Designing, quinazoline based derivatives as FGFR4 selective inhibitors for hepatocellular carcinoma

This repository hosts the tabular dataset used in my thesis, collected on Designing of quinazoline-based derivatives as selective FGFR4 inhibitors for hepatocellular carcinoma (HCC). It includes table's data (original results). Full methodology, data processing steps, and usage instructions mentioned in thesis work.

Table 2: Failed Compounds

S	COMPOUNDS		STRUCTURE	
NO.		R_1	R_2	R ₃
1	19	O HN 32	C ₂ H ₅	O=S=N
2	20	HZ %	CI	O=S=N O
3	21	HZ %	F	O=S=N O
4	22	O H N 32	O _{CH3}	O=S=N O
5	23	HZ %	CF ₃	O=S=N O
6	24	HZ %	Н	O=S=N O
7	25	HZ X	C ₂ H ₅	O=S=NH
8	26	HZ 75	CI	O=S=NH
9	27	O HZ 35	F	O=S=NH

10	28	HN34	O _{CH3}	O=S=NH
11	29	O H	CF ₃	O=S=NH
12	30	O H N 35	Н	0=S=NH
13	61	O S O	C ₂ H ₅	O=S=N O
14	62	O S O	CI	O=S=N O
15	63	O H X	F	O=S=N O
16	64	O H X	O _{`CH3}	O=S=N O
17	65	O H N N N N N N N N N N N N N N N N N N	CF ₃	O=S=N O
18	66	O H X	Н	O=S=N O
19	67	O H X	C ₂ H ₅	O=S=NH
20	68	O TX	CI	O=S=NH
21	69	O H N N	F	O=S=NH
22	70	O S O	O _{CH3}	O=S=NH

23	71	O XX O	CF ₃	O=S=NH
24	72	0/%/O HZ HZ %	Н	O=S=NH
25	97	CI O TY STAN	C ₂ H ₅	O=S=N O
26	98	CI D TY	CI	O=S=N O
27	99	CI TY STAN	F	O=S=N O
28	100		O _{`CH3}	O=S=N O
29	101		CF ₃	O=S=N O
30	102	TZ O	Ι	O=S=N O
31	103	CI C	C ₂ H ₅	O=S=NH
32	104	O ZI	CI	O=S=NH
33	105	CI The state of th	F	0=S=NH
34	106	CI HN 354	O _` CH₃	0=S=NH
35	107	CI TY See	CF ₃	O=S=NH

36	108	CI HN 35	Н	O=S=NH
37	133	F HN &	C ₂ H ₅	O=S=N O
38	134	F HN ×	CI	O=S=N O
39	135	F HZ X	F	O=S=N O
40	136	F HZ X	O _{CH3}	O=S=N O
41	137	F HN X	CF ₃	O=S=N O
42	138	F HN %	Н	O=S=N O
43	139	F HN %	C ₂ H ₅	O=S=NH
44	140	F HN X	CI	O=S=NH
45	141	F HN &	F	O=S=NH
46	142	F HN &	O _{CH3}	O=S=NH
47	143	F HN 3	CF ₃	O=S=NH

48	144	F HN %	Н	O=S=NH
49	169	O HN 32	C ₂ H ₅	O=S=N O
50	170	O IN SE	CI	O=S=N O
51	171	O TZ ZIZ	F	O=S=N O
52	172	O IZ ZIZ	O _{CH3}	O=S=N
53	173	O HN %	O _{CH3}	O=S=N
54	174	O HN 354	Н	O=S=N O
55	175	O HN 34	C ₂ H ₅	0=S=NH
56	176	O HZ HZ	CI	O=S=NH
57	177	O H N N N N N N N N N N N N N N N N N N	F	O=S=NH
58	178	O H N N N N N N N N N N N N N N N N N N	O _{CH3}	O=S=NH
59	179	O HZ X	CF ₃	→ O=S=NH

60	180	O HN 32	Н	O=S=NH
61	205	OHC N	C ₂ H ₅	O=S=N O
62	206	OHC N	CI	O=S=N O
63	207	OHC N	F	O=S=N O
64	208	OHC N	O _{CH3}	O=S=N O
65	209	OHC N X	CF ₃	O=S=N O
66	210	OHC N	Н	O=S=N O
67	211	OHC N	C ₂ H ₅	O=S=NH
68	212	OHC N	CI	O=S=NH
69	213	OHC N	F	O=S=NH
70	214	OHC N	O _{CH3}	O=S=NH
71	215	OHC N	CF ₃	O=S=NH
72	216	OHC N	Н	O=S=NH
73	223	F HZ X	C ₂ H ₅	O=S=NH CH ₃

74	224	F HN &	CI	O=S=NH CH ₃
75	225	F HZ X	F	O=S=NH CH ₃
76	226	EZ EZ O	O _{CH3}	O=S=NH CH ₃
77	227	HZ HO	CF ₃	O=S=NH CH ₃
78	228	HZ HO	Н	O=S=NH CH ₃
79	229	HZ O	C ₂ H ₅	CH ₃ O=S=N CH ₃
80	230	HZ HO	CI	CH ₃ O=S=N CH ₃
81	231	F N N N	F	CH ₃ O=S=N CH ₃
82	232	F Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z	O _{\CH3}	CH ₃ O=S=N CH ₃
83	233	F HZ &	CF ₃	CH ₃ O=S=N CH ₃
84	234	F Z	Н	CH ₃ O=S=N CH ₃
85	235	F HN %	C ₂ H ₅	O=S=NH CH ₃

86	236	F HN 3	CI	O=S=NH CH ₃
87	237	F H N ×	F	O=S=NH CH ₃
88	238	F HZ X	O _{CH3}	O=S=NH CH ₃
89	239	F HN ×	CF ₃	O=S=NH CH ₃
90	240	F HN X	Н	O=S=NH CH ₃
91	247	O H N 33	C ₂ H ₅	O=S=NH CH ₃
92	248	O H N 324	CI	O=S=NH CH ₃
93	249	O H XX	F	O=S=NH CH ₃
94	250	O H N 33	O _{CH3}	O=S=NH CH ₃
95	251	H N N N N N N N N N N N N N N N N N N N	CF ₃	O=S=NH CH ₃
96	252	H N 33	Н	O=S=NH CH ₃
97	253	O H N 3,3,4	C ₂ H ₅	CH ₃ O=S=N CH ₃
98	254	O HN 32 HN 32	CI	CH ₃ O=\$=N CH ₃

99	255	O H X X	F	CH ₃ O=S=N CH ₃
100	256	O S Z Z Z	O CH₃	CH ₃ O=S=N CH ₃
101	257	O	CF ₃	CH ₃ O=S=N CH ₃
102	258	O N X	Н	O=S=N CH ₃
103	259	O N X X	C ₂ H ₅	O=S=NH CH ₃
104	260	O Z	CI	O=S=NH CH ₃
105	261	O N X X	F	O=S=NH CH ₃
106	262	O N X	O _` CH₃	O=S=NH CH ₃
107	263	O N X X	CF ₃	O=S=NH CH ₃
108	264	O ZZ	Н	O=S=NH CH ₃
109	271	OHC N	C ₂ H ₅	O=S=NH CH ₃
110	272	OHC N	CI	O=S=NH CH ₃
111	273	OHC N	F	O=S=NH CH ₃
112	274	OHC N	O _{CH3}	O=S=NH CH ₃

113	275	OHC N	CF ₃	O=S=NH CH ₃
114	276	OHC N	Н	O=S=NH CH ₃
115	277	OHC N	C ₂ H ₅	O=S=N CH ₃
116	278	OHC N	CI	O=S=N CH ₃
117	279	OHC N X	F	CH ₃ O=S=N CH ₃
118	280	OHC N X	O _{CH3}	CH ₃ O=S=N CH ₃
119	281	OHC N	CF ₃	O=S=N CH ₃
120	282	OHC N	Н	O=S=N CH ₃
121	283	OHC N	C ₂ H ₅	O=S=NH CH ₃
122	284	OHC N ze	CI	O=S=NH CH ₃
123	285	OHC N	F	O=S=NH CH ₃
124	286	OHC N	O _{CH3}	O=S=NH CH ₃
125	287	OHC N	CF ₃	O=S=NH CH ₃
126	288	OHC N	Н	O=S=NH CH ₃

127	295	O H N X	C ₂ H ₅	O=S=NH CH ₃
128	296	O H Z Z Z H	CI	O=S=NH CH ₃
129	297	O H N Sy	F	O=S=NH CH ₃
130	298	O HX X	O _{CH3}	O=S=NH CH ₃
131	299	O HX 34	CF ₃	O=S=NH CH ₃
132	300	O HZ XX	Н	O=S=NH CH ₃
133	301	O HZ ZZ	C ₂ H ₅	CH ₃ O=\$=N CH ₃
134	302	O HN 35%	CI	CH ₃ O=\$=N CH ₃
135	303	O H N N N	F	CH ₃ O=S=N CH ₃
136	304	O H N 3 %	O _{CH3}	CH ₃ O=S=N CH ₃
137	305	O HN 24	CF ₃	CH ₃ O=S=N CH ₃
138	306	O HX 34	Н	CH ₃ O=S=N CH ₃
139	307	O HN 3%	C ₂ H ₅	O=S=NH CH ₃

140	308	O HN 22	CI	O=S=NH CH ₃
141	309	O TY SY	F	O=S=NH CH ₃
142	310	O HN 34	O _{CH3}	O=S=NH CH ₃
143	311	O IN SET	CF ₃	O=S=NH CH ₃
144	312	O TZ ZT	Н	O=S=NH CH ₃
145	319	CI The state of th	C ₂ H ₅	O=S=NH CH ₃
146	320	T Z O	CI	O=S=NH CH ₃
147	321	CI The state of th	F	O=S=NH CH ₃
148	322	CI H S	O _{CH3}	O=S=NH CH ₃
149	323	CI The state of th	CF ₃	O=S=NH CH ₃
150	324	CI H S	Н	O=S=NH CH ₃
151	325	CI The state of th	C ₂ H ₅	CH ₃ O=S=N CH ₃
152	326	CI O H N	CI	CH ₃ O=S=N CH ₃

153	327	CI HN 354	F	O=S=N CH ₃
154	328	O ZI	O _{CH3}	CH ₃ O=S=N CH ₃
155	329	CI O H N N N N N N N N N N N N N N N N N N	CF ₃	O=S=N CH ₃
156	330	CI O H N N N N N N N N N N N N N N N N N N	Н	CH ₃ O=S=N CH ₃
157	331	CI O I N	C ₂ H ₅	O=S=NH CH ₃
158	332	CI O I N	CI	O=S=NH CH ₃
159	333	CI O I N	F	O=S=NH CH ₃
160	334	CI O H N See	O _\ CH ₃	O=S=NH CH ₃
161	335	CI O I N	CF ₃	O=S=NH CH ₃
162	336	CI O I No	Н	O=S=NH CH ₃
163	342	0 \$ 0 H X X	Н	O=S=O H ₃ C
164	343	O O ZI	C ₂ H ₅	O=S=NH CH ₃
165	344	O SO TENTO	CI	O=S=NH CH ₃
166	345	O NO	F	O=S=NH CH ₃

167	346	O HN X	O _{CH3}	O=S=NH CH ₃
168	347	O H N N	CF ₃	O=S=NH CH ₃
169	348	O H N O	Н	O=S=NH CH ₃
170	349	O H N N N O	C ₂ H ₅	CH ₃ O=S=N CH ₃
171	350	O S O	CI	CH ₃ CH ₃
172	351	O S O	F	CH ₃ O=S=N CH ₃
173	352	O HN O	O _{CH3}	O=S=N CH ₃
174	353	O H N O	CF ₃	O=S=N CH ₃
175	354	O H N N	Н	O=S=N CH ₃
176	355	O S O	C₂H₅	O=\$=NH CH ₃
177	356	O H N N	CI	O=S=NH CH ₃
178	357	O H N N	F	O=S=NH CH ₃
179	358	O H N N O	O _{CH3}	O=S=NH CH ₃

180	359	O S O	CF ₃	O=\$=NH CH ₃
181	360	O S O	Н	O=S=NH CH ₃

<u>Table 3: Outcome of Primary Screening (Accurate but slow)</u>

Sl No.	Compounds	LF DG score (kcal/mol)
1	38_D	-14.876
2	37_D	-14.777
3	109_D	-14.401
4	55_D	-14.300
5	127_D	-14.289
6	49_D	-14.249
7	2_D	-14.244
8	57_D	-14.226
9	60_D	-14.226
10	42_D	-14.182
11	337_D	-14.142
12	128_D	-14.133
13	1_D	-14.128
14	148_D	-14.122
15	112_D	-14.114
16	43_D	-14.078
17	116_D	-14.068
18	14_D	-14.032
19	150_D	-14.029
20	341_D	-14.020
21	110_D	-14.010
22	111_D	-14.007
23	181_D	-13.984
24	51_D	-13.954
25	338_D	-13.952
26	152_D	-13.949

27	145_D	-13.943
28	4_D	-13.912
29	217_D	-13.873
30	183_D	-13.871
31	13_D	-13.851
32	8_D	-13.845
33	39_D	-13.822
34	113_D	-13.819
35	219_D	-13.817
36	242_D	-13.811
37	146_D	-13.811
38	165_D	-13.798
39	115_D	-13.798
40	114_D	-13.736
41	158_D	-13.730
42	5_D	-13.723
43	18_D	-13.720
44	167_D	-13.719
45	294_D	-13.706
46	120_D	-13.689
47	147_D	-13.683
48	131_D	-13.662
49	121_D	-13.651
50	195_D	-13.648
51	6_D	-13.629
52	52_D	-13.626
53	203_D	-13.624
54	200_D	-13.616
55	162_D	-13.591
56	265_D	-13.582
57	164_D	-13.578
58	241_D	-13.565
59	56_D	-13.511
60	122_D	-13.511
61	126_D	-13.503
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62	193_D	-13.501
63	166_D	-13.500
64	149_D	-13.496
65	187_D	-13.492
66	58_D	-13.490
67	246_D	-13.482
68	222_D	-13.468
69	17_D	-13.465
70	290_D	-13.458
71	50_D	-13.454
72	7_D	-13.454
73	45_D	-13.450
74	161_D	-13.442
75	15_D	-13.435
76	10_D	-13.432
77	289_D	-13.425
78	16_D	-13.424
79	117_D	-13.415
80	220_D	-13.414
81	119_D	-13.414
82	47_D	-13.413
83	35_D	-13.411
84	3_D	-13.407
85	129_D	-13.406
86	46_D	-13.404
87	182_D	-13.398
88	153_D	-13.392
89	34_D	-13.375
90	151_D	-13.375
91	291_D	-13.375
92	221_D	-13.373
93	12_D	-13.364
94	75_D	-13.362
95	160_D	-13.358
96	243_D	-13.353

97	163_D	-13.351
98	130_D	-13.351
99	59_D	-13.344
100	292_D	-13.342
101	32_D	-13.324
102	123_D	-13.320
103	31_D	-13.301
104	270_D	-13.298
105	340_D	-13.295
106	202_D	-13.294
107	118_D	-13.290
108	204_D	-13.282
109	44_D	-13.264
110	132_D	-13.264
111	41_D	-13.263
112	199_D	-13.260
113	156_D	-13.258
114	218_D	-13.255
115	339_D	-13.253
116	157_D	-13.251
117	198_D	-13.245
118	40_D	-13.220
119	154_D	-13.201
120	155_D	-13.195
121	48_D	-13.190
122	159_D	-13.187
123	268_D	-13.181
124	189_D	-13.173
125	11_D	-13.149
126	125_D	-13.143
127	185_D	-13.126
128	245_D	-13.119
129	293_D	-13.107
130	267_D	-13.095
131	188_D	-13.082

132	269_D	-13.077
133	266_D	-13.076
134	9_D	-13.068
135	33_D	-13.048
136	A 40M 1002_D	-13.019

<u>Table 4: Outcome of Secondary Screening (Very Accurate but slow)</u>

SlNo.	Compounds	LFDG Score (kcal/mol)
1	38_D_D	-14.847
2	42_D_D	-14.813
3	37_D_D	-14.722
4	2_D_D	-14.721
5	150_D_D	-14.61
6	1_D_D	-14.534
7	200_D_D	-14.51
8	242_D_D	-14.486
9	146_D_D	-14.48
10	222_D_D	-14.372
11	145_D_D	-14.361
12	17_D_D	-14.33
13	128_D_D	-14.328
14	148_D_D	-14.326
15	338_D_D	-14.312
16	43_D_D	-14.308
17	55_D_D	-14.275
18	165_D_D	-14.26
19	162_D_D	-14.254
20	16_D_D	-14.252
21	182_D_D	-14.232
22	109_D_D	-14.23
23	166_D_D	-14.226
24	161_D_D	-14.214

25	126_D_D	-14.183
26	246_D_D	-14.151
27	160_D_D	-14.106
28	52_D_D	-14.099
29	152_D_D	-14.098
30	198_D_D	-14.095
31	290_D_D	-14.092
32	199_D_D	-14.069
33	14_D_D	-14.059
34	118_D_D	-14.056
35	183_D_D	-14.046
36	18_D_D	-14.04
37	127_D_D	-14.037
38	130_D_D	-14.021
39	13_D_D	-14.016
40	112_D_D	-13.996
41	50_D_D	-13.991
42	117_D_D	-13.989
43	241_D_D	-13.978
44	6_D_D	-13.938
45	204_D_D	-13.931
46	3_D_D	-13.922
47	243_D_D	-13.914
48	111_D_D	-13.913
49	217_D_D	-13.908
50	40_D_D	-13.901
51	266_D_D	-13.894
52	294_D_D	-13.88
53	39_D_D	-13.866
54	121_D_D	-13.853
55	114_D_D	-13.837
56	75_D_D	-13.835
57	154_D_D	-13.833
58	268_D_D	-13.825
59	340_D_D	-13.824

60	185_D_D	-13.822
61	147_D_D	-13.819
62	220_D_D	-13.786
63	31_D_D	-13.778
64	156_D_D	-13.778
65	149_D_D	-13.759
66	32_D_D	-13.744
67	291_D_D	-13.734
68	41_D_D	-13.723
69	292_D_D	-13.71
70	9_D_D	-13.708
71	56_D_D	-13.674
72	265_D_D	-13.64
73	219_D_D	-13.639
74	8_D_D	-13.639
75	35_D_D	-13.638
76	202_D_D	-13.627
77	195_D_D	-13.591
78	116_D_D	-13.583
79	4_D_D	-13.581
80	49_D_D	-13.574
81	51_D_D	-13.562
82	44_D_D	-13.547
83	153_D_D	-13.539
84	59_D_D	-13.535
85	293_D_D	-13.516
86	270_D_D	-13.515
87	7_D_D	-13.464
88	267_D_D	-13.46
89	46_D_D	-13.457
90	155_D_D	-13.446
91	188_D_D	-13.436
92	12_D_D	-13.416
93	337_D_D	-13.413
94	119_D_D	-13.408

95	15_D_D	-13.396
96	57_D_D	-13.387
97	245_D_D	-13.346
98	123_D_D	-13.343
99	187_D_D	-13.332
100	132_D_D	-13.327
101	10_D_D	-13.313
102	115_D_D	-13.283
103	189_D_D	-13.282
104	158_D_D	-13.273
105	131_D_D	-13.244
106	159_D_D	-13.226
107	122_D_D	-13.218
108	181_D_D	-13.208
109	203_D_D	-13.153
110	11_D_D	-13.145
111	269_D_D	-13.132
112	151_D_D	-13.13
113	33_D_D	-13.119
114	5_D_D	-13.079
115	58_D_D	-13.056
116	167_D_D	-13.021
117	221_D_D	-12.922
118	163_D_D	-12.922
119	193_D_D	-12.874
120	339_D_D	-12.851
121	60_D_D	-12.721
122	113_D_D	-12.607
123	341_D_D	-12.519
124	164_D_D	-12.519
125	120_D_D	-12.515
126	34_D_D	-12.504
127	110_D_D	-12.473
128	157_D_D	-12.263
129	47_D_D	-12.233

130	218_D_D	-12.194
131	A 40M 1002_D_D	-12.18
132	45_D_D	-12.127
133	125_D_D	-11.854
134	48_D_D	-11.134
135	289_D_D	-10.959
136	129_D_D	-10.77

Table 5: MMGBSA Calculations

SNO.	Energy	TOTAL	VDWAALS	EEL	EGB	ESURF
	Components:	DG				
1	111_D_D	-70.79	-71.95	-54.17	64.22	-8.89
2	57_D_D	-67.49	-76.56	-54.94	73.3	-9.28
3	47_D_D	-66.97	-75.23	-50.01	67.37	-9.09
4	219_D_D	-66.91	-72.94	-46.12	61.11	-8.96
5	113_D_D	-66.64	-76.1	-81.54	100.14	-9.14
6	195_D_D	-66.62	-71.44	-55.29	68.91	-8.8
7	189_D_D	-65.98	-71.81	-38.94	53.28	-8.52
8	183_D_D	-65.97	-73.2	-52.55	68.54	-8.76
9	109_D_D	-65.91	-74.23	-53.6	70.68	-8.76
10	217_D_D	-65.61	-73.77	-38.54	55.39	-8.68
11	267_D_D	-65.08	-74.29	-37.25	55.06	-8.6
12	51_D_D	-64.89	-75.76	-60.81	80.75	-9.07
13	112_D_D	-64.18	-70.94	-54.43	69.81	-8.62
14	147_D_D	-64.08	-64.67	-63.1	72.63	-8.95
15	121_D_D	-63.99	-73.99	-44.59	63.27	-8.68
16	220_D_D	-63.53	-72.96	-42.51	60.87	-8.92
17	127_D_D	-63.25	-74.47	-45.15	65.15	-8.79
18	115_D_D	-63.23	-71.8	-40.31	57.48	-8.59
19	118_D_D	-62.71	-71.67	-40.11	57.84	-8.76
20	75_D_D	-62.37	-70.64	-51.92	68.64	-8.46
21	123_D_D	-62.07	-73.24	-30.47	50.37	-8.73

22	128_D_D	-61.2	-72.8	-37.91	57.85	-8.34
23	17_D_D	-61.04	-75.76	-30.86	54.43	-8.85
24	243_D_D	-60.82	-75.56	-39.26	62.66	-8.67
25	119_D_D	-60.81	-72.19	-33.39	53.16	-8.38
26	11_D_D	-60.77	-73.15	-31.37	52.22	-8.47
27	163_D_D	-60.77	-75.64	-46.1	69.8	-8.83
28	43_D_D	-60.7	-75.95	-48.6	72.73	-8.89
29	159_D_D	-60.64	-74.18	-40.19	62.59	-8.86
30	122_D_D	-60.44	-73.14	-34.61	55.85	-8.55
31	188_D_D	-60.34	-70.42	-34.8	53.26	-8.38
32	41_D_D	-60.34	-74.22	-43.12	66.06	-9.06
33	222_D_D	-60.09	-72.63	-43.23	64.58	-8.8
34	193_D_D	-59.79	-72.9	-52.81	74.72	-8.8
35	59_D_D	-59.55	-75.92	-54.27	79.55	-8.91
36	130_D_D	-59.52	-73.59	-31.81	54.63	-8.76
37	9_D_D	-59.37	-71.57	-39.15	59.9	-8.55
38	1_D_D	-59.28	-74.5	-43.55	67.48	-8.71
39	55_D_D	-59.18	-75.47	-57.18	82.42	-8.95
40	270_D_D	-59.07	-70.98	-43.53	63.7	-8.26
41	162_D_D	-59.05	-72.7	-52.71	75.1	-8.74
42	50_D_D	-59.05	-73.62	-57.46	80.7	-8.68
43	181_D_D	-59.01	-73.69	-61.01	84.48	-8.79
44	46_D_D	-58.54	-74.68	-53.86	78.77	-8.77
45	49_D_D	-58.25	-73.79	-57.09	81.34	-8.71
46	2_D_D	-58.06	-71.31	-40.5	61.82	-8.06
47	291_D_D	-57.95	-69.12	-46.54	66.51	-8.8
48	110_D_D	-57.93	-68.91	-43.07	62.12	-8.07
49	7_D_D	-57.75	-73.7	-29.67	54.16	-8.54
50	153_D_D	-57.65	-72.76	-31.35	55.13	-8.66
51	37_D_D	-57.41	-73.69	-61.78	86.74	-8.68
52	117_D_D	-57.36	-66.97	-24.56	42.72	-8.55
53	131_D_D	-57.27	-75.81	-26.68	54.06	-8.84

54	185_D_D	-57.23	-73.68	-43.85	68.8	-8.51
55	56_D_D	-57.2	-75.2	-47.8	74.53	-8.73
56	200_D_D	-57.1	-71.12	-43.75	66.12	-8.36
57	187_D_D	-57.09	-71.95	-36.34	59.75	-8.56
58	340_D_D	-57.05	-74.33	-57.41	83.5	-8.82
59	339_D_D	-57.04	-75.39	-25.4	52.57	-8.82
60	38_D_D	-56.95	-71.83	-62.52	85.97	-8.57
61	265_D_D	-56.78	-74.28	-34.04	60.3	-8.77
62	8_D_D	-56.75	-71.63	-32.76	55.79	-8.15
63	202_D_D	-56.66	-71.39	-31.02	54.37	-8.61
64	154_D_D	-56.64	-72.34	-30.38	54.8	-8.73
65	156_D_D	-56.62	-73.07	-31.5	56.43	-8.48
66	120_D_D	-56.53	-68.61	-29.36	49.48	-8.03
67	182_D_D	-56.48	-67.99	-36.06	55.28	-7.71
68	44_D_D	-56.43	-72.91	-33.93	58.55	-8.14
69	292_D_D	-56.12	-73.64	-28.87	55.09	-8.69
70	14_D_D	-56.05	-74.86	-25.29	52.79	-8.69
71	269_D_D	-55.95	-73.41	-36.44	62.35	-8.45
72	165_D_D	-55.88	-74.56	-33.61	61.18	-8.88
73	60_D_D	-55.76	-72.52	-65.94	91.42	-8.71
74	241_D_D	-55.67	-73.94	-29.83	56.63	-8.53
75	32_D_D	-55.63	-72.72	-36.51	62.02	-8.42
76	3_D_D	-55.5	-72.46	-38.72	64.22	-8.54
77	266_D_D	-55.5	-70.15	-25.33	48.06	-8.07
78	290_D_D	-55.45	-74.39	-28.71	56.3	-8.65
79	4_D_D	-55.44	-72.11	-46.98	72.16	-8.51
80	12_D_D	-55.26	-73.71	-22.15	49.19	-8.59
81	18_D_D	-55.24	-76.14	-34.08	63.97	-8.98
82	268_D_D	-55.1	-69.07	-41	63.21	-8.24
83	5_D_D	-54.94	-68.17	-26.09	47.94	-8.61
84	52_D_D	-54.93	-72.26	-61.5	87.56	-8.73
85	126_D_D	-54.52	-73.79	-20.95	49.09	-8.87

86	203_D_D	-54.45	-73.78	-58.76	86.79	-8.71
87	13_D_D	-54.24	-75.35	-20.35	49.94	-8.48
88	34_D_D	-54.19	-72.23	-26.41	52.8	-8.34
89	199_D_D	-54.02	-74.3	-23.07	52.26	-8.91
90	A 40M 1002_D_D	-53.97	-69.98	-26.61	50.55	-7.93
91	152_D_D	-53.86	-71.57	-30.04	56.03	-8.28
92	155_D_D	-53.71	-72.9	-31.34	59.01	-8.47
93	337_D_D	-53.64	-75.18	-32.49	62.89	-8.86
94	341_D_D	-53.21	-71.55	-39.29	66.41	-8.77
95	58_D_D	-53.1	-71.26	-48.18	74.95	-8.62
96	166_D_D	-53.09	-74.99	-32.68	63.48	-8.9
97	160_D_D	-52.92	-72.5	-30.53	58.94	-8.83
98	204_D_D	-52.84	-69.63	-49.08	74.26	-8.39
99	151_D_D	-52.66	-74.63	-23.3	53.67	-8.4
10	338_D_D	-52.58	-74.65	-22.84	53.35	-8.45
101	16_D_D	-52.55	-74.89	-24.76	55.94	-8.83
102	198_D_D	-52.5	-68.25	-30.86	54.53	-7.92
103	33_D_D	-52.13	-73.16	-29.25	58.67	-8.39
104	35_D_D	-51.83	-71.13	-22.09	49.68	-8.29
105	293_D_D	-51.8	-73.75	-33.5	64.17	-8.72
106	246_D_D	-51.4	-72.49	-29.99	59.53	-8.44
107	15_D_D	-51.26	-71.62	-28.7	57.38	-8.32
108	39_D_D	-50.37	-75.14	-38.06	71.85	-9.01
109	10_D_D	-49.63	-69.8	-24.64	52.73	-7.91
110	146_D_D	-49.33	-62.66	-49.8	71.67	-8.55
111	114_D_D	-49.22	-72.21	-34.28	65.68	-8.41
112	161_D_D	-49.13	-69	-41.61	70.16	-8.68
113	167_D_D	-48.9	-75.35	-16.22	50.94	-8.27
114	42_D_D	-48.68	-71.68	-34.2	65.5	-8.3
115	164_D_D	-48.4	-70.39	-26.87	57.25	-8.4
116	294_D_D	-47.96	-65.67	-46.7	72.68	-8.27
117	6_D_D	-47.91	-74.78	-27.55	63.05	-8.64

118	242_D_D	-46.7	-71.54	-29.44	62.85	-8.57
119	157_D_D	-46.27	-66.26	-34.37	62.61	-8.25
120	31_D_D	-45.87	-69.48	-34.79	66.63	-8.23
121	145_D_D	-45.54	-65.43	-45.61	73.95	-8.44
122	158_D_D	-45.48	-71.22	-9.45	43.26	-8.07
123	218_D_D	-45.07	-70.48	-7.89	41.76	-8.46
124	148_D_D	-45.06	-67.68	-33.58	64.69	-8.49
125	116_D_D	-44.96	-69.69	-20.6	53.95	-8.62
126	245_D_D	-44.46	-69.39	-22.45	55.68	-8.3
127	132_D_D	-43.68	-67.18	-24.35	56.09	-8.24
128	149_D_D	-43.36	-63.94	-29.42	58.58	-8.59
129	40_D_D	-41.54	-72.18	-20.84	60.06	-8.59
130	221_D_D	-40.83	-68.27	-23.46	59.45	-8.55
131	150_D_D	-35.87	-67.97	-31.17	71.85	-8.58

Table 6: Detailed Output of Best Compounds

SI NO.	COMPOU NDS	LFdG DOCKING SCORE (kcal/mol)	MMGBSA ΔG (kcal/mol)	RMSD (Å)	INTEREACTION
1	BLU9931	-13.019	-12.18	1.405	A553, D630, SH(C552), C552, L473, L619, R483, V481, V550, K503
2	111	-13.913	-70.79	1.355	A553, D630, SH(C552), C552, L473, L619, T499V481, V550, K503
3	57	-13.387	-67.49	1.422	A553, D630, SH(C552), L473, L619, V481, V550, A501,K503
4	47	-12.233	-66.97	1.672	A553, D630, SH(C552), L473, L619, R483, V550, K471, A501, T499
5	219	-13.639	-66.91	1.349	A553, D630, SH(C552), C552, L473, L619, V481, V550, T499,

					A501, K503, K471
	112	12.607	66.64	1 442	A553, D630, SH(C552), L473,
6	113	-12.607	-66.64	1.443	L619, V550, T499, K503
7	195	-13.591	-66.62	1458	A553, D630, SH(C552), C552,
,	173	-13.371	-00.02	1436	L619, V481, V550, A501, K471
					A553, D630, SH(C552), C552,
8	189	-13.282	-65.98	1.592	L473, L619, V481, V550,
					K503, K471
9	183	-14.046	-65.97	1.398	A553, D630, SH(C552), C552,
	103	1 1.0 10	05.57	1.370	L473, L619, V550
					A553, D630, SH(C552), C552,
10	109	-14.230	-65.91	2.019	L473, L619, V481, V550,
					A501, K503,T499
					A553, D630, SH(C552), C552,
11	217	-13.908	-65.61	1.981	L473, L619V481, V550, T499,
					K503, K471
12	267	-13.460	-65.08	1.486	A553, D630, SH(C552), C552,
12	207	13.100	02.00	11100	L473, L619, V550
13	51	-13.562	-64.89	1.707	D630, V550, L473, N557
14	112	-13.996	-64.18	2.050	D630, V550, V481
15	147	-13.819	-64.08	1.989	D630, SH(C552), L473, L619,
					V550, A501
16	121	-13.853	-63.99	1.380	A553, D630, SH(C552), C552,
					L619, R483, V481, V550, A554
17	220	-13.786	-63.53	2.010	D630, SH(C552), L473, L619,
					V550
18	127	-14.037	-63.25	1.361	A553, D630, SH(C552), C552,
					L619, R483, V481, V550, A554
19	115	-13.283	-63.23	2.005	D630, SH(C552), L473, V481,
					V550, A501
20	118	-14.056	-62.71	2.002	A553, D630, SH(C552), L619,
					V481, V550, A554
21	75	-13.835	-62.37	2.088	D630, SH(C552), L473, V481,
					V550, A501
22	123	-13.343	-62.07	1.530	A553, D630, SH(C552), C552,

					L619, R483, V481, V550, A554
					A553, D630, SH(C552), C552,
23	128	-14.328	-61.20	1.340	L619, R483, V481, V550,
					K503, A554
24	17	-14.330	-61.04	1.342	A553, D630, SH(C552), C552,
24	1 /	-14.330	-01.04	1.342	L619, V481, V550, A554
25	243	-13.914	-60.82	1.341	A553, D630, SH(C552), C552,
23	243	-13.714	-00.82	1.341	L619, V481, V550, K503, A554
26	119	-13.408	-60.81	1.354	A553, D630, SH(C552), C552,
20	119	-13.400	-00.81	1.334	L619, V481, V550
					A553, D630, SH(C552), C552,
27	11	-13.145	-60.77	1.367	L619, R483, V481, V550,
					T499, N557
28	163	-12.922	-60.77	1.421	A553, D630, SH(C552), C552,
20	103	-12.722	-00.77	1.721	L473, L619, V481, V550, A554
					A553, D630, SH(C552), C552,
29	43	-14.308	-60.70	1.406	L619, R483, V481, V550,
					K503, A554
30	159	-13.226	-60.64	2.007	D630, SH(C552), C552, L473,
30	137	13.220	00.01	2.007	V481, V550
31	122	-13.218	-60.44	1.352	A553, D630, SH(C552), C552,
31	122	13.210	00.11	1.332	L473, L619, R483, V481, V550
32	41	-13.723	-60.34	1.398	A553, D630, SH(C552), C552,
32	11	13.723	00.51	1.370	L619, R483, V481, V550
33	188	-13.436	-60.34	1.586	D630, SH(C552), L619, V550,
33	100	13.130	00.51	1.500	N557
34	222	-14.372	-60.09	1.477	D630, SH(C552), C552, L473,
31	222	11.372	00.09	1.177	L619, R483, V481, V550,
					A553, D630, SH(C552), C552,
35	193	-12.874	-59.79	1.454	L619, R483, V481, V550,
					A554, N557
36	59	-13.535	-59.55	1.647	D630, SH(C552), L619, V550,
			22.00	1.017	N557
37	130	-14.021	-59.52	1.355	A553, D630, SH(C552), C552,
	100		0,.02		L619, V481, V550

38 9 -13.708 -59.37 1.384 L473, L619, R483, V481, V550, A554 39 1 -14.534 -59.28 2.675 A553, SH(C552), C552, L619 V550, A501, T499 40 55 -14.275 -59.18 1.701 D630, SH(C552), C552, L473 V550, N557 41 270 -13.515 -59.07 1.111 SH(C552), C552, L619, V550, A554, K555, G556, M524 42 162 -14.254 -59.05 1.452 D630, SH(C552), C552, L473 L619, V550, N557 43 50 -13.991 -59.05 1.706 D630, SH(C552), L619, V550, N557 44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473 V550, N550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552, L652, C552, L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483, A501, N557,	, L619, 9 , L473, , V550, M524 , L473, //550 , V550,	V550, A554 A553, SH(C552), C552, L6 V550, A501, T499 D630, SH(C552), C552, L4 V550, N557 SH(C552), C552, L619, V5 A554, K555, G556, M52 D630, SH(C552), C552, L4	2.675 1.701 1.111	-59.28 -59.18	-14.534	1	
39 1 -14.534 -59.28 2.675 A553, SH(C552), C552, L619 V550, A501, T499 40 55 -14.275 -59.18 1.701 D630, SH(C552), C552, L473 V550, N557 41 270 -13.515 -59.07 1.111 SH(C552), C552, L619, V550 A554, K555, G556, M524 42 162 -14.254 -59.05 1.452 D630, SH(C552), C552, L473 L619, V550 N557 43 50 -13.991 -59.05 1.706 D630, SH(C552), L619, V550 N557 44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473 V550 N550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552, L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483, A501, N557,	9 , L473, , V550, M524 , L473, //550 , V550,	A553, SH(C552), C552, L6 V550, A501, T499 D630, SH(C552), C552, L4 V550, N557 SH(C552), C552, L619, V5 A554, K555, G556, M52 D630, SH(C552), C552, L4	1.701	-59.18		_	39
39 1 -14.534 -59.28 2.675 V550, A501, T499 40 55 -14.275 -59.18 1.701 D630, SH(C552), C552, L473 V550, N557 41 270 -13.515 -59.07 1.111 SH(C552), C552, L619, V550 A554, K555, G556, M524 42 162 -14.254 -59.05 1.452 D630, SH(C552), C552, L473 L619, R483, V481, V550 D630, SH(C552), L619, V550 N557 43 50 -13.991 -59.05 1.706 D630, SH(C552), L619, V550 N557 44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473 V550 N550 N550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 N503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552, L619, R483, V550 N557, K483 A501, N557,	9 , L473, , V550, M524 , L473, //550 , V550,	V550, A501, T499 D630, SH(C552), C552, L4 V550, N557 SH(C552), C552, L619, V5 A554, K555, G556, M52 D630, SH(C552), C552, L4	1.701	-59.18		_	39
40 55 -14.275 -59.18 1.701 D630, SH(C552), C552, L473 V550, N557 41 270 -13.515 -59.07 1.111 SH(C552), C552, L619, V550 A554, K555, G556, M524 42 162 -14.254 -59.05 1.452 D630, SH(C552), C552, L473 L619, R483, V481, V550 D630, SH(C552), L619, V550 N557 43 50 -13.991 -59.05 1.706 D630, SH(C552), L619, V550 N557 N557 44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473 V550 N550 N557 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 N503, A554 N503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552, L619, R483, V550 N557, SH(C552), V550, R483, A501, N557, N557, N557, N557, N557, N557	, L473, , V550, M524 , L473, //550 , V550,	D630, SH(C552), C552, L4 V550, N557 SH(C552), C552, L619, V5 A554, K555, G556, M52 D630, SH(C552), C552, L4	1.701	-59.18		_	39
40 55 -14.275 -59.18 1.701 V550, N557 41 270 -13.515 -59.07 1.111 SH(C552), C552, L619, V550, A554, K555, G556, M524 42 162 -14.254 -59.05 1.452 D630, SH(C552), C552, L473, L619, V550, N557 43 50 -13.991 -59.05 1.706 D630, SH(C552), L619, V550, N557 44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473, V550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552, L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483, A501, N557,	, V550, M524 d, L473, V550 , V550,	V550, N557 SH(C552), C552, L619, V5 A554, K555, G556, M52 D630, SH(C552), C552, L4	1.111		-14.275	55	
V550, N557 V550, N557 SH(C552), C552, L619, V550 A554, K555, G556, M524 SF C59.05 SF C552, L619, V550 A554, K555, G556, M524 SF C619, R483, V481, V550 SF C619, R483, V550	M524 , L473, /550 , V550,	SH(C552), C552, L619, V5 A554, K555, G556, M52 D630, SH(C552), C552, L4	1.111		-14.273	33	40
41 270 -13.515 -59.07 1.111 A554, K555, G556, M524 42 162 -14.254 -59.05 1.452 D630, SH(C552), C552, L473 L619, R483, V481, V550 43 50 -13.991 -59.05 1.706 D630, SH(C552), L619, V550 N557 44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473 V550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552 L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483 A501, N557,	M524 , L473, /550 , V550,	A554, K555, G556, M52 D630, SH(C552), C552, L4		-59.07			40
42 162 -14.254 -59.05 1.452 D630, SH(C552), C552, L473 L619, R483, V481, V550 43 50 -13.991 -59.05 1.706 D630, SH(C552), L619, V550 N557 44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473 V550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C553 L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483 A501, N557,	, L473, /550 , V550,	D630, SH(C552), C552, L4		-37.07	-13 515	270	Δ1
42 162 -14.254 -59.05 1.452 L619, R483, V481, V550 43 50 -13.991 -59.05 1.706 D630, SH(C552), L619, V550 44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473 V550 V550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552, C552, L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483, A501, N557,	/550 , V550,		1.452		-13.313	270	71
L619, R483, V481, V550 D630, SH(C552), L619, V550 N557 A553, D630, SH(C552), L473 V550 A553, D630, SH(C552), C552 L619, R483, V481, V550, K503, A554 A553, D630, SH(C552), C552 L619, R483, V550 A553, D630, SH(C552), C552 L619, R483, V550 A553, SH(C552), V550, R483 A501, N557,	, V550,	L619, R483, V481, V550	1.132	-59.05	-14 254	162	42
43 50 -13.991 -59.05 1.706 N557 44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473 V550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552 L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483 A501, N557,			1	37.03	11.231	102	12
44 181 -13.208 -59.01 1.577 A553, D630, SH(C552), L473 V550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552 L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483 A501, N557,	. L473.	D630, SH(C552), L619, V5	1 706	-59.05	-13 991	50	43
44 181 -13.208 -59.01 1.577 V550 45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552 L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483 A501, N557,	. L473.	N557	1.700	37.03	13.771	30	15
V550 A553, D630, SH(C552), C552 A553, D630, SH(C552), C552 A553, D630, SH(C552), C552 K503, A554 A553, D630, SH(C552), C552 A553, D630, SH(C552), C552 L619, R483, V550 A553, SH(C552), V550, R483 A501, N557,	, ,	A553, D630, SH(C552), L4	1 577	-59.01	-13 208	181	44
45 46 -13.457 -58.54 1.390 L619, R483, V481, V550, K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552 L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483 A501, N557,		V550	1.577	37.01	13.200	101	''
K503, A554 46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552 L619, R483, V550 A553, SH(C552), V550, R483 A501, N557,	, C552,	A553, D630, SH(C552), C5					
46 49 -13.574 -58.25 1.504 A553, D630, SH(C552), C552 L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483 A501, N557,	7550,	L619, R483, V481, V550	1.390	-58.54	-13.457	46	45
46 49 -13.574 -58.25 1.504 L619, R483, V550 47 2 -14.721 -58.06 2.610 A553, SH(C552), V550, R483 A501, N557,		K503, A554					
47 2 -14.721 -58.06 2.610 L619, R483, V550 A553, SH(C552), V550, R483 A501, N557,	, C552,	A553, D630, SH(C552), C5	1.504	-58.25	-13 574	49	46
47 2 -14.721 -58.06 2.610 A501, N557,	0	L619, R483, V550	1.00.	00.20	10.07	.,	
A501, N557,	, R483,	A553, SH(C552), V550, R4	2 610	-58.06	-14 721	2	47
D620 CU(C552) 1 472 1 610		A501, N557,	2.010	20.00	11.721		.,
48 291 -13.734 -57.95 2.041 D630, SH(C332), L473, L619	, L619,	D630, SH(C552), L473, L6	2 041	-57 95	-13 734	291	48
V550, A501		V550, A501	2.0.11	27.50	13.73	271	
49 110 -12.473 -57.93 1.790 A553, SH(C552), C552, V483	, V481,	A553, SH(C552), C552, V ²	1 790	-57 93	-12 473	110	49
V550, V620, N557	7	V550, V620, N557	1.750	37.93	12.173	110	
50 7 -13.464 -57.75 1.363 A553, D630, SH(C552), C552	, C552,	A553, D630, SH(C552), C5	1.363	-57.75	-13 464	7	50
L473, L619, R483, V481, V55	1, V550	L473, L619, R483, V481, V	1.505	37.73	13.101	,	30
51 153 -13.539 -57.65 2.020 D630, SH(C552), C552, L473	, L473,	D630, SH(C552), C552, L4	2 020	-57.65	-13 539	153	51
V481, V550, A554	4	V481, V550, A554	2.020	-57.05	-13.337	133	
52 37 -14.722 -57.41 1.701 A553, D630, SH(C552), C552		A553, D630, SH(C552), C5	1 701	-57 41	-14 722	37	52
L473, V550, G556, N557	, C552,	L473, V550, G556, N55	1.701	-57.41	-14./22	37	32
53 117 -13.989 -57.36 1.815 SH(C552), L473, L619, V481		SH(C552), L473, L619, V4	1 815	-57 36	-13 989	117	53
V550, A554, T499	N557		1.013	37.30	13.707	11/	
54 131 -13.244 -57.27 1.341 A553, D630, SH(C552), C552	N557 , V481,	V550, A554, T499		_		121	54
131	N557 , V481,	r r	1 341	-57 27	_13 244	131	

					A554, K503
55	185	-13.822	-57.23	1.449	A553, D630, SH(C552), C552,
33	103	-13.622	-37.23	1.449	L619, R483, V481, V550,
56	56	-13.674	-57.20	1.688	D630, SH(C552), C552, L619,
30	30	-13.074	-37.20	1.000	L473, V550, N557
57	200	-14.51	-57.10	1.422	A553, D630, SH(C552), C552,
37	200	-14.51	-57.10	1.422	L619, R483, V481, V550
58	187	-13.332	-57.09	1.483	A553, D630, SH(C552), L619,
20	107	15.552	57.05	1.103	V481, V550, A554, N557
59	340	-13.824	-57.05	1.391	A553, D630, SH(C552), C552,
	310	13.021	37.03	1.371	L619, R483, V481, V550, K503
60	339	-12.851	-57.04	1.393	A553, D630, SH(C552), C552,
	337	-12.031	-57.04	1.575	L619, V481, V550, K503
61	38	-14.847	-56.95	1.421	A553, D630, SH(C552), C552,
01	36	-14.047	-30.93	1.721	L473, L619, V481, V550
62	265	-13.64	-56.95	1.568	D630, SH(C552), C552, L473,
02	203	-13.04	-30.73	1.508	V550, G556
63	8	-13.639	-56.78	2.759	A553, SH(C552), C552, L473,
0.5	O	-13.039	-30.76	2.139	L619, R483, V550, T499
64	202	-13.627	-56.75	1.464	A553, SH(C552), C552, L619,
04	202	-13.027	-30.73	1.404	V481, V550, A554,
					A553, D630, SH(C552), C552,
65	154	-13.833	-56.66	1.336	L619, R483, V481, V550,
					A554, K503
66	156	-13.778	-56.64	1.495	D630, SH(C552), C552, L619,
	130	-13.770	-30.04	1.473	L473, R483, V481, V550,
67	120	-12.515	-56.62	1.282	A553, SH(C552), C552, L619,
07	120	-12.313	-30.02	1.202	V481, V550, N557, K555
68	182	-14.232	-56.53	1.505	A553, D630, SH(C552), L473,
00	102	-14.232	-30.33	1.303	L619, R483, V550
69	44	-13.547	-56.48	1.707	A553, D630, SH(C552), C552,
	⊤⊤	-1 <i>3.3</i> 7/	-50.70	1./0/	V550, N557,
70	292	-13.71	-56.43	1.889	D630, SH(C552), L619, V550
71	14	-14.059	-56.12	2.745	A553, D630, SH(C552), C552,
/ 1	17	-1 7. UJ7	-30.12	2.743	L619, R483, V550, A554,

72	269	-13.132	-56.05	1.422	A553, D630, SH(C552), C552,
					L619, R483, V481, V550, A554
73	165	-14.26	-55.95	1.353	A553, D630, SH(C552), C552,
					L619, R483, V481, V550, A554
74	60	-12.721	-55.88	1.045	D630, SH(C552), C552, L473,
					L619, V550, G556
75	241	-13.978	-55.76	2.609	A553, SH(C552), L619, R483,
					V550, A501
					A553, D630, SH(C552), C552,
76	32	-13.744	-55.67	2.677	L473, L619, R483, V481,
					V550, K503
77	3	-13.922	-55.63	2.728	A553, D630, SH(C552), C552,
	3	-13.922	-55.05	2.728	L619, R483, V550, T499
78	266	-13.894	-55.50	1.623	L619, V481, V550,
79	290	-14.092	-55.45	1.971	L473, L619, V550
80	4	12 501	-55.44	2.567	A553, SH(C552), L473, L619,
80	4	-13.581	-33.44	2.307	R483, V550, A501, N557
81	12	-13.416	-55.26	1.384	A553, D630, SH(C552), L619,
01	12	-13.410	-55.20	1.304	R483, V481, V550, K503
82	18	-14.04	-55.24	2.600	SH(C552), L473, R483, V550,
02	16	-14.04	-33.24	2.000	A554, K503, E551
83	268	-13.825	-55.10	1.496	A553, D630, SH(C552), L619,
0.5	200	-13.023	-55.10	1.490	R483, V481, V550, A554
84	5	-13.079	-54.94	3.005	SH(C552), L473, R483, V481,
04	3	-13.079	-34.94	3.003	V550, A501
85	52	-14.099	-54.93	1.421	A553, D630, SH(C552), L619,
83	32	-14.099	-34.93	1.421	R483, V481, V550
96	126	14 102	54.50	1 444	D630, SH(C552), C552, L473,
86	126	-14.183	-54.52	1.444	L619, V550
97	202	12 152	51.15	0.566	A553, D630, SH(C552), L619,
87	203	-13.153	-54.45	0.300	R483, V550, A554, I534
00	12	14.016	54.04	1 271	A553, D630, SH(C552), C552,
88	13	-14.016	-54.24	1.271	L473, L619, V481, V550
90	2.4	12.504	54.10	2.752	A553, SH(C552), C552, L473,
89	34	-12.504	-54.19	2.753	L619, V550, A501
	1	<u>I</u>	<u>I</u>	Í.	ı

90	199	-14.069	-54.02	1.634	D630, SH(C552), C552, L473,
	177	11.009	31.02	1.031	V550, G556

Table 7: Contact Trajectory

SNO.	Bond Type	Ligand Atom	Protein Atom	% Frames Present
1	Hydrophobic	C LIG 293 C	C PRO 126 CG	1.10%
2	Hydrophobic	C LIG 293 C	C LEU 287 CB	1.60%
3	Aromatic-Aromatic	C LIG 293 C	C HIS 291 CG	5.10%
4	Aromatic-Aromatic	C LIG 293 C	C HIS 291 CE1	8.20%
5	Hydrophobic	C LIG 293 C12	C HIS 291 CB	2.70%
6	Aromatic-Aromatic	C LIG 293 C3	C HIS 291 CE1	1.50%
7	Hydrophobic	C LIG 293 C4	C VAL 289 CG2	14.00%
8	Hydrophobic	C LIG 293 C5	C ALA 288 CB	4.90%
9	Hydrophobic	C LIG 293 C5	C VAL 289 CG1	4.20%
10	Hydrophobic	C LIG 293 C5	C VAL 289 CG2	25.80%
11	Hydrophobic	C LIG 293 C7	C VAL 127 CG2	21.80%
12	Hydrophobic	C LIG 293 C7	C ALA 288 CB	17.10%
13	Hydrophobic	C LIG 293 C7	C VAL 289 CG2	18.40%
14	Halogen bond	C LIG 293 CL	C SER 290 O	1.10%
15	Hydrogen bond	C LIG 293 H1	Water	3.50%
16	Hydrogen bond	C LIG 293 H18	Water	31.50%
17	Hydrogen bond	C LIG 293 H19	Water	10.50%
18	Hydrogen bond	C LIG 293 H2	Water	1.50%
19	Hydrogen bond	C LIG 293 N	C NME 292 H	2.20%
20	Hydrogen bond	C LIG 293 N	Water	2.20%
21	Hydrogen bond	C LIG 293 N4	Water	16.40%
22	Hydrogen bond	C LIG 293 O	C VAL 289 H	1.10%
23	Hydrogen bond	C LIG 293 O	C SER 290 HG	1.80%
24	Hydrogen bond	C LIG 293 O	C SER 290 H	4.90%
25	Hydrogen bond	C LIG 293 O	Water	1.30%
26	Hydrogen bond	C LIG 293 O1	C VAL 289 H	1.80%
27	Hydrogen bond	C LIG 293 O1	C SER 290 H	4.40%
28	Hydrogen bond	C LIG 293 O1	Water	26.50%
29	Hydrogen bond	C LIG 293 O2	Water	39.30%
30	Hydrogen bond	C LIG 293 O3	Water	23.30%

31	Hydrophobic	C LIG 293 S1	C ALA 102 CB	87.30%
32	Hydrogen bond	C LIG 293 S1	Water	6.00%
33	Hydrophobic	C LIG 293 S2	C LEU 22 CD1	1.30%
34	Hydrophobic	C LIG 293 S2	C ALA 102 CB	1.80%
			C ASN 105	
35	Sulfur-lone Pair	C LIG 293 S2	OD1	12.50%
36	Hydrogen bond	C LIG 293 S2	Water	1.80%

Table 8: ADME Prediction

• Physicochemical Properties

S NO.	COMPOUNDS	MW	LogP	TPSA	nHA	nHD	nRot
1	1	606.02	4.215	139.81	10	2	9
2	2	606.02	4.215	139.81	10	2	9
3	3	605.05	4.104	135.27	10	2	9
4	4	586.05	4.166	135.27	10	2	9
5	5	621.02	4.531	135.27	10	2	9
6	7	530.06	4.371	105.67	8	2	8
7	8	529.05	4.528	105.67	8	2	8
8	9	548.05	4.473	105.67	8	2	8
9	11	529.05	4.528	105.67	8	2	8
10	12	564.02	4.884	105.67	8	2	8
11	13	529.05	4.528	105.67	8	2	8
12	14	570.05	4.46	122.74	9	2	9
13	17	570.05	4.46	122.74	9	2	9
14	18	589.05	4.253	122.74	9	2	9
15	32	588.04	4.394	122.74	9	2	9
16	34	588.04	4.394	122.74	9	2	9
17	37	575.08	5.044	118.14	10	2	9
18	38	578.08	5.024	108.91	9	2	8
19	41	594.05	5.404	108.91	9	2	8
20	43	559.08	5.051	108.91	9	2	8
21	44	530.06	4.824	105.67	8	2	7
22	46	530.06	4.824	105.67	8	2	7

23	47	498.07	6.196	71.53	6	2	7
24	49	533.04	6.443	71.53	6	2	7
25	50	498.07	6.196	71.53	6	2	7
26	51	547.05	4.491	140.92	10	4	8
27	52	531.05	4.461	131.69	9	4	7
28	55	566.02	4.842	131.69	9	4	7
29	56	531.05	4.461	131.69	9	4	7
30	57	616.08	4.648	138.51	11	2	9
31	59	616.08	4.648	138.51	11	2	9
32	60	588.06	4.272	135.27	10	2	8
33	75	587.06	4.449	135.27	10	2	8
34	109	556.07	5.787	101.13	8	2	8
35	110	574.06	5.832	101.13	8	2	8
36	111	555.07	5.914	101.13	8	2	8
37	112	588.05	4.096	161.29	11	4	8
38	113	634.07	4.861	135.21	11	2	10
39	115	637.08	4.829	125.98	10	2	9
40	117	653.05	5.233	125.98	10	2	9
41	118	618.08	4.871	125.98	10	2	9
42	119	590.06	4.566	122.74	9	2	8
43	120	589.05	4.692	122.74	9	2	8
44	121	624.02	5.075	122.74	9	2	8
45	122	589.05	4.692	122.74	9	2	8
46	123	558.07	5.969	88.6	7	2	8
47	126	573.06	6.016	97.83	8	2	9
48	127	576.06	6.019	88.6	7	2	8
49	128	557.06	6.065	88.6	7	2	8
50	130	557.06	6.065	88.6	7	2	8
51	131	606.04	4.35	157.99	11	4	9
52	147	609.05	4.261	148.76	10	4	8
53	153	590.05	4.321	148.76	10	4	8
54	154	625.02	4.717	148.76	10	4	8
55	156	590.05	4.321	148.76	10	4	8
56	159	594.02	4.287	148.76	10	4	8
57	162	637.06	4.507	143.05	11	2	9
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58	163	652.05	4.595	152.28	12	2	10
59	165	636.05	4.604	143.05	11	2	9
60	181	671.02	4.948	143.05	11	2	9
61	182	636.05	4.604	143.05	11	2	9
62	183	626.03	4.405	139.81	10	2	8
63	185	607.03	4.469	139.81	10	2	8
64	187	642	4.824	139.81	10	2	8
65	188	607.03	4.469	139.81	10	2	8
66	189	575.04	5.762	105.67	8	2	8
67	193	591.03	5.729	114.9	9	2	9
68	195	610.01	6.034	105.67	8	2	8
69	199	575.04	5.762	105.67	8	2	8
70	200	608.02	4.15	165.83	11	4	8
71	202	642.99	4.499	165.83	11	4	8
72	203	637.06	4.619	165.83	11	4	9
73	217	587.06	4.747	131.97	10	2	9
74	219	606.03	5.105	122.74	9	2	8
75	220	601.1	4.772	125.98	10	2	9
76	222	600.09	4.885	125.98	10	2	9
77	241	635.06	5.228	125.98	10	2	9
78	243	600.09	4.885	125.98	10	2	9
79	265	540.08	5.991	88.6	7	2	8
80	266	539.07	6.069	88.6	7	2	8
81	267	558.07	6.024	88.6	7	2	8
82	268	574.04	6.321	88.6	7	2	8
83	269	539.07	6.069	88.6	7	2	8
84	270	573.06	4.23	148.76	10	4	8
85	290	572.06	4.388	148.76	10	4	8
86	291	588.05	4.408	157.99	11	4	9
87	292	591.05	4.319	148.76	10	4	8
88	339	607.03	4.777	148.76	10	4	8
89	340	572.06	4.388	148.76	10	4	8

• ADMET

S NO.	COMPOUNDS	НІА	CYP3A4-inh	hERG	Ames	DILI
1	1	0.037	0.865	0.034	0.007	0.988
2	2	0.037	0.865	0.034	0.007	0.988
3	3	0.02	0.581	0.107	0.169	0.985
4	4	0.052	0.64	0.113	0.14	0.984
5	5	0.022	0.533	0.11	0.112	0.986
6	7	0.029	0.752	0.186	0.246	0.986
7	8	0.059	0.738	0.134	0.113	0.98
8	9	0.047	0.699	0.126	0.121	0.982
9	11	0.059	0.738	0.134	0.113	0.98
10	12	0.041	0.623	0.133	0.092	0.984
11	13	0.059	0.738	0.134	0.113	0.98
12	14	0.02	0.779	0.127	0.037	0.986
13	17	0.02	0.779	0.127	0.037	0.986
14	18	0.013	0.753	0.236	0.187	0.99
15	32	0.021	0.747	0.149	0.096	0.985
16	34	0.021	0.747	0.149	0.096	0.985
17	37	0.367	0.824	0.574	0.065	0.983
18	38	0.346	0.703	0.711	0.189	0.982
19	41	0.218	0.641	0.674	0.055	0.983
20	43	0.382	0.768	0.712	0.068	0.981
21	44	0.053	0.554	0.898	0.11	0.982
22	46	0.053	0.554	0.898	0.11	0.982
23	47	0.305	0.394	0.591	0.702	0.966
24	49	0.147	0.3	0.564	0.674	0.973
25	50	0.305	0.394	0.591	0.702	0.966
26	51	0.066	0.756	0.347	0.192	0.986
27	52	0.077	0.703	0.528	0.195	0.984
28	55	0.045	0.658	0.506	0.176	0.986
29	56	0.077	0.703	0.528	0.195	0.984
30	57	0.112	0.647	0.548	0.061	0.983
31	59	0.112	0.647	0.548	0.061	0.983
32	60	0.008	0.347	0.865	0.119	0.99
33	75	0.024	0.459	0.841	0.058	0.984

34	109	0.028	0.262	0.501	0.726	0.982
35	110	0.049	0.257	0.319	0.626	0.976
36	111	0.074	0.371	0.402	0.472	0.976
37	112	0.034	0.546	0.359	0.107	0.988
38	113	0.112	0.812	0.746	0.104	0.987
39	115	0.102	0.699	0.834	0.235	0.986
40	117	0.057	0.655	0.814	0.082	0.987
41	118	0.105	0.761	0.832	0.099	0.986
42	119	0.012	0.616	0.961	0.321	0.989
43	120	0.019	0.576	0.947	0.144	0.986
44	121	0.013	0.457	0.939	0.122	0.988
45	122	0.019	0.576	0.947	0.144	0.986
46	123	0.028	0.452	0.813	0.788	0.983
47	126	0.059	0.557	0.538	0.648	0.982
48	127	0.041	0.395	0.724	0.691	0.978
49	128	0.048	0.462	0.726	0.651	0.978
50	130	0.048	0.462	0.726	0.651	0.978
51	131	0.027	0.738	0.464	0.255	0.991
52	147	0.028	0.662	0.658	0.374	0.99
53	153	0.03	0.685	0.658	0.225	0.99
54	154	0.02	0.626	0.654	0.207	0.991
55	156	0.03	0.685	0.658	0.225	0.99
56	159	0.069	0.734	0.227	0.253	0.991
57	162	0.084	0.92	0.26	0.004	0.992
58	163	0.227	0.908	0.159	0.004	0.988
59	165	0.18	0.905	0.2	0.004	0.988
60	181	0.131	0.897	0.193	0.004	0.989
61	182	0.18	0.905	0.2	0.004	0.988
62	183	0.03	0.825	0.39	0.004	0.99
63	185	0.03	0.834	0.406	0.004	0.989
64	187	0.025	0.808	0.399	0.004	0.99
65	188	0.03	0.834	0.406	0.004	0.989
66	189	0.117	0.784	0.126	0.006	0.981
67	193	0.144	0.814	0.09	0.006	0.983
68	195	0.066	0.757	0.13	0.005	0.983

69	199	0.117	0.784	0.126	0.006	0.981
70	200	0.04	0.82	0.106	0.004	0.993
71	202	0.032	0.828	0.109	0.003	0.994
72	203	0.037	0.837	0.148	0.004	0.993
73	217	0.015	0.742	0.897	0.023	0.987
74	219	0.014	0.548	0.932	0.019	0.987
75	220	0.045	0.798	0.837	0.038	0.99
76	222	0.098	0.816	0.801	0.025	0.985
77	241	0.066	0.728	0.771	0.017	0.987
78	243	0.098	0.816	0.801	0.025	0.985
79	265	0.032	0.53	0.769	0.564	0.981
80	266	0.064	0.533	0.643	0.271	0.975
81	267	0.054	0.454	0.655	0.401	0.975
82	268	0.036	0.397	0.625	0.246	0.98
83	269	0.064	0.533	0.643	0.271	0.975
84	270	0.012	0.779	0.743	0.091	0.994
85	290	0.024	0.722	0.563	0.033	0.99
86	291	0.02	0.766	0.349	0.034	0.991
87	292	0.02	0.713	0.575	0.077	0.991
88	339	0.02	0.707	0.544	0.032	0.991
89	340	0.024	0.722	0.563	0.033	0.99