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

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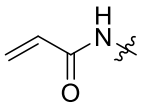
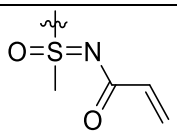
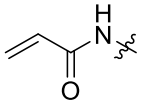
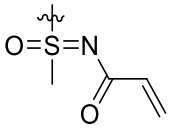
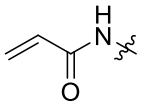
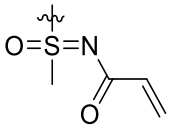
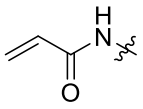
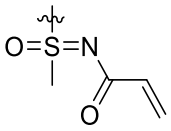
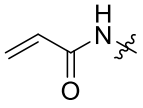
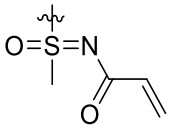
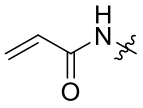
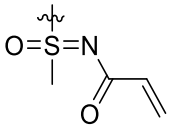
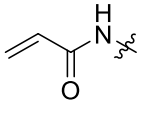
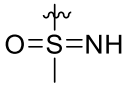
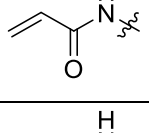
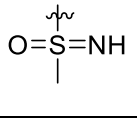
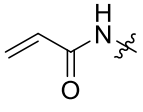
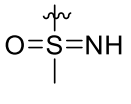
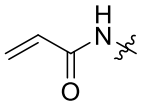
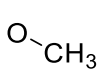
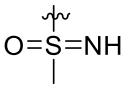
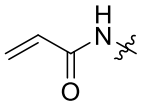
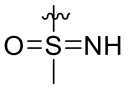
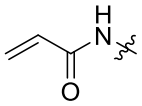
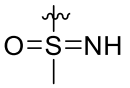
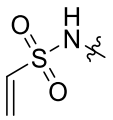
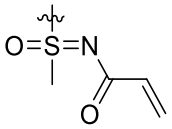
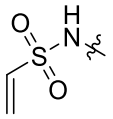
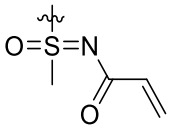
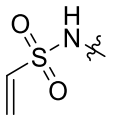
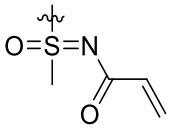
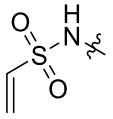
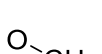
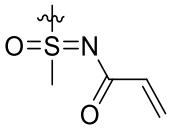
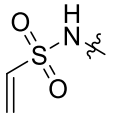
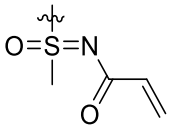
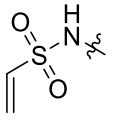
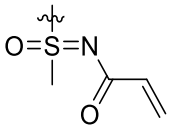
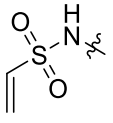
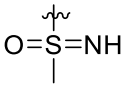
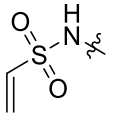
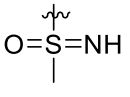
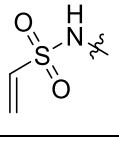
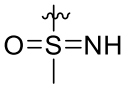
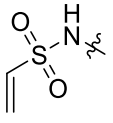
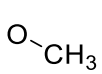
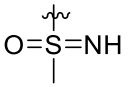
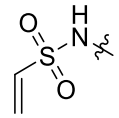
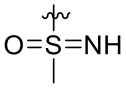
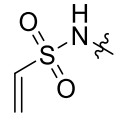
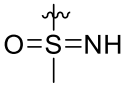
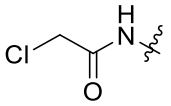
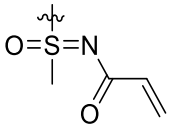
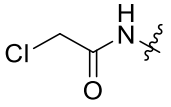
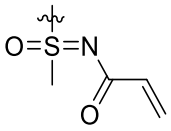
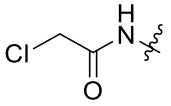
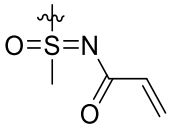
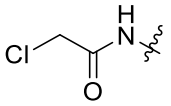
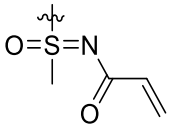
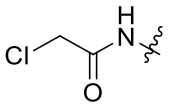
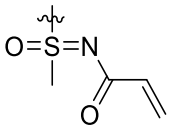
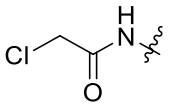
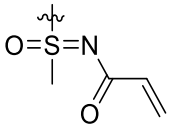
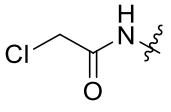
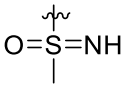
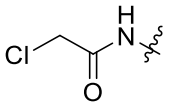
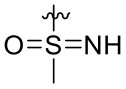
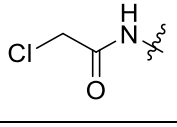
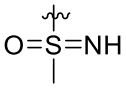
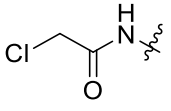
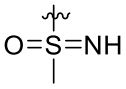
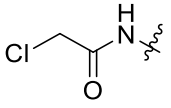
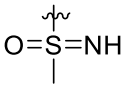
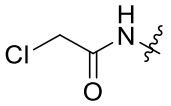
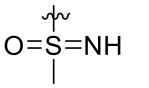
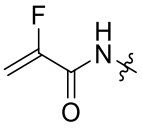
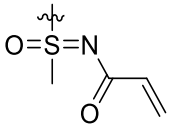
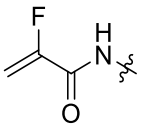
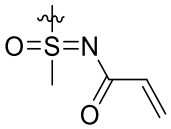
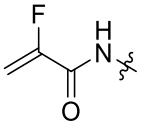
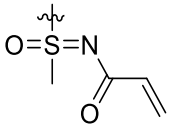
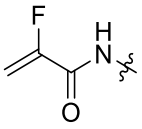
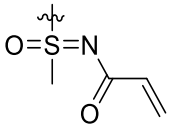
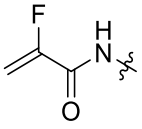
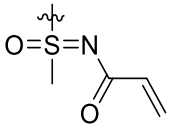
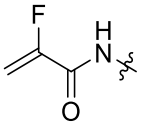
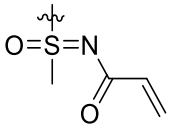
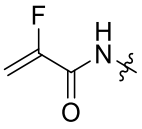
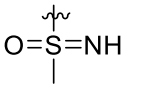
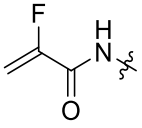
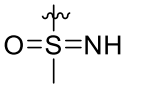
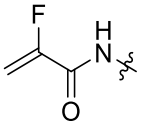
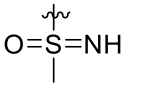
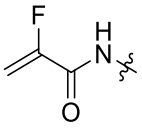
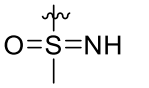
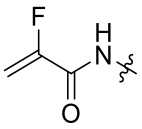
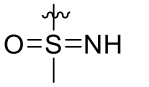
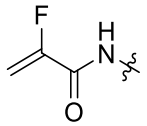
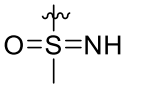
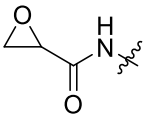
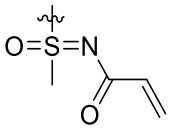
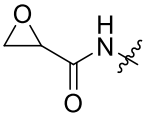
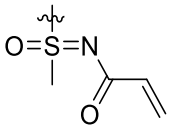
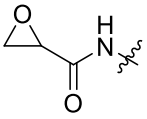
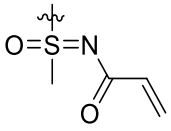
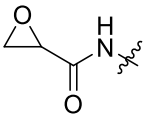
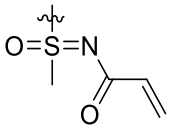
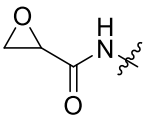
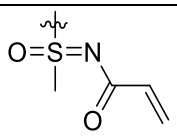
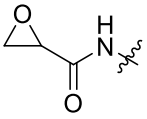
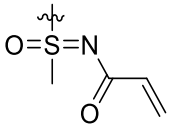
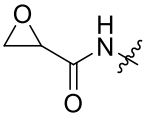
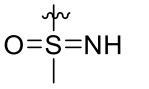
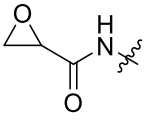
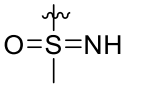
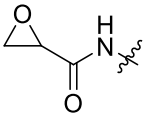
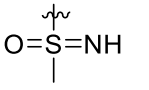
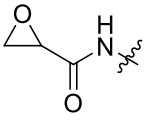
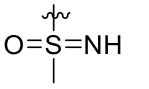
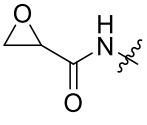
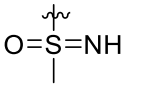
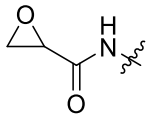
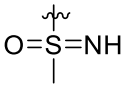
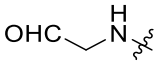
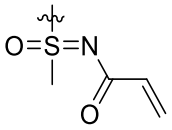
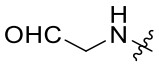
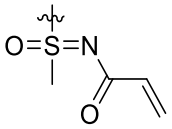
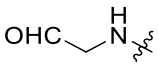
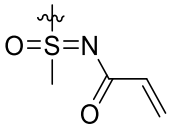
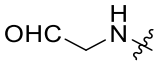
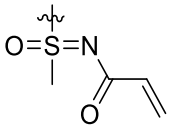
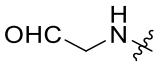
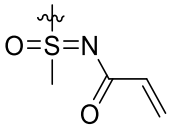
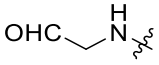
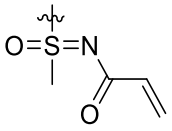
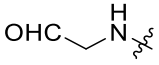
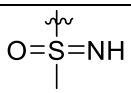
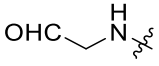
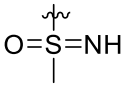
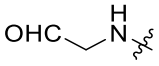
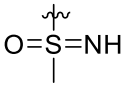
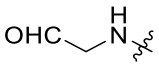
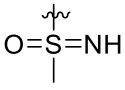
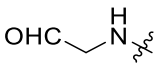
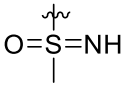
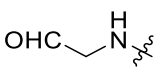
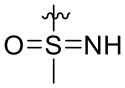
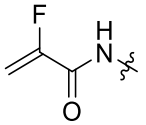
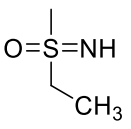
1	19		C_2H_5	
2	20		Cl	
3	21		F	
4	22		O_{CH_3}	
5	23		CF_3	
6	24		H	
7	25		C_2H_5	
8	26		Cl	
9	27		F	

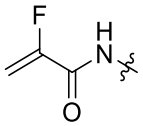
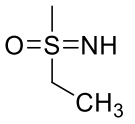
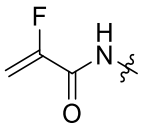
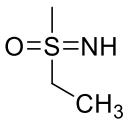
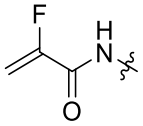
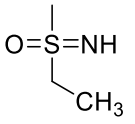
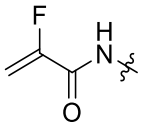
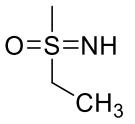
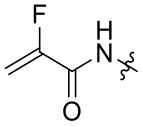
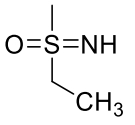
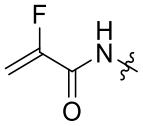
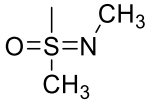
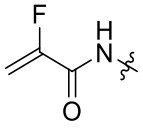
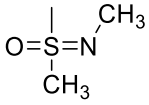
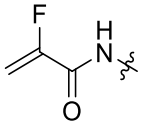
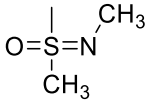
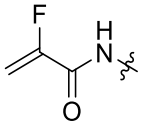
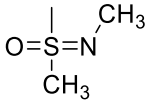
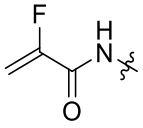
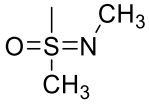
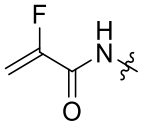
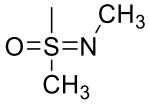
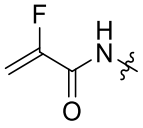
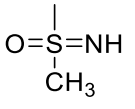
10	28			
11	29		CF_3	
12	30		H	
13	61		C_2H_5	
14	62		Cl	
15	63		F	
16	64			
17	65		CF_3	
18	66		H	
19	67		C_2H_5	
20	68		Cl	
21	69		F	
22	70			

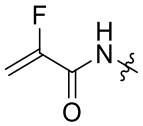
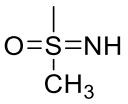
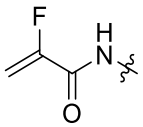
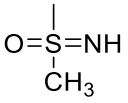
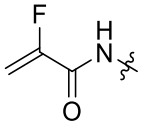
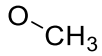
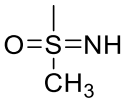
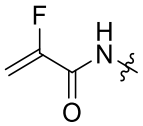
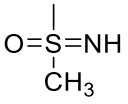
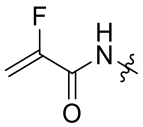
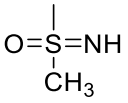
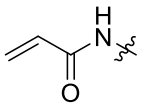
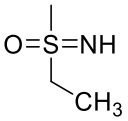
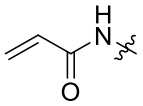
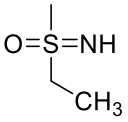
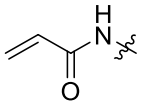
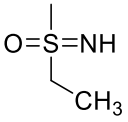
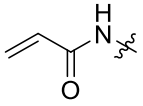
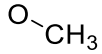
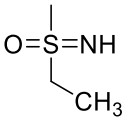
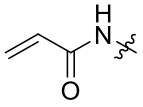
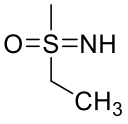
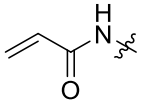
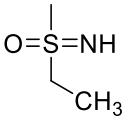
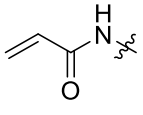
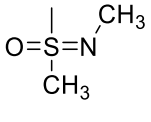
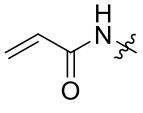
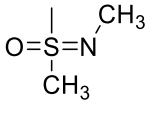
23	71		CF_3	
24	72		H	
25	97		C_2H_5	
26	98		Cl	
27	99		F	
28	100		O_{CH_3}	
29	101		CF_3	
30	102		H	
31	103		C_2H_5	
32	104		Cl	
33	105		F	
34	106		O_{CH_3}	
35	107		CF_3	

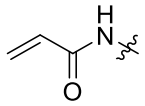
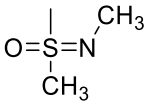
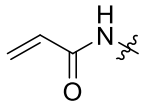
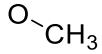
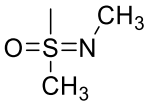
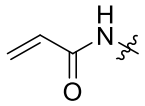
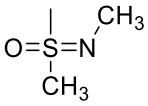
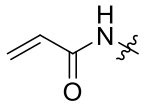
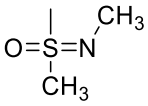
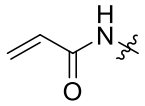
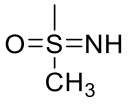
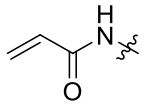
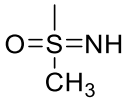
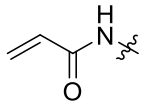
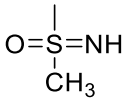
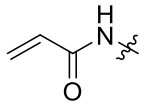
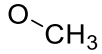
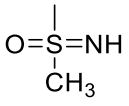
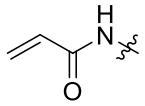
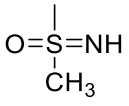
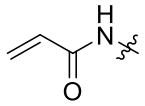
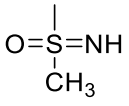
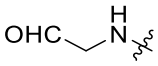
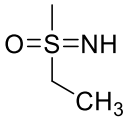
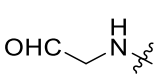
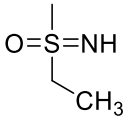
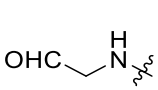
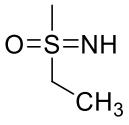
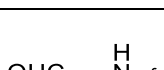
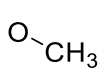
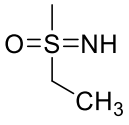
36	108		H	
37	133		C_2H_5	
38	134		Cl	
39	135		F	
40	136		O_{CH_3}	
41	137		CF_3	
42	138		H	
43	139		C_2H_5	
44	140		Cl	
45	141		F	
46	142		O_{CH_3}	
47	143		CF_3	

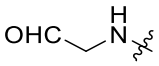
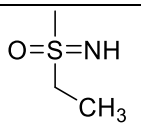
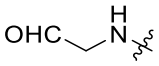
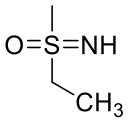
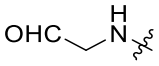
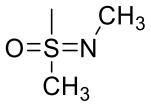
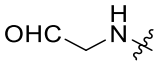
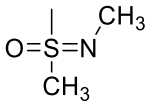
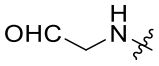
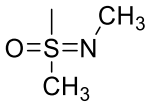
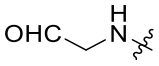
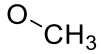
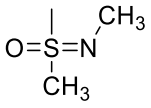
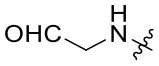
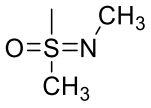
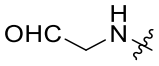
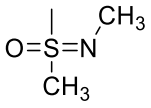
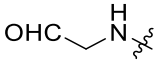
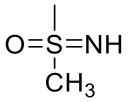
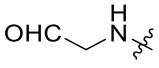
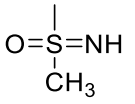
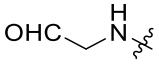
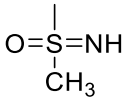
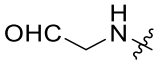
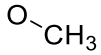
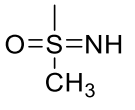
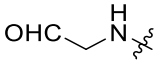
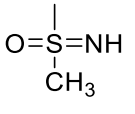
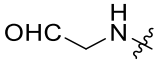
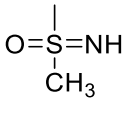
48	144		H	
49	169		C_2H_5	
50	170		Cl	
51	171		F	
52	172		O_{CH_3}	
53	173		O_{CH_3}	
54	174		H	
55	175		C_2H_5	
56	176		Cl	
57	177		F	
58	178		O_{CH_3}	
59	179		CF_3	

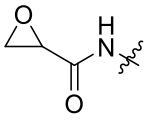
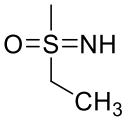
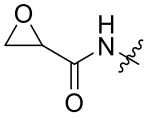
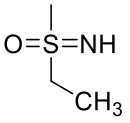
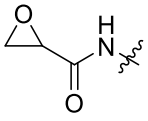
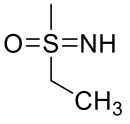
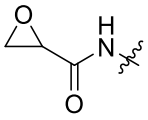
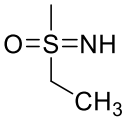
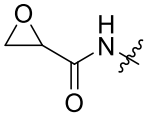
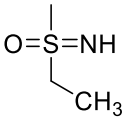
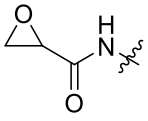
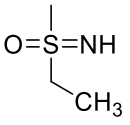
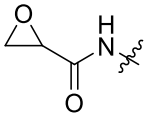
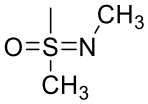
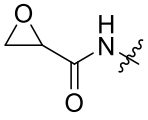
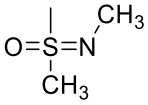
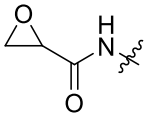
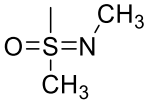
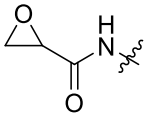
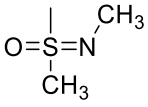
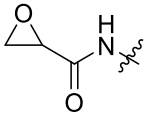
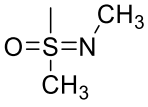
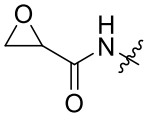
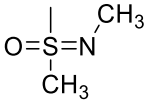
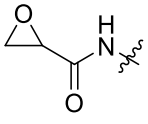
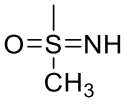
60	180		H	
61	205		C_2H_5	
62	206		Cl	
63	207		F	
64	208			
65	209		CF_3	
66	210		H	
67	211		C_2H_5	
68	212		Cl	
69	213		F	
70	214			
71	215		CF_3	
72	216		H	
73	223		C_2H_5	

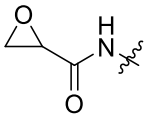
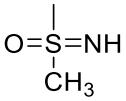
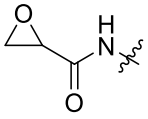
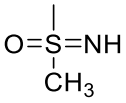
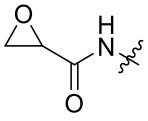
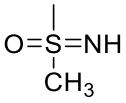
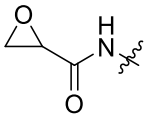
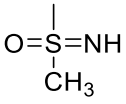
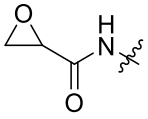
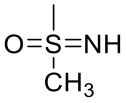
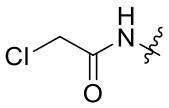
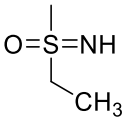
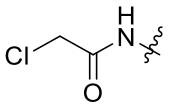
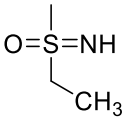
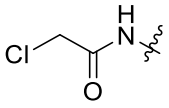
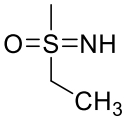
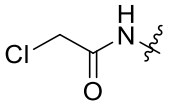
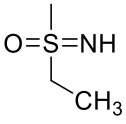
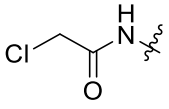
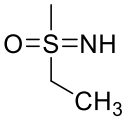
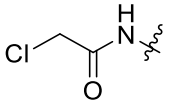
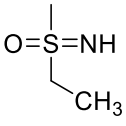
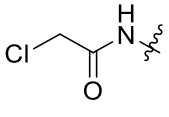
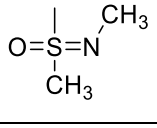
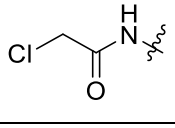
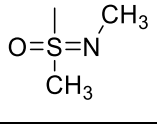
74	224		Cl	
75	225		F	
76	226			
77	227		CF_3	
78	228		H	
79	229		C_2H_5	
80	230		Cl	
81	231		F	
82	232			
83	233		CF_3	
84	234		H	
85	235		C_2H_5	

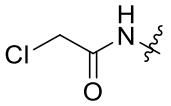
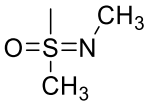
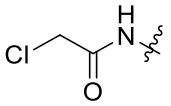
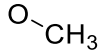
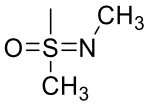
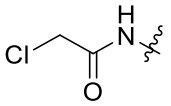
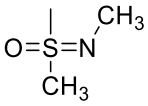
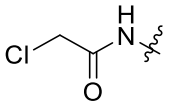
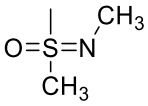
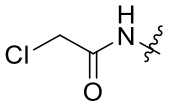
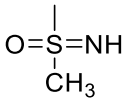
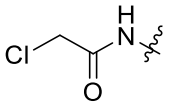
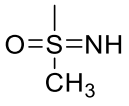
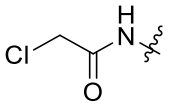
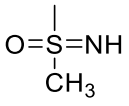
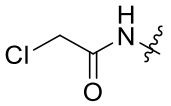
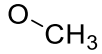
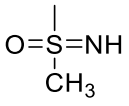
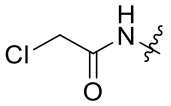
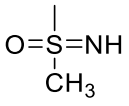
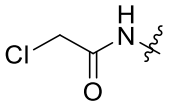
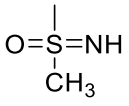
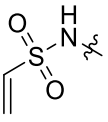
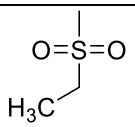
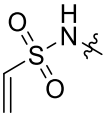
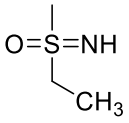
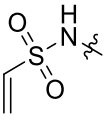
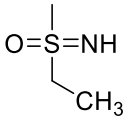
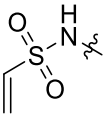
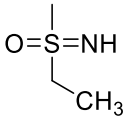
86	236		Cl	
87	237		F	
88	238			
89	239		CF_3	
90	240		H	
91	247		C_2H_5	
92	248		Cl	
93	249		F	
94	250			
95	251		CF_3	
96	252		H	
97	253		C_2H_5	
98	254		Cl	

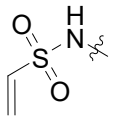
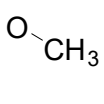
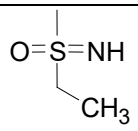
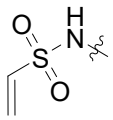
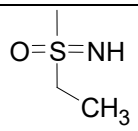
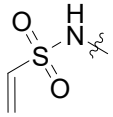
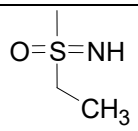
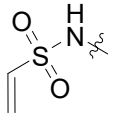
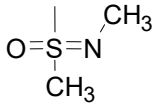
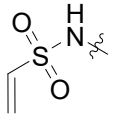
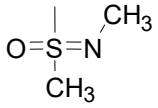
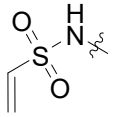
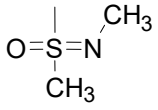
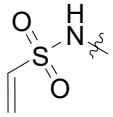
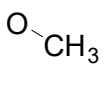
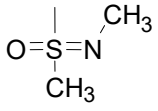
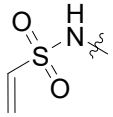
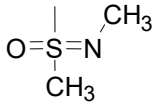
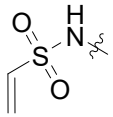
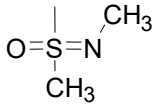
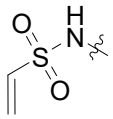
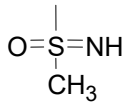
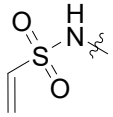
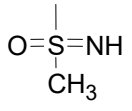
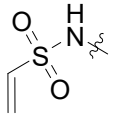
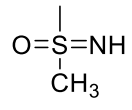
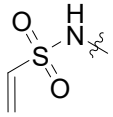
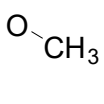
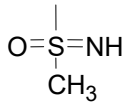
99	255		F	
100	256			
101	257		CF_3	
102	258		H	
103	259		C_2H_5	
104	260		Cl	
105	261		F	
106	262			
107	263		CF_3	
108	264		H	
109	271		C_2H_5	
110	272		Cl	
111	273		F	
112	274			

113	275		CF_3	
114	276		H	
115	277		C_2H_5	
116	278		Cl	
117	279		F	
118	280			
119	281		CF_3	
120	282		H	
121	283		C_2H_5	
122	284		Cl	
123	285		F	
124	286			
125	287		CF_3	
126	288		H	

127	295		C_2H_5	
128	296		Cl	
129	297		F	
130	298		O_{CH_3}	
131	299		CF_3	
132	300		H	
133	301		C_2H_5	
134	302		Cl	
135	303		F	
136	304		O_{CH_3}	
137	305		CF_3	
138	306		H	
139	307		C_2H_5	

140	308		Cl	
141	309		F	
142	310			
143	311		CF_3	
144	312		H	
145	319		C_2H_5	
146	320		Cl	
147	321		F	
148	322			
149	323		CF_3	
150	324		H	
151	325		C_2H_5	
152	326		Cl	

153	327		F	
154	328			
155	329		CF_3	
156	330		H	
157	331		C_2H_5	
158	332		Cl	
159	333		F	
160	334			
161	335		CF_3	
162	336		H	
163	342		H	
164	343		C_2H_5	
165	344		Cl	
166	345		F	

167	346			
168	347		CF_3	
169	348		H	
170	349		C_2H_5	
171	350		Cl	
172	351		F	
173	352			
174	353		CF_3	
175	354		H	
176	355		C_2H_5	
177	356		Cl	
178	357		F	
179	358			

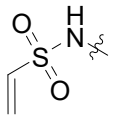
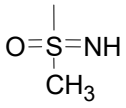
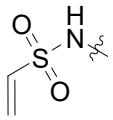
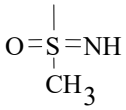
180	359		CF_3	
181	360		H	

Table 3 : Outcome of Primary Screening (Accurate but slow)

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

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

Table 4 : Outcome of Secondary Screening (Very Accurate but slow)

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 Components:	TOTAL DG	VDWAALS	EEL	EGB	ESURF
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

Sl NO.	**COMPOUNDS**	**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
6	113	-12.607	-66.64	1.443	A553, D630, SH(C552), L473, L619, V550, T499, K503
7	195	-13.591	-66.62	1458	A553, D630, SH(C552), C552, L619, V481, V550, A501, K471
8	189	-13.282	-65.98	1.592	A553, D630, SH(C552), C552, L473, L619, V481, V550, K503, K471
9	183	-14.046	-65.97	1.398	A553, D630, SH(C552), C552, L473, L619, V550
10	109	-14.230	-65.91	2.019	A553, D630, SH(C552), C552, L473, L619, V481, V550, A501, K503,T499
11	217	-13.908	-65.61	1.981	A553, D630, SH(C552), C552, L473, L619V481, V550, T499, K503, K471
12	267	-13.460	-65.08	1.486	A553, D630, SH(C552), C552, 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
23	128	-14.328	-61.20	1.340	A553, D630, SH(C552), C552, L619, R483, V481, V550, K503, A554
24	17	-14.330	-61.04	1.342	A553, D630, SH(C552), C552, L619, V481, V550, A554
25	243	-13.914	-60.82	1.341	A553, D630, SH(C552), C552, L619, V481, V550, K503, A554
26	119	-13.408	-60.81	1.354	A553, D630, SH(C552), C552, L619, V481, V550
27	11	-13.145	-60.77	1.367	A553, D630, SH(C552), C552, L619, R483, V481, V550, T499, N557
28	163	-12.922	-60.77	1.421	A553, D630, SH(C552), C552, L473, L619, V481, V550, A554
29	43	-14.308	-60.70	1.406	A553, D630, SH(C552), C552, L619, R483, V481, V550, K503, A554
30	159	-13.226	-60.64	2.007	D630, SH(C552), C552, L473, V481, V550
31	122	-13.218	-60.44	1.352	A553, D630, SH(C552), C552, L473, L619, R483, V481, V550
32	41	-13.723	-60.34	1.398	A553, D630, SH(C552), C552, L619, R483, V481, V550
33	188	-13.436	-60.34	1.586	D630, SH(C552), L619, V550, N557
34	222	-14.372	-60.09	1.477	D630, SH(C552), C552, L473, L619, R483, V481, V550,
35	193	-12.874	-59.79	1.454	A553, D630, SH(C552), C552, L619, R483, V481, V550, A554, N557
36	59	-13.535	-59.55	1.647	D630, SH(C552), L619, V550, N557
37	130	-14.021	-59.52	1.355	A553, D630, SH(C552), C552, L619, V481, V550

38	9	-13.708	-59.37	1.384	A553, D630, SH(C552), C552, 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, 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	A553, D630, SH(C552), C552, 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,
48	291	-13.734	-57.95	2.041	D630, SH(C552), L473, L619, V550, A501
49	110	-12.473	-57.93	1.790	A553, SH(C552), C552, V481, V550, V620, N557
50	7	-13.464	-57.75	1.363	A553, D630, SH(C552), C552, L473, L619, R483, V481, V550
51	153	-13.539	-57.65	2.020	D630, SH(C552), C552, L473, V481, V550, A554
52	37	-14.722	-57.41	1.701	A553, D630, SH(C552), C552, L473, V550, G556, N557
53	117	-13.989	-57.36	1.815	SH(C552), L473, L619, V481, V550, A554, T499
54	131	-13.244	-57.27	1.341	A553, D630, SH(C552), C552, L619, R483, V481, V550,

					A554, K503
55	185	-13.822	-57.23	1.449	A553, D630, SH(C552), C552, L619, R483, V481, V550,
56	56	-13.674	-57.20	1.688	D630, SH(C552), C552, L619, L473, V550, N557
57	200	-14.51	-57.10	1.422	A553, D630, SH(C552), C552, L619, R483, V481, V550
58	187	-13.332	-57.09	1.483	A553, D630, SH(C552), L619, V481, V550, A554, N557
59	340	-13.824	-57.05	1.391	A553, D630, SH(C552), C552, L619, R483, V481, V550, K503
60	339	-12.851	-57.04	1.393	A553, D630, SH(C552), C552, L619, V481, V550, K503
61	38	-14.847	-56.95	1.421	A553, D630, SH(C552), C552, L473, L619, V481, V550
62	265	-13.64	-56.95	1.568	D630, SH(C552), C552, L473, V550, G556
63	8	-13.639	-56.78	2.759	A553, SH(C552), C552, L473, L619, R483, V550, T499
64	202	-13.627	-56.75	1.464	A553, SH(C552), C552, L619, V481, V550, A554,
65	154	-13.833	-56.66	1.336	A553, D630, SH(C552), C552, L619, R483, V481, V550, A554, K503
66	156	-13.778	-56.64	1.495	D630, SH(C552), C552, L619, L473, R483, V481, V550,
67	120	-12.515	-56.62	1.282	A553, SH(C552), C552, L619, V481, V550, N557, K555
68	182	-14.232	-56.53	1.505	A553, D630, SH(C552), L473, L619, R483, V550
69	44	-13.547	-56.48	1.707	A553, D630, SH(C552), C552, 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, 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
76	32	-13.744	-55.67	2.677	A553, D630, SH(C552), C552, L473, L619, R483, V481, V550, K503
77	3	-13.922	-55.63	2.728	A553, D630, SH(C552), C552, 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	-13.581	-55.44	2.567	A553, SH(C552), L473, L619, R483, V550, A501, N557
81	12	-13.416	-55.26	1.384	A553, D630, SH(C552), L619, R483, V481, V550, K503
82	18	-14.04	-55.24	2.600	SH(C552), L473, R483, V550, A554, K503, E551
83	268	-13.825	-55.10	1.496	A553, D630, SH(C552), L619, R483, V481, V550, A554
84	5	-13.079	-54.94	3.005	SH(C552), L473, R483, V481, V550, A501
85	52	-14.099	-54.93	1.421	A553, D630, SH(C552), L619, R483, V481, V550
86	126	-14.183	-54.52	1.444	D630, SH(C552), C552, L473, L619, V550
87	203	-13.153	-54.45	0.566	A553, D630, SH(C552), L619, R483, V550, A554, I534
88	13	-14.016	-54.24	1.271	A553, D630, SH(C552), C552, L473, L619, V481, V550
89	34	-12.504	-54.19	2.753	A553, SH(C552), C552, L473, L619, V550, A501

90	199	-14.069	-54.02	1.634	D630, SH(C552), C552, L473, 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%
35	Sulfur-lone Pair	C LIG 293 S2	C ASN 105 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

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	HIA	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