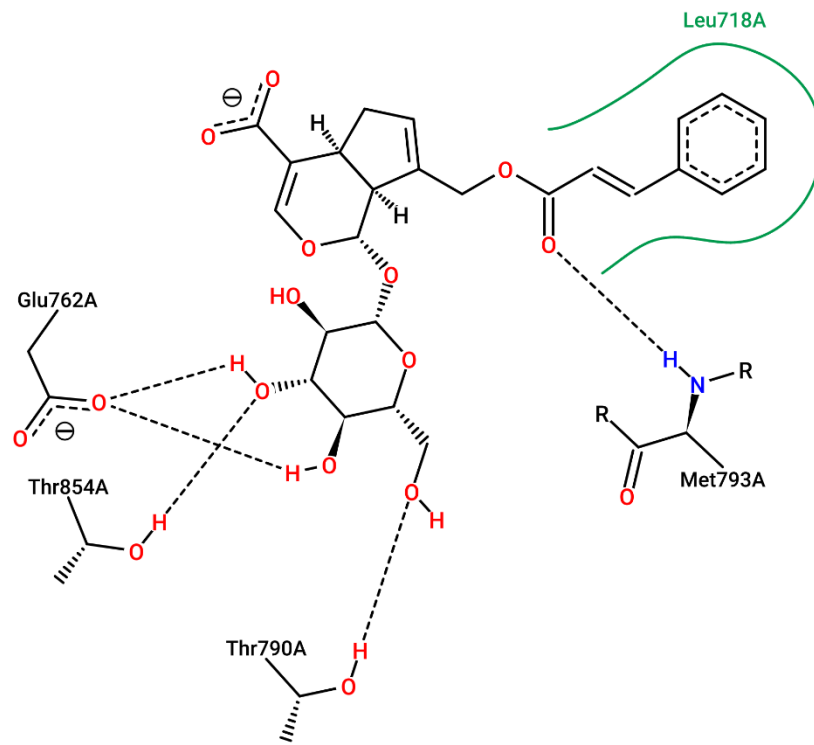


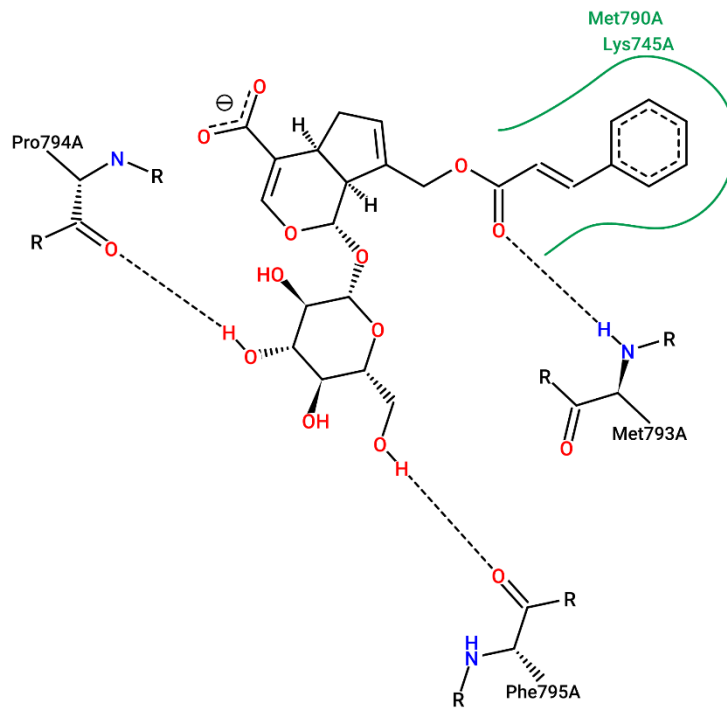
Ligand	GOLD score 1M17: erlotinib WT 100 runs	GOLD score 4I22: Gefitinib dMT (L858R+T790M) 100 runs	GOLD score 6LUD: Osimertinib tMT (L858R/T790M/ C797S) 100 runs
erlotinib	76.91	79.11	69.64
Gefitinib	90.16	94.6	81.11
Osimertinib	78.37	82.43	73.06
247	26.46	25.98	25.14
305	29.38	27.7	26.08
555	31.19	29.69	30.6
1780	71.24	69.9	67.42
14328	36.64	37.19	36.31
71034	46.44	47.35	43.53
188274	68.18	70.62	67.84
445638	58.66	62.6	57.65
637563	34.7	35.98	33.95
2822141	55.43	56.3	52.13
5280373	52.55	54.02	53.27
5280378	51.92	52.9	49.48
5283387	63.09	67.53	58.98
5318650	55.52	53.55	52.45
5319484	65.41	70.74	71.01
5708351	54.08	54.38	56
9543603	69.69	73.95	70.09
9911823	49.63	49.85	44.25
23786390	78.12	72.61	71.1
129651991	66.03	70.39	63.3
346864890	62.29	67.61	59.35
NP-003294	59.14	61.33	58.84
NP-006862	65.69	57.23	62.78
NP-009051	59.91	59.01	57.97

23786390

1. WT



2. Double MT



3.

