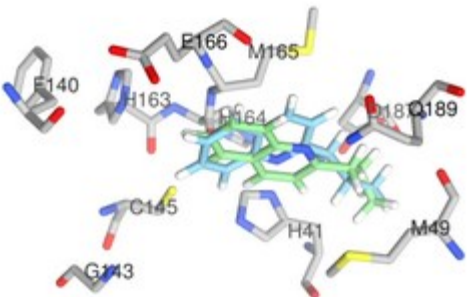
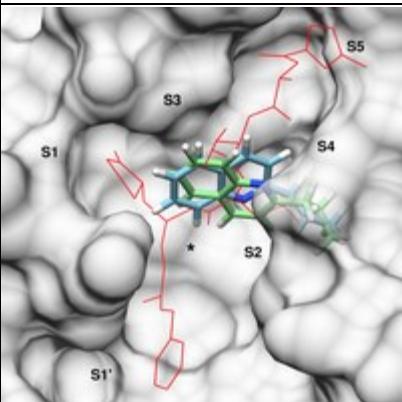
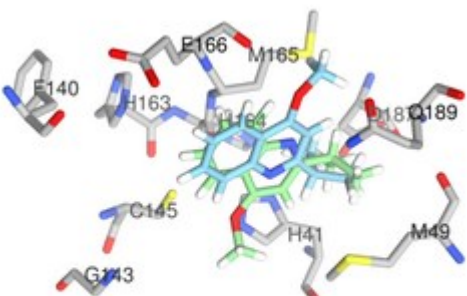
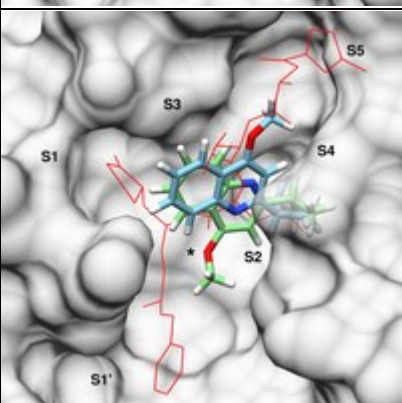
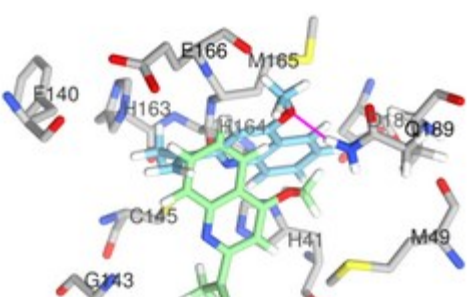
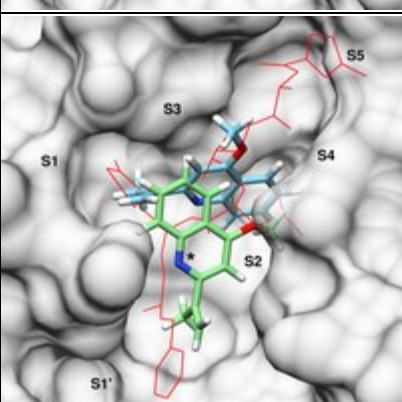
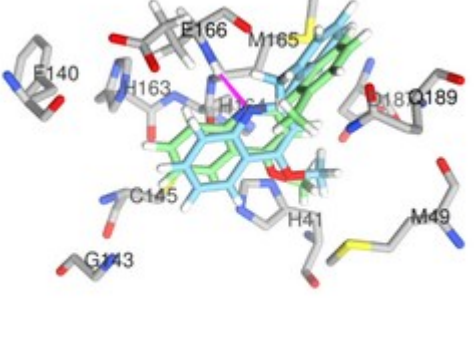
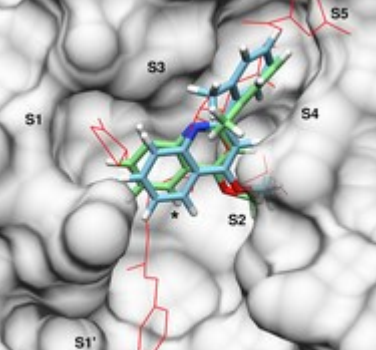
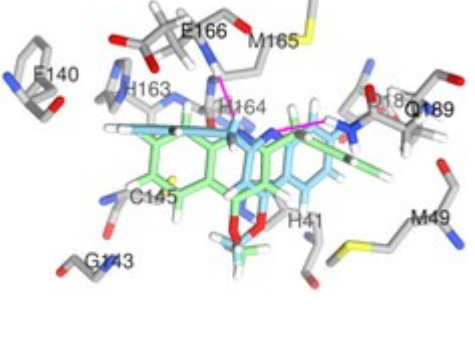
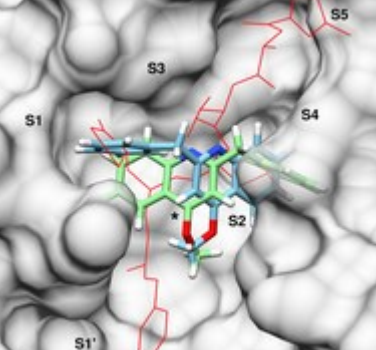
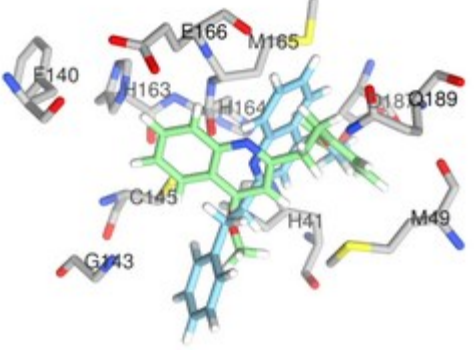
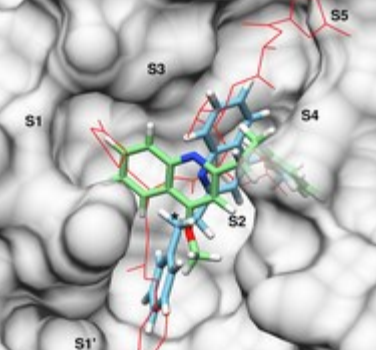
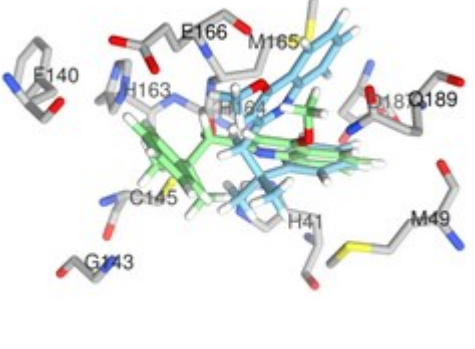
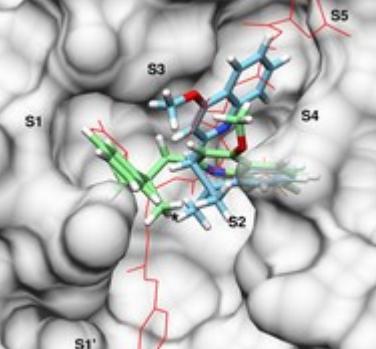
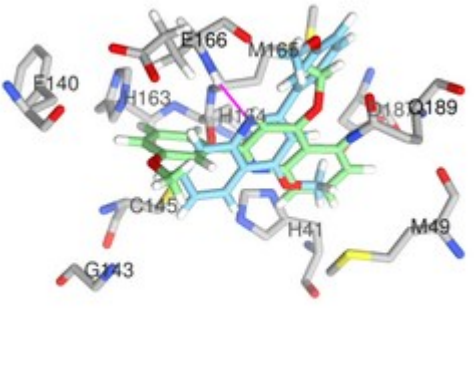
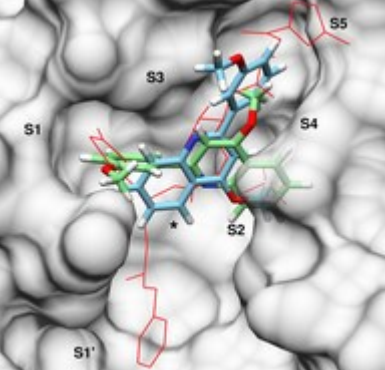
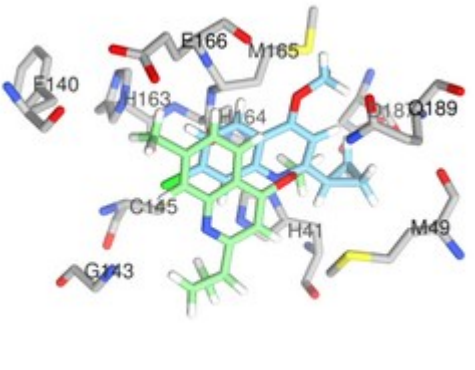
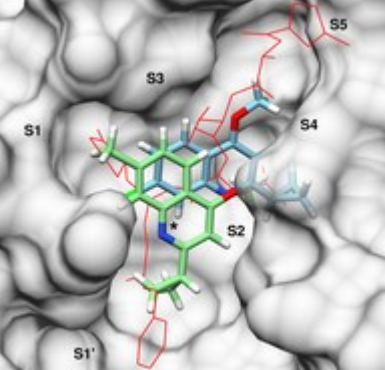
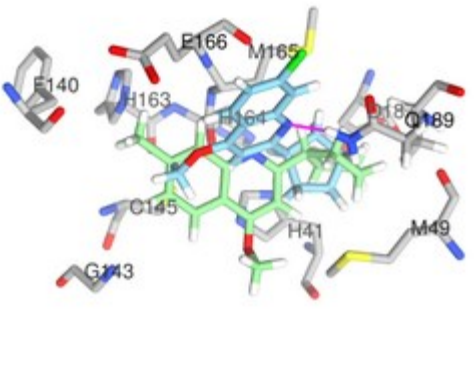
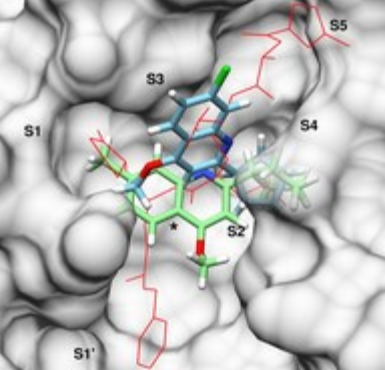
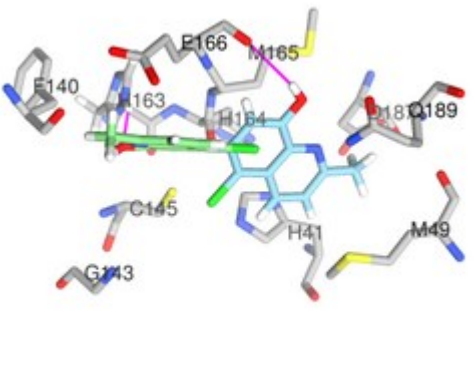
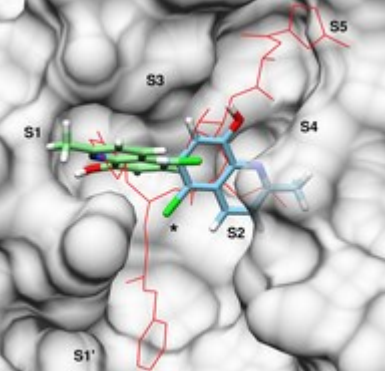
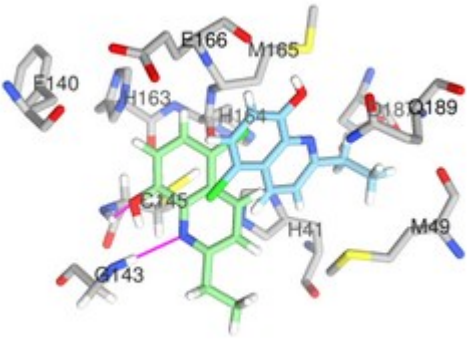
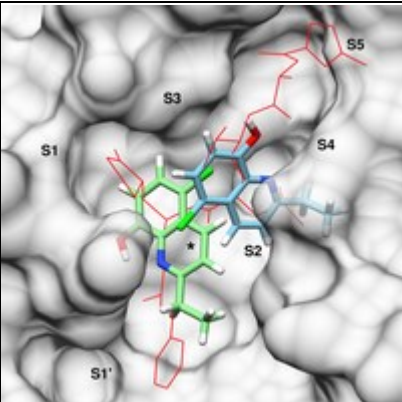
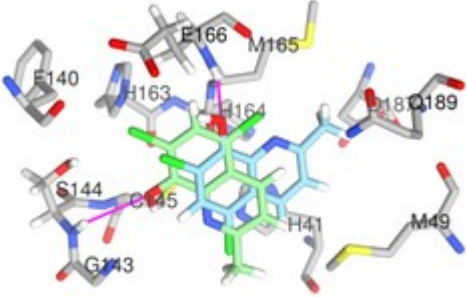
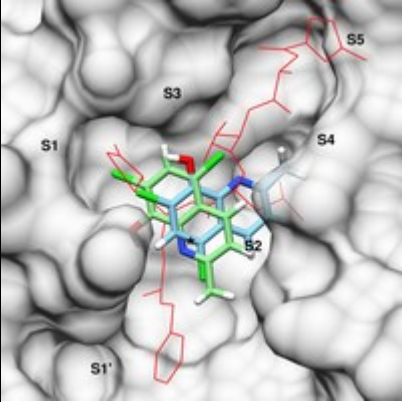
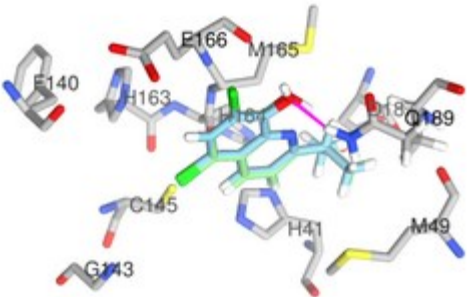
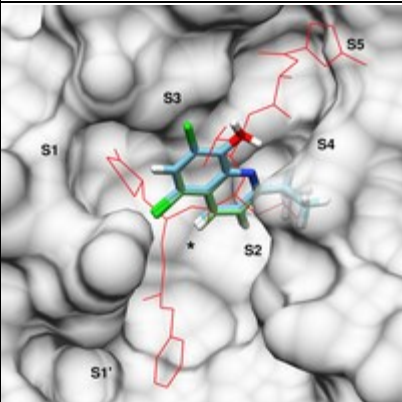
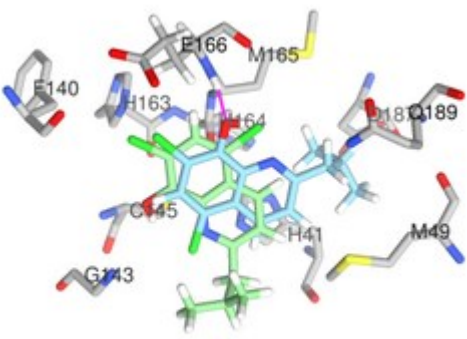
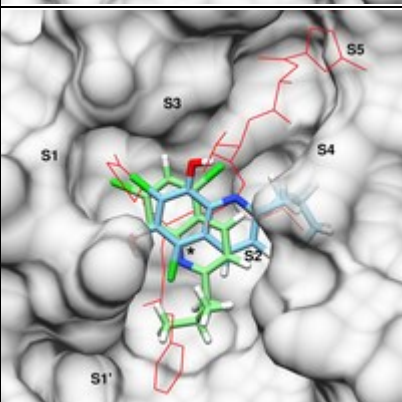


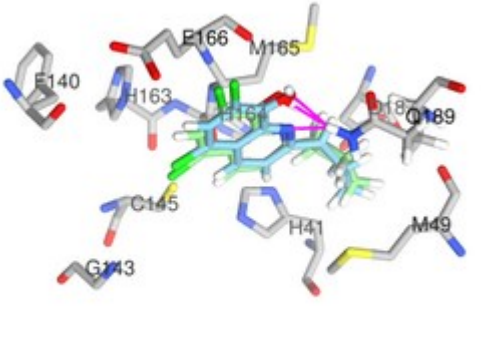
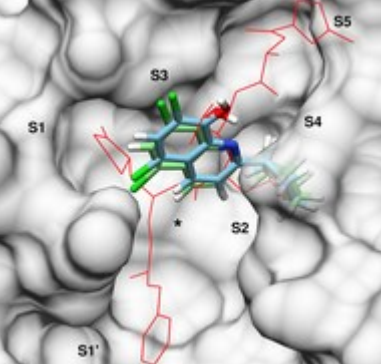
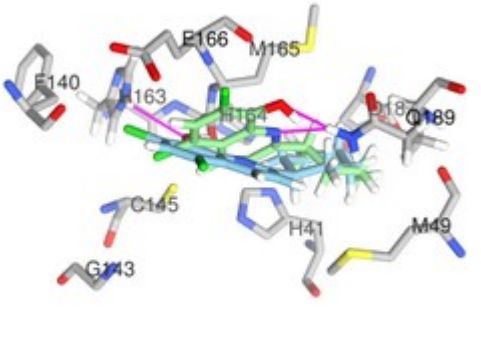
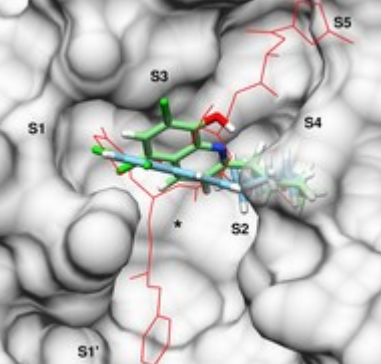
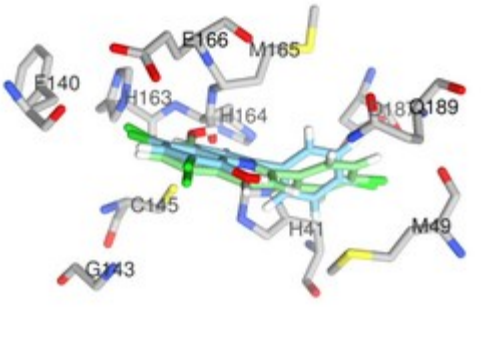
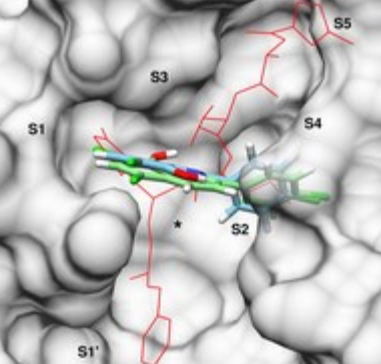
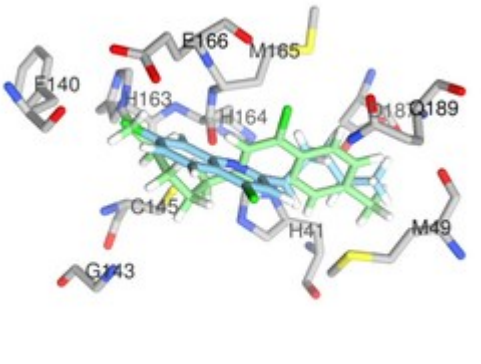
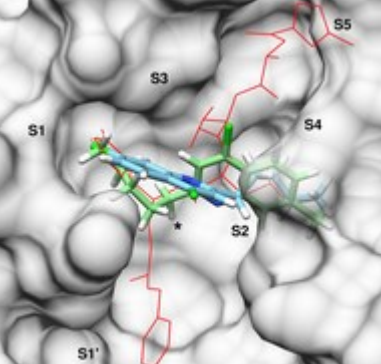
Table S3. Docking energy scores and lowest-energy poses for the compounds considered in this study.

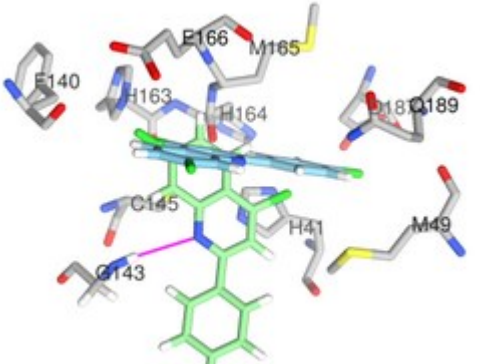
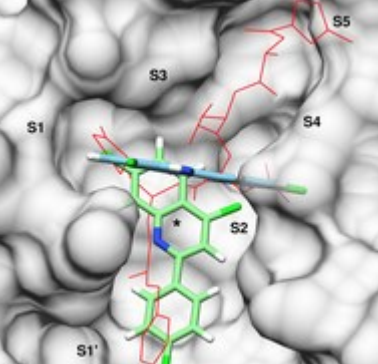
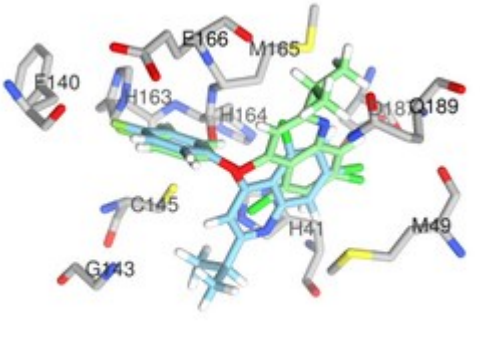
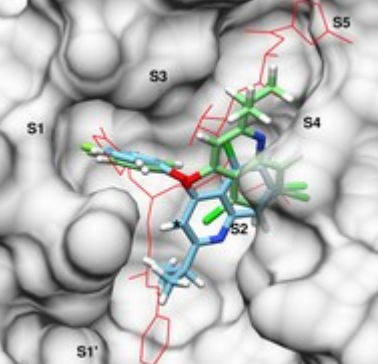
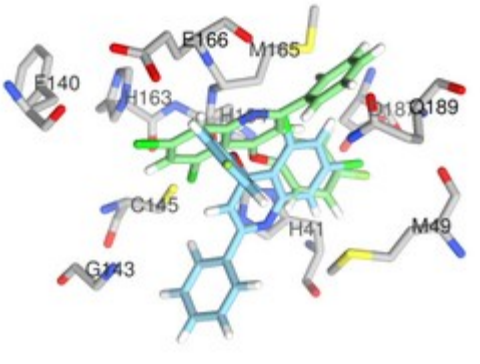
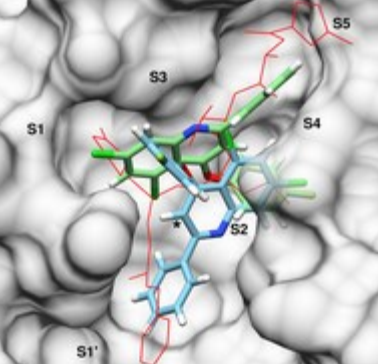
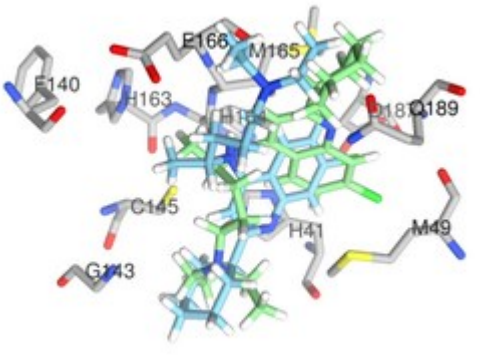
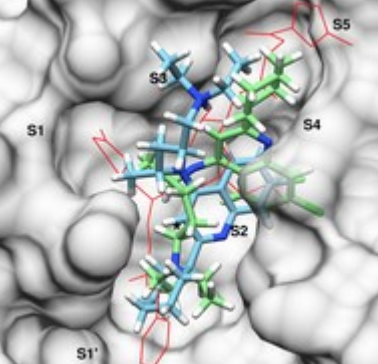
Compound	Energy scores (kcal/mol)		Pose comparison Blue = DOCK, Green = Smina	
	DOCK GBSA	Smina	Non-covalent interactions	Surface Red wire = N3 orientation
PQ	-25.8	-8.5		
1	-25.6	-8.3		
2	-25.3	-7.8		

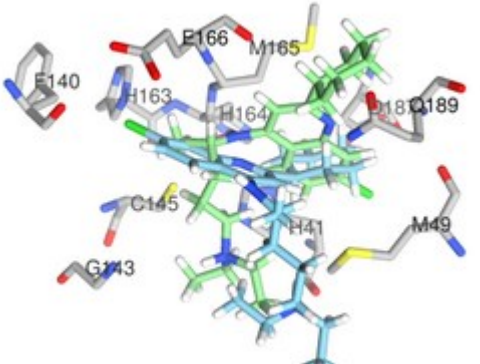
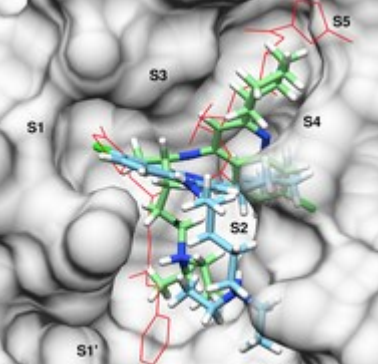
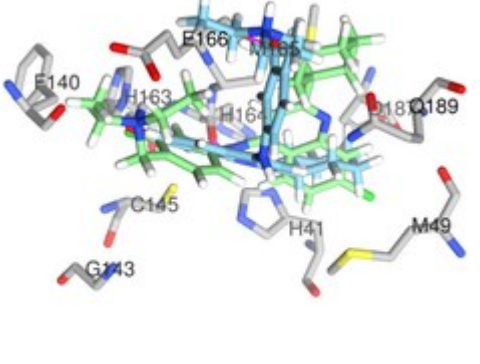
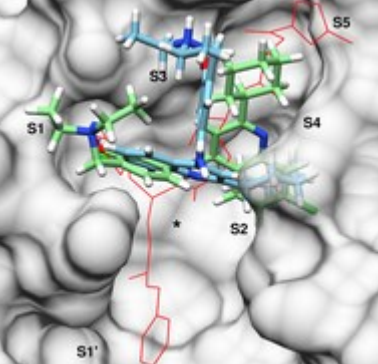
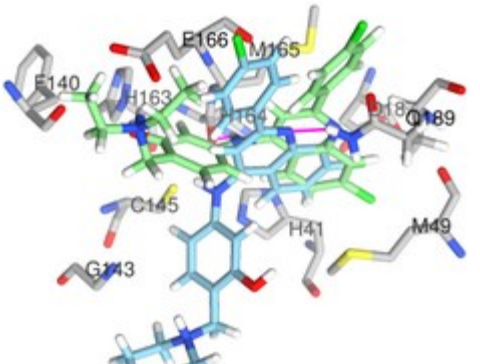
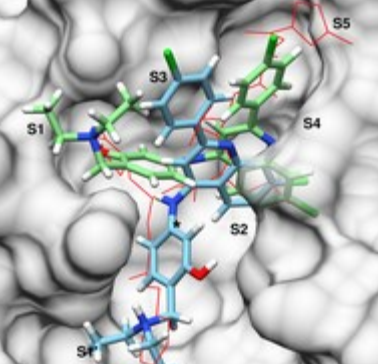
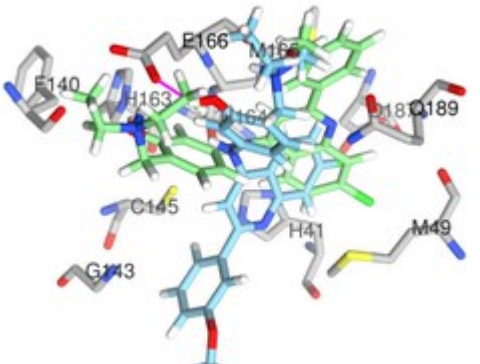
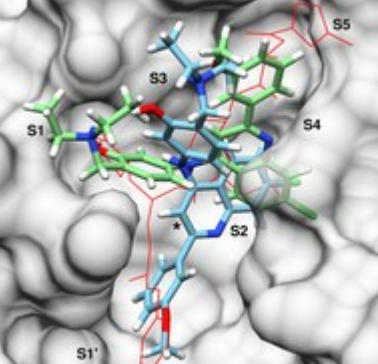
3	-24.9	-9.0		
4	-28.2	-10.2		
5	-27.6	-10.0		
6	-30.1	-10.7		

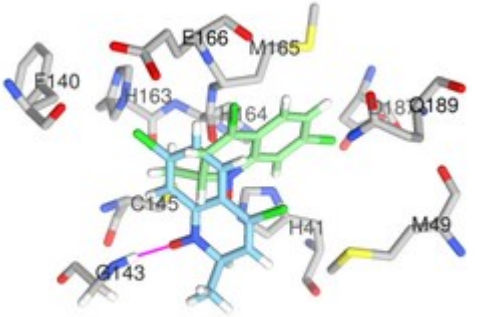
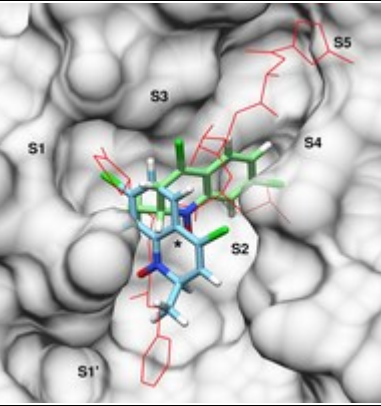
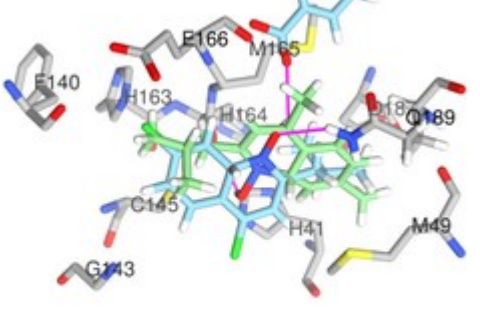
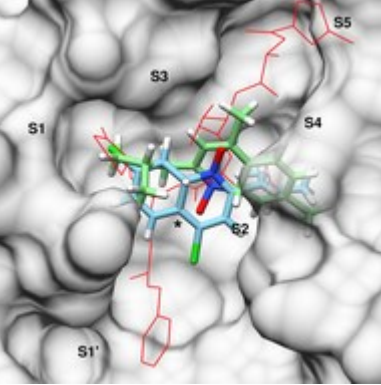
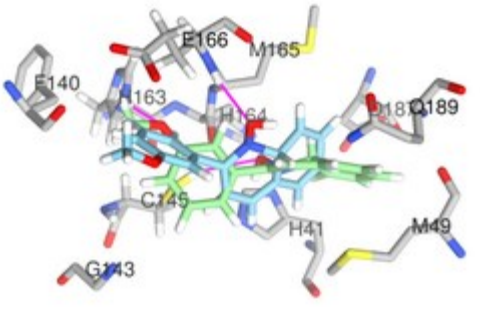
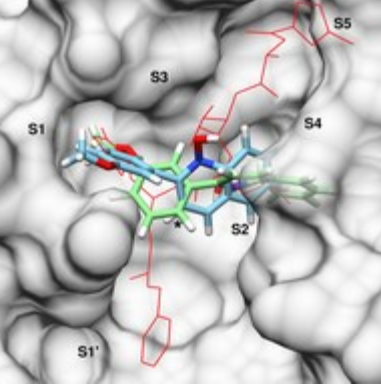
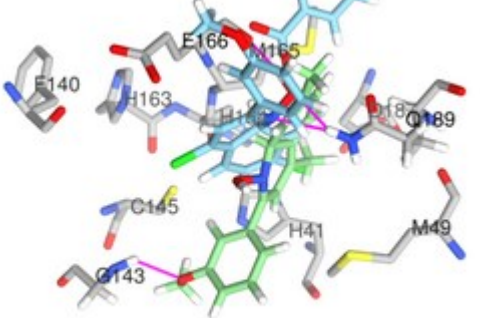
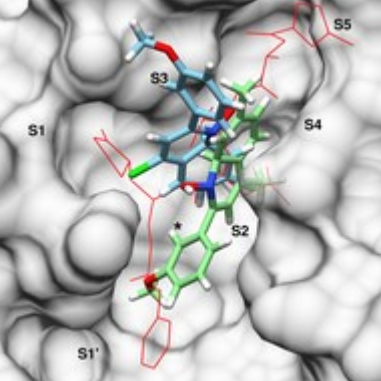
7	-25.5	-9.0		
8	-28.0	-8.5		
9	-29.7	-9.8		
10	-21.2	-8.1		

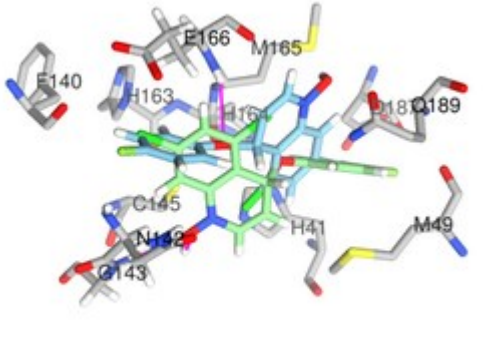
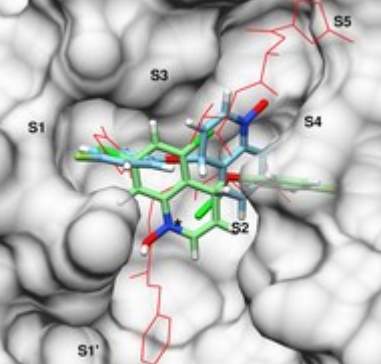
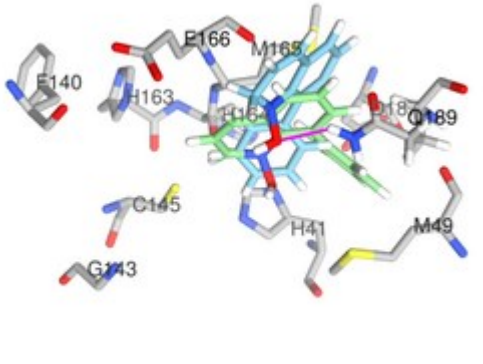
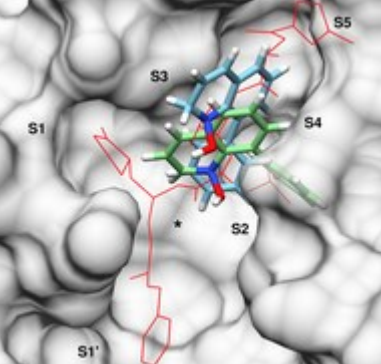
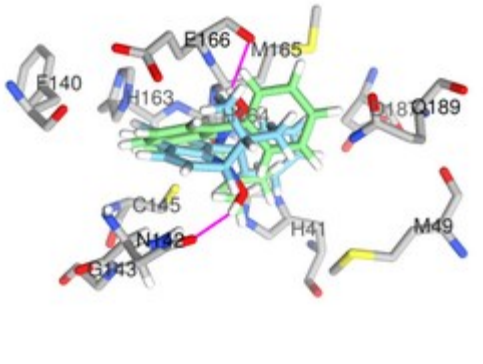
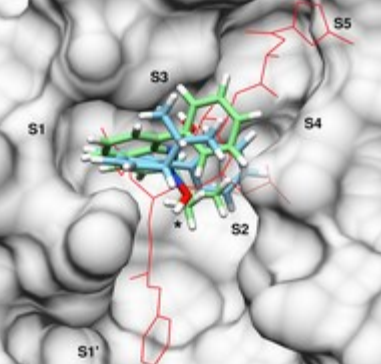
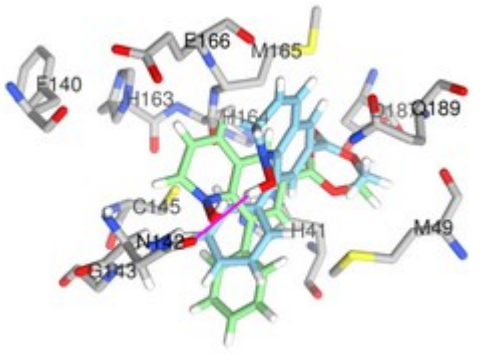
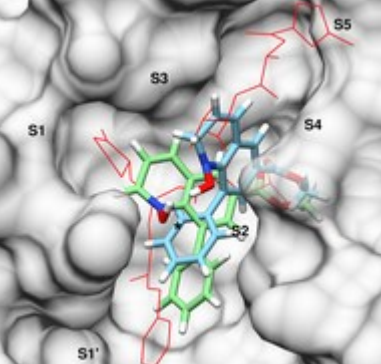
11	-24.2	-8.5		
12	-25.3	-8.7		
13	-28.7	-9.6		
14	-29.1	-8.5		

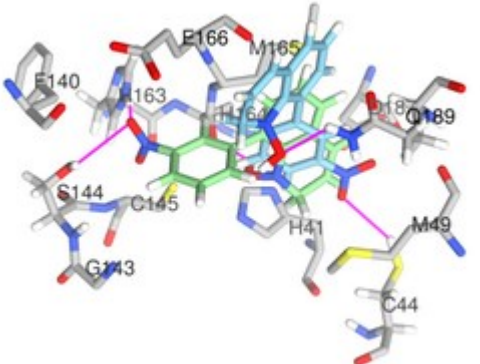
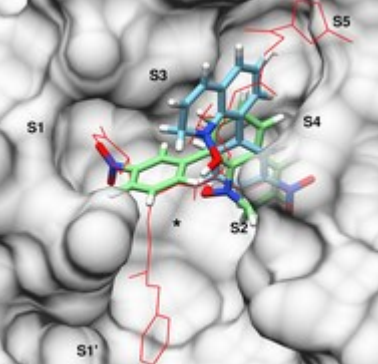
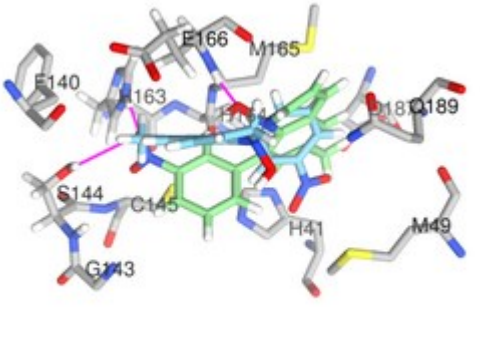
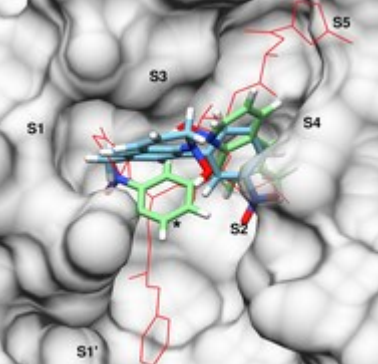
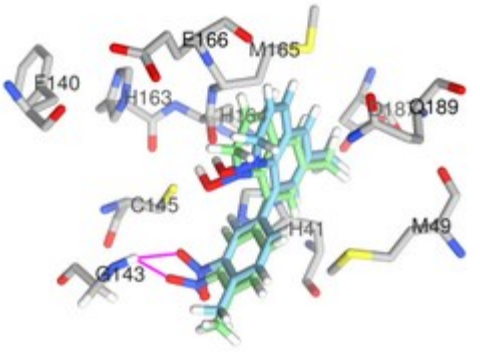
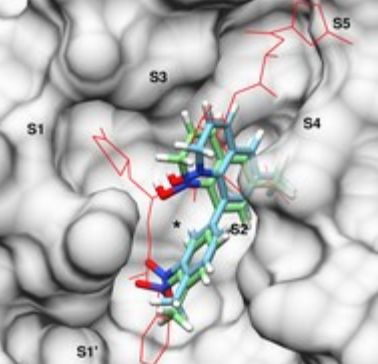
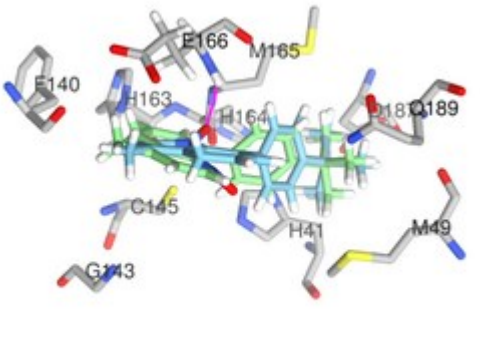
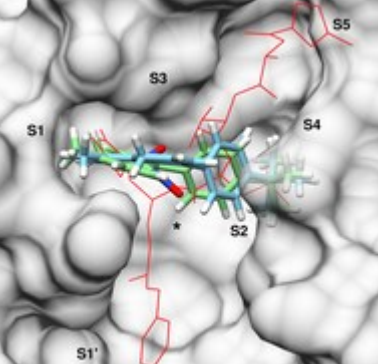
15	-31.4	-9.5		
16	-28.1	-9.3		
17	-29.1	-11.4		
18	-32.3	-8.7		

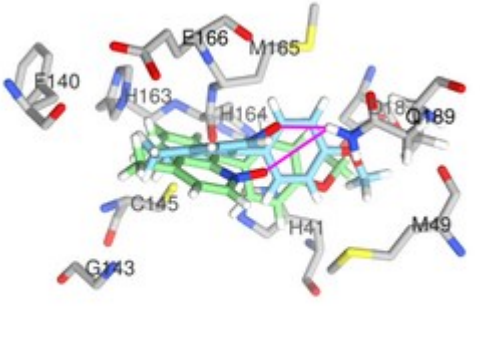
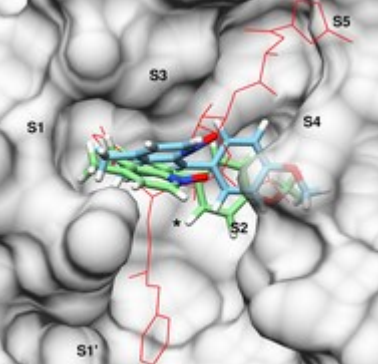
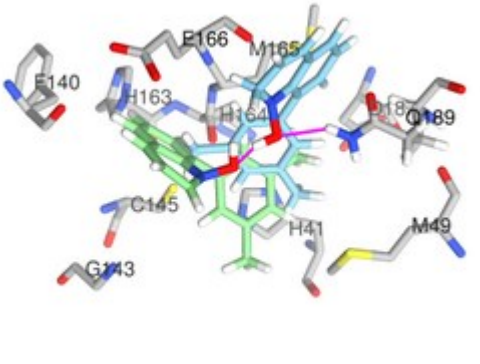
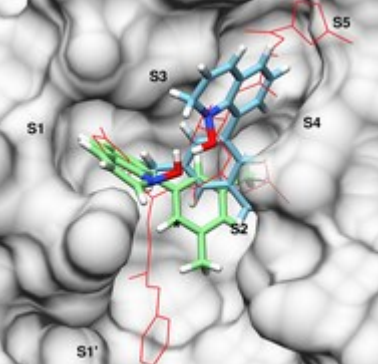
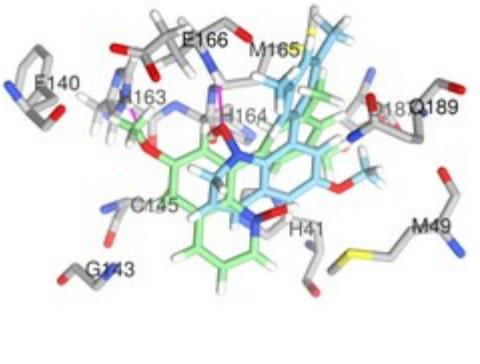
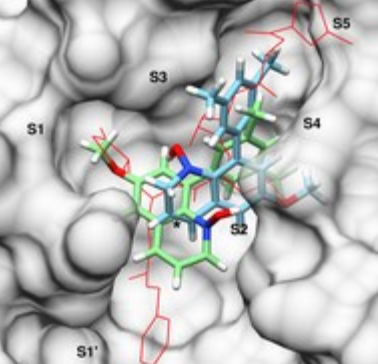
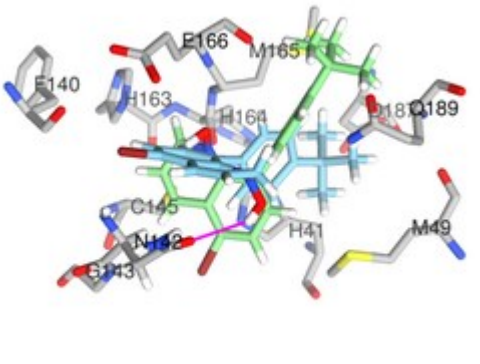
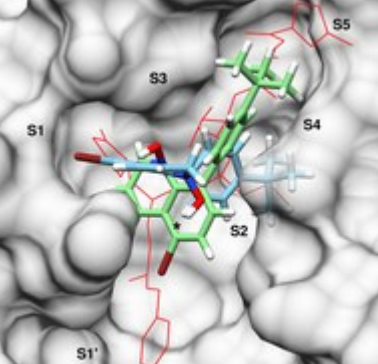
19	-29.0	-8.8		
20	-33.0	-10.3		
21	-32.4	-12.5		
22_R	-38.5	-10.0		

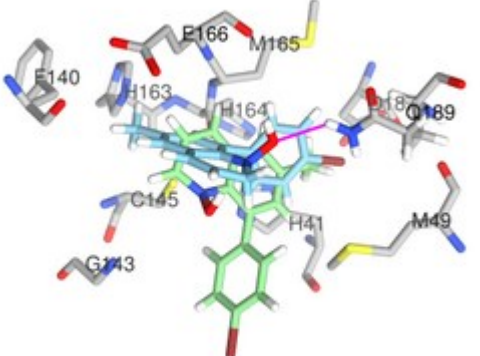
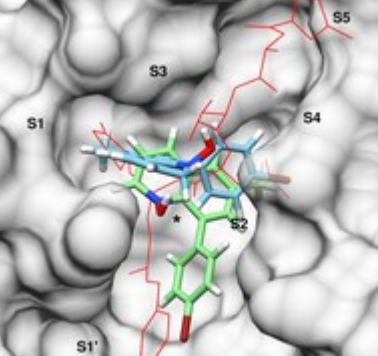
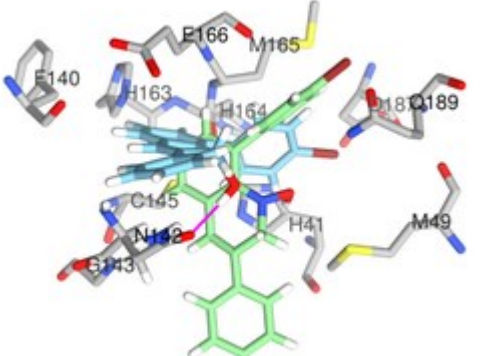
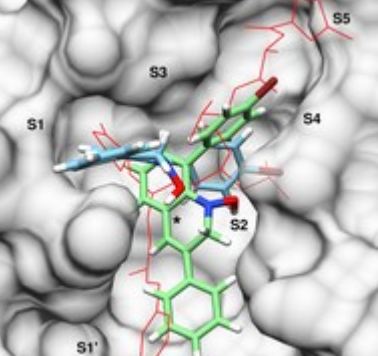
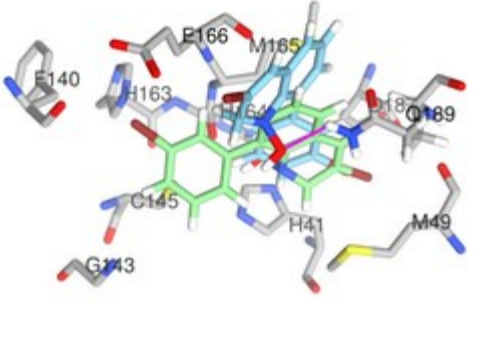
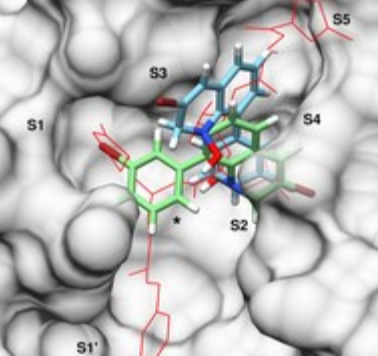
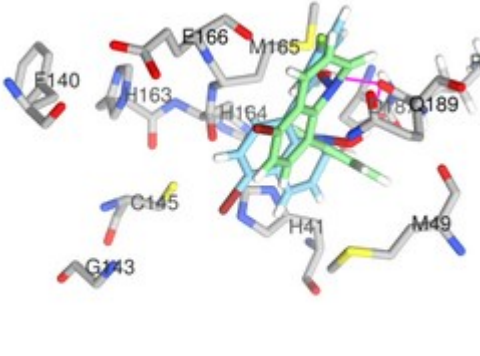
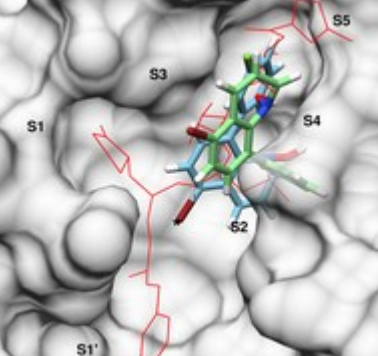
22_S	-39.2	-9.8		
23	-37.1	-11.1		
24	-36.2	-11.9		
25	-35.9	-11.2		

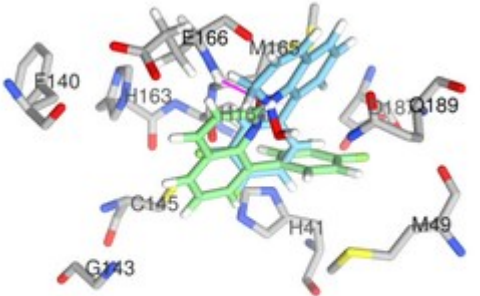
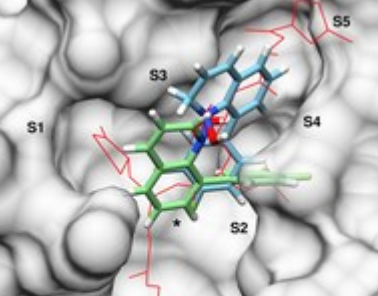
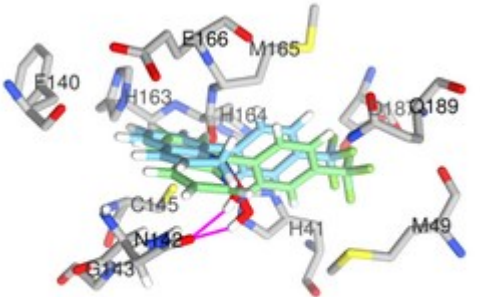
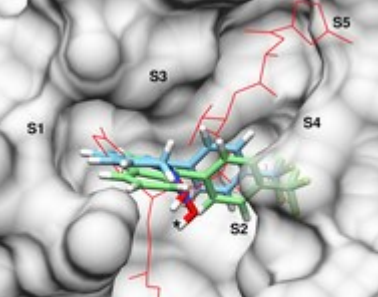
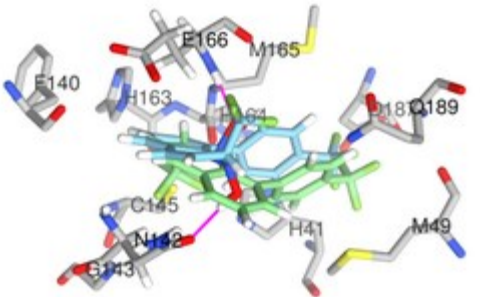
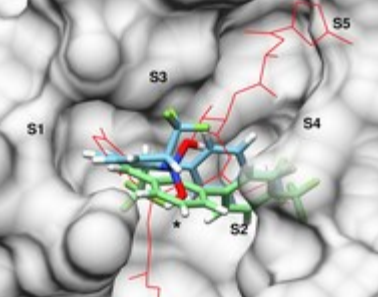
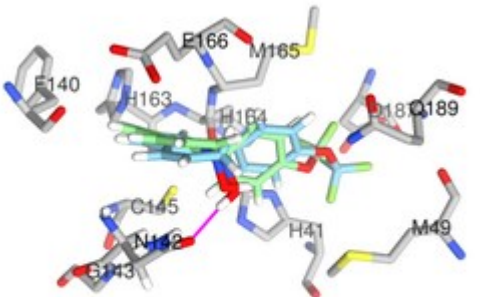
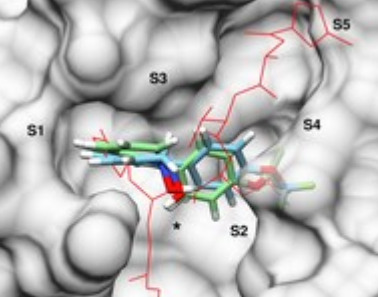
26	-21.5	-8.6		
27	-32.2	-10.4		
28	-25.6	-9.9		
29	-28.8	-8.3		

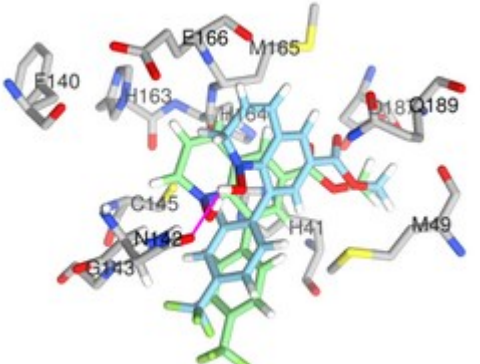
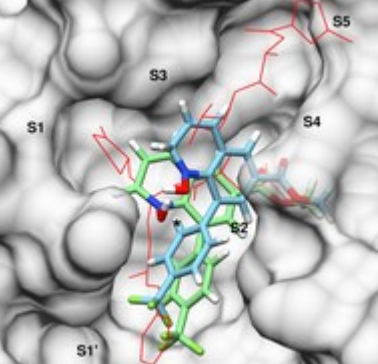
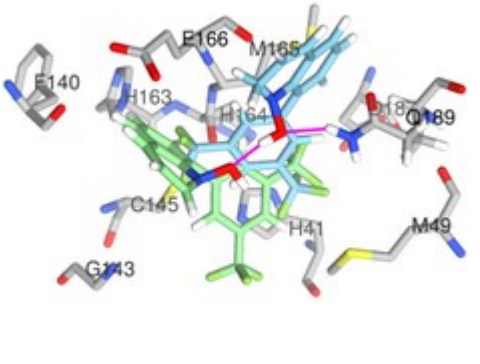
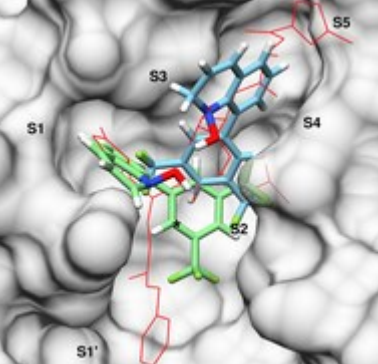
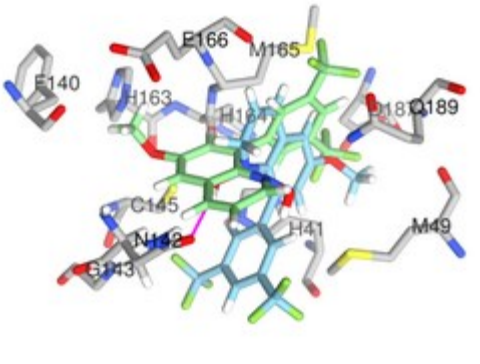
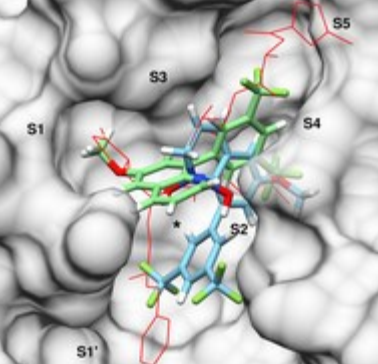
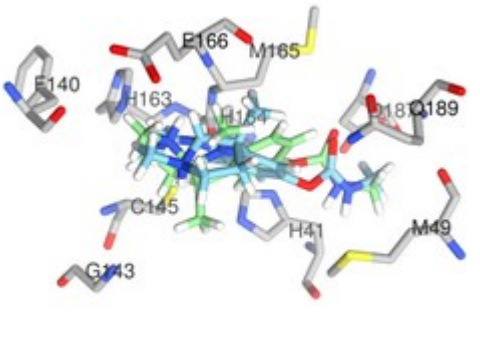
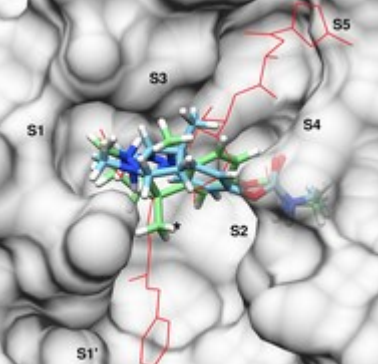
30	-29.3	-11.1		
31	-22.9	-9.7		
32	-22.3	-8.7		
33	-28.1	-9.4		

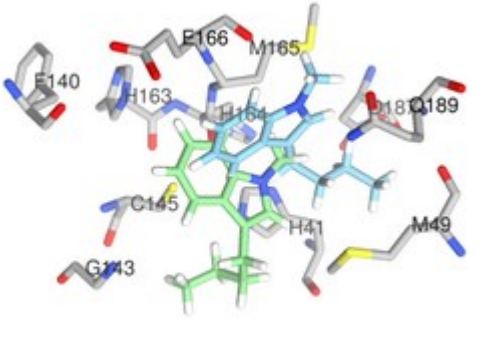
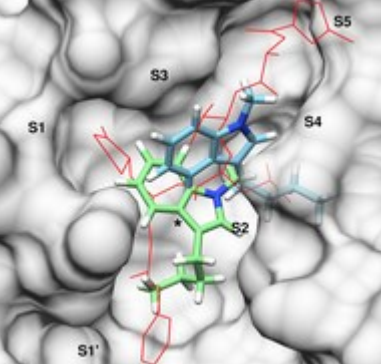
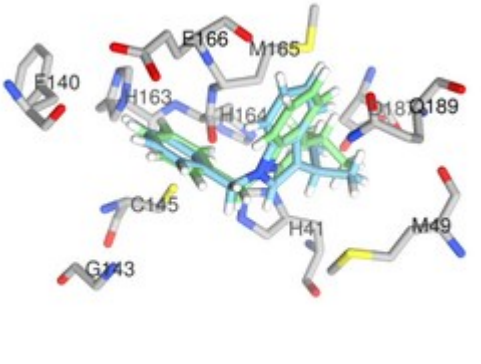
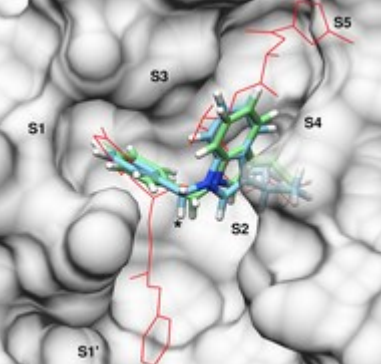
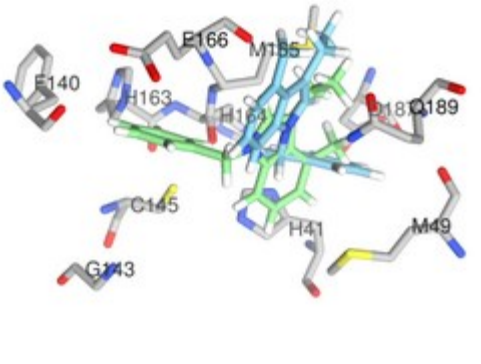
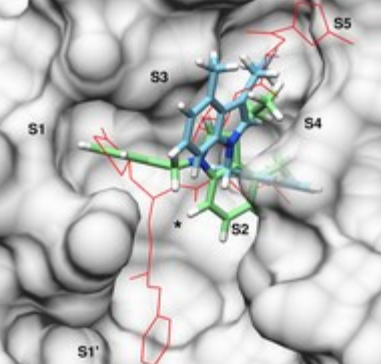
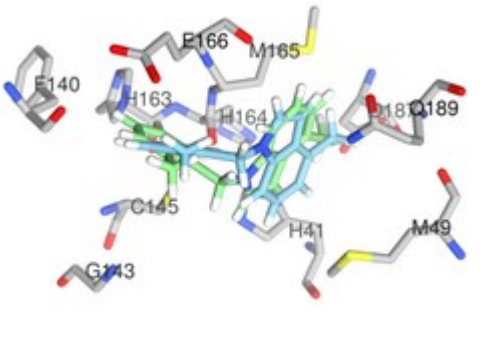
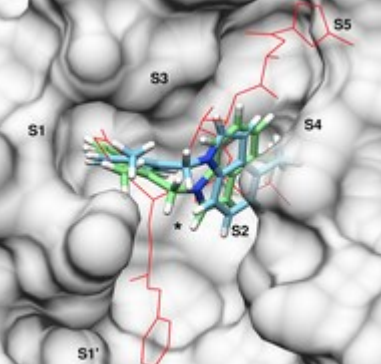
34	-29.4	-10.1		
35	-27.3	-11.1		
36	-30.6	-9.1		
37	-22.6	-10.5		

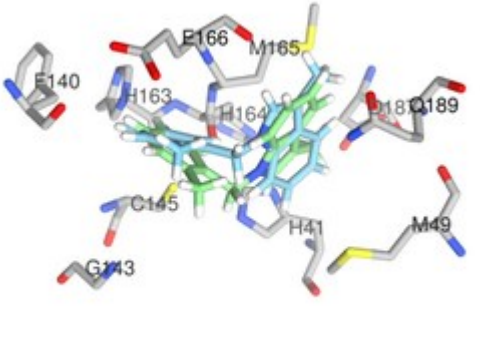
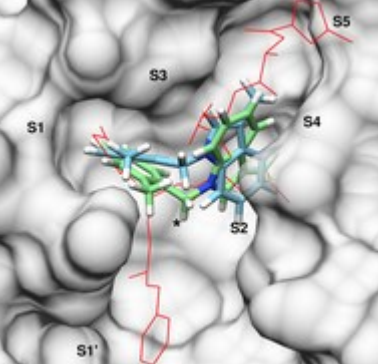
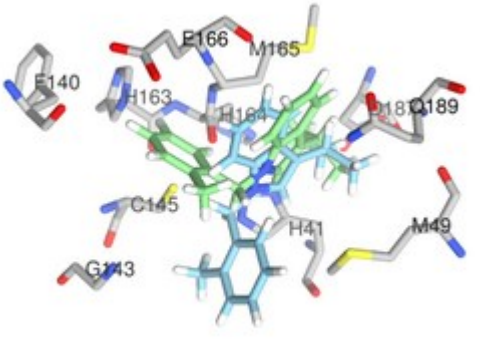
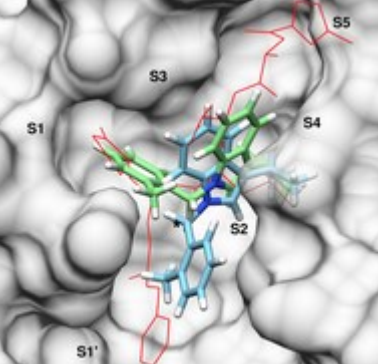
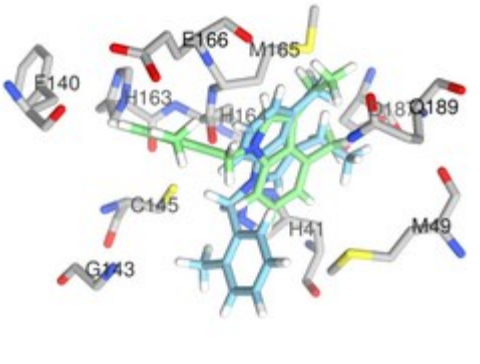
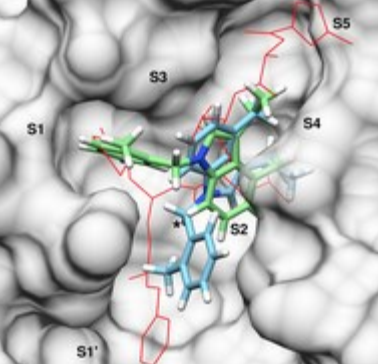
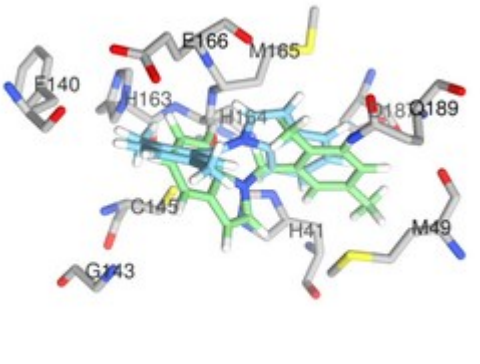
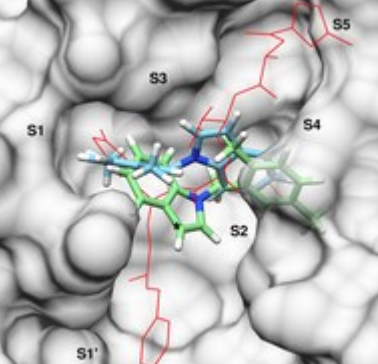
38	-23.0	-8.3		
39	-28.5	-9.3		
40	-30.0	-10.0		
41	-27.5	-9.0		

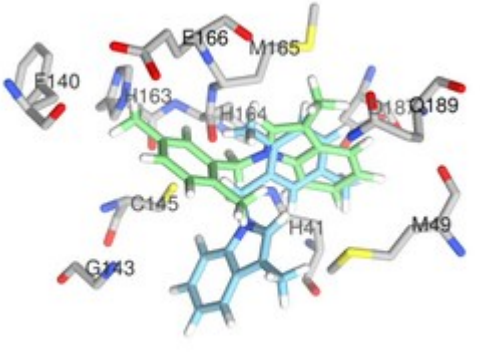
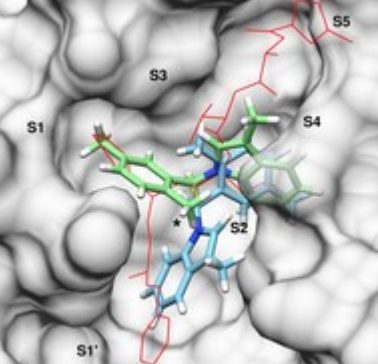
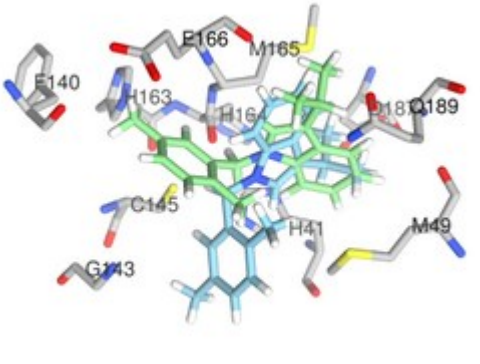
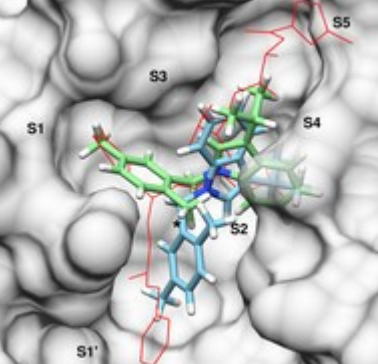
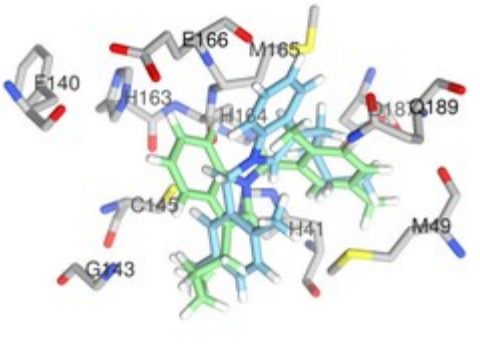
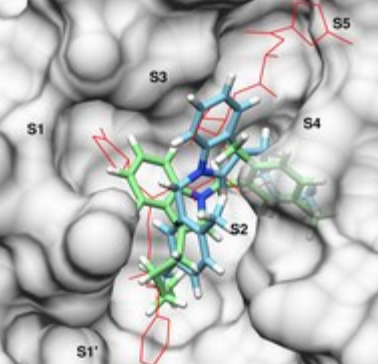
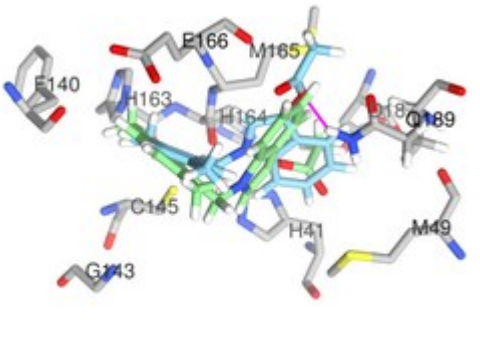
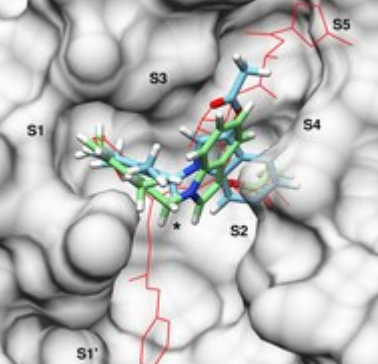
42	-29.2	-9.3		
43	-29.7	-9.5		
44	-30.2	-10.4		
45	-23.9	-10.2		

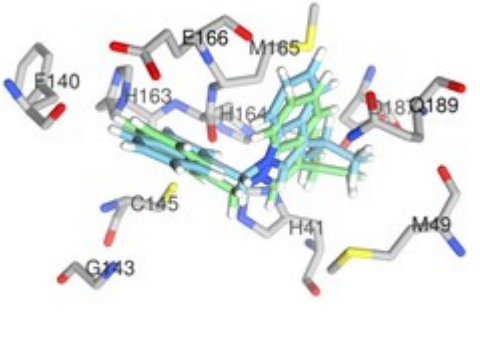
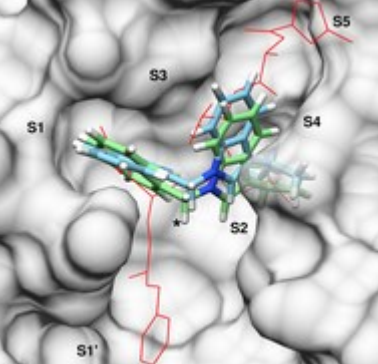
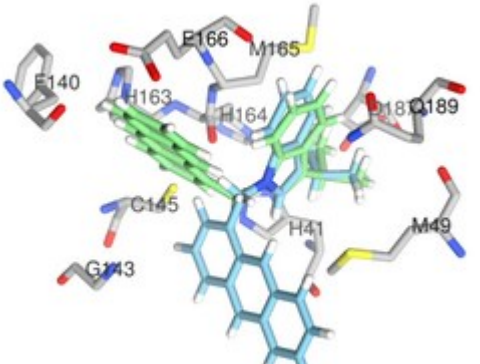
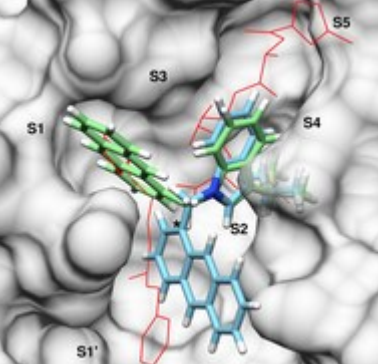
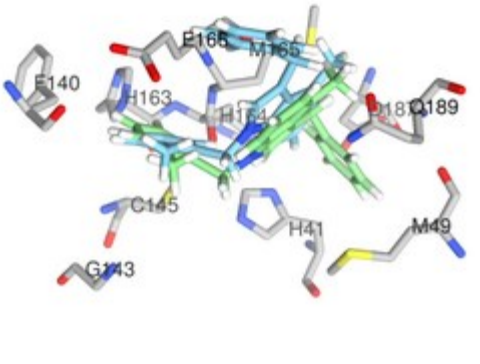
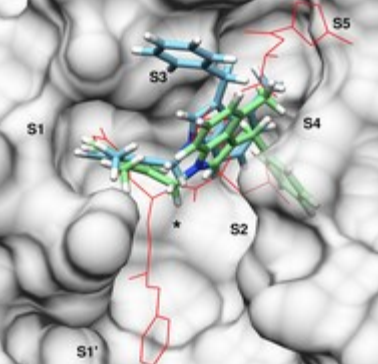
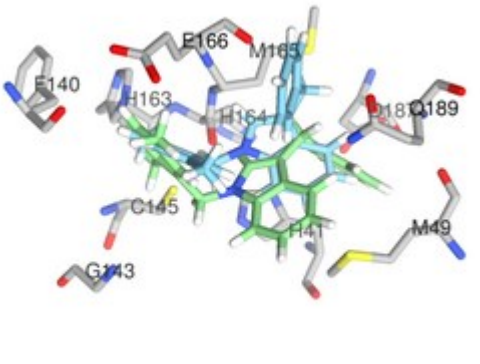
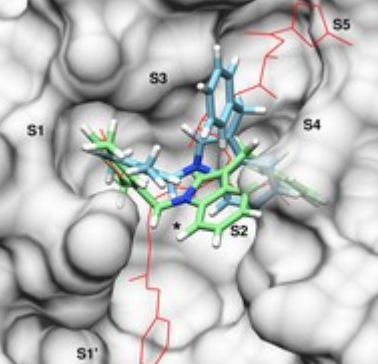
46	-23.2	-10.2		
47	-28.5	-9.2		
48	-29.7	-10.9		
49	-30.2	-10.4		

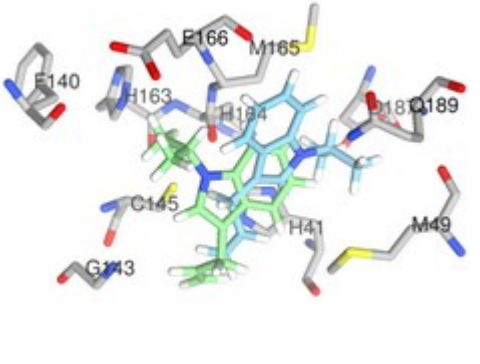
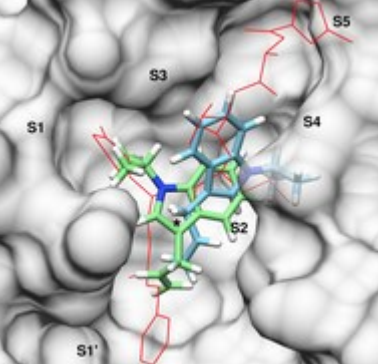
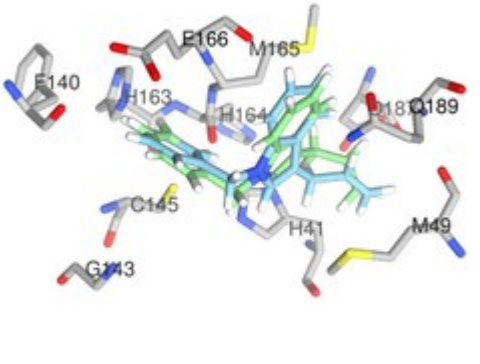
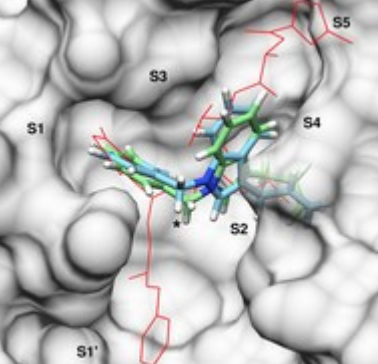
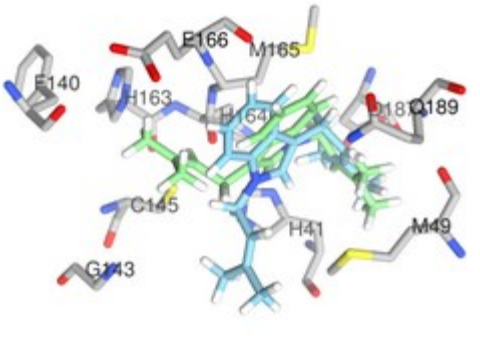
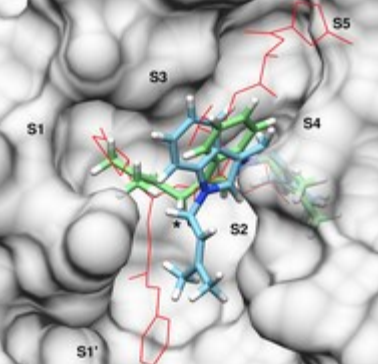
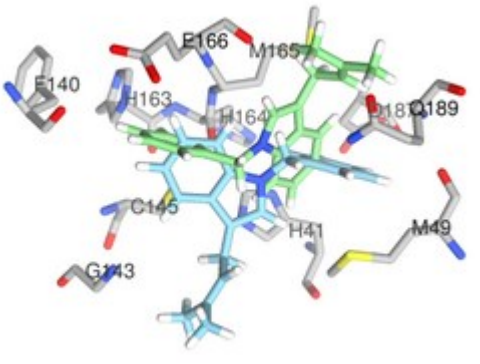
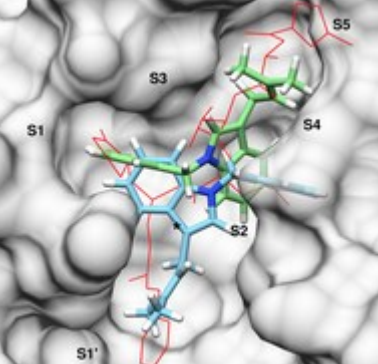
50	-30.1	-10.4		
51	-27.4	-10.6		
52	-30.6	-10.3		
PS	-26.5	-10.1		

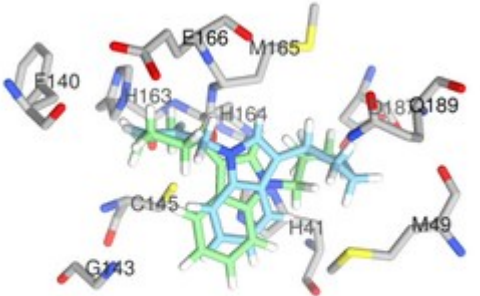
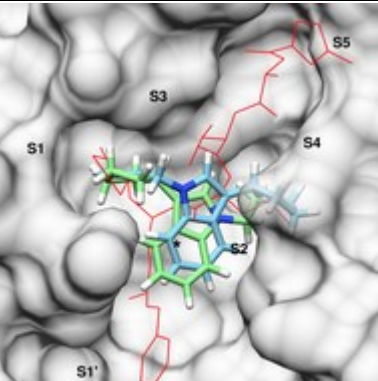
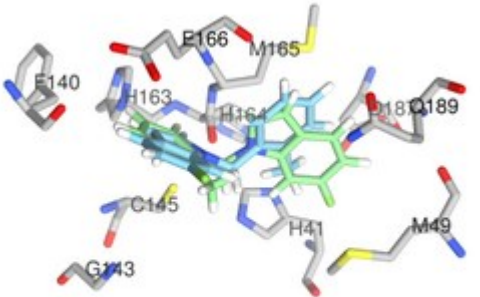
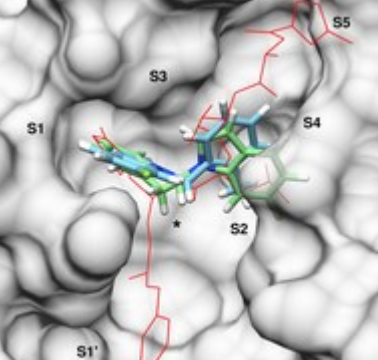
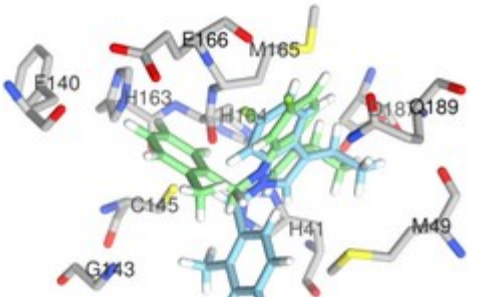
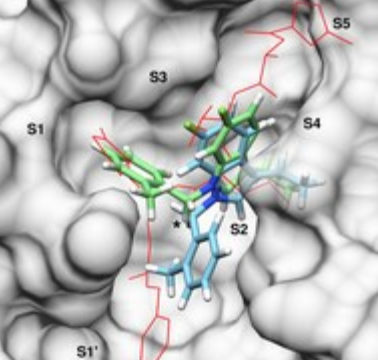
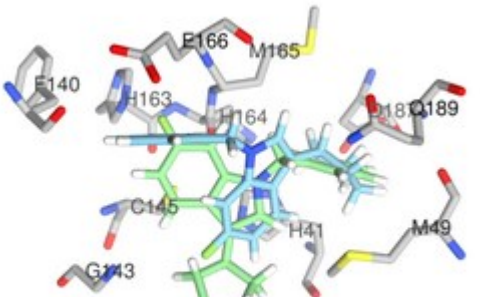
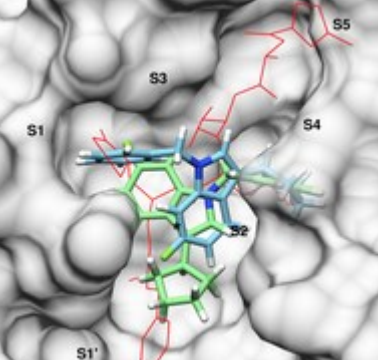
53	-28.6	-6.7		
54	-31.1	-9.1		
55	-30.5	-9.1		
56	-26.4	-8.9		

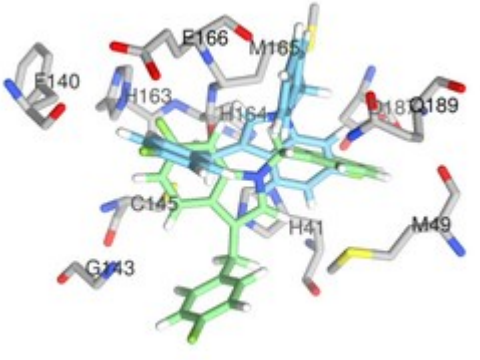
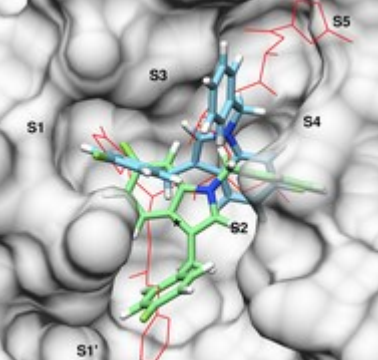
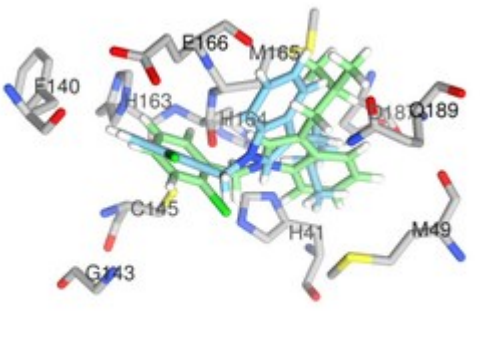
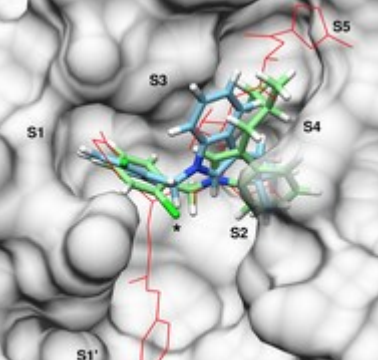
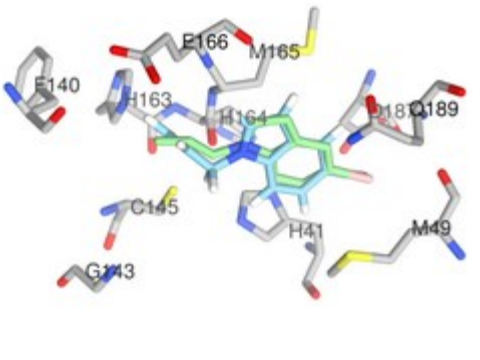
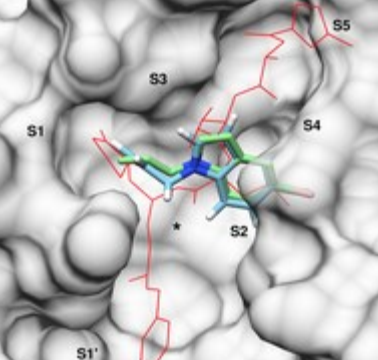
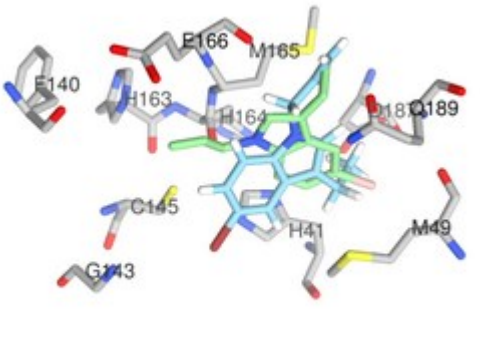
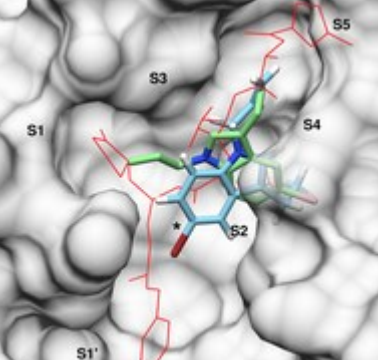
57	-28.3	-8.4		
58	-30.7	-9.0		
59	-29.6	-8.7		
60	-28.0	-9.5		

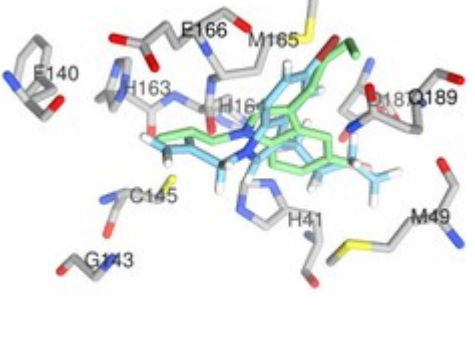
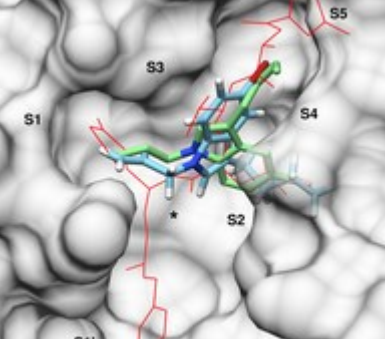
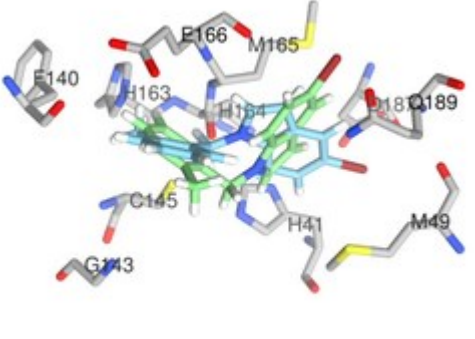
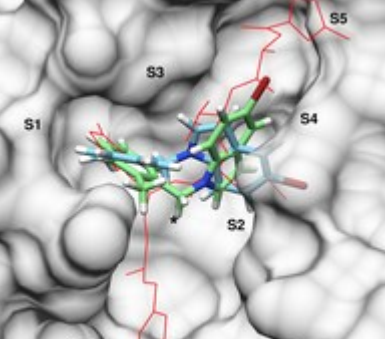
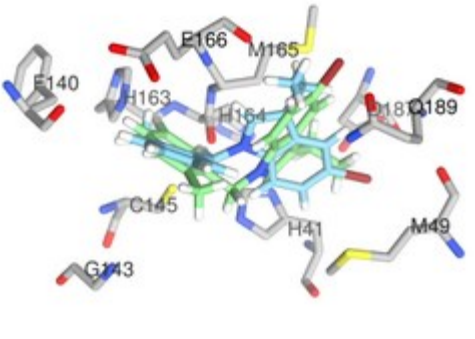
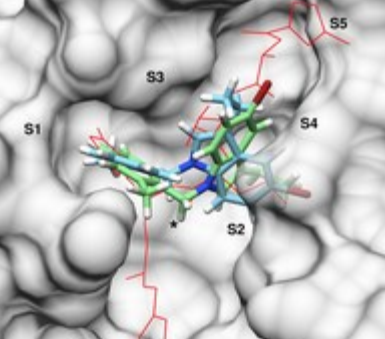
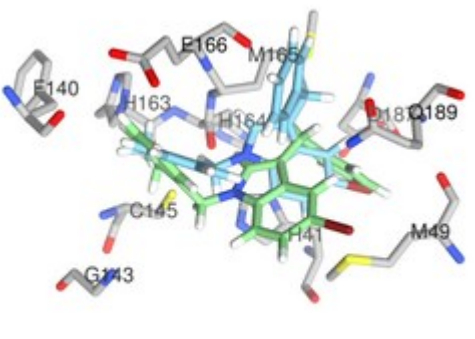
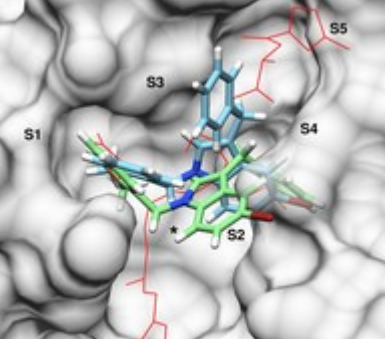
61	-28.6	-9.8		
62	-31.9	-9.6		
63	-32.9	-9.3		
64	-31.3	-9.6		

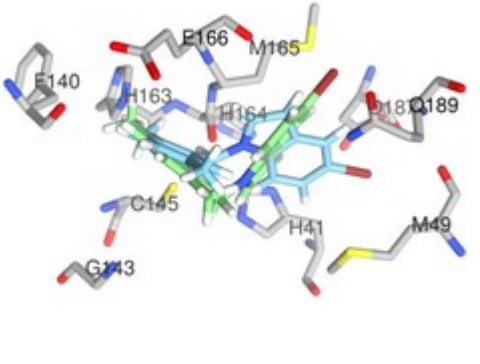
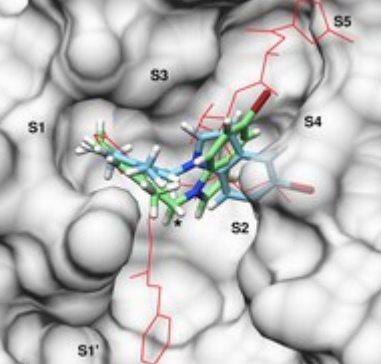
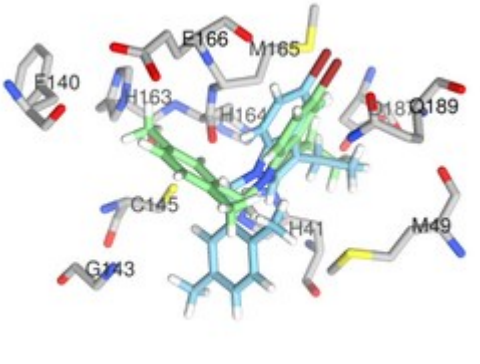
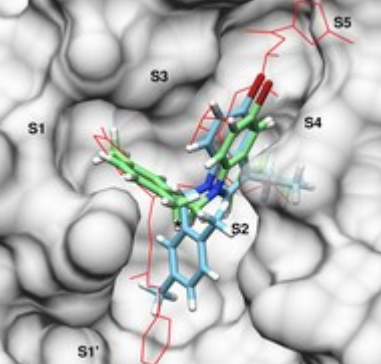
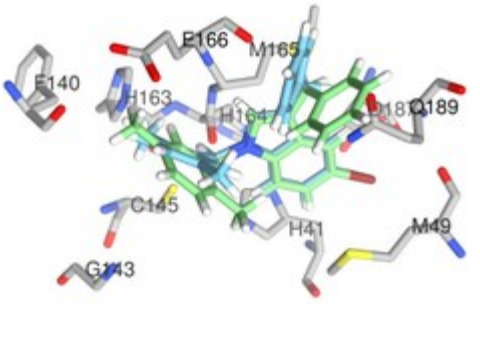
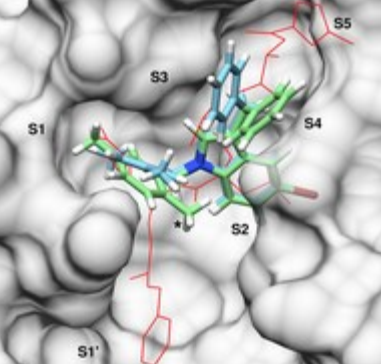
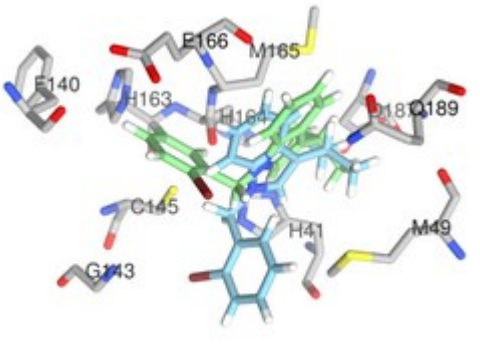
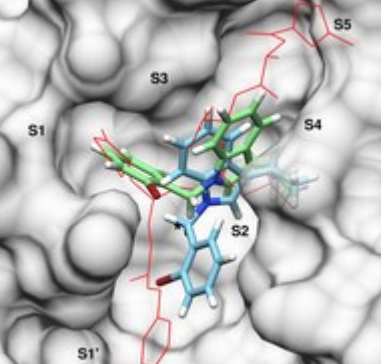
65	-31.7	-11.2		
66	-33.0	-13.0		
67	-27.0	-11.8		
68	-29.9	-11.5		

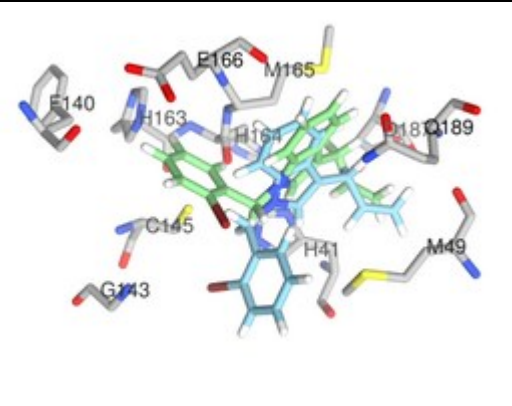
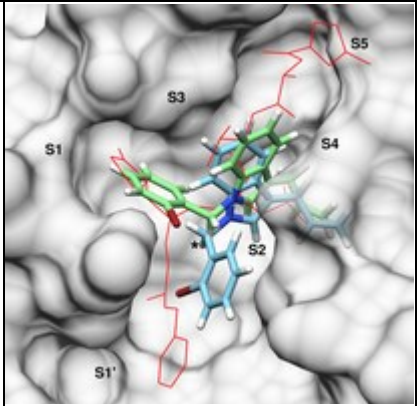
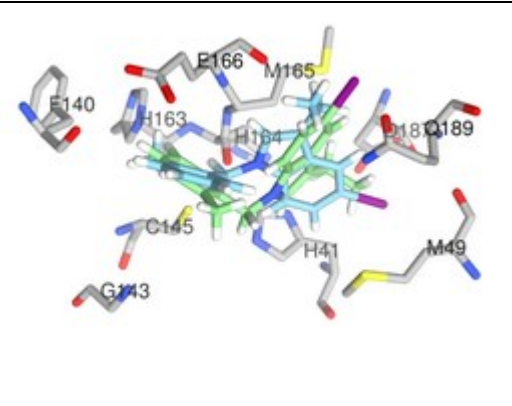
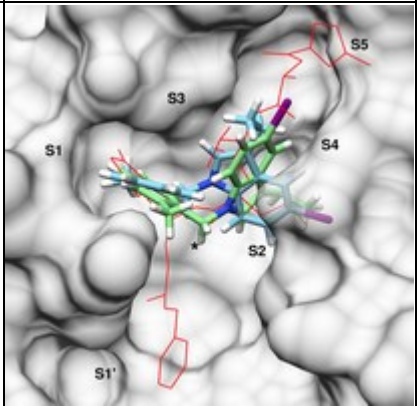
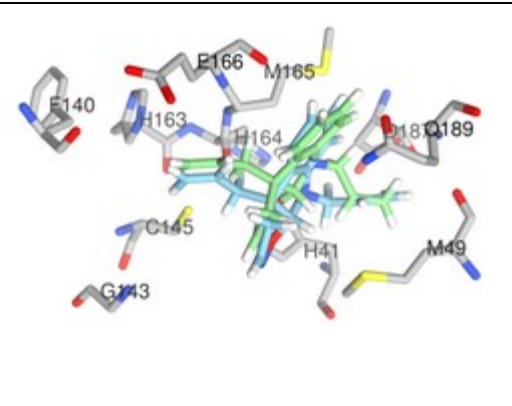
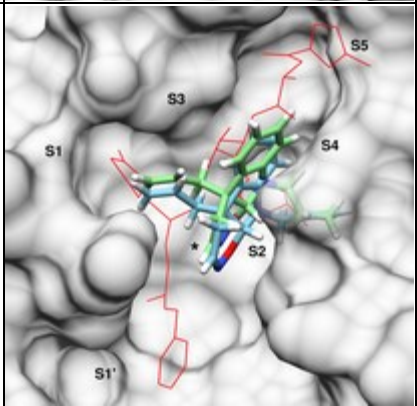
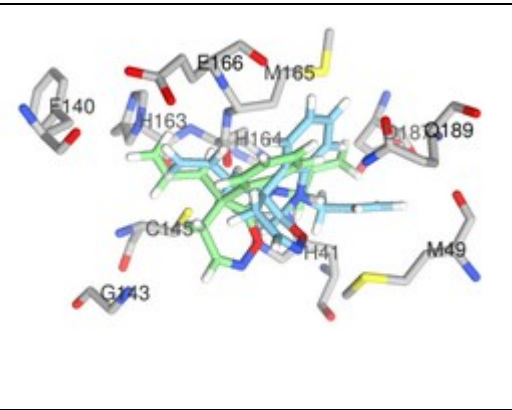
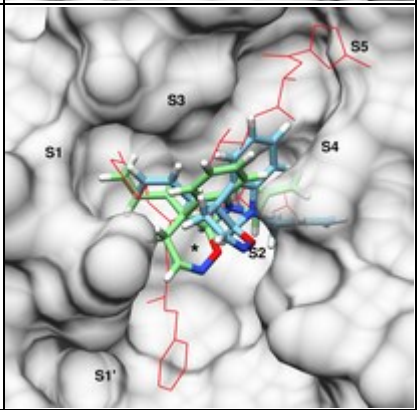
69	-26.4	-8.4		
70	-31.3	-8.7		
71	-30.6	-9.8		
72	-28.5	-9.3		

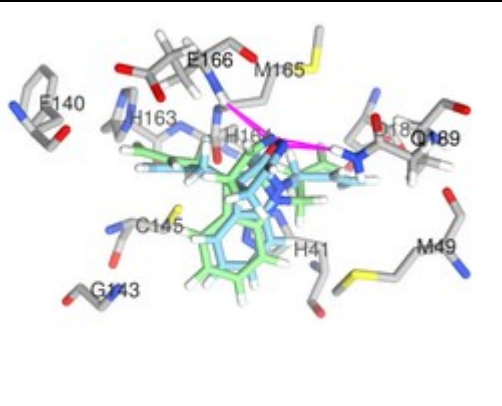
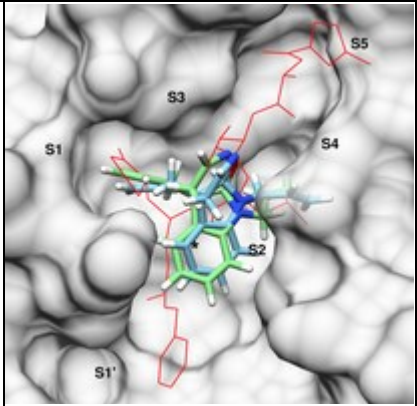
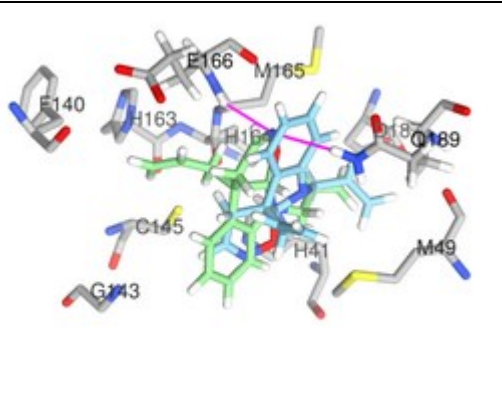
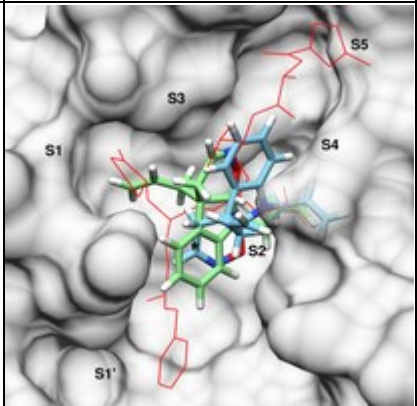
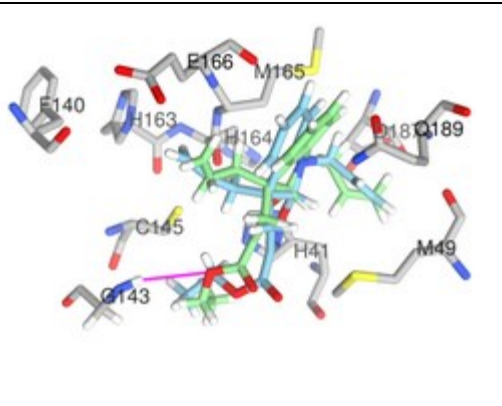
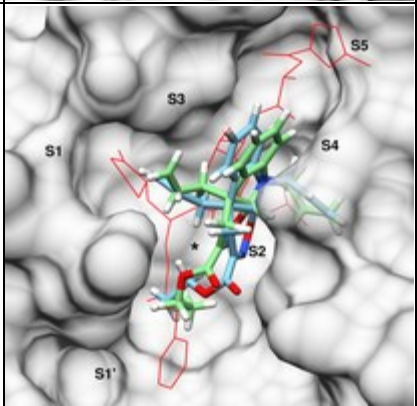
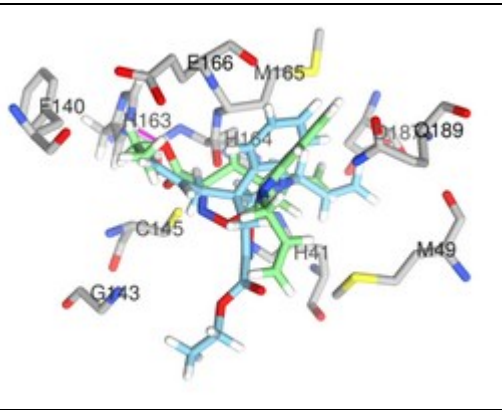
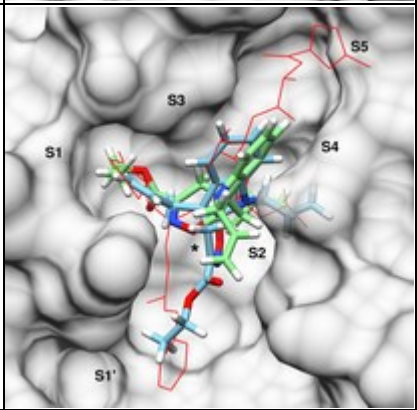
73	-30.6	-8.6		
74	-25.9	-8.8		
75	-28.8	-9.6		
76	-34.7	-10.0		

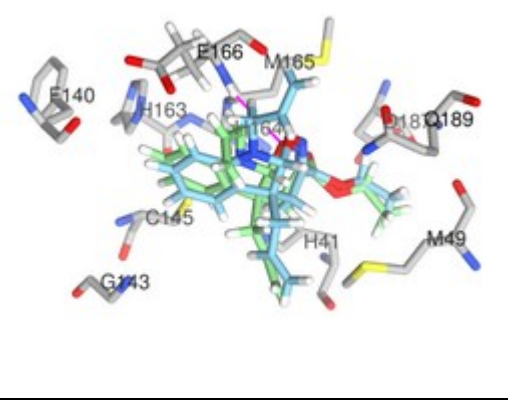
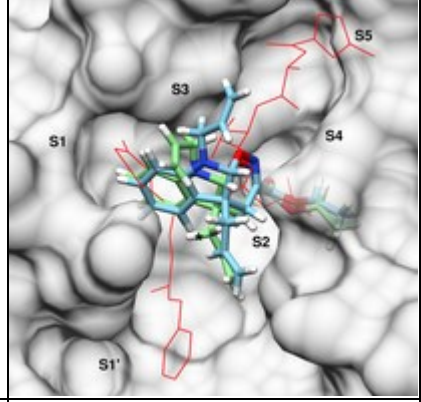
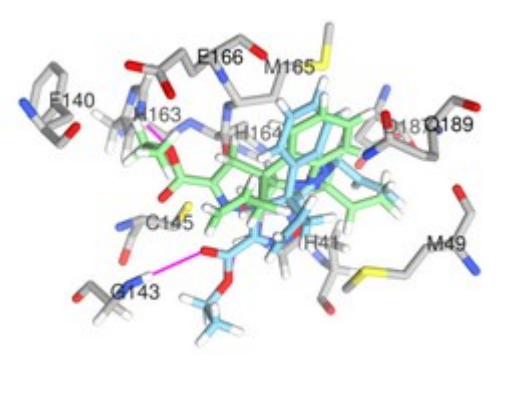
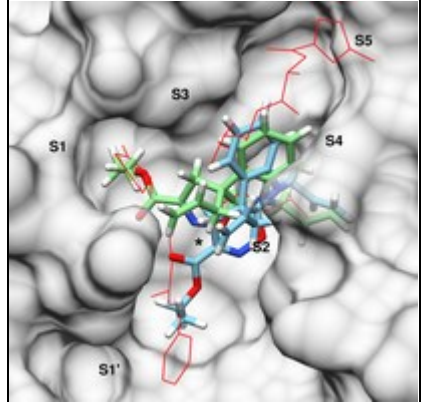
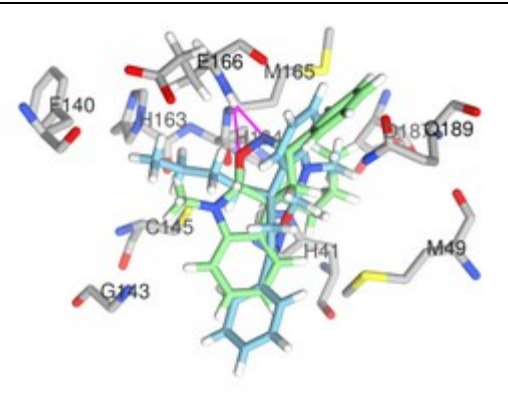
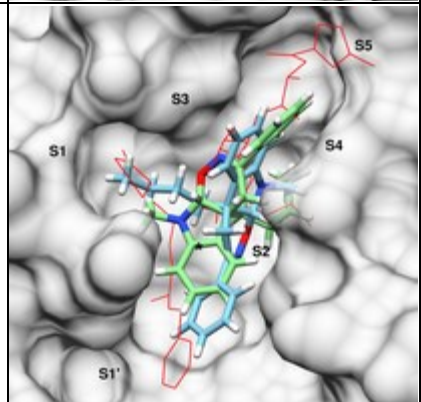
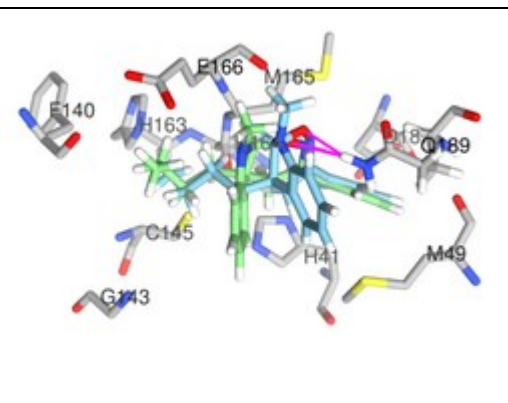
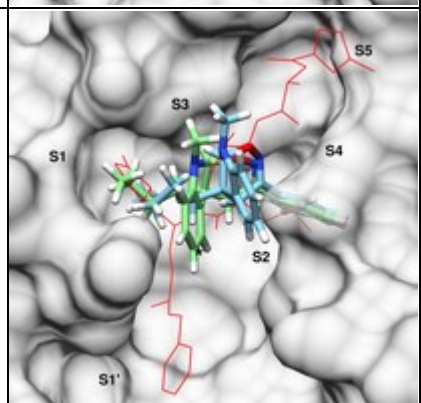
77	-30.8	-10.9		
78	-32.8	-10.4		
79	-28.1	-7.3		
80	-28.9	-8.5		

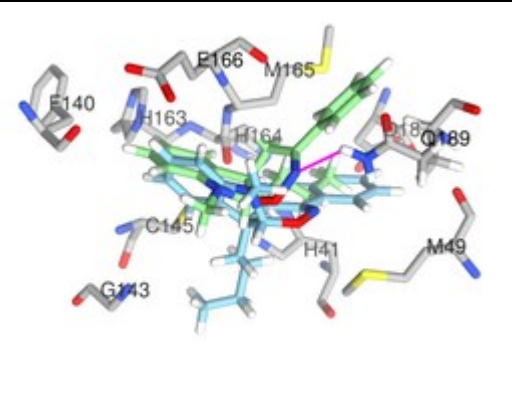
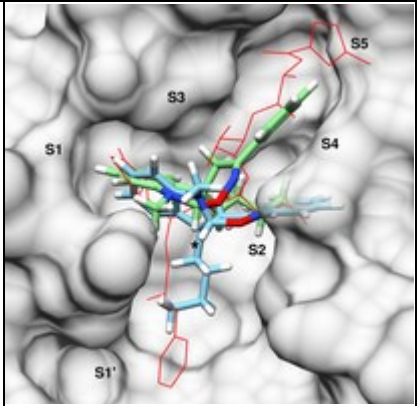
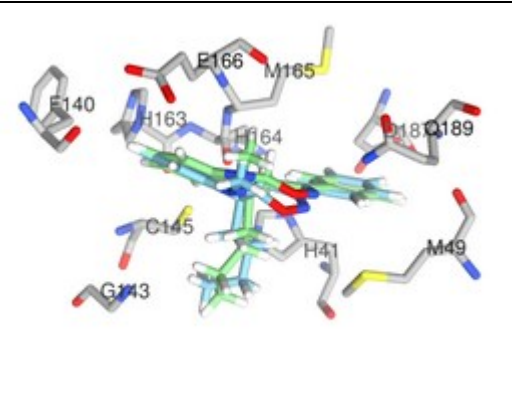
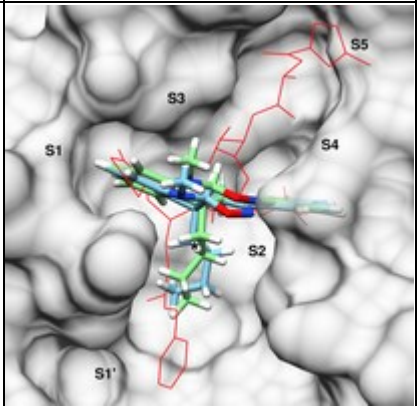
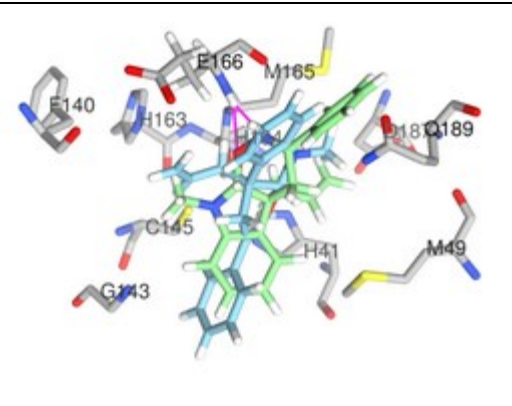
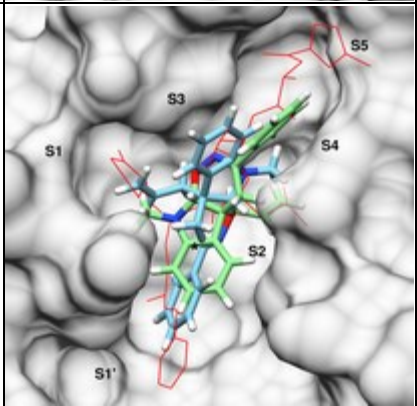
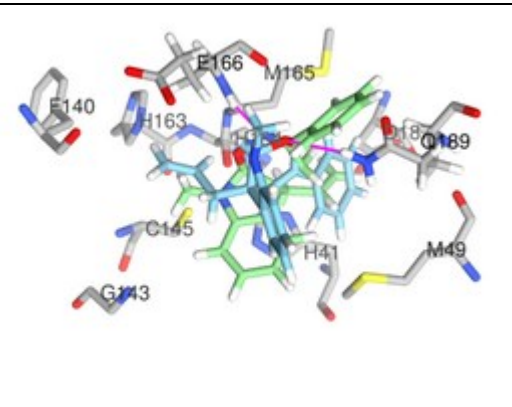
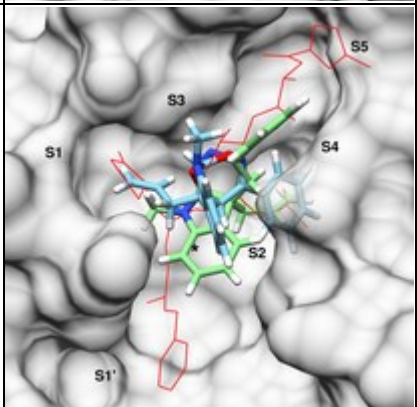
81	-33.3	-8.2		
82	-33.5	-8.5		
83	-33.9	-9.0		
84	-37.3	-12.9		

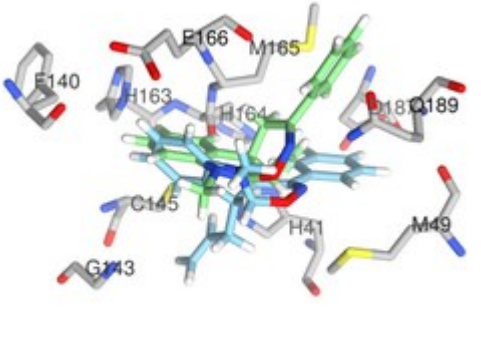
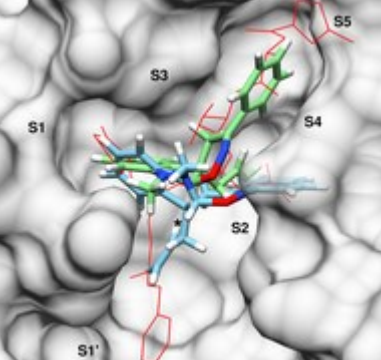
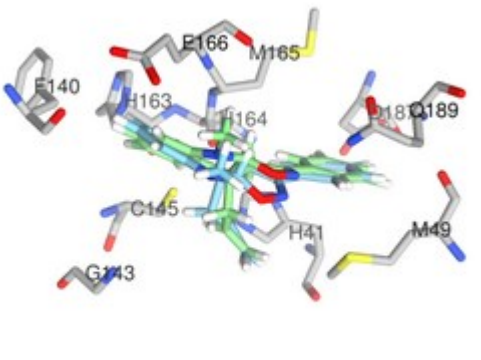
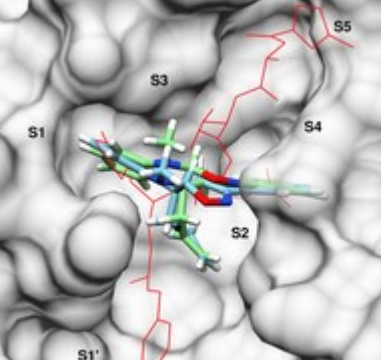
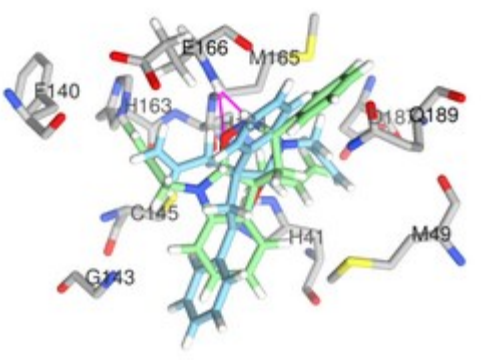
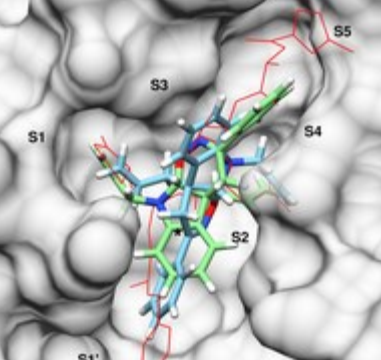
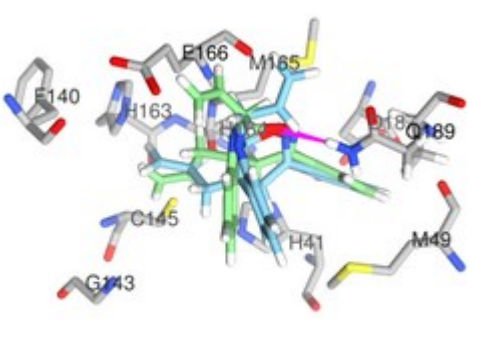
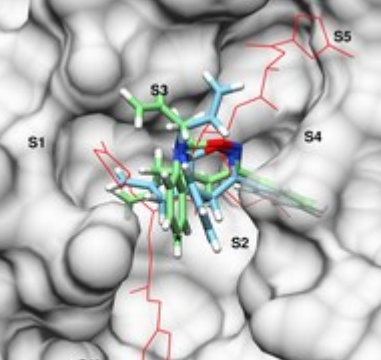
85	-33.2	-8.4		
86	-35.0	-8.6		
87	-38.0	-11.9		
88	-33.5	-9.1		

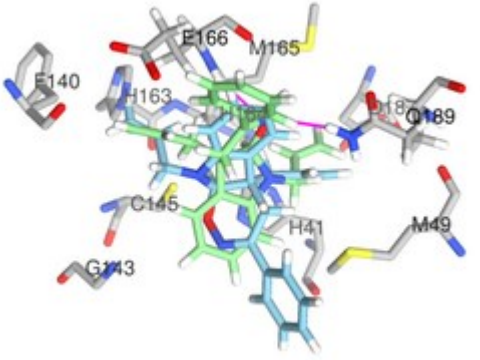
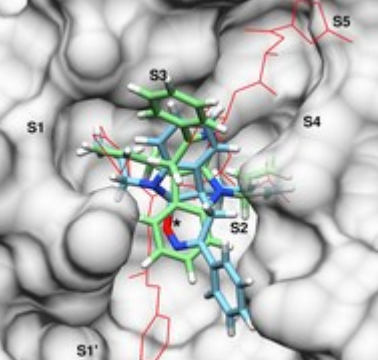
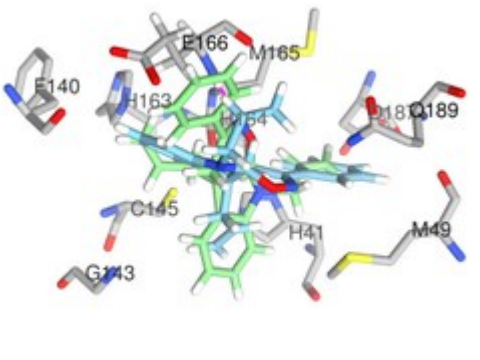
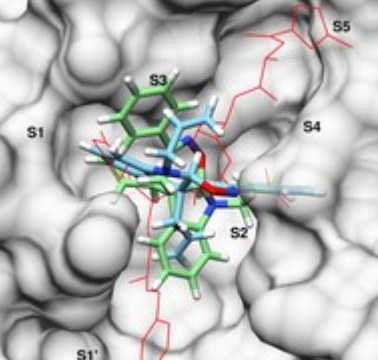
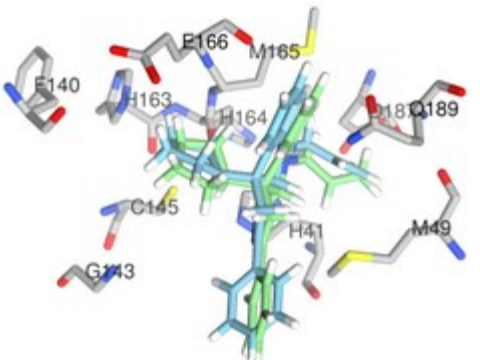
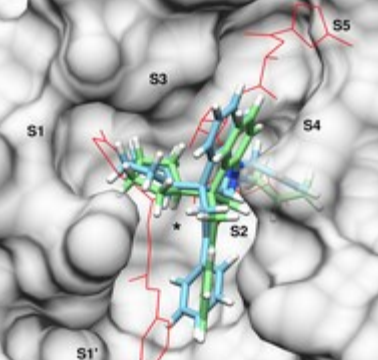
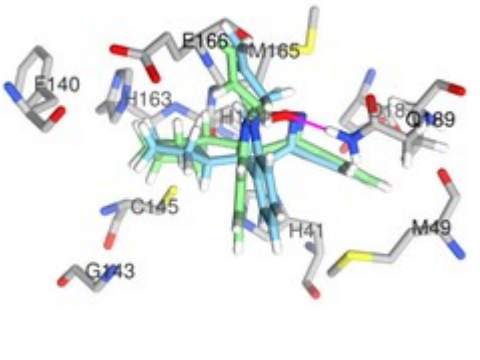
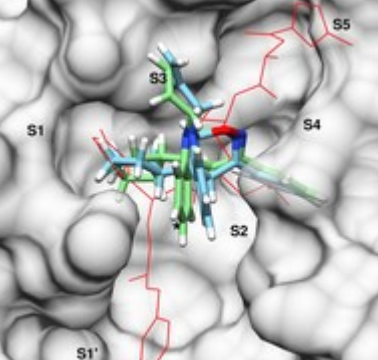
89	-33.6	-8.9		
90	-34.7	-9.4		
91_SR	-30.2	-8.4		
91_SS	-26.6	-7.8		

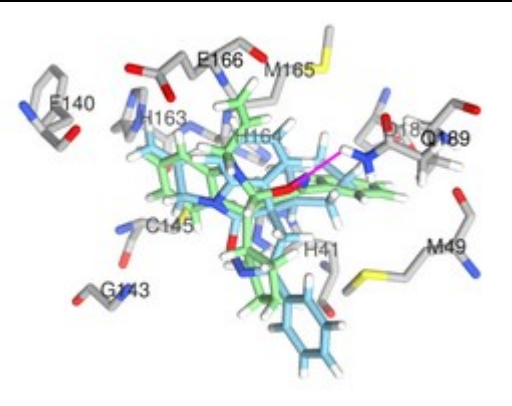
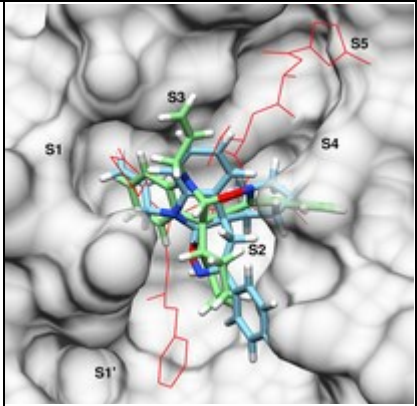
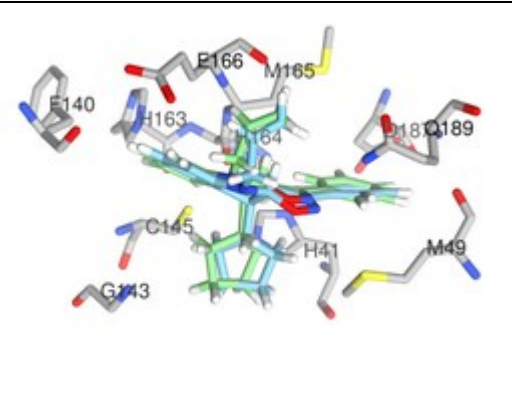
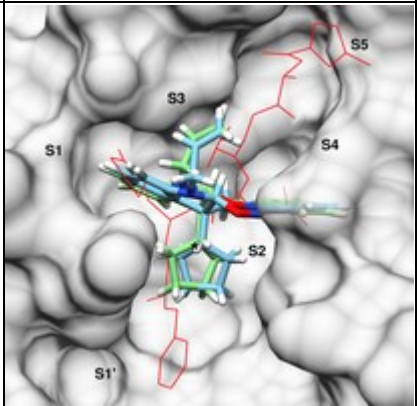
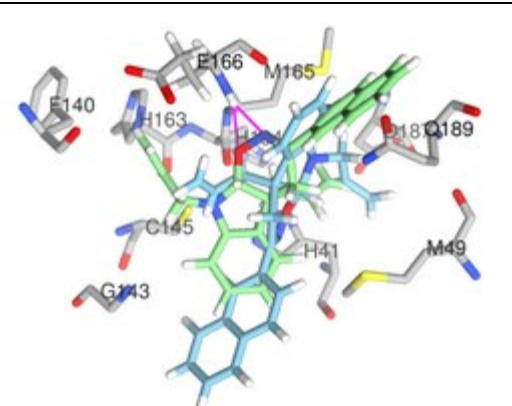
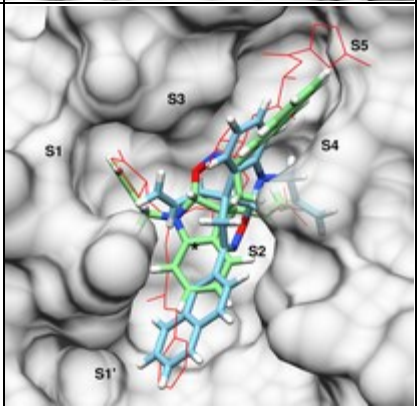
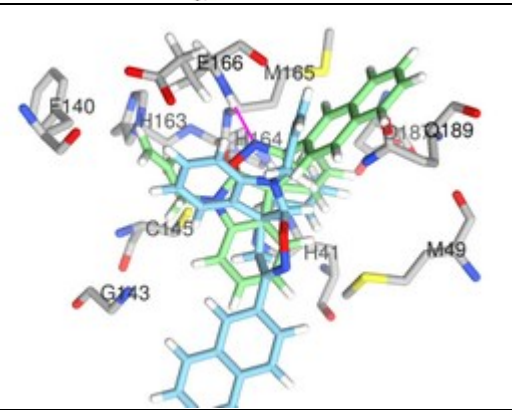
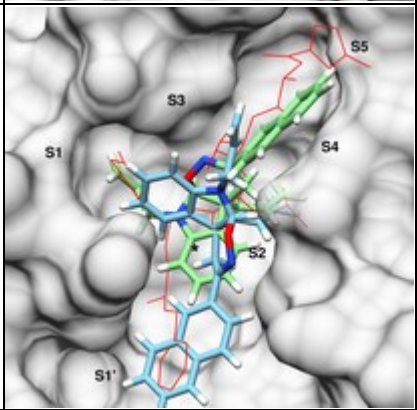
91_RR	-25.7	-9.3		
91_RS	-27.6	-7.5		
92_SR	-31.6	-8.8		
92_SS	-32.8	-8.7		

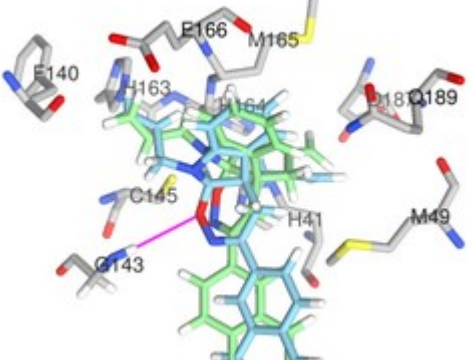
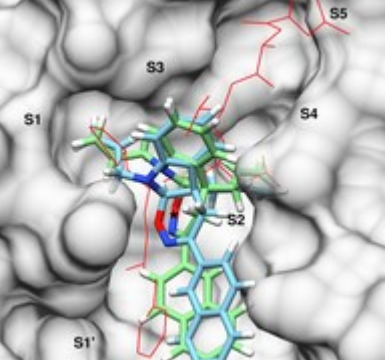
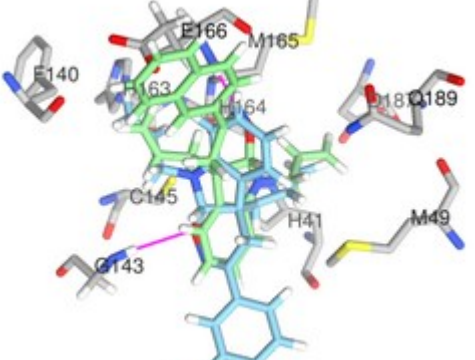
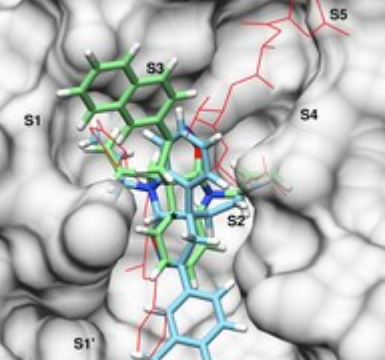
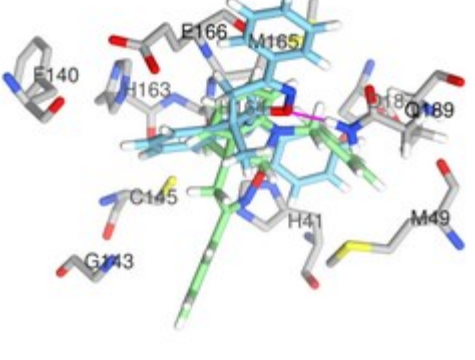
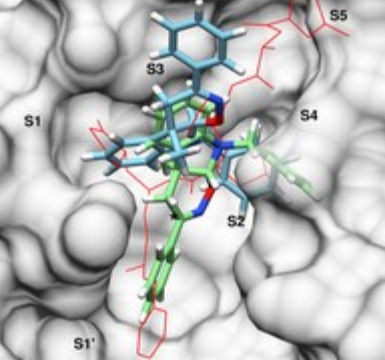
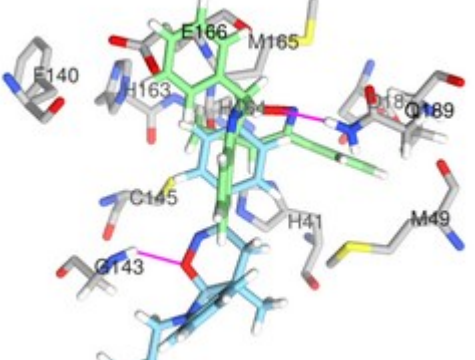
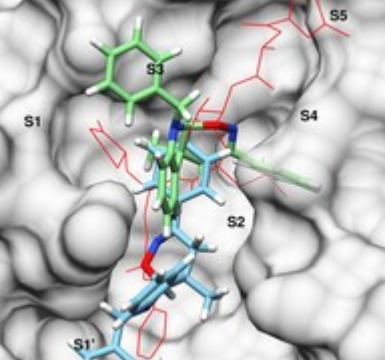
92_RR	-31.2	-8.6		
92_RS	-33.3	-10.3		
93_SR	-31.8	-9.7		
93_SS	-31.8	-11.3		

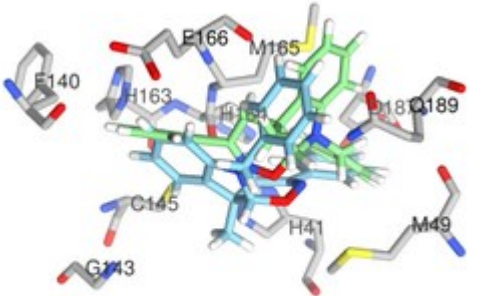
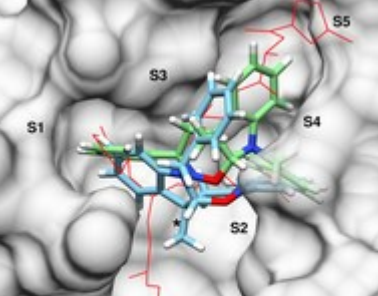
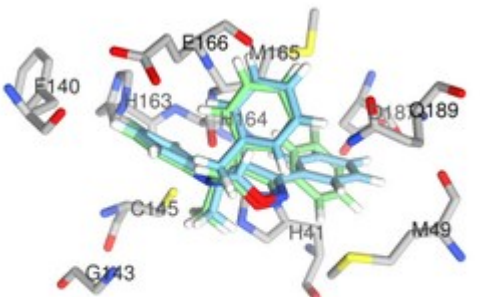
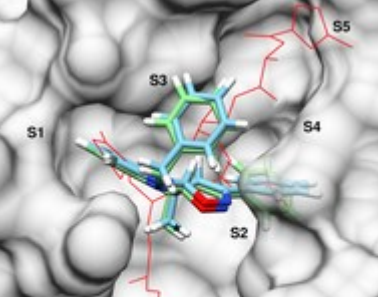
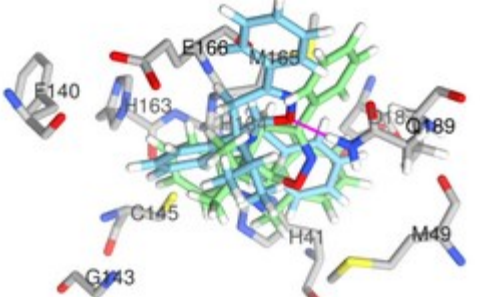
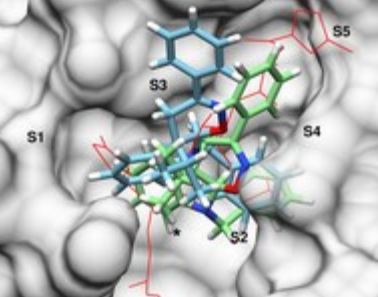
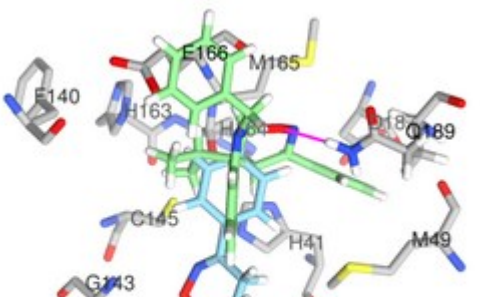
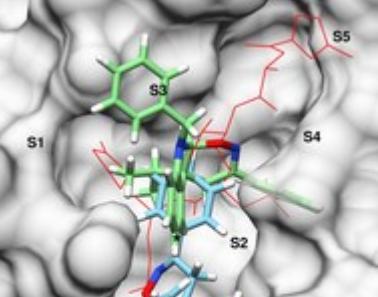
93_RR	-32.8	-9.5		
93_RS	-34.4	-9.3		
94_SR	-27.9	-10.1		
94_SS	-26.2	-9.2		

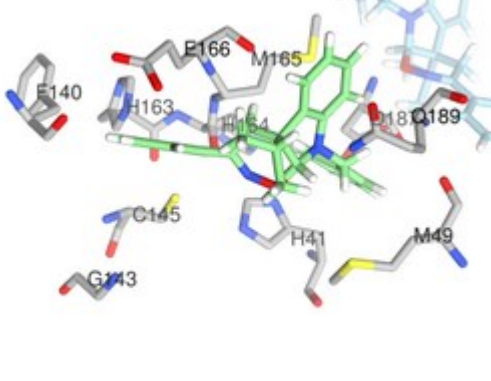
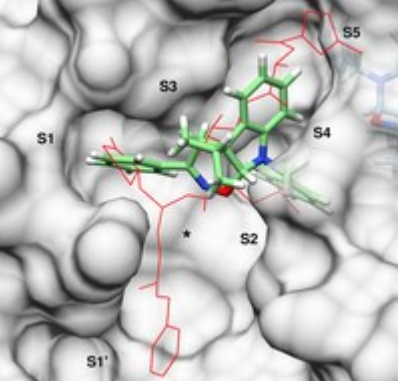
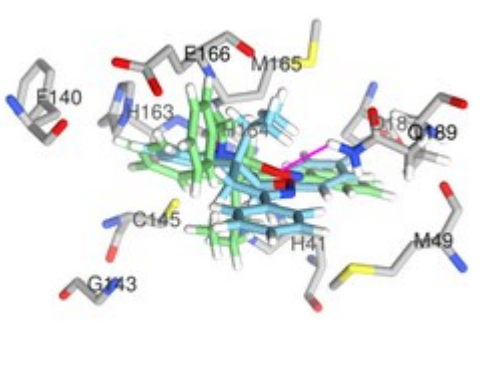
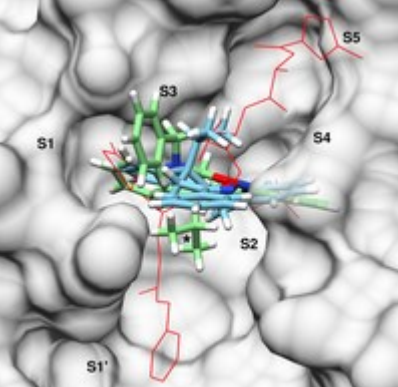
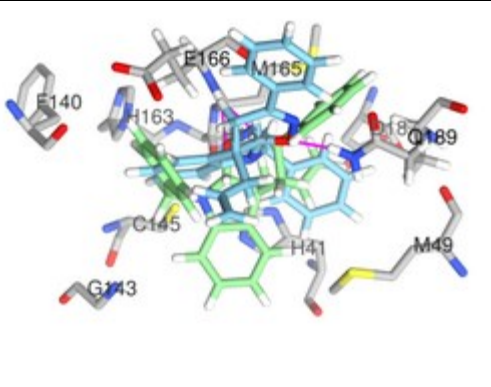
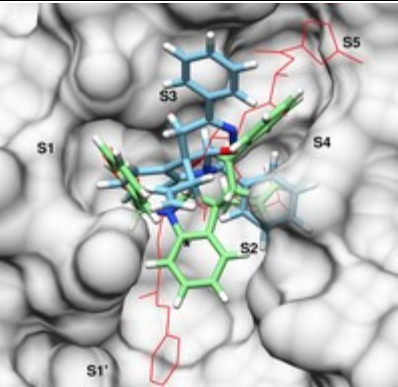
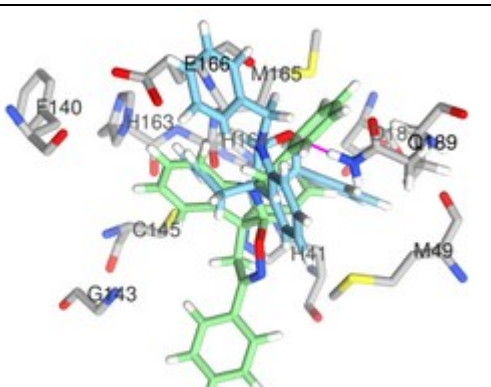
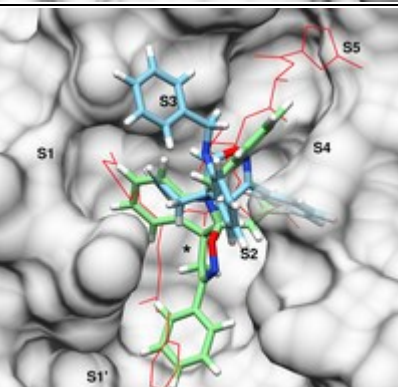
94_RR	-28.6	-9.3		
94_RS	-28.8	-11.1		
95_SR	-32.4	-9.7		
95_SS	-30.4	-9.8		

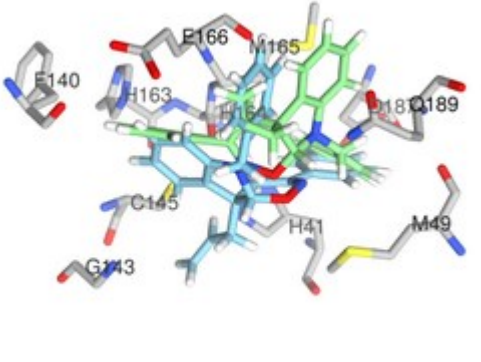
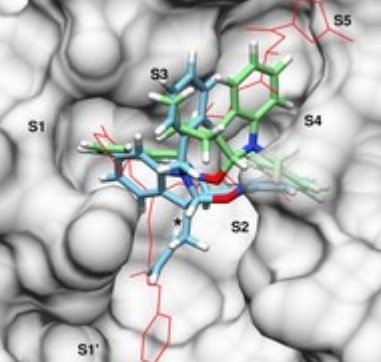
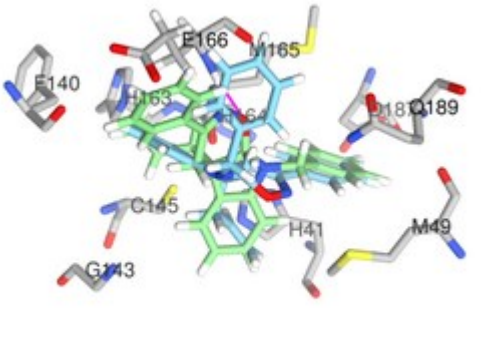
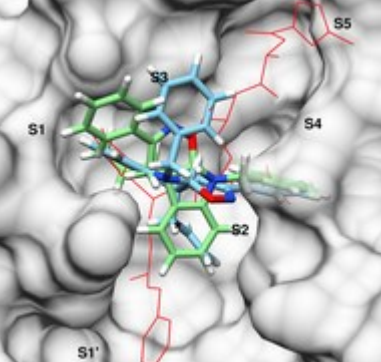
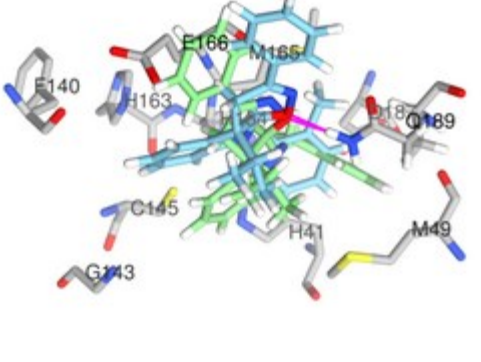
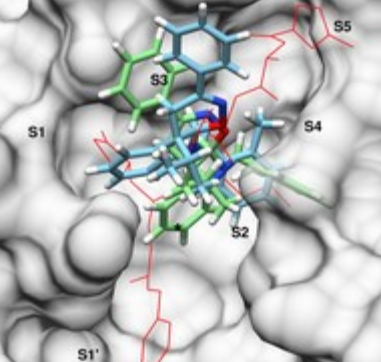
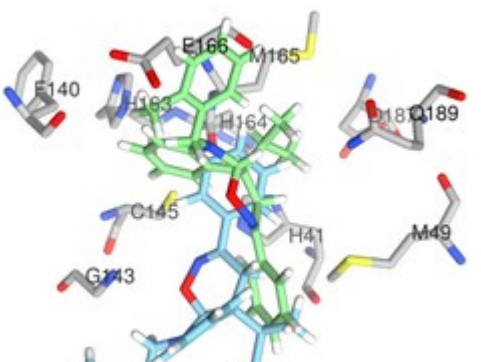
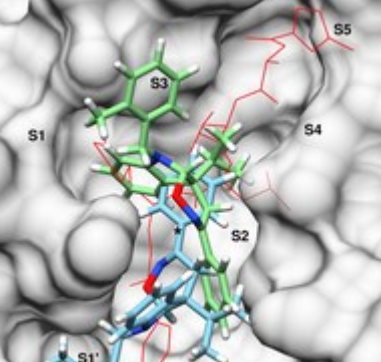
95_RR	-30.6	-9.1		
95_RS	-31.2	-9.0		
96_RR	-34.0	-9.7		
96_RS	-33.6	-10.5		

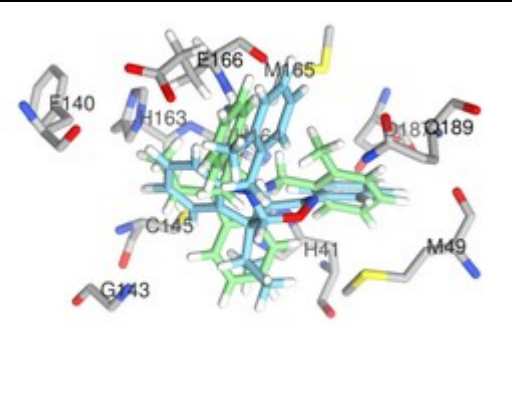
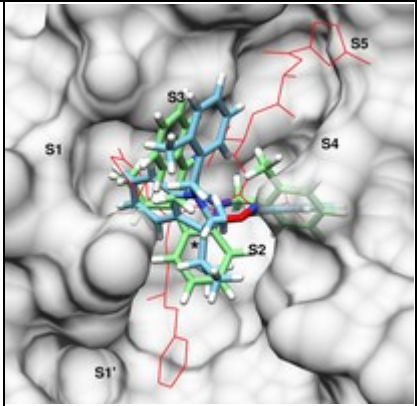
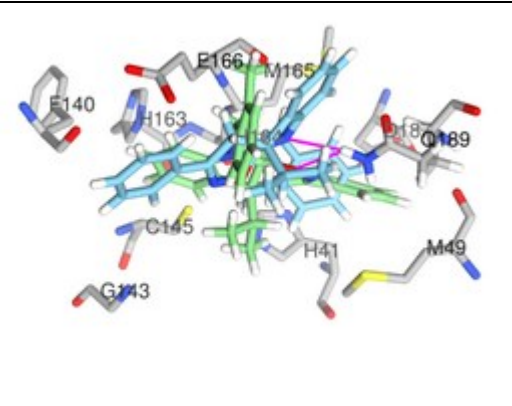
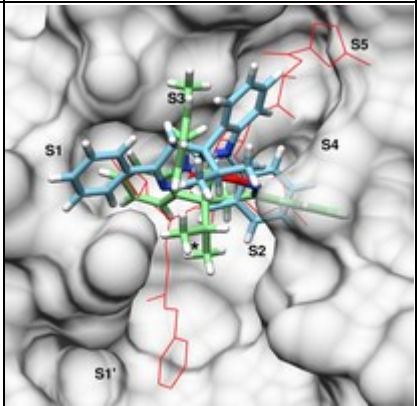
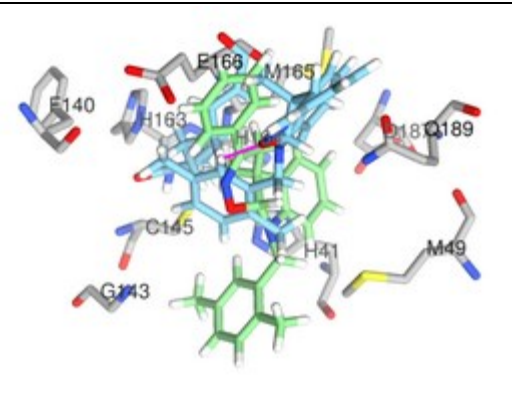
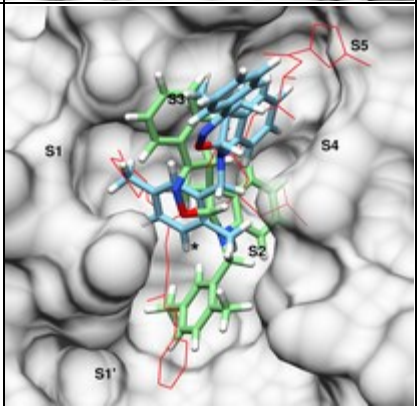
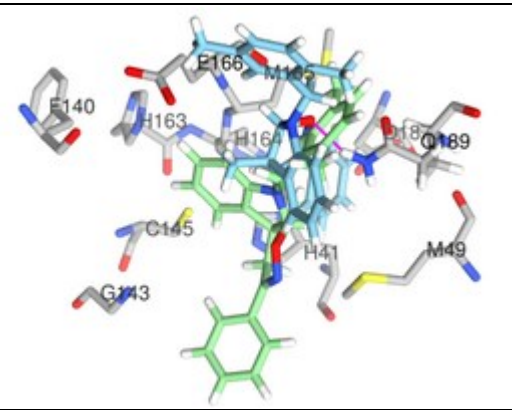
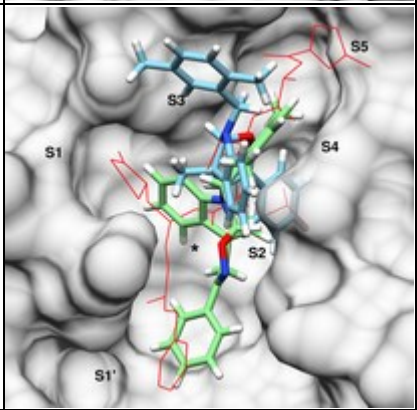
96_SR	-30.2	-10.4		
96_SS	-29.4	-10.8		
97_SR	-37.4	-10.5		
97_SS	-32.9	-9.8		

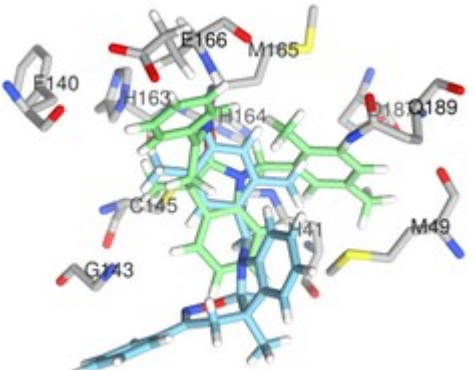
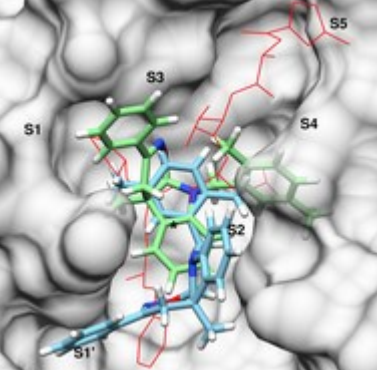
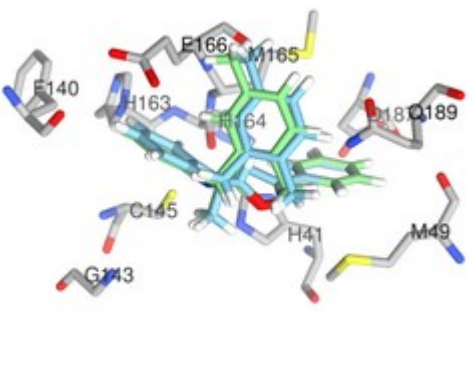
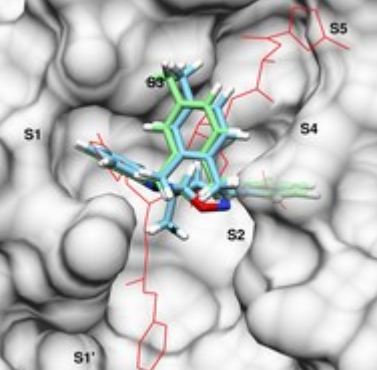
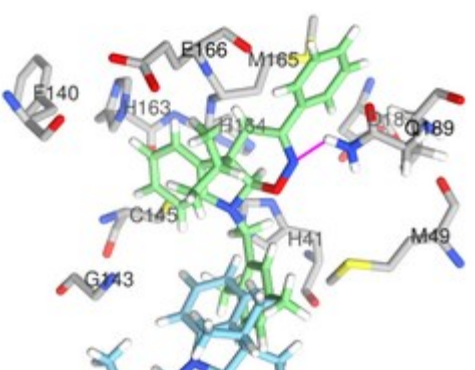
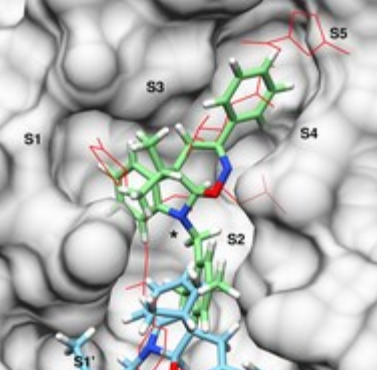
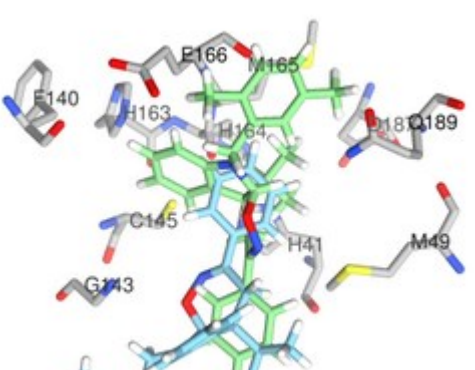
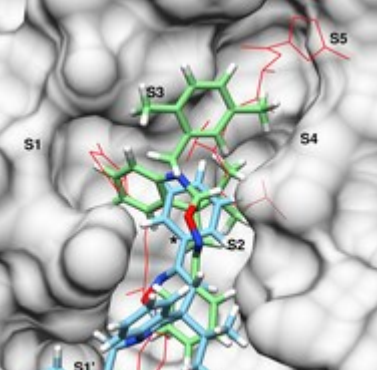
97_RR	-34.0	-10.0		
97_RS	-35.5	-9.7		
98_SR	-29.4	-10.7		
98_SS	-31.2	-11.0		

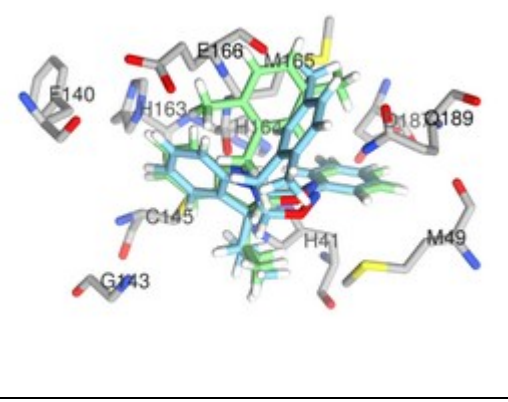
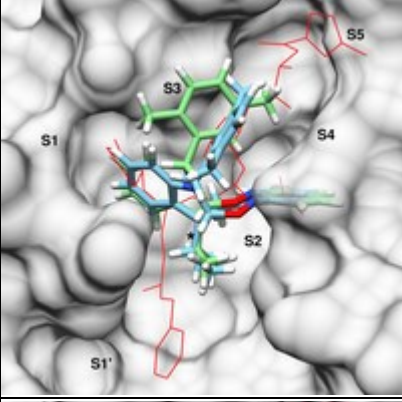
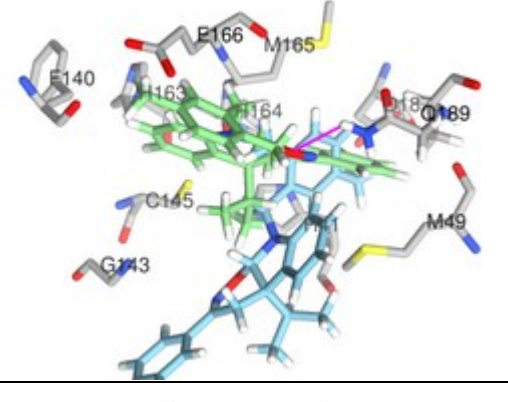
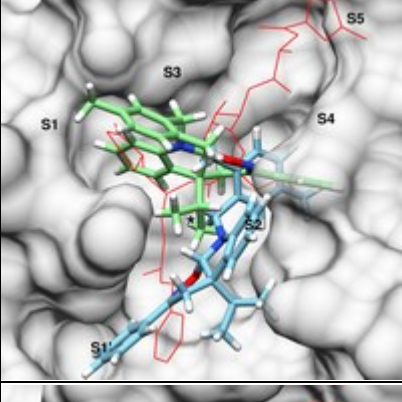
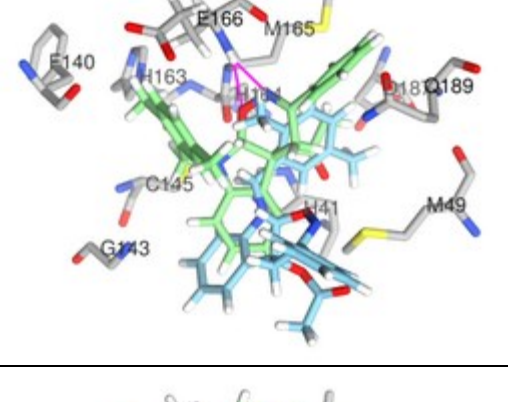
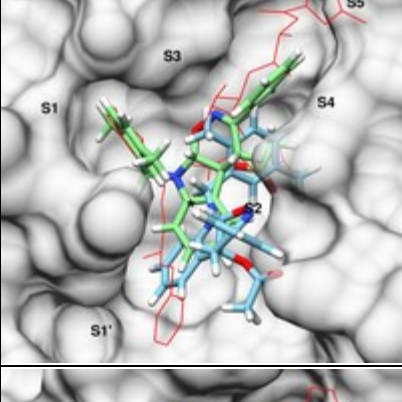
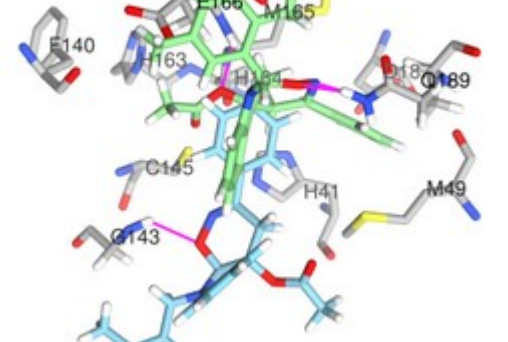
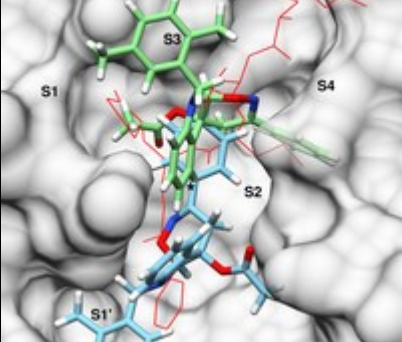
98_RR	-29.4	-12.8		
98_RS	-30.0	-10.7		
99_RR	-30.2	-12.2		
99_RS	-32.5	-11.3		

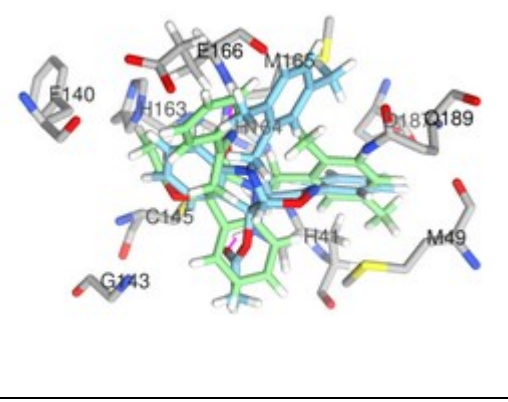
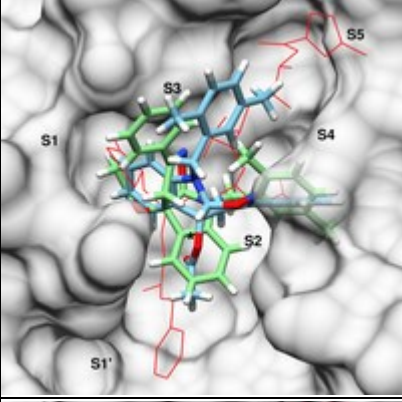
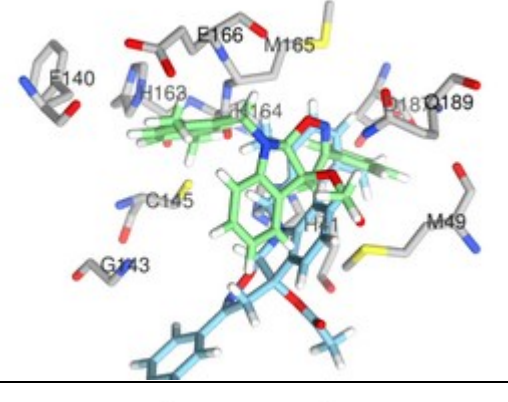
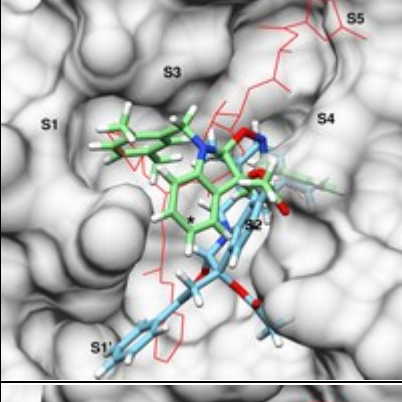
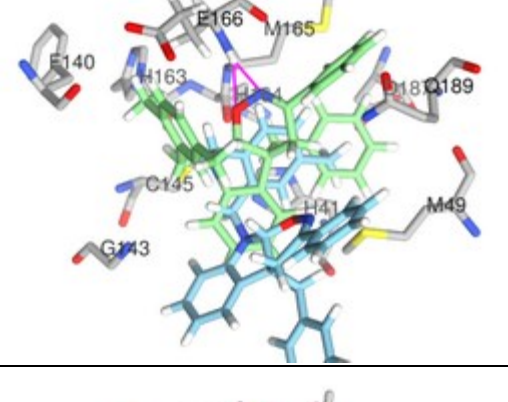
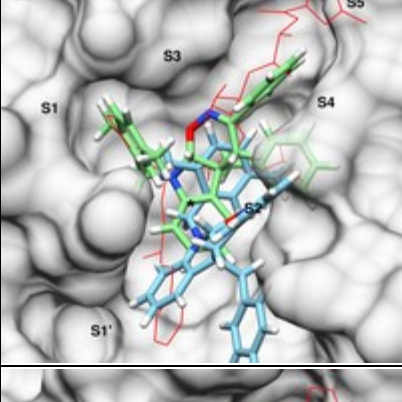
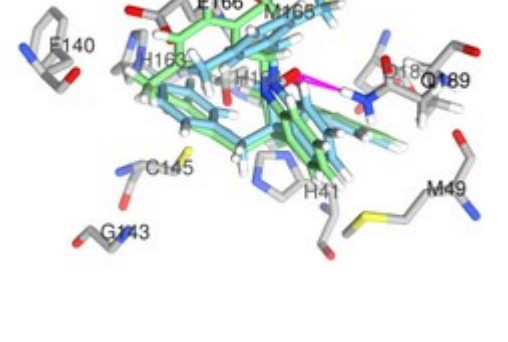
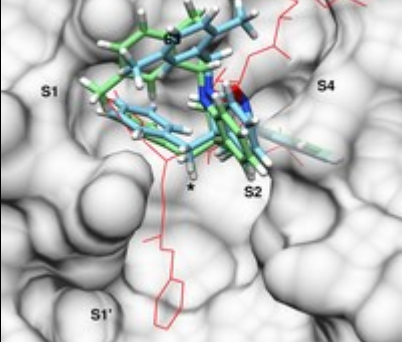
99_SR	-26.5	-13.4		
99_SS	-29.6	-11.4		
100_SR	-30.2	-11.6		
100_SS	-31.5	-9.8		

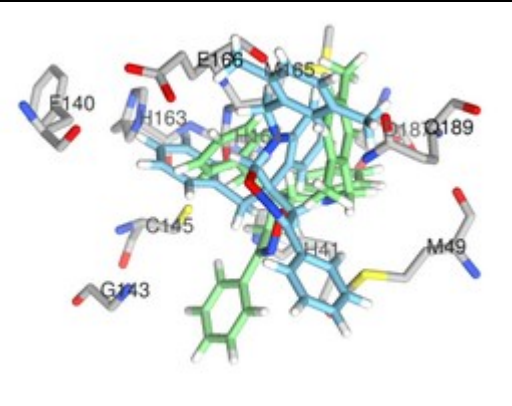
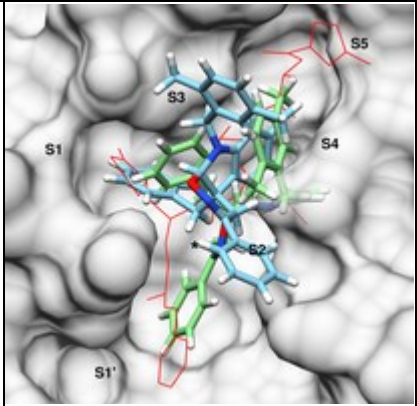
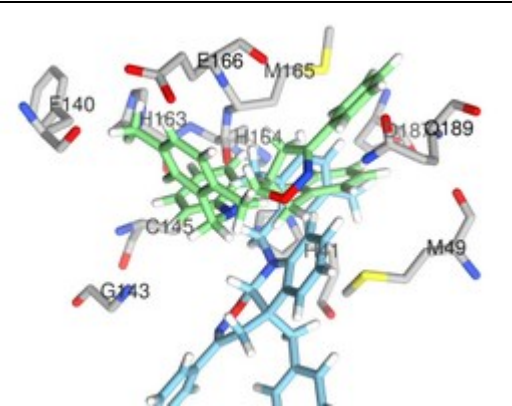
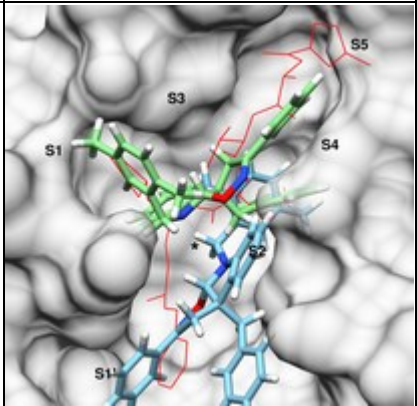
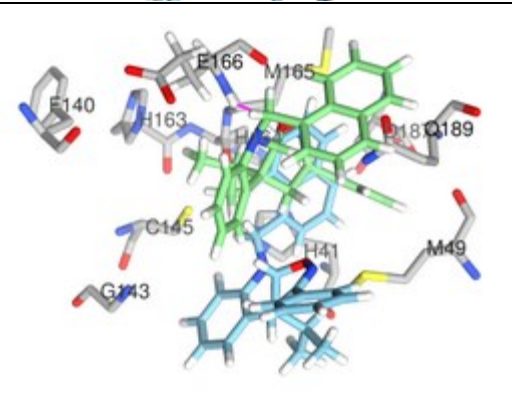
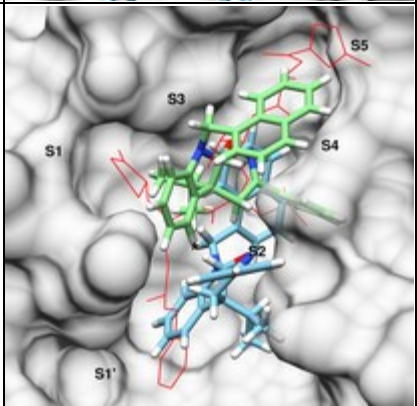
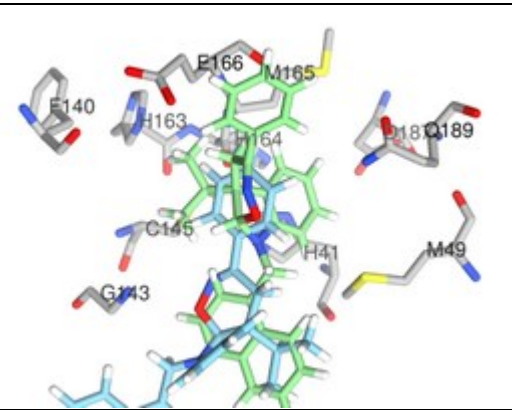
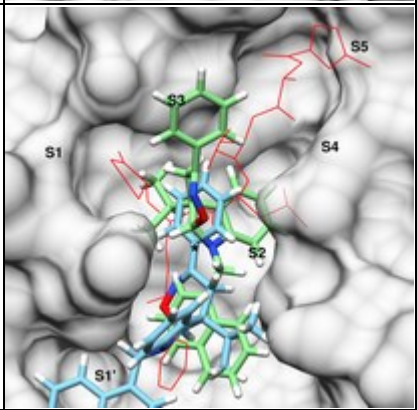
100_RR	-31.8	-12.3		
100_RS	-31.1	-9.8		
101_RR	-29.6	-11.0		
101_RS	-33.0	-10.2		

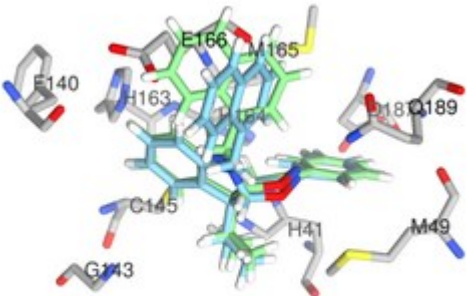
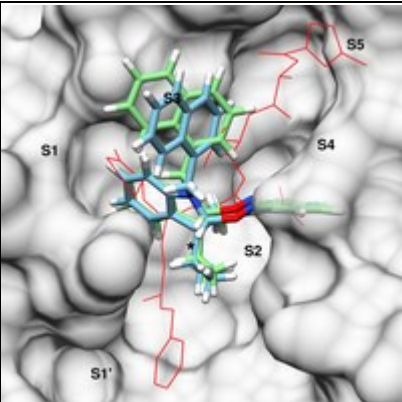
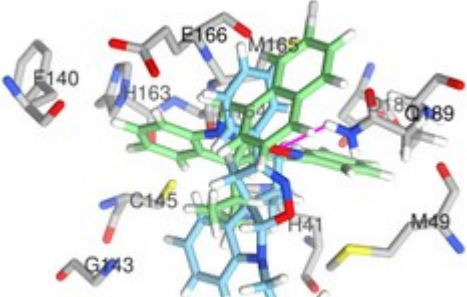
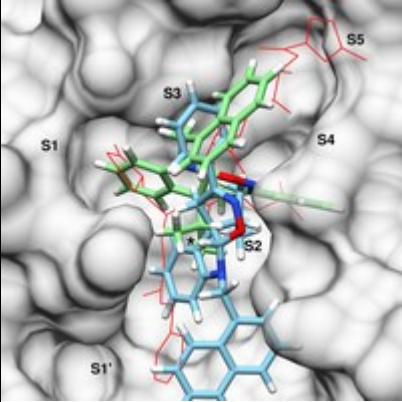
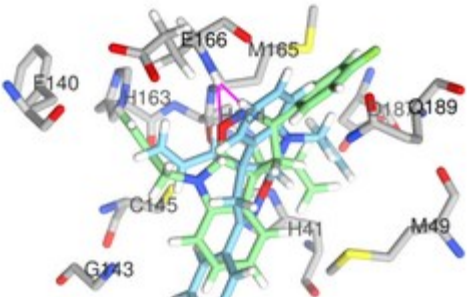
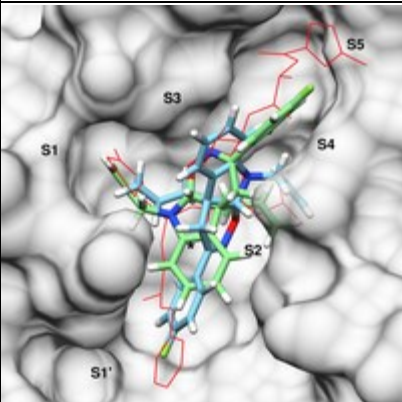
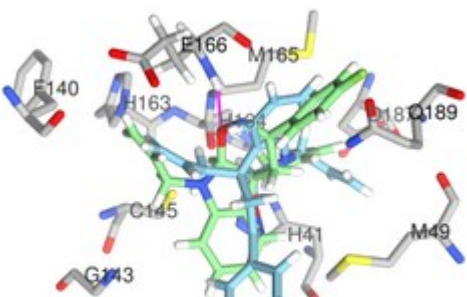
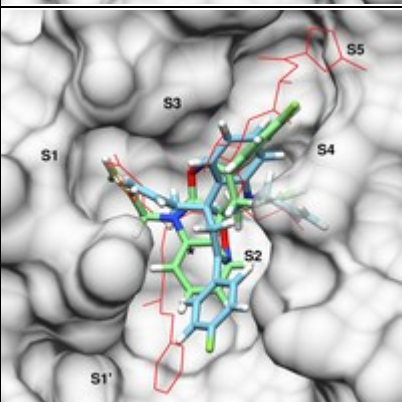
101_SR	-33.2	-11.1		
101_SS	-25.9	-10.8		
102_SR	-25.7	-9.7		
102_SS	-31.7	-10.7		

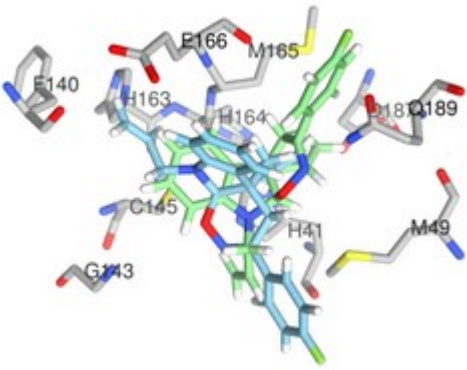
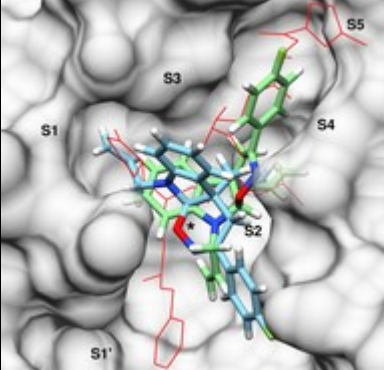
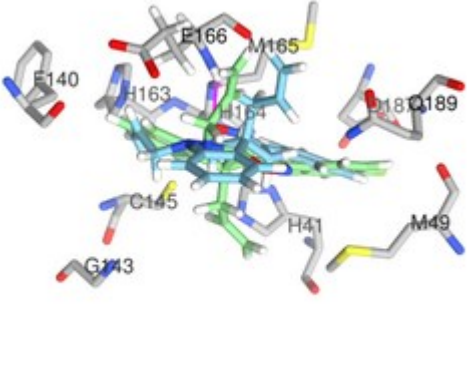
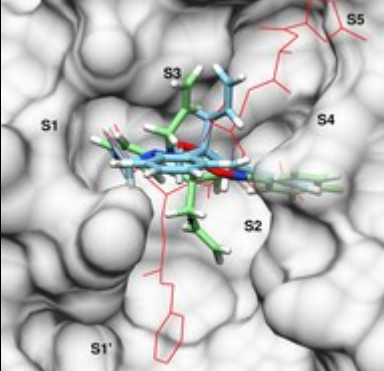
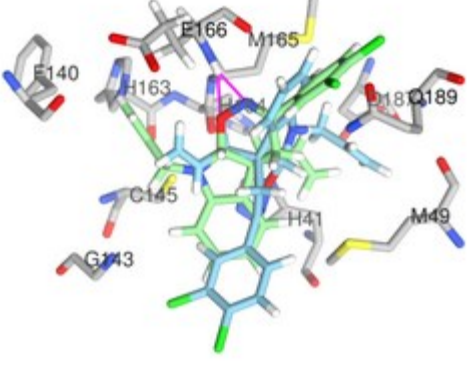
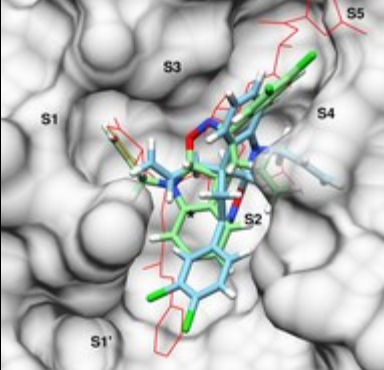
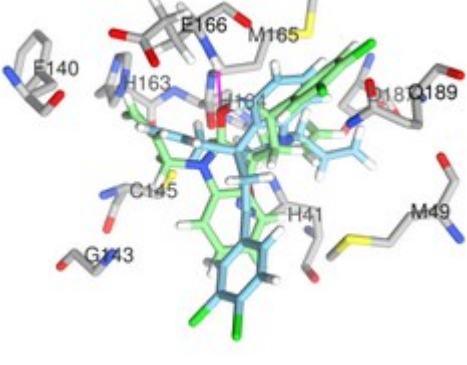
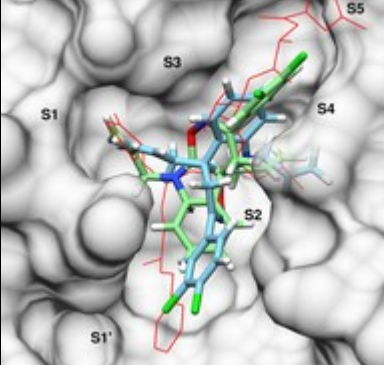
102_RR	-28.6	-12.5		
102_RS	-31.0	-11.5		
103_RR	-26.0	-11.0		
103_RS	-32.3	-10.4		

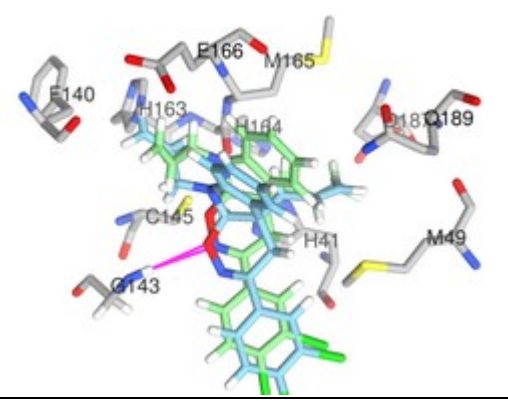
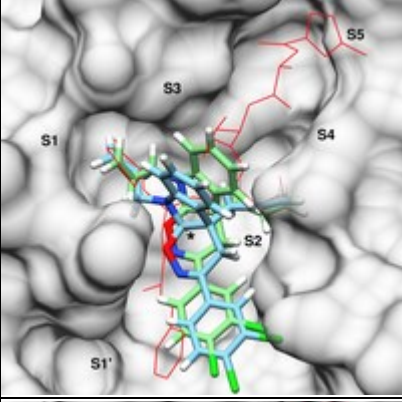
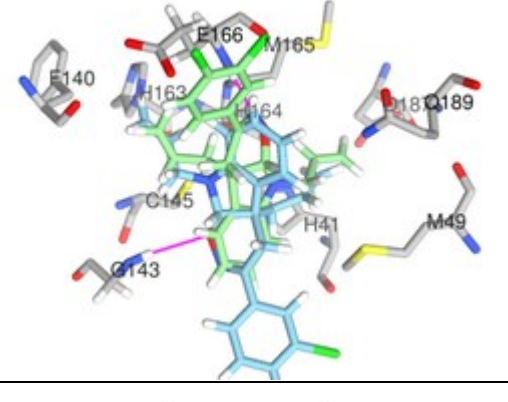
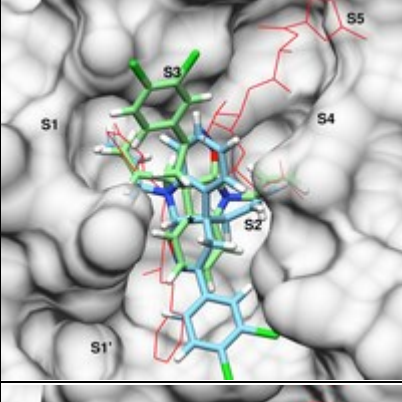
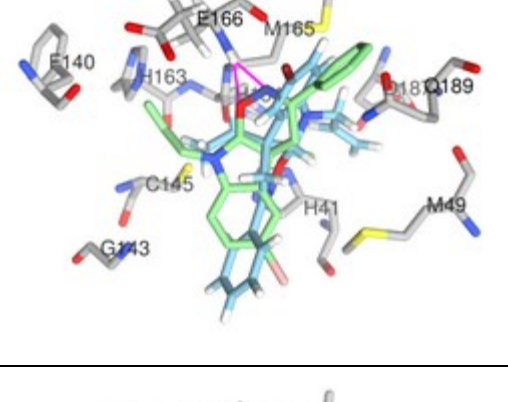
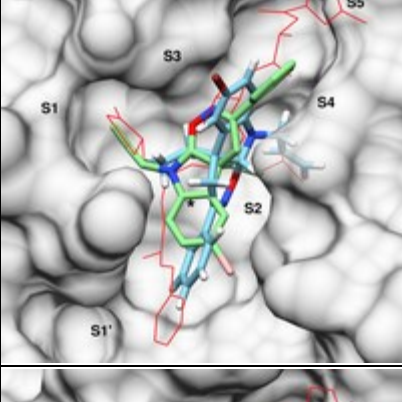
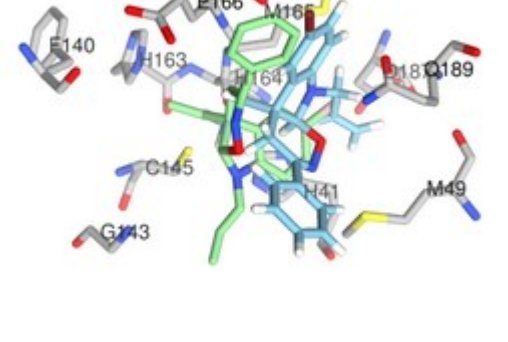
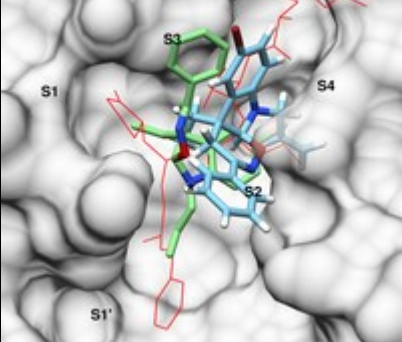
103_SR	-34.0	-11.1		
103_SS	-32.6	-11.7		
104_RR	-31.5	-12.3		
104_RS	-35.9	-12.1		

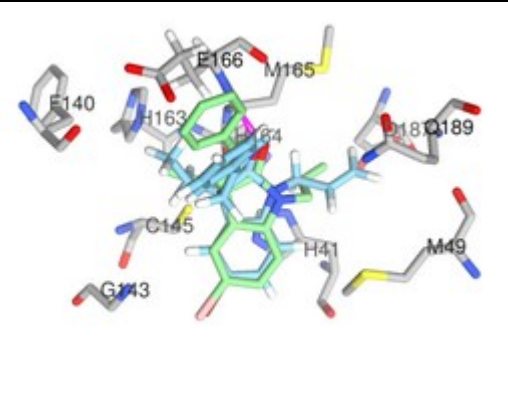
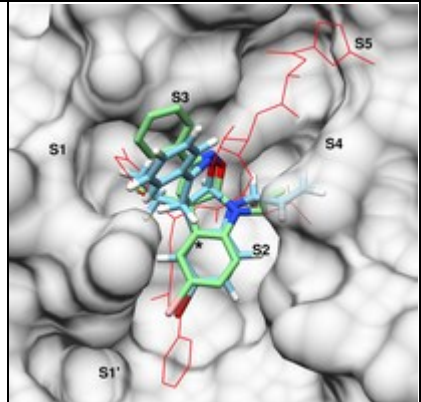
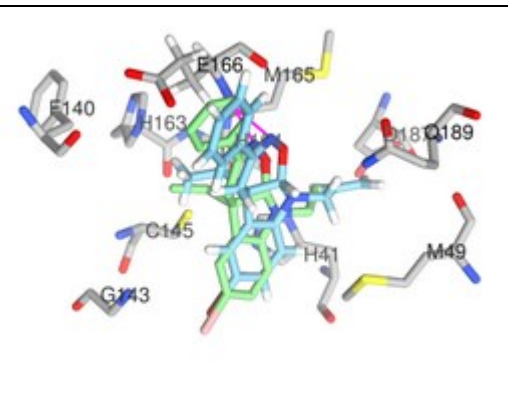
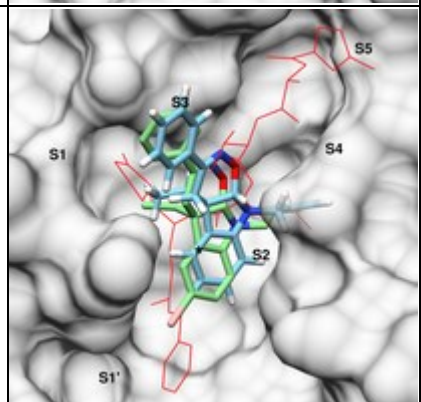
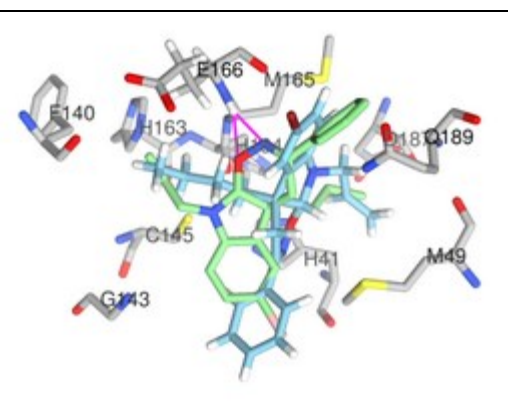
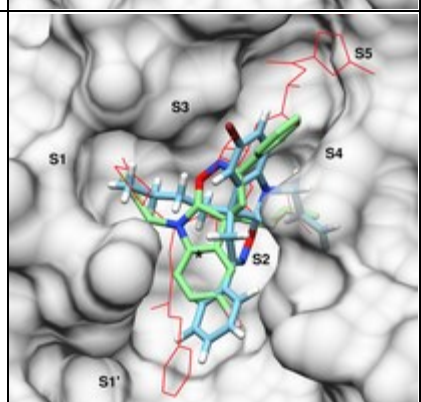
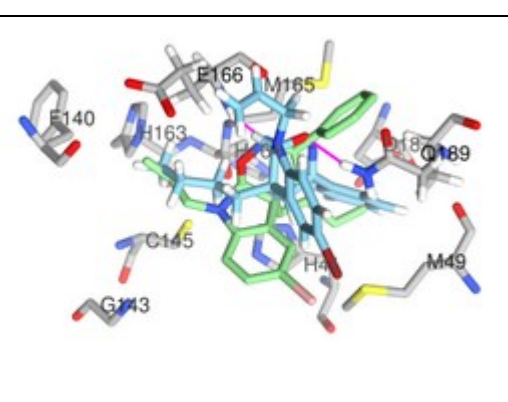
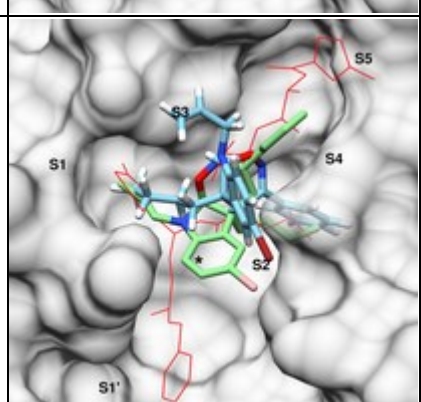
104_SR	-33.6	-12.7		
104_SS	-35.5	-11.0		
105_SR	-32.4	-13.1		
105_SS	-33.1	-11.8		

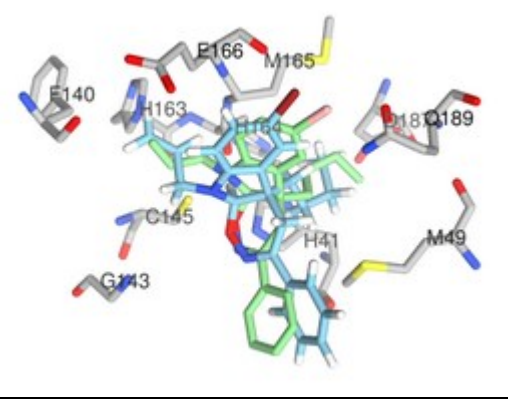
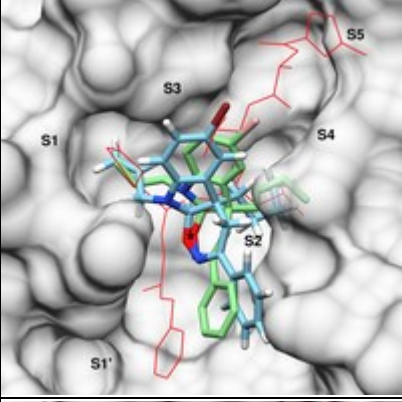
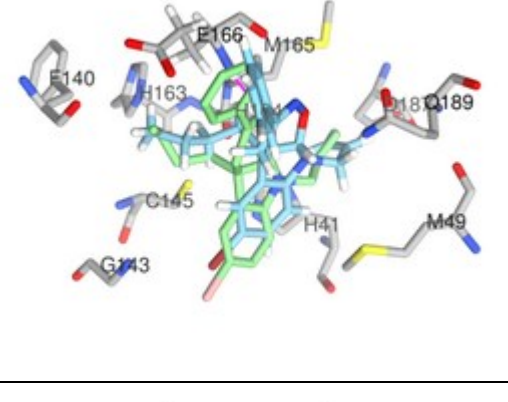
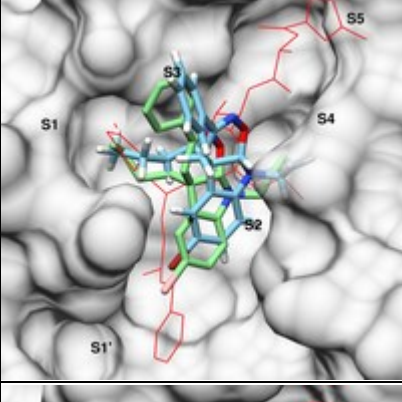
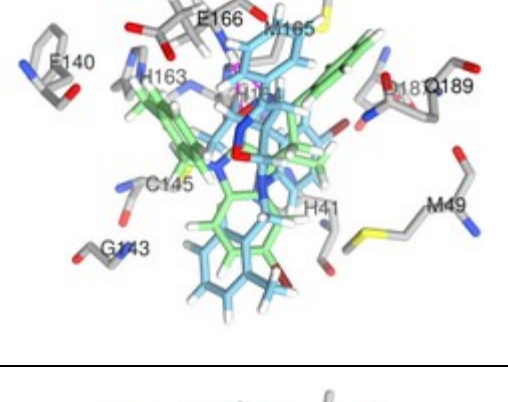
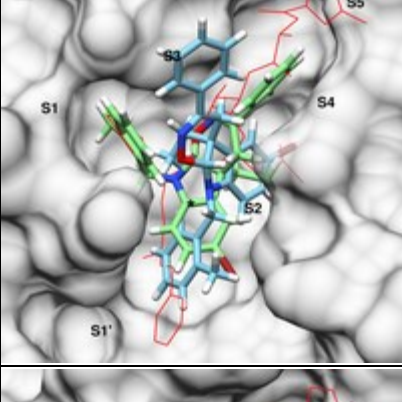
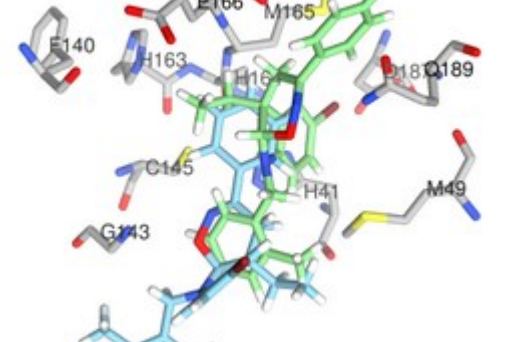
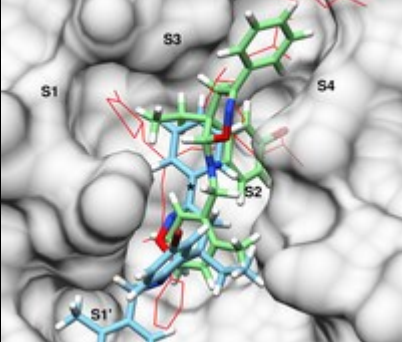
105_RR	-30.2	-12.8		
105_RS	-36.2	-12.3		
106_RR	-30.2	-11.7		
106_RS	-34.3	-10.6		

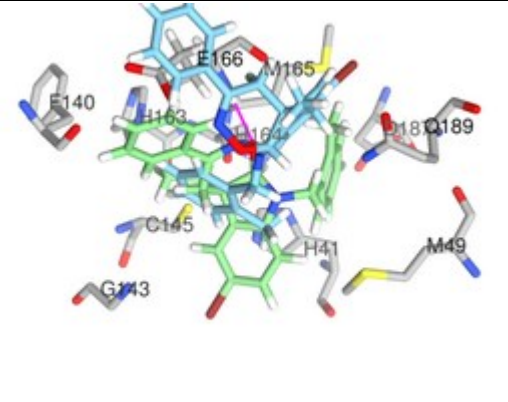
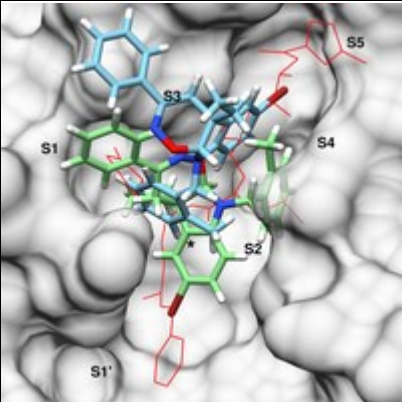
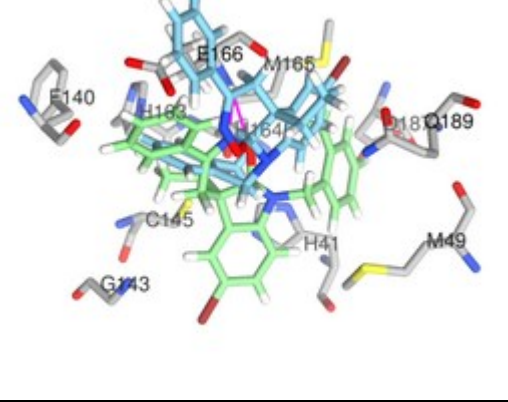
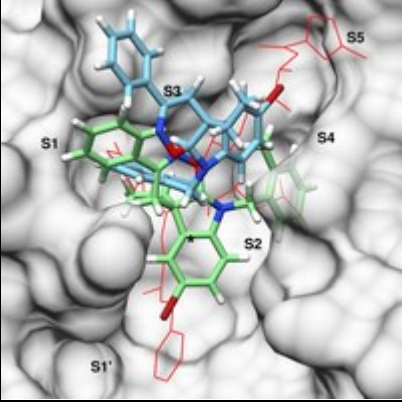
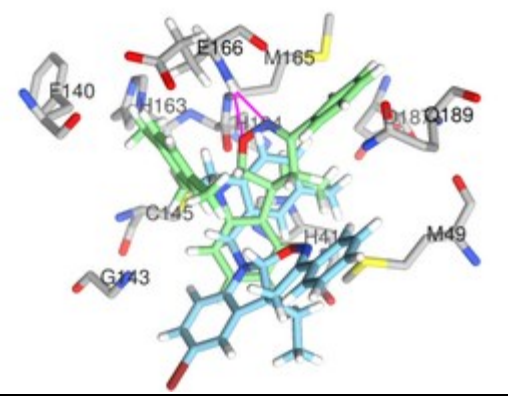
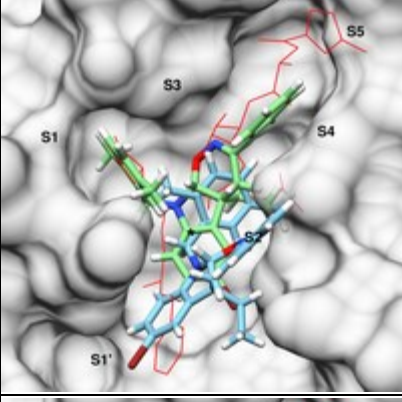
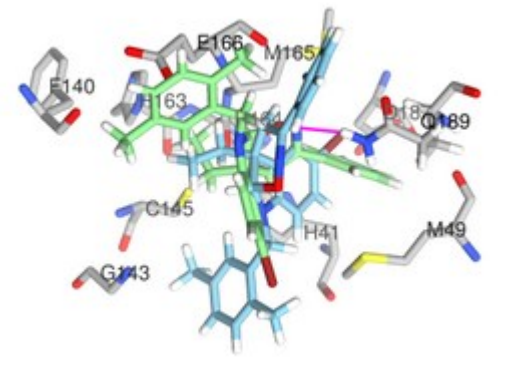
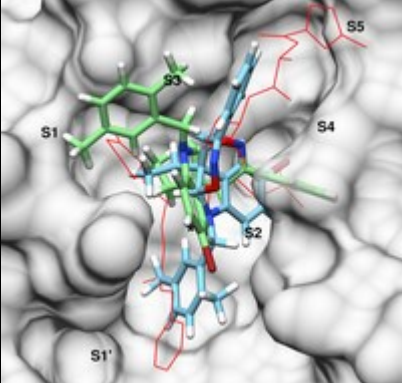
106_SR	-33.4	-11.3		
106_SS	-28.4	-11.8		
107_SR	-32.6	-10.0		
107_SS	-32.1	-9.8		

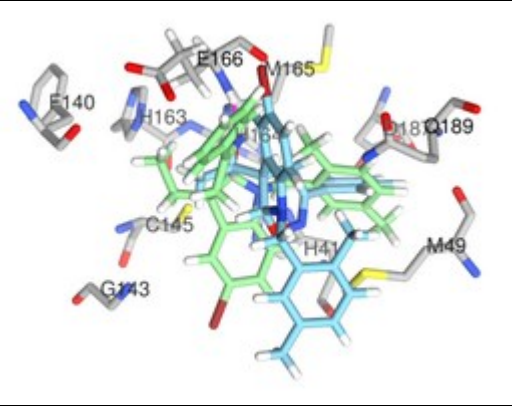
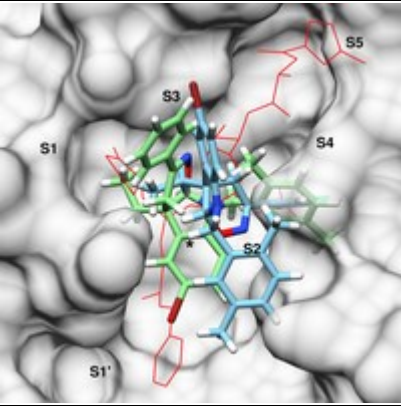
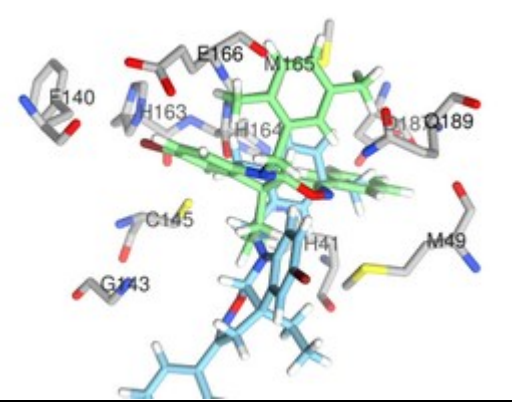
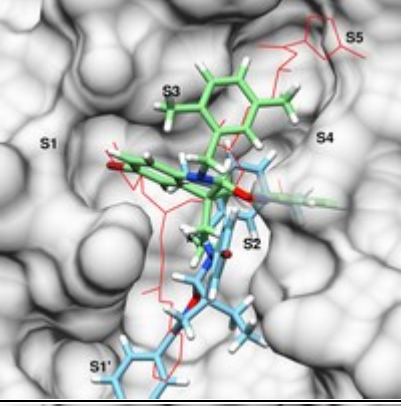
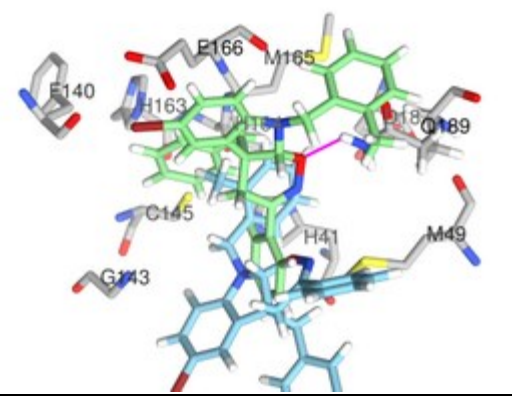
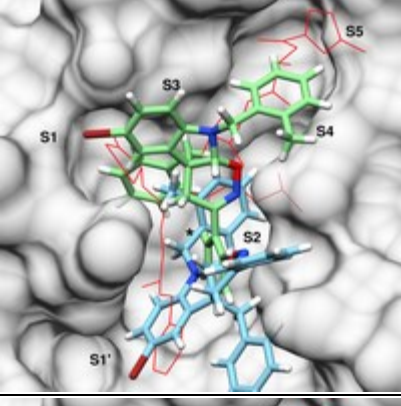
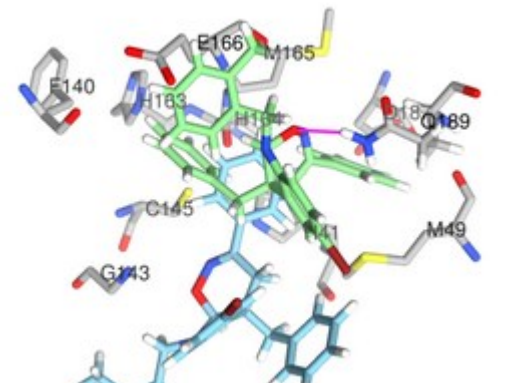
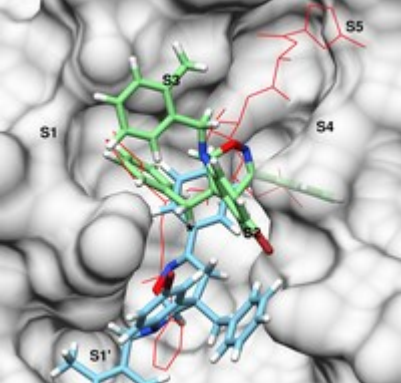
107_RR	-30.2	-10.2		
107_RS	-28.7	-10.4		
108_SR	-36.3	-10.6		
108_SS	-33.7	-9.8		

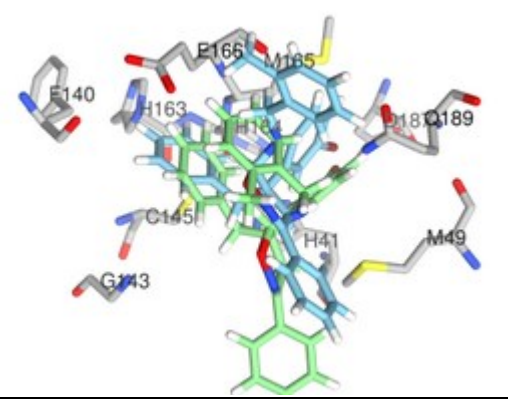
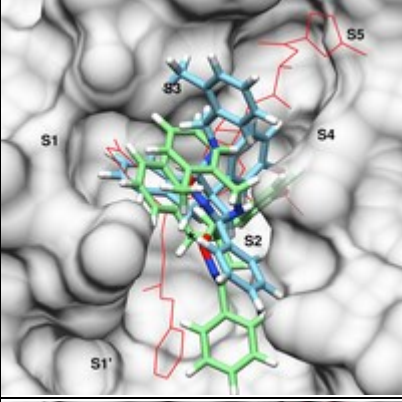
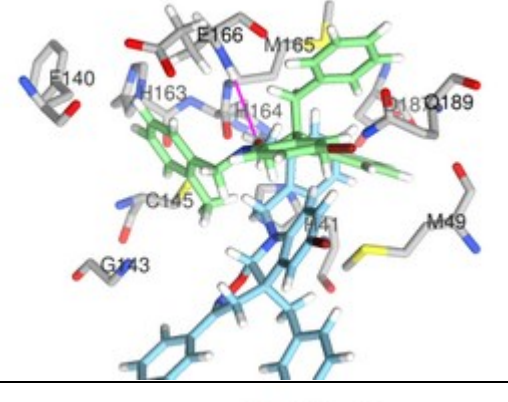
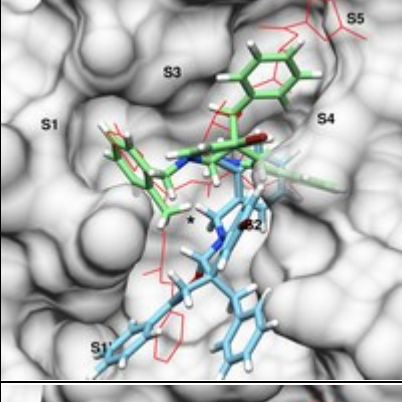
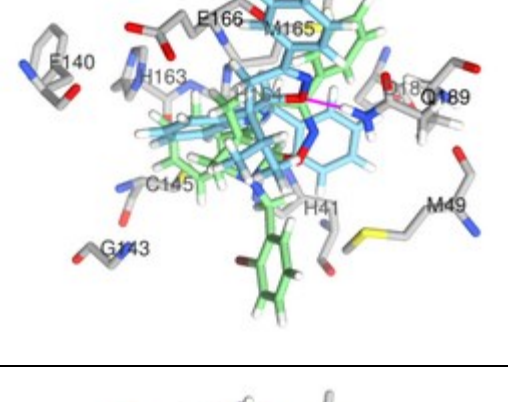
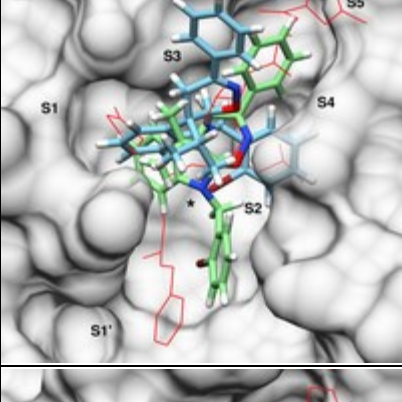
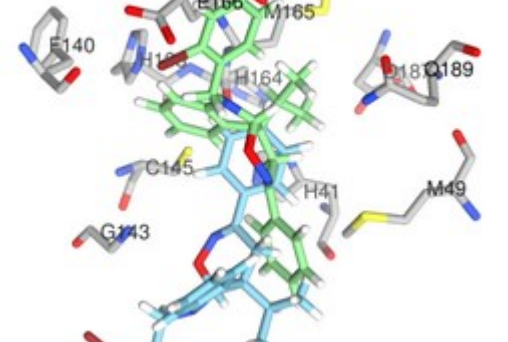
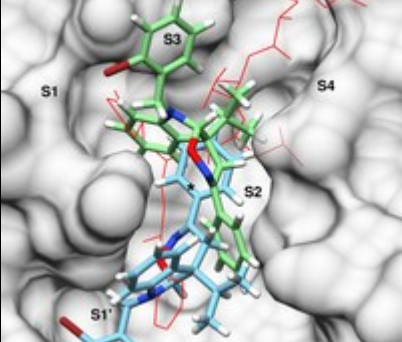
108_RR	-34.3	-9.9		
108_RS	-34.8	-9.3		
109_SR	-33.5	-9.1		
109_SS	-31.2	-8.9		

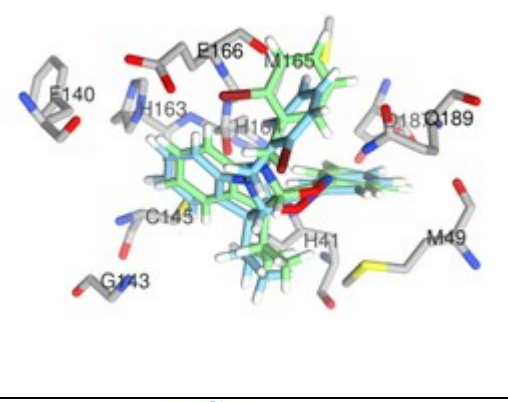
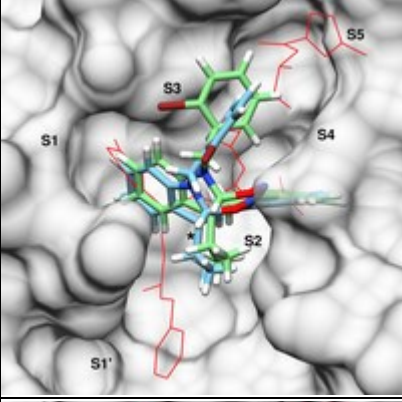
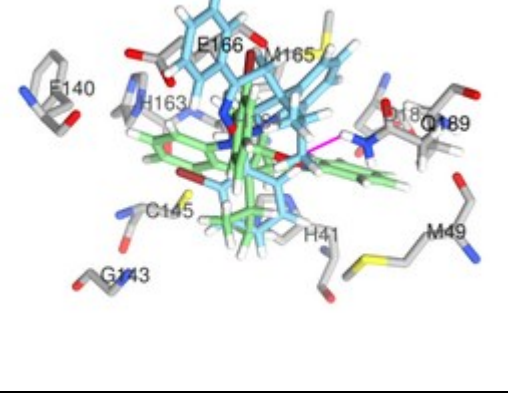
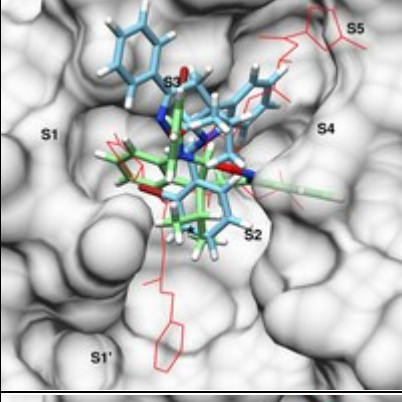
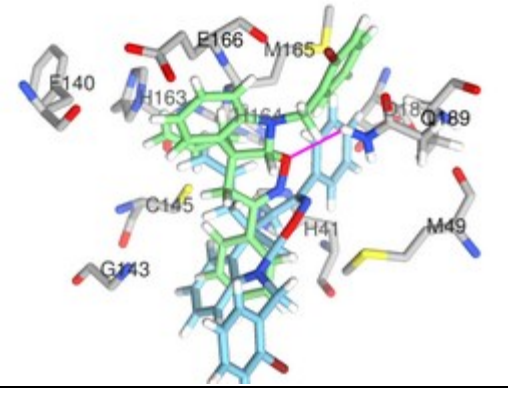
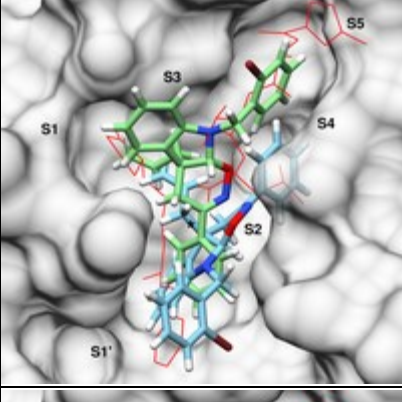
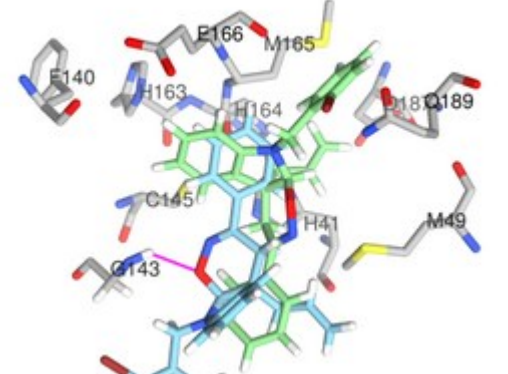
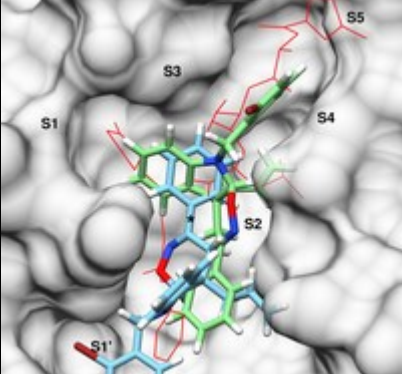
109_RR	-30.6	-9.1		
109_RS	-29.6	-9.1		
110_SR	-39.1	-10.4		
110_SS	-35.2	-10.1		

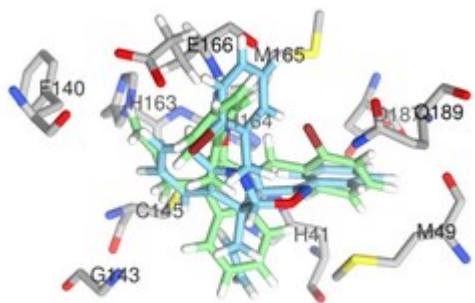
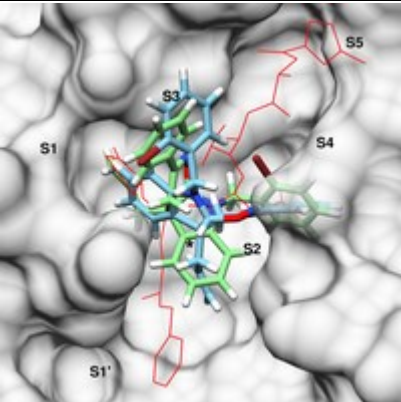
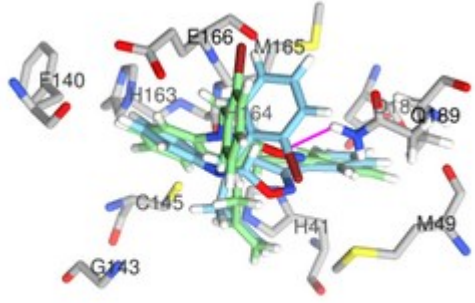
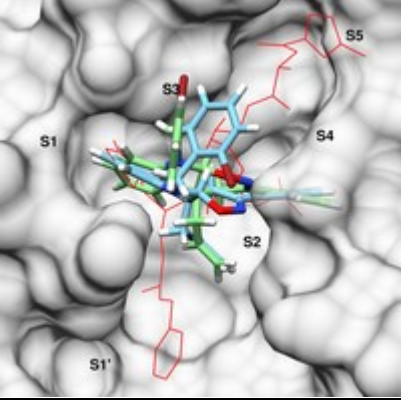
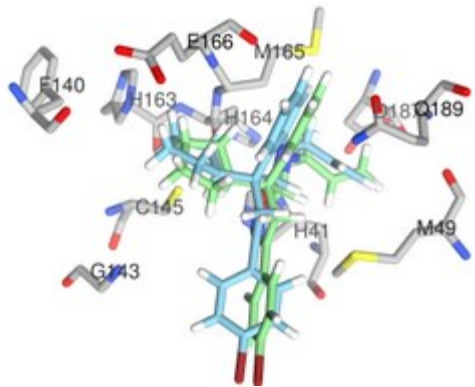
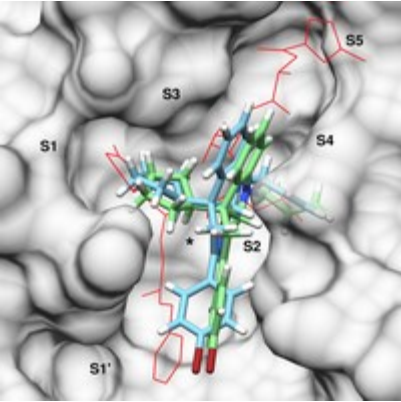
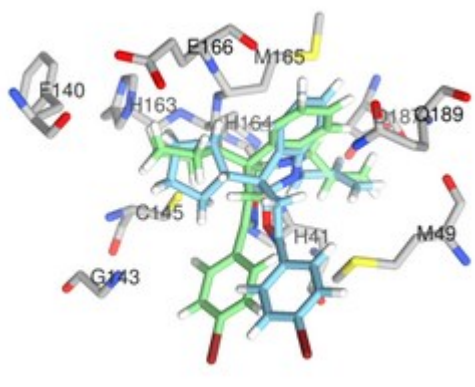
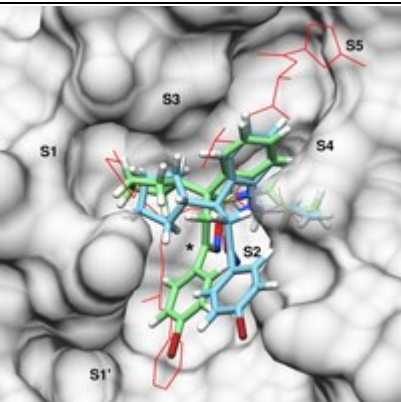
110_RR	-33.3	-9.6		
110_RS	-32.5	-8.9		
111_SR	-29.3	-12.4		
111_SS	-33.0	-9.9		

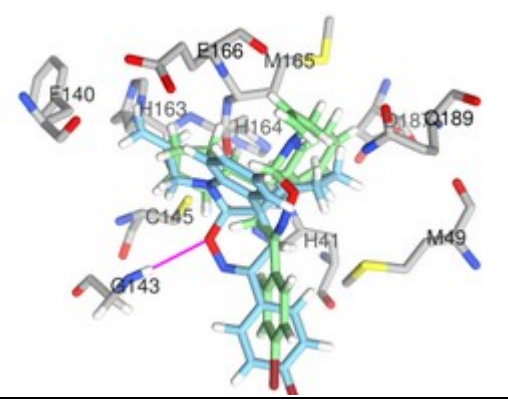
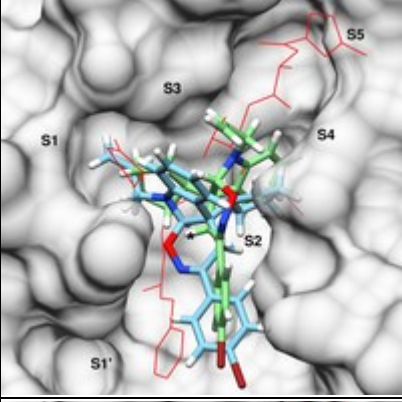
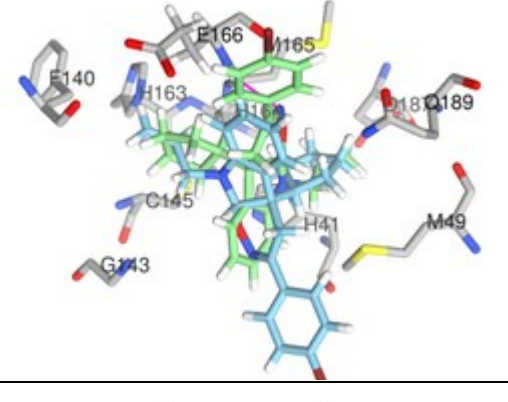
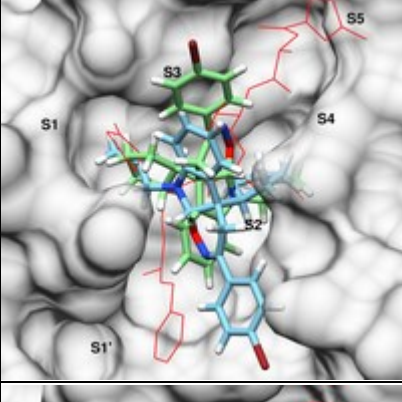
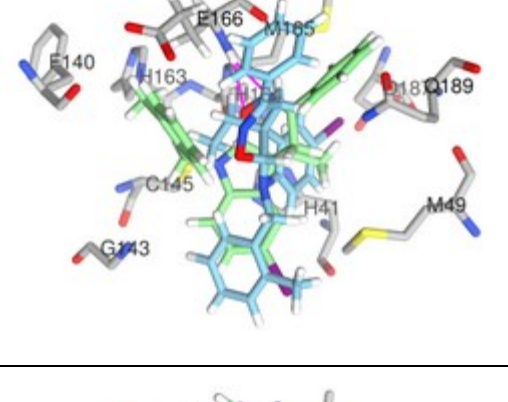
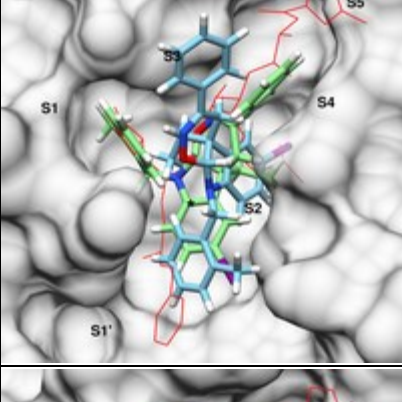
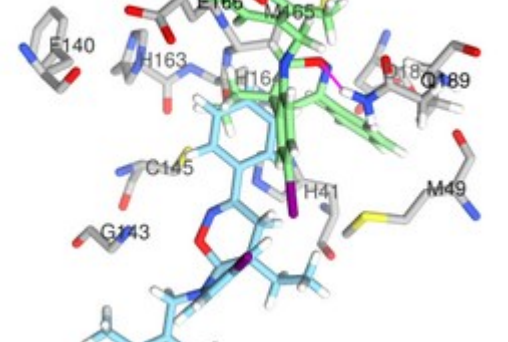
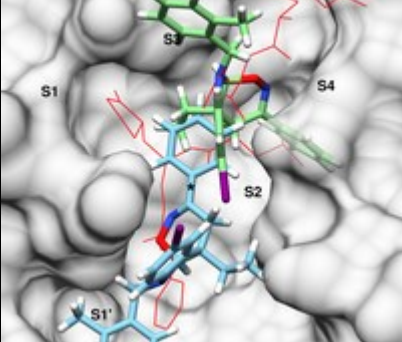
111_RR	-27.1	-10.7		
111_RS	-29.8	-10.2		
112_SR	-30.7	-12.4		
112_SS	-33.2	-11.4		

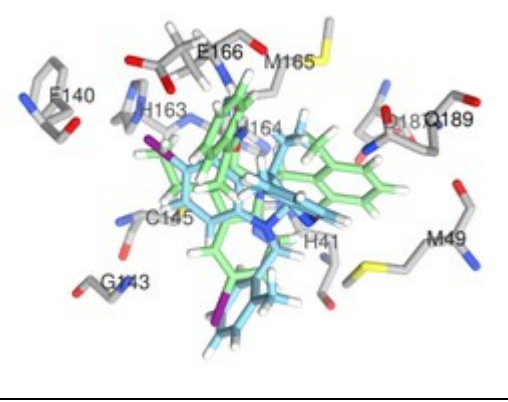
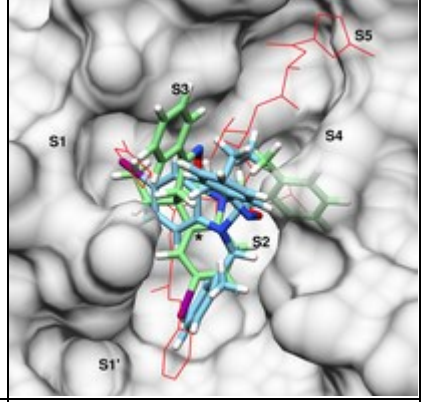
112_RR	-29.4	-12.1		
112_RS	-33.2	-11.7		
113_SR	-29.9	-10.8		
113_SS	-35.4	-11.3		

113_RR	-31.8	-10.7		
113_RS	-31.6	-12.5		
114_RR	-31.2	-10.4		
114_RS	-32.3	-9.9		

114_SR	-33.4	-10.5		
114_SS	-27.0	-11.7		
115_SR	-29.5	-10.2		
115_SS	-36.0	-10.0		

115_RR	-33.5	-10.5		
115_RS	-32.2	-11.1		
116_RR	-34.9	-9.8		
116_RS	-31.2	-10.8		

116_SR	-36.5	-9.9		
116_SS	-30.2	-9.9		
117_SR	-28.0	-12.3		
117_SS	-33.5	-10.3		

117_RR	-26.0	-11.6		
117_RS	-29.9	-11.6	