

Discriminatory Analysis Based Molecular Docking Study for in Silico Identification of Epigallocatechin-3-Gallate (EGCG) Derivatives as B-Raf^{V600E} Inhibitors

Huazhou Ying^a, Jiangfeng Xie^a, Xingguo Liu^c, Tingting Yao^a, Xiaowu Dong^{a,*}, Chunqi Hu^{a,b,*}

^aZhejiang Province Key Laboratory of Anti-Cancer Drug Research, College of Pharmaceutical Sciences, Zhejiang University, Hangzhou, P. R. China

^bCollege of chemistry & chemical engineering, Shaoxing University, Shaoxing, P. R. China

^cSchool of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou, P. R. China

*Corresponding authors: Tel. (Fax.): +86 571 88981051; E-mail: dongxw@zju.edu.cn (X.-W.D.)

Tel. (Fax.):+86 575 88341521; E-mail: hucq@usx.edu.cn (C.-Q.H.)

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Table S1. The RMSD value to initial conformation and the distance of key interaction between amino acids and compound B2 during molecular simulation

Time (ps)	RMSD to Initial conformation	Asn580	Ser465	Thr529	Asp594
1	0	2.10309	1.85221	2.48572	2.16216
2	0.327081	2.27527	1.90372	2.47689	2.07962
3	0.342812	2.33681	2.02199	2.30957	2.35817
4	0.343872	2.12421	2.17086	2.13705	2.191
5	0.346473	2.04436	2.2064	2.2984	2.16941
6	0.361804	2.30169	1.96946	2.30806	2.32111
7	0.377348	2.14015	2.04723	2.63601	2.33673
8	0.378959	2.19714	1.86436	2.59542	2.33941
9	0.403311	2.05692	1.95564	2.4586	2.3151
10	0.386298	2.30969	1.99075	2.4914	2.29592
11	0.397295	2.14794	1.88706	2.43406	2.29961
12	0.403206	2.2597	2.05866	2.23453	2.63771
13	0.425985	1.99367	1.8216	2.4793	2.16245
14	0.424949	2.22958	2.08595	2.32972	2.57492
15	0.420985	2.04932	2.03613	2.1566	2.28165
16	0.428006	2.37268	2.17165	2.25382	2.09109
17	0.44374	2.57857	2.18199	2.02578	2.28809
18	0.461298	2.38295	2.33961	2.31787	2.32384
19	0.463659	2.23533	1.94589	2.09096	2.01865
20	0.442608	2.08376	1.95388	2.12831	2.0538
21	0.415041	2.30278	1.93484	2.05323	2.11558
22	0.45242	2.44341	2.19115	2.19706	2.12907
23	0.470275	2.06969	2.13713	2.04279	2.19415
24	0.463664	2.47542	2.17328	2.03173	2.19333
25	0.439221	2.1609	2.10421	2.1064	2.04231
26	0.45647	2.24185	2.13757	2.05182	2.05004
27	0.445968	2.14823	1.80823	1.97233	2.32369
28	0.454061	2.24229	2.16958	2.16958	2.29769
29	0.468596	2.27876	1.94845	2.16554	2.51288
30	0.48711	2.32084	2.27101	2.199	2.13955
31	0.466004	2.1425	1.97261	2.3051	2.02298
32	0.481056	2.24167	2.14702	2.15872	2.22733
33	0.47124	2.22818	2.07575	1.95185	2.18552
34	0.487767	2.13711	1.98497	2.1792	2.09457
35	0.478126	2.1226	1.96071	2.19193	2.07845
36	0.489124	2.19834	2.3395	2.1322	2.29731
37	0.478334	2.20779	1.87697	2.19705	2.24515
38	0.507639	1.98629	1.95304	2.18616	2.08055
39	0.510523	2.14559	2.18184	2.11182	2.05124
40	0.527983	2.20072	2.00368	1.85411	2.31741
41	0.479647	2.15526	2.11314	2.04782	2.13128
42	0.493319	2.4617	2.10269	2.11853	2.15132

43	0.496812	2.13599	2.12774	2.05702	2.36619
44	0.488574	2.07637	2.07591	2.00125	2.13739
45	0.486903	2.20556	2.26019	2.05634	2.02211
46	0.497694	2.25032	1.97118	2.02305	2.50498
47	0.497628	2.1004	2.09665	2.11484	2.46131
48	0.514364	2.16533	1.78571	2.24609	2.1308
49	0.506773	2.10827	2.17804	2.1323	2.31522
50	0.518464	2.03888	1.8555	2.02162	2.3283
51	0.522408	2.18155	1.97466	1.90258	2.14131
52	0.520529	2.15232	2.07749	2.34469	2.30942
53	0.505798	2.29996	2.31668	2.30286	2.42123
54	0.505895	2.15308	1.92651	2.19193	2.07158
55	0.536841	2.007	2.01226	2.04488	2.10934
56	0.546971	2.36911	2.02542	2.04264	2.08296
57	0.562872	2.25079	2.13627	2.0024	2.27886
58	0.55261	2.18643	2.26862	2.06138	2.43409
59	0.554626	2.245	2.15965	1.90339	2.16006
60	0.551587	2.29973	2.06972	2.07259	2.34849
61	0.571252	2.2716	2.13079	2.40114	2.22754
62	0.607678	2.24166	1.97995	2.15699	2.40491
63	0.567959	2.26998	2.11118	2.22569	2.25665
64	0.572572	2.12101	1.97295	2.10942	2.16215
65	0.579539	2.13954	1.95533	2.1933	2.27311
66	0.569807	2.23901	2.06156	2.13701	2.32566
67	0.569025	2.13698	2.12125	2.06354	2.07879
68	0.572006	2.25165	1.8012	2.11974	2.40414
69	0.590473	2.30758	1.91109	1.98195	2.314
70	0.592807	2.15851	2.04781	2.07435	2.17654
71	0.578991	2.15316	1.89188	1.99444	2.02362
72	0.564587	2.0828	2.09007	2.12615	2.69626
73	0.562127	2.07517	2.13703	2.19211	2.29231
74	0.568081	2.2322	1.93741	2.11543	2.36029
75	0.565109	2.22899	2.04479	2.18293	2.27492
76	0.578589	2.29843	2.36726	1.94663	2.30149
77	0.580521	2.07189	2.10981	2.0802	2.21423
78	0.565116	2.13638	1.99176	2.26233	2.06933
79	0.564714	2.07994	2.04704	2.13513	1.99177
80	0.600336	2.10877	2.20788	2.06477	2.20916
81	0.576447	1.87797	2.30584	2.16135	2.16286
82	0.573538	2.07854	2.06409	2.11634	2.44338
83	0.579197	2.04208	2.14183	2.06013	2.35638
84	0.580457	1.87888	1.97802	2.20957	2.54202
85	0.57048	1.88479	1.98002	2.292	2.07255
86	0.588566	2.29331	1.97505	1.94879	2.32715
87	0.588419	2.1691	1.85857	1.97258	2.14501
88	0.588176	2.19134	2.13252	2.04401	2.48473
89	0.589969	2.0435	2.06268	1.92482	2.25432

90	0.575708	2.37484	1.80872	2.0538	2.21982
91	0.562014	2.13375	2.29161	1.93574	2.30225
92	0.572795	2.10376	2.19221	2.0328	2.39053
93	0.596169	2.20914	2.1254	2.05661	2.17017
94	0.581682	2.21374	2.13686	2.19232	2.12777
95	0.580252	2.21551	2.27592	2.03049	2.08014
96	0.555971	2.21147	1.86168	2.08073	2.14338
97	0.585844	2.1389	2.09245	1.87973	1.97121
98	0.588514	2.10455	2.11708	2.06418	2.21667
99	0.616093	2.08905	2.05866	1.89207	2.21912
100	0.578307	2.14691	1.96038	1.96841	2.36804
101	0.607153	2.18471	2.0684	1.98311	2.42231
102	0.590724	2.10993	1.88972	1.83447	2.29183
103	0.568244	2.16994	2.05582	1.92446	2.18765
104	0.604553	2.24608	1.96512	2.05129	2.06826
105	0.575962	2.04352	1.93824	1.95416	2.15461
106	0.586333	2.14698	1.89765	2.13683	2.3792
107	0.584148	2.23512	1.90323	2.34969	2.25361
108	0.567647	2.28405	1.98788	2.13974	2.14051
109	0.597374	2.01528	2.02585	1.92105	2.103
110	0.578845	2.02258	2.07903	2.24195	2.46049
111	0.577741	2.34616	1.95801	1.95763	2.296
112	0.584363	2.27748	2.14644	2.03744	2.08675
113	0.589352	2.35648	2.2949	2.0469	2.31306
114	0.574492	1.87337	2.18464	2.36545	2.32089
115	0.584733	2.26471	1.99317	1.93499	2.04
116	0.578872	2.23656	2.01605	2.00317	2.10448
117	0.583543	2.06055	2.02125	1.94813	2.27852
118	0.573665	2.2461	2.23505	1.95584	2.34943
119	0.591416	1.87012	2.05096	2.04622	2.24566
120	0.610862	2.0085	2.04653	2.08909	2.22897
121	0.575994	1.91187	1.91154	1.90346	2.17847
122	0.572932	2.08954	1.89458	2.08487	2.05044
123	0.57941	2.21212	1.91071	2.04312	2.18577
124	0.577481	2.2573	1.96674	2.10067	2.05276
125	0.575834	2.21389	1.90143	1.9695	2.44876
126	0.562963	2.17509	1.89155	2.166	2.37354
127	0.587655	2.22346	2.15609	2.03353	2.19466
128	0.5658	2.0839	2.0018	2.23453	2.12667
129	0.586401	2.07063	2.0353	2.11275	2.55331
130	0.552523	2.40862	2.11806	2.34276	2.17393
131	0.568518	1.97637	2.11659	2.26949	2.30358
132	0.573388	2.10281	2.0404	2.16751	2.32774
133	0.557372	2.01041	1.9734	2.02656	2.15873
134	0.562452	2.14083	1.908	2.16727	2.40506
135	0.587844	1.99834	2.37056	1.96822	2.1488
136	0.572841	2.17763	2.10404	2.23062	2.17839

137	0.581347	2.11607	2.25636	1.97309	2.39833
138	0.568914	2.24592	1.8305	2.54122	2.80559
139	0.592272	2.30909	2.06973	2.13735	2.09732
140	0.585661	1.93514	2.01869	2.2796	2.39506
141	0.571246	2.05149	2.09866	2.00379	2.25985
142	0.58007	1.98964	1.85532	1.96671	2.17897
143	0.57534	2.04355	2.20001	2.20732	2.1978
144	0.575734	2.28744	2.21283	2.13509	2.23519
145	0.567947	2.13489	2.48113	2.03787	2.50066
146	0.557105	1.97883	2.03889	2.04774	2.32629
147	0.590294	1.93305	1.90199	2.01643	2.19518
148	0.587607	2.14936	1.97228	2.06472	2.13572
149	0.577064	2.02262	1.80309	2.01498	2.13364
150	0.574358	2.06281	2.16207	2.15411	2.07316
151	0.57377	1.96434	1.79221	1.94495	2.13049
152	0.589599	2.18602	2.09961	2.1836	2.16874
153	0.558175	2.05117	2.08063	1.99082	2.26008
154	0.584048	2.07322	1.84502	2.31034	2.45471
155	0.578117	2.03166	2.11643	2.07211	2.28295
156	0.604928	2.22272	2.10537	2.24214	2.16024
157	0.587372	2.25381	1.96721	2.13017	2.12893
158	0.566907	2.18148	2.16264	1.98094	2.25047
159	0.58275	2.04906	2.11722	1.79558	2.0201
160	0.592276	1.86335	2.10419	2.02514	2.11115
161	0.575853	1.89503	1.88323	2.01669	2.10808
162	0.584481	1.99778	1.95479	2.10799	2.43948
163	0.586614	2.15053	2.3199	2.21559	2.3187
164	0.59267	2.30144	2.17638	1.86836	2.02993
165	0.603243	2.1147	2.26278	1.92182	2.37442
166	0.593837	2.09142	2.24961	2.10366	2.27166
167	0.588854	2.3195	2.05255	1.94935	2.21849
168	0.58193	2.23799	1.99853	2.12606	2.14271
169	0.601458	2.08112	2.17642	1.98457	2.34346
170	0.577146	2.17283	1.91001	1.95742	2.26382
171	0.603622	2.09188	1.91228	1.99445	2.26793
172	0.582985	2.05233	1.94186	1.92741	2.19942
173	0.578078	2.08074	2.01774	1.99479	2.11061
174	0.572824	1.90099	1.85983	2.0947	2.26264
175	0.572617	1.96765	1.90547	2.16658	2.08891
176	0.582412	2.14629	2.05745	2.3667	2.20821
177	0.59613	1.89213	1.93382	2.12425	2.25046
178	0.573288	2.29762	1.90053	2.09449	2.27116
179	0.582387	2.43018	2.05393	1.79402	2.43723
180	0.607444	2.16694	2.08811	1.9112	2.24866
181	0.576488	2.14531	1.90857	2.04965	2.37617
182	0.59711	2.19943	1.99405	2.13507	2.19416
183	0.580663	2.03904	2.05064	1.95858	2.35789

184	0.606024	2.18969	2.09953	2.01516	2.15183
185	0.598531	2.04769	2.16976	2.12785	2.19443
186	0.59113	2.00429	1.87532	2.13418	2.0132
187	0.611974	2.08415	2.28241	1.95722	2.08471
188	0.563025	2.16296	2.30296	1.85401	2.1187
189	0.586163	2.02897	2.07063	2.17132	2.11101
190	0.598072	1.89611	1.93759	1.95441	2.17832
191	0.585573	2.2872	2.05313	2.0654	2.4874
192	0.587632	2.03977	2.03388	1.91062	2.44384
193	0.577284	1.87776	2.0068	1.99877	2.1708
194	0.584273	2.00124	2.03973	1.89972	2.26383
195	0.599001	2.16449	2.1594	2.0486	2.44968
196	0.613103	2.17657	1.86876	1.95525	2.19755
197	0.579989	2.07827	2.07025	1.91881	2.29328
198	0.594641	2.15125	2.03146	1.85036	2.19204
199	0.603645	2.17093	2.06109	1.90754	2.16934
200	0.576534	2.1736	2.1262	2.28404	2.30104
201	0.612111	2.21594	2.14544	1.9189	2.32676
202	0.582857	2.13304	1.81816	2.27399	2.41088
203	0.579415	1.94277	1.98159	2.14679	2.48037
204	0.59151	2.09775	2.1517	2.16109	2.14206
205	0.577699	1.96673	2.17131	2.11135	2.21394
206	0.600785	2.04161	1.88286	1.91501	2.25669
207	0.590139	2.06743	2.08539	2.05091	2.38257
208	0.594016	1.93692	2.09428	2.40359	2.27686
209	0.581285	2.09455	1.85986	2.10525	2.22601
210	0.587768	2.29876	2.07144	2.03075	2.36202
211	0.581022	2.27489	2.00855	2.10461	2.14472
212	0.602213	2.0271	1.91405	2.02347	2.29431
213	0.587671	1.9624	2.0071	2.05668	2.24051
214	0.598327	1.84428	1.87894	2.1531	2.10916
215	0.582532	2.01714	1.93229	1.95451	2.10072
216	0.583901	2.26022	2.06314	2.01521	2.30638
217	0.597256	1.90808	1.89597	1.94419	2.23243
218	0.591472	2.0085	1.84877	2.06956	2.14723
219	0.579394	2.08885	1.82622	2.10307	2.53825
220	0.580305	2.08424	1.98261	2.23324	2.18855
221	0.565861	2.13102	1.88236	2.12113	2.13695
222	0.59276	2.18671	2.09503	2.00777	2.24974
223	0.579384	2.16802	1.93052	1.74886	2.18639
224	0.589932	1.872	1.9924	2.08953	2.17081
225	0.580012	2.26403	2.0047	1.87845	2.16665
226	0.584097	2.13611	2.25619	2.26959	2.40524
227	0.576354	2.21234	1.91377	2.1583	2.46422
228	0.56112	2.22444	1.99968	2.17269	2.22094
229	0.59774	2.217	2.0067	1.88096	2.40314
230	0.595066	2.04647	2.10982	2.12683	2.27647

231	0.565931	1.99556	1.95377	2.02354	2.18203
232	0.623375	1.98008	2.30546	1.94145	1.91651
233	0.583632	2.27349	2.09585	2.07348	2.23611
234	0.591011	2.14043	1.97894	1.97431	2.20945
235	0.595602	2.15274	1.8826	1.97914	2.22628
236	0.589564	2.02778	1.8753	2.06411	2.08794
237	0.576789	1.93778	2.01437	2.0709	2.2391
238	0.580074	2.20302	1.99081	2.06377	2.19943
239	0.58801	2.23194	2.24364	2.05063	2.21979
240	0.603867	1.99767	1.83129	2.17124	2.49221
241	0.610649	2.07704	1.76896	1.93531	2.02281
242	0.571716	1.94157	2.17673	2.1719	2.36976
243	0.583108	2.17829	1.92617	2.00652	2.34506
244	0.587883	2.27098	2.01242	2.08687	2.21106
245	0.600741	1.94247	1.93195	2.00309	2.11032
246	0.592717	2.0417	2.03543	2.02013	2.18053
247	0.623393	1.97981	2.20724	1.9453	1.97061
248	0.596654	2.16886	2.01326	2.14891	2.10236
249	0.614295	2.03175	1.92154	2.02186	2.2272
250	0.605565	2.07288	2.0089	2.11326	2.44465
251	0.630305	2.15265	2.00591	2.02624	2.16142
252	0.599055	1.9208	1.98006	1.96423	2.18896
253	0.614021	2.05326	1.9409	2.02771	2.18144
254	0.598225	2.03252	2.13534	2.0633	2.11452
255	0.596374	2.33578	2.26422	2.14335	2.48853
256	0.58162	2.24026	1.98542	2.1266	2.10554
257	0.591744	2.03289	2.1473	2.00397	2.2147
258	0.584496	2.31338	1.90715	1.93636	2.20364
259	0.612276	2.29974	1.88664	1.93287	2.22408
260	0.590275	2.15418	1.98321	1.96491	2.08248
261	0.589835	1.99956	1.87559	1.9372	2.46559
262	0.5862	2.05922	2.12155	2.04993	2.45896
263	0.581088	1.93437	1.85189	2.15165	2.3288
264	0.577288	2.10392	1.9179	2.10508	2.18889
265	0.596772	2.01982	1.79491	2.24544	2.22313
266	0.589787	2.08782	2.08754	2.03263	2.34241
267	0.594633	2.01586	1.76653	1.99682	2.34656
268	0.577346	2.21528	2.05427	1.81648	2.36617
269	0.582516	2.18521	2.03294	2.06781	2.13284
270	0.596213	2.3052	2.06769	2.20596	2.34971
271	0.58114	2.16765	2.02339	1.92848	2.28803
272	0.587242	2.02801	1.91659	1.97094	2.38698
273	0.581629	2.15086	1.91117	2.20307	2.26912
274	0.591295	2.25483	2.30258	1.937	2.37532
275	0.584695	2.22732	2.01482	1.96447	2.11904
276	0.584256	2.0769	1.87591	1.97105	2.10862
277	0.589374	2.16193	2.16229	2.04723	2.49716

278	0.60268	2.13811	1.98181	1.96006	2.24944
279	0.598858	2.13018	2.20687	2.00689	2.50441
280	0.605166	1.99001	1.85308	1.9822	2.62131
281	0.593502	2.12075	1.98931	1.95917	2.17454
282	0.602931	2.29692	1.96872	2.0434	2.24506
283	0.594474	2.18616	2.04599	2.01561	2.27162
284	0.60766	2.11253	1.98079	2.25019	2.26622
285	0.584226	2.05	2.04594	1.92485	2.4673
286	0.601981	1.83029	2.10158	1.96091	2.15725
287	0.583622	1.93384	1.86421	1.98412	2.18457
288	0.595517	2.04609	1.78872	2.08491	2.1251
289	0.567625	1.98992	2.03195	2.23604	2.17039
290	0.59081	1.93235	1.95331	2.05698	2.47579
291	0.590672	2.17946	1.80968	1.8805	2.60994
292	0.592101	1.96351	2.02977	1.90813	2.18108
293	0.57651	1.97996	1.95373	2.14424	2.34801
294	0.591593	2.21002	2.16487	1.9839	2.09417
295	0.602219	2.12131	2.03627	1.84434	2.20892
296	0.577211	2.2059	2.07634	1.87591	2.39943
297	0.579664	2.13548	1.9687	2.0956	2.13139
298	0.588983	2.05352	2.03083	1.95622	2.47406
299	0.601428	2.22582	2.19072	1.92237	2.29103
300	0.599579	2.05294	2.13586	1.8979	2.65733
301	0.606018	2.04779	1.94566	1.9443	2.03053
302	0.601818	2.03102	2.15274	2.16671	2.26049
303	0.58456	2.2656	1.91906	2.0901	2.21328
304	0.576331	1.99168	1.97091	2.10505	2.43787
305	0.576632	2.05634	1.88761	2.10114	2.20035
306	0.599302	2.11251	2.04007	2.18187	2.17233
307	0.587141	2.34398	1.897	2.10941	2.33535
308	0.588559	2.06498	1.86149	2.08886	2.41477
309	0.590702	2.22322	2.05478	2.11561	2.25595
310	0.59281	2.03306	1.90336	2.19821	2.38008
311	0.592335	2.13269	2.04564	1.93513	2.30365
312	0.579915	2.28459	1.98389	1.98568	2.25713
313	0.581451	2.1997	2.01282	2.05003	2.20993
314	0.614787	2.08457	2.09711	1.95171	2.04291
315	0.596354	2.19617	1.92351	1.96543	2.16833
316	0.608998	2.12487	1.96703	2.01377	2.12404
317	0.59565	2.18241	1.9511	1.92245	2.29885
318	0.611073	2.20742	2.24474	1.91154	2.23768
319	0.593987	2.11914	2.0029	2.12726	2.53693
320	0.588794	2.01392	1.90895	2.18696	2.23515
321	0.603079	1.9482	1.93728	1.99149	2.24187
322	0.60559	2.23472	2.07414	2.03355	2.40794
323	0.601664	2.22177	2.18005	1.99033	2.34535
324	0.599449	2.10105	2.15606	1.98181	2.38012

325	0.602735	2.17141	2.09703	2.08768	2.33767
326	0.57459	2.19315	2.17195	2.07313	2.61659
327	0.589479	2.20557	1.9794	2.05839	2.11221
328	0.581432	2.37359	2.05787	2.03041	2.30037
329	0.581915	2.28358	1.88979	1.90983	2.23928
330	0.589309	2.29296	1.98938	2.09383	2.28806
331	0.601279	2.11831	1.93852	1.98295	2.35262
332	0.58359	2.0257	1.90418	2.09394	2.28926
333	0.617834	2.05866	2.12519	1.98977	2.49707
334	0.609174	2.20701	2.12814	2.049	2.42393
335	0.609362	1.98749	1.9708	2.00545	2.09981
336	0.566792	2.17776	1.89455	2.05781	2.45348
337	0.582374	2.27128	2.03119	2.01201	2.42084
338	0.604167	2.21835	2.21622	1.96184	2.53348
339	0.584545	2.20831	2.03658	2.01843	2.18552
340	0.604843	2.09451	1.9329	2.04063	2.1904
341	0.600415	2.04803	2.08676	1.9308	2.14386
342	0.586627	2.08343	2.01413	1.85829	2.18238
343	0.593319	2.01946	1.88388	1.98028	2.31269
344	0.606989	2.06356	1.93372	2.12387	2.05705
345	0.594944	2.06767	2.11434	1.89048	2.44206
346	0.587222	2.20357	1.89954	1.99912	2.14305
347	0.575766	2.13726	1.98968	2.22558	2.26609
348	0.605955	2.07813	1.99239	1.94055	2.02148
349	0.586437	2.22475	2.17151	1.97116	2.40681
350	0.587039	2.22599	1.92881	2.09337	2.43068
351	0.594467	2.10421	1.9568	1.80037	2.17541
352	0.618785	1.94842	2.02483	2.12804	2.25848
353	0.578948	2.21667	2.08364	2.05323	2.48462
354	0.599458	2.24991	2.00769	1.92998	2.12937
355	0.597371	2.40029	2.04023	1.89157	2.31158
356	0.584388	2.07064	2.29941	2.08484	2.49413
357	0.618703	2.21768	1.92644	2.05509	2.14686
358	0.603929	2.05504	2.08637	2.08933	2.25177
359	0.593166	1.93159	2.02416	2.13211	2.18411
360	0.603791	2.26859	1.92153	1.90749	2.21462
361	0.578154	2.1599	1.97808	1.99763	2.31091
362	0.571092	2.2006	1.94743	1.89767	2.37833
363	0.599975	2.10321	2.17874	1.87403	2.20133
364	0.60235	2.19898	1.88922	2.13303	1.9305
365	0.593747	2.09246	1.83565	2.12192	2.35424
366	0.57897	2.37487	1.82862	1.86093	2.2768
367	0.585013	2.20282	2.19866	1.84108	2.14539
368	0.579132	2.08519	1.98491	1.88665	2.24285
369	0.587829	2.08374	1.93827	2.04303	2.26943
370	0.585952	1.98854	2.13358	2.1755	2.26534
371	0.579709	1.98088	2.23098	2.03572	2.3189

372	0.600422	2.1896	2.08884	1.92451	2.26193
373	0.593104	2.01082	2.13177	1.93302	2.2355
374	0.608281	1.9746	1.97474	1.93762	2.45411
375	0.59967	1.94418	2.19838	1.99548	2.39522
376	0.604617	2.23956	1.8448	1.89799	2.28393
377	0.583167	2.05859	2.15791	2.01219	2.20491
378	0.592724	2.08163	1.88879	2.16852	2.22124
379	0.593878	2.08796	2.06017	2.00306	2.33478
380	0.562002	2.09803	2.05435	2.03153	2.16806
381	0.59693	2.31569	1.86315	2.03281	2.25973
382	0.585615	2.27688	2.0613	2.01483	2.2115
383	0.568549	2.22097	2.10969	1.99629	2.39685
384	0.589486	2.05005	2.13753	2.06568	2.04302
385	0.574781	2.05616	2.0457	2.00523	2.4582
386	0.613944	2.02994	2.04426	2.00605	2.07002
387	0.605885	1.87174	1.98373	2.08912	2.22936
388	0.58327	2.08461	2.05426	2.02183	2.34895
389	0.569199	2.09948	2.31918	2.13213	2.16181
390	0.609639	2.08351	1.93625	1.97106	2.23103
391	0.584726	2.177	1.87353	2.03556	2.24527
392	0.591024	2.29022	2.00194	2.03414	2.03512
393	0.552061	2.057	1.83007	1.90922	2.4703
394	0.600118	2.06761	1.94491	1.94822	2.12961
395	0.586646	2.09199	1.82197	1.95179	2.27387
396	0.580697	2.15823	1.98502	2.08999	2.33177
397	0.584429	2.05298	2.16356	1.9608	2.14341
398	0.592416	2.31144	2.15329	1.95169	2.3614
399	0.589432	2.17313	1.86301	2.04814	2.64385
400	0.61046	1.92172	2.20885	1.90015	2.03056
401	0.60764	2.25941	2.05477	2.13898	2.0202
402	0.599913	2.21642	1.82487	2.24246	2.10977
403	0.597503	2.13991	2.05404	1.83737	2.31613
404	0.602186	2.17643	2.12221	2.0912	2.28596
405	0.592845	2.2644	2.208	2.0448	2.17124
406	0.604005	2.36417	1.86159	2.01813	2.21473
407	0.584573	2.09884	1.98417	2.06293	2.2751
408	0.607821	2.13311	2.05469	2.1061	2.20433
409	0.590755	2.35363	2.03297	2.13683	2.46618
410	0.595399	2.17265	2.02398	2.09413	2.29864
411	0.601986	2.07209	1.87706	1.94877	2.0893
412	0.609514	2.28354	2.29989	1.97074	2.52058
413	0.584473	2.06244	2.0217	2.28907	2.31684
414	0.610135	2.20235	1.85096	1.93341	2.35807
415	0.581469	2.08829	2.14988	2.12386	2.27738
416	0.588275	2.25463	2.08684	2.08638	2.34909
417	0.600488	2.36514	2.00378	2.01155	2.61463
418	0.588339	2.21791	1.97127	2.12041	2.14843

419	0.596832	2.15615	1.85795	1.91338	2.31745
420	0.575909	2.16861	2.01696	1.95995	2.06671
421	0.593825	2.01953	2.15694	2.03557	2.17271
422	0.575055	2.42585	2.21008	1.94241	2.22131
423	0.576201	2.12983	1.91979	2.03499	2.41116
424	0.571877	2.07018	2.19958	2.24206	2.44792
425	0.57976	2.0948	1.96954	1.9175	2.34408
426	0.572091	2.14661	1.81516	1.99206	2.33105
427	0.589089	2.26727	1.92483	2.0706	2.44418
428	0.559261	2.32759	2.01163	1.98501	2.3497
429	0.591722	2.13604	2.11866	1.91191	2.26798
430	0.602458	2.17137	2.22031	2.05612	2.07805
431	0.581478	2.12284	1.99865	1.85195	2.29282
432	0.56861	2.10823	1.8465	2.02722	2.52823
433	0.588664	2.03535	1.92276	2.09333	2.22557
434	0.599784	2.25969	1.88675	2.03395	2.31453
435	0.588952	2.28444	2.29936	2.22649	2.16867
436	0.615237	2.07953	2.12878	1.93647	2.36419
437	0.593487	1.97979	1.81649	1.89991	2.27325
438	0.604788	1.91715	1.91689	1.97625	2.46634
439	0.58695	2.1893	1.8739	1.93395	2.32607
440	0.587477	2.3239	2.03042	1.95047	2.41218
441	0.59166	2.16583	1.8655	1.96044	2.14943
442	0.601739	2.02504	2.00364	1.94667	2.51119
443	0.593272	2.11763	1.85985	2.03874	2.29924
444	0.598757	2.25551	1.97967	2.18775	2.5386
445	0.594592	2.23676	2.06741	1.99106	2.36012
446	0.624326	2.07549	1.98259	2.05594	2.24458
447	0.596905	2.24441	2.10018	2.20258	2.12074
448	0.596369	2.40489	2.31696	2.09084	2.30958
449	0.598628	2.25935	2.01474	1.95733	2.26486
450	0.5867	2.13376	1.88066	1.93079	2.644
451	0.609225	2.09431	1.83029	1.97273	2.4487
452	0.582795	2.12355	1.87763	1.90628	2.29278
453	0.587298	2.04117	2.11648	2.17805	2.1665
454	0.582928	2.32126	1.86727	2.1818	2.33217
455	0.586838	2.19306	1.82884	1.88688	2.19404
456	0.572842	2.15944	1.91327	1.99582	2.18326
457	0.617299	2.26362	1.94826	2.17859	2.10425
458	0.591284	2.12674	1.97976	1.87036	2.42033
459	0.597177	2.30604	1.99323	1.88177	2.29234
460	0.578619	2.29666	2.06991	1.96666	2.25585
461	0.607447	2.12751	2.00107	1.90755	2.5642
462	0.590106	2.06379	1.917	2.01751	2.16457
463	0.592944	2.35688	2.04883	1.96246	2.3217
464	0.581892	2.25946	2.05039	1.94613	2.28648
465	0.594702	2.03881	1.97624	2.12818	2.07988

466	0.574798	2.23246	2.01655	2.33926	2.37073
467	0.584243	2.21167	2.0836	2.06763	2.40775
468	0.593141	2.11401	1.89984	2.2165	2.49589
469	0.59152	2.06999	1.94518	1.86218	2.08698
470	0.571294	2.28594	2.14812	1.98995	2.35179
471	0.592291	2.13853	1.92196	1.97798	2.20943
472	0.604534	2.16684	1.8349	1.98267	2.26079
473	0.59794	1.88833	1.96682	1.999	2.18734
474	0.594304	2.02204	2.14597	1.93355	2.13378
475	0.597586	2.09251	1.90326	2.147	2.21506
476	0.596795	2.09118	2.10238	2.05831	2.04979
477	0.594761	2.15703	1.97738	1.8834	2.27744
478	0.587484	2.21642	1.96134	2.00787	2.32094
479	0.591915	2.15829	1.85568	2.00228	2.19904
480	0.606416	2.06632	1.99854	2.13536	2.31617
481	0.595923	2.17558	2.1543	1.99474	2.23842
482	0.603927	1.99693	2.0837	2.01169	2.28529
483	0.609366	2.11532	1.88928	1.94782	2.26702
484	0.60415	2.17744	1.97522	2.12688	2.43127
485	0.605139	2.15022	2.01351	2.1068	2.49663
486	0.600905	2.08488	1.92394	1.90661	2.27432
487	0.60732	2.27292	2.23546	2.17492	2.50076
488	0.619674	2.36928	1.90226	2.06043	2.06775
489	0.584152	2.2597	2.0807	1.96463	2.26595
490	0.611941	2.07896	2.01067	2.1662	2.21646
491	0.611301	2.20246	2.08912	1.9056	2.56035
492	0.599522	2.11678	2.13707	1.89683	2.21074
493	0.614323	2.19071	2.00948	1.88273	2.22573
494	0.631673	1.93865	2.18468	2.14041	2.56547
495	0.595308	2.14292	2.19912	1.95708	2.32254
496	0.631944	2.17691	2.1051	2.07307	2.30456
497	0.60097	2.26796	1.78054	2.07305	2.31984
498	0.615924	2.16789	1.9208	2.0056	2.40289
499	0.61734	2.23757	1.82632	2.29858	2.22715
500	0.597696	1.99806	1.9138	2.04846	2.59912

Table S2 The calculated interaction Energies between key amino acids with compound B2.

Residue	Interaction Energy (kcal/mol)	VDW Interaction Energy (kcal/mol)	Electrostatic Interaction Energy (kcal/mol)
ILE463	-0.465755	-0.686452	0.220697
SER465	-6.35264	-1.03352	-5.31912
GLY466	0.361418	0.511949	-0.150531
SER467	-2.19322	-1.15918	-1.03404
GLY469	-0.383314	-0.364588	-0.018726
VAL471	-4.01348	-3.7658	-0.247676
ALA481	3.91651	2.32972	1.58679
VAL482	-1.93395	-0.973147	-0.960803
LYS483	-3.02184	-4.33051	1.30867
LEU505	-0.666395	-0.68215	0.015755
THR508	-0.476311	-0.15722	-0.319091
ILE513	-1.68874	-0.988537	-0.7002
LEU514	0.09377	-1.61357	1.70734
PHE516	-1.5932	-1.80606	0.212857
ILE527	-2.26064	-2.31129	0.050648
THR529	-8.07468	-2.96084	-5.11384
GLN530	-0.182578	-0.311711	0.129133
TRP531	-1.61059	-0.807157	-0.803432
SER536	-0.867384	-0.395526	-0.471858
HIS574	-1.69591	-0.204016	-1.49189
LYS578	0.357014	-0.406427	0.763441
ASN580	-6.35264	-2.05672	-8.26572
ASN581	-3.98578	-0.683102	-3.30268
PHE583	-4.27368	-3.75329	-0.520393
ILE592	-0.285262	-0.429245	0.143983
GLY593	-3.43332	-1.84039	-1.59293
ASP594	-5.08437	-2.26056	-2.82381
PHE595	-2.10401	-2.04291	-0.061102
GLY596	-0.38845	-0.522046	0.133596