEMBL1304839	-6.2	2959	eMol16056885	-6.2	3010	eMol36015132	-6.1
2909:	CHEMBL50303	-6.2	2960	eMol16379583	-6.2	3011	eMol36015606	-6.1
2910:	eMol1221018	-6.2	2961	eMol18551360	-6.2	3012	eMol36016612	-6.1
2911:	eMol13484898	-6.2	2962	eMol18877796	-6.2	3013	eMol36888187	-6.1
2912:	eMol19032400	-6.2	2963	eMol2234154	-6.2	3014	eMol4550433	-6.1
2913:	eMol232791660	-6.2	2964	eMol27202790	-6.2	3015	eMol4709963	-6.1
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2915:	eMol24453864	-6.2	2966	eMol30719809	-6.2	3017	eMol5444433	-6.1
2916:	eMol25810033	-6.2	2967	eMol36015730	-6.2	3018	eMol5538292	-6.1
2917:	eMol26251102	-6.2	2968	eMol43995579	-6.2	3019	eMol684014	-6.1
2918:	eMol27187020	-6.2	2969	eMol559945	-6.2	3020	eMol7287216	-6.1
2919:	eMol27202450	-6.2	2970	eMol681842	-6.2	3021	CHEMBL3805895	-6.1
2920:	eMol301525116	-6.2	2971	eMol7288900	-6.2	3022	CHEMBL47554	-6.1
2921:	eMol3536592	-6.2	2972	eMol8858539	-6.2	3023	eMol11677024	-6.1
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2923:	eMol36015826	-6.2	2974	CHEMBL19730	-6.1	3025	eMol2306401	-6.1
2924:	eMol36016552	-6.2	2975	CHEMBL3945396	-6.1	3026	eMol24113837	-6.1
2925:	eMol36016678	-6.2	2976	CHEMBL52119	-6.1	3027	eMol24659819	-6.1
2926:	eMol36733945	-6.2	2977	CHEMBL53036	-6.1	3028	eMol2467293	-6.1
2927:	eMol4731515	-6.2	2978	eMol13858043	-6.1	3029	eMol27187350	-6.1
2928:	eMol5444853	-6.2	2979	eMol16379067	-6.1	3030	eMol34126716	-6.1
2929:	eMol579572	-6.2	2980	eMol20347647	-6.1	3031	eMol36015312	-6.1
2930:	CHEMBL184051	-6.2	2981	eMol27045587	-6.1	3032	eMol36909907	-6.1
2931:	CHEMBL297908	-6.2	2982	eMol279157786	-6.1	3033	eMol43744868	-6.1
2932:	CHEMBL3644257	-6.2	2983	eMol316931780	-6.1	3034	eMol44045654	-6.1
2933:	CHEMBL52963	-6.2	2984	eMol32246751	-6.1	3035	eMol5444329	-6.1
2904:	eMol43704543	-6.2	2955	eMol5444939	-6.2	3006	eMol27202772	-6.1

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
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3038:	CHEMBL298261	-6.1	3089	eMol561665	-6.1	3140	eMol5444855	-6.1
3039:	CHEMBL3417657	-6.1	3090	eMol562441	-6.1	3141	CHEMBL1415373	-6.1
3040:	eMol16379633	-6.1	3091	eMol8310757	-6.1	3142	CHEMBL1548408	-6.1
3041:	eMol16795339	-6.1	3092	eMol98685524	-6.1	3143	CHEMBL3088320	-6.1
3042:	eMol26348928	-6.1	3093:	CHEMBL1307530	-6.1	3144	eMol1035519	-6.1
3043:	eMol27202834	-6.1	3094:	CHEMBL1437582	-6.1	3145	eMol1226533	-6.1
3044:	eMol27202854	-6.1	3095:	CHEMBL3417630	-6.1	3146	eMol13084309	-6.1
3045:	eMol2993561	-6.1	3096	CHEMBL54011	-6.1	3147	eMol16351861	-6.1
3046:	eMol29970720	-6.1	3097	eMol2208787	-6.1	3148	eMol18930908	-6.1
3047:	eMol3315627	-6.1	3098	eMol2222259	-6.1	3149	eMol1990456	-6.1
3048:	eMol3398875	-6.1	3099	eMol2306586	-6.1	3150	eMol20382752	-6.1
3049:	eMol35670480	-6.1	3100	eMol27186988	-6.1	3151	eMol27485968	-6.1
3050:	eMol36016424	-6.1	3101	eMol27187200	-6.1	3152	eMol29991603	-6.1
3051:	eMol36016438	-6.1	3102	eMol27202436	-6.1	3153	eMol300148591	-6.1
3052:	eMol36016640	-6.1	3103	eMol27202928	-6.1	3154	eMol3052111	-6.1
3053:	eMol36016646	-6.1	3104	eMol27202930	-6.1	3155	eMol317379879	-6.1
3054:	eMol5444611	-6.1	3105	eMol2742270	-6.1	3156	eMol32245541	-6.1
3055:	eMol5445001	-6.1	3106	eMol27490349	-6.1	3157	eMol32246329	-6.1
3056:	eMol5538612	-6.1	3107	eMol2992536	-6.1	3158	eMol36733917	-6.1
3057:	eMol7280788	-6.1	3108	eMol3315543	-6.1	3159	eMol43789927	-6.1
3058:	eMol7293044	-6.1	3109	eMol36015534	-6.1	3160	eMol4388901	-6.1
3059:	eMol8858469	-6.1	3110	eMol36015810	-6.1	3161	eMol4716784	-6.1
3060:	eMol936598	-6.1	3111	eMol36016554	-6.1	3162	eMol49902893	-6.1
3061:	eMol98721312	-6.1	3112	eMol36898000	-6.1	3163	eMol5444615	-6.1
3062:	CHEMBL1520424	-6.1	3113	eMol44590310	-6.1	3164	eMol5444647	-6.1
3063:	CHEMBL1711522	-6.1	3114	eMol4694279	-6.1	3165	eMol5538248	-6.1
3064:	CHEMBL1885709	-6.1	3115	eMol4702837	-6.1	3166	eMol5538440	-6.1
3065:	CHEMBL3417648	-6.1	3116	eMol49186053	-6.1	3167	eMol5827739	-6.1
3066:	CHEMBL45717	-6.1	3117	eMol5538746	-6.1	3168	eMol629457	-6.1
3067:	eMol11936467	-6.1	3118:	CHEMBL1406694	-6.1	3169	CHEMBL1449112	-6.1
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3069:	eMol20374348	-6.1	3120	eMol16374583	-6.1	3171	CHEMBL3417642	-6.1
3070:	eMol2213399	-6.1	3121	eMol179170457	-6.1	3172	CHEMBL3951235	-6.1
3071:	eMol24428010	-6.1	3122	eMol2209089	-6.1	3173	eMol16374795	-6.1
3072:	eMol24652558	-6.1	3123	eMol23993871	-6.1	3174	eMol16379071	-6.1
3073:	eMol25775757	-6.1	3124	eMol25782469	-6.1	3175	eMol19385162	-6.1
3074:	eMol25877073	-6.1	3125	eMol26656725	-6.1	3176	eMol1975589	-6.1
3075:	eMol27187348	-6.1	3126	eMol27202784	-6.1	3177	eMol25816245	-6.1
3076:	eMol27202434	-6.1	3127	eMol27490351	-6.1	3178	eMol27182636	-6.1
3077:	eMol27202832	-6.1	3128	eMol28321918	-6.1	3179	eMol27202482	-6.1
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3079:	eMol3053706	-6.1	3130	eMol3264054	-6.1	3181	eMol3063576	-6.1
3080:	eMol3400337	-6.1	3131	eMol36015426	-6.1	3182	eMol3091693	-6.1
3081:	eMol36015978	-6.1	3132	eMol36015510	-6.1	3183	eMol3397107	-6.1
3082:	eMol36016626	-6.1	3133	eMol36016666	-6.1	3184	eMol36015988	-6.1
3083:	eMol43686132	-6.1	3134	eMol36734197	-6.1	3185	eMol36016416	-6.1
3084:	eMol4477570	-6.1	3135	eMol36913018	-6.1	3186	eMol4694992	-6.1
3085:	eMol45696249	-6.1	3136	eMol43752173	-6.1	3187	eMol5444391	-6.1
3086:	eMol4573222	-6.1	3137	eMol43780890	-6.1	3188	eMol5444525	-6.1
3057:	eMol7280788	-6.1	3108	eMol3315543	-6.1	3159	eMol43789927	-6.1

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
3189	eMol5444779	-6.1	3240	eMol20337436	-6.0	3291	eMol25784125	-6.0
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3191	eMol566446	-6.1	3242	eMol24109710	-6.0	3293	eMol27202954	-6.0
3192	eMol587772	-6.1	3243	eMol24484845	-6.0	3294	eMol31758530	-6.0
3193	eMol7288156	-6.1	3244	eMol24526125	-6.0	3295	eMol32245537	-6.0
3194	CHEMBL1572860	-6.1	3245	eMol25810047	-6.0	3296	eMol3316876	-6.0
3195	CHEMBL1736020	-6.1	3246	eMol26141668	-6.0	3297	eMol3423798	-6.0
3196	eMol11049916	-6.1	3247	eMol27187296	-6.0	3298	eMol36016292	-6.0
3197	eMol14071710	-6.1	3248	eMol313096295	-6.0	3299	eMol36636761	-6.0
3198	eMol17487545	-6.1	3249	eMol3457575	-6.0	3300	eMol43745160	-6.0
3199	eMol193274204	-6.1	3250	eMol36015690	-6.0	3301	eMol43757701	-6.0
3200	eMol2130267	-6.1	3251	eMol45560599	-6.0	3302	eMol45687695	-6.0
3201	eMol25784121	-6.1	3252	eMol5444609	-6.0	3303	eMol565260	-6.0
3202	eMol26244399	-6.1	3253	eMol6812204	-6.0	3304	eMol579976	-6.0
3203	eMol27202830	-6.1	3254	CHEMBL1320203	-6.0	3305	eMol6546367	-6.0
3204	eMol27490347	-6.1	3255	CHEMBL1492493	-6.0	3306	eMol7266946	-6.0
3205	eMol3048978	-6.1	3256	CHEMBL296457	-6.0	3307	CHEMBL1333010	-6.0
3206	eMol3318318	-6.1	3257	eMol101721903	-6.0	3308	CHEMBL1875720	-6.0
3207	eMol3460521	-6.1	3258	eMol11063247	-6.0	3309	CHEMBL3926487	-6.0
3208	eMol36015668	-6.1	3259	eMol11827681	-6.0	3310	eMol11920572	-6.0
3209	eMol36015710	-6.1	3260	eMol11908175	-6.0	3311	eMol11924298	-6.0
3210	eMol75947178	-6.1	3261	eMol18841974	-6.0	3312	eMol13536327	-6.0
3211	CHEMBL1390719	-6.0	3262	eMol24170571	-6.0	3313	eMol16378913	-6.0
3212	CHEMBL300718	-6.0	3263	eMol2498271	-6.0	3314	eMol16379715	-6.0
3213	eMol12034278	-6.0	3264	eMol25823463	-6.0	3315	eMol16379733	-6.0
3214	eMol13870199	-6.0	3265	eMol25881352	-6.0	3316	eMol19031541	-6.0
3215	eMol16374761	-6.0	3266	eMol27495723	-6.0	3317	eMol26339153	-6.0
3216	eMol16668429	-6.0	3267	eMol2992822	-6.0	3318	eMol27187016	-6.0
3217	eMol1684723	-6.0	3268	eMol32247779	-6.0	3319	eMol27202318	-6.0
3218	eMol17487345	-6.0	3269	eMol36015604	-6.0	3320	eMol27202480	-6.0
3219	eMol19041072	-6.0	3270	eMol3651370	-6.0	3321	eMol3460171	-6.0
3220	eMol19076610	-6.0	3271	eMol36898006	-6.0	3322	eMol3492428	-6.0
3221	eMol19567048	-6.0	3272	eMol43744852	-6.0	3323	eMol36015722	-6.0
3222	eMol206907990	-6.0	3273	eMol43779180	-6.0	3324	eMol36015958	-6.0
3223	eMol22755694	-6.0	3274	eMol5777105	-6.0	3325	eMol4382848	-6.0
3224	eMol24004870	-6.0	3275	eMol579208	-6.0	3326	eMol4395800	-6.0
3225	eMol24113537	-6.0	3276	eMol7270508	-6.0	3327	eMol4693783	-6.0
3226	eMol25583051	-6.0	3277	eMol98536537	-6.0	3328	eMol5444503	-6.0
3227	eMol27182870	-6.0	3278	CHEMBL1475496	-6.0	3329	eMol935476	-6.0
3228	eMol27202840	-6.0	3279	CHEMBL1488729	-6.0	3330	CHEMBL3417626	-6.0
3229	eMol27202972	-6.0	3280	CHEMBL1536346	-6.0	3331	CHEMBL3444374	-6.0
3230	eMol33328676	-6.0	3281	CHEMBL43557	-6.0	3332	CHEMBL3806217	-6.0
3231	eMol3397089	-6.0	3282	eMol1149945	-6.0	3333	CHEMBL43877	-6.0
3232	eMol36010135	-6.0	3283	eMol1415846	-6.0	3334	eMol172296216	-6.0
3233	eMol36015936	-6.0	3284	eMol16378909	-6.0	3335	eMol206976528	-6.0
3234	eMol36733947	-6.0	3285	eMol16407976	-6.0	3336	eMol2212585	-6.0
3235	eMol43747061	-6.0	3286	eMol18831935	-6.0	3337	eMol2438554	-6.0
3236	eMol4383786	-6.0	3287	eMol18923614	-6.0	3338	eMol26141626	-6.0
3237	eMol46210774	-6.0	3288	eMol2232828	-6.0	3339	eMol27045489	-6.0
3238	eMol5444499	-6.0	3289	eMol23999017	-6.0	3340	eMol3277055	-6.0
3239	CHEMBL3417625	-6.0	3290	eMol24113623	-6.0	3341	eMol3351148	-6.0
3210	eMol75947178	-6.1	3261	eMol18841974	-6.0	3312	eMol13536327	-6.0

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
3342:	eMol3395457	-6.0	3393	eMol2992524	-6.0	3444	eMol4544980	-6.0
3343:	eMol3499188	-6.0	3394	eMol3111079	-6.0	3445	eMol4694293	-6.0
3344:	eMol35670178	-6.0	3395	eMol3119032	-6.0	3446	eMol4711170	-6.0
3345:	eMol36015970	-6.0	3396	eMol32245409	-6.0	3447	eMol5444385	-6.0
3346:	eMol36016116	-6.0	3397	eMol32246319	-6.0	3448	eMol5444405	-6.0
3347:	eMol36733931	-6.0	3398	eMol3254168	-6.0	3449	eMol5444553	-6.0
3348:	eMol36733937	-6.0	3399	eMol33344239	-6.0	3450	eMol7276298	-6.0
3349:	eMol36888153	-6.0	3400	eMol36016004	-6.0	3451	eMol7283516	-6.0
3350:	eMol44073193	-6.0	3401	eMol36016280	-6.0	3452	eMol72989932	-6.0
3351:	eMol5444923	-6.0	3402	eMol36016538	-6.0	3453	eMol8853953	-6.0
3352:	eMol6546369	-6.0	3403	eMol560173	-6.0	3454	eMol97962232	-6.0
3353:	eMol674701	-6.0	3404	eMol566772	-6.0	3455	eMol98985756	-6.0
3354:	eMol936508	-6.0	3405	eMol7289978	-6.0	3456	CHEMBL1347075	-5.9
3355:	CHEMBL85147	-6.0	3406	CHEMBL1391450	-6.0	3457	CHEMBL85119	-5.9
3356:	eMol11071012	-6.0	3407	CHEMBL361653	-6.0	3458	eMol1201940	-5.9
3357:	eMol11828091	-6.0	3408	CHEMBL3805543	-6.0	3459	eMol1749926	-5.9
3358:	eMol16379193	-6.0	3409	CHEMBL3805810	-6.0	3460	eMol25938161	-5.9
3359:	eMol16379649	-6.0	3410	CHEMBL46620	-6.0	3461	eMol26141630	-5.9
3360:	eMol16379827	-6.0	3411	eMol11896654	-6.0	3462	eMol27202850	-5.9
3361:	eMol16379865	-6.0	3412	eMol11939765	-6.0	3463	eMol3252276	-5.9
3362:	eMol27490343	-6.0	3413	eMol1681159	-6.0	3464	eMol36015366	-5.9
3363:	eMol29662423	-6.0	3414	eMol27045563	-6.0	3465	eMol36015634	-5.9
3364:	eMol32247207	-6.0	3415	eMol27182530	-6.0	3466	eMol36015670	-5.9
3365:	eMol3585513	-6.0	3416	eMol27186992	-6.0	3467	eMol36015736	-5.9
3366:	eMol36015644	-6.0	3417	eMol27202822	-6.0	3468	eMol36016548	-5.9
3367:	eMol36015744	-6.0	3418	eMol32014360	-6.0	3469	eMol3651372	-5.9
3368:	eMol36016290	-6.0	3419	eMol3255018	-6.0	3470	eMol43716255	-5.9
3369:	eMol36016638	-6.0	3420	eMol36015696	-6.0	3471	eMol5444409	-5.9
3370:	eMol36619357	-6.0	3421	eMol36016016	-6.0	3472	eMol5444919	-5.9
3371:	eMol44073265	-6.0	3422	eMol36016644	-6.0	3473	eMol5447791	-5.9
3372:	eMol44131056	-6.0	3423	eMol43772250	-6.0	3474	eMol5538604	-5.9
3373:	eMol4473164	-6.0	3424	eMol48938138	-6.0	3475	eMol5538882	-5.9
3374:	eMol5444511	-6.0	3425	eMol5444323	-6.0	3476	eMol579138	-5.9
3375:	eMol5444837	-6.0	3426	eMol5444513	-6.0	3477	eMol7263572	-5.9
3376:	eMol5444857	-6.0	3427	eMol7277736	-6.0	3478	eMol7280576	-5.9
3377:	eMol5538878	-6.0	3428	CHEMBL1482443	-6.0	3479	CHEMBL1327048	-5.9
3378:	eMol6829772	-6.0	3429	eMol24428102	-6.0	3480	CHEMBL1453502	-5.9
3379:	eMol7272446	-6.0	3430	eMol25814749	-6.0	3481	CHEMBL1462195	-5.9
3380:	eMol1026757	-6.0	3431	eMol26241386	-6.0	3482	CHEMBL3417620	-5.9
3381:	eMol1077066	-6.0	3432	eMol27182364	-6.0	3483	CHEMBL46368	-5.9
3382:	eMol1198254	-6.0	3433	eMol27202432	-6.0	3484	eMol1448893	-5.9
3383:	eMol16374763	-6.0	3434	eMol27490299	-6.0	3485	eMol16379635	-5.9
3384:	eMol1878750	-6.0	3435	eMol27490305	-6.0	3486	eMol16379679	-5.9
3385:	eMol2388279	-6.0	3436	eMol29272184	-6.0	3487	eMol16379795	-5.9
3386:	eMol25797963	-6.0	3437	eMol3073582	-6.0	3488	eMol23982156	-5.9
3387:	eMol25813429	-6.0	3438	eMol3461011	-6.0	3489	eMol25797945	-5.9
3388:	eMol25814739	-6.0	3439	eMol36015992	-6.0	3490	eMol2709463	-5.9
3389:	eMol26333881	-6.0	3440	eMol36898040	-6.0	3491	eMol27202860	-5.9
3390:	eMol27045581	-6.0	3441	eMol43757699	-6.0	3492	eMol29274292	-5.9
3391:	eMol27202534	-6.0	3442	eMol43771188	-6.0	3493	eMol30117396	-5.9
3392:	eMol27202944	-6.0	3443	eMol44012299	-6.0	3494	eMol30308489	-5.9
3363:	eMol29662423	-6.0	3414	eMol27045563	-6.0	3465	eMol36015634	-5.9

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
3495	eMol31758354	-5.9	3546	eMol48996032	-5.9	3597	eMol2045101	-5.9
3496	eMol32245651	-5.9	3547	eMol5445039	-5.9	3598	eMol26141652	-5.9
3497	eMol3308467	-5.9	3548	eMol5527763	-5.9	3599	eMol2992478	-5.9
3498	eMol36016558	-5.9	3549	eMol560175	-5.9	3600	eMol3007749	-5.9
3499	eMol36016632	-5.9	3550	eMol7285010	-5.9	3601	eMol36010137	-5.9
3500	eMol36733927	-5.9	3551	CHEMBL1409464	-5.9	3602	eMol36010139	-5.9
3501	eMol43745052	-5.9	3552	CHEMBL1503062	-5.9	3603	eMol36016014	-5.9
3502	eMol43772256	-5.9	3553	CHEMBL3417622	-5.9	3604	eMol43420012	-5.9
3503	eMol43775420	-5.9	3554	CHEMBL3417651	-5.9	3605	eMol43691638	-5.9
3504	eMol44519731	-5.9	3555	CHEMBL3627819	-5.9	3606	eMol4708865	-5.9
3505	eMol5444325	-5.9	3556	CHEMBL3805842	-5.9	3607	eMol5444505	-5.9
3506	eMol5444521	-5.9	3557	CHEMBL42254	-5.9	3608	eMol5444929	-5.9
3507	eMol5444937	-5.9	3558	eMol16375243	-5.9	3609	eMol8599848	-5.9
3508	eMol6798950	-5.9	3559	eMol16757822	-5.9	3610	eMol98035511	-5.9
3509	eMol7669354	-5.9	3560	eMol18832810	-5.9	3611	eMol98295135	-5.9
3510	eMol8858445	-5.9	3561	eMol2045239	-5.9	3612	CHEMBL116635	-5.9
3511	CHEMBL1368478	-5.9	3562	eMol206984662	-5.9	3613	CHEMBL1480909	-5.9
3512	CHEMBL1497366	-5.9	3563	eMol24102384	-5.9	3614	CHEMBL1570569	-5.9
3513	eMol16056937	-5.9	3564	eMol27202524	-5.9	3615	CHEMBL184700	-5.9
3514	eMol19076760	-5.9	3565	eMol3061940	-5.9	3616	CHEMBL3806223	-5.9
3515	eMol206993232	-5.9	3566	eMol3525797	-5.9	3617	eMol11897152	-5.9
3516	eMol24110312	-5.9	3567	eMol36015428	-5.9	3618	eMol16351881	-5.9
3517	eMol25816331	-5.9	3568	eMol36016012	-5.9	3619	eMol16374603	-5.9
3518	eMol27187010	-5.9	3569	eMol36016152	-5.9	3620	eMol19076762	-5.9
3519	eMol27202218	-5.9	3570	eMol43731528	-5.9	3621	eMol206977250	-5.9
3520	eMol27202946	-5.9	3571	eMol43745064	-5.9	3622	eMol27115416	-5.9
3521	eMol30083536	-5.9	3572	eMol48982458	-5.9	3623	eMol27187292	-5.9
3522	eMol3245586	-5.9	3573	eMol581336	-5.9	3624	eMol27202396	-5.9
3523	eMol3379409	-5.9	3574	eMol679602	-5.9	3625	eMol32247059	-5.9
3524	eMol36015702	-5.9	3575	eMol76020498	-5.9	3626	eMol34126722	-5.9
3525	eMol36016164	-5.9	3576	eMol956537	-5.9	3627	eMol36015618	-5.9
3526	eMol36016634	-5.9	3577	eMol98451737	-5.9	3628	eMol36015938	-5.9
3527	eMol36016662	-5.9	3578	CHEMBL3251278	-5.9	3629	eMol36015990	-5.9
3528	eMol43745897	-5.9	3579	CHEMBL3303662	-5.9	3630	eMol36016532	-5.9
3529	eMol5444915	-5.9	3580	CHEMBL3417623	-5.9	3631	eMol5538886	-5.9
3530	eMol6770480	-5.9	3581	CHEMBL3417653	-5.9	3632	eMol5747647	-5.9
3531	eMol6844944	-5.9	3582	CHEMBL52027	-5.9	3633	eMol7276176	-5.9
3532	eMol7276886	-5.9	3583	eMol206962509	-5.9	3634	CHEMBL1416395	-5.9
3533	eMol7294930	-5.9	3584	eMol27202438	-5.9	3635	CHEMBL1529015	-5.9
3534	CHEMBL1559259	-5.9	3585	eMol32246641	-5.9	3636	CHEMBL3417619	-5.9
3535	eMol11905852	-5.9	3586	eMol34147555	-5.9	3637	CHEMBL3818256	-5.9
3536	eMol16378915	-5.9	3587	eMol5444389	-5.9	3638	eMol20351100	-5.9
3537	eMol27490283	-5.9	3588	eMol5538744	-5.9	3639	eMol2123188	-5.9
3538	eMol277684421	-5.9	3589	eMol685354	-5.9	3640	eMol2194421	-5.9
3539	eMol3120283	-5.9	3590	CHEMBL1323430	-5.9	3641	eMol25895035	-5.9
3540	eMol32417568	-5.9	3591	CHEMBL42492	-5.9	3642	eMol27202376	-5.9
3541	eMol3484149	-5.9	3592	CHEMBL50183	-5.9	3643	eMol27202820	-5.9
3542	eMol36015388	-5.9	3593	eMol101338171	-5.9	3644	eMol2992538	-5.9
3543	eMol3628332	-5.9	3594	eMol16379655	-5.9	3645	eMol32551016	-5.9
3544	eMol43779182	-5.9	3595	eMol16755860	-5.9	3646	eMol36010119	-5.9
3545	eMol43943035	-5.9	3596	eMol17182671	-5.9	3647	eMol36015538	-5.9

Table S1. *Continued.*

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
3648:	eMol36015946	-5.9	3699	eMol7273458	-5.8	3750	eMol16801545	-5.8
3649:	eMol36016624	-5.9	3700	CHEMBL296471	-5.8	3751	eMol233065671	-5.8
3650:	eMol4396702	-5.9	3701	CHEMBL3805423	-5.8	3752	eMol24102744	-5.8
3651:	eMol5444965	-5.9	3702	eMol16375283	-5.8	3753	eMol25808001	-5.8
3652:	eMol5445015	-5.9	3703	eMol16379191	-5.8	3754	eMol25810019	-5.8
3653:	CHEMBL2180424	-5.9	3704	eMol179165020	-5.8	3755	eMol27045477	-5.8
3654:	CHEMBL3417644	-5.9	3705	eMol27187196	-5.8	3756	eMol27186986	-5.8
3655:	eMol11492617	-5.9	3706	eMol27202942	-5.8	3757	eMol27187058	-5.8
3656:	eMol11651355	-5.9	3707	eMol29272178	-5.8	3758	eMol30499969	-5.8
3657:	eMol13457575	-5.9	3708	eMol3015060	-5.8	3759	eMol32246797	-5.8
3658:	eMol1991716	-5.9	3709	eMol36015446	-5.8	3760	eMol32259086	-5.8
3659:	eMol2234330	-5.9	3710	eMol36016136	-5.8	3761	eMol3247755	-5.8
3660:	eMol24116061	-5.9	3711	eMol36016418	-5.8	3762	eMol3473706	-5.8
3661:	eMol27045573	-5.9	3712	eMol36016576	-5.8	3763	eMol36015394	-5.8
3662:	eMol27202826	-5.9	3713	eMol36016630	-5.8	3764	eMol36015628	-5.8
3663:	eMol3060124	-5.9	3714	eMol43758409	-5.8	3765	eMol36733921	-5.8
3664:	eMol35670746	-5.9	3715	eMol566748	-5.8	3766	eMol43779178	-5.8
3665:	eMol36015662	-5.9	3716	eMol7297616	-5.8	3767	eMol4718807	-5.8
3666:	eMol43749023	-5.9	3717	eMol8599285	-5.8	3768	eMol6844630	-5.8
3667:	eMol45705052	-5.9	3718	CHEMBL1412503	-5.8	3769	eMol7265596	-5.8
3668:	eMol5444781	-5.9	3719	CHEMBL1596292	-5.8	3770	eMol7280232	-5.8
3669:	eMol5444941	-5.9	3720	CHEMBL3805156	-5.8	3771	CHEMBL1386169	-5.8
3670:	eMol560295	-5.9	3721	eMol16351969	-5.8	3772	CHEMBL1612982	-5.8
3671:	eMol7262416	-5.9	3722	eMol17485771	-5.8	3773	eMol11910455	-5.8
3672:	eMol7275912	-5.9	3723	eMol2330945	-5.8	3774	eMol1201944	-5.8
3673:	CHEMBL1349955	-5.8	3724	eMol25784525	-5.8	3775	eMol16379757	-5.8
3674:	CHEMBL1551011	-5.8	3725	eMol27045549	-5.8	3776	eMol18837122	-5.8
3675:	CHEMBL298186	-5.8	3726	eMol27202372	-5.8	3777	eMol2211247	-5.8
3676:	CHEMBL36436	-5.8	3727	eMol27202464	-5.8	3778	eMol24102224	-5.8
3677:	eMol16056895	-5.8	3728	eMol27202824	-5.8	3779	eMol25810025	-5.8
3678:	eMol16351863	-5.8	3729	eMol279062638	-5.8	3780	eMol29946079	-5.8
3679:	eMol16379727	-5.8	3730	eMol34126654	-5.8	3781	eMol29970678	-5.8
3680:	eMol18567164	-5.8	3731	eMol36015418	-5.8	3782	eMol32246637	-5.8
3681:	eMol18915564	-5.8	3732	eMol36888077	-5.8	3783	eMol3243276	-5.8
3682:	eMol20337406	-5.8	3733	eMol3707337	-5.8	3784	eMol3378047	-5.8
3683:	eMol27349471	-5.8	3734	eMol43686098	-5.8	3785	eMol36015404	-5.8
3684:	eMol32245395	-5.8	3735	eMol4479471	-5.8	3786	eMol43692862	-5.8
3685:	eMol34173242	-5.8	3736	eMol560051	-5.8	3787	eMol43757807	-5.8
3686:	eMol3445274	-5.8	3737	eMol579892	-5.8	3788	CHEMBL1528422	-5.8
3687:	eMol36015524	-5.8	3738	eMol5803186	-5.8	3789	CHEMBL2355657	-5.8
3688:	eMol36016276	-5.8	3739	eMol8311949	-5.8	3790	eMol11949268	-5.8
3689:	eMol36016286	-5.8	3740	eMol935358	-5.8	3791	eMol16385658	-5.8
3690:	eMol36734015	-5.8	3741	ChEBI120532	-5.8	3792	eMol17487549	-5.8
3691:	eMol44831971	-5.8	3742	CHEMBL1484192	-5.8	3793	eMol18899622	-5.8
3692:	eMol5444441	-5.8	3743	CHEMBL1501308	-5.8	3794	eMol23736354	-5.8
3693:	eMol5444873	-5.8	3744	CHEMBL1541968	-5.8	3795	eMol24062462	-5.8
3694:	eMol54877800	-5.8	3745	CHEMBL44983	-5.8	3796	eMol25946128	-5.8
3695:	eMol5538872	-5.8	3746	eMol1114360	-5.8	3797	eMol289941373	-5.8
3696:	eMol5538874	-5.8	3747	eMol11942269	-5.8	3798	eMol29272180	-5.8
3697:	eMol624279	-5.8	3748	eMol1346671	-5.8	3799	eMol3458277	-5.8
3698:	eMol7268950	-5.8	3749	eMol1454694	-5.8	3800	eMol36015676	-5.8
3669:	eMol5444941	-5.9	3720	CHEMBL3805156	-5.8	3771	CHEMBL1386169	-5.8

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
3801:	eMol43757795	-5.8	3852:	eMol3203801	-5.8	3903:	eMol5444651	-5.7
3802:	eMol4439491	-5.8	3853:	eMol32867972	-5.8	3904:	eMol5538230	-5.7
3803:	eMol5444737	-5.8	3854:	eMol3518209	-5.8	3905:	eMol5538572	-5.7
3804:	eMol5538750	-5.8	3855:	eMol36015982	-5.8	3906:	eMol578940	-5.7
3805:	eMol11897144	-5.8	3856:	eMol36016550	-5.8	3907:	eMol8858379	-5.7
3806:	eMol179165023	-5.8	3857:	eMol36888147	-5.8	3908:	eMol98677038	-5.7
3807:	eMol18880257	-5.8	3858:	eMol43224757	-5.8	3909:	CHEMBL1430145	-5.7
3808:	eMol23016524	-5.8	3859:	eMol560067	-5.8	3910:	eMol101341286	-5.7
3809:	eMol24053582	-5.8	3860:	eMol587732	-5.8	3911:	eMol16378087	-5.7
3810:	eMol26762435	-5.8	3861:	eMol7290742	-5.8	3912:	eMol1748573	-5.7
3811:	eMol36015302	-5.8	3862:	eMol1456137	-5.8	3913:	eMol179164950	-5.7
3812:	eMol36015768	-5.8	3863:	eMol16351587	-5.8	3914:	eMol24427988	-5.7
3813:	eMol36015964	-5.8	3864:	eMol16379197	-5.8	3915:	eMol24538112	-5.7
3814:	eMol42925185	-5.8	3865:	eMol24428322	-5.8	3916:	eMol2478254	-5.7
3815:	eMol45932363	-5.8	3866:	eMol25150648	-5.8	3917:	eMol26273901	-5.7
3816:	eMol5444833	-5.8	3867:	eMol27115412	-5.8	3918:	eMol3389097	-5.7
3817:	eMol560053	-5.8	3868:	eMol29947096	-5.8	3919:	eMol3517782	-5.7
3818:	CHEMBL1414275	-5.8	3869:	eMol3118180	-5.8	3920:	eMol36016636	-5.7
3819:	CHEMBL46990	-5.8	3870:	eMol32245479	-5.8	3921:	eMol36733951	-5.7
3820:	eMol1120516	-5.8	3871:	eMol32246741	-5.8	3922:	eMol43709145	-5.7
3821:	eMol1149913	-5.8	3872:	eMol3473526	-5.8	3923:	eMol43754301	-5.7
3822:	eMol16379631	-5.8	3873:	eMol36015738	-5.8	3924:	eMol43780754	-5.7
3823:	eMol1684016	-5.8	3874:	eMol36015818	-5.8	3925:	eMol5444835	-5.7
3824:	eMol177240154	-5.8	3875:	eMol43777018	-5.8	3926:	eMol5538900	-5.7
3825:	eMol1996956	-5.8	3876:	eMol44070271	-5.8	3927:	eMol555458	-5.7
3826:	eMol26291695	-5.8	3877:	eMol5527727	-5.8	3928:	eMol581338	-5.7
3827:	eMol2708943	-5.8	3878:	eMol5538566	-5.8	3929:	eMol681870	-5.7
3828:	eMol27485958	-5.8	3879:	eMol7272094	-5.8	3930:	CHEMBL1323102	-5.7
3829:	eMol300748351	-5.8	3880:	CHEMBL299758	-5.7	3931:	CHEMBL3251274	-5.7
3830:	eMol33328686	-5.8	3881:	eMol1456572	-5.7	3932:	CHEMBL3302804	-5.7
3831:	eMol3377803	-5.8	3882:	eMol15983238	-5.7	3933:	CHEMBL3417656	-5.7
3832:	eMol3550246	-5.8	3883:	eMol16378895	-5.7	3934:	CHEMBL3805990	-5.7
3833:	eMol36015998	-5.8	3884:	eMol29274406	-5.7	3935:	eMol11905834	-5.7
3834:	eMol36016402	-5.8	3885:	eMol29945943	-5.7	3936:	eMol1201942	-5.7
3835:	eMol36016570	-5.8	3886:	eMol29987856	-5.7	3937:	eMol19834537	-5.7
3836:	eMol36734157	-5.8	3887:	eMol3063065	-5.7	3938:	eMol2009845	-5.7
3837:	eMol43706397	-5.8	3888:	eMol316607523	-5.7	3939:	eMol206994786	-5.7
3838:	eMol4569646	-5.8	3889:	eMol32246223	-5.7	3940:	eMol24659537	-5.7
3839:	eMol4769967	-5.8	3890:	eMol33328746	-5.7	3941:	eMol25017853	-5.7
3840:	eMol581218	-5.8	3891:	eMol3453673	-5.7	3942:	eMol27202858	-5.7
3841:	eMol7707303	-5.8	3892:	eMol36016288	-5.7	3943:	eMol276247962	-5.7
3842:	CHEMBL295198	-5.8	3893:	eMol36888099	-5.7	3944:	eMol29574834	-5.7
3843:	CHEMBL3805373	-5.8	3894:	eMol7260540	-5.7	3945:	eMol300994022	-5.7
3844:	eMol16352275	-5.8	3895:	CHEMBL1999927	-5.7	3946:	eMol32245663	-5.7
3845:	eMol16375907	-5.8	3896:	CHEMBL3417647	-5.7	3947:	eMol36010097	-5.7
3846:	eMol16379189	-5.8	3897:	eMol1129158	-5.7	3948:	eMol36016430	-5.7
3847:	eMol1754894	-5.8	3898:	eMol16375745	-5.7	3949:	eMol36016530	-5.7
3848:	eMol19874354	-5.8	3899:	eMol27187224	-5.7	3950:	eMol42728099	-5.7
3849:	eMol2490920	-5.8	3900:	eMol27202940	-5.7	3951:	eMol43678570	-5.7
3850:	eMol27115418	-5.8	3901:	eMol3165472	-5.7	3952:	eMol43747049	-5.7
3851:	eMol3091717	-5.8	3902:	eMol36015334	-5.7	3953:	eMol45908565	-5.7
3822:	eMol16379631	-5.8	3873:	eMol36015738	-5.8	3924:	eMol43780754	-5.7

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
3954:	CHEMBL1512259	-5.7	4005	eMol36015836	-5.7	4056	eMol1266027	-5.7
3955:	eMol11980724	-5.7	4006	eMol36015850	-5.7	4057	eMol15983254	-5.7
3956:	eMol179165017	-5.7	4007	eMol36016436	-5.7	4058	eMol16351885	-5.7
3957:	eMol179330987	-5.7	4008	eMol44059490	-5.7	4059	eMol24080844	-5.7
3958:	eMol2405173	-5.7	4009	eMol45789241	-5.7	4060	eMol24147635	-5.7
3959:	eMol257850519	-5.7	4010	eMol5444653	-5.7	4061	eMol2709017	-5.7
3960:	eMol30682572	-5.7	4011	eMol5444731	-5.7	4062	eMol27182526	-5.7
3961:	eMol31873562	-5.7	4012	CHEMBL37887	-5.7	4063	eMol29272194	-5.7
3962:	eMol3191734	-5.7	4013	CHEMBL3805719	-5.7	4064	eMol29956351	-5.7
3963:	eMol4124876	-5.7	4014	CHEMBL42510	-5.7	4065	eMol32089964	-5.7
3964:	eMol4492362	-5.7	4015	CHEMBL44909	-5.7	4066	eMol3315429	-5.7
3965:	eMol5444793	-5.7	4016	eMol13870135	-5.7	4067	eMol3402145	-5.7
3966:	eMol7293790	-5.7	4017	eMol16379739	-5.7	4068	eMol34147575	-5.7
3967:	eMol98035508	-5.7	4018	eMol18936964	-5.7	4069	eMol3581283	-5.7
3968:	CHEMBL1413103	-5.7	4019	eMol25825133	-5.7	4070	eMol3581435	-5.7
3969:	CHEMBL1443164	-5.7	4020	eMol26264984	-5.7	4071	eMol36015408	-5.7
3970:	CHEMBL1701550	-5.7	4021	eMol29963253	-5.7	4072	eMol36015966	-5.7
3971:	CHEMBL3251265	-5.7	4022	eMol32245227	-5.7	4073	eMol36016002	-5.7
3972:	CHEMBL3303952	-5.7	4023	eMol32246219	-5.7	4074	eMol36016272	-5.7
3973:	CHEMBL3962862	-5.7	4024	eMol3314151	-5.7	4075	eMol36016600	-5.7
3974:	eMol16379537	-5.7	4025	eMol3450783	-5.7	4076	eMol5538560	-5.7
3975:	eMol16776762	-5.7	4026	eMol36015858	-5.7	4077	eMol679756	-5.7
3976:	eMol206992985	-5.7	4027	eMol36016000	-5.7	4078	CHEMBL3417631	-5.6
3977:	eMol24423982	-5.7	4028	eMol36016006	-5.7	4079	eMol13396536	-5.6
3978:	eMol25881320	-5.7	4029	eMol36016420	-5.7	4080	eMol19269633	-5.6
3979:	eMol2666505	-5.7	4030	eMol36016616	-5.7	4081	eMol24113033	-5.6
3980:	eMol2881396	-5.7	4031	eMol36888165	-5.7	4082	eMol2588259	-5.6
3981:	eMol31758390	-5.7	4032	eMol43747057	-5.7	4083	eMol26132226	-5.6
3982:	eMol32245285	-5.7	4033	eMol43751241	-5.7	4084	eMol300090481	-5.6
3983:	eMol3246420	-5.7	4034	eMol43754319	-5.7	4085	eMol36016404	-5.6
3984:	eMol32738498	-5.7	4035	eMol46563820	-5.7	4086	eMol36016426	-5.6
3985:	eMol3323420	-5.7	4036	eMol581354	-5.7	4087	eMol43731600	-5.6
3986:	eMol3581639	-5.7	4037	CHEMBL1408481	-5.7	4088	eMol5444643	-5.6
3987:	eMol50316116	-5.7	4038	CHEMBL413095	-5.7	4089	eMol5444921	-5.6
3988:	eMol5538600	-5.7	4039	eMol16379791	-5.7	4090	eMol587912	-5.6
3989:	eMol5538748	-5.7	4040	eMol1764260	-5.7	4091	eMol681846	-5.6
3990:	eMol5803268	-5.7	4041	eMol2005049	-5.7	4092	eMol6844632	-5.6
3991:	eMol6546341	-5.7	4042	eMol3059233	-5.7	4093	CHEMBL1299662	-5.6
3992:	eMol670804	-5.7	4043	eMol3165424	-5.7	4094	CHEMBL3417624	-5.6
3993:	eMol678803	-5.7	4044	eMol32245281	-5.7	4095	CHEMBL45997	-5.6
3994:	eMol101338165	-5.7	4045	eMol36015704	-5.7	4096	eMol16351805	-5.6
3995:	eMol11383493	-5.7	4046	eMol36015852	-5.7	4097	eMol18567168	-5.6
3996:	eMol11689326	-5.7	4047	eMol36733943	-5.7	4098	eMol24111627	-5.6
3997:	eMol14012794	-5.7	4048	eMol3707309	-5.7	4099	eMol24428014	-5.6
3998:	eMol16379805	-5.7	4049	eMol43692886	-5.7	4100	eMol27452042	-5.6
3999:	eMol23989036	-5.7	4050	eMol5444927	-5.7	4101	eMol27485950	-5.6
4000:	eMol26287348	-5.7	4051	eMol565392	-5.7	4102	eMol2961107	-5.6
4001:	eMol27115428	-5.7	4052	eMol579530	-5.7	4103	eMol3063476	-5.6
4002:	eMol27187212	-5.7	4053	CHEMBL289053	-5.7	4104	eMol3222998	-5.6
4003:	eMol3154639	-5.7	4054	CHEMBL398633	-5.7	4105	eMol32247631	-5.6
4004:	eMol36015698	-5.7	4055	eMol1098662	-5.7	4106	eMol3652708	-5.6
3975:	eMol16776762	-5.7	4026	eMol36015858	-5.7	4077	eMol679756	-5.7

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
4107	eMol5444825	-5.6	4158	eMol5444741	-5.6	4209	eMol34117146	-5.6
4108	eMol5538422	-5.6	4159	eMol5444821	-5.6	4210	eMol36015370	-5.6
4109	eMol7276046	-5.6	4160	eMol7262778	-5.6	4211	eMol36016628	-5.6
4110	eMol7720322	-5.6	4161	eMol936680	-5.6	4212	eMol36734039	-5.6
4111	eMol8227994	-5.6	4162	eMol11067809	-5.6	4213	eMol43716279	-5.6
4112	eMol99154804	-5.6	4163	eMol13406955	-5.6	4214	eMol44027807	-5.6
4113	CHEMBL1363412	-5.6	4164	eMol13856757	-5.6	4215	eMol5538274	-5.6
4114	CHEMBL185819	-5.6	4165	eMol15983296	-5.6	4216	eMol5538596	-5.6
4115	CHEMBL298877	-5.6	4166	eMol16378849	-5.6	4217	eMol561929	-5.6
4116	CHEMBL3805394	-5.6	4167	eMol16387280	-5.6	4218	eMol7297548	-5.6
4117	eMol1035451	-5.6	4168	eMol3118142	-5.6	4219	CHEMBL1361934	-5.6
4118	eMol16374525	-5.6	4169	eMol3471424	-5.6	4220	CHEMBL1409728	-5.6
4119	eMol17177598	-5.6	4170	eMol3531069	-5.6	4221	CHEMBL1502873	-5.6
4120	eMol23985110	-5.6	4171	eMol36015660	-5.6	4222	CHEMBL287739	-5.6
4121	eMol34103732	-5.6	4172	eMol36016568	-5.6	4223	CHEMBL46580	-5.6
4122	eMol3554360	-5.6	4173	eMol5538442	-5.6	4224	eMol11071094	-5.6
4123	eMol36015348	-5.6	4174	eMol562339	-5.6	4225	eMol16374967	-5.6
4124	eMol36015412	-5.6	4175	CHEMBL1333939	-5.6	4226	eMol1755498	-5.6
4125	eMol36015666	-5.6	4176	eMol15961299	-5.6	4227	eMol1996958	-5.6
4126	eMol36016406	-5.6	4177	eMol16387194	-5.6	4228	eMol2312222	-5.6
4127	eMol36016414	-5.6	4178	eMol3091455	-5.6	4229	eMol25936931	-5.6
4128	eMol5476123	-5.6	4179	eMol36016010	-5.6	4230	eMol3091595	-5.6
4129	eMol5538734	-5.6	4180	eMol36016434	-5.6	4231	eMol3165452	-5.6
4130	eMol579888	-5.6	4181	eMol36016536	-5.6	4232	eMol3247843	-5.6
4131	eMol581332	-5.6	4182	eMol53746272	-5.6	4233	eMol3252590	-5.6
4132	eMol98984071	-5.6	4183	eMol5444841	-5.6	4234	eMol36015332	-5.6
4133	CHEMBL46221	-5.6	4184	eMol561465	-5.6	4235	eMol36015708	-5.6
4134	eMol100505980	-5.6	4185	CHEMBL277367	-5.6	4236	eMol36016660	-5.6
4135	eMol11772107	-5.6	4186	eMol11665251	-5.6	4237	eMol565358	-5.6
4136	eMol1411602	-5.6	4187	eMol11857514	-5.6	4238	eMol7274020	-5.6
4137	eMol16351787	-5.6	4188	eMol16379199	-5.6	4239	eMol7289486	-5.6
4138	eMol1681157	-5.6	4189	eMol23169915	-5.6	4240	CHEMBL1310951	-5.5
4139	eMol24512694	-5.6	4190	eMol27490353	-5.6	4241	CHEMBL3192694	-5.5
4140	eMol27182632	-5.6	4191	eMol2992804	-5.6	4242	eMol11996719	-5.5
4141	eMol30248265	-5.6	4192	eMol3192660	-5.6	4243	eMol16715583	-5.5
4142	eMol36015996	-5.6	4193	eMol36015824	-5.6	4244	eMol179164999	-5.5
4143	eMol36016400	-5.6	4194	eMol36015868	-5.6	4245	eMol207218450	-5.5
4144	eMol6120463	-5.6	4195	eMol36016048	-5.6	4246	eMol24000041	-5.5
4145	eMol7261208	-5.6	4196	eMol5444555	-5.6	4247	eMol24659823	-5.5
4146	eMol11939349	-5.6	4197	eMol5444745	-5.6	4248	eMol25948294	-5.5
4147	eMol16379137	-5.6	4198	eMol5444823	-5.6	4249	eMol26236444	-5.5
4148	eMol177226996	-5.6	4199	eMol588330	-5.6	4250	eMol300233846	-5.5
4149	eMol18917833	-5.6	4200	eMol935616	-5.6	4251	eMol3394121	-5.5
4150	eMol189971515	-5.6	4201	eMol98750076	-5.6	4252	eMol36016028	-5.5
4151	eMol2277798	-5.6	4202	CHEMBL1538079	-5.6	4253	eMol36016620	-5.5
4152	eMol24659539	-5.6	4203	eMol1125948	-5.6	4254	eMol36888107	-5.5
4153	eMol2888718	-5.6	4204	eMol11942097	-5.6	4255	eMol43753923	-5.5
4154	eMol31758306	-5.6	4205	eMol16379641	-5.6	4256	eMol4495299	-5.5
4155	eMol36015682	-5.6	4206	eMol24107019	-5.6	4257	CHEMBL37758	-5.5
4156	eMol36016284	-5.6	4207	eMol3320388	-5.6	4258	eMol1259454	-5.5
4157	eMol43747097	-5.6	4208	eMol3375755	-5.6	4259	eMol13444090	-5.5
4128	eMol5476123	-5.6	4179	eMol36016010	-5.6	4230	eMol3091595	-5.6

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
4260:	eMol16656843	-5.5	4311	eMol5538580	-5.5	4362	CHEMBL108678	-5.5
4261:	eMol16786048	-5.5	4312	eMol5829456	-5.5	4363	eMol11922227	-5.5
4262:	eMol24117398	-5.5	4313	eMol11900836	-5.5	4364	eMol16379571	-5.5
4263:	eMol26298847	-5.5	4314	eMol13464851	-5.5	4365	eMol2466422	-5.5
4264:	eMol27045473	-5.5	4315	eMol16274923	-5.5	4366	eMol30662258	-5.5
4265:	eMol27485926	-5.5	4316	eMol17485889	-5.5	4367	eMol32245953	-5.5
4266:	eMol2991951	-5.5	4317	eMol1753662	-5.5	4368	eMol33328728	-5.5
4267:	eMol3105499	-5.5	4318	eMol2399769	-5.5	4369	eMol36015664	-5.5
4268:	eMol49047598	-5.5	4319	eMol27115434	-5.5	4370	eMol36016428	-5.5
4269:	eMol6514227	-5.5	4320	eMol30576034	-5.5	4371	eMol36016432	-5.5
4270:	eMol7291792	-5.5	4321	eMol679702	-5.5	4372	eMol36016556	-5.5
4271:	CHEMBL1994932	-5.5	4322	eMol7261308	-5.5	4373	eMol43745168	-5.5
4272:	CHEMBL2238498	-5.5	4323	eMol7281506	-5.5	4374	eMol43757693	-5.5
4273:	CHEMBL37829	-5.5	4324	eMol7639977	-5.5	4375	eMol5444867	-5.5
4274:	eMol16351803	-5.5	4325	CHEMBL276947	-5.5	4376	eMol7285922	-5.5
4275:	eMol24115063	-5.5	4326	CHEMBL3251273	-5.5	4377	CHEMBL1583040	-5.5
4276:	eMol317058156	-5.5	4327	CHEMBL3304410	-5.5	4378	eMol1764760	-5.5
4277:	eMol31758520	-5.5	4328	eMol13542776	-5.5	4379	eMol25621652	-5.5
4278:	eMol32480666	-5.5	4329	eMol26236690	-5.5	4380	eMol2992506	-5.5
4279:	eMol36015612	-5.5	4330	eMol2992800	-5.5	4381	eMol36015382	-5.5
4280:	eMol36015686	-5.5	4331	eMol3247471	-5.5	4382	eMol36015720	-5.5
4281:	eMol36016408	-5.5	4332	eMol3385015	-5.5	4383	eMol43754663	-5.5
4282:	eMol5538598	-5.5	4333	eMol36015374	-5.5	4384	eMol5444327	-5.5
4283:	eMol560297	-5.5	4334	eMol4260980	-5.5	4385	eMol579954	-5.5
4284:	eMol6514345	-5.5	4335	eMol43745020	-5.5	4386	eMol587978	-5.5
4285:	eMol695171	-5.5	4336	eMol5444341	-5.5	4387	eMol7271458	-5.5
4286:	CHEMBL1524621	-5.5	4337	eMol5444625	-5.5	4388	eMol8267093	-5.5
4287:	CHEMBL3954127	-5.5	4338	eMol5444785	-5.5	4389	CHEMBL283373	-5.4
4288:	eMol179170445	-5.5	4339	eMol6810339	-5.5	4390	CHEMBL287914	-5.4
4289:	eMol27202924	-5.5	4340	eMol7262724	-5.5	4391	CHEMBL3908563	-5.4
4290:	eMol36624923	-5.5	4341	CHEMBL3251272	-5.5	4392	CHEMBL43067	-5.4
4291:	eMol43692860	-5.5	4342	CHEMBL3302444	-5.5	4393	eMol2212509	-5.4
4292:	eMol5538490	-5.5	4343	eMol11936155	-5.5	4394	eMol23982998	-5.4
4293:	eMol5538498	-5.5	4344	eMol13998590	-5.5	4395	eMol33345106	-5.4
4294:	eMol5538876	-5.5	4345	eMol1764882	-5.5	4396	eMol36898042	-5.4
4295:	eMol581300	-5.5	4346	eMol23625944	-5.5	4397	eMol5444787	-5.4
4296:	eMol7277304	-5.5	4347	eMol24006861	-5.5	4398	CHEMBL1363639	-5.4
4297:	CHEMBL277894	-5.5	4348	eMol24432113	-5.5	4399	eMol13518872	-5.4
4298:	eMol1120542	-5.5	4349	eMol29944972	-5.5	4400	eMol13924352	-5.4
4299:	eMol16379651	-5.5	4350	eMol3594414	-5.5	4401	eMol16782365	-5.4
4300:	eMol2462968	-5.5	4351	eMol36015376	-5.5	4402	eMol1749616	-5.4
4301:	eMol2477726	-5.5	4352	eMol36015648	-5.5	4403	eMol24174701	-5.4
4302:	eMol26295378	-5.5	4353	eMol36733923	-5.5	4404	eMol25656108	-5.4
4303:	eMol27187222	-5.5	4354	eMol36733929	-5.5	4405	eMol27187262	-5.4
4304:	eMol29274294	-5.5	4355	eMol43686126	-5.5	4406	eMol32247525	-5.4
4305:	eMol31307202	-5.5	4356	eMol43716311	-5.5	4407	eMol32247621	-5.4
4306:	eMol36015652	-5.5	4357	eMol43754317	-5.5	4408	eMol3252534	-5.4
4307:	eMol36016274	-5.5	4358	eMol4566462	-5.5	4409	eMol36015678	-5.4
4308:	eMol43222155	-5.5	4359	eMol5444755	-5.5	4410	eMol5444333	-5.4
4309:	eMol43691644	-5.5	4360	eMol936264	-5.5	4411	eMol5444729	-5.4
4310:	eMol5538280	-5.5	4361	eMol99058638	-5.5	4412	CHEMBL1582944	-5.4
4281:	eMol36016408	-5.5	4332	eMol3385015	-5.5	4383	eMol43754663	-5.5

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
4413:	CHEMBL1979224	-5.4	4464:	eMol587792	-5.4	4515:	eMol1125956	-5.3
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4415:	eMol1684436	-5.4	4466:	eMol17485765	-5.4	4517:	eMol27045263	-5.3
4416:	eMol1830750	-5.4	4467:	eMol2221159	-5.4	4518:	eMol3165074	-5.3
4417:	eMol24145924	-5.4	4468:	eMol23993395	-5.4	4519:	eMol32246169	-5.3
4418:	eMol26141646	-5.4	4469:	eMol2493592	-5.4	4520:	eMol3392027	-5.3
4419:	eMol31653406	-5.4	4470:	eMol3253524	-5.4	4521:	eMol48982489	-5.3
4420:	eMol31758546	-5.4	4471:	eMol36015566	-5.4	4522:	eMol5444437	-5.3
4421:	eMol3232593	-5.4	4472:	eMol36016606	-5.4	4523:	eMol7273880	-5.3
4422:	eMol3376557	-5.4	4473:	eMol3652688	-5.4	4524:	ChEBI114898	-5.3
4423:	eMol36015354	-5.4	4474:	eMol5538576	-5.4	4525:	CHEMBL1499477	-5.3
4424:	eMol36015750	-5.4	4475:	eMol15267850	-5.4	4526:	CHEMBL1902366	-5.3
4425:	eMol36016658	-5.4	4476:	eMol2992496	-5.4	4527:	eMol16379689	-5.3
4426:	eMol36016664	-5.4	4477:	eMol36015638	-5.4	4528:	eMol1682729	-5.3
4427:	eMol3649917	-5.4	4478:	eMol36015700	-5.4	4529:	eMol17485891	-5.3
4428:	eMol43746057	-5.4	4479:	eMol36016038	-5.4	4530:	eMol2022679	-5.3
4429:	eMol4594606	-5.4	4480:	eMol36016562	-5.4	4531:	eMol2227456	-5.3
4430:	eMol5527725	-5.4	4481:	eMol36734195	-5.4	4532:	eMol36015360	-5.3
4431:	eMol5538492	-5.4	4482:	eMol43744884	-5.4	4533:	eMol36015932	-5.3
4432:	eMol565570	-5.4	4483:	eMol4423161	-5.4	4534:	eMol36015980	-5.3
4433:	eMol7290874	-5.4	4484:	eMol7287028	-5.4	4535:	eMol36016682	-5.3
4434:	eMol8066827	-5.4	4485:	CHEMBL1346627	-5.4	4536:	eMol684044	-5.3
4435:	CHEMBL2298707	-5.4	4486:	CHEMBL1387694	-5.4	4537:	CHEMBL3099880	-5.3
4436:	eMol16370291	-5.4	4487:	eMol1675470	-5.4	4538:	eMol1237709	-5.3
4437:	eMol24471123	-5.4	4488:	eMol1683990	-5.4	4539:	eMol16809465	-5.3
4438:	eMol2588265	-5.4	4489:	eMol17487547	-5.4	4540:	eMol17485449	-5.3
4439:	eMol277677811	-5.4	4490:	eMol2597902	-5.4	4541:	eMol18836616	-5.3
4440:	eMol43368571	-5.4	4491:	eMol27045547	-5.4	4542:	eMol2010041	-5.3
4441:	eMol5538278	-5.4	4492:	eMol27485948	-5.4	4543:	eMol3303379	-5.3
4442:	eMol7297608	-5.4	4493:	eMol3139546	-5.4	4544:	eMol3521216	-5.3
4443:	CHEMBL1573972	-5.4	4494:	eMol31397858	-5.4	4545:	eMol36015444	-5.3
4444:	eMol11908173	-5.4	4495:	eMol3393477	-5.4	4546:	eMol4551419	-5.3
4445:	eMol11943144	-5.4	4496:	eMol36015834	-5.4	4547:	eMol5444861	-5.3
4446:	eMol17014756	-5.4	4497:	eMol36016544	-5.4	4548:	eMol5538554	-5.3
4447:	eMol27187264	-5.4	4498:	eMol36016560	-5.4	4549:	eMol7279368	-5.3
4448:	eMol2889626	-5.4	4499:	eMol36016588	-5.4	4550:	CHEMBL3402872	-5.3
4449:	eMol2992808	-5.4	4500:	CHEMBL3251275	-5.4	4551:	eMol11935855	-5.3
4450:	eMol3248581	-5.4	4501:	CHEMBL3303239	-5.4	4552:	eMol13496736	-5.3
4451:	eMol36015194	-5.4	4502:	eMol11070671	-5.4	4553:	eMol32245321	-5.3
4452:	eMol43754741	-5.4	4503:	eMol16379435	-5.4	4554:	eMol3239805	-5.3
4453:	eMol15983236	-5.4	4504:	eMol1993386	-5.4	4555:	eMol579118	-5.3
4454:	eMol27391996	-5.4	4505:	eMol27372647	-5.4	4556:	CHEMBL3443924	-5.3
4455:	eMol2891570	-5.4	4506:	eMol2992522	-5.4	4557:	eMol2992834	-5.3
4456:	eMol30576050	-5.4	4507:	eMol43749015	-5.4	4558:	eMol30081384	-5.3
4457:	eMol31364087	-5.4	4508:	eMol44058047	-5.4	4559:	eMol36015362	-5.3
4458:	eMol31758386	-5.4	4509:	eMol6779880	-5.4	4560:	eMol36015380	-5.3
4459:	eMol3426910	-5.4	4510:	eMol7259888	-5.4	4561:	eMol36015828	-5.3
4460:	eMol36015378	-5.4	4511:	CHEMBL1196711	-5.3	4562:	eMol43753953	-5.3
4461:	eMol36015680	-5.4	4512:	CHEMBL1424773	-5.3	4563:	eMol936600	-5.3
4462:	eMol36015830	-5.4	4513:	CHEMBL557974	-5.3	4564:	CHEMBL1452604	-5.3
4463:	eMol43731224	-5.4	4514:	eMol11070944	-5.3	4565:	eMol27485924	-5.3
4434:	eMol8066827	-5.4	4485:	CHEMBL1346627	-5.4	4536:	eMol684044	-5.3

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
4566:	eMol34103616	-5.3	4617	eMol2002540	-5.2	4668	eMol3648258	-5.2
4567:	eMol36016534	-5.3	4618	eMol20381014	-5.2	4669	eMol43747071	-5.2
4568:	eMol3651748	-5.3	4619	eMol2992534	-5.2	4670	eMol560063	-5.2
4569:	eMol5538602	-5.3	4620	eMol31758600	-5.2	4671	eMol587500	-5.2
4570:	eMol566474	-5.3	4621	eMol32246589	-5.2	4672	eMol6844634	-5.2
4571:	CHEMBL1325614	-5.3	4622	eMol36015440	-5.2	4673	CHEMBL1365141	-5.2
4572:	CHEMBL3417629	-5.3	4623	eMol36016674	-5.2	4674	eMol11939763	-5.2
4573:	eMol12034280	-5.3	4624	eMol36734167	-5.2	4675	eMol13857973	-5.2
4574:	eMol13857885	-5.3	4625	eMol5538428	-5.2	4676	eMol16679965	-5.2
4575:	eMol30739818	-5.3	4626	eMol5538740	-5.2	4677	eMol2265196	-5.2
4576:	eMol33341133	-5.3	4627	eMol5538868	-5.2	4678	eMol2992510	-5.2
4577:	eMol36016656	-5.3	4628	eMol679604	-5.2	4679	eMol3082150	-5.2
4578:	eMol43686130	-5.3	4629	eMol936278	-5.2	4680	eMol3254728	-5.2
4579:	eMol5444461	-5.3	4630:	CHEMBL1495305	-5.2	4681	eMol36015816	-5.2
4580:	eMol5444743	-5.3	4631:	CHEMBL1525394	-5.2	4682	eMol36015860	-5.2
4581:	eMol684462	-5.3	4632	eMol1372989	-5.2	4683	eMol44131054	-5.2
4582:	eMol1415332	-5.3	4633	eMol15983294	-5.2	4684	eMol5445009	-5.2
4583:	eMol2169394	-5.3	4634	eMol16385722	-5.2	4685	CHEMBL1336366	-5.2
4584:	eMol27187412	-5.3	4635	eMol1676313	-5.2	4686	eMol16370277	-5.2
4585:	eMol36015780	-5.3	4636	eMol17191180	-5.2	4687	eMol16390223	-5.2
4586:	eMol4935076	-5.3	4637	eMol36016672	-5.2	4688	eMol3115949	-5.2
4587:	eMol5538556	-5.3	4638	eMol36619339	-5.2	4689	eMol3331199	-5.2
4588:	eMol5538702	-5.3	4639	eMol43747041	-5.2	4690	eMol36015728	-5.2
4589:	eMol27490291	-5.3	4640	eMol4878607	-5.2	4691	eMol43789559	-5.2
4590:	eMol3061651	-5.3	4641	eMol5444935	-5.2	4692	CHEMBL2297261	-5.2
4591:	eMol36015352	-5.3	4642	eMol5538754	-5.2	4693	eMol1027541	-5.2
4592:	eMol36015724	-5.3	4643	eMol9931089	-5.2	4694	eMol16379645	-5.2
4593:	eMol36319682	-5.3	4644	eMol24113059	-5.2	4695	eMol16379767	-5.2
4594:	eMol36733935	-5.3	4645	eMol32247521	-5.2	4696	eMol27485960	-5.2
4595:	eMol43368191	-5.3	4646	eMol3775394	-5.2	4697	eMol3177115	-5.2
4596:	eMol43781742	-5.3	4647	eMol43744984	-5.2	4698	eMol33751194	-5.2
4597:	eMol5538282	-5.3	4648	eMol48997350	-5.2	4699	eMol36733949	-5.2
4598:	eMol7278884	-5.3	4649	eMol5444629	-5.2	4700	eMol43013812	-5.2
4599:	CHEMBL1421596	-5.3	4650	eMol100986457	-5.2	4701	eMol44458391	-5.2
4600:	eMol16387248	-5.3	4651	eMol18832597	-5.2	4702	eMol579214	-5.2
4601:	eMol16407996	-5.3	4652	eMol27492270	-5.2	4703	eMol13542782	-5.2
4602:	eMol3037268	-5.3	4653	eMol3245754	-5.2	4704	eMol1454684	-5.2
4603:	eMol3247263	-5.3	4654	eMol3331425	-5.2	4705	eMol24083372	-5.2
4604:	eMol43744870	-5.3	4655	eMol36015622	-5.2	4706	eMol2459471	-5.2
4605:	eMol5444749	-5.3	4656	eMol44089932	-5.2	4707	eMol3245382	-5.2
4606:	eMol5538772	-5.3	4657	eMol4419462	-5.2	4708	eMol36015706	-5.2
4607:	eMol1114358	-5.2	4658	eMol5538426	-5.2	4709	eMol5444395	-5.2
4608:	eMol16379753	-5.2	4659	eMol7281382	-5.2	4710	eMol588046	-5.2
4609:	eMol3118150	-5.2	4660:	CHEMBL1503758	-5.2	4711	eMol7260062	-5.2
4610:	eMol3418906	-5.2	4661:	CHEMBL3932469	-5.2	4712	eMol7274732	-5.2
4611:	eMol36015536	-5.2	4662	eMol11908179	-5.2	4713	eMol16379859	-5.1
4612:	eMol36015994	-5.2	4663	eMol1674472	-5.2	4714	eMol1677693	-5.1
4613:	eMol36016670	-5.2	4664	eMol1682797	-5.2	4715	eMol24100950	-5.1
4614:	eMol7284830	-5.2	4665	eMol3001067	-5.2	4716	eMol5785086	-5.1
4615:	eMol16390201	-5.2	4666	eMol31758466	-5.2	4717	eMol7282482	-5.1
4616:	eMol1678749	-5.2	4667	eMol3176687	-5.2	4718	eMol98766494	-5.1
4587:	eMol5538556	-5.3	4638:	eMol36619339	-5.2	4689	eMol3331199	-5.2

Table S1. Continued.

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
4719:	CHEMBL3942503	-5.1	4770:	eMol36015624	-5.1	4821:	eMol1035461	-5.0
4720:	eMol115038	-5.1	4771:	eMol43747053	-5.1	4822:	eMol1448879	-5.0
4721:	eMol18813395	-5.1	4772:	eMol5538342	-5.1	4823:	eMol179170454	-5.0
4722:	eMol24657929	-5.1	4773:	eMol624285	-5.1	4824:	eMol29917277	-5.0
4723:	eMol3380771	-5.1	4774:	eMol13480687	-5.1	4825:	eMol3523628	-5.0
4724:	eMol36010363	-5.1	4775:	eMol29917279	-5.1	4826:	eMol5538888	-5.0
4725:	eMol7291634	-5.1	4776:	eMol3059181	-5.1	4827:	eMol16379829	-5.0
4726:	CHEMBL3251277	-5.1	4777:	eMol49213685	-5.1	4828:	eMol23996477	-5.0
4727:	CHEMBL3302547	-5.1	4778:	eMol5538756	-5.1	4829:	eMol3032190	-5.0
4728:	eMol15983244	-5.1	4779:	CHEMBL43621	-5.1	4830:	eMol3200820	-5.0
4729:	eMol32246675	-5.1	4780:	eMol11821373	-5.1	4831:	eMol36016668	-5.0
4730:	eMol3245798	-5.1	4781:	eMol23999589	-5.1	4832:	eMol48304474	-5.0
4731:	eMol3523620	-5.1	4782:	eMol2709467	-5.1	4833:	eMol13512590	-5.0
4732:	eMol3648256	-5.1	4783:	eMol3249517	-5.1	4834:	eMol29274280	-5.0
4733:	eMol50319429	-5.1	4784:	eMol34126726	-5.1	4835:	eMol43754827	-5.0
4734:	eMol5538276	-5.1	4785:	eMol3480399	-5.1	4836:	eMol44073147	-5.0
4735:	eMol8455240	-5.1	4786:	eMol3503186	-5.1	4837:	eMol3493996	-5.0
4736:	eMol1319937	-5.1	4787:	eMol36015986	-5.1	4838:	eMol36015336	-5.0
4737:	eMol3048384	-5.1	4788:	eMol43744964	-5.1	4839:	eMol36015782	-5.0
4738:	eMol32245889	-5.1	4789:	eMol11864402	-5.0	4840:	eMol3648252	-5.0
4739:	eMol36016618	-5.1	4790:	eMol3112215	-5.0	4841:	eMol2409053	-5.0
4740:	eMol43745176	-5.1	4791:	eMol31758416	-5.0	4842:	eMol27485956	-5.0
4741:	eMol23999013	-5.1	4792:	eMol32247467	-5.0	4843:	eMol29917275	-5.0
4742:	eMol2992486	-5.1	4793:	eMol36016130	-5.0	4844:	eMol33342600	-5.0
4743:	eMol3214250	-5.1	4794:	eMol43013800	-5.0	4845:	eMol9959049	-5.0
4744:	eMol32246429	-5.1	4795:	eMol43743404	-5.0	4846:	CHEMBL1543282	-4.9
4745:	eMol3652086	-5.1	4796:	eMol76019788	-5.0	4847:	eMol1454660	-4.9
4746:	eMol5444397	-5.1	4797:	CHEMBL1976112	-5.0	4848:	eMol34206915	-4.9
4747:	eMol6833538	-5.1	4798:	CHEMBL601797	-5.0	4849:	eMol3658197	-4.9
4748:	eMol7283790	-5.1	4799:	eMol17014760	-5.0	4850:	eMol29645389	-4.9
4749:	CHEMBL1351050	-5.1	4800:	eMol2001487	-5.0	4851:	eMol43013872	-4.9
4750:	eMol13520613	-5.1	4801:	eMol3091469	-5.0	4852:	eMol44080938	-4.9
4751:	eMol31758260	-5.1	4802:	eMol3376021	-5.0	4853:	eMol5538486	-4.9
4752:	eMol3252718	-5.1	4803:	CHEMBL1388432	-5.0	4854:	CHEMBL1386751	-4.9
4753:	eMol3523624	-5.1	4804:	eMol16385660	-5.0	4855:	CHEMBL1701256	-4.9
4754:	eMol43780908	-5.1	4805:	eMol2889322	-5.0	4856:	eMol17487551	-4.9
4755:	eMol4422602	-5.1	4806:	eMol2992528	-5.0	4857:	eMol2881728	-4.9
4756:	eMol4459106	-5.1	4807:	eMol36015500	-5.0	4858:	eMol32236794	-4.9
4757:	eMol6833971	-5.1	4808:	eMol36016528	-5.0	4859:	eMol5444551	-4.9
4758:	eMol13539183	-5.1	4809:	eMol16379787	-5.0	4860:	eMol15089032	-4.9
4759:	eMol2167461	-5.1	4810:	eMol31364085	-5.0	4861:	eMol36898088	-4.9
4760:	eMol3651756	-5.1	4811:	eMol32246255	-5.0	4862:	eMol43730460	-4.9
4761:	eMol5538438	-5.1	4812:	eMol43691630	-5.0	4863:	eMol5444447	-4.9
4762:	eMol5538742	-5.1	4813:	eMol4904340	-5.0	4864:	eMol5444733	-4.9
4763:	eMol11465601	-5.1	4814:	CHEMBL1500721	-5.0	4865:	eMol587738	-4.9
4764:	eMol16813507	-5.1	4815:	CHEMBL3919247	-5.0	4866:	CHEMBL3910321	-4.9
4765:	eMol2264316	-5.1	4816:	eMol11329944	-5.0	4867:	eMol31653504	-4.9
4766:	eMol316832342	-5.1	4817:	eMol17014768	-5.0	4868:	eMol32246579	-4.9
4767:	eMol32246257	-5.1	4818:	eMol18922892	-5.0	4869:	eMol36015636	-4.9
4768:	eMol33380364	-5.1	4819:	eMol43746043	-5.0	4870:	eMol36016146	-4.9
4769:	eMol36015504	-5.1	4820:	CHEMBL1452793	-5.0	4871:	eMol50340675	-4.9
4740:	eMol43745176	-5.1	4791:	eMol31758416	-5.0	4842:	eMol27485956	-5.0

Table S1. *Continued.*

No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)	No.	Compound Name/Code	Docking Score (kcal/mol)
4872	eMol5514743	-4.9	4915	eMol7276588	-4.8	4958	eMol2048663	-4.6
4873	eMol29942864	-4.9	4916	eMol36733899	-4.8	4959	eMol36015726	-4.6
4874	eMol36015626	-4.9	4917	CHEMBL1313582	-4.8	4960	eMol11952112	-4.6
4875	eMol36016008	-4.9	4918	eMol3048390	-4.8	4961	eMol16379883	-4.5
4876	eMol36887773	-4.9	4919	eMol5444751	-4.8	4962	eMol43691660	-4.5
4877	eMol43747101	-4.9	4920	eMol5538494	-4.8	4963	eMol5538884	-4.5
4878	eMol98058053	-4.9	4921	eMol5538738	-4.8	4964	eMol24006030	-4.5
4879	eMol36015732	-4.9	4922	eMol560365	-4.8	4965	eMol1676695	-4.5
4880	eMol43757853	-4.9	4923	CHEMBL1311188	-4.8	4966	eMol36015856	-4.5
4881	eMol11681118	-4.9	4924	eMol2992480	-4.8	4967	eMol8238421	-4.5
4882	eMol16379853	-4.9	4925	eMol1684765	-4.7	4968	eMol1178884	-4.5
4883	eMol2501901	-4.9	4926	eMol3145070	-4.7	4969	eMol27348310	-4.5
4884	eMol2992824	-4.9	4927	eMol3512950	-4.7	4970	eMol1266023	-4.5
4885	eMol32245269	-4.9	4928	eMol11747245	-4.7	4971	eMol5538892	-4.5
4886	eMol679700	-4.9	4929	eMol17014766	-4.7	4972	eMol32246633	-4.4
4887	eMol24110832	-4.8	4930	eMol16799937	-4.7	4973	eMol29274282	-4.4
4888	eMol31758564	-4.8	4931	eMol30288722	-4.7	4974	eMol43415245	-4.4
4889	eMol32245319	-4.8	4932	eMol32246207	-4.7	4975	eMol48312056	-4.4
4890	eMol32247457	-4.8	4933	eMol1454680	-4.7	4976	eMol5785084	-4.4
4891	eMol3419044	-4.8	4934	eMol16378089	-4.7	4977	eMol43746069	-4.4
4892	eMol5514745	-4.8	4935	eMol5444411	-4.7	4978	eMol30647010	-4.3
4902	eMol4448867	-4.8	4945	CHEMBL1406150	-4.6	4988	eMol17199912	-4.2
4903	eMol5444829	-4.8	4946	eMol1114366	-4.6	4989	CHEMBL3928151	-4.1
4904	eMol5444859	-4.8	4947	eMol16378097	-4.6	4990	CHEMBL1525899	-4.1
4905	eMol29274296	-4.8	4948	eMol3254458	-4.6	4991	eMol1471822	-4.1
4906	eMol5538890	-4.8	4949	eMol3473340	-4.6	4992	eMol32247517	-4.0
4907	eMol98068785	-4.8	4950	eMol3652896	-4.6	4993	CHEMBL3194843	-4.0
4908	eMol3257328	-4.8	4951	eMol5538910	-4.6	4994	eMol1023917	-4.0
4909	eMol33316910	-4.8	4952	eMol13469491	-4.6	4995	eMol207114346	-4.0
4910	eMol36016680	-4.8	4953	eMol27492328	-4.6	4996	eMol36015960	-4.0
4911	eMol3710762	-4.8	4954	eMol44548742	-4.6	4997	eMol5785216	-4.0
4912	eMol43759025	-4.8	4955	eMol5538894	-4.6	4998	eMol36731517	-3.9
4913	eMol5444435	-4.8	4956	eMol5444403	-4.6	4999	eMol13803787	-3.8
4914	eMol5538246	-4.8	4957	eMol43789551	-4.6	5000	eMol31758544	-3.7

^a Duplicated compounds with identical InChKey could be observed.

Table S2. Estimated conventional and intermediate docking scores (in kcal/mol) for QNZ and the top 1000 potent allosteric inhibitors against mutated PBP2a allosteric site in acidic medium.^a

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
	QNZ	-6.9	-8.0	50	eMol22447774	-8.5	-8.7
1	eMol19266609	-7.9	-9.5	51	eMol19076742	-8.6	-8.7
2	eMol24519694	-9.0	-9.5	52	CHEMBL1215650	-8.5	-8.7
3	eMol26313117	-8.9	-9.4	53	CHEMBL1579061	-8.5	-8.7
4	eMol24389393	-7.9	-9.4	54	eMol26269394	-8.5	-8.7
5	CHEMBL1214717	-9.4	-9.4	55	eMol31781482	-8.7	-8.6
6	eMol29587310	-9.4	-9.4	56	eMol23157132	-8.4	-8.6
7	eMol45585846	-9.4	-9.4	57	CHEMBL1215649	-8.5	-8.6
8	eMol23239806	-9.3	-9.4	58	eMol26196316	-8.5	-8.6
9	CHEMBL1214718	-9.2	-9.3	59	eMol30646140	-7.7	-8.6
10	eMol29597031	-9.2	-9.3	60	eMol72993476	-7.7	-8.6
11	eMol31786896	-8.4	-9.3	61	CHEMBL3818129	-8.5	-8.6
12	eMol45585848	-9.2	-9.3	62	eMol26319231	-8.2	-8.6
13	eMol23186178	-9.1	-9.3	63	eMol300994534	-8.4	-8.6
14	eMol2403964	-8.7	-9.3	64	eMol48938145	-8.4	-8.6
15	eMol19076714	-8.4	-9.2	65	CHEMBL1214713	-8.2	-8.6
16	eMol31297102	-7.9	-9.2	66	CHEMBL1384683	-8.2	-8.6
17	eMol26293960	-8.1	-9.2	67	eMol26270654	-8.2	-8.6
18	eMol19076718	-8.9	-9.1	68	eMol29633913	-7.8	-8.6
19	CHEMBL1534883	-9.0	-9.1	69	eMol33366267	-7.9	-8.6
20	eMol1344114	-9.0	-9.1	70	eMol45622743	-7.8	-8.6
21	eMol18542844	-9.1	-9.1	71	eMol75958504	-7.9	-8.6
22	CHEMBL3819187	-7.8	-9.1	72	eMol23246696	-8.5	-8.6
23	eMol30323633	-9.0	-9.1	73	CHEMBL1558437	-8.2	-8.6
24	CHEMBL1214794	-8.9	-9.0	74	eMol26242050	-8.1	-8.6
25	eMol26196290	-8.9	-9.0	75	eMol30671942	-7.9	-8.5
26	eMol45585824	-8.9	-9.0	76	eMol26242034	-8.2	-8.5
27	CHEMBL1214938	-8.7	-9.0	77	eMol26242042	-7.6	-8.5
28	eMol20375178	-8.7	-9.0	78	eMol23175530	-8.3	-8.5
29	eMol30323569	-8.6	-9.0	79	CHEMBL3805924	-8.3	-8.5
30	CHEMBL3818732	-8.0	-9.0	80	CHEMBL4103504	-8.3	-8.5
31	eMol30341049	-8.8	-8.9	81	eMol24428240	-7.2	-8.5
32	eMol43906045	-8.8	-8.9	82	eMol24519844	-8.4	-8.5
33	eMol26437582	-8.2	-8.9	83	eMol23181799	-8.3	-8.4
34	eMol19076712	-8.9	-8.9	84	eMol26242044	-8.3	-8.4
35	eMol20378769	-8.7	-8.9	85	eMol579568	-8.4	-8.4
36	CHEMBL3818584	-8.3	-8.9	86	eMol23239141	-8.3	-8.4
37	eMol3021959	-7.1	-8.9	87	CHEMBL1215080	-8.4	-8.4
38	eMol18542846	-8.8	-8.8	88	eMol23243407	-8.2	-8.4
39	eMol20342262	-7.9	-8.8	89	eMol43906059	-8.4	-8.4
40	eMol1166007	-8.7	-8.8	90	eMol587826	-8.2	-8.4
41	eMol26242018	-8.0	-8.8	91	eMol588192	-8.2	-8.4
42	eMol19076754	-8.6	-8.8	92	eMol25810077	-7.9	-8.4
43	eMol20337486	-8.8	-8.8	93	eMol27202240	-8.4	-8.4
44	eMol20379909	-8.8	-8.8	94	eMol679826	-8.3	-8.4
45	CHEMBL1215648	-8.6	-8.7	95	CHEMBL3818035	-7.9	-8.4
46	eMol26196326	-8.6	-8.7	96	eMol36912832	-7.9	-8.4
47	eMol45585842	-8.6	-8.7	97	eMol43906055	-8.0	-8.4
48	eMol23241028	-8.6	-8.7	98	eMol18962382	-8.4	-8.4
49	eMol23190351	-7.9	-8.7	99	eMol27202910	-8.3	-8.4

Table S2. *Continued.*

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
100	eMol31532412	-8.3	-8.4	152	eMol681936	-8.2	-8.2
101	eMol25810075	-8.3	-8.4	153	CHEMBL508966	-8.1	-8.2
102	eMol26264570	-8.1	-8.4	154	eMol1755402	-8.0	-8.2
103	eMol26313223	-8.3	-8.4	155	eMol24530483	-8.2	-8.2
104	eMol30248263	-8.0	-8.4	156	eMol26242038	-7.9	-8.2
105	CHEMBL1214647	-8.1	-8.4	157	eMol26320021	-7.4	-8.2
106	eMol679820	-7.2	-8.4	158	eMol566488	-8.1	-8.2
107	CHEMBL1215003	-8.2	-8.3	159	CHEMBL1215578	-8.0	-8.2
108	CHEMBL3817888	-8.1	-8.3	160	CHEMBL3818775	-8.2	-8.2
109	eMol193446288	-8.3	-8.3	161	eMol27252412	-8.1	-8.2
110	eMol27202248	-8.4	-8.3	162	eMol299980544	-8.2	-8.2
111	eMol43906053	-8.2	-8.3	163	eMol679822	-8.0	-8.2
112	CHEMBL3818572	-8.0	-8.3	164	eMol956623	-8.2	-8.2
113	CHEMBL395193	-8.3	-8.3	165	eMol11920256	-8.1	-8.2
114	eMol18542848	-8.3	-8.3	166	eMol23178762	-8.1	-8.2
115	eMol2992792	-8.1	-8.3	167	eMol48982653	-7.7	-8.2
116	eMol6263471	-8.2	-8.3	168	CHEMBL1215797	-8.0	-8.2
117	eMol26242022	-7.9	-8.3	169	eMol18550846	-8.1	-8.2
118	eMol43731476	-7.6	-8.3	170	eMol20377597	-8.0	-8.2
119	eMol46480173	-8.2	-8.3	171	eMol4566508	-7.3	-8.2
120	eMol19076598	-7.3	-8.3	172	eMol26314779	-8.1	-8.2
121	eMol20347873	-8.2	-8.3	173	eMol4558540	-8.0	-8.2
122	eMol206926236	-8.2	-8.3	174	CHEMBL3819481	-7.9	-8.2
123	eMol300094331	-8.2	-8.3	175	eMol20368046	-8.1	-8.2
124	eMol300154219	-7.3	-8.3	176	eMol23147497	-8.1	-8.2
125	eMol25810083	-8.3	-8.3	177	eMol26330545	-8.2	-8.2
126	eMol26242032	-7.9	-8.3	178	eMol29565259	-7.8	-8.2
127	eMol25810071	-8.3	-8.3	179	eMol45585838	-7.8	-8.2
128	eMol46365626	-8.2	-8.3	180	eMol679824	-8.0	-8.2
129	eMol566574	-8.1	-8.3	181	CHEMBL1214648	-8.0	-8.2
130	eMol27406062	-7.8	-8.3	182	CHEMBL1215004	-7.7	-8.2
131	CHEMBL1214935	-8.1	-8.3	183	eMol26242024	-7.7	-8.2
132	CHEMBL3818929	-8.2	-8.3	184	eMol26242026	-7.8	-8.2
133	CHEMBL518358	-8.2	-8.3	185	eMol26242052	-7.3	-8.2
134	eMol43906051	-8.1	-8.3	186	eMol29587306	-7.7	-8.2
135	CHEMBL1214936	-8.2	-8.3	187	eMol45585836	-7.7	-8.2
136	eMol26196312	-8.2	-8.3	188	eMol679556	-8.0	-8.2
137	eMol26314331	-7.5	-8.3	189	CHEMBL3582082	-7.3	-8.1
138	eMol30017880	-7.4	-8.3	190	eMol20361212	-8.1	-8.1
139	eMol45585832	-8.2	-8.3	191	eMol37002179	-7.4	-8.1
140	eMol25819217	-8.3	-8.2	192	eMol4562556	-8.1	-8.1
141	eMol26809774	-8.2	-8.2	193	eMol4578697	-7.3	-8.1
142	eMol27202258	-8.3	-8.2	194	eMol45935562	-7.5	-8.1
143	eMol46490873	-8.1	-8.2	195	eMol565850	-7.0	-8.1
144	eMol26314565	-8.2	-8.2	196	CHEMBL1601398	-8.0	-8.1
145	eMol1088331	-8.2	-8.2	197	CHEMBL3582080	-7.9	-8.1
146	eMol13856171	-8.0	-8.2	198	eMol2507718	-8.0	-8.1
147	eMol29653471	-8.2	-8.2	199	eMol256911679	-8.0	-8.1
148	eMol30323345	-9.8	-8.2	200	eMol27202348	-8.1	-8.1
149	eMol43731530	-7.3	-8.2	201	eMol301527162	-8.0	-8.1
150	eMol45622745	-8.2	-8.2	202	eMol4518648	-8.1	-8.1
151	eMol46480165	-8.2	-8.2	203	eMol4552519	-8.0	-8.1

Table S2. *Continued.*

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
204	eMol4446697	-7.7	-8.1	256	eMol25810089	-8.0	-8.0
205	eMol4577396	-8.0	-8.1	257	eMol26242040	-7.8	-8.0
206	eMol177199339	-7.9	-8.1	258	eMol26242048	-7.6	-8.0
207	eMol27202252	-8.0	-8.1	259	eMol26309353	-7.9	-8.0
208	eMol300994251	-7.9	-8.1	260	eMol4381378	-7.9	-8.0
209	eMol36912834	-8.0	-8.1	261	eMol4581546	-7.8	-8.0
210	eMol48768479	-7.9	-8.1	262	eMol50556474	-7.5	-8.0
211	eMol579756	-8.0	-8.1	263	CHEMBL2259942	-7.8	-8.0
212	eMol580072	-8.0	-8.1	264	CHEMBL3819363	-7.4	-8.0
213	eMol4566756	-7.9	-8.1	265	eMol26311024	-7.7	-8.0
214	eMol27202760	-8.0	-8.1	266	eMol43757885	-7.6	-8.0
215	eMol27202916	-7.2	-8.1	267	eMol679670	-8.0	-8.0
216	eMol29634797	-7.6	-8.1	268	CHEMBL1632342	-7.2	-8.0
217	CHEMBL1214941	-8.6	-8.1	269	eMol206910852	-7.9	-8.0
218	eMol25784531	-7.1	-8.1	270	eMol233046940	-7.7	-8.0
219	eMol27091674	-8.0	-8.1	271	eMol26313085	-7.5	-8.0
220	eMol679550	-7.9	-8.1	272	eMol46363574	-7.9	-8.0
221	CHEMBL1443074	-8.0	-8.1	273	eMol679552	-7.9	-8.0
222	eMol18940433	-8.0	-8.1	274	CHEMBL3818377	-8.4	-8.0
223	eMol27091498	-8.0	-8.1	275	eMol206911267	-7.9	-8.0
224	eMol20378767	-7.9	-8.1	276	eMol46480254	-7.9	-8.0
225	eMol27091442	-7.9	-8.1	277	eMol679664	-8.0	-8.0
226	eMol565798	-8.1	-8.1	278	eMol26263266	-7.0	-7.9
227	eMol29638777	-7.8	-8.1	280	eMol4579587	-7.7	-7.9
228	eMol4397966	-8.0	-8.1	281	eMol46210804	-7.6	-7.9
229	eMol45622749	-7.8	-8.1	282	eMol25908513	-7.9	-7.9
230	eMol579718	-8.0	-8.1	283	eMol27202994	-7.9	-7.9
231	eMol179164947	-7.8	-8.0	279	eMol4116278	-7.7	-7.9
232	eMol27202242	-8.0	-8.0	284	eMol4552457	-7.8	-7.9
233	eMol27202948	-7.4	-8.0	285	eMol565168	-8.6	-7.9
234	eMol18551342	-8.0	-8.0	286	eMol1035565	-7.9	-7.9
235	eMol206992517	-8.0	-8.0	287	eMol26259383	-7.3	-7.9
236	eMol25966646	-7.9	-8.0	288	eMol679554	-7.8	-7.9
237	eMol4549830	-7.3	-8.0	289	eMol26315830	-7.8	-7.9
238	CHEMBL3805841	-7.7	-8.0	290	eMol46480212	-7.8	-7.9
239	eMol1035521	-7.9	-8.0	291	eMol4726858	-7.6	-7.9
240	CHEMBL1214934	-7.0	-8.0	292	eMol566288	-7.8	-7.9
241	eMol26262168	-7.0	-8.0	293	eMol587628	-7.9	-7.9
242	eMol28321864	-8.0	-8.0	294	CHEMBL3817906	-7.7	-7.9
243	eMol681814	-7.9	-8.0	295	CHEMBL3819338	-7.6	-7.9
244	CHEMBL1215082	-7.4	-8.0	296	eMol24313582	-7.8	-7.9
245	CHEMBL485839	-8.0	-8.0	297	eMol26242046	-8.0	-7.9
246	eMol43906047	-7.9	-8.0	298	eMol27202958	-7.7	-7.9
247	eMol43906057	-7.4	-8.0	299	eMol27202992	-7.8	-7.9
248	eMol46367311	-7.8	-8.0	300	eMol4555657	-7.8	-7.9
249	eMol581308	-7.9	-8.0	301	eMol4572924	-7.8	-7.9
250	CHEMBL2259943	-7.9	-8.0	302	eMol56752349	-7.9	-7.9
251	eMol4581322	-8.0	-8.0	303	eMol587646	-7.5	-7.9
252	CHEMBL2259944	-8.0	-8.0	304	eMol43745241	-7.5	-7.9
253	eMol20342220	-7.8	-8.0	305	eMol4389171	-7.8	-7.9
254	eMol20342278	-7.9	-8.0	306	eMol579044	-7.4	-7.9
255	eMol25810001	-7.9	-8.0	307	CHEMBL1528362	-7.7	-7.9

Table S2. *Continued.*

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
308	eMol179164959	-7.9	-7.9	360	eMol4740224	-7.8	-7.8
309	eMol19076348	-7.7	-7.9	361	eMol588388	-7.6	-7.8
310	CHEMBL3819186	-7.8	-7.9	362	eMol561887	-7.8	-7.8
311	eMol26251042	-7.8	-7.9	363	eMol23202652	-7.8	-7.8
312	CHEMBL3819597	-7.8	-7.9	364	CHEMBL3818582	-7.1	-7.8
313	eMol26311238	-7.7	-7.9	365	eMol1429356	-7.3	-7.8
314	eMol4555647	-7.8	-7.9	366	eMol17203477	-7.5	-7.8
315	CHEMBL1212961	-7.8	-7.9	367	eMol19076364	-7.7	-7.8
316	eMol18550688	-7.8	-7.9	368	eMol46365712	-7.6	-7.8
317	eMol19267414	-7.8	-7.9	369	eMol566118	-7.5	-7.8
318	eMol193447787	-7.5	-7.9	370	eMol679668	-7.5	-7.8
319	eMol24029848	-7.5	-7.9	371	eMol8267101	-7.6	-7.8
320	eMol26242054	-7.4	-7.9	372	eMol26312078	-7.5	-7.8
321	eMol300136046	-7.8	-7.9	373	eMol300445092	-7.7	-7.8
322	eMol681860	-7.7	-7.9	374	eMol30665797	-7.7	-7.8
323	CHEMBL1215006	-7.3	-7.8	375	eMol43744848	-7.7	-7.8
324	eMol20342268	-7.7	-7.8	376	CHEMBL3817850	-7.7	-7.8
325	eMol24520354	-7.8	-7.8	377	eMol20342205	-7.7	-7.8
326	eMol27202956	-8.1	-7.8	378	eMol27202264	-7.7	-7.8
327	eMol299966748	-7.3	-7.8	379	eMol206985996	-7.7	-7.7
328	eMol314064301	-7.8	-7.8	380	eMol25965034	-7.7	-7.7
329	eMol50301465	-7.2	-7.8	381	eMol26310961	-7.7	-7.7
330	CHEMBL1215081	-7.9	-7.8	382	eMol27202268	-7.6	-7.7
331	CHEMBL1215803	-7.6	-7.8	383	eMol43906067	-7.5	-7.7
332	CHEMBL3819140	-7.6	-7.8	384	eMol25810163	-7.6	-7.7
333	eMol206970196	-7.8	-7.8	385	eMol3103759	-7.6	-7.7
334	eMol24525196	-7.7	-7.8	386	eMol58034831	-7.7	-7.7
335	eMol26196328	-7.9	-7.8	387	eMol581076	-7.4	-7.7
336	eMol4090808	-7.3	-7.8	388	eMol179165002	-7.7	-7.7
337	eMol45585844	-7.9	-7.8	389	eMol179165014	-7.7	-7.7
338	eMol4579154	-7.8	-7.8	390	eMol20337448	-7.2	-7.7
339	eMol4580802	-7.7	-7.8	391	eMol23249723	-7.7	-7.7
340	eMol562493	-7.7	-7.8	392	eMol3318312	-7.6	-7.7
341	eMol679666	-7.7	-7.8	393	eMol588272	-7.4	-7.7
342	CHEMBL1214861	-7.8	-7.8	394	eMol26141700	-7.7	-7.7
343	CHEMBL1371074	-7.7	-7.8	395	eMol27202980	-7.4	-7.7
344	eMol23208796	-7.2	-7.8	396	CHEMBL1214645	-7.3	-7.7
345	eMol24511821	-7.7	-7.8	397	CHEMBL517897	-7.7	-7.7
346	eMol25813417	-7.8	-7.8	398	eMol25955419	-7.7	-7.7
347	eMol27202742	-7.7	-7.8	399	eMol27202996	-7.3	-7.7
348	eMol566380	-7.9	-7.8	400	eMol7667302	-7.7	-7.7
349	CHEMBL323866	-7.6	-7.8	401	eMol935898	-7.2	-7.7
350	eMol208103615	-7.8	-7.8	402	CHEMBL485838	-7.6	-7.7
351	eMol26242036	-7.4	-7.8	403	eMol26189153	-7.4	-7.7
352	eMol35699388	-7.2	-7.8	404	eMol26356948	-7.4	-7.7
353	eMol35717814	-7.3	-7.8	405	eMol588168	-7.3	-7.7
354	eMol4413761	-7.7	-7.8	406	eMol27203000	-7.4	-7.7
355	CHEMBL2403015	-7.8	-7.8	407	eMol43745056	-7.3	-7.7
356	CHEMBL3819445	-8.1	-7.8	408	eMol25810081	-7.1	-7.7
357	eMol16374637	-7.5	-7.8	409	eMol3060078	-7.6	-7.7
358	eMol1751766	-7.5	-7.8	410	eMol45701494	-7.5	-7.7
359	eMol3427847	-7.5	-7.8	411	eMol16683412	-7.5	-7.7
329	eMol50301465	-7.2	-7.8	381	eMol26310961	-7.7	-7.7

Table S2. *Continued.*

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
412	eMol26405201	-7.5	-7.7	464	eMol43730464	-7.2	-7.6
413	eMol27202262	-7.6	-7.7	465	eMol4551561	-7.5	-7.6
414	eMol43731776	-7.1	-7.7	466	eMol4577787	-7.6	-7.6
415	eMol565754	-7.5	-7.7	467	eMol588256	-7.5	-7.6
416	eMol233088901	-7.5	-7.6	468	eMol9919488	-7.4	-7.6
417	eMol4574833	-7.6	-7.6	469	CHEMBL117642	-7.4	-7.6
418	eMol1675430	-7.6	-7.6	470	CHEMBL511010	-7.4	-7.6
419	eMol1764190	-7.3	-7.6	471	eMol25896479	-7.5	-7.6
420	eMol25784115	-7.6	-7.6	472	eMol43906063	-7.9	-7.6
421	eMol32369766	-7.6	-7.6	473	eMol46400681	-7.5	-7.6
422	CHEMBL3818012	-7.5	-7.6	474	eMol8238281	-7.3	-7.6
423	CHEMBL520033	-7.5	-7.6	475	CHEMBL1994876	-7.4	-7.5
424	eMol27202960	-7.5	-7.6	476	CHEMBL250917	-7.5	-7.5
425	eMol4075283	-7.3	-7.6	477	CHEMBL3817957	-7.5	-7.5
426	eMol4587779	-7.5	-7.6	478	eMol1679768	-7.5	-7.5
427	eMol956409	-7.6	-7.6	479	eMol27202984	-7.3	-7.5
428	eMol24116475	-7.5	-7.6	480	eMol4480890	-7.5	-7.5
429	eMol26327269	-7.6	-7.6	481	eMol45708568	-7.2	-7.5
430	eMol32812942	-7.4	-7.6	482	eMol1025907	-7.4	-7.5
431	eMol6753441	-7.5	-7.6	483	eMol18940061	-7.5	-7.5
432	eMol944638	-7.6	-7.6	484	eMol206875270	-7.4	-7.5
433	eMol1429358	-7.5	-7.6	485	eMol299962831	-7.4	-7.5
434	eMol179177638	-7.4	-7.6	486	CHEMBL1584455	-7.5	-7.5
435	eMol25909178	-7.7	-7.6	487	CHEMBL3819326	-7.5	-7.5
436	eMol46480052	-7.6	-7.6	488	eMol23250559	-7.5	-7.5
437	CHEMBL3818704	-7.4	-7.6	489	eMol25810127	-7.5	-7.5
438	CHEMBL397391	-7.3	-7.6	490	eMol4386746	-7.5	-7.5
439	eMol32246523	-7.2	-7.6	491	eMol45944068	-7.5	-7.5
440	eMol561655	-7.3	-7.6	492	CHEMBL1499977	-7.4	-7.5
441	eMol588102	-7.6	-7.6	493	CHEMBL3805023	-7.4	-7.5
442	eMol7635480	-7.6	-7.6	494	CHEMBL462179	-7.9	-7.5
443	CHEMBL114364	-7.5	-7.6	495	eMol1040103	-7.5	-7.5
444	eMol18958642	-7.6	-7.6	496	eMol181128729	-7.4	-7.5
445	eMol24058094	-7.4	-7.6	497	eMol19266607	-7.5	-7.5
446	eMol46509913	-7.1	-7.6	498	eMol25937897	-7.4	-7.5
447	eMol46509917	-7.6	-7.6	499	eMol26255667	-7.5	-7.5
448	eMol5779489	-7.6	-7.6	500	eMol27202250	-7.4	-7.5
449	eMol587808	-7.4	-7.6	501	eMol27202902	-7.4	-7.5
450	eMol588228	-7.2	-7.6	502	eMol2993022	-7.4	-7.5
451	CHEMBL117438	-7.2	-7.6	503	eMol300014864	-7.5	-7.5
452	CHEMBL1423402	-7.1	-7.6	504	eMol46479990	-7.5	-7.5
453	eMol206987969	-7.5	-7.6	505	eMol565838	-7.3	-7.5
454	eMol2130046	-7.2	-7.6	506	CHEMBL116817	-7.2	-7.5
455	eMol36904288	-7.1	-7.6	507	eMol206908008	-7.5	-7.5
456	eMol4448933	-7.5	-7.6	508	eMol206985560	-7.5	-7.5
457	eMol5444969	-7.2	-7.6	509	eMol24520756	-7.4	-7.5
458	eMol935130	-7.5	-7.6	510	eMol25902291	-7.2	-7.5
459	CHEMBL1214868	-7.6	-7.6	511	eMol276247970	-7.3	-7.5
460	CHEMBL3818515	-7.5	-7.6	512	eMol300990951	-7.3	-7.5
461	eMol20377433	-7.6	-7.6	513	eMol3317346	-7.2	-7.5
462	eMol26683947	-7.6	-7.6	514	eMol4485131	-7.3	-7.5
463	eMol28321866	-7.5	-7.6	515	eMol4725672	-7.4	-7.5

Table S2. *Continued.*

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
516:	CHEMBL1360793	-7.4	-7.5	568	eMol4706083	-7.2	-7.4
517:	CHEMBL602627	-7.5	-7.5	569	eMol16352353	-7.4	-7.4
518:	eMol20356176	-7.4	-7.5	570	eMol24519100	-7.0	-7.4
519:	eMol25816251	-7.5	-7.5	571	eMol26327656	-7.4	-7.4
520:	eMol27091590	-7.3	-7.5	572	eMol27338418	-7.4	-7.4
521:	eMol4521223	-7.4	-7.5	573	eMol46210806	-7.4	-7.4
522:	eMol4567258	-7.5	-7.5	574	eMol48597407	-7.1	-7.4
523:	eMol45935466	-7.5	-7.5	575:	CHEMBL3818933	-7.3	-7.4
524:	eMol684240	-7.3	-7.5	576	eMol1324430	-7.3	-7.4
525:	CHEMBL1988177	-7.4	-7.5	577	eMol18551352	-7.2	-7.4
526:	eMol25903079	-7.4	-7.5	578	eMol2166708	-7.1	-7.4
527:	eMol25965334	-7.4	-7.5	579	eMol23246986	-7.2	-7.4
528:	eMol26250892	-7.3	-7.5	580	eMol2385157	-7.3	-7.4
529:	eMol45928112	-7.4	-7.5	581	eMol25902329	-7.4	-7.4
530:	eMol46528447	-7.5	-7.5	582	eMol26219237	-7.2	-7.4
531:	CHEMBL116408	-7.3	-7.5	583	eMol26246365	-7.4	-7.4
532:	eMol20354197	-7.4	-7.5	584	eMol4572232	-7.1	-7.4
533:	eMol2880336	-7.3	-7.5	585	eMol935636	-7.2	-7.4
534:	eMol49384601	-7.5	-7.5	586:	CHEMBL3805378	-7.4	-7.4
535:	eMol75932399	-7.4	-7.5	587:	CHEMBL3819459	-7.0	-7.4
536:	eMol20337444	-7.5	-7.5	588:	CHEMBL3819532	-7.4	-7.4
537:	eMol24419686	-7.2	-7.5	589	eMol25903125	-7.4	-7.4
538:	eMol27202290	-7.5	-7.5	590	eMol32812998	-7.1	-7.4
539:	eMol3535618	-7.5	-7.5	591	eMol32813226	-7.2	-7.4
540:	eMol579714	-7.3	-7.5	592	eMol32813234	-7.2	-7.4
541:	eMol24526444	-7.3	-7.5	593	eMol46479912	-7.4	-7.4
542:	eMol27187406	-7.5	-7.5	594	eMol4934666	-7.4	-7.4
543:	eMol27202402	-7.4	-7.5	595	eMol936420	-7.1	-7.4
544:	eMol31760166	-7.2	-7.5	596:	CHEMBL1402619	-7.4	-7.4
545:	eMol46480026	-7.4	-7.5	597:	CHEMBL3818910	-7.3	-7.4
546:	eMol46480194	-7.7	-7.5	598	eMol1040791	-7.3	-7.4
547:	eMol2408165	-7.1	-7.4	599	eMol16351683	-7.4	-7.4
548:	eMol33346433	-7.1	-7.4	600	eMol206921779	-7.2	-7.4
549:	eMol565478	-7.4	-7.4	601	eMol25810171	-7.4	-7.4
550:	CHEMBL455639	-7.3	-7.4	602	eMol26324339	-7.3	-7.4
551:	eMol1149869	-7.0	-7.4	603	eMol27202936	-7.4	-7.4
552:	eMol18550714	-7.2	-7.4	604	eMol4739467	-7.4	-7.4
553:	eMol23247039	-7.4	-7.4	605	eMol72578631	-7.0	-7.4
554:	eMol24524408	-7.4	-7.4	606	eMol1678605	-7.3	-7.4
555:	eMol4708971	-7.3	-7.4	607	eMol19076750	-7.3	-7.4
556:	eMol588158	-7.3	-7.4	608	eMol24520553	-7.1	-7.4
557:	eMol936632	-7.2	-7.4	609	eMol24538139	-7.3	-7.4
558:	eMol956403	-7.4	-7.4	610	eMol25829045	-7.2	-7.4
559:	CHEMBL3818229	-7.2	-7.4	611	eMol26936203	-7.4	-7.4
560:	eMol16056893	-7.2	-7.4	612	eMol27202398	-7.2	-7.4
561:	eMol20378545	-7.4	-7.4	613	eMol276247952	-7.3	-7.4
562:	eMol24427986	-7.0	-7.4	614	eMol300978663	-7.3	-7.4
563:	eMol25918241	-7.3	-7.4	615	eMol4490859	-7.2	-7.4
564:	eMol26316348	-7.4	-7.4	616	eMol46445765	-7.2	-7.4
565:	eMol4565043	-7.0	-7.4	617	eMol206850549	-7.3	-7.4
566:	eMol46479157	-7.4	-7.4	618	eMol207259512	-7.3	-7.4
567:	eMol46479980	-7.4	-7.4	619	eMol299991997	-7.3	-7.4
537:	eMol24419686	-7.2	-7.5	589	eMol25903125	-7.4	-7.4

Table S2. *Continued.*

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
620:	eMol4732807	-7.3	-7.4	672	eMol43731198	-7.1	-7.3
621:	eMol956477	-7.3	-7.4	673	eMol566406	-7.2	-7.3
622:	CHEMBL3818171	-7.1	-7.4	674	eMol588242	-7.7	-7.3
623:	CHEMBL579620	-7.2	-7.4	675	CHEMBL3805665	-7.1	-7.3
624:	eMol1683032	-7.3	-7.4	676	CHEMBL3819311	-7.2	-7.3
625:	eMol20337442	-7.1	-7.4	677	CHEMBL38330	-7.1	-7.3
626:	eMol2141753	-7.2	-7.4	678	eMol11071566	-7.3	-7.3
627:	eMol25968613	-7.2	-7.4	679	eMol206964256	-7.3	-7.3
628:	eMol26245604	-7.3	-7.4	680	eMol23206884	-7.3	-7.3
629:	eMol27202970	-7.3	-7.4	681	eMol24520802	-7.3	-7.3
630:	eMol4606566	-7.2	-7.4	682	eMol25771182	-7.3	-7.3
631:	eMol4715267	-7.3	-7.4	683	eMol25907499	-7.3	-7.3
632:	eMol4728946	-7.3	-7.4	684	eMol25913211	-7.3	-7.3
633:	CHEMBL114005	-7.1	-7.3	685	eMol26262902	-7.3	-7.3
634:	eMol18961180	-7.2	-7.3	686	eMol316831112	-7.2	-7.3
635:	eMol19076404	-7.4	-7.3	687	eMol4433627	-7.2	-7.3
636:	eMol206907968	-7.3	-7.3	688	eMol4580053	-7.5	-7.3
637:	eMol24520050	-7.3	-7.3	689	eMol24532024	-7.3	-7.3
638:	eMol316344188	-7.3	-7.3	690	eMol25958221	-7.2	-7.3
639:	eMol44673597	-7.3	-7.3	691	eMol26264151	-7.1	-7.3
640:	eMol4698359	-7.4	-7.3	692	eMol26300005	-7.2	-7.3
641:	eMol4718679	-7.2	-7.3	693	eMol26326968	-7.3	-7.3
642:	eMol17203597	-7.0	-7.3	694	eMol26936207	-7.2	-7.3
643:	eMol180102976	-7.3	-7.3	695	eMol27187414	-7.1	-7.3
644:	eMol25797977	-7.3	-7.3	696	eMol27202912	-7.3	-7.3
645:	eMol29649914	-7.3	-7.3	697	eMol579510	-7.1	-7.3
646:	eMol4477952	-7.3	-7.3	698	eMol935864	-7.6	-7.3
647:	eMol45622753	-7.3	-7.3	699	CHEMBL113923	-7.1	-7.3
648:	CHEMBL115809	-7.3	-7.3	700	CHEMBL47157	-7.2	-7.3
649:	CHEMBL116634	-7.3	-7.3	701	eMol179164953	-7.2	-7.3
650:	eMol17192354	-7.2	-7.3	702	eMol20380394	-7.1	-7.3
651:	eMol179164956	-7.2	-7.3	703	eMol2330950	-7.3	-7.3
652:	eMol23242679	-7.3	-7.3	704	eMol25902283	-7.3	-7.3
653:	eMol25901925	-7.3	-7.3	705	eMol26285150	-7.3	-7.3
654:	eMol25936279	-7.3	-7.3	706	eMol27187400	-7.1	-7.3
655:	eMol26230266	-7.3	-7.3	707	eMol46400679	-7.3	-7.3
656:	eMol26315986	-7.3	-7.3	708	eMol4713307	-7.2	-7.3
657:	eMol27252901	-7.3	-7.3	709	CHEMBL4099863	-7.2	-7.3
658:	eMol4713633	-7.3	-7.3	710	eMol24521048	-7.3	-7.3
659:	CHEMBL3819196	-7.1	-7.3	711	eMol25966304	-7.3	-7.3
660:	eMol16797514	-8.1	-7.3	712	eMol27202388	-7.3	-7.3
661:	eMol19076688	-7.3	-7.3	713	eMol27202918	-7.2	-7.3
662:	eMol20375154	-7.3	-7.3	714	eMol46400677	-7.2	-7.3
663:	eMol26300049	-7.3	-7.3	715	eMol4709495	-7.2	-7.3
664:	eMol46370139	-7.3	-7.3	716	CHEMBL1302012	-7.1	-7.3
665:	eMol51435800	-7.5	-7.3	717	CHEMBL2297150	-7.0	-7.3
666:	CHEMBL1383006	-7.1	-7.3	718	CHEMBL326628	-7.2	-7.3
667:	eMol17202599	-7.1	-7.3	719	CHEMBL3817866	-7.2	-7.3
668:	eMol180102764	-7.2	-7.3	720	CHEMBL3818856	-7.1	-7.3
669:	eMol23191317	-7.3	-7.3	721	CHEMBL577676	-7.2	-7.3
670:	eMol2409922	-7.2	-7.3	722	CHEMBL585981	-7.2	-7.3
671:	eMol26251302	-7.1	-7.3	723	eMol1120546	-7.2	-7.3
641:	eMol4718679	-7.2	-7.3	693	eMol26326968	-7.3	-7.3

Table S2. *Continued.*

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
724:	eMol18866942	-7.1	-7.3	776	eMol45133343	-7.2	-7.2
725:	eMol24113359	-7.2	-7.3	777	eMol46491554	-7.2	-7.2
726:	eMol25825125	-7.2	-7.3	778	eMol588078	-7.1	-7.2
727:	eMol26250339	-7.1	-7.3	779	eMol7265152	-7.6	-7.2
728:	eMol26285928	-7.2	-7.3	780	eMol22370884	-7.2	-7.2
729:	eMol26314361	-7.2	-7.3	781	eMol24521662	-7.2	-7.2
730:	eMol26569999	-7.2	-7.3	782	eMol24526765	-7.1	-7.2
731:	eMol29987858	-7.0	-7.3	783	eMol2517109	-7.1	-7.2
732:	eMol4408548	-7.2	-7.3	784	eMol25963663	-7.2	-7.2
733:	eMol44127206	-7.4	-7.3	785	eMol26328784	-7.2	-7.2
734:	eMol46479958	-7.2	-7.3	786	eMol27202280	-7.1	-7.2
735:	eMol4726520	-7.2	-7.3	787	eMol27202496	-7.1	-7.2
736:	CHEMBL296691	-7.2	-7.2	788	eMol27202506	-7.2	-7.2
737:	eMol19076602	-7.2	-7.2	789	eMol27202540	-7.2	-7.2
738:	eMol24520240	-7.2	-7.2	790	eMol30744925	-7.3	-7.2
739:	eMol24521330	-7.2	-7.2	791	eMol4146706	-7.1	-7.2
740:	eMol25902049	-7.1	-7.2	792	eMol43744846	-7.1	-7.2
741:	eMol26285666	-7.2	-7.2	793	eMol46400687	-7.2	-7.2
742:	eMol26314117	-7.1	-7.2	794	eMol46479996	-7.2	-7.2
743:	eMol27202754	-7.2	-7.2	795	eMol5672543	-7.1	-7.2
744:	eMol2768990	-7.2	-7.2	796	CHEMBL3805042	-7.2	-7.2
745:	eMol29665906	-7.1	-7.2	797	CHEMBL3806178	-7.2	-7.2
746:	eMol43731202	-7.7	-7.2	798	CHEMBL3818209	-7.1	-7.2
747:	eMol46370137	-7.2	-7.2	799	eMol18550720	-7.2	-7.2
748:	eMol566256	-7.5	-7.2	800	eMol206987841	-7.0	-7.2
749:	eMol956435	-7.3	-7.2	801	eMol23201309	-7.2	-7.2
750:	CHEMBL1559857	-7.1	-7.2	802	eMol25819233	-7.1	-7.2
751:	CHEMBL3806097	-7.2	-7.2	803	eMol26314895	-7.1	-7.2
752:	CHEMBL3806218	-7.1	-7.2	804	eMol26315041	-7.0	-7.2
753:	eMol16351673	-7.1	-7.2	805	eMol27202282	-7.1	-7.2
754:	eMol18516265	-7.2	-7.2	806	eMol27202756	-7.2	-7.2
755:	eMol18550716	-7.1	-7.2	807	CHEMBL1562035	-7.1	-7.2
756:	eMol23241510	-7.2	-7.2	808	eMol25912447	-7.1	-7.2
757:	eMol25770408	-7.2	-7.2	809	eMol26277244	-7.2	-7.2
758:	eMol26289047	-7.2	-7.2	810	eMol26292416	-7.2	-7.2
759:	eMol27045407	-7.2	-7.2	811	eMol26316052	-7.2	-7.2
760:	eMol27202350	-7.2	-7.2	812	eMol27202358	-7.2	-7.2
761:	eMol27202914	-7.2	-7.2	813	CHEMBL34185	-7.1	-7.2
762:	eMol43746869	-7.2	-7.2	814	CHEMBL3818747	-7.1	-7.2
763:	eMol5444645	-7.1	-7.2	815	eMol2208925	-7.5	-7.2
764:	eMol5847921	-7.2	-7.2	816	eMol2308510	-7.0	-7.2
765:	CHEMBL1552848	-7.1	-7.2	817	eMol23152351	-7.0	-7.2
766:	CHEMBL247353	-7.1	-7.2	818	eMol23170772	-7.2	-7.2
767:	CHEMBL4079984	-7.2	-7.2	819	eMol25810099	-7.2	-7.2
768:	eMol18860491	-7.5	-7.2	820	eMol26289870	-7.2	-7.2
769:	eMol19076828	-7.0	-7.2	821	eMol26310907	-7.2	-7.2
770:	eMol2115166	-7.1	-7.2	822	eMol27202410	-7.2	-7.2
771:	eMol26293580	-7.1	-7.2	823	eMol27202762	-7.2	-7.2
772:	eMol27045405	-7.2	-7.2	824	eMol206964558	-7.1	-7.2
773:	eMol27202232	-7.1	-7.2	825	eMol23185851	-7.1	-7.2
774:	eMol27202920	-7.2	-7.2	826	eMol23241342	-7.2	-7.2
775:	eMol30322739	-7.2	-7.2	827	eMol24518463	-7.2	-7.2

Table S2. *Continued.*

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
828:	eMol26330383	-7.2	-7.2	880:	eMol25816255	-7.0	-7.1
829:	eMol26936201	-7.1	-7.2	881:	eMol26276632	-7.1	-7.1
830:	eMol27045521	-7.2	-7.2	882:	CHEMBL1551922	-7.1	-7.1
831:	eMol36016142	-7.1	-7.2	883:	CHEMBL3818499	-7.1	-7.1
832:	eMol46545587	-7.1	-7.2	884:	CHEMBL3818977	-7.1	-7.1
833:	eMol24428006	-7.1	-7.2	885:	eMol206990555	-7.1	-7.1
834:	eMol25770418	-7.1	-7.2	886:	eMol24524699	-7.1	-7.1
835:	eMol26310653	-7.0	-7.2	887:	eMol25771206	-7.1	-7.1
836:	eMol26315688	-7.1	-7.2	888:	eMol26286396	-7.1	-7.1
837:	eMol560303	-7.1	-7.2	889:	eMol26311934	-7.4	-7.1
838:	CHEMBL3805407	-7.1	-7.2	890:	eMol26312838	-7.1	-7.1
839:	eMol24519079	-7.2	-7.2	891:	eMol26314721	-7.3	-7.1
840:	eMol24521248	-7.1	-7.2	892:	eMol27202336	-7.1	-7.1
841:	eMol26189151	-7.1	-7.2	893:	eMol27202362	-7.1	-7.1
842:	eMol26292060	-7.1	-7.2	894:	eMol30104228	-7.1	-7.1
843:	eMol26310839	-7.1	-7.2	895:	eMol43731200	-8.0	-7.1
844:	eMol26314359	-7.1	-7.2	896:	CHEMBL3804857	-7.1	-7.1
845:	eMol26936209	-7.1	-7.2	897:	eMol1165997	-7.1	-7.1
846:	eMol45932769	-7.1	-7.2	898:	eMol16352193	-7.0	-7.1
847:	eMol46534208	-7.1	-7.2	899:	eMol19076826	-7.1	-7.1
848:	eMol6263477	-7.1	-7.2	900:	eMol206920578	-7.1	-7.1
849:	eMol106491702	-7.1	-7.1	901:	eMol2231344	-7.2	-7.1
850:	eMol16351675	-7.1	-7.1	902:	eMol25924517	-7.1	-7.1
851:	eMol19076732	-7.0	-7.1	903:	eMol25966294	-7.1	-7.1
852:	eMol206980481	-7.1	-7.1	904:	eMol316862506	-7.1	-7.1
853:	eMol23242609	-7.1	-7.1	905:	CHEMBL299107	-7.1	-7.1
854:	eMol26313449	-7.1	-7.1	906:	CHEMBL3804866	-7.1	-7.1
855:	eMol26319543	-7.1	-7.1	907:	CHEMBL3818626	-7.0	-7.1
856:	CHEMBL1414265	-7.1	-7.1	908:	eMol15983174	-7.0	-7.1
857:	eMol1156520	-7.2	-7.1	909:	eMol1748795	-7.7	-7.1
858:	eMol20344945	-7.1	-7.1	910:	eMol24520023	-7.1	-7.1
859:	eMol206965980	-7.1	-7.1	911:	eMol24531798	-7.1	-7.1
860:	eMol26270766	-7.1	-7.1	912:	eMol25913057	-7.1	-7.1
861:	eMol26276502	-7.1	-7.1	913:	eMol26288955	-7.1	-7.1
862:	eMol4491662	-7.1	-7.1	914:	eMol26326313	-7.1	-7.1
863:	CHEMBL1394809	-7.0	-7.1	915:	eMol31278496	-7.1	-7.1
864:	eMol16351677	-7.1	-7.1	916:	eMol46400683	-7.0	-7.1
865:	eMol18542840	-7.1	-7.1	917:	eMol566142	-7.4	-7.1
866:	eMol20380392	-7.1	-7.1	918:	eMol579926	-7.1	-7.1
867:	eMol206843436	-7.0	-7.1	919:	CHEMBL1439596	-7.1	-7.1
868:	eMol24428326	-7.4	-7.1	920:	CHEMBL550397	-7.1	-7.1
869:	eMol25790309	-7.1	-7.1	921:	eMol20378615	-7.1	-7.1
870:	eMol26331720	-7.1	-7.1	922:	eMol24430231	-7.1	-7.1
871:	eMol26350850	-7.1	-7.1	923:	eMol24531722	-7.1	-7.1
872:	eMol26570001	-7.1	-7.1	924:	eMol26314551	-7.0	-7.1
873:	eMol27187440	-7.1	-7.1	925:	eMol4709315	-7.0	-7.1
874:	eMol45935468	-7.1	-7.1	926:	eMol6157528	-7.0	-7.1
875:	eMol588368	-7.1	-7.1	927:	CHEMBL1215796	-7.1	-7.1
876:	CHEMBL3818347	-7.0	-7.1	928:	eMol19076734	-7.0	-7.1
877:	eMol1035551	-7.1	-7.1	929:	eMol20310561	-7.1	-7.1
878:	eMol18550722	-7.1	-7.1	930:	eMol206849669	-7.1	-7.1
879:	eMol19076370	-7.0	-7.1	931:	eMol25945602	-7.1	-7.1
849:	eMol106491702	-7.1	-7.1	901:	eMol2231344	-7.2	-7.1

Table S2. *Continued.*

No.	Compound Name/Code	Docking score (kcal/mol)		No.	Compound Name/Code	Docking score (kcal/mol)	
		Conventional	Intermediate			Conventional	Intermediate
932:	eMol299994300	-7.1	-7.1	967	eMol43731774	-7.2	-6.9
933:	eMol300089978	-7.1	-7.1	968	eMol3018072	-7.4	-6.9
934:	eMol956263	-7.1	-7.1	969	eMol316351191	-7.5	-6.9
935:	CHEMBL1373990	-7.0	-7.1	970	eMol206964210	-7.0	-6.8
936:	eMol16379841	-7.0	-7.1	971	eMol27115486	-7.3	-6.8
937:	eMol1752196	-7.0	-7.1	972	eMol23244410	-7.1	-6.8
938:	eMol25895011	-7.0	-7.1	973	eMol33339294	-7.1	-6.7
939:	eMol25913175	-7.1	-7.1	974	eMol2992508	-7.6	-6.7
940:	eMol26524217	-7.0	-7.1	975	eMol4732869	-7.1	-6.7
941:	eMol3033983	-7.1	-7.1	976	CHEMBL395117	-7.1	-6.6
942:	eMol207355370	-7.3	-7.0	977	eMol4738130	-7.2	-6.6
943:	eMol25895009	-7.0	-7.0	978	eMol25895023	-7.3	-6.5
944:	eMol679754	-7.1	-7.0	979	eMol27380659	-7.8	-6.5
945:	CHEMBL3818366	-7.0	-7.0	980	eMol1149947	-7.3	-6.5
946:	eMol206965358	-7.0	-7.0	981	eMol27202380	-7.1	-6.5
947:	eMol25901881	-7.0	-7.0	982	eMol33346435	-7.2	-6.5
948:	eMol26299531	-7.0	-7.0	983	CHEMBL82690	-7.4	-6.3
949:	eMol26324447	-7.0	-7.0	984	eMol11690694	-7.5	-6.3
950:	eMol27202422	-7.1	-7.0	985	eMol1764376	-7.6	-6.2
951:	eMol3775722	-7.0	-7.0	986	eMol2992482	-8.1	-6.2
952:	CHEMBL1900041	-7.0	-7.0	987	eMol2194316	-7.1	-6.1
953:	CHEMBL3804880	-7.0	-7.0	988	eMol16375743	-7.1	-6.1
954:	eMol181109768	-7.2	-7.0	989	eMol36016132	-7.1	-6.0
955:	eMol20356657	-7.0	-7.0	990	eMol16351883	-7.1	-5.8
956:	CHEMBL2297667	-7.0	-7.0	991	eMol179165005	-7.3	-5.8
957:	eMol4388132	-7.4	-7.0	992	eMol587916	-7.1	-5.7
958:	eMol27202320	-7.0	-7.0	993	eMol43745829	-7.3	-5.7
959:	eMol25903659	-7.1	-7.0	994	eMol2992488	-7.6	-5.6
960:	eMol44548966	-7.2	-7.0	995	eMol24493983	-7.4	-5.5
961:	eMol565918	-7.2	-6.9	996	eMol24427880	-7.4	-5.4
962:	eMol206909136	-7.1	-6.9	997	eMol5444883	-7.1	-5.3
963:	eMol581304	-7.3	-6.9	998	eMol31358919	-7.3	-5.3
964:	eMol46411087	-7.4	-6.9	999	eMol3181655	-7.1	-5.1
965:	CHEMBL1591720	-7.1	-6.9	1000	CHEMBL1214720	-8.8	-5.1
966:	eMol27202778	-7.1	-6.9				

^a Data ranked based on the intermediate docking scores.

Table S3. Estimated conventional, intermediate, and Expensive docking scores for QNZ and the top 250 potent allosteric inhibitors against mutated PBP2a allosteric site in acidic medium.^a

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Conventional	Intermediate	Expensive			Conventional	Intermediate	Expensive
	QNZ	-6.9	-8.0	-8.3	63	eMol30323633	-9.0	-9.1	-8.2
1	eMol26313223	-8.3	-8.4	-10.0	64	CHEMBL1214938	-8.7	-9.0	-8.2
2	eMol26437582	-8.2	-8.9	-9.9	65	eMol20375178	-8.7	-9.0	-8.2
3	eMol26314565	-8.2	-8.2	-9.6	66	eMol30323569	-8.6	-9.0	-8.2
4	eMol26313117	-8.9	-9.4	-9.5	67	eMol30341049	-8.8	-8.9	-8.2
5	eMol26293960	-8.1	-9.2	-9.4	68	eMol43906045	-8.8	-8.9	-8.2
6	eMol3021959	-7.1	-8.9	-9.4	69	CHEMBL3818584	-8.3	-8.9	-8.2
7	eMol29597031	-9.2	-9.3	-9.3	70	eMol20378769	-8.7	-8.9	-8.2
8	eMol26269394	-8.5	-8.7	-9.1	71	eMol20342262	-7.9	-8.8	-8.2
9	eMol27202760	-8.0	-8.1	-9.1	72	eMol19076712	-8.9	-8.9	-8.2
10	eMol26242018	-8.0	-8.8	-9.0	73	eMol18542846	-8.8	-8.8	-8.2
11	eMol29633913	-7.8	-8.6	-8.9	74	CHEMBL1214941	-8.6	-8.1	-8.1
12	CHEMBL1215080	-8.4	-8.4	-8.9	75	eMol1166007	-8.7	-8.8	-8.1
13	eMol27252412	-8.1	-8.2	-8.7	76	CHEMBL3805841	-7.7	-8.0	-8.1
14	eMol30017880	-7.4	-8.3	-8.7	77	eMol20337486	-8.8	-8.8	-8.1
15	eMol26319231	-8.2	-8.6	-8.7	78	eMol23190351	-7.9	-8.7	-8.1
16	eMol26264570	-8.1	-8.4	-8.7	79	eMol19076754	-8.6	-8.8	-8.1
17	eMol300094331	-8.2	-8.3	-8.7	80	eMol31781482	-8.7	-8.6	-8.1
18	eMol29565259	-7.8	-8.2	-8.6	81	CHEMBL1215649	-8.5	-8.6	-8.1
19	eMol27406062	-7.8	-8.3	-8.6	82	eMol26196316	-8.5	-8.6	-8.1
20	eMol299980544	-8.2	-8.2	-8.6	83	eMol33366267	-7.9	-8.6	-8.1
21	eMol27202252	-8.0	-8.1	-8.6	84	eMol75958504	-7.9	-8.6	-8.1
22	eMol29634797	-7.6	-8.1	-8.6	85	CHEMBL1215648	-8.6	-8.7	-8.1
23	eMol27202248	-8.4	-8.3	-8.6	86	eMol20379909	-8.8	-8.8	-8.1
24	CHEMBL1215082	-7.4	-8.0	-8.5	87	eMol26196326	-8.6	-8.7	-8.1
25	eMol26242042	-7.6	-8.5	-8.5	88	eMol45585842	-8.6	-8.7	-8.1
26	eMol300154219	-7.3	-8.3	-8.5	89	eMol23241028	-8.6	-8.7	-8.1
27	eMol26242026	-7.8	-8.2	-8.4	90	eMol45622743	-7.8	-8.6	-8.1
28	eMol26330545	-8.2	-8.2	-8.4	91	CHEMBL1215650	-8.5	-8.7	-8.1
29	eMol27091674	-8.0	-8.1	-8.4	92	CHEMBL1579061	-8.5	-8.7	-8.1
30	CHEMBL1215004	-7.7	-8.2	-8.4	93	eMol30646140	-7.7	-8.6	-8.1
31	eMol27091498	-8.0	-8.1	-8.4	94	eMol72993476	-7.7	-8.6	-8.1
32	eMol29587306	-7.7	-8.2	-8.4	95	eMol22447774	-8.5	-8.7	-8.1
33	eMol26314779	-8.1	-8.2	-8.3	96	eMol30248263	-8.0	-8.4	-8.0
34	eMol27202948	-7.4	-8.0	-8.3	97	eMol19076742	-8.6	-8.7	-8.0
35	eMol301527162	-8.0	-8.1	-8.3	98	eMol23157132	-8.4	-8.6	-8.0
36	eMol19266609	-7.9	-9.5	-8.2	99	eMol26242050	-8.1	-8.6	-8.0
37	eMol24519694	-9.0	-9.5	-8.2	100	CHEMBL1214713	-8.2	-8.6	-8.0
38	CHEMBL1443074	-8.0	-8.1	-8.2	101	CHEMBL1384683	-8.2	-8.6	-8.0
39	eMol18940433	-8.0	-8.1	-8.2	102	CHEMBL1558437	-8.2	-8.6	-8.0
40	CHEMBL1214717	-9.4	-9.4	-8.2	103	CHEMBL3818129	-8.5	-8.6	-8.0
41	eMol29587310	-9.4	-9.4	-8.2	104	eMol26270654	-8.2	-8.6	-8.0
42	eMol45585846	-9.4	-9.4	-8.2	105	eMol300994534	-8.4	-8.6	-8.0
43	eMol24389393	-7.9	-9.4	-8.2	106	eMol48938145	-8.4	-8.6	-8.0
44	eMol23239806	-9.3	-9.4	-8.2	107	eMol30671942	-7.9	-8.5	-8.0
45	CHEMBL1214718	-9.2	-9.3	-8.2	108	eMol23246696	-8.5	-8.6	-8.0
46	eMol45585848	-9.2	-9.3	-8.2	109	eMol26242044	-8.3	-8.4	-8.0
47	eMol31786896	-8.4	-9.3	-8.2	110	eMol36912832	-7.9	-8.4	-8.0
48	eMol2403964	-8.7	-9.3	-8.2	111	eMol26242034	-8.2	-8.5	-7.9
49	eMol23186178	-9.1	-9.3	-8.2	112	CHEMBL3805924	-8.3	-8.5	-7.9
50	eMol31297102	-7.9	-9.2	-8.2	113	eMol23175530	-8.3	-8.5	-7.9
51	eMol19076714	-8.4	-9.2	-8.2	114	eMol24519844	-8.4	-8.5	-7.9
52	eMol19076718	-8.9	-9.1	-8.2	115	CHEMBL3582080	-7.9	-8.1	-7.9
53	eMol18542844	-9.1	-9.1	-8.2	116	eMol1344114	-9.0	-9.1	-7.9
54	CHEMBL1214794	-8.9	-9.0	-8.2	117	eMol26242032	-7.9	-8.3	-7.9
55	eMol25810077	-7.9	-8.4	-8.2	118	eMol43906059	-8.4	-8.4	-7.9
56	eMol26196290	-8.9	-9.0	-8.2	119	eMol23243407	-8.2	-8.4	-7.9
57	eMol45585824	-8.9	-9.0	-8.2	120	eMol43906055	-8.0	-8.4	-7.9
58	CHEMBL3819187	-7.8	-9.1	-8.2	121	eMol579568	-8.4	-8.4	-7.8
59	CHEMBL3818732	-8.0	-9.0	-8.2	122	eMol23239141	-8.3	-8.4	-7.8
60	eMol26262168	-7.0	-8.0	-8.2	123	eMol588192	-8.2	-8.4	-7.8
61	eMol29638777	-7.8	-8.1	-8.2	124	CHEMBL4103504	-8.3	-8.5	-7.8
62	eMol46480173	-8.2	-8.3	-8.2	125	eMol23181799	-8.3	-8.4	-7.8

Table S3. *Continued.*

No.	Compound Name/Code	Docking Score (kcal/mol)			No.	Compound Name/Code	Docking Score (kcal/mol)		
		Conventional	Intermediate	Expensive			Conventional	Intermediate	Expensive
126	eMol587826	-8.2	-8.4	-7.8	189	eMol4566508	-7.3	-8.2	-7.6
127	eMol679826	-8.3	-8.4	-7.8	190	eMol20368046	-8.1	-8.2	-7.6
128	eMol27202910	-8.3	-8.4	-7.8	191	eMol23147497	-8.1	-8.2	-7.6
129	CHEMBL3818572	-8.0	-8.3	-7.8	192	eMol679824	-8.0	-8.2	-7.6
130	eMol18962382	-8.4	-8.4	-7.8	193	eMol24428240	-7.2	-8.5	-7.6
131	eMol27202240	-8.4	-8.4	-7.8	194	eMol37002179	-7.4	-8.1	-7.6
132	eMol679820	-7.2	-8.4	-7.8	195	eMol45585838	-7.8	-8.2	-7.6
133	eMol31532412	-8.3	-8.4	-7.8	196	CHEMBL1601398	-8.0	-8.1	-7.6
134	CHEMBL1215003	-8.2	-8.3	-7.8	197	eMol2507718	-8.0	-8.1	-7.6
135	eMol25810075	-8.3	-8.4	-7.8	198	eMol26242024	-7.7	-8.2	-7.6
136	eMol2992792	-8.1	-8.3	-7.8	199	eMol4558540	-8.0	-8.2	-7.6
137	eMol43731476	-7.6	-8.3	-7.8	200	eMol256911679	-8.0	-8.1	-7.6
138	eMol43906053	-8.2	-8.3	-7.8	201	eMol4562556	-8.1	-8.1	-7.6
139	CHEMBL395193	-8.3	-8.3	-7.8	202	eMol45935562	-7.5	-8.1	-7.6
140	eMol193446288	-8.3	-8.3	-7.8	203	eMol565850	-7.0	-8.1	-7.6
141	eMol26242022	-7.9	-8.3	-7.8	204	eMol579756	-8.0	-8.1	-7.6
142	CHEMBL3817888	-8.1	-8.3	-7.7	205	eMol20361212	-8.1	-8.1	-7.5
143	eMol18542848	-8.3	-8.3	-7.7	206	eMol4446697	-7.7	-8.1	-7.5
144	eMol20347873	-8.2	-8.3	-7.7	207	eMol25784531	-7.1	-8.1	-7.5
145	eMol206926236	-8.2	-8.3	-7.7	208	eMol27202348	-8.1	-8.1	-7.5
146	eMol45622749	-7.8	-8.1	-7.7	209	eMol4518648	-8.1	-8.1	-7.5
147	eMol25810071	-8.3	-8.3	-7.7	210	eMol177199339	-7.9	-8.1	-7.5
148	eMol6263471	-8.2	-8.3	-7.7	211	eMol300994251	-7.9	-8.1	-7.5
149	CHEMBL1214647	-8.1	-8.4	-7.7	212	eMol45585836	-7.7	-8.2	-7.5
150	eMol19076598	-7.3	-8.3	-7.7	213	eMol4577396	-8.0	-8.1	-7.5
151	eMol25810083	-8.3	-8.3	-7.7	214	eMol48768479	-7.9	-8.1	-7.5
152	eMol46490873	-8.1	-8.2	-7.7	215	eMol4566756	-7.9	-8.1	-7.5
153	eMol46365626	-8.2	-8.3	-7.7	216	eMol20378767	-7.9	-8.1	-7.5
154	eMol566574	-8.1	-8.3	-7.7	217	eMol580072	-8.0	-8.1	-7.5
155	CHEMBL3818929	-8.2	-8.3	-7.7	218	eMol179164947	-7.8	-8.0	-7.5
156	CHEMBL518358	-8.2	-8.3	-7.7	219	eMol46367311	-7.8	-8.0	-7.5
157	eMol13856171	-8.0	-8.2	-7.7	220	eMol565798	-8.1	-8.1	-7.5
158	eMol26809774	-8.2	-8.2	-7.7	221	eMol27091442	-7.9	-8.1	-7.5
159	CHEMBL1214935	-8.1	-8.3	-7.7	222	eMol27202916	-7.2	-8.1	-7.5
160	eMol26242038	-7.9	-8.2	-7.7	223	eMol4397966	-8.0	-8.1	-7.5
161	eMol26314331	-7.5	-8.3	-7.7	224	eMol679550	-7.9	-8.1	-7.5
162	eMol43906051	-8.1	-8.3	-7.7	225	CHEMBL1214934	-7.0	-8.0	-7.5
163	CHEMBL1214936	-8.2	-8.3	-7.7	226	eMol25966646	-7.9	-8.0	-7.5
164	eMol26196312	-8.2	-8.3	-7.7	227	eMol27202242	-8.0	-8.0	-7.5
165	eMol27202258	-8.3	-8.2	-7.7	228	eMol28321864	-8.0	-8.0	-7.4
166	eMol45585832	-8.2	-8.3	-7.7	229	eMol4549830	-7.3	-8.0	-7.4
167	eMol681936	-8.2	-8.2	-7.7	230	eMol1035521	-7.9	-8.0	-7.4
168	eMol25819217	-8.3	-8.2	-7.6	231	eMol206992517	-8.0	-8.0	-7.4
169	eMol26320021	-7.4	-8.2	-7.6	232	eMol579718	-8.0	-8.1	-7.4
170	eMol30323345	-9.8	-8.2	-7.6	233	eMol581308	-7.9	-8.0	-7.4
171	eMol43731530	-7.3	-8.2	-7.6	234	CHEMBL485839	-8.0	-8.0	-7.4
172	eMol46480165	-8.2	-8.2	-7.6	235	eMol43906047	-7.9	-8.0	-7.4
173	eMol1088331	-8.2	-8.2	-7.6	236	eMol43906057	-7.4	-8.0	-7.4
174	eMol1755402	-8.0	-8.2	-7.6	237	eMol681814	-7.9	-8.0	-7.4
175	eMol23178762	-8.1	-8.2	-7.6	238	CHEMBL2259943	-7.9	-8.0	-7.4
176	CHEMBL3819481	-7.9	-8.2	-7.6	239	eMol36912834	-8.0	-8.1	-7.4
177	CHEMBL1215578	-8.0	-8.2	-7.6	240	eMol26242052	-7.3	-8.2	-7.4
178	CHEMBL1215797	-8.0	-8.2	-7.6	241	eMol18551342	-8.0	-8.0	-7.4
179	CHEMBL508966	-8.1	-8.2	-7.6	242	eMol4578697	-7.3	-8.1	-7.4
180	eMol20377597	-8.0	-8.2	-7.6	243	eMol4552519	-8.0	-8.1	-7.4
181	eMol24530483	-8.2	-8.2	-7.6	244	CHEMBL3818035	-7.9	-8.4	-7.4
182	eMol29653471	-8.2	-8.2	-7.6	245	eMol679822	-8.0	-8.2	-7.4
183	eMol45622745	-8.2	-8.2	-7.6	246	CHEMBL1214648	-8.0	-8.2	-7.4
184	eMol48982653	-7.7	-8.2	-7.6	247	CHEMBL3582082	-7.3	-8.1	-7.4
185	eMol566488	-8.1	-8.2	-7.6	248	CHEMBL3818775	-8.2	-8.2	-7.4
186	eMol679556	-8.0	-8.2	-7.6	249	eMol11920256	-8.1	-8.2	-7.4
187	eMol956623	-8.2	-8.2	-7.6	250	CHEMBL1534883	-9.0	-9.1	-7.4
188	eMol18550846	-8.1	-8.2	-7.6					

^aData ranked based on the Expensive docking score.

Table S4. Estimated conventional, intermediate, and expensive docking scores, MM-GBSA//MM binding energies and binding features of AMBER-based minimized structures for QNZ and the top 35 potent inhibitors against mutated PBP2a allosteric site in acidic medium.^a

No.	Compound Name/Code	Docking score (kcal/mol)			MM-GBSA//MM binding energy (kcal/mol)	Binding Features ^b
		Conventional	Intermediate	Expensive		
1	QNZ	-6.9	-8.0	-8.3	-31.4	VAL277 (2.28 Å), GLU294 (1.57 Å), LYS316 (2.60, 2.72 Å)
2	eMol26313223	-8.3	-8.4	-10.0	-39.6	LYS146 (1.89 Å), LYS273 (1.94, 2.21 Å), LYS316 (2.19 Å)
3	eMol26314565	-8.2	-8.2	-9.6	-39.1	LYS146 (1.97 Å), LYS273 (2.03 Å), LYS316 (3.08 Å)
4	eMol26437582	-8.2	-8.9	-9.9	-38.2	GLU294 (1.59 Å), LYS316 (1.82 Å), LYS146 (2.14 Å)
5	eMol29634797	-7.6	-8.1	-8.6	-37.1	LYS273 (1.77, 2.46 Å), ASP295 (1.61 Å), LYS316 (1.92 Å)
6	eMol29597031	-9.2	-9.3	-9.3	-35.2	LYS146 (2.21 Å), VAL277 (1.98 Å), GLU294 (1.62 Å), LYS316 (1.80 Å)
7	eMol29633913	-7.8	-8.6	-8.9	-34.2	GLU294 (1.67 Å), LYS316 (1.83 Å)
8	eMol26314779	-8.1	-8.2	-8.3	-34.2	LYS146 (2.10 Å), LYS273 (1.90 Å), LYS316 (2.85 Å)
9	eMol26269394	-8.5	-8.7	-9.1	-31.6	LYS146 (2.01 Å), LYS273 (2.02 Å), GLU294 (1.57 Å), LYS316 (1.79 Å)
10	eMol27252412	-8.1	-8.2	-8.7	-29.8	LYS316 (2.24 Å)
11	eMol300094331	-8.2	-8.3	-8.7	-29.6	GLU294 (1.60 Å), LYS316 (1.99 Å)
12	eMol30017880	-7.4	-8.3	-8.7	-29.3	TYR105 (2.04 Å), LYS146 (2.16 Å), GLU294 (1.58 Å), LYS316 (1.86 Å)
13	eMol26242018	-8.0	-8.8	-9.0	-29.1	LYS146 (2.16 Å), GLU294 (1.58 Å), LYS316 (1.86 Å)
14	eMol27091498	-8.0	-8.1	-8.4	-29.1	LYS273 (1.92 Å), ASP295 (1.97 Å), LYS316 (1.99 Å)
15	eMol26313117	-8.9	-9.4	-9.5	-29.0	LYS146 (2.21 Å), ASP295 (2.01 Å), LYS316 (1.90 Å)
16	eMol27406062	-7.8	-8.3	-8.6	-28.6	LYS146 (2.07 Å), LYS273 (1.99 Å), GLU294 (1.60 Å), ASP295 (2.60 Å), LYS316 (1.85 Å)
17	eMol27091674	-8.0	-8.1	-8.4	-28.4	LYS273 (1.92 Å), ASP295 (1.99 Å), LYS316 (1.97 Å)

Table S4. Continued.

No.	Compound Name/Code	Docking score (kcal/mol)			MM-GBSA/MM binding energy (kcal/mol)	Binding Features ^b
		Conventional	Intermediate	Expensive		
18	eMol26242042	-7.6	-8.5	-8.5	-28.2	LYS146 (2.22 Å), LYS273 (2.01 Å), ASP295 (2.13 Å), LYS316 (1.86 Å)
19	eMol26242026	-7.8	-8.2	-8.4	-27.9	LYS146 (2.21 Å), LYS273 (1.99 Å), ASP295 (2.09 Å), LYS316 (1.86 Å)
20	eMol301527162	-8.0	-8.1	-8.3	-27.8	LYS273 (1.89 Å), ASP295 (1.92, 2.83 Å), LYS316 (2.36, 3.02, 3.04, 3.07 Å)
21	eMol26293960	-8.1	-9.2	-9.4	-27.4	LYS146 (2.31 Å), ASP295 (2.12 Å), LYS316 (1.90 Å)
22	eMol3021959	-7.1	-8.9	-9.4	-27.1	LYS316 (1.86 Å)
23	CHEMBL1215004	-7.7	-8.2	-8.4	-26.7	LYS146 (2.24 Å), HIS293 (2.89 Å), GLU294 (1.62 Å), ASP295 (2.04 Å), LYS316 (1.80 Å)
24	CHEMBL1215080	-8.4	-8.4	-8.9	-26.4	LYS146 (1.99 Å), LYS273 (2.01 Å), GLU294 (1.56 Å), LYS316 (1.80 Å)
25	eMol26262168	-7.0	-8.0	-8.5	-26.3	LYS146 (2.22 Å), GLU294 (1.61 Å), LYS316 (1.80 Å)
26	CHEMBL1215082	-7.4	-8.0	-8.5	-25.5	LYS146 (1.97 Å), LYS273 (2.17 Å), GLU294 (1.56 Å), LYS316 (1.81 Å)
27	eMol29565259	-7.8	-8.2	-8.6	-25.1	LYS146 (1.98 Å), LYS273 (1.95, 2.96 Å), GLU294 (1.57 Å), LYS316 (1.81 Å)
28	eMol26330545	-8.2	-8.2	-8.4	-25.1	LYS273 (2.06 Å), LYS316 (1.98 Å)
29	eMol27202248	-8.4	-8.3	-8.6	-24.5	LYS273 (2.15 Å), LYS316 (2.01 Å)
30	eMol27202760	-8.0	-8.1	-9.1	-24.5	LYS273 (1.94 Å), LYS316 (1.92 Å)
31	eMol26264570	-8.1	-8.4	-8.7	-24.3	LYS273 (2.00, 2.02 Å), GLU294 (1.62 Å), LYS316 (1.83 Å)
32	eMol27202948	-7.4	-8.0	-8.3	-24.0	LYS273 (2.30 Å), ASP295 (2.18 Å), LYS316 (2.59 Å)
33	eMol27202252	-8.0	-8.1	-8.6	-23.3	LYS316 (1.89 Å)
34	eMol299980544	-8.2	-8.2	-8.6	-23.2	LYS316 (1.96 Å)
35	eMol26319231	-8.2	-8.6	-8.7	-22.9	LYS273 (2.01 Å), LYS316 (1.95 Å)
36	eMol300154219	-7.3	-8.3	-8.5	-21.0	LYS273 (1.92, 2.45 Å), ASP295 (2.21 Å), LYS316 (2.51 Å)

^aData ranked based on the MM-GBSA/MM binding energy. ^bOnly hydrogen bonds (in Å) were displayed.