

Electronic Supplementary Information

The Impact of *Mycobacterium tuberculosis gyrB* Point Mutations on 6-Fluoroquinolones Resistance Profile: *in silico* Mutagenesis and Structure-based Assessment

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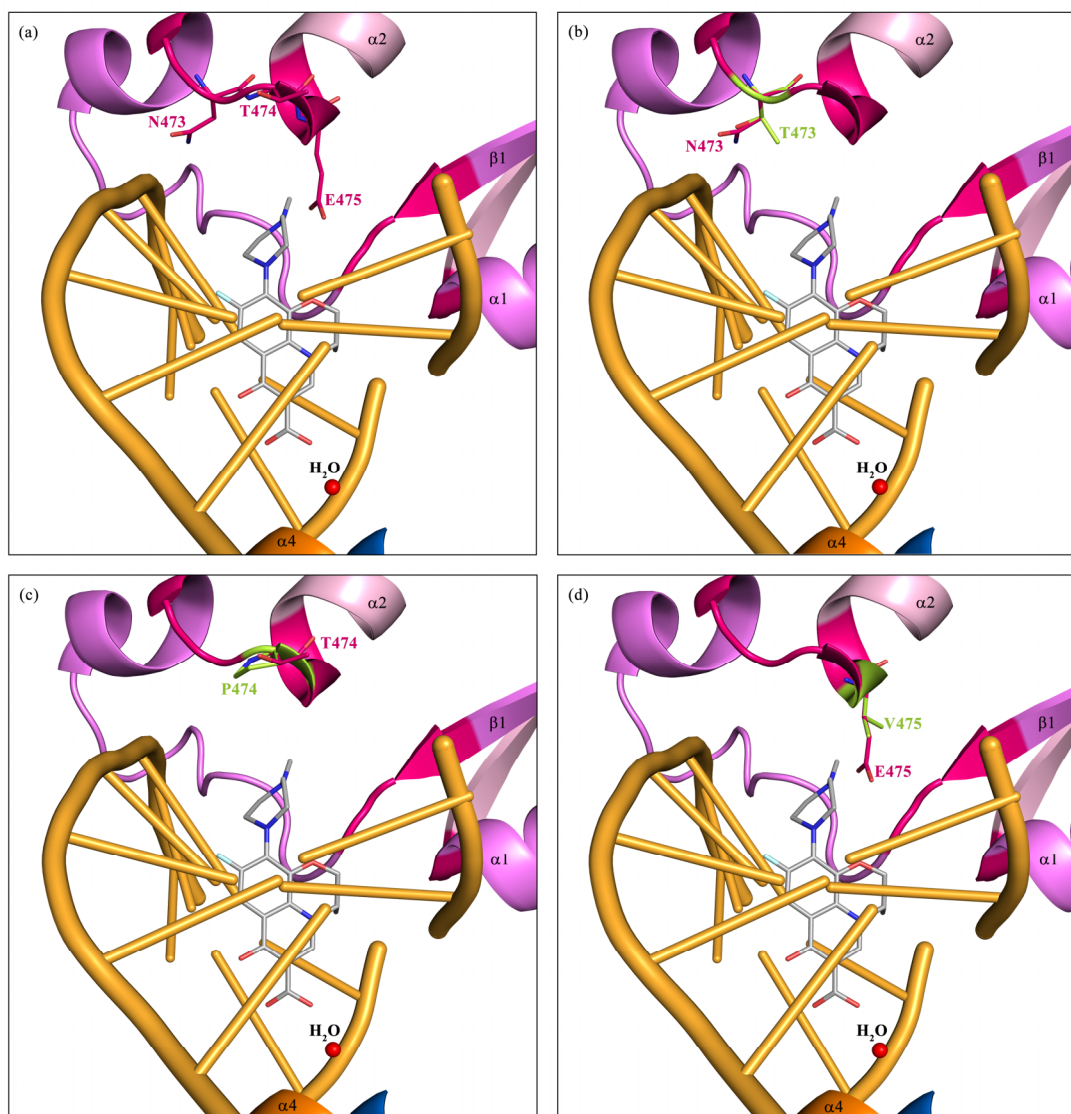


Figure S1 Close view of the *gyrB* hot spot region within our previously published *M. tuberculosis*-DNA gyrase protein homology model 3K9F_{mod}³⁹ and the corresponding mutant models produced by *in silico* mutagenesis: (a) wild-type H37Rv model (3K9F_{mod})³⁹, (b) N473T_{mod} model, (c) T474P_{mod} model, and (d) E475V_{mod} model. The unaffected amino acid residues (N473, T474, and E475; stick representation) are colored in hot pink, while their quinolone-caused alterations (T473, P474, and V475; stick representation) in light green (Table 2). The DNA molecule is depicted in solid orange, the water molecule used in the docking calculations as solid red sphere, and the co-crystallized intercalated ligand LFX is represented in native atomic colors.

Table S1 The results obtained after the Level 1 Boolean-based (T/F (true/false)) clustering (Geometry assessment) of the *ExpLib* dock poses within the QBP of each *M. tuberculosis*-DNA gyrase protein model: a) wild-type 3K9F_{mod},³⁹ b) N473T_{mod}, c) T474P_{mod}, and d) E475V_{mod}.

a) 3K9F_{mod}.

Cluster ID	DOCK POSE	MICexp	GSF	VO (T/F)	VF (T/F)	NMPF (4-5)	Result (T/F)
1	Structure001 ExpLibOpt sdf 1 dock3	3.0000	67.12	T	T	2	F
	Structure001 ExpLibOpt sdf 1 dock1	3.0000	66.63	T	F	0	F
	Structure001 ExpLibOpt sdf 1 dock2	3.0000	66.39	T	F	0	F
2	Structure002 ExpLibOpt sdf 2 dock9	0.0115	67.26	F	F	1	F
	Structure002 ExpLibOpt sdf 2 dock4	0.0115	66.93	T	T	5	T
	Structure002 ExpLibOpt sdf 2 dock2	0.0115	66.89	F	F	1	F
	Structure002 ExpLibOpt sdf 2 dock8	0.0115	66.86	F	F	1	F
	Structure002 ExpLibOpt sdf 2 dock3	0.0115	66.82	T	T	5	T
	Structure002 ExpLibOpt sdf 2 dock1	0.0115	66.74	F	F	1	F
	Structure002 ExpLibOpt sdf 2 dock5	0.0115	66.65	T	T	5	T
	Structure002 ExpLibOpt sdf 2 dock7	0.0115	66.48	T	T	5	T
	Structure002 ExpLibOpt sdf 2 dock6	0.0115	66.31	T	T	2	F
	Structure002 ExpLibOpt sdf 2 dock10	0.0115	65.76	T	T	5	T
	Structure003 ExpLibOpt sdf 3 dock2	0.3000	61.76	T	T	4	T
3	Structure003 ExpLibOpt sdf 3 dock3	0.3000	60.34	T	T	5	T
	Structure003 ExpLibOpt sdf 3 dock1	0.3000	59.27	T	T	5	T
4	Structure004 ExpLibOpt sdf 4 dock1	0.0100	62.61	T	T	5	T
	Structure004 ExpLibOpt sdf 4 dock2	0.0100	62.39	T	T	5	T
	Structure004 ExpLibOpt sdf 4 dock3	0.0100	61.79	T	T	4	T
5	Structure005 ExpLibOpt sdf 5 dock2	0.3000	63.28	F	F	0	F
	Structure005 ExpLibOpt sdf 5 dock4	0.3000	61.37	T	T	4	T
	Structure005 ExpLibOpt sdf 5 dock9	0.3000	61.12	F	F	1	F
	Structure005 ExpLibOpt sdf 5 dock6	0.3000	60.49	T	T	5	T
	Structure005 ExpLibOpt sdf 5 dock10	0.3000	60.36	T	T	4	T

	Structure005 ExpLibOpt sdf 5 dock1	0.3000	60.11	T	T	5	T
	Structure005 ExpLibOpt sdf 5 dock8	0.3000	59.56	T	T	5	T
	Structure005 ExpLibOpt sdf 5 dock5	0.3000	59.15	T	T	5	T
	Structure005 ExpLibOpt sdf 5 dock7	0.3000	58.90	T	T	5	T
	Structure005 ExpLibOpt sdf 5 dock3	0.3000	58.42	T	T	4	T
6	Structure006 ExpLibOpt sdf 6 dock1	0.1200	65.06	T	F	2	F
	Structure006 ExpLibOpt sdf 6 dock2	0.1200	64.84	T	F	2	F
	Structure006 ExpLibOpt sdf 6 dock3	0.1200	64.53	T	F	1	F
7	Structure007 ExpLibOpt sdf 7 dock9	3.5000	64.77	F	F	2	F
	Structure007 ExpLibOpt sdf 7 dock2	3.5000	64.37	F	F	2	F
	Structure007 ExpLibOpt sdf 7 dock3	3.5000	63.64	T	F	1	F
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	Structure007 ExpLibOpt sdf 7 dock8	3.5000	63.35	T	T	4	T
	Structure007 ExpLibOpt sdf 7 dock5	3.5000	63.11	T	F	0	F
	Structure007 ExpLibOpt sdf 7 dock1	3.5000	63.06	T	T	4	T
	Structure007 ExpLibOpt sdf 7 dock6	3.5000	63.02	T	T	3	F
	Structure007 ExpLibOpt sdf 7 dock7	3.5000	62.60	T	T	3	F
	Structure007 ExpLibOpt sdf 7 dock4	3.5000	62.30	T	T	4	T
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	Structure008 ExpLibOpt sdf 8 dock1	0.1000	68.52	T	T	4	T
	Structure008 ExpLibOpt sdf 8 dock3	0.1000	68.16	T	T	4	T
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	Structure009 ExpLibOpt sdf 9 dock2	1.4000	67.73	F	F	0	F
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	Structure009 ExpLibOpt sdf 9 dock10	1.4000	64.39	F	F	0	F
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	Structure009 ExpLibOpt sdf 9 dock3	1.4000	63.60	F	F	1	F
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	Structure013 ExpLibOpt sdf 13 dock3	1.6000	58.84	T	F	1	F
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	Structure037 ExpLibOpt sdf 37 dock6	0.1250	71.49	T	T	3	F
	Structure037 ExpLibOpt sdf 37 dock5	0.1250	71.10	T	T	4	T
	Structure037 ExpLibOpt sdf 37 dock10	0.1250	70.35	F	F	0	F

	Structure037 ExpLibOpt sdf 37 dock4	0.1250	70.04	T	F	2	F
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	Structure037 ExpLibOpt sdf 37 dock9	0.1250	69.71	T	F	2	F
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	Structure039 ExpLibOpt sdf 39 dock8	0.1100	64.96	T	T	5	T
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	Structure040 ExpLibOpt sdf 40 dock4	0.0120	65.74	T	F	3	F
41	Structure040 ExpLibOpt sdf 40 dock1	0.0120	60.68	F	F	2	F
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	Structure042 ExpLibOpt sdf 42 dock1	0.0160	74.76	T	F	1	F
43	Structure042 ExpLibOpt sdf 42 dock2	0.0160	74.60	T	F	1	F
	Structure043 ExpLibOpt sdf 43 dock2	0.6000	65.52	F	F	0	F
	Structure043 ExpLibOpt sdf 43 dock10	0.6000	65.38	F	T	0	F
	Structure043 ExpLibOpt sdf 43 dock4	0.6000	64.49	F	F	2	F
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	Structure050 ExpLibOpt sdf 50 dock1	0.0016	74.35	T	F	3	F
	Structure050 ExpLibOpt sdf 50 dock9	0.0016	72.04	F	F	0	F
	Structure050 ExpLibOpt sdf 50 dock7	0.0016	71.70	F	F	1	F
	Structure050 ExpLibOpt sdf 50 dock5	0.0016	71.05	F	F	3	F

51	Structure051 ExpLibOpt sdf 51 dock2	6.3000	79.55	T	T	4	T
	Structure051 ExpLibOpt sdf 51 dock3	6.3000	77.48	T	T	4	T
	Structure051 ExpLibOpt sdf 51 dock1	6.3000	76.22	T	F	4	F
52	Structure052 ExpLibOpt sdf 52 dock3	6.5700	82.29	T	T	5	T
	Structure052 ExpLibOpt sdf 52 dock4	6.5700	79.78	T	T	3	F
	Structure052 ExpLibOpt sdf 52 dock1	6.5700	79.30	T	T	3	F
	Structure052 ExpLibOpt sdf 52 dock2	6.5700	74.87	F	F	0	F
53	Structure053 ExpLibOpt sdf 53 dock5	5.2000	87.45	F	F	0	F
	Structure053 ExpLibOpt sdf 53 dock7	5.2000	82.97	T	T	4	T
	Structure053 ExpLibOpt sdf 53 dock1	5.2000	82.74	F	F	0	F
	Structure053 ExpLibOpt sdf 53 dock9	5.2000	77.03	F	F	0	F
	Structure053 ExpLibOpt sdf 53 dock4	5.2000	74.71	F	F	0	F
	Structure053 ExpLibOpt sdf 53 dock8	5.2000	74.66	F	F	1	F
	Structure053 ExpLibOpt sdf 53 dock3	5.2000	71.98	F	F	0	F
	Structure053 ExpLibOpt sdf 53 dock6	5.2000	68.37	F	F	0	F
	Structure053 ExpLibOpt sdf 53 dock10	5.2000	65.95	F	F	0	F
	Structure053 ExpLibOpt sdf 53 dock2	5.2000	62.87	F	F	0	F
54	Structure054 ExpLibOpt sdf 54 dock6	6.9000	91.03	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock9	6.9000	89.25	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock8	6.9000	84.98	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock4	6.9000	84.69	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock7	6.9000	77.02	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock10	6.9000	76.09	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock2	6.9000	72.82	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock1	6.9000	72.07	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock3	6.9000	71.64	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock5	6.9000	68.16	F	F	0	F
55	Structure055 ExpLibOpt sdf 55 dock1	6.4500	86.05	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock8	6.4500	85.98	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock4	6.4500	83.44	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock2	6.4500	82.20	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock7	6.4500	79.73	F	F	0	F

	Structure055 ExpLibOpt sdf 55 dock9	6.4500	79.28	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock3	6.4500	77.45	T	T	5	T
	Structure055 ExpLibOpt sdf 55 dock6	6.4500	73.03	T	F	3	F
	Structure055 ExpLibOpt sdf 55 dock5	6.4500	71.99	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock10	6.4500	71.28	F	F	0	F
56	Structure056 ExpLibOpt sdf 56 dock3	6.7000	85.93	F	F	0	F
	Structure056 ExpLibOpt sdf 56 dock10	6.7000	83.05	T	T	1	F
	Structure056 ExpLibOpt sdf 56 dock5	6.7000	80.67	F	F	0	F
	Structure056 ExpLibOpt sdf 56 dock6	6.7000	75.92	F	F	1	F
	Structure056 ExpLibOpt sdf 56 dock4	6.7000	71.69	F	F	1	F
	Structure056 ExpLibOpt sdf 56 dock7	6.7000	71.62	F	F	1	F
	Structure056 ExpLibOpt sdf 56 dock8	6.7000	70.18	F	F	0	F
	Structure056 ExpLibOpt sdf 56 dock9	6.7000	69.11	F	F	0	F
	Structure056 ExpLibOpt sdf 56 dock1	6.7000	67.41	F	F	1	F
57	Structure056 ExpLibOpt sdf 56 dock2	6.7000	66.69	F	F	1	F
	Structure057 ExpLibOpt sdf 57 dock3	6.3000	90.11	F	F	0	F
	Structure057 ExpLibOpt sdf 57 dock2	6.3000	88.02	F	F	0	F
	Structure057 ExpLibOpt sdf 57 dock4	6.3000	82.86	F	F	0	F
58	Structure057 ExpLibOpt sdf 57 dock1	6.3000	82.73	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock2	6.2600	92.67	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock1	6.2600	90.28	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock10	6.2600	89.66	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock7	6.2600	86.49	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock9	6.2600	75.12	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock6	6.2600	72.24	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock5	6.2600	71.57	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock4	6.2600	71.36	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock3	6.2600	70.45	F	F	0	F
59	Structure058 ExpLibOpt sdf 58 dock8	6.2600	62.54	F	F	1	F
	Structure059 ExpLibOpt sdf 59 dock4	6.9200	91.15	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock1	6.9200	89.96	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock7	6.9200	88.88	F	F	0	F

	Structure059 ExpLibOpt sdf 59 dock9	6.9200	85.18	T	T	5	T
	Structure059 ExpLibOpt sdf 59 dock10	6.9200	80.88	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock6	6.9200	73.15	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock5	6.9200	71.21	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock2	6.9200	69.54	F	F	1	F
	Structure059 ExpLibOpt sdf 59 dock3	6.9200	65.15	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock8	6.9200	63.31	F	F	1	F
60	Structure060 ExpLibOpt sdf 60 dock2	0.0300	75.92	T	T	4	T
	Structure060 ExpLibOpt sdf 60 dock3	0.0300	75.69	T	T	4	T
	Structure060 ExpLibOpt sdf 60 dock1	0.0300	70.62	T	T	3	F
61	Structure061 ExpLibOpt sdf 61 dock2	3.2000	63.12	T	T	4	T
	Structure061 ExpLibOpt sdf 61 dock1	3.2000	62.64	T	T	4	T
	Structure061 ExpLibOpt sdf 61 dock3	3.2000	62.49	T	T	4	T
62	Structure062 ExpLibOpt sdf 62 dock3	0.1250	74.16	T	T	5	T
	Structure062 ExpLibOpt sdf 62 dock2	0.1250	73.40	T	T	5	T
	Structure062 ExpLibOpt sdf 62 dock1	0.1250	72.83	T	T	5	T
63	Structure063 ExpLibOpt sdf 63 dock5	0.5000	73.67	T	T	5	T
	Structure063 ExpLibOpt sdf 63 dock3	0.5000	73.18	T	T	2	F
	Structure063 ExpLibOpt sdf 63 dock7	0.5000	73.09	T	T	3	F
	Structure063 ExpLibOpt sdf 63 dock4	0.5000	72.81	T	T	5	T
	Structure063 ExpLibOpt sdf 63 dock1	0.5000	72.49	T	T	2	F
	Structure063 ExpLibOpt sdf 63 dock6	0.5000	71.86	T	T	4	T
	Structure063 ExpLibOpt sdf 63 dock2	0.5000	66.94	F	F	1	F
64	Structure064 ExpLibOpt sdf 64 dock3	0.0300	78.65	T	T	3	F
	Structure064 ExpLibOpt sdf 64 dock1	0.0300	78.53	T	T	3	F
	Structure064 ExpLibOpt sdf 64 dock2	0.0300	78.32	T	T	3	F
65	Structure065 ExpLibOpt sdf 65 dock3	0.7800	77.81	T	T	5	T
	Structure065 ExpLibOpt sdf 65 dock1	0.7800	77.16	T	T	3	F
	Structure065 ExpLibOpt sdf 65 dock2	0.7800	74.77	T	T	5	T
66	Structure066 ExpLibOpt sdf 66 dock6	0.7800	82.53	T	T	2	F
	Structure066 ExpLibOpt sdf 66 dock2	0.7800	81.50	T	T	3	F
	Structure066 ExpLibOpt sdf 66 dock5	0.7800	80.71	T	T	5	T

	Structure066 ExpLibOpt sdf 66 dock1	0.7800	77.75	T	T	5	T
	Structure066 ExpLibOpt sdf 66 dock4	0.7800	76.07	T	T	3	F
	Structure066 ExpLibOpt sdf 66 dock3	0.7800	75.78	F	F	1	F
67	Structure067 ExpLibOpt sdf 67 dock4	6.2500	83.39	F	F	0	F
	Structure067 ExpLibOpt sdf 67 dock5	6.2500	82.77	F	F	0	F
	Structure067 ExpLibOpt sdf 67 dock10	6.2500	77.02	T	T	1	F
	Structure067 ExpLibOpt sdf 67 dock2	6.2500	75.42	T	T	5	T
	Structure067 ExpLibOpt sdf 67 dock1	6.2500	75.25	F	F	0	F
	Structure067 ExpLibOpt sdf 67 dock7	6.2500	73.97	F	F	0	F
	Structure067 ExpLibOpt sdf 67 dock3	6.2500	73.76	T	T	5	T
	Structure067 ExpLibOpt sdf 67 dock6	6.2500	72.60	T	T	2	F
	Structure067 ExpLibOpt sdf 67 dock8	6.2500	72.33	T	T	5	T
	Structure067 ExpLibOpt sdf 67 dock9	6.2500	71.07	T	T	5	T
68	Structure068 ExpLibOpt sdf 68 dock5	0.7800	80.59	T	T	3	F
	Structure068 ExpLibOpt sdf 68 dock8	0.7800	78.33	T	T	5	T
	Structure068 ExpLibOpt sdf 68 dock3	0.7800	77.50	T	T	5	T
	Structure068 ExpLibOpt sdf 68 dock10	0.7800	76.33	F	F	1	F
	Structure068 ExpLibOpt sdf 68 dock4	0.7800	76.27	T	T	5	T
	Structure068 ExpLibOpt sdf 68 dock1	0.7800	75.18	F	F	0	F
	Structure068 ExpLibOpt sdf 68 dock6	0.7800	75.04	T	T	3	F
	Structure068 ExpLibOpt sdf 68 dock7	0.7800	74.89	T	T	3	F
	Structure068 ExpLibOpt sdf 68 dock2	0.7800	74.65	F	F	0	F
	Structure068 ExpLibOpt sdf 68 dock9	0.7800	69.73	F	F	0	F
69	Structure069 ExpLibOpt sdf 69 dock8	1.5600	79.74	F	F	0	F
	Structure069 ExpLibOpt sdf 69 dock5	1.5600	78.60	T	T	5	T
	Structure069 ExpLibOpt sdf 69 dock1	1.5600	78.23	T	T	5	T
	Structure069 ExpLibOpt sdf 69 dock2	1.5600	76.92	F	F	0	F
	Structure069 ExpLibOpt sdf 69 dock9	1.5600	76.71	F	F	0	F
	Structure069 ExpLibOpt sdf 69 dock6	1.5600	76.59	T	T	5	T
	Structure069 ExpLibOpt sdf 69 dock10	1.5600	76.37	T	T	2	F
	Structure069 ExpLibOpt sdf 69 dock4	1.5600	75.77	T	T	3	F
	Structure069 ExpLibOpt sdf 69 dock7	1.5600	74.50	T	F	0	F

	Structure069 ExpLibOpt sdf 69 dock3	1.5600	71.94	F	F	0	F
70	Structure070 ExpLibOpt sdf 70 dock8	1.5600	84.99	F	F	0	F
	Structure070 ExpLibOpt sdf 70 dock1	1.5600	76.85	F	F	2	F
	Structure070 ExpLibOpt sdf 70 dock10	1.5600	76.16	T	T	5	T
	Structure070 ExpLibOpt sdf 70 dock7	1.5600	75.45	T	T	5	T
	Structure070 ExpLibOpt sdf 70 dock6	1.5600	75.30	F	F	0	F
	Structure070 ExpLibOpt sdf 70 dock4	1.5600	75.24	F	F	1	F
	Structure070 ExpLibOpt sdf 70 dock9	1.5600	74.64	T	T	3	F
	Structure070 ExpLibOpt sdf 70 dock5	1.5600	73.76	F	F	0	F
	Structure070 ExpLibOpt sdf 70 dock2	1.5600	73.01	T	T	3	F
	Structure070 ExpLibOpt sdf 70 dock3	1.5600	69.58	F	F	1	F
71	Structure071 ExpLibOpt sdf 71 dock1	3.1300	88.58	F	F	0	F
	Structure071 ExpLibOpt sdf 71 dock6	3.1300	87.49	F	F	0	F
	Structure071 ExpLibOpt sdf 71 dock3	3.1300	83.63	F	F	0	F
	Structure071 ExpLibOpt sdf 71 dock4	3.1300	80.14	T	T	5	T
	Structure071 ExpLibOpt sdf 71 dock2	3.1300	79.36	F	F	0	F
	Structure071 ExpLibOpt sdf 71 dock5	3.1300	77.91	T	T	5	T
72	Structure072 ExpLibOpt sdf 72 dock10	7.1200	85.19	F	F	0	F
	Structure072 ExpLibOpt sdf 72 dock1	7.1200	83.65	F	F	1	F
	Structure072 ExpLibOpt sdf 72 dock7	7.1200	82.86	T	T	3	F
	Structure072 ExpLibOpt sdf 72 dock5	7.1200	81.81	T	T	5	T
	Structure072 ExpLibOpt sdf 72 dock8	7.1200	79.88	F	F	1	F
	Structure072 ExpLibOpt sdf 72 dock4	7.1200	79.02	T	T	3	F
	Structure072 ExpLibOpt sdf 72 dock3	7.1200	79.01	F	F	0	F
	Structure072 ExpLibOpt sdf 72 dock6	7.1200	77.21	T	T	5	T
	Structure072 ExpLibOpt sdf 72 dock9	7.1200	76.19	F	F	1	F
	Structure072 ExpLibOpt sdf 72 dock2	7.1200	75.47	F	F	1	F
73	Structure073 ExpLibOpt sdf 73 dock3	0.0600	67.36	T	T	5	T
	Structure073 ExpLibOpt sdf 73 dock1	0.0600	67.01	T	T	5	T
	Structure073 ExpLibOpt sdf 73 dock2	0.0600	66.90	T	T	5	T
74	Structure074 ExpLibOpt sdf 74 dock2	0.7800	74.49	T	T	3	F
	Structure074 ExpLibOpt sdf 74 dock1	0.7800	73.48	T	T	4	T

	Structure074 ExpLibOpt sdf 74 dock3	0.7800	72.01	T	T	4	T
75	Structure075 ExpLibOpt sdf 75 dock1	0.0625	66.45	T	F	1	F
	Structure075 ExpLibOpt sdf 75 dock3	0.0625	66.44	T	T	2	F
	Structure075 ExpLibOpt sdf 75 dock2	0.0625	64.90	T	T	1	F
76	Structure076 ExpLibOpt sdf 76 dock3	0.1250	73.56	T	T	4	T
	Structure076 ExpLibOpt sdf 76 dock2	0.1250	73.11	T	T	4	T
	Structure076 ExpLibOpt sdf 76 dock1	0.1250	72.13	T	T	4	T
77	Structure077 ExpLibOpt sdf 77 dock2	6.2500	77.85	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock7	6.2500	77.21	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock5	6.2500	76.18	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock3	6.2500	74.78	T	T	5	T
	Structure077 ExpLibOpt sdf 77 dock4	6.2500	73.28	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock6	6.2500	72.99	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock1	6.2500	71.56	T	T	5	T
78	Structure078 ExpLibOpt sdf 78 dock1	3.1300	70.43	T	T	5	T
	Structure078 ExpLibOpt sdf 78 dock3	3.1300	70.27	T	T	2	F
	Structure078 ExpLibOpt sdf 78 dock2	3.1300	69.92	T	T	5	T
79	Structure079 ExpLibOpt sdf 79 dock4	3.1300	79.15	T	T	3	F
	Structure079 ExpLibOpt sdf 79 dock5	3.1300	77.71	T	T	2	F
	Structure079 ExpLibOpt sdf 79 dock3	3.1300	76.96	T	T	2	F
	Structure079 ExpLibOpt sdf 79 dock1	3.1300	76.82	F	F	0	F
	Structure079 ExpLibOpt sdf 79 dock10	3.1300	70.01	F	F	0	F
	Structure079 ExpLibOpt sdf 79 dock8	3.1300	68.44	T	T	5	T
	Structure079 ExpLibOpt sdf 79 dock7	3.1300	68.37	T	T	5	T
	Structure079 ExpLibOpt sdf 79 dock6	3.1300	68.10	F	F	0	F
	Structure079 ExpLibOpt sdf 79 dock9	3.1300	67.48	F	T	3	F
	Structure079 ExpLibOpt sdf 79 dock2	3.1300	64.46	F	F	0	F
80	Structure080 ExpLibOpt sdf 80 dock2	1.5600	81.21	T	F	1	F
	Structure080 ExpLibOpt sdf 80 dock3	1.5600	80.48	T	F	1	F
	Structure080 ExpLibOpt sdf 80 dock1	1.5600	80.34	T	F	1	F
81	Structure081 ExpLibOpt sdf 81 dock2	0.3900	70.52	T	T	4	T
	Structure081 ExpLibOpt sdf 81 dock5	0.3900	70.48	F	F	1	F

	Structure081 ExpLibOpt sdf 81 dock4	0.3900	70.09	T	T	4	T
	Structure081 ExpLibOpt sdf 81 dock6	0.3900	69.98	F	F	1	F
	Structure081 ExpLibOpt sdf 81 dock10	0.3900	69.97	F	F	0	F
	Structure081 ExpLibOpt sdf 81 dock3	0.3900	69.63	F	F	0	F
	Structure081 ExpLibOpt sdf 81 dock1	0.3900	69.33	T	T	4	T
	Structure081 ExpLibOpt sdf 81 dock8	0.3900	68.94	F	F	1	F
	Structure081 ExpLibOpt sdf 81 dock7	0.3900	68.71	F	F	1	F
	Structure081 ExpLibOpt sdf 81 dock9	0.3900	65.49	T	T	2	F
82	Structure082 ExpLibOpt sdf 82 dock9	0.0030	86.85	F	F	0	F
	Structure082 ExpLibOpt sdf 82 dock8	0.0030	79.75	F	F	0	F
	Structure082 ExpLibOpt sdf 82 dock1	0.0030	75.14	T	T	5	T
	Structure082 ExpLibOpt sdf 82 dock5	0.0030	73.08	F	F	2	F
	Structure082 ExpLibOpt sdf 82 dock2	0.0030	73.07	F	F	1	F
	Structure082 ExpLibOpt sdf 82 dock7	0.0030	72.98	T	F	1	F
	Structure082 ExpLibOpt sdf 82 dock6	0.0030	72.45	T	T	3	F
	Structure082 ExpLibOpt sdf 82 dock3	0.0030	71.98	F	F	1	F
	Structure082 ExpLibOpt sdf 82 dock10	0.0030	66.75	F	F	1	F
	Structure082 ExpLibOpt sdf 82 dock4	0.0030	66.04	T	T	5	T
83	Structure083 ExpLibOpt sdf 83 dock5	0.0027	87.74	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock10	0.0027	87.50	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock2	0.0027	83.92	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock3	0.0027	83.83	T	T	5	T
	Structure083 ExpLibOpt sdf 83 dock6	0.0027	83.73	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock9	0.0027	82.47	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock1	0.0027	82.45	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock7	0.0027	82.24	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock4	0.0027	73.38	F	T	2	F
	Structure083 ExpLibOpt sdf 83 dock8	0.0027	66.97	F	F	0	F
84	Structure084 ExpLibOpt sdf 84 dock10	0.0026	81.99	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock3	0.0026	81.69	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock5	0.0026	78.57	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock8	0.0026	76.72	F	F	2	F

	Structure084 ExpLibOpt sdf 84 dock7	0.0026	76.27	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock1	0.0026	72.65	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock2	0.0026	65.30	F	F	1	F
	Structure084 ExpLibOpt sdf 84 dock9	0.0026	63.16	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock6	0.0026	61.92	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock4	0.0026	60.08	F	F	1	F
85	Structure085 ExpLibOpt sdf 85 dock9	0.0027	85.29	F	F	0	F
	Structure085 ExpLibOpt sdf 85 dock7	0.0027	82.22	F	F	0	F
	Structure085 ExpLibOpt sdf 85 dock1	0.0027	79.20	F	F	0	F
	Structure085 ExpLibOpt sdf 85 dock4	0.0027	74.85	F	F	2	F
	Structure085 ExpLibOpt sdf 85 dock6	0.0027	74.57	F	F	1	F
	Structure085 ExpLibOpt sdf 85 dock5	0.0027	74.14	F	F	0	F
	Structure085 ExpLibOpt sdf 85 dock3	0.0027	73.91	F	F	0	F
	Structure085 ExpLibOpt sdf 85 dock2	0.0027	73.73	T	T	2	F
86	Structure085 ExpLibOpt sdf 85 dock8	0.0027	67.87	F	F	1	F
	Structure086 ExpLibOpt sdf 86 dock2	0.0012	87.92	F	F	0	F
	Structure086 ExpLibOpt sdf 86 dock1	0.0012	87.13	F	F	0	F
	Structure086 ExpLibOpt sdf 86 dock6	0.0012	86.29	F	F	0	F
	Structure086 ExpLibOpt sdf 86 dock4	0.0012	81.60	T	T	5	T
	Structure086 ExpLibOpt sdf 86 dock5	0.0012	80.62	F	F	0	F
87	Structure086 ExpLibOpt sdf 86 dock3	0.0012	79.91	F	F	1	F
	Structure087 ExpLibOpt sdf 87 dock5	0.0012	80.88	F	F	0	F
	Structure087 ExpLibOpt sdf 87 dock6	0.0012	79.11	F	T	2	F
	Structure087 ExpLibOpt sdf 87 dock9	0.0012	77.78	F	F	1	F
	Structure087 ExpLibOpt sdf 87 dock2	0.0012	76.58	F	F	0	F
	Structure087 ExpLibOpt sdf 87 dock1	0.0012	73.84	F	F	2	F
	Structure087 ExpLibOpt sdf 87 dock8	0.0012	72.27	F	F	0	F
	Structure087 ExpLibOpt sdf 87 dock10	0.0012	72.05	F	F	1	F
	Structure087 ExpLibOpt sdf 87 dock3	0.0012	71.93	F	F	0	F
	Structure087 ExpLibOpt sdf 87 dock7	0.0012	64.18	F	F	0	F
88	Structure087 ExpLibOpt sdf 87 dock4	0.0012	57.54	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock2	0.0014	78.44	F	F	0	F

	Structure088 ExpLibOpt sdf 88 dock1	0.0014	75.99	F	F	1	F
	Structure088 ExpLibOpt sdf 88 dock6	0.0014	73.17	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock7	0.0014	73.16	T	T	5	T
	Structure088 ExpLibOpt sdf 88 dock5	0.0014	68.97	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock8	0.0014	68.33	F	F	2	F
	Structure088 ExpLibOpt sdf 88 dock4	0.0014	66.62	F	F	1	F
	Structure088 ExpLibOpt sdf 88 dock3	0.0014	63.83	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock9	0.0014	61.55	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock10	0.0014	50.13	F	F	0	F
89	Structure089 ExpLibOpt sdf 89 dock4	0.0108	83.20	F	F	0	F
	Structure089 ExpLibOpt sdf 89 dock9	0.0108	82.16	F	F	1	F
	Structure089 ExpLibOpt sdf 89 dock5	0.0108	75.33	F	F	2	F
	Structure089 ExpLibOpt sdf 89 dock10	0.0108	74.27	F	F	0	F
	Structure089 ExpLibOpt sdf 89 dock2	0.0108	73.09	T	T	4	T
	Structure089 ExpLibOpt sdf 89 dock8	0.0108	70.18	F	F	0	F
	Structure089 ExpLibOpt sdf 89 dock1	0.0108	65.45	F	F	0	F
	Structure089 ExpLibOpt sdf 89 dock7	0.0108	59.33	T	F	0	F
	Structure089 ExpLibOpt sdf 89 dock6	0.0108	56.53	F	F	0	F
90	Structure089 ExpLibOpt sdf 89 dock3	0.0108	52.71	F	F	0	F
	Structure090 ExpLibOpt sdf 90 dock5	0.0029	90.73	F	F	0	F
	Structure090 ExpLibOpt sdf 90 dock9	0.0029	81.36	F	F	1	F
	Structure090 ExpLibOpt sdf 90 dock6	0.0029	79.56	F	F	1	F
	Structure090 ExpLibOpt sdf 90 dock3	0.0029	77.66	F	F	1	F
	Structure090 ExpLibOpt sdf 90 dock2	0.0029	74.88	F	F	0	F
	Structure090 ExpLibOpt sdf 90 dock1	0.0029	74.69	F	F	0	F
	Structure090 ExpLibOpt sdf 90 dock4	0.0029	73.98	F	F	1	F
	Structure090 ExpLibOpt sdf 90 dock8	0.0029	72.60	T	T	5	T
	Structure090 ExpLibOpt sdf 90 dock10	0.0029	70.77	F	F	0	F
91	Structure090 ExpLibOpt sdf 90 dock7	0.0029	70.61	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock6	0.0014	93.13	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock7	0.0014	93.03	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock5	0.0014	78.87	F	F	0	F

	Structure091 ExpLibOpt sdf 91 dock3	0.0014	77.10	F	F	2	F
	Structure091 ExpLibOpt sdf 91 dock8	0.0014	74.86	T	F	0	F
	Structure091 ExpLibOpt sdf 91 dock4	0.0014	73.50	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock10	0.0014	72.51	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock9	0.0014	69.82	F	F	2	F
	Structure091 ExpLibOpt sdf 91 dock2	0.0014	57.32	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock1	0.0014	56.30	F	F	0	F
92	Structure092 ExpLibOpt sdf 92 dock4	6.2500	80.24	F	F	1	F
	Structure092 ExpLibOpt sdf 92 dock9	6.2500	79.68	F	F	1	F
	Structure092 ExpLibOpt sdf 92 dock3	6.2500	78.97	F	F	1	F
	Structure092 ExpLibOpt sdf 92 dock8	6.2500	77.82	T	T	2	F
	Structure092 ExpLibOpt sdf 92 dock5	6.2500	76.97	T	T	5	T
	Structure092 ExpLibOpt sdf 92 dock7	6.2500	75.30	F	F	0	F
	Structure092 ExpLibOpt sdf 92 dock2	6.2500	74.41	F	F	0	F
	Structure092 ExpLibOpt sdf 92 dock1	6.2500	73.65	T	T	2	F
93	Structure092 ExpLibOpt sdf 92 dock6	6.2500	72.32	T	T	3	F
	Structure093 ExpLibOpt sdf 93 dock3	0.1250	76.68	T	T	1	F
	Structure093 ExpLibOpt sdf 93 dock4	0.1250	76.02	T	T	3	F
	Structure093 ExpLibOpt sdf 93 dock1	0.1250	75.81	T	T	3	F
94	Structure093 ExpLibOpt sdf 93 dock2	0.1250	72.87	T	T	3	F
	Structure094 ExpLibOpt sdf 94 dock4	3.1300	101.17	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock1	3.1300	83.34	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock8	3.1300	82.29	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock9	3.1300	81.62	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock3	3.1300	79.94	F	F	1	F
	Structure094 ExpLibOpt sdf 94 dock2	3.1300	79.36	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock6	3.1300	73.69	F	F	1	F
	Structure094 ExpLibOpt sdf 94 dock10	3.1300	72.23	F	F	1	F
	Structure094 ExpLibOpt sdf 94 dock5	3.1300	68.03	F	F	1	F
95	Structure094 ExpLibOpt sdf 94 dock7	3.1300	53.25	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock10	0.7800	100.39	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock3	0.7800	89.65	F	F	0	F

	Structure095 ExpLibOpt sdf 95 dock4	0.7800	89.24	F	F	1	F
	Structure095 ExpLibOpt sdf 95 dock7	0.7800	88.05	F	F	1	F
	Structure095 ExpLibOpt sdf 95 dock8	0.7800	86.57	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock1	0.7800	85.41	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock9	0.7800	82.60	F	F	1	F
	Structure095 ExpLibOpt sdf 95 dock5	0.7800	74.12	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock6	0.7800	73.51	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock2	0.7800	44.65	F	F	0	F
96	Structure096 ExpLibOpt sdf 96 dock9	0.7800	77.69	F	F	1	F
	Structure096 ExpLibOpt sdf 96 dock7	0.7800	76.70	T	T	5	T
	Structure096 ExpLibOpt sdf 96 dock3	0.7800	75.87	F	F	0	F
	Structure096 ExpLibOpt sdf 96 dock6	0.7800	75.64	T	T	5	T
	Structure096 ExpLibOpt sdf 96 dock2	0.7800	74.74	F	F	0	F
	Structure096 ExpLibOpt sdf 96 dock10	0.7800	74.14	T	F	1	F
	Structure096 ExpLibOpt sdf 96 dock8	0.7800	73.96	T	T	4	T
	Structure096 ExpLibOpt sdf 96 dock1	0.7800	71.94	F	F	0	F
	Structure096 ExpLibOpt sdf 96 dock5	0.7800	66.79	F	F	0	F
	Structure096 ExpLibOpt sdf 96 dock4	0.7800	65.04	F	F	0	F
97	Structure097 ExpLibOpt sdf 97 dock8	0.7800	80.82	T	T	5	T
	Structure097 ExpLibOpt sdf 97 dock7	0.7800	80.64	T	T	5	T
	Structure097 ExpLibOpt sdf 97 dock3	0.7800	77.47	T	T	5	T
	Structure097 ExpLibOpt sdf 97 dock4	0.7800	76.56	F	F	1	F
	Structure097 ExpLibOpt sdf 97 dock1	0.7800	75.61	F	F	0	F
	Structure097 ExpLibOpt sdf 97 dock5	0.7800	71.85	F	F	0	F
	Structure097 ExpLibOpt sdf 97 dock6	0.7800	71.33	F	F	0	F
	Structure097 ExpLibOpt sdf 97 dock2	0.7800	67.65	F	F	0	F
98	Structure098 ExpLibOpt sdf 98 dock2	0.0060	71.41	T	F	1	F
	Structure098 ExpLibOpt sdf 98 dock1	0.0060	71.17	T	F	0	F
	Structure098 ExpLibOpt sdf 98 dock3	0.0060	70.51	T	F	2	F
99	Structure099 ExpLibOpt sdf 99 dock2	0.0060	70.46	T	T	4	T
	Structure099 ExpLibOpt sdf 99 dock3	0.0060	69.87	T	T	4	T
	Structure099 ExpLibOpt sdf 99 dock1	0.0060	69.74	T	T	4	T

100	Structure100 ExpLibOpt sdf 100 dock3	0.0130	64.27	T	T	2	F
	Structure100 ExpLibOpt sdf 100 dock1	0.0130	64.20	T	T	2	F
	Structure100 ExpLibOpt sdf 100 dock2	0.0130	61.90	T	T	2	F
101	Structure101 ExpLibOpt sdf 101 dock4	0.0060	73.24	T	T	1	F
	Structure101 ExpLibOpt sdf 101 dock3	0.0060	73.15	T	T	2	F
	Structure101 ExpLibOpt sdf 101 dock1	0.0060	72.77	T	T	3	F
	Structure101 ExpLibOpt sdf 101 dock2	0.0060	72.70	T	T	4	T
102	Structure102 ExpLibOpt sdf 102 dock1	0.0010	60.91	T	F	1	F
	Structure102 ExpLibOpt sdf 102 dock2	0.0010	60.76	T	F	1	F
	Structure102 ExpLibOpt sdf 102 dock3	0.0010	59.68	T	F	2	F
103	Structure103 ExpLibOpt sdf 103 dock2	0.0020	74.24	T	T	4	T
	Structure103 ExpLibOpt sdf 103 dock1	0.0020	74.05	T	T	4	T
	Structure103 ExpLibOpt sdf 103 dock3	0.0020	73.46	T	F	0	F
104	Structure104 ExpLibOpt sdf 104 dock8	0.0130	61.73	F	F	0	F
	Structure104 ExpLibOpt sdf 104 dock2	0.0130	61.47	F	F	0	F
	Structure104 ExpLibOpt sdf 104 dock3	0.0130	60.60	F	F	0	F
	Structure104 ExpLibOpt sdf 104 dock1	0.0130	59.53	T	F	1	F
	Structure104 ExpLibOpt sdf 104 dock7	0.0130	59.31	T	F	2	F
	Structure104 ExpLibOpt sdf 104 dock6	0.0130	59.27	T	F	1	F
	Structure104 ExpLibOpt sdf 104 dock5	0.0130	59.19	T	F	1	F
	Structure104 ExpLibOpt sdf 104 dock4	0.0130	57.30	F	F	1	F
105	Structure105 ExpLibOpt sdf 105 dock2	0.0060	71.20	T	T	3	F
	Structure105 ExpLibOpt sdf 105 dock1	0.0060	70.86	T	T	3	F
	Structure105 ExpLibOpt sdf 105 dock3	0.0060	70.32	T	T	3	F
106	Structure106 ExpLibOpt sdf 106 dock1	0.0250	73.81	T	T	5	T
	Structure106 ExpLibOpt sdf 106 dock3	0.0250	73.49	T	T	5	T
	Structure106 ExpLibOpt sdf 106 dock2	0.0250	73.06	T	T	5	T
107	Structure107 ExpLibOpt sdf 107 dock3	0.0300	63.10	T	F	1	F
	Structure107 ExpLibOpt sdf 107 dock1	0.0300	61.21	T	T	3	F
	Structure107 ExpLibOpt sdf 107 dock5	0.0300	60.90	T	T	3	F
	Structure107 ExpLibOpt sdf 107 dock6	0.0300	60.40	T	F	2	F
	Structure107 ExpLibOpt sdf 107 dock4	0.0300	59.80	T	T	3	F

	Structure107 ExpLibOpt sdf 107 dock10	0.0300	59.10	T	T	5	T
	Structure107 ExpLibOpt sdf 107 dock7	0.0300	58.79	T	F	3	F
	Structure107 ExpLibOpt sdf 107 dock9	0.0300	58.44	T	T	2	F
	Structure107 ExpLibOpt sdf 107 dock2	0.0300	56.24	T	T	2	F
	Structure107 ExpLibOpt sdf 107 dock8	0.0300	54.92	T	T	3	F
108	Structure108 ExpLibOpt sdf 108 dock10	0.0600	71.15	T	T	5	T
	Structure108 ExpLibOpt sdf 108 dock1	0.0600	70.91	T	T	5	T
	Structure108 ExpLibOpt sdf 108 dock7	0.0600	70.30	T	T	2	F
	Structure108 ExpLibOpt sdf 108 dock4	0.0600	69.86	T	T	2	F
	Structure108 ExpLibOpt sdf 108 dock2	0.0600	69.71	T	T	2	F
	Structure108 ExpLibOpt sdf 108 dock9	0.0600	69.63	T	F	1	F
	Structure108 ExpLibOpt sdf 108 dock3	0.0600	69.36	T	T	5	T
	Structure108 ExpLibOpt sdf 108 dock8	0.0600	69.00	T	T	5	T
	Structure108 ExpLibOpt sdf 108 dock5	0.0600	68.84	T	T	5	T
109	Structure109 ExpLibOpt sdf 109 dock1	0.2000	65.28	T	T	5	T
	Structure109 ExpLibOpt sdf 109 dock3	0.2000	62.97	T	T	5	T
	Structure109 ExpLibOpt sdf 109 dock2	0.2000	62.75	T	T	4	T
110	Structure110 ExpLibOpt sdf 110 dock1	0.3900	73.04	T	T	5	T
	Structure110 ExpLibOpt sdf 110 dock2	0.3900	72.84	T	T	5	T
	Structure110 ExpLibOpt sdf 110 dock3	0.3900	72.43	T	T	5	T
111	Structure111 ExpLibOpt sdf 111 dock4	0.7800	69.88	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock5	0.7800	69.23	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock3	0.7800	69.08	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock2	0.7800	67.76	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock1	0.7800	67.67	T	T	5	T
112	Structure112 ExpLibOpt sdf 112 dock2	1.5600	67.07	T	T	2	F
	Structure112 ExpLibOpt sdf 112 dock3	1.5600	67.01	T	T	2	F
	Structure112 ExpLibOpt sdf 112 dock1	1.5600	66.58	T	T	2	F
113	Structure113 ExpLibOpt sdf 113 dock1	0.3900	66.01	T	T	2	F
	Structure113 ExpLibOpt sdf 113 dock3	0.3900	64.38	T	T	2	F
	Structure113 ExpLibOpt sdf 113 dock2	0.3900	63.93	T	T	5	T

114	Structure114 ExpLibOpt sdf 114 dock5	0.1000	86.82	T	T	5	T
	Structure114 ExpLibOpt sdf 114 dock2	0.1000	86.51	T	T	5	T
	Structure114 ExpLibOpt sdf 114 dock1	0.1000	86.13	T	T	5	T
	Structure114 ExpLibOpt sdf 114 dock4	0.1000	76.46	T	T	4	T
	Structure114 ExpLibOpt sdf 114 dock3	0.1000	76.10	T	T	4	T
115	Structure115 ExpLibOpt sdf 115 dock1	0.1000	76.53	T	T	5	T
	Structure115 ExpLibOpt sdf 115 dock2	0.1000	75.97	T	T	5	T
	Structure115 ExpLibOpt sdf 115 dock3	0.1000	75.28	T	T	5	T
116	Structure116 ExpLibOpt sdf 116 dock2	0.1000	73.77	F	F	2	F
	Structure116 ExpLibOpt sdf 116 dock4	0.1000	73.76	F	F	1	F
	Structure116 ExpLibOpt sdf 116 dock1	0.1000	73.23	F	F	1	F
	Structure116 ExpLibOpt sdf 116 dock3	0.1000	67.14	T	T	1	F
117	Structure117 ExpLibOpt sdf 117 dock3	0.2000	63.96	T	T	1	F
	Structure117 ExpLibOpt sdf 117 dock4	0.2000	63.74	T	T	5	T
	Structure117 ExpLibOpt sdf 117 dock1	0.2000	62.54	T	T	5	T
	Structure117 ExpLibOpt sdf 117 dock2	0.2000	61.02	T	T	4	T
118	Structure118 ExpLibOpt sdf 118 dock3	0.0015	67.63	T	F	0	F
	Structure118 ExpLibOpt sdf 118 dock1	0.0015	67.48	T	F	1	F
	Structure118 ExpLibOpt sdf 118 dock2	0.0015	67.43	T	F	0	F
119	Structure119 ExpLibOpt sdf 119 dock2	0.0250	76.75	T	T	4	T
	Structure119 ExpLibOpt sdf 119 dock1	0.0250	75.73	T	T	4	T
	Structure119 ExpLibOpt sdf 119 dock3	0.0250	75.69	T	T	4	T
120	Structure120 ExpLibOpt sdf 120 dock1	0.3900	76.32	T	T	5	T
	Structure120 ExpLibOpt sdf 120 dock3	0.3900	74.07	T	T	5	T
	Structure120 ExpLibOpt sdf 120 dock2	0.3900	73.81	T	T	5	T
121	Structure121 ExpLibOpt sdf 121 dock4	0.0125	75.82	F	F	0	F
	Structure121 ExpLibOpt sdf 121 dock10	0.0125	69.67	F	F	0	F
	Structure121 ExpLibOpt sdf 121 dock5	0.0125	66.89	F	F	1	F
	Structure121 ExpLibOpt sdf 121 dock3	0.0125	60.12	T	T	2	F
	Structure121 ExpLibOpt sdf 121 dock6	0.0125	50.27	F	F	0	F
	Structure121 ExpLibOpt sdf 121 dock9	0.0125	37.59	F	F	0	F
	Structure121 ExpLibOpt sdf 121 dock8	0.0125	36.59	F	F	0	F

	Structure121 ExpLibOpt sdf 121 dock1	0.0125	35.76	F	F	0	F
	Structure121 ExpLibOpt sdf 121 dock7	0.0125	35.47	F	F	0	F
	Structure121 ExpLibOpt sdf 121 dock2	0.0125	33.25	F	F	0	F
122	Structure122 ExpLibOpt sdf 122 dock4	0.3900	64.34	F	F	1	F
	Structure122 ExpLibOpt sdf 122 dock3	0.3900	57.85	F	F	1	F
	Structure122 ExpLibOpt sdf 122 dock5	0.3900	57.40	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock7	0.3900	56.80	T	F	1	F
	Structure122 ExpLibOpt sdf 122 dock1	0.3900	51.66	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock10	0.3900	50.13	T	F	0	F
	Structure122 ExpLibOpt sdf 122 dock2	0.3900	48.27	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock6	0.3900	47.29	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock9	0.3900	45.80	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock8	0.3900	38.95	F	F	0	F
123	Structure123 ExpLibOpt sdf 123 dock6	0.3900	63.43	F	F	1	F
	Structure123 ExpLibOpt sdf 123 dock4	0.3900	59.27	F	F	1	F
	Structure123 ExpLibOpt sdf 123 dock5	0.3900	57.90	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock1	0.3900	56.57	T	F	0	F
	Structure123 ExpLibOpt sdf 123 dock2	0.3900	55.34	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock7	0.3900	47.06	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock3	0.3900	38.99	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock9	0.3900	25.87	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock8	0.3900	23.10	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock10	0.3900	16.98	F	F	0	F
124	Structure124 ExpLibOpt sdf 124 dock8	0.2000	80.75	T	T	3	F
	Structure124 ExpLibOpt sdf 124 dock5	0.2000	65.73	F	F	1	F
	Structure124 ExpLibOpt sdf 124 dock10	0.2000	56.66	F	F	0	F
	Structure124 ExpLibOpt sdf 124 dock1	0.2000	55.35	F	F	0	F
	Structure124 ExpLibOpt sdf 124 dock7	0.2000	54.12	F	F	0	F
	Structure124 ExpLibOpt sdf 124 dock3	0.2000	53.96	F	F	0	F
	Structure124 ExpLibOpt sdf 124 dock9	0.2000	53.45	F	F	0	F
	Structure124 ExpLibOpt sdf 124 dock4	0.2000	50.69	F	F	0	F
	Structure124 ExpLibOpt sdf 124 dock2	0.2000	50.45	F	F	0	F

	Structure124 ExpLibOpt sdf 124 dock6	0.2000	45.93	F	F	1	F
125	Structure125 ExpLibOpt sdf 125 dock5	0.2000	66.44	F	F	0	F
	Structure125 ExpLibOpt sdf 125 dock4	0.2000	58.77	F	F	0	F
	Structure125 ExpLibOpt sdf 125 dock2	0.2000	57.15	F	F	0	F
	Structure125 ExpLibOpt sdf 125 dock1	0.2000	45.78	F	F	0	F
	Structure125 ExpLibOpt sdf 125 dock3	0.2000	45.36	F	F	0	F
126	Structure126 ExpLibOpt sdf 126 dock9	0.3900	67.69	F	F	0	F
	Structure126 ExpLibOpt sdf 126 dock3	0.3900	67.48	F	F	0	F
	Structure126 ExpLibOpt sdf 126 dock7	0.3900	62.04	F	F	1	F
	Structure126 ExpLibOpt sdf 126 dock8	0.3900	61.78	F	F	0	F
	Structure126 ExpLibOpt sdf 126 dock6	0.3900	59.50	F	F	0	F
	Structure126 ExpLibOpt sdf 126 dock1	0.3900	59.48	F	F	0	F
	Structure126 ExpLibOpt sdf 126 dock5	0.3900	55.82	F	F	0	F
	Structure126 ExpLibOpt sdf 126 dock10	0.3900	54.83	F	F	0	F
	Structure126 ExpLibOpt sdf 126 dock4	0.3900	47.70	F	F	0	F
	Structure126 ExpLibOpt sdf 126 dock2	0.3900	42.67	F	F	0	F
127	Structure127 ExpLibOpt sdf 127 dock7	0.7800	64.74	F	F	1	F
	Structure127 ExpLibOpt sdf 127 dock3	0.7800	52.47	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock6	0.7800	52.15	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock9	0.7800	47.69	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock5	0.7800	44.78	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock1	0.7800	40.36	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock2	0.7800	37.81	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock8	0.7800	37.39	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock4	0.7800	36.39	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock10	0.7800	35.30	F	F	0	F
128	Structure128 ExpLibOpt sdf 128 dock2	0.1000	83.45	T	T	5	T
	Structure128 ExpLibOpt sdf 128 dock9	0.1000	81.99	T	T	3	F
	Structure128 ExpLibOpt sdf 128 dock1	0.1000	78.04	F	F	0	F
	Structure128 ExpLibOpt sdf 128 dock8	0.1000	73.08	T	F	0	F
	Structure128 ExpLibOpt sdf 128 dock10	0.1000	66.67	F	F	1	F
	Structure128 ExpLibOpt sdf 128 dock7	0.1000	58.88	F	F	0	F

	Structure128 ExpLibOpt sdf 128 dock5	0.1000	58.85	F	F	1	F
	Structure128 ExpLibOpt sdf 128 dock3	0.1000	52.98	F	F	0	F
	Structure128 ExpLibOpt sdf 128 dock6	0.1000	52.13	F	F	0	F
	Structure128 ExpLibOpt sdf 128 dock4	0.1000	49.59	F	F	0	F
129	Structure129 ExpLibOpt sdf 129 dock8	0.2000	76.24	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock2	0.2000	72.83	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock6	0.2000	58.56	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock10	0.2000	50.82	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock1	0.2000	45.27	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock5	0.2000	40.72	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock3	0.2000	36.93	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock7	0.2000	35.14	F	F	1	F
	Structure129 ExpLibOpt sdf 129 dock4	0.2000	30.15	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock9	0.2000	30.04	F	F	0	F
130	Structure130 ExpLibOpt sdf 130 dock2	0.3900	74.12	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock7	0.3900	70.03	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock1	0.3900	57.29	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock8	0.3900	54.03	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock9	0.3900	52.99	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock5	0.3900	52.46	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock6	0.3900	50.52	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock10	0.3900	49.91	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock4	0.3900	46.22	F	F	0	F
131	Structure131 ExpLibOpt sdf 131 dock8	0.7800	69.35	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock7	0.7800	59.34	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock4	0.7800	58.47	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock9	0.7800	52.82	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock1	0.7800	42.70	T	F	0	F
	Structure131 ExpLibOpt sdf 131 dock3	0.7800	35.02	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock2	0.7800	32.67	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock6	0.7800	24.13	F	F	0	F

	Structure131 ExpLibOpt sdf 131 dock10	0.7800	16.10	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock5	0.7800	10.23	F	F	0	F
132	Structure132 ExpLibOpt sdf 132 dock4	0.7800	83.19	T	T	2	F
	Structure132 ExpLibOpt sdf 132 dock3	0.7800	73.20	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock5	0.7800	72.61	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock10	0.7800	66.56	F	F	1	F
	Structure132 ExpLibOpt sdf 132 dock1	0.7800	61.69	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock7	0.7800	49.74	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock6	0.7800	47.20	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock8	0.7800	45.90	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock9	0.7800	45.49	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock2	0.7800	33.66	F	F	0	F
133	Structure133 ExpLibOpt sdf 133 dock7	0.1000	84.75	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock4	0.1000	75.55	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock6	0.1000	73.85	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock5	0.1000	71.82	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock2	0.1000	69.51	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock3	0.1000	59.90	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock1	0.1000	55.09	F	F	0	F
134	Structure134 ExpLibOpt sdf 134 dock10	0.1000	76.54	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock2	0.1000	73.21	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock1	0.1000	72.45	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock5	0.1000	72.11	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock4	0.1000	69.61	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock7	0.1000	64.28	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock6	0.1000	64.15	F	F	1	F
	Structure134 ExpLibOpt sdf 134 dock8	0.1000	59.70	F	F	1	F
	Structure134 ExpLibOpt sdf 134 dock9	0.1000	57.66	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock3	0.1000	22.75	F	F	0	F
135	Structure135 ExpLibOpt sdf 135 dock4	0.1000	96.66	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock7	0.1000	89.09	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock2	0.1000	85.36	F	F	0	F

	Structure135 ExpLibOpt sdf 135 dock1	0.1000	74.13	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock3	0.1000	73.39	F	F	1	F
	Structure135 ExpLibOpt sdf 135 dock8	0.1000	63.37	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock6	0.1000	60.08	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock5	0.1000	53.00	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock10	0.1000	46.92	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock9	0.1000	37.72	F	F	1	F
136	Structure136 ExpLibOpt sdf 136 dock8	1.2600	89.06	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock3	1.2600	79.53	T	F	0	F
	Structure136 ExpLibOpt sdf 136 dock9	1.2600	78.00	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock1	1.2600	71.13	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock6	1.2600	68.23	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock5	1.2600	66.40	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock2	1.2600	65.41	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock4	1.2600	65.30	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock7	1.2600	60.77	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock10	1.2600	60.27	F	F	0	F
137	Structure137 ExpLibOpt sdf 137 dock2	1.3000	88.03	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock5	1.3000	80.95	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock3	1.3000	76.90	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock7	1.3000	75.37	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock8	1.3000	74.54	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock9	1.3000	69.96	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock1	1.3000	68.72	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock4	1.3000	63.59	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock10	1.3000	62.73	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock6	1.3000	46.93	F	F	0	F
138	Structure138 ExpLibOpt sdf 138 dock7	0.0031	86.80	F	F	0	F
	Structure138 ExpLibOpt sdf 138 dock3	0.0031	78.62	F	F	1	F
	Structure138 ExpLibOpt sdf 138 dock9	0.0031	78.09	F	F	2	F
	Structure138 ExpLibOpt sdf 138 dock6	0.0031	74.75	T	T	4	T
	Structure138 ExpLibOpt sdf 138 dock10	0.0031	74.37	F	F	2	F

	Structure138 ExpLibOpt sdf 138 dock1	0.0031	72.79	F	F	1	F
	Structure138 ExpLibOpt sdf 138 dock2	0.0031	69.94	F	F	1	F
	Structure138 ExpLibOpt sdf 138 dock4	0.0031	69.34	T	T	5	T
	Structure138 ExpLibOpt sdf 138 dock5	0.0031	69.21	T	T	5	T
	Structure138 ExpLibOpt sdf 138 dock8	0.0031	67.77	F	F	2	F
139	Structure139 ExpLibOpt sdf 139 dock2	0.3300	74.79	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock9	0.3300	73.93	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock1	0.3300	70.29	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock7	0.3300	69.20	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock5	0.3300	69.03	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock4	0.3300	67.79	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock3	0.3300	66.12	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock10	0.3300	65.36	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock8	0.3300	64.55	F	F	0	F
140	Structure140 ExpLibOpt sdf 140 dock6	0.3300	62.67	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock8	0.1600	79.38	F	F	1	F
	Structure140 ExpLibOpt sdf 140 dock7	0.1600	73.23	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock6	0.1600	69.11	F	F	2	F
	Structure140 ExpLibOpt sdf 140 dock2	0.1600	67.97	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock9	0.1600	65.99	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock3	0.1600	64.26	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock1	0.1600	63.40	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock5	0.1600	63.30	F	F	0	F
141	Structure140 ExpLibOpt sdf 140 dock10	0.1600	62.94	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock4	0.1600	59.26	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock7	0.3200	87.16	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock4	0.3200	86.94	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock5	0.3200	86.46	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock1	0.3200	85.77	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock2	0.3200	84.61	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock6	0.3200	79.52	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock3	0.3200	73.76	F	F	0	F

142	Structure142 ExpLibOpt sdf 142 dock4	0.0400	66.70	F	F	0	F
	Structure142 ExpLibOpt sdf 142 dock3	0.0400	64.99	F	F	0	F
	Structure142 ExpLibOpt sdf 142 dock5	0.0400	60.93	F	F	0	F
	Structure142 ExpLibOpt sdf 142 dock1	0.0400	55.10	F	F	0	F
	Structure142 ExpLibOpt sdf 142 dock2	0.0400	42.13	F	F	0	F
143	Structure143 ExpLibOpt sdf 143 dock1	0.7800	77.72	T	F	0	F
	Structure143 ExpLibOpt sdf 143 dock6	0.7800	72.74	F	F	0	F
	Structure143 ExpLibOpt sdf 143 dock7	0.7800	72.55	F	F	0	F
	Structure143 ExpLibOpt sdf 143 dock3	0.7800	68.95	F	F	0	F
	Structure143 ExpLibOpt sdf 143 dock2	0.7800	68.18	F	F	0	F
	Structure143 ExpLibOpt sdf 143 dock10	0.7800	67.24	F	F	0	F
	Structure143 ExpLibOpt sdf 143 dock5	0.7800	66.88	F	F	0	F
	Structure143 ExpLibOpt sdf 143 dock4	0.7800	64.05	F	F	0	F
	Structure143 ExpLibOpt sdf 143 dock8	0.7800	63.39	F	F	0	F
144	Structure143 ExpLibOpt sdf 143 dock9	0.7800	62.11	F	F	0	F
	Structure144 ExpLibOpt sdf 144 dock3	0.2000	80.32	T	T	5	T
	Structure144 ExpLibOpt sdf 144 dock9	0.2000	77.64	F	F	1	F
	Structure144 ExpLibOpt sdf 144 dock10	0.2000	71.25	F	F	0	F
	Structure144 ExpLibOpt sdf 144 dock5	0.2000	70.56	F	F	0	F
	Structure144 ExpLibOpt sdf 144 dock1	0.2000	68.16	F	F	0	F
	Structure144 ExpLibOpt sdf 144 dock6	0.2000	67.93	F	F	1	F
	Structure144 ExpLibOpt sdf 144 dock8	0.2000	66.32	F	F	0	F
	Structure144 ExpLibOpt sdf 144 dock4	0.2000	65.90	T	F	3	F
145	Structure144 ExpLibOpt sdf 144 dock2	0.2000	58.77	F	F	0	F
	Structure144 ExpLibOpt sdf 144 dock7	0.2000	45.03	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock6	0.1000	84.68	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock10	0.1000	80.98	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock5	0.1000	67.09	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock4	0.1000	58.24	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock1	0.1000	53.48	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock2	0.1000	48.15	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock3	0.1000	47.45	F	F	0	F

Structure145 ExpLibOpt sdf 145 dock8	0.1000	46.51	F	F	0	F
Structure145 ExpLibOpt sdf 145 dock7	0.1000	42.89	F	F	0	F
Structure145 ExpLibOpt sdf 145 dock9	0.1000	22.11	F	F	0	F

Legend	
GSF	GOLDScore Fitness Function
VO	Visual Orientation
VF	Visual Fitness
NMPF	Number of Matching Pharmacophoric Features

b) N473T_{mod}.

Cluster ID	DOCK POSE	MICexp	GSF	VO (T/F)	VF (T/F)	NMPF (4-5)	Result (T/F)
1	Structure001 ExpLibOpt sdf 1 dock1	3.0000	70.81	T	T	5	T
	Structure001 ExpLibOpt sdf 1 dock2	3.0000	69.67	T	T	4	T
	Structure001 ExpLibOpt sdf 1 dock4	3.0000	69.45	T	T	4	T
2	Structure002 ExpLibOpt sdf 2 dock3	0.0115	67.49	T	F	1	F
	Structure002 ExpLibOpt sdf 2 dock1	0.0115	67.43	T	F	1	F
	Structure002 ExpLibOpt sdf 2 dock5	0.0115	67.38	T	F	1	F
3	Structure003 ExpLibOpt sdf 3 dock6	0.3000	64.91	T	F	0	F
	Structure003 ExpLibOpt sdf 3 dock3	0.3000	64.81	T	F	1	F
	Structure003 ExpLibOpt sdf 3 dock2	0.3000	62.40	T	F	1	F
4	Structure004 ExpLibOpt sdf 4 dock3	0.0100	64.38	F	F	1	F
	Structure004 ExpLibOpt sdf 4 dock2	0.0100	64.07	F	F	1	F
	Structure004 ExpLibOpt sdf 4 dock1	0.0100	63.86	F	F	0	F
5	Structure005 ExpLibOpt sdf 5 dock1	0.3000	66.24	F	F	0	F
	Structure005 ExpLibOpt sdf 5 dock6	0.3000	63.12	F	F	0	F
	Structure005 ExpLibOpt sdf 5 dock2	0.3000	61.27	T	F	2	F
6	Structure006 ExpLibOpt sdf 6 dock1	0.1200	65.38	T	F	1	F
	Structure006 ExpLibOpt sdf 6 dock3	0.1200	65.37	F	F	1	F
	Structure006 ExpLibOpt sdf 6 dock2	0.1200	65.13	F	F	1	F
7	Structure007 ExpLibOpt sdf 7 dock9	3.5000	64.09	F	F	1	F
	Structure007 ExpLibOpt sdf 7 dock1	3.5000	63.70	T	T	4	T
	Structure007 ExpLibOpt sdf 7 dock5	3.5000	63.23	T	T	5	T
8	Structure008 ExpLibOpt sdf 8 dock1	0.1000	66.80	T	T	5	T
	Structure008 ExpLibOpt sdf 8 dock3	0.1000	66.62	T	T	5	T
	Structure008 ExpLibOpt sdf 8 dock2	0.1000	66.58	T	T	5	T
9	Structure009 ExpLibOpt sdf 9 dock6	1.4000	64.60	F	F	0	F
	Structure009 ExpLibOpt sdf 9 dock4	1.4000	64.14	F	F	0	F
	Structure009 ExpLibOpt sdf 9 dock2	1.4000	63.77	F	F	0	F
10	Structure010 ExpLibOpt sdf 10 dock3	3.2000	64.47	T	T	5	T
	Structure010 ExpLibOpt sdf 10 dock1	3.2000	64.25	T	F	0	F

	Structure010 ExpLibOpt sdf 10 dock2	3.2000	63.88	T	T	5	T
11	Structure011 ExpLibOpt sdf 11 dock2	0.0500	73.27	T	T	4	T
	Structure011 ExpLibOpt sdf 11 dock3	0.0500	73.17	T	F	3	F
	Structure011 ExpLibOpt sdf 11 dock1	0.0500	71.82	T	T	5	T
12	Structure012 ExpLibOpt sdf 12 dock1	0.5000	79.05	T	T	5	T
	Structure012 ExpLibOpt sdf 12 dock2	0.5000	78.52	T	T	5	T
	Structure012 ExpLibOpt sdf 12 dock3	0.5000	76.44	T	F	2	F
13	Structure013 ExpLibOpt sdf 13 dock3	1.6000	59.22	T	F	1	F
	Structure013 ExpLibOpt sdf 13 dock1	1.6000	59.04	T	F	2	F
	Structure013 ExpLibOpt sdf 13 dock2	1.6000	57.92	T	F	3	F
14	Structure014 ExpLibOpt sdf 14 dock1	0.5000	75.87	F	F	1	F
	Structure014 ExpLibOpt sdf 14 dock4	0.5000	71.74	T	T	4	T
	Structure014 ExpLibOpt sdf 14 dock5	0.5000	71.17	T	T	4	T
15	Structure015 ExpLibOpt sdf 15 dock5	0.5000	65.86	F	F	0	F
	Structure015 ExpLibOpt sdf 15 dock2	0.5000	65.63	F	F	0	F
	Structure015 ExpLibOpt sdf 15 dock1	0.5000	63.42	T	F	1	F
16	Structure016 ExpLibOpt sdf 16 dock2	2.0000	61.33	F	F	2	F
	Structure016 ExpLibOpt sdf 16 dock4	2.0000	61.20	F	F	2	F
	Structure016 ExpLibOpt sdf 16 dock1	2.0000	61.01	F	F	2	F
17	Structure017 ExpLibOpt sdf 17 dock1	0.5000	75.94	T	T	5	T
	Structure017 ExpLibOpt sdf 17 dock2	0.5000	75.93	T	T	5	T
	Structure017 ExpLibOpt sdf 17 dock3	0.5000	72.22	T	T	5	T
18	Structure018 ExpLibOpt sdf 18 dock4	0.5000	64.75	F	F	0	F
	Structure018 ExpLibOpt sdf 18 dock1	0.5000	64.45	F	F	1	F
	Structure018 ExpLibOpt sdf 18 dock2	0.5000	64.42	F	F	0	F
19	Structure019 ExpLibOpt sdf 19 dock2	0.2500	74.83	F	F	0	F
	Structure019 ExpLibOpt sdf 19 dock3	0.2500	74.10	F	F	0	F
	Structure019 ExpLibOpt sdf 19 dock1	0.2500	73.29	F	F	1	F
20	Structure020 ExpLibOpt sdf 20 dock1	0.0100	67.89	T	T	4	T
	Structure020 ExpLibOpt sdf 20 dock2	0.0100	67.80	T	T	4	T
	Structure020 ExpLibOpt sdf 20 dock3	0.0100	67.22	T	T	4	T
21	Structure021 ExpLibOpt sdf 21 dock3	0.0310	78.48	T	T	5	T

	Structure021 ExpLibOpt sdf 21 dock2	0.0310	78.35	T	T	5	T
	Structure021 ExpLibOpt sdf 21 dock1	0.0310	78.14	T	T	5	T
22	Structure022 ExpLibOpt sdf 22 dock3	0.0100	70.54	T	T	4	T
	Structure022 ExpLibOpt sdf 22 dock1	0.0100	70.18	T	T	5	T
	Structure022 ExpLibOpt sdf 22 dock2	0.0100	66.69	F	T	2	F
23	Structure023 ExpLibOpt sdf 23 dock4	0.0100	63.02	T	T	4	T
	Structure023 ExpLibOpt sdf 23 dock2	0.0100	62.84	T	T	4	T
	Structure023 ExpLibOpt sdf 23 dock1	0.0100	62.77	T	T	4	T
24	Structure024 ExpLibOpt sdf 24 dock7	0.9000	80.29	T	T	4	T
	Structure024 ExpLibOpt sdf 24 dock2	0.9000	78.60	T	F	2	F
	Structure024 ExpLibOpt sdf 24 dock4	0.9000	76.97	T	T	4	T
25	Structure025 ExpLibOpt sdf 25 dock3	0.1250	69.27	T	T	5	T
	Structure025 ExpLibOpt sdf 25 dock1	0.1250	69.26	T	T	5	T
	Structure025 ExpLibOpt sdf 25 dock2	0.1250	68.49	T	T	5	T
26	Structure026 ExpLibOpt sdf 26 dock1	0.3000	65.01	T	F	3	F
	Structure026 ExpLibOpt sdf 26 dock2	0.3000	64.56	T	T	5	T
	Structure026 ExpLibOpt sdf 26 dock3	0.3000	64.12	T	F	1	F
27	Structure027 ExpLibOpt sdf 27 dock2	0.1200	71.05	T	F	0	F
	Structure027 ExpLibOpt sdf 27 dock3	0.1200	70.26	T	F	0	F
	Structure027 ExpLibOpt sdf 27 dock1	0.1200	69.73	T	F	0	F
28	Structure028 ExpLibOpt sdf 28 dock1	0.0040	62.91	T	F	0	F
	Structure028 ExpLibOpt sdf 28 dock3	0.0040	61.82	T	F	0	F
	Structure028 ExpLibOpt sdf 28 dock2	0.0040	61.01	T	F	2	F
29	Structure029 ExpLibOpt sdf 29 dock1	2.0000	75.71	T	T	4	T
	Structure029 ExpLibOpt sdf 29 dock3	2.0000	75.68	T	T	4	T
	Structure029 ExpLibOpt sdf 29 dock2	2.0000	75.25	T	T	4	T
30	Structure030 ExpLibOpt sdf 30 dock1	0.3900	65.53	T	F	2	F
	Structure030 ExpLibOpt sdf 30 dock2	0.3900	64.56	T	F	2	F
	Structure030 ExpLibOpt sdf 30 dock3	0.3900	64.37	T	F	2	F
31	Structure031 ExpLibOpt sdf 31 dock1	0.0600	73.42	T	T	5	T
	Structure031 ExpLibOpt sdf 31 dock2	0.0600	72.60	T	T	5	T
	Structure031 ExpLibOpt sdf 31 dock3	0.0600	69.64	T	T	5	T

32	Structure032 ExpLibOpt sdf 32 dock1	0.3900	72.21	F	F	1	F
	Structure032 ExpLibOpt sdf 32 dock2	0.3900	71.54	F	F	1	F
	Structure032 ExpLibOpt sdf 32 dock3	0.3900	70.00	T	F	2	F
33	Structure033 ExpLibOpt sdf 33 dock3	0.3900	72.90	F	F	0	F
	Structure033 ExpLibOpt sdf 33 dock1	0.3900	71.65	F	F	1	F
	Structure033 ExpLibOpt sdf 33 dock2	0.3900	70.23	T	F	1	F
34	Structure034 ExpLibOpt sdf 34 dock6	0.7800	72.02	T	T	5	T
	Structure034 ExpLibOpt sdf 34 dock5	0.7800	71.27	T	T	5	T
	Structure034 ExpLibOpt sdf 34 dock8	0.7800	70.51	T	T	5	T
35	Structure035 ExpLibOpt sdf 35 dock2	0.7800	71.59	T	T	5	T
	Structure035 ExpLibOpt sdf 35 dock1	0.7800	71.05	T	T	3	F
	Structure035 ExpLibOpt sdf 35 dock3	0.7800	70.72	T	T	5	T
36	Structure036 ExpLibOpt sdf 36 dock2	0.7800	67.07	T	T	5	T
	Structure036 ExpLibOpt sdf 36 dock1	0.7800	66.50	T	T	5	T
	Structure036 ExpLibOpt sdf 36 dock3	0.7800	65.18	T	T	5	T
37	Structure037 ExpLibOpt sdf 37 dock9	0.1250	70.64	T	T	4	T
	Structure037 ExpLibOpt sdf 37 dock1	0.1250	70.64	T	T	4	T
	Structure037 ExpLibOpt sdf 37 dock6	0.1250	70.45	T	F	2	F
38	Structure038 ExpLibOpt sdf 38 dock1	0.0020	71.61	T	T	4	T
	Structure038 ExpLibOpt sdf 38 dock2	0.0020	70.60	T	T	4	T
	Structure038 ExpLibOpt sdf 38 dock3	0.0020	70.14	T	T	4	T
39	Structure039 ExpLibOpt sdf 39 dock1	0.1100	65.63	T	T	5	T
	Structure039 ExpLibOpt sdf 39 dock3	0.1100	65.11	T	T	5	T
	Structure039 ExpLibOpt sdf 39 dock2	0.1100	64.96	T	T	5	T
40	Structure040 ExpLibOpt sdf 40 dock1	0.0120	67.45	T	T	5	T
	Structure040 ExpLibOpt sdf 40 dock3	0.0120	66.47	T	T	5	T
	Structure040 ExpLibOpt sdf 40 dock2	0.0120	65.00	T	T	5	T
41	Structure041 ExpLibOpt sdf 41 dock3	0.2500	66.18	T	T	4	T
	Structure041 ExpLibOpt sdf 41 dock4	0.2500	66.05	T	T	4	T
	Structure041 ExpLibOpt sdf 41 dock1	0.2500	64.75	T	T	4	T
42	Structure042 ExpLibOpt sdf 42 dock2	0.0160	74.63	T	T	4	T
	Structure042 ExpLibOpt sdf 42 dock1	0.0160	74.11	T	T	3	F

	Structure042 ExpLibOpt sdf 42 dock3	0.0160	73.89	T	T	3	F
43	Structure043 ExpLibOpt sdf 43 dock1	0.6000	67.82	T	F	1	F
	Structure043 ExpLibOpt sdf 43 dock3	0.6000	67.69	T	F	1	F
	Structure043 ExpLibOpt sdf 43 dock2	0.6000	65.45	T	T	4	T
	Structure044 ExpLibOpt sdf 44 dock1	0.3900	59.31	T	T	5	T
44	Structure044 ExpLibOpt sdf 44 dock2	0.3900	58.98	T	T	4	T
	Structure044 ExpLibOpt sdf 44 dock3	0.3900	58.62	T	F	2	F
45	Structure045 ExpLibOpt sdf 45 dock1	0.3000	71.65	T	T	5	T
	Structure045 ExpLibOpt sdf 45 dock2	0.3000	71.38	T	T	5	T
	Structure045 ExpLibOpt sdf 45 dock3	0.3000	71.04	T	T	5	T
46	Structure046 ExpLibOpt sdf 46 dock1	0.0300	70.63	T	T	5	T
	Structure046 ExpLibOpt sdf 46 dock2	0.0300	70.17	T	T	5	T
	Structure046 ExpLibOpt sdf 46 dock3	0.0300	68.98	T	T	5	T
47	Structure047 ExpLibOpt sdf 47 dock1	0.1250	70.78	T	F	2	F
	Structure047 ExpLibOpt sdf 47 dock3	0.1250	70.40	T	F	3	F
	Structure047 ExpLibOpt sdf 47 dock2	0.1250	70.37	T	T	5	T
48	Structure048 ExpLibOpt sdf 48 dock2	0.1250	66.93	T	T	5	T
	Structure048 ExpLibOpt sdf 48 dock3	0.1250	66.82	T	F	1	F
	Structure048 ExpLibOpt sdf 48 dock1	0.1250	66.22	T	T	5	T
49	Structure049 ExpLibOpt sdf 49 dock1	0.5000	74.55	T	T	4	T
	Structure049 ExpLibOpt sdf 49 dock3	0.5000	74.32	T	T	4	T
	Structure049 ExpLibOpt sdf 49 dock2	0.5000	73.90	T	T	4	T
50	Structure050 ExpLibOpt sdf 50 dock9	0.0016	88.44	F	F	0	F
	Structure050 ExpLibOpt sdf 50 dock1	0.0016	84.75	F	F	0	F
	Structure050 ExpLibOpt sdf 50 dock8	0.0016	80.37	F	F	1	F
51	Structure051 ExpLibOpt sdf 51 dock7	6.3000	82.11	T	F	3	F
	Structure051 ExpLibOpt sdf 51 dock2	6.3000	81.54	T	F	0	F
	Structure051 ExpLibOpt sdf 51 dock6	6.3000	80.26	T	F	1	F
52	Structure052 ExpLibOpt sdf 52 dock9	6.5700	82.96	F	F	0	F
	Structure052 ExpLibOpt sdf 52 dock10	6.5700	81.04	T	F	3	F
	Structure052 ExpLibOpt sdf 52 dock6	6.5700	80.33	T	T	5	T
53	Structure053 ExpLibOpt sdf 53 dock3	5.2000	89.76	F	F	0	F

	Structure053 ExpLibOpt sdf 53 dock2	5.2000	86.77	F	F	0	F
	Structure053 ExpLibOpt sdf 53 dock10	5.2000	85.86	F	F	0	F
54	Structure054 ExpLibOpt sdf 54 dock4	6.9000	93.60	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock2	6.9000	90.39	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock8	6.9000	89.42	T	F	3	F
55	Structure055 ExpLibOpt sdf 55 dock10	6.4500	83.27	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock7	6.4500	81.38	T	F	3	F
	Structure055 ExpLibOpt sdf 55 dock1	6.4500	77.41	F	F	0	F
56	Structure056 ExpLibOpt sdf 56 dock3	6.7000	87.29	T	F	0	F
	Structure056 ExpLibOpt sdf 56 dock4	6.7000	86.30	T	F	3	F
	Structure056 ExpLibOpt sdf 56 dock8	6.7000	85.77	F	F	0	F
57	Structure057 ExpLibOpt sdf 57 dock2	6.3000	91.95	F	F	0	F
	Structure057 ExpLibOpt sdf 57 dock1	6.3000	90.22	F	F	0	F
	Structure057 ExpLibOpt sdf 57 dock9	6.3000	89.59	F	F	0	F
58	Structure058 ExpLibOpt sdf 58 dock3	6.2600	92.71	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock9	6.2600	90.28	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock8	6.2600	82.87	F	F	0	F
59	Structure059 ExpLibOpt sdf 59 dock4	6.9200	91.37	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock5	6.9200	90.85	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock9	6.9200	88.57	F	F	0	F
60	Structure060 ExpLibOpt sdf 60 dock2	0.0300	76.54	T	T	4	T
	Structure060 ExpLibOpt sdf 60 dock1	0.0300	75.82	T	T	4	T
	Structure060 ExpLibOpt sdf 60 dock3	0.0300	75.23	T	T	4	T
61	Structure061 ExpLibOpt sdf 61 dock5	3.2000	66.24	F	F	1	F
	Structure061 ExpLibOpt sdf 61 dock6	3.2000	66.13	F	F	1	F
	Structure061 ExpLibOpt sdf 61 dock9	3.2000	63.12	T	T	4	T
62	Structure062 ExpLibOpt sdf 62 dock1	0.1250	74.79	T	T	5	T
	Structure062 ExpLibOpt sdf 62 dock3	0.1250	73.20	T	T	5	T
	Structure062 ExpLibOpt sdf 62 dock2	0.1250	71.94	T	T	5	T
63	Structure063 ExpLibOpt sdf 63 dock7	0.5000	75.50	T	F	4	F
	Structure063 ExpLibOpt sdf 63 dock5	0.5000	74.73	T	F	1	F
	Structure063 ExpLibOpt sdf 63 dock10	0.5000	74.56	T	F	3	F

64	Structure064 ExpLibOpt sdf 64 dock3	0.0300	78.62	T	T	3	F
	Structure064 ExpLibOpt sdf 64 dock4	0.0300	78.51	T	T	3	F
	Structure064 ExpLibOpt sdf 64 dock2	0.0300	78.26	T	T	3	F
65	Structure065 ExpLibOpt sdf 65 dock1	0.7800	77.72	F	F	0	F
	Structure065 ExpLibOpt sdf 65 dock4	0.7800	77.68	T	T	5	T
	Structure065 ExpLibOpt sdf 65 dock7	0.7800	77.53	T	T	5	T
66	Structure066 ExpLibOpt sdf 66 dock1	0.7800	83.44	T	F	1	F
	Structure066 ExpLibOpt sdf 66 dock2	0.7800	82.90	T	T	5	T
	Structure066 ExpLibOpt sdf 66 dock7	0.7800	82.60	T	F	4	F
67	Structure067 ExpLibOpt sdf 67 dock3	6.2500	78.52	F	F	1	F
	Structure067 ExpLibOpt sdf 67 dock2	6.2500	77.08	T	T	5	T
	Structure067 ExpLibOpt sdf 67 dock6	6.2500	75.40	T	F	0	F
68	Structure068 ExpLibOpt sdf 68 dock1	0.7800	86.46	T	F	0	F
	Structure068 ExpLibOpt sdf 68 dock3	0.7800	81.87	T	T	5	T
	Structure068 ExpLibOpt sdf 68 dock2	0.7800	77.18	T	T	5	T
69	Structure069 ExpLibOpt sdf 69 dock1	1.5600	83.55	T	F	4	F
	Structure069 ExpLibOpt sdf 69 dock7	1.5600	82.44	F	F	0	F
	Structure069 ExpLibOpt sdf 69 dock9	1.5600	79.52	T	F	2	F
70	Structure070 ExpLibOpt sdf 70 dock1	1.5600	83.63	F	F	0	F
	Structure070 ExpLibOpt sdf 70 dock9	1.5600	83.55	F	F	0	F
	Structure070 ExpLibOpt sdf 70 dock3	1.5600	79.06	T	F	5	F
71	Structure071 ExpLibOpt sdf 71 dock7	3.1300	86.75	F	F	0	F
	Structure071 ExpLibOpt sdf 71 dock9	3.1300	84.52	F	F	0	F
	Structure071 ExpLibOpt sdf 71 dock6	3.1300	81.73	T	T	5	T
72	Structure072 ExpLibOpt sdf 72 dock1	7.1200	81.41	T	T	5	T
	Structure072 ExpLibOpt sdf 72 dock6	7.1200	79.52	T	F	3	F
	Structure072 ExpLibOpt sdf 72 dock9	7.1200	79.42	T	T	5	T
73	Structure073 ExpLibOpt sdf 73 dock1	0.0600	66.64	T	T	5	T
	Structure073 ExpLibOpt sdf 73 dock3	0.0600	66.35	T	T	5	T
	Structure073 ExpLibOpt sdf 73 dock2	0.0600	65.28	T	F	5	F
74	Structure074 ExpLibOpt sdf 74 dock4	0.7800	75.51	T	T	4	T
	Structure074 ExpLibOpt sdf 74 dock2	0.7800	73.38	T	T	4	T

	Structure074 ExpLibOpt sdf 74 dock3	0.7800	71.02	T	T	4	T
75	Structure075 ExpLibOpt sdf 75 dock1	0.0625	67.34	T	F	2	F
	Structure075 ExpLibOpt sdf 75 dock2	0.0625	66.89	T	F	2	F
	Structure075 ExpLibOpt sdf 75 dock3	0.0625	65.44	T	F	1	F
	Structure075 ExpLibOpt sdf 75 dock3	0.0625	65.44	T	F	1	F
76	Structure076 ExpLibOpt sdf 76 dock3	0.1250	72.58	T	T	4	T
	Structure076 ExpLibOpt sdf 76 dock2	0.1250	72.40	T	T	4	T
	Structure076 ExpLibOpt sdf 76 dock1	0.1250	68.85	T	F	0	F
77	Structure077 ExpLibOpt sdf 77 dock1	6.2500	79.83	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock10	6.2500	78.74	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock5	6.2500	78.47	F	F	0	F
78	Structure078 ExpLibOpt sdf 78 dock1	3.1300	70.05	T	T	5	T
	Structure078 ExpLibOpt sdf 78 dock2	3.1300	69.83	T	F	3	F
	Structure078 ExpLibOpt sdf 78 dock3	3.1300	69.35	T	F	3	F
79	Structure079 ExpLibOpt sdf 79 dock5	3.1300	80.33	F	F	0	F
	Structure079 ExpLibOpt sdf 79 dock8	3.1300	80.16	F	F	0	F
	Structure079 ExpLibOpt sdf 79 dock1	3.1300	79.93	T	F	2	F
80	Structure080 ExpLibOpt sdf 80 dock2	1.5600	83.59	T	F	1	F
	Structure080 ExpLibOpt sdf 80 dock1	1.5600	83.41	T	F	1	F
	Structure080 ExpLibOpt sdf 80 dock3	1.5600	83.20	T	F	1	F
81	Structure081 ExpLibOpt sdf 81 dock1	0.3900	70.95	F	F	1	F
	Structure081 ExpLibOpt sdf 81 dock4	0.3900	70.26	F	F	0	F
	Structure081 ExpLibOpt sdf 81 dock2	0.3900	69.76	F	F	0	F
82	Structure082 ExpLibOpt sdf 82 dock5	0.0030	92.30	F	F	0	F
	Structure082 ExpLibOpt sdf 82 dock1	0.0030	80.92	T	T	5	T
	Structure082 ExpLibOpt sdf 82 dock10	0.0030	78.40	F	F	1	F
83	Structure083 ExpLibOpt sdf 83 dock2	0.0027	89.72	T	F	5	F
	Structure083 ExpLibOpt sdf 83 dock1	0.0027	86.67	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock7	0.0027	84.91	F	F	0	F
84	Structure084 ExpLibOpt sdf 84 dock5	0.0026	85.50	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock10	0.0026	81.51	F	F	1	F
	Structure084 ExpLibOpt sdf 84 dock2	0.0026	80.70	T	F	3	F
85	Structure085 ExpLibOpt sdf 85 dock2	0.0027	83.64	F	F	0	F

	Structure085 ExpLibOpt sdf 85 dock3	0.0027	81.94	F	F	1	F
	Structure085 ExpLibOpt sdf 85 dock9	0.0027	79.59	T	T	5	T
86	Structure086 ExpLibOpt sdf 86 dock5	0.0012	89.29	T	F	3	F
	Structure086 ExpLibOpt sdf 86 dock7	0.0012	89.19	F	F	0	F
	Structure086 ExpLibOpt sdf 86 dock6	0.0012	87.76	F	F	0	F
87	Structure087 ExpLibOpt sdf 87 dock1	0.0012	85.30	F	F	0	F
	Structure087 ExpLibOpt sdf 87 dock3	0.0012	81.78	F	F	0	F
	Structure087 ExpLibOpt sdf 87 dock9	0.0012	79.97	F	F	1	F
88	Structure088 ExpLibOpt sdf 88 dock1	0.0014	78.99	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock2	0.0014	78.44	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock10	0.0014	78.37	F	F	0	F
89	Structure089 ExpLibOpt sdf 89 dock9	0.0108	87.87	F	F	0	F
	Structure089 ExpLibOpt sdf 89 dock3	0.0108	79.90	F	F	0	F
	Structure089 ExpLibOpt sdf 89 dock8	0.0108	77.99	F	F	0	F
90	Structure090 ExpLibOpt sdf 90 dock3	0.0029	81.84	F	F	0	F
	Structure090 ExpLibOpt sdf 90 dock9	0.0029	80.49	F	F	0	F
	Structure090 ExpLibOpt sdf 90 dock5	0.0029	73.86	F	F	1	F
91	Structure091 ExpLibOpt sdf 91 dock10	0.0014	91.26	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock4	0.0014	86.40	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock3	0.0014	83.52	F	F	0	F
92	Structure092 ExpLibOpt sdf 92 dock8	6.2500	84.49	F	F	0	F
	Structure092 ExpLibOpt sdf 92 dock6	6.2500	81.11	T	F	1	F
	Structure092 ExpLibOpt sdf 92 dock2	6.2500	80.81	T	T	5	T
93	Structure093 ExpLibOpt sdf 93 dock2	0.1250	77.85	T	T	3	F
	Structure093 ExpLibOpt sdf 93 dock1	0.1250	77.73	T	T	3	F
	Structure093 ExpLibOpt sdf 93 dock3	0.1250	77.32	T	T	3	F
94	Structure094 ExpLibOpt sdf 94 dock9	3.1300	94.44	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock8	3.1300	86.64	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock4	3.1300	85.38	F	F	0	F
95	Structure095 ExpLibOpt sdf 95 dock4	0.7800	101.41	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock2	0.7800	99.74	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock3	0.7800	98.03	F	F	0	F

96	Structure096 ExpLibOpt sdf 96 dock3	0.7800	84.92	T	F	1	F
	Structure096 ExpLibOpt sdf 96 dock5	0.7800	83.62	T	F	2	F
	Structure096 ExpLibOpt sdf 96 dock9	0.7800	82.03	T	F	3	F
97	Structure097 ExpLibOpt sdf 97 dock3	0.7800	87.51	T	F	1	F
	Structure097 ExpLibOpt sdf 97 dock4	0.7800	83.05	T	T	5	T
	Structure097 ExpLibOpt sdf 97 dock9	0.7800	82.09	T	T	5	T
98	Structure098 ExpLibOpt sdf 98 dock2	0.0060	69.81	T	F	1	F
	Structure098 ExpLibOpt sdf 98 dock3	0.0060	69.27	T	F	1	F
	Structure098 ExpLibOpt sdf 98 dock1	0.0060	68.94	T	F	2	F
99	Structure099 ExpLibOpt sdf 99 dock3	0.0060	71.49	T	T	4	T
	Structure099 ExpLibOpt sdf 99 dock1	0.0060	71.22	T	T	4	T
	Structure099 ExpLibOpt sdf 99 dock2	0.0060	69.23	T	T	4	T
100	Structure100 ExpLibOpt sdf 100 dock2	0.0130	65.98	T	F	0	F
	Structure100 ExpLibOpt sdf 100 dock1	0.0130	65.60	T	F	1	F
	Structure100 ExpLibOpt sdf 100 dock3	0.0130	60.94	T	T	4	T
101	Structure101 ExpLibOpt sdf 101 dock2	0.0060	73.61	T	T	4	T
	Structure101 ExpLibOpt sdf 101 dock1	0.0060	73.32	T	T	4	T
	Structure101 ExpLibOpt sdf 101 dock3	0.0060	72.76	T	F	4	F
102	Structure102 ExpLibOpt sdf 102 dock1	0.0010	62.17	F	F	0	F
	Structure102 ExpLibOpt sdf 102 dock3	0.0010	60.65	T	F	1	F
	Structure102 ExpLibOpt sdf 102 dock2	0.0010	60.02	T	F	1	F
103	Structure103 ExpLibOpt sdf 103 dock1	0.0020	73.64	T	T	4	T
	Structure103 ExpLibOpt sdf 103 dock2	0.0020	72.70	T	F	0	F
	Structure103 ExpLibOpt sdf 103 dock3	0.0020	72.69	T	F	0	F
104	Structure104 ExpLibOpt sdf 104 dock3	0.0130	62.75	T	F	1	F
	Structure104 ExpLibOpt sdf 104 dock2	0.0130	61.98	T	F	1	F
	Structure104 ExpLibOpt sdf 104 dock4	0.0130	59.46	T	F	1	F
105	Structure105 ExpLibOpt sdf 105 dock3	0.0060	70.89	T	T	4	T
	Structure105 ExpLibOpt sdf 105 dock1	0.0060	70.67	T	T	4	T
	Structure105 ExpLibOpt sdf 105 dock2	0.0060	70.64	T	T	4	T
106	Structure106 ExpLibOpt sdf 106 dock3	0.0250	72.79	T	T	5	T
	Structure106 ExpLibOpt sdf 106 dock2	0.0250	72.70	T	T	5	T

	Structure106 ExpLibOpt sdf 106 dock1	0.0250	72.57	T	T	5	T
107	Structure107 ExpLibOpt sdf 107 dock3	0.0300	65.56	F	F	1	F
	Structure107 ExpLibOpt sdf 107 dock2	0.0300	65.16	F	F	0	F
	Structure107 ExpLibOpt sdf 107 dock1	0.0300	65.11	T	F	1	F
108	Structure108 ExpLibOpt sdf 108 dock6	0.0600	72.19	T	T	5	T
	Structure108 ExpLibOpt sdf 108 dock2	0.0600	71.82	T	T	5	T
	Structure108 ExpLibOpt sdf 108 dock8	0.0600	70.95	T	T	5	T
109	Structure109 ExpLibOpt sdf 109 dock2	0.2000	62.96	T	T	5	T
	Structure109 ExpLibOpt sdf 109 dock4	0.2000	62.21	T	T	5	T
	Structure109 ExpLibOpt sdf 109 dock1	0.2000	61.65	T	F	2	F
110	Structure110 ExpLibOpt sdf 110 dock3	0.3900	73.59	T	T	5	T
	Structure110 ExpLibOpt sdf 110 dock2	0.3900	72.22	T	T	5	T
	Structure110 ExpLibOpt sdf 110 dock1	0.3900	71.87	T	T	5	T
111	Structure111 ExpLibOpt sdf 111 dock3	0.7800	69.18	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock2	0.7800	67.83	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock1	0.7800	66.60	T	T	5	T
112	Structure112 ExpLibOpt sdf 112 dock3	1.5600	68.43	T	T	5	T
	Structure112 ExpLibOpt sdf 112 dock1	1.5600	68.19	T	T	5	T
	Structure112 ExpLibOpt sdf 112 dock2	1.5600	64.90	T	T	5	T
113	Structure113 ExpLibOpt sdf 113 dock3	0.3900	63.59	T	F	2	F
	Structure113 ExpLibOpt sdf 113 dock1	0.3900	63.46	T	T	5	T
	Structure113 ExpLibOpt sdf 113 dock2	0.3900	61.56	T	T	5	T
114	Structure114 ExpLibOpt sdf 114 dock1	0.1000	87.56	T	T	5	T
	Structure114 ExpLibOpt sdf 114 dock3	0.1000	86.82	T	T	5	T
	Structure114 ExpLibOpt sdf 114 dock2	0.1000	86.32	T	T	5	T
115	Structure115 ExpLibOpt sdf 115 dock1	0.1000	85.65	T	T	5	T
	Structure115 ExpLibOpt sdf 115 dock4	0.1000	85.23	T	T	5	T
	Structure115 ExpLibOpt sdf 115 dock6	0.1000	82.10	T	T	5	T
116	Structure116 ExpLibOpt sdf 116 dock3	0.1000	74.17	F	F	0	F
	Structure116 ExpLibOpt sdf 116 dock4	0.1000	73.84	F	F	1	F
	Structure116 ExpLibOpt sdf 116 dock1	0.1000	73.09	F	F	1	F
117	Structure117 ExpLibOpt sdf 117 dock3	0.2000	66.32	T	F	1	F

	Structure117 ExpLibOpt sdf 117 dock1	0.2000	63.29	T	F	1	F
	Structure117 ExpLibOpt sdf 117 dock2	0.2000	61.25	T	F	3	F
118	Structure118 ExpLibOpt sdf 118 dock1	0.0015	69.24	T	F	1	F
	Structure118 ExpLibOpt sdf 118 dock3	0.0015	69.21	T	F	1	F
	Structure118 ExpLibOpt sdf 118 dock2	0.0015	69.11	T	F	1	F
119	Structure119 ExpLibOpt sdf 119 dock2	0.0250	75.69	T	T	4	T
	Structure119 ExpLibOpt sdf 119 dock3	0.0250	75.41	T	F	2	F
	Structure119 ExpLibOpt sdf 119 dock1	0.0250	74.84	T	T	4	T
120	Structure120 ExpLibOpt sdf 120 dock3	0.3900	72.87	T	T	5	T
	Structure120 ExpLibOpt sdf 120 dock6	0.3900	71.19	T	T	5	T
	Structure120 ExpLibOpt sdf 120 dock8	0.3900	70.53	T	T	4	T
121	Structure121 ExpLibOpt sdf 121 dock8	0.0125	92.34	T	F	2	F
	Structure121 ExpLibOpt sdf 121 dock1	0.0125	89.54	T	F	2	F
	Structure121 ExpLibOpt sdf 121 dock7	0.0125	84.20	F	F	0	F
122	Structure122 ExpLibOpt sdf 122 dock10	0.3900	62.77	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock7	0.3900	59.39	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock6	0.3900	58.14	T	F	0	F
123	Structure123 ExpLibOpt sdf 123 dock8	0.3900	56.66	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock3	0.3900	55.87	F	F	1	F
	Structure123 ExpLibOpt sdf 123 dock5	0.3900	53.17	F	F	0	F
124	Structure124 ExpLibOpt sdf 124 dock6	0.2000	84.77	T	F	3	F
	Structure124 ExpLibOpt sdf 124 dock9	0.2000	81.61	T	T	5	T
	Structure124 ExpLibOpt sdf 124 dock10	0.2000	64.23	F	F	0	F
125	Structure125 ExpLibOpt sdf 125 dock3	0.2000	67.03	F	F	2	F
	Structure125 ExpLibOpt sdf 125 dock10	0.2000	63.21	F	F	1	F
	Structure125 ExpLibOpt sdf 125 dock2	0.2000	62.31	F	F	0	F
126	Structure126 ExpLibOpt sdf 126 dock8	0.3900	87.01	T	T	5	T
	Structure126 ExpLibOpt sdf 126 dock2	0.3900	82.77	T	T	5	T
	Structure126 ExpLibOpt sdf 126 dock10	0.3900	78.90	F	F	1	F
127	Structure127 ExpLibOpt sdf 127 dock10	0.7800	85.33	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock6	0.7800	81.28	T	F	3	F
	Structure127 ExpLibOpt sdf 127 dock8	0.7800	63.99	F	F	0	F

128	Structure128 ExpLibOpt sdf 128 dock7	0.1000	88.89	T	T	5	T
	Structure128 ExpLibOpt sdf 128 dock8	0.1000	85.72	T	T	5	T
	Structure128 ExpLibOpt sdf 128 dock1	0.1000	85.71	T	T	5	T
129	Structure129 ExpLibOpt sdf 129 dock6	0.2000	89.84	T	F	3	F
	Structure129 ExpLibOpt sdf 129 dock10	0.2000	82.09	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock2	0.2000	68.15	F	F	0	F
130	Structure130 ExpLibOpt sdf 130 dock1	0.3900	62.92	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock7	0.3900	62.48	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock6	0.3900	61.97	F	F	0	F
131	Structure131 ExpLibOpt sdf 131 dock1	0.7800	67.16	F	F	1	F
	Structure131 ExpLibOpt sdf 131 dock2	0.7800	66.45	F	F	1	F
	Structure131 ExpLibOpt sdf 131 dock8	0.7800	63.46	F	F	0	F
132	Structure132 ExpLibOpt sdf 132 dock2	0.7800	83.93	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock8	0.7800	82.12	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock5	0.7800	80.28	F	F	0	F
133	Structure133 ExpLibOpt sdf 133 dock6	0.1000	79.92	F	F	1	F
	Structure133 ExpLibOpt sdf 133 dock3	0.1000	78.49	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock4	0.1000	73.11	F	F	0	F
134	Structure134 ExpLibOpt sdf 134 dock5	0.1000	79.58	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock2	0.1000	77.34	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock10	0.1000	73.98	F	F	0	F
135	Structure135 ExpLibOpt sdf 135 dock3	0.1000	88.48	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock7	0.1000	80.79	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock4	0.1000	78.99	F	F	0	F
136	Structure136 ExpLibOpt sdf 136 dock6	1.2600	80.51	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock8	1.2600	80.00	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock5	1.2600	78.89	F	F	0	F
137	Structure137 ExpLibOpt sdf 137 dock1	1.3000	83.16	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock6	1.3000	75.38	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock4	1.3000	75.28	F	F	0	F
138	Structure138 ExpLibOpt sdf 138 dock3	0.0031	82.20	F	F	0	F
	Structure138 ExpLibOpt sdf 138 dock1	0.0031	78.12	F	F	0	F

	Structure138 ExpLibOpt sdf 138 dock9	0.0031	74.21	T	T	5	T
139	Structure139 ExpLibOpt sdf 139 dock2	0.3300	79.36	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock5	0.3300	77.65	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock1	0.3300	77.52	F	F	0	F
140	Structure140 ExpLibOpt sdf 140 dock2	0.1600	83.07	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock5	0.1600	79.63	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock4	0.1600	79.40	F	F	0	F
141	Structure141 ExpLibOpt sdf 141 dock10	0.3200	86.59	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock3	0.3200	84.35	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock1	0.3200	84.09	F	F	0	F
142	Structure142 ExpLibOpt sdf 142 dock2	0.0400	78.10	F	F	0	F
	Structure142 ExpLibOpt sdf 142 dock8	0.0400	75.71	F	F	0	F
	Structure142 ExpLibOpt sdf 142 dock3	0.0400	75.47	F	F	0	F
143	Structure143 ExpLibOpt sdf 143 dock1	0.7800	83.09	T	F	3	F
	Structure143 ExpLibOpt sdf 143 dock8	0.7800	75.61	F	F	0	F
	Structure143 ExpLibOpt sdf 143 dock6	0.7800	74.53	T	T	5	T
144	Structure144 ExpLibOpt sdf 144 dock1	0.2000	83.42	T	F	3	F
	Structure144 ExpLibOpt sdf 144 dock2	0.2000	73.31	T	F	3	F
	Structure144 ExpLibOpt sdf 144 dock3	0.2000	63.78	T	F	3	F
145	Structure145 ExpLibOpt sdf 145 dock7	0.1000	95.34	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock4	0.1000	87.74	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock6	0.1000	79.57	F	F	0	F

Legend	
GSF	GOLDScore Fitness Function
VO	Visual Orientation
VF	Visual Fitness
NMPF	Number of Matching Pharmacophoric Features

c) T474P_{mod.}

Cluster ID	DOCK POSE	MICexp	GSF	VO (T/F)	VF (T/F)	NMPF (4-5)	Result (T/F)
1	Structure001 ExpLibOpt sdf 1 dock2	3.0000	68.57	T	T	2	F
	Structure001 ExpLibOpt sdf 1 dock6	3.0000	68.27	T	T	2	F
	Structure001 ExpLibOpt sdf 1 dock4	3.0000	68.12	T	T	2	F
2	Structure002 ExpLibOpt sdf 2 dock10	0.0115	67.85	F	F	1	F
	Structure002 ExpLibOpt sdf 2 dock8	0.0115	67.84	F	F	1	F
	Structure002 ExpLibOpt sdf 2 dock2	0.0115	67.31	F	F	1	F
3	Structure003 ExpLibOpt sdf 3 dock2	0.3000	61.96	T	T	5	T
	Structure003 ExpLibOpt sdf 3 dock3	0.3000	60.83	T	T	5	T
	Structure003 ExpLibOpt sdf 3 dock4	0.3000	60.37	T	F	3	F
4	Structure004 ExpLibOpt sdf 4 dock1	0.0100	62.75	T	T	5	T
	Structure004 ExpLibOpt sdf 4 dock2	0.0100	61.84	T	T	5	T
	Structure004 ExpLibOpt sdf 4 dock3	0.0100	61.67	T	T	5	T
5	Structure005 ExpLibOpt sdf 5 dock2	0.3000	61.83	T	F	2	F
	Structure005 ExpLibOpt sdf 5 dock3	0.3000	61.69	T	F	2	F
	Structure005 ExpLibOpt sdf 5 dock1	0.3000	61.60	T	F	2	F
6	Structure006 ExpLibOpt sdf 6 dock2	0.1200	65.02	F	F	1	F
	Structure006 ExpLibOpt sdf 6 dock4	0.1200	64.89	F	F	1	F
	Structure006 ExpLibOpt sdf 6 dock3	0.1200	64.60	F	F	2	F
7	Structure007 ExpLibOpt sdf 7 dock3	3.5000	64.22	F	F	1	F
	Structure007 ExpLibOpt sdf 7 dock5	3.5000	64.04	T	T	3	F
	Structure007 ExpLibOpt sdf 7 dock7	3.5000	63.82	T	T	3	F
8	Structure008 ExpLibOpt sdf 8 dock2	0.1000	69.00	T	T	4	T
	Structure008 ExpLibOpt sdf 8 dock1	0.1000	67.92	T	T	4	T
	Structure008 ExpLibOpt sdf 8 dock3	0.1000	66.37	T	T	4	T
9	Structure009 ExpLibOpt sdf 9 dock8	1.4000	65.10	F	F	1	F
	Structure009 ExpLibOpt sdf 9 dock2	1.4000	64.99	T	F	1	F
	Structure009 ExpLibOpt sdf 9 dock1	1.4000	64.52	F	F	0	F
10	Structure010 ExpLibOpt sdf 10 dock3	3.2000	64.41	T	T	4	T
	Structure010 ExpLibOpt sdf 10 dock2	3.2000	64.12	T	T	5	T

	Structure010 ExpLibOpt sdf 10 dock1	3.2000	63.44	T	T	4	T
11	Structure011 ExpLibOpt sdf 11 dock6	0.0500	70.41	T	F	3	F
	Structure011 ExpLibOpt sdf 11 dock4	0.0500	70.11	T	F	2	F
	Structure011 ExpLibOpt sdf 11 dock2	0.0500	69.07	T	T	4	T
12	Structure012 ExpLibOpt sdf 12 dock1	0.5000	79.82	T	T	5	T
	Structure012 ExpLibOpt sdf 12 dock3	0.5000	79.57	T	T	5	T
	Structure012 ExpLibOpt sdf 12 dock2	0.5000	79.45	T	T	5	T
13	Structure013 ExpLibOpt sdf 13 dock2	1.6000	58.90	T	F	1	F
	Structure013 ExpLibOpt sdf 13 dock1	1.6000	57.89	T	F	3	F
	Structure013 ExpLibOpt sdf 13 dock4	1.6000	57.74	T	F	2	F
14	Structure014 ExpLibOpt sdf 14 dock9	0.5000	72.92	F	F	1	F
	Structure014 ExpLibOpt sdf 14 dock2	0.5000	71.04	T	F	2	F
	Structure014 ExpLibOpt sdf 14 dock3	0.5000	70.22	T	F	2	F
15	Structure015 ExpLibOpt sdf 15 dock1	0.5000	62.27	T	T	4	T
	Structure015 ExpLibOpt sdf 15 dock3	0.5000	61.98	T	T	4	T
	Structure015 ExpLibOpt sdf 15 dock2	0.5000	61.87	T	F	2	F
16	Structure016 ExpLibOpt sdf 16 dock5	2.0000	63.05	F	F	0	F
	Structure016 ExpLibOpt sdf 16 dock4	2.0000	62.07	F	F	0	F
	Structure016 ExpLibOpt sdf 16 dock6	2.0000	61.62	F	F	0	F
17	Structure017 ExpLibOpt sdf 17 dock2	0.5000	76.72	T	T	5	T
	Structure017 ExpLibOpt sdf 17 dock1	0.5000	76.50	T	T	5	T
	Structure017 ExpLibOpt sdf 17 dock3	0.5000	76.44	T	T	5	T
18	Structure018 ExpLibOpt sdf 18 dock8	0.5000	62.65	F	F	1	F
	Structure018 ExpLibOpt sdf 18 dock6	0.5000	62.37	T	F	1	F
	Structure018 ExpLibOpt sdf 18 dock1	0.5000	62.04	T	F	3	F
19	Structure019 ExpLibOpt sdf 19 dock2	0.2500	75.10	F	F	0	F
	Structure019 ExpLibOpt sdf 19 dock3	0.2500	74.64	F	F	0	F
	Structure019 ExpLibOpt sdf 19 dock1	0.2500	74.20	F	F	0	F
20	Structure020 ExpLibOpt sdf 20 dock2	0.0100	67.73	T	T	4	T
	Structure020 ExpLibOpt sdf 20 dock3	0.0100	66.59	T	T	4	T
	Structure020 ExpLibOpt sdf 20 dock1	0.0100	64.85	T	T	4	T
21	Structure021 ExpLibOpt sdf 21 dock3	0.0310	77.50	T	T	5	T

	Structure021 ExpLibOpt sdf 21 dock2	0.0310	77.45	T	T	5	T
	Structure021 ExpLibOpt sdf 21 dock1	0.0310	77.10	T	T	5	T
22	Structure022 ExpLibOpt sdf 22 dock4	0.0100	70.64	T	T	5	T
	Structure022 ExpLibOpt sdf 22 dock1	0.0100	69.93	T	T	5	T
	Structure022 ExpLibOpt sdf 22 dock2	0.0100	67.99	T	T	5	T
23	Structure023 ExpLibOpt sdf 23 dock2	0.0100	63.46	T	T	4	T
	Structure023 ExpLibOpt sdf 23 dock1	0.0100	63.25	T	T	4	T
	Structure023 ExpLibOpt sdf 23 dock3	0.0100	61.71	T	T	4	T
24	Structure024 ExpLibOpt sdf 24 dock4	0.9000	72.04	F	F	0	F
	Structure024 ExpLibOpt sdf 24 dock1	0.9000	71.31	F	F	0	F
	Structure024 ExpLibOpt sdf 24 dock2	0.9000	69.87	F	F	1	F
25	Structure025 ExpLibOpt sdf 25 dock1	0.1250	71.44	T	T	5	T
	Structure025 ExpLibOpt sdf 25 dock3	0.1250	70.19	T	F	3	F
	Structure025 ExpLibOpt sdf 25 dock2	0.1250	69.34	T	T	5	T
26	Structure026 ExpLibOpt sdf 26 dock1	0.3000	64.86	T	T	5	T
	Structure026 ExpLibOpt sdf 26 dock2	0.3000	64.62	T	T	5	T
	Structure026 ExpLibOpt sdf 26 dock3	0.3000	64.53	T	T	5	T
27	Structure027 ExpLibOpt sdf 27 dock9	0.1200	64.59	T	F	1	F
	Structure027 ExpLibOpt sdf 27 dock4	0.1200	63.87	F	F	1	F
	Structure027 ExpLibOpt sdf 27 dock1	0.1200	63.73	T	T	5	T
28	Structure028 ExpLibOpt sdf 28 dock9	0.0040	67.03	F	F	0	F
	Structure028 ExpLibOpt sdf 28 dock3	0.0040	66.54	F	F	0	F
	Structure028 ExpLibOpt sdf 28 dock5	0.0040	63.25	F	F	1	F
29	Structure029 ExpLibOpt sdf 29 dock4	2.0000	75.38	T	T	4	T
	Structure029 ExpLibOpt sdf 29 dock6	2.0000	75.23	T	T	4	T
	Structure029 ExpLibOpt sdf 29 dock7	2.0000	74.83	T	T	4	T
30	Structure030 ExpLibOpt sdf 30 dock2	0.3900	63.67	T	T	5	T
	Structure030 ExpLibOpt sdf 30 dock3	0.3900	63.52	T	T	5	T
	Structure030 ExpLibOpt sdf 30 dock1	0.3900	62.38	T	T	5	T
31	Structure031 ExpLibOpt sdf 31 dock1	0.0600	71.70	T	T	5	T
	Structure031 ExpLibOpt sdf 31 dock2	0.0600	70.53	T	T	5	T
	Structure031 ExpLibOpt sdf 31 dock3	0.0600	69.98	T	T	5	T

32	Structure032 ExpLibOpt sdf 32 dock1	0.3900	66.98	T	F	2	F
	Structure032 ExpLibOpt sdf 32 dock3	0.3900	66.86	T	F	2	F
	Structure032 ExpLibOpt sdf 32 dock2	0.3900	64.54	T	F	1	F
33	Structure033 ExpLibOpt sdf 33 dock8	0.3900	69.64	T	F	1	F
	Structure033 ExpLibOpt sdf 33 dock3	0.3900	69.29	T	F	1	F
	Structure033 ExpLibOpt sdf 33 dock7	0.3900	68.93	T	F	1	F
34	Structure034 ExpLibOpt sdf 34 dock1	0.7800	71.10	T	F	1	F
	Structure034 ExpLibOpt sdf 34 dock3	0.7800	70.70	T	F	1	F
	Structure034 ExpLibOpt sdf 34 dock5	0.7800	70.41	T	F	1	F
35	Structure035 ExpLibOpt sdf 35 dock3	0.7800	71.09	T	T	5	T
	Structure035 ExpLibOpt sdf 35 dock1	0.7800	69.70	T	T	5	T
	Structure035 ExpLibOpt sdf 35 dock2	0.7800	69.57	T	T	5	T
36	Structure036 ExpLibOpt sdf 36 dock4	0.7800	67.90	T	T	5	T
	Structure036 ExpLibOpt sdf 36 dock1	0.7800	67.41	T	T	5	T
	Structure036 ExpLibOpt sdf 36 dock3	0.7800	65.06	T	T	5	T
37	Structure037 ExpLibOpt sdf 37 dock3	0.1250	72.55	F	F	0	F
	Structure037 ExpLibOpt sdf 37 dock1	0.1250	71.66	T	F	2	F
	Structure037 ExpLibOpt sdf 37 dock4	0.1250	71.66	T	F	2	F
38	Structure038 ExpLibOpt sdf 38 dock1	0.0020	72.90	T	T	4	T
	Structure038 ExpLibOpt sdf 38 dock2	0.0020	72.57	T	T	4	T
	Structure038 ExpLibOpt sdf 38 dock3	0.0020	71.66	T	T	4	T
39	Structure039 ExpLibOpt sdf 39 dock1	0.1100	66.25	T	F	3	F
	Structure039 ExpLibOpt sdf 39 dock9	0.1100	65.76	T	F	4	F
	Structure039 ExpLibOpt sdf 39 dock10	0.1100	65.31	T	T	5	T
40	Structure040 ExpLibOpt sdf 40 dock3	0.0120	66.43	T	T	4	T
	Structure040 ExpLibOpt sdf 40 dock1	0.0120	65.84	T	T	5	T
	Structure040 ExpLibOpt sdf 40 dock4	0.0120	65.51	T	T	5	T
41	Structure041 ExpLibOpt sdf 41 dock1	0.2500	67.50	T	T	4	T
	Structure041 ExpLibOpt sdf 41 dock2	0.2500	66.95	T	T	4	T
	Structure041 ExpLibOpt sdf 41 dock3	0.2500	66.60	T	F	3	F
42	Structure042 ExpLibOpt sdf 42 dock1	0.0160	75.60	T	F	2	F
	Structure042 ExpLibOpt sdf 42 dock2	0.0160	74.05	T	T	3	F

	Structure042 ExpLibOpt sdf 42 dock3	0.0160	73.81	T	T	3	F
43	Structure043 ExpLibOpt sdf 43 dock1	0.6000	64.38	F	F	1	F
	Structure043 ExpLibOpt sdf 43 dock4	0.6000	64.31	F	F	1	F
	Structure043 ExpLibOpt sdf 43 dock3	0.6000	62.80	F	F	0	F
	Structure043 ExpLibOpt sdf 43 dock3	0.6000	62.80	F	F	0	F
44	Structure044 ExpLibOpt sdf 44 dock1	0.3900	61.02	T	T	5	T
	Structure044 ExpLibOpt sdf 44 dock3	0.3900	60.54	T	T	5	T
	Structure044 ExpLibOpt sdf 44 dock2	0.3900	59.73	T	T	4	T
45	Structure045 ExpLibOpt sdf 45 dock2	0.3000	68.30	T	T	5	T
	Structure045 ExpLibOpt sdf 45 dock3	0.3000	67.93	T	T	5	T
	Structure045 ExpLibOpt sdf 45 dock1	0.3000	67.85	T	T	5	T
46	Structure046 ExpLibOpt sdf 46 dock2	0.0300	69.90	T	T	5	T
	Structure046 ExpLibOpt sdf 46 dock1	0.0300	69.67	T	T	5	T
	Structure046 ExpLibOpt sdf 46 dock3	0.0300	69.64	T	T	5	T
47	Structure047 ExpLibOpt sdf 47 dock1	0.1250	71.63	T	T	5	T
	Structure047 ExpLibOpt sdf 47 dock2	0.1250	70.43	T	F	3	F
	Structure047 ExpLibOpt sdf 47 dock3	0.1250	70.02	T	T	5	T
48	Structure048 ExpLibOpt sdf 48 dock2	0.1250	67.37	T	T	5	T
	Structure048 ExpLibOpt sdf 48 dock1	0.1250	67.25	T	T	5	T
	Structure048 ExpLibOpt sdf 48 dock3	0.1250	66.99	T	T	5	T
49	Structure049 ExpLibOpt sdf 49 dock2	0.5000	77.57	T	F	2	F
	Structure049 ExpLibOpt sdf 49 dock9	0.5000	76.85	T	T	4	T
	Structure049 ExpLibOpt sdf 49 dock10	0.5000	76.09	T	F	3	F
50	Structure050 ExpLibOpt sdf 50 dock5	0.0016	79.63	F	F	0	F
	Structure050 ExpLibOpt sdf 50 dock3	0.0016	77.27	F	F	1	F
	Structure050 ExpLibOpt sdf 50 dock9	0.0016	74.29	T	T	5	T
51	Structure051 ExpLibOpt sdf 51 dock5	6.3000	77.62	T	T	5	T
	Structure051 ExpLibOpt sdf 51 dock3	6.3000	76.89	F	F	0	F
	Structure051 ExpLibOpt sdf 51 dock2	6.3000	76.64	T	F	2	F
52	Structure052 ExpLibOpt sdf 52 dock3	6.5700	80.94	T	T	5	T
	Structure052 ExpLibOpt sdf 52 dock2	6.5700	79.46	T	T	5	T
	Structure052 ExpLibOpt sdf 52 dock4	6.5700	79.13	T	T	5	T
53	Structure053 ExpLibOpt sdf 53 dock4	5.2000	95.68	F	F	0	F

	Structure053 ExpLibOpt sdf 53 dock9	5.2000	86.73	F	F	1	F
	Structure053 ExpLibOpt sdf 53 dock7	5.2000	82.45	F	F	0	F
54	Structure054 ExpLibOpt sdf 54 dock9	6.9000	92.29	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock2	6.9000	91.69	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock10	6.9000	88.97	F	F	0	F
55	Structure055 ExpLibOpt sdf 55 dock1	6.4500	83.25	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock5	6.4500	83.02	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock4	6.4500	82.73	F	F	0	F
56	Structure056 ExpLibOpt sdf 56 dock4	6.7000	84.95	F	F	0	F
	Structure056 ExpLibOpt sdf 56 dock7	6.7000	83.28	F	F	0	F
	Structure056 ExpLibOpt sdf 56 dock9	6.7000	80.62	F	F	0	F
57	Structure057 ExpLibOpt sdf 57 dock1	6.3000	88.63	F	F	0	F
	Structure057 ExpLibOpt sdf 57 dock10	6.3000	86.10	F	F	0	F
	Structure057 ExpLibOpt sdf 57 dock9	6.3000	84.50	F	F	0	F
58	Structure058 ExpLibOpt sdf 58 dock10	6.2600	93.99	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock1	6.2600	92.03	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock5	6.2600	90.57	F	F	0	F
59	Structure059 ExpLibOpt sdf 59 dock5	6.9200	88.39	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock3	6.9200	86.22	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock8	6.9200	82.16	F	F	0	F
60	Structure060 ExpLibOpt sdf 60 dock2	0.0300	77.50	T	T	4	T
	Structure060 ExpLibOpt sdf 60 dock1	0.0300	77.34	T	T	4	T
	Structure060 ExpLibOpt sdf 60 dock3	0.0300	76.86	T	T	4	T
61	Structure061 ExpLibOpt sdf 61 dock3	3.2000	65.89	F	F	1	F
	Structure061 ExpLibOpt sdf 61 dock4	3.2000	62.89	T	T	4	T
	Structure061 ExpLibOpt sdf 61 dock7	3.2000	62.65	T	T	4	T
62	Structure062 ExpLibOpt sdf 62 dock2	0.1250	74.09	T	T	5	T
	Structure062 ExpLibOpt sdf 62 dock3	0.1250	73.93	T	T	5	T
	Structure062 ExpLibOpt sdf 62 dock1	0.1250	73.80	T	T	5	T
63	Structure063 ExpLibOpt sdf 63 dock9	0.5000	72.87	F	F	0	F
	Structure063 ExpLibOpt sdf 63 dock4	0.5000	72.13	T	T	5	T
	Structure063 ExpLibOpt sdf 63 dock8	0.5000	71.75	T	T	5	T

64	Structure064 ExpLibOpt sdf 64 dock1	0.0300	81.18	T	T	3	F
	Structure064 ExpLibOpt sdf 64 dock3	0.0300	80.89	T	T	3	F
	Structure064 ExpLibOpt sdf 64 dock2	0.0300	79.85	T	T	3	F
65	Structure065 ExpLibOpt sdf 65 dock10	0.7800	82.05	F	F	0	F
	Structure065 ExpLibOpt sdf 65 dock4	0.7800	81.21	F	F	0	F
	Structure065 ExpLibOpt sdf 65 dock5	0.7800	80.37	F	F	0	F
66	Structure066 ExpLibOpt sdf 66 dock7	0.7800	84.61	F	F	0	F
	Structure066 ExpLibOpt sdf 66 dock4	0.7800	81.28	F	F	0	F
	Structure066 ExpLibOpt sdf 66 dock5	0.7800	79.52	F	F	0	F
67	Structure067 ExpLibOpt sdf 67 dock5	6.2500	79.61	F	F	0	F
	Structure067 ExpLibOpt sdf 67 dock8	6.2500	77.70	F	F	0	F
	Structure067 ExpLibOpt sdf 67 dock2	6.2500	76.20	F	F	0	F
68	Structure068 ExpLibOpt sdf 68 dock1	0.7800	80.09	T	F	2	F
	Structure068 ExpLibOpt sdf 68 dock3	0.7800	78.28	F	F	0	F
	Structure068 ExpLibOpt sdf 68 dock2	0.7800	78.12	T	T	5	T
69	Structure069 ExpLibOpt sdf 69 dock6	1.5600	82.53	F	F	0	F
	Structure069 ExpLibOpt sdf 69 dock10	1.5600	80.60	F	F	0	F
	Structure069 ExpLibOpt sdf 69 dock9	1.5600	78.04	T	T	5	T
70	Structure070 ExpLibOpt sdf 70 dock3	1.5600	76.69	F	F	1	F
	Structure070 ExpLibOpt sdf 70 dock1	1.5600	71.89	F	F	1	F
	Structure070 ExpLibOpt sdf 70 dock2	1.5600	71.72	F	F	1	F
71	Structure071 ExpLibOpt sdf 71 dock8	3.1300	87.72	F	F	0	F
	Structure071 ExpLibOpt sdf 71 dock3	3.1300	86.75	F	F	0	F
	Structure071 ExpLibOpt sdf 71 dock9	3.1300	80.48	T	T	5	T
72	Structure072 ExpLibOpt sdf 72 dock3	7.1200	80.51	F	F	0	F
	Structure072 ExpLibOpt sdf 72 dock2	7.1200	80.28	F	F	0	F
	Structure072 ExpLibOpt sdf 72 dock1	7.1200	79.58	F	F	0	F
73	Structure073 ExpLibOpt sdf 73 dock1	0.0600	69.39	T	T	5	T
	Structure073 ExpLibOpt sdf 73 dock2	0.0600	68.37	T	T	5	T
	Structure073 ExpLibOpt sdf 73 dock3	0.0600	66.68	T	T	5	T
74	Structure074 ExpLibOpt sdf 74 dock3	0.7800	74.20	T	T	4	T
	Structure074 ExpLibOpt sdf 74 dock2	0.7800	74.15	T	T	4	T

	Structure074 ExpLibOpt sdf 74 dock1	0.7800	74.14	T	F	3	F
75	Structure075 ExpLibOpt sdf 75 dock4	0.0625	67.45	T	T	2	F
	Structure075 ExpLibOpt sdf 75 dock1	0.0625	67.38	T	T	2	F
	Structure075 ExpLibOpt sdf 75 dock2	0.0625	66.92	T	T	2	F
	Structure075 ExpLibOpt sdf 75 dock3	0.0625	66.92	T	T	2	F
76	Structure076 ExpLibOpt sdf 76 dock2	0.1250	71.98	T	T	4	T
	Structure076 ExpLibOpt sdf 76 dock3	0.1250	71.39	T	T	4	T
	Structure076 ExpLibOpt sdf 76 dock1	0.1250	70.75	T	T	4	T
77	Structure077 ExpLibOpt sdf 77 dock9	6.2500	80.64	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock4	6.2500	80.36	F	F	1	F
	Structure077 ExpLibOpt sdf 77 dock5	6.2500	76.58	T	T	5	T
78	Structure078 ExpLibOpt sdf 78 dock3	3.1300	71.40	T	T	5	T
	Structure078 ExpLibOpt sdf 78 dock1	3.1300	70.51	T	T	5	T
	Structure078 ExpLibOpt sdf 78 dock2	3.1300	67.81	T	T	4	T
79	Structure079 ExpLibOpt sdf 79 dock5	3.1300	75.65	F	F	1	F
	Structure079 ExpLibOpt sdf 79 dock3	3.1300	72.07	F	F	0	F
	Structure079 ExpLibOpt sdf 79 dock9	3.1300	71.61	T	T	4	T
80	Structure080 ExpLibOpt sdf 80 dock1	1.5600	82.24	T	F	1	F
	Structure080 ExpLibOpt sdf 80 dock4	1.5600	82.20	T	F	1	F
	Structure080 ExpLibOpt sdf 80 dock5	1.5600	81.17	T	F	1	F
81	Structure081 ExpLibOpt sdf 81 dock1	0.3900	70.37	T	T	4	T
	Structure081 ExpLibOpt sdf 81 dock3	0.3900	70.00	T	T	4	T
	Structure081 ExpLibOpt sdf 81 dock2	0.3900	69.73	T	T	4	T
82	Structure082 ExpLibOpt sdf 82 dock4	0.0030	77.03	F	F	0	F
	Structure082 ExpLibOpt sdf 82 dock9	0.0030	76.13	T	T	5	T
	Structure082 ExpLibOpt sdf 82 dock1	0.0030	75.17	F	F	1	F
83	Structure083 ExpLibOpt sdf 83 dock6	0.0027	86.83	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock3	0.0027	85.59	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock5	0.0027	85.10	F	F	0	F
84	Structure084 ExpLibOpt sdf 84 dock5	0.0026	85.86	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock2	0.0026	81.17	F	F	1	F
	Structure084 ExpLibOpt sdf 84 dock8	0.0026	79.23	F	F	0	F
85	Structure085 ExpLibOpt sdf 85 dock1	0.0027	90.04	F	F	0	F

	Structure085 ExpLibOpt sdf 85 dock4	0.0027	78.29	F	F	0	F
	Structure085 ExpLibOpt sdf 85 dock7	0.0027	76.85	F	F	0	F
86	Structure086 ExpLibOpt sdf 86 dock2	0.0012	87.36	F	F	0	F
	Structure086 ExpLibOpt sdf 86 dock5	0.0012	84.83	F	F	0	F
	Structure086 ExpLibOpt sdf 86 dock4	0.0012	83.20	F	F	0	F
87	Structure087 ExpLibOpt sdf 87 dock9	0.0012	85.28	F	F	1	F
	Structure087 ExpLibOpt sdf 87 dock10	0.0012	79.18	F	F	1	F
	Structure087 ExpLibOpt sdf 87 dock3	0.0012	78.30	F	F	1	F
88	Structure088 ExpLibOpt sdf 88 dock5	0.0014	80.12	F	F	1	F
	Structure088 ExpLibOpt sdf 88 dock7	0.0014	78.36	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock1	0.0014	77.61	F	F	0	F
89	Structure089 ExpLibOpt sdf 89 dock7	0.0108	84.32	F	F	1	F
	Structure089 ExpLibOpt sdf 89 dock5	0.0108	81.20	F	F	1	F
	Structure089 ExpLibOpt sdf 89 dock1	0.0108	80.05	F	F	1	F
90	Structure090 ExpLibOpt sdf 90 dock7	0.0029	92.35	F	F	0	F
	Structure090 ExpLibOpt sdf 90 dock1	0.0029	85.91	F	F	1	F
	Structure090 ExpLibOpt sdf 90 dock10	0.0029	77.94	F	F	0	F
91	Structure091 ExpLibOpt sdf 91 dock10	0.0014	92.17	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock8	0.0014	86.07	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock6	0.0014	83.55	F	F	1	F
92	Structure092 ExpLibOpt sdf 92 dock4	6.2500	78.28	F	F	0	F
	Structure092 ExpLibOpt sdf 92 dock2	6.2500	76.85	T	T	4	T
	Structure092 ExpLibOpt sdf 92 dock3	6.2500	74.24	T	T	5	T
93	Structure093 ExpLibOpt sdf 93 dock2	0.1250	77.39	T	F	2	F
	Structure093 ExpLibOpt sdf 93 dock1	0.1250	77.09	T	F	1	F
	Structure093 ExpLibOpt sdf 93 dock4	0.1250	76.87	T	F	1	F
94	Structure094 ExpLibOpt sdf 94 dock6	3.1300	105.50	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock4	3.1300	104.33	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock7	3.1300	103.04	F	F	0	F
95	Structure095 ExpLibOpt sdf 95 dock8	0.7800	89.62	F	F	1	F
	Structure095 ExpLibOpt sdf 95 dock10	0.7800	81.76	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock7	0.7800	81.57	F	F	0	F

96	Structure096 ExpLibOpt sdf 96 dock6	0.7800	78.87	T	T	5	T
	Structure096 ExpLibOpt sdf 96 dock1	0.7800	78.72	T	T	5	T
	Structure096 ExpLibOpt sdf 96 dock4	0.7800	78.42	F	F	0	F
97	Structure097 ExpLibOpt sdf 97 dock6	0.7800	82.72	T	T	5	T
	Structure097 ExpLibOpt sdf 97 dock7	0.7800	82.51	T	T	5	T
	Structure097 ExpLibOpt sdf 97 dock4	0.7800	82.05	T	T	5	T
98	Structure098 ExpLibOpt sdf 98 dock2	0.0060	69.19	T	F	2	F
	Structure098 ExpLibOpt sdf 98 dock1	0.0060	67.27	T	F	1	F
	Structure098 ExpLibOpt sdf 98 dock3	0.0060	66.83	T	F	2	F
99	Structure099 ExpLibOpt sdf 99 dock1	0.0060	71.26	T	T	4	T
	Structure099 ExpLibOpt sdf 99 dock3	0.0060	70.50	T	T	4	T
	Structure099 ExpLibOpt sdf 99 dock2	0.0060	69.69	T	T	4	T
100	Structure100 ExpLibOpt sdf 100 dock3	0.0130	63.48	T	T	4	T
	Structure100 ExpLibOpt sdf 100 dock1	0.0130	62.89	T	T	4	T
	Structure100 ExpLibOpt sdf 100 dock2	0.0130	61.87	T	T	4	T
101	Structure101 ExpLibOpt sdf 101 dock6	0.0060	74.73	T	T	4	T
	Structure101 ExpLibOpt sdf 101 dock5	0.0060	74.60	T	T	4	T
	Structure101 ExpLibOpt sdf 101 dock3	0.0060	73.94	T	T	4	T
102	Structure102 ExpLibOpt sdf 102 dock3	0.0010	61.54	T	F	1	F
	Structure102 ExpLibOpt sdf 102 dock2	0.0010	61.25	T	F	2	F
	Structure102 ExpLibOpt sdf 102 dock1	0.0010	58.42	T	F	3	F
103	Structure103 ExpLibOpt sdf 103 dock2	0.0020	75.59	T	T	4	T
	Structure103 ExpLibOpt sdf 103 dock1	0.0020	74.83	T	T	4	T
	Structure103 ExpLibOpt sdf 103 dock3	0.0020	74.35	T	T	4	T
104	Structure104 ExpLibOpt sdf 104 dock5	0.0130	62.22	F	F	0	F
	Structure104 ExpLibOpt sdf 104 dock7	0.0130	61.38	F	F	1	F
	Structure104 ExpLibOpt sdf 104 dock3	0.0130	60.92	T	F	1	F
105	Structure105 ExpLibOpt sdf 105 dock1	0.0060	71.54	T	F	3	F
	Structure105 ExpLibOpt sdf 105 dock2	0.0060	69.88	T	T	4	T
	Structure105 ExpLibOpt sdf 105 dock3	0.0060	67.69	T	T	4	T
106	Structure106 ExpLibOpt sdf 106 dock3	0.0250	74.05	T	T	5	T
	Structure106 ExpLibOpt sdf 106 dock2	0.0250	73.93	T	T	5	T

	Structure106 ExpLibOpt sdf 106 dock1	0.0250	73.31	T	T	5	T
107	Structure107 ExpLibOpt sdf 107 dock4	0.0300	63.13	T	F	2	F
	Structure107 ExpLibOpt sdf 107 dock10	0.0300	61.63	T	F	3	F
	Structure107 ExpLibOpt sdf 107 dock7	0.0300	59.54	T	T	4	T
	Structure107 ExpLibOpt sdf 107 dock3	0.0300	59.54	T	T	4	T
108	Structure108 ExpLibOpt sdf 108 dock3	0.0600	71.19	T	F	2	F
	Structure108 ExpLibOpt sdf 108 dock1	0.0600	70.30	T	T	5	T
	Structure108 ExpLibOpt sdf 108 dock2	0.0600	70.26	T	T	5	T
109	Structure109 ExpLibOpt sdf 109 dock2	0.2000	64.09	T	T	5	T
	Structure109 ExpLibOpt sdf 109 dock1	0.2000	64.06	T	T	4	T
	Structure109 ExpLibOpt sdf 109 dock3	0.2000	62.21	T	F	3	F
110	Structure110 ExpLibOpt sdf 110 dock1	0.3900	73.31	T	T	5	T
	Structure110 ExpLibOpt sdf 110 dock2	0.3900	73.03	T	T	5	T
	Structure110 ExpLibOpt sdf 110 dock3	0.3900	72.95	T	T	5	T
111	Structure111 ExpLibOpt sdf 111 dock10	0.7800	70.45	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock4	0.7800	70.38	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock3	0.7800	69.79	T	T	5	T
112	Structure112 ExpLibOpt sdf 112 dock2	1.5600	68.02	T	F	3	F
	Structure112 ExpLibOpt sdf 112 dock1	1.5600	68.02	T	F	3	F
	Structure112 ExpLibOpt sdf 112 dock3	1.5600	67.97	T	F	3	F
113	Structure113 ExpLibOpt sdf 113 dock1	0.3900	63.81	T	F	4	F
	Structure113 ExpLibOpt sdf 113 dock3	0.3900	62.11	T	F	4	F
	Structure113 ExpLibOpt sdf 113 dock10	0.3900	61.86	T	F	3	F
114	Structure114 ExpLibOpt sdf 114 dock1	0.1000	79.32	T	F	2	F
	Structure114 ExpLibOpt sdf 114 dock2	0.1000	78.41	T	T	5	T
	Structure114 ExpLibOpt sdf 114 dock4	0.1000	67.61	T	F	2	F
115	Structure115 ExpLibOpt sdf 115 dock2	0.1000	77.35	T	T	5	T
	Structure115 ExpLibOpt sdf 115 dock3	0.1000	76.77	T	T	5	T
	Structure115 ExpLibOpt sdf 115 dock1	0.1000	76.65	T	T	5	T
116	Structure116 ExpLibOpt sdf 116 dock1	0.1000	74.24	F	F	0	F
	Structure116 ExpLibOpt sdf 116 dock4	0.1000	73.75	F	F	0	F
	Structure116 ExpLibOpt sdf 116 dock6	0.1000	73.62	F	F	0	F
117	Structure117 ExpLibOpt sdf 117 dock2	0.2000	63.98	T	T	5	T

	Structure117 ExpLibOpt sdf 117 dock1	0.2000	63.82	T	T	5	T
	Structure117 ExpLibOpt sdf 117 dock3	0.2000	63.62	T	T	5	T
118	Structure118 ExpLibOpt sdf 118 dock3	0.0015	64.07	T	F	2	F
	Structure118 ExpLibOpt sdf 118 dock1	0.0015	62.17	T	T	2	F
	Structure118 ExpLibOpt sdf 118 dock2	0.0015	61.05	T	T	2	F
119	Structure119 ExpLibOpt sdf 119 dock3	0.0250	76.57	T	T	4	T
	Structure119 ExpLibOpt sdf 119 dock1	0.0250	76.48	T	T	4	T
	Structure119 ExpLibOpt sdf 119 dock2	0.0250	76.08	T	T	4	T
120	Structure120 ExpLibOpt sdf 120 dock3	0.3900	72.63	T	F	5	F
	Structure120 ExpLibOpt sdf 120 dock4	0.3900	72.58	T	T	5	T
	Structure120 ExpLibOpt sdf 120 dock7	0.3900	72.10	T	T	5	T
121	Structure121 ExpLibOpt sdf 121 dock2	0.0125	78.97	F	F	0	F
	Structure121 ExpLibOpt sdf 121 dock10	0.0125	77.06	F	F	0	F
	Structure121 ExpLibOpt sdf 121 dock9	0.0125	76.58	F	F	0	F
122	Structure122 ExpLibOpt sdf 122 dock4	0.3900	70.56	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock6	0.3900	66.51	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock2	0.3900	63.49	F	F	1	F
123	Structure123 ExpLibOpt sdf 123 dock2	0.3900	73.53	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock1	0.3900	66.84	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock9	0.3900	58.84	F	F	0	F
124	Structure124 ExpLibOpt sdf 124 dock10	0.2000	69.58	F	F	1	F
	Structure124 ExpLibOpt sdf 124 dock2	0.2000	69.48	F	F	1	F
	Structure124 ExpLibOpt sdf 124 dock3	0.2000	68.94	F	F	1	F
125	Structure125 ExpLibOpt sdf 125 dock9	0.2000	67.04	F	F	0	F
	Structure125 ExpLibOpt sdf 125 dock3	0.2000	59.61	F	F	0	F
	Structure125 ExpLibOpt sdf 125 dock1	0.2000	45.07	F	F	0	F
126	Structure126 ExpLibOpt sdf 126 dock7	0.3900	79.01	F	F	1	F
	Structure126 ExpLibOpt sdf 126 dock9	0.3900	73.10	F	F	1	F
	Structure126 ExpLibOpt sdf 126 dock10	0.3900	70.16	F	F	1	F
127	Structure127 ExpLibOpt sdf 127 dock4	0.7800	90.83	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock10	0.7800	86.86	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock8	0.7800	74.12	F	F	0	F

128	Structure128 ExpLibOpt sdf 128 dock4	0.1000	84.31	T	T	5	T
	Structure128 ExpLibOpt sdf 128 dock6	0.1000	73.63	F	F	0	F
	Structure128 ExpLibOpt sdf 128 dock9	0.1000	71.81	F	F	1	F
129	Structure129 ExpLibOpt sdf 129 dock1	0.2000	81.33	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock10	0.2000	78.07	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock6	0.2000	60.29	F	F	0	F
130	Structure130 ExpLibOpt sdf 130 dock1	0.3900	58.51	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock4	0.3900	54.88	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock5	0.3900	51.89	F	F	1	F
131	Structure131 ExpLibOpt sdf 131 dock10	0.7800	79.97	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock1	0.7800	79.82	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock7	0.7800	70.16	F	F	0	F
132	Structure132 ExpLibOpt sdf 132 dock7	0.7800	66.11	F	F	1	F
	Structure132 ExpLibOpt sdf 132 dock9	0.7800	63.40	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock1	0.7800	63.07	F	F	1	F
133	Structure133 ExpLibOpt sdf 133 dock10	0.1000	81.16	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock5	0.1000	80.06	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock2	0.1000	77.67	F	F	0	F
134	Structure134 ExpLibOpt sdf 134 dock1	0.1000	97.87	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock10	0.1000	83.88	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock5	0.1000	72.26	F	F	0	F
135	Structure135 ExpLibOpt sdf 135 dock5	0.1000	92.24	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock6	0.1000	79.83	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock1	0.1000	79.44	F	F	0	F
136	Structure136 ExpLibOpt sdf 136 dock7	1.2600	85.45	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock4	1.2600	82.69	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock3	1.2600	73.13	F	F	0	F
137	Structure137 ExpLibOpt sdf 137 dock2	1.3000	83.78	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock3	1.3000	78.93	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock6	1.3000	74.31	F	F	0	F
138	Structure138 ExpLibOpt sdf 138 dock9	0.0031	88.27	F	F	0	F
	Structure138 ExpLibOpt sdf 138 dock5	0.0031	86.05	F	F	0	F

	Structure138 ExpLibOpt sdf 138 dock6	0.0031	76.30	F	F	1	F
139	Structure139 ExpLibOpt sdf 139 dock9	0.3300	76.41	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock2	0.3300	73.33	F	F	1	F
	Structure139 ExpLibOpt sdf 139 dock10	0.3300	73.07	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock10	0.3300	73.07	F	F	0	F
140	Structure140 ExpLibOpt sdf 140 dock9	0.1600	85.35	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock8	0.1600	85.29	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock4	0.1600	80.28	F	F	0	F
141	Structure141 ExpLibOpt sdf 141 dock10	0.3200	82.85	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock1	0.3200	76.62	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock5	0.3200	76.25	F	F	0	F
142	Structure142 ExpLibOpt sdf 142 dock1	0.0400	87.23	F	F	1	F
	Structure142 ExpLibOpt sdf 142 dock2	0.0400	79.53	F	F	0	F
	Structure142 ExpLibOpt sdf 142 dock4	0.0400	76.28	F	F	1	F
143	Structure143 ExpLibOpt sdf 143 dock1	0.7800	77.61	T	T	5	T
	Structure143 ExpLibOpt sdf 143 dock4	0.7800	76.24	T	T	5	T
	Structure143 ExpLibOpt sdf 143 dock3	0.7800	74.71	F	F	0	F
144	Structure144 ExpLibOpt sdf 144 dock2	0.2000	79.96	T	T	5	T
	Structure144 ExpLibOpt sdf 144 dock3	0.2000	76.68	T	F	3	F
	Structure144 ExpLibOpt sdf 144 dock6	0.2000	69.04	T	T	5	T
145	Structure145 ExpLibOpt sdf 145 dock1	0.1000	97.59	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock4	0.1000	87.21	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock2	0.1000	87.14	F	F	0	F

Legend	
GSF	GOLDScore Fitness Function
VO	Visual Orientation
VF	Visual Fitness
NMPF	Number of Matching Pharmacophoric Features

d) E475V_{mod}.

Cluster ID	DOCK POSE	MICexp	GSF	VO (T/F)	VF (T/F)	NMPF (4-5)	Result (T/F)
1	Structure001 ExpLibOpt sdf 1 dock1	3.0000	66.86	T	F	1	F
	Structure001 ExpLibOpt sdf 1 dock3	3.0000	66.55	T	F	1	F
	Structure001 ExpLibOpt sdf 1 dock2	3.0000	66.41	T	F	1	F
2	Structure002 ExpLibOpt sdf 2 dock4	0.0115	66.74	T	T	5	T
	Structure002 ExpLibOpt sdf 2 dock3	0.0115	66.57	T	T	5	T
	Structure002 ExpLibOpt sdf 2 dock2	0.0115	66.44	T	T	5	T
3	Structure003 ExpLibOpt sdf 3 dock1	0.3000	61.43	T	T	5	T
	Structure003 ExpLibOpt sdf 3 dock3	0.3000	61.08	T	T	5	T
	Structure003 ExpLibOpt sdf 3 dock2	0.3000	60.82	T	T	5	T
4	Structure004 ExpLibOpt sdf 4 dock4	0.0100	62.91	T	T	5	T
	Structure004 ExpLibOpt sdf 4 dock3	0.0100	62.71	T	T	5	T
	Structure004 ExpLibOpt sdf 4 dock2	0.0100	62.38	T	T	5	T
5	Structure005 ExpLibOpt sdf 5 dock1	0.3000	64.25	F	F	0	F
	Structure005 ExpLibOpt sdf 5 dock4	0.3000	62.59	F	F	1	F
	Structure005 ExpLibOpt sdf 5 dock6	0.3000	61.10	T	F	4	F
6	Structure006 ExpLibOpt sdf 6 dock2	0.1200	64.87	F	F	1	F
	Structure006 ExpLibOpt sdf 6 dock3	0.1200	64.65	T	F	1	F
	Structure006 ExpLibOpt sdf 6 dock1	0.1200	64.23	T	F	1	F
7	Structure007 ExpLibOpt sdf 7 dock3	3.5000	63.69	T	T	4	T
	Structure007 ExpLibOpt sdf 7 dock2	3.5000	63.33	T	T	3	F
	Structure007 ExpLibOpt sdf 7 dock1	3.5000	63.26	T	T	4	T
8	Structure008 ExpLibOpt sdf 8 dock2	0.1000	68.27	T	T	4	T
	Structure008 ExpLibOpt sdf 8 dock1	0.1000	68.07	T	T	4	T
	Structure008 ExpLibOpt sdf 8 dock3	0.1000	67.48	T	T	4	T
9	Structure009 ExpLibOpt sdf 9 dock2	1.4000	64.35	F	F	0	F
	Structure009 ExpLibOpt sdf 9 dock1	1.4000	64.03	F	F	0	F
	Structure009 ExpLibOpt sdf 9 dock3	1.4000	63.78	F	F	0	F
10	Structure010 ExpLibOpt sdf 10 dock2	3.2000	64.62	T	T	4	T
	Structure010 ExpLibOpt sdf 10 dock1	3.2000	64.60	T	T	4	T

	Structure010 ExpLibOpt sdf 10 dock3	3.2000	63.90	T	T	4	T
11	Structure011 ExpLibOpt sdf 11 dock1	0.0500	69.09	T	T	3	F
	Structure011 ExpLibOpt sdf 11 dock3	0.0500	68.03	T	T	4	T
	Structure011 ExpLibOpt sdf 11 dock2	0.0500	67.83	T	T	4	T
	Structure012 ExpLibOpt sdf 12 dock1	0.5000	79.52	T	T	5	T
12	Structure012 ExpLibOpt sdf 12 dock3	0.5000	79.47	T	T	5	T
	Structure012 ExpLibOpt sdf 12 dock2	0.5000	79.04	T	T	5	T
	Structure013 ExpLibOpt sdf 13 dock3	1.6000	59.15	T	F	1	F
13	Structure013 ExpLibOpt sdf 13 dock4	1.6000	58.47	T	F	1	F
	Structure013 ExpLibOpt sdf 13 dock5	1.6000	58.35	T	F	3	F
	Structure014 ExpLibOpt sdf 14 dock1	0.5000	70.57	T	F	4	F
14	Structure014 ExpLibOpt sdf 14 dock5	0.5000	67.15	T	F	3	F
	Structure014 ExpLibOpt sdf 14 dock2	0.5000	65.72	T	T	4	T
	Structure015 ExpLibOpt sdf 15 dock1	0.5000	63.52	T	F	3	F
15	Structure015 ExpLibOpt sdf 15 dock3	0.5000	63.27	T	F	2	F
	Structure015 ExpLibOpt sdf 15 dock2	0.5000	61.50	T	F	3	F
	Structure016 ExpLibOpt sdf 16 dock3	2.0000	62.70	F	F	0	F
16	Structure016 ExpLibOpt sdf 16 dock10	2.0000	62.35	F	F	1	F
	Structure016 ExpLibOpt sdf 16 dock2	2.0000	62.29	F	F	1	F
	Structure017 ExpLibOpt sdf 17 dock2	0.5000	76.46	T	T	5	T
17	Structure017 ExpLibOpt sdf 17 dock3	0.5000	76.08	T	T	5	T
	Structure017 ExpLibOpt sdf 17 dock1	0.5000	75.78	T	T	5	T
	Structure018 ExpLibOpt sdf 18 dock7	0.5000	61.38	F	F	1	F
18	Structure018 ExpLibOpt sdf 18 dock9	0.5000	61.12	T	T	5	T
	Structure018 ExpLibOpt sdf 18 dock6	0.5000	60.77	T	T	4	T
	Structure019 ExpLibOpt sdf 19 dock1	0.2500	71.55	F	F	0	F
19	Structure019 ExpLibOpt sdf 19 dock3	0.2500	71.51	F	F	0	F
	Structure019 ExpLibOpt sdf 19 dock2	0.2500	70.72	F	F	1	F
	Structure020 ExpLibOpt sdf 20 dock2	0.0100	67.39	T	T	4	T
20	Structure020 ExpLibOpt sdf 20 dock1	0.0100	67.02	T	T	4	T
	Structure020 ExpLibOpt sdf 20 dock3	0.0100	66.80	T	T	4	T
21	Structure021 ExpLibOpt sdf 21 dock1	0.0310	77.49	T	T	5	T

	Structure021 ExpLibOpt sdf 21 dock2	0.0310	76.44	T	T	5	T
	Structure021 ExpLibOpt sdf 21 dock3	0.0310	74.96	T	T	5	T
22	Structure022 ExpLibOpt sdf 22 dock5	0.0100	69.66	T	T	5	T
	Structure022 ExpLibOpt sdf 22 dock2	0.0100	68.66	T	F	4	F
	Structure022 ExpLibOpt sdf 22 dock6	0.0100	68.37	T	T	5	T
23	Structure023 ExpLibOpt sdf 23 dock4	0.0100	62.90	T	T	4	T
	Structure023 ExpLibOpt sdf 23 dock2	0.0100	62.28	T	T	5	T
	Structure023 ExpLibOpt sdf 23 dock5	0.0100	61.60	T	T	4	T
24	Structure024 ExpLibOpt sdf 24 dock5	0.9000	74.66	T	F	3	F
	Structure024 ExpLibOpt sdf 24 dock2	0.9000	74.01	T	F	2	F
	Structure024 ExpLibOpt sdf 24 dock1	0.9000	71.78	F	F	0	F
25	Structure025 ExpLibOpt sdf 25 dock2	0.1250	70.73	T	F	3	F
	Structure025 ExpLibOpt sdf 25 dock3	0.1250	70.51	T	F	5	F
	Structure025 ExpLibOpt sdf 25 dock1	0.1250	69.26	T	F	4	F
26	Structure026 ExpLibOpt sdf 26 dock3	0.3000	64.41	T	F	5	F
	Structure026 ExpLibOpt sdf 26 dock1	0.3000	64.39	T	F	4	F
	Structure026 ExpLibOpt sdf 26 dock2	0.3000	63.87	T	T	5	T
27	Structure027 ExpLibOpt sdf 27 dock6	0.1200	72.60	F	F	0	F
	Structure027 ExpLibOpt sdf 27 dock1	0.1200	67.07	F	F	0	F
	Structure027 ExpLibOpt sdf 27 dock4	0.1200	66.17	F	F	1	F
28	Structure028 ExpLibOpt sdf 28 dock3	0.0040	67.00	F	F	0	F
	Structure028 ExpLibOpt sdf 28 dock5	0.0040	66.01	F	F	0	F
	Structure028 ExpLibOpt sdf 28 dock4	0.0040	65.92	F	F	1	F
29	Structure029 ExpLibOpt sdf 29 dock1	2.0000	75.35	T	T	4	T
	Structure029 ExpLibOpt sdf 29 dock3	2.0000	75.14	T	T	4	T
	Structure029 ExpLibOpt sdf 29 dock8	2.0000	74.83	T	T	4	T
30	Structure030 ExpLibOpt sdf 30 dock3	0.3900	67.87	T	F	2	F
	Structure030 ExpLibOpt sdf 30 dock1	0.3900	67.74	T	F	3	F
	Structure030 ExpLibOpt sdf 30 dock2	0.3900	66.74	T	T	5	T
31	Structure031 ExpLibOpt sdf 31 dock2	0.0600	69.94	T	T	5	T
	Structure031 ExpLibOpt sdf 31 dock3	0.0600	69.74	T	T	5	T
	Structure031 ExpLibOpt sdf 31 dock1	0.0600	68.69	T	T	5	T

32	Structure032 ExpLibOpt sdf 32 dock1	0.3900	65.46	T	F	2	F
	Structure032 ExpLibOpt sdf 32 dock5	0.3900	64.97	T	F	1	F
	Structure032 ExpLibOpt sdf 32 dock6	0.3900	64.28	T	F	2	F
33	Structure033 ExpLibOpt sdf 33 dock5	0.3900	68.47	T	F	1	F
	Structure033 ExpLibOpt sdf 33 dock2	0.3900	68.36	F	F	0	F
	Structure033 ExpLibOpt sdf 33 dock3	0.3900	67.69	T	F	1	F
34	Structure034 ExpLibOpt sdf 34 dock2	0.7800	70.30	T	F	1	F
	Structure034 ExpLibOpt sdf 34 dock7	0.7800	69.97	T	F	1	F
	Structure034 ExpLibOpt sdf 34 dock6	0.7800	69.87	F	F	1	F
35	Structure035 ExpLibOpt sdf 35 dock1	0.7800	71.22	T	T	5	T
	Structure035 ExpLibOpt sdf 35 dock2	0.7800	69.34	T	F	3	F
	Structure035 ExpLibOpt sdf 35 dock3	0.7800	67.85	T	T	5	T
36	Structure036 ExpLibOpt sdf 36 dock1	0.7800	67.72	T	T	5	T
	Structure036 ExpLibOpt sdf 36 dock2	0.7800	67.47	T	T	5	T
	Structure036 ExpLibOpt sdf 36 dock3	0.7800	67.03	T	T	5	T
37	Structure037 ExpLibOpt sdf 37 dock6	0.1250	71.30	T	T	4	T
	Structure037 ExpLibOpt sdf 37 dock7	0.1250	70.55	T	T	4	T
	Structure037 ExpLibOpt sdf 37 dock2	0.1250	69.02	T	T	4	T
38	Structure038 ExpLibOpt sdf 38 dock2	0.0020	72.09	T	F	4	F
	Structure038 ExpLibOpt sdf 38 dock4	0.0020	71.35	T	T	4	T
	Structure038 ExpLibOpt sdf 38 dock6	0.0020	70.55	T	T	4	T
39	Structure039 ExpLibOpt sdf 39 dock1	0.1100	65.84	T	F	5	F
	Structure039 ExpLibOpt sdf 39 dock8	0.1100	64.63	T	T	5	T
	Structure039 ExpLibOpt sdf 39 dock7	0.1100	64.44	T	F	5	F
40	Structure040 ExpLibOpt sdf 40 dock3	0.0120	66.58	T	F	4	F
	Structure040 ExpLibOpt sdf 40 dock2	0.0120	66.17	T	F	3	F
	Structure040 ExpLibOpt sdf 40 dock1	0.0120	65.33	T	F	5	F
41	Structure041 ExpLibOpt sdf 41 dock1	0.2500	66.90	T	T	4	T
	Structure041 ExpLibOpt sdf 41 dock2	0.2500	66.88	T	F	3	F
	Structure041 ExpLibOpt sdf 41 dock3	0.2500	66.18	T	T	4	T
42	Structure042 ExpLibOpt sdf 42 dock3	0.0160	73.85	T	F	4	F
	Structure042 ExpLibOpt sdf 42 dock2	0.0160	72.91	T	T	3	F

	Structure042 ExpLibOpt sdf 42 dock1	0.0160	72.00	T	T	3	F
43	Structure043 ExpLibOpt sdf 43 dock1	0.6000	65.63	T	F	1	F
	Structure043 ExpLibOpt sdf 43 dock6	0.6000	65.53	F	F	0	F
	Structure043 ExpLibOpt sdf 43 dock10	0.6000	64.95	T	F	0	F
	Structure044 ExpLibOpt sdf 44 dock3	0.3900	61.97	F	F	1	F
44	Structure044 ExpLibOpt sdf 44 dock10	0.3900	61.06	F	F	1	F
	Structure044 ExpLibOpt sdf 44 dock7	0.3900	60.35	T	T	5	T
45	Structure045 ExpLibOpt sdf 45 dock1	0.3000	69.74	T	F	1	F
	Structure045 ExpLibOpt sdf 45 dock5	0.3000	68.88	T	F	1	F
	Structure045 ExpLibOpt sdf 45 dock4	0.3000	68.81	T	F	1	F
46	Structure046 ExpLibOpt sdf 46 dock3	0.0300	69.60	T	T	5	T
	Structure046 ExpLibOpt sdf 46 dock2	0.0300	69.53	T	T	5	T
	Structure046 ExpLibOpt sdf 46 dock1	0.0300	69.47	T	T	5	T
47	Structure047 ExpLibOpt sdf 47 dock1	0.1250	71.35	T	F	2	F
	Structure047 ExpLibOpt sdf 47 dock2	0.1250	70.86	T	F	5	F
	Structure047 ExpLibOpt sdf 47 dock3	0.1250	70.13	T	T	5	T
48	Structure048 ExpLibOpt sdf 48 dock2	0.1250	66.99	T	T	5	T
	Structure048 ExpLibOpt sdf 48 dock1	0.1250	66.61	T	F	2	F
	Structure048 ExpLibOpt sdf 48 dock3	0.1250	66.43	T	T	5	T
49	Structure049 ExpLibOpt sdf 49 dock5	0.5000	76.32	T	T	4	T
	Structure049 ExpLibOpt sdf 49 dock3	0.5000	76.13	T	T	4	T
	Structure049 ExpLibOpt sdf 49 dock8	0.5000	74.64	T	T	4	T
50	Structure050 ExpLibOpt sdf 50 dock1	0.0016	84.13	F	F	0	F
	Structure050 ExpLibOpt sdf 50 dock5	0.0016	78.40	T	F	5	F
	Structure050 ExpLibOpt sdf 50 dock9	0.0016	75.65	T	F	4	F
51	Structure051 ExpLibOpt sdf 51 dock1	6.3000	79.95	T	F	2	F
	Structure051 ExpLibOpt sdf 51 dock2	6.3000	79.91	T	F	3	F
	Structure051 ExpLibOpt sdf 51 dock6	6.3000	79.70	T	F	3	F
52	Structure052 ExpLibOpt sdf 52 dock10	6.5700	79.60	T	T	5	T
	Structure052 ExpLibOpt sdf 52 dock1	6.5700	78.77	T	F	2	F
	Structure052 ExpLibOpt sdf 52 dock2	6.5700	78.75	F	F	1	F
53	Structure053 ExpLibOpt sdf 53 dock5	5.2000	89.59	F	F	0	F

	Structure053 ExpLibOpt sdf 53 dock8	5.2000	86.64	F	F	0	F
	Structure053 ExpLibOpt sdf 53 dock6	5.2000	85.30	F	F	0	F
54	Structure054 ExpLibOpt sdf 54 dock5	6.9000	99.19	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock10	6.9000	91.25	F	F	0	F
	Structure054 ExpLibOpt sdf 54 dock3	6.9000	86.73	F	F	0	F
55	Structure055 ExpLibOpt sdf 55 dock5	6.4500	86.17	T	F	2	F
	Structure055 ExpLibOpt sdf 55 dock6	6.4500	83.53	F	F	0	F
	Structure055 ExpLibOpt sdf 55 dock7	6.4500	83.35	T	F	3	F
56	Structure056 ExpLibOpt sdf 56 dock10	6.7000	86.04	F	F	0	F
	Structure056 ExpLibOpt sdf 56 dock7	6.7000	85.89	F	F	0	F
	Structure056 ExpLibOpt sdf 56 dock5	6.7000	84.19	F	F	0	F
57	Structure057 ExpLibOpt sdf 57 dock3	6.3000	87.75	F	F	0	F
	Structure057 ExpLibOpt sdf 57 dock5	6.3000	84.55	F	F	0	F
	Structure057 ExpLibOpt sdf 57 dock7	6.3000	80.40	T	F	4	F
58	Structure058 ExpLibOpt sdf 58 dock2	6.2600	90.35	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock8	6.2600	89.22	F	F	0	F
	Structure058 ExpLibOpt sdf 58 dock4	6.2600	87.83	F	F	0	F
59	Structure059 ExpLibOpt sdf 59 dock10	6.9200	87.00	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock8	6.9200	86.98	F	F	0	F
	Structure059 ExpLibOpt sdf 59 dock5	6.9200	83.39	T	F	3	F
60	Structure060 ExpLibOpt sdf 60 dock3	0.0300	75.70	T	T	4	T
	Structure060 ExpLibOpt sdf 60 dock2	0.0300	75.22	T	T	4	T
	Structure060 ExpLibOpt sdf 60 dock1	0.0300	70.12	T	T	4	T
61	Structure061 ExpLibOpt sdf 61 dock8	3.2000	66.48	F	F	1	F
	Structure061 ExpLibOpt sdf 61 dock4	3.2000	66.43	F	F	1	F
	Structure061 ExpLibOpt sdf 61 dock2	3.2000	66.04	F	F	0	F
62	Structure062 ExpLibOpt sdf 62 dock1	0.1250	73.04	T	T	5	T
	Structure062 ExpLibOpt sdf 62 dock3	0.1250	72.70	T	T	5	T
	Structure062 ExpLibOpt sdf 62 dock2	0.1250	71.37	T	T	5	T
63	Structure063 ExpLibOpt sdf 63 dock2	0.5000	74.44	T	F	2	F
	Structure063 ExpLibOpt sdf 63 dock4	0.5000	74.00	T	T	5	T
	Structure063 ExpLibOpt sdf 63 dock3	0.5000	73.28	T	T	5	T

64	Structure064 ExpLibOpt sdf 64 dock2	0.0300	78.34	T	T	3	F
	Structure064 ExpLibOpt sdf 64 dock1	0.0300	76.81	T	T	3	F
	Structure064 ExpLibOpt sdf 64 dock3	0.0300	75.67	T	T	3	F
65	Structure065 ExpLibOpt sdf 65 dock3	0.7800	82.48	T	F	2	F
	Structure065 ExpLibOpt sdf 65 dock2	0.7800	81.89	T	F	3	F
	Structure065 ExpLibOpt sdf 65 dock6	0.7800	80.21	T	F	2	F
66	Structure066 ExpLibOpt sdf 66 dock3	0.7800	83.99	F	F	0	F
	Structure066 ExpLibOpt sdf 66 dock8	0.7800	81.47	F	F	0	F
	Structure066 ExpLibOpt sdf 66 dock4	0.7800	80.34	T	F	2	F
67	Structure067 ExpLibOpt sdf 67 dock8	6.2500	77.97	F	F	0	F
	Structure067 ExpLibOpt sdf 67 dock4	6.2500	75.05	T	F	3	F
	Structure067 ExpLibOpt sdf 67 dock1	6.2500	74.72	T	F	1	F
68	Structure068 ExpLibOpt sdf 68 dock2	0.7800	82.46	T	F	2	F
	Structure068 ExpLibOpt sdf 68 dock9	0.7800	80.95	T	F	3	F
	Structure068 ExpLibOpt sdf 68 dock1	0.7800	77.27	T	T	5	T
69	Structure069 ExpLibOpt sdf 69 dock2	1.5600	77.87	T	T	5	T
	Structure069 ExpLibOpt sdf 69 dock4	1.5600	76.95	T	T	3	F
	Structure069 ExpLibOpt sdf 69 dock3	1.5600	75.80	T	T	5	T
70	Structure070 ExpLibOpt sdf 70 dock7	1.5600	83.73	F	F	0	F
	Structure070 ExpLibOpt sdf 70 dock2	1.5600	78.20	T	F	3	F
	Structure070 ExpLibOpt sdf 70 dock9	1.5600	76.69	T	F	5	F
71	Structure071 ExpLibOpt sdf 71 dock1	3.1300	80.47	T	T	5	T
	Structure071 ExpLibOpt sdf 71 dock10	3.1300	80.21	T	T	5	T
	Structure071 ExpLibOpt sdf 71 dock7	3.1300	79.01	T	T	5	T
72	Structure072 ExpLibOpt sdf 72 dock2	7.1200	86.84	F	F	0	F
	Structure072 ExpLibOpt sdf 72 dock8	7.1200	86.63	T	F	2	F
	Structure072 ExpLibOpt sdf 72 dock4	7.1200	81.25	T	T	5	T
73	Structure073 ExpLibOpt sdf 73 dock1	0.0600	68.99	T	T	5	T
	Structure073 ExpLibOpt sdf 73 dock2	0.0600	66.80	T	T	5	T
	Structure073 ExpLibOpt sdf 73 dock4	0.0600	64.99	T	T	5	T
74	Structure074 ExpLibOpt sdf 74 dock2	0.7800	73.04	T	F	4	F
	Structure074 ExpLibOpt sdf 74 dock3	0.7800	72.20	T	T	4	T

	Structure074 ExpLibOpt sdf 74 dock1	0.7800	71.90	T	T	4	T
75	Structure075 ExpLibOpt sdf 75 dock5	0.0625	68.16	F	F	0	F
	Structure075 ExpLibOpt sdf 75 dock7	0.0625	68.14	T	F	1	F
	Structure075 ExpLibOpt sdf 75 dock1	0.0625	67.59	T	F	1	F
76	Structure076 ExpLibOpt sdf 76 dock3	0.1250	72.75	T	T	4	T
	Structure076 ExpLibOpt sdf 76 dock2	0.1250	72.09	T	T	4	T
	Structure076 ExpLibOpt sdf 76 dock1	0.1250	71.96	T	T	4	T
77	Structure077 ExpLibOpt sdf 77 dock5	6.2500	79.34	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock1	6.2500	77.97	F	F	0	F
	Structure077 ExpLibOpt sdf 77 dock7	6.2500	76.30	F	F	0	F
78	Structure078 ExpLibOpt sdf 78 dock2	3.1300	70.03	T	T	5	T
	Structure078 ExpLibOpt sdf 78 dock3	3.1300	69.88	T	T	5	T
	Structure078 ExpLibOpt sdf 78 dock1	3.1300	69.61	T	T	5	T
79	Structure079 ExpLibOpt sdf 79 dock1	3.1300	81.68	T	F	1	F
	Structure079 ExpLibOpt sdf 79 dock5	3.1300	72.28	T	T	5	T
	Structure079 ExpLibOpt sdf 79 dock4	3.1300	72.07	F	F	0	F
80	Structure080 ExpLibOpt sdf 80 dock6	1.5600	81.38	T	T	5	T
	Structure080 ExpLibOpt sdf 80 dock1	1.5600	81.10	T	T	5	T
	Structure080 ExpLibOpt sdf 80 dock2	1.5600	80.82	T	T	5	T
81	Structure081 ExpLibOpt sdf 81 dock2	0.3900	70.87	F	F	1	F
	Structure081 ExpLibOpt sdf 81 dock3	0.3900	70.43	F	F	1	F
	Structure081 ExpLibOpt sdf 81 dock1	0.3900	69.87	F	F	1	F
82	Structure082 ExpLibOpt sdf 82 dock6	0.0030	81.44	F	F	0	F
	Structure082 ExpLibOpt sdf 82 dock9	0.0030	78.99	T	F	4	F
	Structure082 ExpLibOpt sdf 82 dock8	0.0030	76.71	T	F	3	F
83	Structure083 ExpLibOpt sdf 83 dock2	0.0027	86.41	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock8	0.0027	86.35	F	F	0	F
	Structure083 ExpLibOpt sdf 83 dock7	0.0027	84.61	F	F	0	F
84	Structure084 ExpLibOpt sdf 84 dock5	0.0026	81.88	F	F	0	F
	Structure084 ExpLibOpt sdf 84 dock7	0.0026	78.72	F	F	1	F
	Structure084 ExpLibOpt sdf 84 dock3	0.0026	77.83	F	F	1	F
85	Structure085 ExpLibOpt sdf 85 dock5	0.0027	83.51	F	F	0	F

	Structure085 ExpLibOpt sdf 85 dock2	0.0027	82.44	F	F	1	F
	Structure085 ExpLibOpt sdf 85 dock6	0.0027	79.69	T	F	5	F
86	Structure086 ExpLibOpt sdf 86 dock4	0.0012	86.18	T	F	3	F
	Structure086 ExpLibOpt sdf 86 dock5	0.0012	84.99	F	F	0	F
	Structure086 ExpLibOpt sdf 86 dock2	0.0012	82.91	T	F	3	F
87	Structure087 ExpLibOpt sdf 87 dock7	0.0012	80.37	T	T	5	T
	Structure087 ExpLibOpt sdf 87 dock6	0.0012	79.50	T	T	5	T
	Structure087 ExpLibOpt sdf 87 dock3	0.0012	77.15	F	F	0	F
88	Structure088 ExpLibOpt sdf 88 dock5	0.0014	84.88	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock7	0.0014	82.56	F	F	0	F
	Structure088 ExpLibOpt sdf 88 dock1	0.0014	80.69	F	F	1	F
89	Structure089 ExpLibOpt sdf 89 dock6	0.0108	81.14	T	T	3	F
	Structure089 ExpLibOpt sdf 89 dock10	0.0108	80.43	F	F	1	F
	Structure089 ExpLibOpt sdf 89 dock9	0.0108	78.14	F	F	1	F
90	Structure090 ExpLibOpt sdf 90 dock5	0.0029	92.75	F	F	0	F
	Structure090 ExpLibOpt sdf 90 dock6	0.0029	88.47	F	F	0	F
	Structure090 ExpLibOpt sdf 90 dock3	0.0029	87.04	F	F	0	F
91	Structure091 ExpLibOpt sdf 91 dock7	0.0014	82.67	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock4	0.0014	82.01	F	F	0	F
	Structure091 ExpLibOpt sdf 91 dock2	0.0014	78.86	F	F	0	F
92	Structure092 ExpLibOpt sdf 92 dock2	6.2500	80.11	F	F	1	F
	Structure092 ExpLibOpt sdf 92 dock1	6.2500	80.03	F	F	0	F
	Structure092 ExpLibOpt sdf 92 dock4	6.2500	79.21	T	T	3	F
93	Structure093 ExpLibOpt sdf 93 dock3	0.1250	76.63	T	T	1	F
	Structure093 ExpLibOpt sdf 93 dock1	0.1250	76.61	T	T	3	F
	Structure093 ExpLibOpt sdf 93 dock5	0.1250	76.30	T	T	3	F
94	Structure094 ExpLibOpt sdf 94 dock1	3.1300	100.74	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock8	3.1300	98.27	F	F	0	F
	Structure094 ExpLibOpt sdf 94 dock3	3.1300	94.95	F	F	0	F
95	Structure095 ExpLibOpt sdf 95 dock9	0.7800	88.70	F	F	0	F
	Structure095 ExpLibOpt sdf 95 dock1	0.7800	88.02	F	F	1	F
	Structure095 ExpLibOpt sdf 95 dock7	0.7800	87.93	F	F	0	F

96	Structure096 ExpLibOpt sdf 96 dock1	0.7800	78.55	T	T	5	T
	Structure096 ExpLibOpt sdf 96 dock5	0.7800	78.07	F	F	0	F
	Structure096 ExpLibOpt sdf 96 dock4	0.7800	77.19	T	T	5	T
97	Structure097 ExpLibOpt sdf 97 dock4	0.7800	81.92	T	F	3	F
	Structure097 ExpLibOpt sdf 97 dock6	0.7800	79.09	F	F	1	F
	Structure097 ExpLibOpt sdf 97 dock8	0.7800	79.03	F	F	0	F
98	Structure098 ExpLibOpt sdf 98 dock2	0.0060	70.85	T	F	1	F
	Structure098 ExpLibOpt sdf 98 dock1	0.0060	70.72	T	F	1	F
	Structure098 ExpLibOpt sdf 98 dock3	0.0060	70.00	T	F	2	F
99	Structure099 ExpLibOpt sdf 99 dock2	0.0060	69.89	T	T	4	T
	Structure099 ExpLibOpt sdf 99 dock3	0.0060	69.33	T	T	4	T
	Structure099 ExpLibOpt sdf 99 dock1	0.0060	69.31	T	T	4	T
100	Structure100 ExpLibOpt sdf 100 dock3	0.0130	64.69	T	F	2	F
	Structure100 ExpLibOpt sdf 100 dock4	0.0130	63.48	T	F	2	F
	Structure100 ExpLibOpt sdf 100 dock2	0.0130	60.59	T	T	4	T
101	Structure101 ExpLibOpt sdf 101 dock2	0.0060	73.64	T	T	4	T
	Structure101 ExpLibOpt sdf 101 dock1	0.0060	73.63	T	T	4	T
	Structure101 ExpLibOpt sdf 101 dock3	0.0060	72.43	T	T	4	T
102	Structure102 ExpLibOpt sdf 102 dock3	0.0010	63.04	F	F	1	F
	Structure102 ExpLibOpt sdf 102 dock6	0.0010	61.12	F	F	1	F
	Structure102 ExpLibOpt sdf 102 dock10	0.0010	60.78	T	F	2	F
103	Structure103 ExpLibOpt sdf 103 dock4	0.0020	74.63	T	F	1	F
	Structure103 ExpLibOpt sdf 103 dock2	0.0020	74.59	T	T	4	T
	Structure103 ExpLibOpt sdf 103 dock7	0.0020	73.19	T	T	4	T
104	Structure104 ExpLibOpt sdf 104 dock4	0.0130	61.23	F	F	1	F
	Structure104 ExpLibOpt sdf 104 dock8	0.0130	61.04	F	F	0	F
	Structure104 ExpLibOpt sdf 104 dock2	0.0130	60.90	F	F	0	F
105	Structure105 ExpLibOpt sdf 105 dock1	0.0060	70.87	T	F	3	F
	Structure105 ExpLibOpt sdf 105 dock2	0.0060	70.04	T	T	4	T
	Structure105 ExpLibOpt sdf 105 dock3	0.0060	69.33	T	T	4	T
106	Structure106 ExpLibOpt sdf 106 dock2	0.0250	73.58	T	T	5	T
	Structure106 ExpLibOpt sdf 106 dock1	0.0250	73.46	T	T	5	T

	Structure106 ExpLibOpt sdf 106 dock3	0.0250	73.30	T	T	5	T
107	Structure107 ExpLibOpt sdf 107 dock1	0.0300	59.82	F	F	0	F
	Structure107 ExpLibOpt sdf 107 dock8	0.0300	59.81	T	F	1	F
	Structure107 ExpLibOpt sdf 107 dock7	0.0300	58.72	F	F	1	F
108	Structure108 ExpLibOpt sdf 108 dock1	0.0600	70.69	T	T	5	T
	Structure108 ExpLibOpt sdf 108 dock6	0.0600	70.39	T	T	5	T
	Structure108 ExpLibOpt sdf 108 dock4	0.0600	70.31	T	F	2	F
109	Structure109 ExpLibOpt sdf 109 dock1	0.2000	66.00	T	F	3	F
	Structure109 ExpLibOpt sdf 109 dock3	0.2000	62.06	T	F	4	F
	Structure109 ExpLibOpt sdf 109 dock4	0.2000	61.72	T	T	5	T
110	Structure110 ExpLibOpt sdf 110 dock3	0.3900	72.82	T	T	5	T
	Structure110 ExpLibOpt sdf 110 dock1	0.3900	72.58	T	F	4	F
	Structure110 ExpLibOpt sdf 110 dock2	0.3900	71.78	T	T	5	T
111	Structure111 ExpLibOpt sdf 111 dock1	0.7800	69.63	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock7	0.7800	69.41	T	T	5	T
	Structure111 ExpLibOpt sdf 111 dock2	0.7800	68.22	T	T	5	T
112	Structure112 ExpLibOpt sdf 112 dock1	1.5600	67.08	T	T	5	T
	Structure112 ExpLibOpt sdf 112 dock5	1.5600	66.80	T	F	3	F
	Structure112 ExpLibOpt sdf 112 dock9	1.5600	66.75	T	F	3	F
113	Structure113 ExpLibOpt sdf 113 dock2	0.3900	63.78	T	T	5	T
	Structure113 ExpLibOpt sdf 113 dock6	0.3900	62.49	T	T	5	T
	Structure113 ExpLibOpt sdf 113 dock4	0.3900	61.93	T	F	3	F
114	Structure114 ExpLibOpt sdf 114 dock3	0.1000	77.63	T	F	4	F
	Structure114 ExpLibOpt sdf 114 dock1	0.1000	75.66	T	T	5	T
	Structure114 ExpLibOpt sdf 114 dock4	0.1000	75.58	T	T	5	T
115	Structure115 ExpLibOpt sdf 115 dock1	0.1000	77.56	T	T	5	T
	Structure115 ExpLibOpt sdf 115 dock2	0.1000	76.48	T	T	5	T
	Structure115 ExpLibOpt sdf 115 dock4	0.1000	76.34	T	T	5	T
116	Structure116 ExpLibOpt sdf 116 dock1	0.1000	74.11	F	F	0	F
	Structure116 ExpLibOpt sdf 116 dock2	0.1000	73.73	F	F	1	F
	Structure116 ExpLibOpt sdf 116 dock3	0.1000	71.72	F	F	1	F
117	Structure117 ExpLibOpt sdf 117 dock2	0.2000	63.88	T	T	5	T

	Structure117 ExpLibOpt sdf 117 dock3	0.2000	63.45	T	T	5	T
	Structure117 ExpLibOpt sdf 117 dock1	0.2000	60.65	T	T	5	T
118	Structure118 ExpLibOpt sdf 118 dock3	0.0015	67.88	T	F	0	F
	Structure118 ExpLibOpt sdf 118 dock1	0.0015	67.66	T	F	0	F
	Structure118 ExpLibOpt sdf 118 dock4	0.0015	67.18	T	F	0	F
119	Structure119 ExpLibOpt sdf 119 dock2	0.0250	76.53	T	T	3	F
	Structure119 ExpLibOpt sdf 119 dock3	0.0250	75.80	T	T	4	T
	Structure119 ExpLibOpt sdf 119 dock1	0.0250	74.96	T	T	4	T
120	Structure120 ExpLibOpt sdf 120 dock1	0.3900	76.30	T	F	5	F
	Structure120 ExpLibOpt sdf 120 dock3	0.3900	73.11	T	F	5	F
	Structure120 ExpLibOpt sdf 120 dock2	0.3900	68.16	T	F	3	F
121	Structure121 ExpLibOpt sdf 121 dock8	0.0125	68.28	F	F	0	F
	Structure121 ExpLibOpt sdf 121 dock3	0.0125	68.20	T	F	2	F
	Structure121 ExpLibOpt sdf 121 dock2	0.0125	63.51	F	F	0	F
122	Structure122 ExpLibOpt sdf 122 dock9	0.3900	71.44	T	T	5	T
	Structure122 ExpLibOpt sdf 122 dock1	0.3900	64.55	F	F	0	F
	Structure122 ExpLibOpt sdf 122 dock2	0.3900	63.01	F	F	0	F
123	Structure123 ExpLibOpt sdf 123 dock3	0.3900	69.01	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock10	0.3900	63.77	F	F	0	F
	Structure123 ExpLibOpt sdf 123 dock1	0.3900	57.13	F	F	1	F
124	Structure124 ExpLibOpt sdf 124 dock6	0.2000	81.19	T	F	2	F
	Structure124 ExpLibOpt sdf 124 dock10	0.2000	65.66	F	F	0	F
	Structure124 ExpLibOpt sdf 124 dock9	0.2000	62.63	F	F	0	F
125	Structure125 ExpLibOpt sdf 125 dock2	0.2000	67.85	F	F	1	F
	Structure125 ExpLibOpt sdf 125 dock4	0.2000	67.64	F	F	0	F
	Structure125 ExpLibOpt sdf 125 dock8	0.2000	66.24	F	F	0	F
126	Structure126 ExpLibOpt sdf 126 dock3	0.3900	86.14	T	F	2	F
	Structure126 ExpLibOpt sdf 126 dock4	0.3900	84.85	F	F	0	F
	Structure126 ExpLibOpt sdf 126 dock7	0.3900	83.51	T	T	4	T
127	Structure127 ExpLibOpt sdf 127 dock2	0.7800	82.16	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock6	0.7800	80.74	F	F	0	F
	Structure127 ExpLibOpt sdf 127 dock7	0.7800	62.19	F	F	1	F

128	Structure128 ExpLibOpt sdf 128 dock2	0.1000	81.74	F	F	1	F
	Structure128 ExpLibOpt sdf 128 dock4	0.1000	81.68	T	T	5	T
	Structure128 ExpLibOpt sdf 128 dock7	0.1000	76.90	F	F	0	F
129	Structure129 ExpLibOpt sdf 129 dock7	0.2000	67.60	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock2	0.2000	57.23	F	F	0	F
	Structure129 ExpLibOpt sdf 129 dock10	0.2000	54.36	F	F	0	F
130	Structure130 ExpLibOpt sdf 130 dock10	0.3900	76.77	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock1	0.3900	56.70	F	F	0	F
	Structure130 ExpLibOpt sdf 130 dock8	0.3900	52.23	F	F	0	F
131	Structure131 ExpLibOpt sdf 131 dock1	0.7800	80.69	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock7	0.7800	70.57	F	F	0	F
	Structure131 ExpLibOpt sdf 131 dock9	0.7800	62.04	F	F	0	F
132	Structure132 ExpLibOpt sdf 132 dock2	0.7800	76.32	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock3	0.7800	72.73	F	F	0	F
	Structure132 ExpLibOpt sdf 132 dock9	0.7800	54.97	F	F	0	F
133	Structure133 ExpLibOpt sdf 133 dock2	0.1000	89.97	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock10	0.1000	88.47	F	F	0	F
	Structure133 ExpLibOpt sdf 133 dock7	0.1000	77.53	F	F	0	F
134	Structure134 ExpLibOpt sdf 134 dock7	0.1000	92.62	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock4	0.1000	83.05	F	F	0	F
	Structure134 ExpLibOpt sdf 134 dock9	0.1000	79.13	F	F	0	F
135	Structure135 ExpLibOpt sdf 135 dock7	0.1000	89.63	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock6	0.1000	83.20	F	F	0	F
	Structure135 ExpLibOpt sdf 135 dock5	0.1000	82.04	F	F	0	F
136	Structure136 ExpLibOpt sdf 136 dock3	1.2600	87.44	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock8	1.2600	78.07	F	F	0	F
	Structure136 ExpLibOpt sdf 136 dock5	1.2600	75.79	F	F	0	F
137	Structure137 ExpLibOpt sdf 137 dock4	1.3000	89.63	T	F	1	F
	Structure137 ExpLibOpt sdf 137 dock10	1.3000	84.25	F	F	0	F
	Structure137 ExpLibOpt sdf 137 dock9	1.3000	82.95	F	F	0	F
138	Structure138 ExpLibOpt sdf 138 dock2	0.0031	77.32	F	F	1	F
	Structure138 ExpLibOpt sdf 138 dock1	0.0031	76.64	F	F	0	F

	Structure138 ExpLibOpt sdf 138 dock5	0.0031	76.18	F	F	1	F
139	Structure139 ExpLibOpt sdf 139 dock1	0.3300	78.85	T	F	2	F
	Structure139 ExpLibOpt sdf 139 dock7	0.3300	75.96	F	F	1	F
	Structure139 ExpLibOpt sdf 139 dock3	0.3300	73.91	F	F	0	F
	Structure139 ExpLibOpt sdf 139 dock5	0.3300	73.91	F	F	0	F
140	Structure140 ExpLibOpt sdf 140 dock1	0.1600	82.41	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock7	0.1600	80.26	F	F	0	F
	Structure140 ExpLibOpt sdf 140 dock5	0.1600	78.19	F	F	0	F
141	Structure141 ExpLibOpt sdf 141 dock3	0.3200	87.71	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock10	0.3200	81.78	F	F	0	F
	Structure141 ExpLibOpt sdf 141 dock7	0.3200	80.61	F	F	0	F
142	Structure142 ExpLibOpt sdf 142 dock1	0.0400	93.12	F	F	1	F
	Structure142 ExpLibOpt sdf 142 dock5	0.0400	74.85	F	F	1	F
	Structure142 ExpLibOpt sdf 142 dock3	0.0400	71.45	F	F	1	F
143	Structure143 ExpLibOpt sdf 143 dock6	0.7800	78.38	T	T	5	T
	Structure143 ExpLibOpt sdf 143 dock8	0.7800	74.11	T	F	0	F
	Structure143 ExpLibOpt sdf 143 dock3	0.7800	71.66	T	T	5	T
144	Structure144 ExpLibOpt sdf 144 dock9	0.2000	81.67	T	F	1	F
	Structure144 ExpLibOpt sdf 144 dock3	0.2000	79.27	T	T	5	T
	Structure144 ExpLibOpt sdf 144 dock4	0.2000	78.60	T	T	5	T
145	Structure145 ExpLibOpt sdf 145 dock5	0.1000	99.41	F	F	0	F
	Structure145 ExpLibOpt sdf 145 dock3	0.1000	98.05	F	F	1	F
	Structure145 ExpLibOpt sdf 145 dock7	0.1000	87.06	F	F	0	F

Legend	
GSF	GOLDScore Fitness Function
VO	Visual Orientation
VF	Visual Fitness
NMPF	Number of Matching Pharmacophoric Features

Table S2. The results obtained after the Level 1 Boolean-based (T/F (true/false)) clustering (Geometry assessment) of the combinatorially-generated drug-like 6-FQ binding poses (*CombiLibHits*) for the constructed *gyrB* mutant models: a) N473T_{mod}, b) T474P_{mod}, and c) E475V_{mod}.

a) N473T_{mod}.

Cluster ID	DOCK POSE	MICpred_combi	GSF	VO (T/F)	VF (T/F)	NMPF (4-5)	Result (T/F)
CIP'-024-176	CIP'-024-176 CombiLibHits sdf 1 dock2	0.0250	80.32	T	F	2	F
	CIP'-024-176 CombiLibHits sdf 1 dock1	0.0250	79.62	T	F	2	F
	CIP'-024-176 CombiLibHits sdf 1 dock3	0.0250	79.59	T	F	2	F
CIP'-028-002	CIP'-028-002 CombiLibHits sdf 2 dock1	0.0499	86.91	T	F	2	F
	CIP'-028-002 CombiLibHits sdf 2 dock7	0.0499	86.52	T	T	4	T
	CIP'-028-002 CombiLibHits sdf 2 dock10	0.0499	85.67	T	T	4	T
CIP'-028-018	CIP'-028-018 CombiLibHits sdf 3 dock3	0.0300	82.21	F	F	0	F
	CIP'-028-018 CombiLibHits sdf 3 dock2	0.0300	80.87	F	F	0	F
	CIP'-028-018 CombiLibHits sdf 3 dock1	0.0300	78.71	F	F	0	F
CIP'-028-055	CIP'-028-055 CombiLibHits sdf 4 dock2	0.0234	94.05	T	T	4	T
	CIP'-028-055 CombiLibHits sdf 4 dock3	0.0234	93.57	T	T	4	T
	CIP'-028-055 CombiLibHits sdf 4 dock1	0.0234	93.44	T	T	4	T
CIP'-028-059	CIP'-028-059 CombiLibHits sdf 5 dock3	0.0499	87.58	F	F	1	F
	CIP'-028-059 CombiLibHits sdf 5 dock1	0.0499	87.19	F	F	1	F
	CIP'-028-059 CombiLibHits sdf 5 dock2	0.0499	86.75	F	F	1	F
CIP'-028-073	CIP'-028-073 CombiLibHits sdf 6 dock3	0.0021	88.03	T	T	4	T
	CIP'-028-073 CombiLibHits sdf 6 dock1	0.0021	87.79	T	F	2	F
	CIP'-028-073 CombiLibHits sdf 6 dock2	0.0021	86.52	T	F	2	F
CIP'-028-113	CIP'-028-113 CombiLibHits sdf 7 dock3	0.0499	90.60	T	T	4	T
	CIP'-028-113 CombiLibHits sdf 7 dock2	0.0499	90.34	T	T	4	T
	CIP'-028-113 CombiLibHits sdf 7 dock1	0.0499	89.81	T	T	4	T
CIP'-028-128	CIP'-028-128 CombiLibHits sdf 8 dock4	0.0021	90.64	T	T	4	T

	CIP'-028-128 CombiLibHits sdf 8 dock1	0.0021	89.83	T	T	4	T
	CIP'-028-128 CombiLibHits sdf 8 dock2	0.0021	89.63	T	T	4	T
CIP'-028-148	CIP'-028-148 CombiLibHits sdf 9 dock1	0.0499	87.54	T	F	3	F
	CIP'-028-148 CombiLibHits sdf 9 dock2	0.0499	85.80	T	F	1	F
	CIP'-028-148 CombiLibHits sdf 9 dock3	0.0499	84.72	T	T	4	T
CIP'-028-149	CIP'-028-149 CombiLibHits sdf 10 dock8	0.0021	88.35	F	F	0	F
	CIP'-028-149 CombiLibHits sdf 10 dock10	0.0021	86.77	F	F	0	F
	CIP'-028-149 CombiLibHits sdf 10 dock3	0.0021	86.71	T	T	4	T
CIP'-028-154	CIP'-028-154 CombiLibHits sdf 11 dock2	0.0021	89.93	T	T	4	T
	CIP'-028-154 CombiLibHits sdf 11 dock3	0.0021	89.58	T	F	3	F
	CIP'-028-154 CombiLibHits sdf 11 dock5	0.0021	89.33	T	T	4	T
CIP'-036-057	CIP'-036-057 CombiLibHits sdf 12 dock3	0.0021	86.33	T	F	4	F
	CIP'-036-057 CombiLibHits sdf 12 dock1	0.0021	86.09	T	T	4	T
	CIP'-036-057 CombiLibHits sdf 12 dock4	0.0021	85.22	T	F	3	F
CIP'-036-059	CIP'-036-059 CombiLibHits sdf 13 dock1	0.0021	89.98	T	F	1	F
	CIP'-036-059 CombiLibHits sdf 13 dock2	0.0021	89.98	T	F	1	F
	CIP'-036-059 CombiLibHits sdf 13 dock3	0.0021	89.16	T	F	1	F
CIP'-036-092	CIP'-036-092 CombiLibHits sdf 14 dock2	0.0250	90.35	T	F	1	F
	CIP'-036-092 CombiLibHits sdf 14 dock3	0.0250	90.24	T	F	1	F
	CIP'-036-092 CombiLibHits sdf 14 dock4	0.0250	87.97	T	F	1	F
CIP'-046-018	CIP'-046-018 CombiLibHits sdf 15 dock9	0.0300	95.58	T	F	1	F
	CIP'-046-018 CombiLibHits sdf 15 dock3	0.0300	84.31	T	F	1	F
	CIP'-046-018 CombiLibHits sdf 15 dock6	0.0300	82.91	T	F	0	F
CIP'-046-069	CIP'-046-069 CombiLibHits sdf 16 dock8	0.0300	82.92	F	F	0	F
	CIP'-046-069 CombiLibHits sdf 16 dock4	0.0300	82.27	F	F	0	F
	CIP'-046-069 CombiLibHits sdf 16 dock7	0.0300	78.24	T	F	2	F
CIP'-046-149	CIP'-046-149 CombiLibHits sdf 17 dock2	0.0311	87.18	T	F	2	F
	CIP'-046-149 CombiLibHits sdf 17 dock1	0.0311	84.42	T	F	2	F
	CIP'-046-149 CombiLibHits sdf 17 dock7	0.0311	76.13	T	F	2	F
CIP'-046-156	CIP'-046-156 CombiLibHits sdf 18 dock5	0.0311	85.72	T	F	2	F
	CIP'-046-156 CombiLibHits sdf 18 dock1	0.0311	80.95	F	F	1	F
	CIP'-046-156 CombiLibHits sdf 18 dock7	0.0311	78.76	F	F	1	F

CIP'-059-176	CIP'-059-176 CombiLibHits sdf 19 dock3	0.0329	81.20	T	T	4	T
	CIP'-059-176 CombiLibHits sdf 19 dock1	0.0329	80.60	T	T	4	T
	CIP'-059-176 CombiLibHits sdf 19 dock6	0.0329	80.57	T	T	4	T
CIP'-060-169	CIP'-060-169 CombiLibHits sdf 20 dock3	0.0499	87.41	F	F	1	F
	CIP'-060-169 CombiLibHits sdf 20 dock5	0.0499	86.78	F	F	1	F
	CIP'-060-169 CombiLibHits sdf 20 dock6	0.0499	86.08	F	F	1	F
CIP'-095-057	CIP'-095-057 CombiLibHits sdf 21 dock2	0.0021	91.83	T	T	4	T
	CIP'-095-057 CombiLibHits sdf 21 dock3	0.0021	91.11	T	T	4	T
	CIP'-095-057 CombiLibHits sdf 21 dock4	0.0021	90.45	T	T	4	T
CIP'-095-059	CIP'-095-059 CombiLibHits sdf 22 dock3	0.0021	94.47	F	F	1	F
	CIP'-095-059 CombiLibHits sdf 22 dock1	0.0021	94.26	F	F	1	F
	CIP'-095-059 CombiLibHits sdf 22 dock4	0.0021	92.69	F	F	1	F
CIP'-095-073	CIP'-095-073 CombiLibHits sdf 23 dock5	0.0401	93.43	T	T	4	T
	CIP'-095-073 CombiLibHits sdf 23 dock3	0.0401	93.06	T	T	4	T
	CIP'-095-073 CombiLibHits sdf 23 dock4	0.0401	92.86	T	F	3	F
CIP'-095-177	CIP'-095-177 CombiLibHits sdf 24 dock3	0.0401	94.97	T	F	3	F
	CIP'-095-177 CombiLibHits sdf 24 dock5	0.0401	94.56	T	F	3	F
	CIP'-095-177 CombiLibHits sdf 24 dock1	0.0401	94.18	T	F	3	F
CIP'-095-183	CIP'-095-183 CombiLibHits sdf 25 dock6	0.0401	93.24	T	T	4	T
	CIP'-095-183 CombiLibHits sdf 25 dock5	0.0401	92.23	T	F	4	F
	CIP'-095-183 CombiLibHits sdf 25 dock4	0.0401	91.86	T	F	4	F
CIP'-100-073	CIP'-100-073 CombiLibHits sdf 26 dock1	0.0329	87.91	T	T	4	T
	CIP'-100-073 CombiLibHits sdf 26 dock2	0.0329	87.81	T	T	4	T
	CIP'-100-073 CombiLibHits sdf 26 dock3	0.0329	87.64	T	F	2	F
CIP-028-056	CIP-028-056 CombiLibHits sdf 27 dock5	0.0021	86.41	T	F	2	F
	CIP-028-056 CombiLibHits sdf 27 dock7	0.0021	85.59	T	F	2	F
	CIP-028-056 CombiLibHits sdf 27 dock1	0.0021	85.17	F	F	2	F
CIP-028-066	CIP-028-066 CombiLibHits sdf 28 dock7	0.0300	90.47	F	F	0	F
	CIP-028-066 CombiLibHits sdf 28 dock2	0.0300	87.56	T	F	3	F
	CIP-028-066 CombiLibHits sdf 28 dock8	0.0300	86.79	T	T	4	T
CIP-028-082	CIP-028-082 CombiLibHits sdf 29 dock1	0.0300	97.48	T	T	4	T
	CIP-028-082 CombiLibHits sdf 29 dock2	0.0300	97.41	T	T	4	T

	CIP-028-082 CombiLibHits sdf 29 dock3	0.0300	90.80	T	T	4	T
CIP-028-083	CIP-028-083 CombiLibHits sdf 30 dock1	0.0499	85.56	T	F	4	F
	CIP-028-083 CombiLibHits sdf 30 dock3	0.0499	85.22	T	F	2	F
	CIP-028-083 CombiLibHits sdf 30 dock4	0.0499	85.19	T	F	1	F
CIP-028-102	CIP-028-102 CombiLibHits sdf 31 dock1	0.0130	80.68	T	F	1	F
	CIP-028-102 CombiLibHits sdf 31 dock6	0.0130	80.53	T	F	1	F
	CIP-028-102 CombiLibHits sdf 31 dock4	0.0130	80.50	T	F	1	F
CIP-036-096	CIP-036-096 CombiLibHits sdf 32 dock1	0.0250	83.06	T	F	1	F
	CIP-036-096 CombiLibHits sdf 32 dock3	0.0250	82.37	T	F	1	F
	CIP-036-096 CombiLibHits sdf 32 dock2	0.0250	80.66	T	F	1	F
CIP-037-090	CIP-037-090 CombiLibHits sdf 33 dock1	0.0130	92.35	T	F	1	F
	CIP-037-090 CombiLibHits sdf 33 dock3	0.0130	91.33	T	F	1	F
	CIP-037-090 CombiLibHits sdf 33 dock2	0.0130	86.52	T	F	0	F
CIP-049-083	CIP-049-083 CombiLibHits sdf 34 dock2	0.0130	94.54	F	F	0	F
	CIP-049-083 CombiLibHits sdf 34 dock4	0.0130	93.52	F	F	0	F
	CIP-049-083 CombiLibHits sdf 34 dock5	0.0130	91.98	F	F	0	F
CIP-049-096	CIP-049-096 CombiLibHits sdf 35 dock2	0.0329	84.44	T	T	4	T
	CIP-049-096 CombiLibHits sdf 35 dock5	0.0329	83.90	T	T	4	T
	CIP-049-096 CombiLibHits sdf 35 dock6	0.0329	83.86	T	T	4	T
CIP-049-101	CIP-049-101 CombiLibHits sdf 36 dock1	0.0401	86.75	T	F	1	F
	CIP-049-101 CombiLibHits sdf 36 dock3	0.0401	86.43	T	F	1	F
	CIP-049-101 CombiLibHits sdf 36 dock2	0.0401	84.41	T	T	4	T
CIP-059-096	CIP-059-096 CombiLibHits sdf 37 dock9	0.0250	86.00	T	F	1	F
	CIP-059-096 CombiLibHits sdf 37 dock7	0.0250	85.63	T	F	1	F
	CIP-059-096 CombiLibHits sdf 37 dock10	0.0250	84.72	T	F	1	F
CIP-059-102	CIP-059-102 CombiLibHits sdf 38 dock8	0.0250	85.39	T	F	1	F
	CIP-059-102 CombiLibHits sdf 38 dock4	0.0250	84.86	T	F	1	F
	CIP-059-102 CombiLibHits sdf 38 dock5	0.0250	83.97	T	F	1	F
CIP-060-090	CIP-060-090 CombiLibHits sdf 39 dock1	0.0499	86.41	F	F	0	F
	CIP-060-090 CombiLibHits sdf 39 dock9	0.0499	86.15	F	F	0	F
	CIP-060-090 CombiLibHits sdf 39 dock10	0.0499	86.09	F	F	0	F
CIP-096-098	CIP-096-098 CombiLibHits sdf 40 dock1	0.0401	86.61	T	T	4	T

	CIP-096-098 CombiLibHits sdf 40 dock3	0.0401	85.35	T	T	4	T
	CIP-096-098 CombiLibHits sdf 40 dock2	0.0401	84.97	T	T	4	T
CIP-101-101	CIP-101-101 CombiLibHits sdf 41 dock2	0.0401	84.96	T	F	2	F
	CIP-101-101 CombiLibHits sdf 41 dock7	0.0401	84.67	T	F	2	F
	CIP-101-101 CombiLibHits sdf 41 dock5	0.0401	84.51	T	F	1	F
MOX'-016-005	MOX'-016-005 CombiLibHits sdf 42 dock1	0.0499	82.62	T	F	0	F
	MOX'-016-005 CombiLibHits sdf 42 dock3	0.0499	81.79	T	F	0	F
	MOX'-016-005 CombiLibHits sdf 42 dock2	0.0499	81.60	T	F	0	F
MOX'-016-116	MOX'-016-116 CombiLibHits sdf 43 dock1	0.0499	83.94	T	F	2	F
	MOX'-016-116 CombiLibHits sdf 43 dock3	0.0499	83.81	T	T	3	F
	MOX'-016-116 CombiLibHits sdf 43 dock2	0.0499	79.24	T	F	2	F
MOX'-016-137	MOX'-016-137 CombiLibHits sdf 44 dock2	0.0300	89.54	T	T	3	F
	MOX'-016-137 CombiLibHits sdf 44 dock3	0.0300	89.24	T	T	4	T
	MOX'-016-137 CombiLibHits sdf 44 dock1	0.0300	88.71	T	T	4	T
MOX'-028-116	MOX'-028-116 CombiLibHits sdf 45 dock1	0.0130	86.34	T	T	4	T
	MOX'-028-116 CombiLibHits sdf 45 dock7	0.0130	82.94	T	T	4	T
	MOX'-028-116 CombiLibHits sdf 45 dock8	0.0130	82.13	T	F	2	F
MOX'-039-005	MOX'-039-005 CombiLibHits sdf 46 dock5	0.0499	82.47	T	T	4	T
	MOX'-039-005 CombiLibHits sdf 46 dock1	0.0499	82.32	T	T	4	T
	MOX'-039-005 CombiLibHits sdf 46 dock3	0.0499	82.12	T	T	4	T
MOX'-060-033	MOX'-060-033 CombiLibHits sdf 47 dock5	0.0401	80.08	T	T	4	T
	MOX'-060-033 CombiLibHits sdf 47 dock2	0.0401	76.41	T	T	4	T
	MOX'-060-033 CombiLibHits sdf 47 dock3	0.0401	76.18	T	T	4	T
MOX'-065-050	MOX'-065-050 CombiLibHits sdf 48 dock3	0.0401	87.63	T	F	1	F
	MOX'-065-050 CombiLibHits sdf 48 dock1	0.0401	87.00	T	F	2	F
	MOX'-065-050 CombiLibHits sdf 48 dock2	0.0401	84.71	T	F	1	F

Legend	
GSF	GOLDScore Fitness Function
VO	Visual Orientation
VF	Visual Fitness
NMPF	Number of Matching Pharmacophoric Features

b) T474P_{mod}.

Cluster ID	DOCK POSE	MICpred_combi	GSF	VO (T/F)	VF (T/F)	NMPF (4-5)	Result (T/F)
CIP'-024-176	CIP'-024-176 CombiLibHits sdf 1 dock3	0.0250	80.03	T	F	2	F
	CIP'-024-176 CombiLibHits sdf 1 dock2	0.0250	79.98	T	T	4	T
	CIP'-024-176 CombiLibHits sdf 1 dock1	0.0250	77.23	T	F	2	F
CIP'-028-002	CIP'-028-002 CombiLibHits sdf 2 dock2	0.0499	89.04	T	T	4	T
	CIP'-028-002 CombiLibHits sdf 2 dock1	0.0499	88.35	T	T	4	T
	CIP'-028-002 CombiLibHits sdf 2 dock4	0.0499	86.02	T	T	4	T
CIP'-028-018	CIP'-028-018 CombiLibHits sdf 3 dock9	0.0300	95.59	T	F	2	F
	CIP'-028-018 CombiLibHits sdf 3 dock8	0.0300	85.54	T	F	2	F
	CIP'-028-018 CombiLibHits sdf 3 dock1	0.0300	84.11	T	F	0	F
CIP'-028-055	CIP'-028-055 CombiLibHits sdf 4 dock2	0.0234	96.06	T	T	3	F
	CIP'-028-055 CombiLibHits sdf 4 dock3	0.0234	94.07	T	T	4	T
	CIP'-028-055 CombiLibHits sdf 4 dock1	0.0234	92.54	T	F	3	F
CIP'-028-059	CIP'-028-059 CombiLibHits sdf 5 dock10	0.0499	86.21	F	F	1	F
	CIP'-028-059 CombiLibHits sdf 5 dock6	0.0499	85.09	T	T	4	T
	CIP'-028-059 CombiLibHits sdf 5 dock4	0.0499	85.02	T	F	2	F
CIP'-028-073	CIP'-028-073 CombiLibHits sdf 6 dock1	0.0021	87.33	T	T	4	T
	CIP'-028-073 CombiLibHits sdf 6 dock2	0.0021	86.74	T	T	4	T
	CIP'-028-073 CombiLibHits sdf 6 dock4	0.0021	86.26	T	T	4	T
CIP'-028-113	CIP'-028-113 CombiLibHits sdf 7 dock4	0.0499	89.75	F	F	1	F
	CIP'-028-113 CombiLibHits sdf 7 dock2	0.0499	86.45	F	F	0	F
	CIP'-028-113 CombiLibHits sdf 7 dock1	0.0499	86.00	F	F	0	F
CIP'-028-128	CIP'-028-128 CombiLibHits sdf 8 dock6	0.0021	95.38	F	F	0	F
	CIP'-028-128 CombiLibHits sdf 8 dock1	0.0021	88.62	F	F	0	F
	CIP'-028-128 CombiLibHits sdf 8 dock9	0.0021	88.10	T	T	4	T
CIP'-028-148	CIP'-028-148 CombiLibHits sdf 9 dock2	0.0499	85.89	T	T	4	T
	CIP'-028-148 CombiLibHits sdf 9 dock5	0.0499	85.88	T	F	2	F
	CIP'-028-148 CombiLibHits sdf 9 dock3	0.0499	83.55	T	F	1	F
CIP'-028-149	CIP'-028-149 CombiLibHits sdf 10 dock4	0.0021	88.08	F	F	0	F

CIP'-028-154	CIP'-028-149 CombiLibHits sdf 10 dock6	0.0021	86.02	F	F	0	F
	CIP'-028-149 CombiLibHits sdf 10 dock7	0.0021	83.08	F	F	0	F
	CIP'-028-154 CombiLibHits sdf 11 dock1	0.0021	91.36	F	F	1	F
	CIP'-028-154 CombiLibHits sdf 11 dock2	0.0021	87.98	T	F	3	F
	CIP'-028-154 CombiLibHits sdf 11 dock9	0.0021	87.65	T	F	1	F
CIP'-036-057	CIP'-036-057 CombiLibHits sdf 12 dock1	0.0021	84.48	T	T	4	T
	CIP'-036-057 CombiLibHits sdf 12 dock3	0.0021	83.65	T	T	4	T
	CIP'-036-057 CombiLibHits sdf 12 dock2	0.0021	83.16	T	T	4	T
CIP'-036-059	CIP'-036-059 CombiLibHits sdf 13 dock2	0.0021	91.17	T	F	1	F
	CIP'-036-059 CombiLibHits sdf 13 dock1	0.0021	91.09	T	F	1	F
	CIP'-036-059 CombiLibHits sdf 13 dock3	0.0021	90.84	T	F	1	F
CIP'-036-092	CIP'-036-092 CombiLibHits sdf 14 dock1	0.0250	86.19	T	T	3	F
	CIP'-036-092 CombiLibHits sdf 14 dock6	0.0250	85.96	T	T	4	T
	CIP'-036-092 CombiLibHits sdf 14 dock5	0.0250	85.07	F	F	0	F
CIP'-046-018	CIP'-046-018 CombiLibHits sdf 15 dock10	0.0300	95.59	T	F	2	F
	CIP'-046-018 CombiLibHits sdf 15 dock8	0.0300	93.48	T	F	2	F
	CIP'-046-018 CombiLibHits sdf 15 dock9	0.0300	90.12	T	F	2	F
CIP'-046-069	CIP'-046-069 CombiLibHits sdf 16 dock3	0.0300	85.78	F	F	0	F
	CIP'-046-069 CombiLibHits sdf 16 dock9	0.0300	79.67	T	F	1	F
	CIP'-046-069 CombiLibHits sdf 16 dock7	0.0300	78.81	F	F	0	F
CIP'-046-149	CIP'-046-149 CombiLibHits sdf 17 dock2	0.0311	85.94	T	T	4	T
	CIP'-046-149 CombiLibHits sdf 17 dock5	0.0311	85.42	T	F	1	F
	CIP'-046-149 CombiLibHits sdf 17 dock1	0.0311	85.27	T	T	4	T
CIP'-046-156	CIP'-046-156 CombiLibHits sdf 18 dock1	0.0311	86.23	T	F	2	F
	CIP'-046-156 CombiLibHits sdf 18 dock7	0.0311	80.78	T	T	4	T
	CIP'-046-156 CombiLibHits sdf 18 dock10	0.0311	80.41	T	F	3	F
CIP'-059-176	CIP'-059-176 CombiLibHits sdf 19 dock5	0.0329	83.25	T	F	1	F
	CIP'-059-176 CombiLibHits sdf 19 dock2	0.0329	82.37	F	F	1	F
	CIP'-059-176 CombiLibHits sdf 19 dock10	0.0329	81.38	T	T	4	T
CIP'-060-169	CIP'-060-169 CombiLibHits sdf 20 dock7	0.0499	84.73	T	F	1	F
	CIP'-060-169 CombiLibHits sdf 20 dock2	0.0499	84.68	T	F	1	F
	CIP'-060-169 CombiLibHits sdf 20 dock3	0.0499	84.67	F	F	0	F

CIP'-095-057	CIP'-095-057 CombiLibHits sdf 21 dock1	0.0021	86.99	T	T	4	T
	CIP'-095-057 CombiLibHits sdf 21 dock3	0.0021	86.48	T	F	0	F
	CIP'-095-057 CombiLibHits sdf 21 dock2	0.0021	85.38	T	F	2	F
CIP'-095-059	CIP'-095-059 CombiLibHits sdf 22 dock8	0.0021	93.62	T	F	1	F
	CIP'-095-059 CombiLibHits sdf 22 dock1	0.0021	93.29	T	F	1	F
	CIP'-095-059 CombiLibHits sdf 22 dock6	0.0021	92.95	T	F	1	F
CIP'-095-073	CIP'-095-073 CombiLibHits sdf 23 dock4	0.0401	92.04	T	T	4	T
	CIP'-095-073 CombiLibHits sdf 23 dock5	0.0401	91.98	T	T	4	T
	CIP'-095-073 CombiLibHits sdf 23 dock2	0.0401	90.13	T	T	4	T
CIP'-095-177	CIP'-095-177 CombiLibHits sdf 24 dock9	0.0401	91.01	T	T	4	T
	CIP'-095-177 CombiLibHits sdf 24 dock4	0.0401	90.85	T	T	4	T
	CIP'-095-177 CombiLibHits sdf 24 dock5	0.0401	90.47	T	F	1	F
CIP'-095-183	CIP'-095-183 CombiLibHits sdf 25 dock1	0.0401	94.31	T	F	4	F
	CIP'-095-183 CombiLibHits sdf 25 dock2	0.0401	91.65	T	T	4	T
	CIP'-095-183 CombiLibHits sdf 25 dock3	0.0401	87.40	T	T	4	T
CIP'-100-073	CIP'-100-073 CombiLibHits sdf 26 dock10	0.0329	89.48	T	T	4	T
	CIP'-100-073 CombiLibHits sdf 26 dock6	0.0329	89.01	T	T	4	T
	CIP'-100-073 CombiLibHits sdf 26 dock9	0.0329	88.62	T	T	4	T
CIP-028-056	CIP-028-056 CombiLibHits sdf 27 dock7	0.0021	89.80	T	F	2	F
	CIP-028-056 CombiLibHits sdf 27 dock8	0.0021	87.34	T	F	2	F
	CIP-028-056 CombiLibHits sdf 27 dock10	0.0021	87.06	T	F	2	F
CIP-028-066	CIP-028-066 CombiLibHits sdf 28 dock1	0.0300	90.82	T	F	0	F
	CIP-028-066 CombiLibHits sdf 28 dock8	0.0300	90.26	F	F	0	F
	CIP-028-066 CombiLibHits sdf 28 dock10	0.0300	87.76	F	F	0	F
CIP-028-082	CIP-028-082 CombiLibHits sdf 29 dock4	0.0300	97.90	T	T	4	T
	CIP-028-082 CombiLibHits sdf 29 dock2	0.0300	96.85	T	T	4	T
	CIP-028-082 CombiLibHits sdf 29 dock3	0.0300	96.82	T	F	3	F
CIP-028-083	CIP-028-083 CombiLibHits sdf 30 dock10	0.0499	86.25	T	F	2	F
	CIP-028-083 CombiLibHits sdf 30 dock2	0.0499	84.44	T	F	2	F
	CIP-028-083 CombiLibHits sdf 30 dock1	0.0499	84.10	T	T	4	T
CIP-028-102	CIP-028-102 CombiLibHits sdf 31 dock5	0.0130	81.55	T	F	1	F
	CIP-028-102 CombiLibHits sdf 31 dock3	0.0130	80.90	T	F	1	F

	CIP-028-102 CombiLibHits sdf 31 dock8	0.0130	80.32	T	T	4	T
CIP-036-096	CIP-036-096 CombiLibHits sdf 32 dock1	0.0250	80.86	T	T	4	T
	CIP-036-096 CombiLibHits sdf 32 dock8	0.0250	80.45	T	T	4	T
	CIP-036-096 CombiLibHits sdf 32 dock6	0.0250	80.35	T	T	4	T
	CIP-036-096 CombiLibHits sdf 32 dock6	0.0250	80.35	T	T	4	T
CIP-037-090	CIP-037-090 CombiLibHits sdf 33 dock1	0.0130	90.34	T	F	3	F
	CIP-037-090 CombiLibHits sdf 33 dock5	0.0130	88.31	T	F	2	F
	CIP-037-090 CombiLibHits sdf 33 dock6	0.0130	87.88	T	F	2	F
CIP-049-083	CIP-049-083 CombiLibHits sdf 34 dock4	0.0130	93.23	F	F	0	F
	CIP-049-083 CombiLibHits sdf 34 dock5	0.0130	90.41	F	F	0	F
	CIP-049-083 CombiLibHits sdf 34 dock1	0.0130	89.99	F	F	0	F
CIP-049-096	CIP-049-096 CombiLibHits sdf 35 dock2	0.0329	85.58	T	T	4	T
	CIP-049-096 CombiLibHits sdf 35 dock1	0.0329	85.09	T	T	4	T
	CIP-049-096 CombiLibHits sdf 35 dock6	0.0329	84.85	T	T	4	T
CIP-049-101	CIP-049-101 CombiLibHits sdf 36 dock3	0.0401	83.99	T	F	2	F
	CIP-049-101 CombiLibHits sdf 36 dock1	0.0401	83.79	T	F	0	F
	CIP-049-101 CombiLibHits sdf 36 dock2	0.0401	83.49	T	F	2	F
CIP-059-096	CIP-059-096 CombiLibHits sdf 37 dock3	0.0250	84.96	T	F	1	F
	CIP-059-096 CombiLibHits sdf 37 dock5	0.0250	83.99	T	F	2	F
	CIP-059-096 CombiLibHits sdf 37 dock9	0.0250	83.96	T	F	1	F
CIP-059-102	CIP-059-102 CombiLibHits sdf 38 dock6	0.0250	85.72	F	F	0	F
	CIP-059-102 CombiLibHits sdf 38 dock5	0.0250	85.48	F	F	0	F
	CIP-059-102 CombiLibHits sdf 38 dock7	0.0250	83.69	T	F	1	F
CIP-060-090	CIP-060-090 CombiLibHits sdf 39 dock2	0.0499	88.36	F	F	2	F
	CIP-060-090 CombiLibHits sdf 39 dock9	0.0499	86.34	F	F	2	F
	CIP-060-090 CombiLibHits sdf 39 dock4	0.0499	85.67	F	F	0	F
CIP-096-098	CIP-096-098 CombiLibHits sdf 40 dock2	0.0401	84.49	T	T	4	T
	CIP-096-098 CombiLibHits sdf 40 dock7	0.0401	84.04	T	F	1	F
	CIP-096-098 CombiLibHits sdf 40 dock5	0.0401	83.63	T	T	4	T
CIP-101-101	CIP-101-101 CombiLibHits sdf 41 dock4	0.0401	87.47	T	F	2	F
	CIP-101-101 CombiLibHits sdf 41 dock3	0.0401	87.07	T	T	4	T
	CIP-101-101 CombiLibHits sdf 41 dock2	0.0401	85.77	T	F	2	F
MOX'-016-005	MOX'-016-005 CombiLibHits sdf 42 dock3	0.0499	85.01	F	F	0	F

	MOX'-016-005 CombiLibHits sdf 42 dock9	0.0499	84.86	T	F	4	F
	MOX'-016-005 CombiLibHits sdf 42 dock1	0.0499	84.12	T	T	4	T
MOX'-016-116	MOX'-016-116 CombiLibHits sdf 43 dock6	0.0499	85.20	T	T	3	F
	MOX'-016-116 CombiLibHits sdf 43 dock1	0.0499	84.96	T	T	4	T
	MOX'-016-116 CombiLibHits sdf 43 dock4	0.0499	79.19	T	F	1	F
MOX'-016-137	MOX'-016-137 CombiLibHits sdf 44 dock2	0.0300	90.86	T	T	4	T
	MOX'-016-137 CombiLibHits sdf 44 dock5	0.0300	87.49	T	T	4	T
	MOX'-016-137 CombiLibHits sdf 44 dock1	0.0300	84.24	T	T	4	T
MOX'-028-116	MOX'-028-116 CombiLibHits sdf 45 dock3	0.0130	87.27	T	T	4	T
	MOX'-028-116 CombiLibHits sdf 45 dock4	0.0130	86.69	T	T	4	T
	MOX'-028-116 CombiLibHits sdf 45 dock10	0.0130	85.68	T	T	4	T
MOX'-039-005	MOX'-039-005 CombiLibHits sdf 46 dock2	0.0499	84.48	T	T	4	T
	MOX'-039-005 CombiLibHits sdf 46 dock6	0.0499	83.37	T	F	3	F
	MOX'-039-005 CombiLibHits sdf 46 dock4	0.0499	81.67	T	F	4	F
MOX'-060-033	MOX'-060-033 CombiLibHits sdf 47 dock9	0.0401	83.72	T	T	4	T
	MOX'-060-033 CombiLibHits sdf 47 dock4	0.0401	82.52	T	T	4	T
	MOX'-060-033 CombiLibHits sdf 47 dock7	0.0401	79.88	T	T	4	T
MOX'-065-050	MOX'-065-050 CombiLibHits sdf 48 dock5	0.0401	88.93	T	F	2	F
	MOX'-065-050 CombiLibHits sdf 48 dock2	0.0401	86.16	T	F	2	F
	MOX'-065-050 CombiLibHits sdf 48 dock7	0.0401	85.92	T	T	4	T

Legend	
GSF	GOLDScore Fitness Function
VO	Visual Orientation
VF	Visual Fitness
NMPF	Number of Matching Pharmacophoric Features

c) E475V_{mod}.

Cluster ID	DOCK POSE	MICpred_combi	GSF	VO (T/F)	VF (T/F)	NMPF (4-5)	Result (T/F)
CIP'-024-176	CIP'-024-176 CombiLibHits sdf 1 dock1	0.0250	80.53	T	T	4	T
	CIP'-024-176 CombiLibHits sdf 1 dock2	0.0250	79.73	T	F	3	F
	CIP'-024-176 CombiLibHits sdf 1 dock3	0.0250	79.58	T	F	2	F
CIP'-028-002	CIP'-028-002 CombiLibHits sdf 2 dock3	0.0499	88.35	T	F	2	F
	CIP'-028-002 CombiLibHits sdf 2 dock2	0.0499	86.78	T	T	4	T
	CIP'-028-002 CombiLibHits sdf 2 dock1	0.0499	86.67	T	T	4	T
CIP'-028-018	CIP'-028-018 CombiLibHits sdf 3 dock10	0.0300	86.31	T	F	1	F
	CIP'-028-018 CombiLibHits sdf 3 dock7	0.0300	84.54	T	T	4	T
	CIP'-028-018 CombiLibHits sdf 3 dock9	0.0300	83.92	T	F	3	F
CIP'-028-055	CIP'-028-055 CombiLibHits sdf 4 dock1	0.0234	90.86	T	F	4	F
	CIP'-028-055 CombiLibHits sdf 4 dock2	0.0234	90.09	T	T	4	T
	CIP'-028-055 CombiLibHits sdf 4 dock3	0.0234	89.46	T	F	2	F
CIP'-028-059	CIP'-028-059 CombiLibHits sdf 5 dock2	0.0499	84.66	T	F	1	F
	CIP'-028-059 CombiLibHits sdf 5 dock3	0.0499	83.91	T	F	2	F
	CIP'-028-059 CombiLibHits sdf 5 dock4	0.0499	82.42	T	F	1	F
CIP'-028-073	CIP'-028-073 CombiLibHits sdf 6 dock2	0.0021	88.26	T	T	4	T
	CIP'-028-073 CombiLibHits sdf 6 dock3	0.0021	86.72	T	T	4	T
	CIP'-028-073 CombiLibHits sdf 6 dock1	0.0021	86.70	T	F	2	F
CIP'-028-113	CIP'-028-113 CombiLibHits sdf 7 dock1	0.0499	89.75	T	T	4	T
	CIP'-028-113 CombiLibHits sdf 7 dock3	0.0499	88.37	T	T	4	T
	CIP'-028-113 CombiLibHits sdf 7 dock2	0.0499	87.46	T	T	4	T
CIP'-028-128	CIP'-028-128 CombiLibHits sdf 8 dock3	0.0021	93.51	F	F	1	F
	CIP'-028-128 CombiLibHits sdf 8 dock8	0.0021	93.50	F	F	1	F
	CIP'-028-128 CombiLibHits sdf 8 dock6	0.0021	87.56	T	T	4	T
CIP'-028-148	CIP'-028-148 CombiLibHits sdf 9 dock5	0.0499	85.24	T	F	2	F
	CIP'-028-148 CombiLibHits sdf 9 dock2	0.0499	84.33	T	T	4	T
	CIP'-028-148 CombiLibHits sdf 9 dock1	0.0499	83.80	T	F	2	F
CIP'-028-149	CIP'-028-149 CombiLibHits sdf 10 dock6	0.0021	87.57	F	F	0	F

	CIP'-028-149 CombiLibHits sdf 10 dock9	0.0021	87.04	T	T	4	T
	CIP'-028-149 CombiLibHits sdf 10 dock3	0.0021	85.51	T	F	2	F
CIP'-028-154	CIP'-028-154 CombiLibHits sdf 11 dock1	0.0021	88.91	T	T	4	T
	CIP'-028-154 CombiLibHits sdf 11 dock2	0.0021	87.93	T	T	4	T
	CIP'-028-154 CombiLibHits sdf 11 dock4	0.0021	87.88	T	T	4	T
	CIP'-028-154 CombiLibHits sdf 11 dock3	0.0021	87.88	T	T	4	T
CIP'-036-057	CIP'-036-057 CombiLibHits sdf 12 dock2	0.0021	84.06	T	F	3	F
	CIP'-036-057 CombiLibHits sdf 12 dock3	0.0021	83.78	T	F	3	F
	CIP'-036-057 CombiLibHits sdf 12 dock1	0.0021	83.37	T	T	4	T
CIP'-036-059	CIP'-036-059 CombiLibHits sdf 13 dock1	0.0021	88.51	T	F	1	F
	CIP'-036-059 CombiLibHits sdf 13 dock5	0.0021	88.50	T	F	1	F
	CIP'-036-059 CombiLibHits sdf 13 dock4	0.0021	87.40	T	F	1	F
CIP'-036-092	CIP'-036-092 CombiLibHits sdf 14 dock1	0.0250	86.78	T	F	2	F
	CIP'-036-092 CombiLibHits sdf 14 dock3	0.0250	85.04	T	T	4	T
	CIP'-036-092 CombiLibHits sdf 14 dock5	0.0250	84.75	T	F	3	F
CIP'-046-018	CIP'-046-018 CombiLibHits sdf 15 dock7	0.0300	89.03	T	T	4	T
	CIP'-046-018 CombiLibHits sdf 15 dock1	0.0300	78.95	F	F	0	F
	CIP'-046-018 CombiLibHits sdf 15 dock3	0.0300	78.07	F	F	0	F
CIP'-046-069	CIP'-046-069 CombiLibHits sdf 16 dock2	0.0300	81.77	F	F	0	F
	CIP'-046-069 CombiLibHits sdf 16 dock5	0.0300	80.94	F	F	2	F
	CIP'-046-069 CombiLibHits sdf 16 dock3	0.0300	77.03	F	F	1	F
CIP'-046-149	CIP'-046-149 CombiLibHits sdf 17 dock3	0.0311	85.75	F	F	0	F
	CIP'-046-149 CombiLibHits sdf 17 dock2	0.0311	78.27	F	F	0	F
	CIP'-046-149 CombiLibHits sdf 17 dock9	0.0311	77.22	F	F	1	F
CIP'-046-156	CIP'-046-156 CombiLibHits sdf 18 dock1	0.0311	84.30	T	F	4	F
	CIP'-046-156 CombiLibHits sdf 18 dock6	0.0311	82.23	T	F	2	F
	CIP'-046-156 CombiLibHits sdf 18 dock3	0.0311	79.89	F	F	1	F
CIP'-059-176	CIP'-059-176 CombiLibHits sdf 19 dock2	0.0329	80.27	T	F	2	F
	CIP'-059-176 CombiLibHits sdf 19 dock1	0.0329	80.19	T	T	4	T
	CIP'-059-176 CombiLibHits sdf 19 dock4	0.0329	79.99	T	T	4	T
CIP'-060-169	CIP'-060-169 CombiLibHits sdf 20 dock1	0.0499	83.09	T	F	1	F
	CIP'-060-169 CombiLibHits sdf 20 dock2	0.0499	82.42	T	F	2	F
	CIP'-060-169 CombiLibHits sdf 20 dock4	0.0499	82.00	T	F	2	F

CIP'-095-057	CIP'-095-057 CombiLibHits sdf 21 dock7	0.0021	87.58	T	F	1	F
	CIP'-095-057 CombiLibHits sdf 21 dock2	0.0021	87.21	T	T	4	T
	CIP'-095-057 CombiLibHits sdf 21 dock6	0.0021	86.85	T	T	4	T
CIP'-095-059	CIP'-095-059 CombiLibHits sdf 22 dock3	0.0021	90.79	T	F	2	F
	CIP'-095-059 CombiLibHits sdf 22 dock2	0.0021	90.32	T	T	4	T
	CIP'-095-059 CombiLibHits sdf 22 dock4	0.0021	90.30	T	T	4	T
CIP'-095-073	CIP'-095-073 CombiLibHits sdf 23 dock1	0.0401	93.04	T	T	4	T
	CIP'-095-073 CombiLibHits sdf 23 dock4	0.0401	92.80	T	T	4	T
	CIP'-095-073 CombiLibHits sdf 23 dock3	0.0401	91.26	T	F	3	F
CIP'-095-177	CIP'-095-177 CombiLibHits sdf 24 dock1	0.0401	91.59	T	F	0	F
	CIP'-095-177 CombiLibHits sdf 24 dock6	0.0401	91.01	T	T	4	T
	CIP'-095-177 CombiLibHits sdf 24 dock3	0.0401	90.75	T	T	4	T
CIP'-095-183	CIP'-095-183 CombiLibHits sdf 25 dock1	0.0401	95.69	T	T	4	T
	CIP'-095-183 CombiLibHits sdf 25 dock3	0.0401	94.54	T	F	3	F
	CIP'-095-183 CombiLibHits sdf 25 dock5	0.0401	94.35	T	T	4	T
CIP'-100-073	CIP'-100-073 CombiLibHits sdf 26 dock1	0.0329	89.43	T	T	4	T
	CIP'-100-073 CombiLibHits sdf 26 dock3	0.0329	87.49	T	T	4	T
	CIP'-100-073 CombiLibHits sdf 26 dock4	0.0329	87.18	T	T	4	T
CIP-028-056	CIP-028-056 CombiLibHits sdf 27 dock4	0.0021	86.15	T	F	3	F
	CIP-028-056 CombiLibHits sdf 27 dock3	0.0021	85.52	T	F	2	F
	CIP-028-056 CombiLibHits sdf 27 dock2	0.0021	84.32	T	F	1	F
CIP-028-066	CIP-028-066 CombiLibHits sdf 28 dock8	0.0300	93.85	T	F	1	F
	CIP-028-066 CombiLibHits sdf 28 dock4	0.0300	86.75	F	F	0	F
	CIP-028-066 CombiLibHits sdf 28 dock6	0.0300	82.63	F	F	2	F
CIP-028-082	CIP-028-082 CombiLibHits sdf 29 dock3	0.0300	95.37	T	F	3	F
	CIP-028-082 CombiLibHits sdf 29 dock1	0.0300	95.18	T	F	3	F
	CIP-028-082 CombiLibHits sdf 29 dock2	0.0300	92.24	T	T	4	T
CIP-028-083	CIP-028-083 CombiLibHits sdf 30 dock1	0.0499	85.14	T	F	2	F
	CIP-028-083 CombiLibHits sdf 30 dock3	0.0499	84.64	T	F	3	F
	CIP-028-083 CombiLibHits sdf 30 dock4	0.0499	82.27	T	F	2	F
CIP-028-102	CIP-028-102 CombiLibHits sdf 31 dock10	0.0130	80.80	T	F	4	F
	CIP-028-102 CombiLibHits sdf 31 dock2	0.0130	80.22	T	T	4	T

	CIP-028-102 CombiLibHits sdf 31 dock6	0.0130	79.71	T	F	3	F
CIP-036-096	CIP-036-096 CombiLibHits sdf 32 dock1	0.0250	80.68	T	T	4	T
	CIP-036-096 CombiLibHits sdf 32 dock2	0.0250	80.01	T	T	4	T
	CIP-036-096 CombiLibHits sdf 32 dock9	0.0250	79.76	T	F	4	F
CIP-037-090	CIP-037-090 CombiLibHits sdf 33 dock1	0.0130	92.52	F	F	0	F
	CIP-037-090 CombiLibHits sdf 33 dock4	0.0130	91.19	F	F	0	F
	CIP-037-090 CombiLibHits sdf 33 dock7	0.0130	91.18	F	F	1	F
CIP-049-083	CIP-049-083 CombiLibHits sdf 34 dock5	0.0130	93.56	F	F	0	F
	CIP-049-083 CombiLibHits sdf 34 dock6	0.0130	93.18	F	F	0	F
	CIP-049-083 CombiLibHits sdf 34 dock3	0.0130	88.62	T	T	4	T
CIP-049-096	CIP-049-096 CombiLibHits sdf 35 dock4	0.0329	85.23	T	T	4	T
	CIP-049-096 CombiLibHits sdf 35 dock6	0.0329	84.31	T	F	4	F
	CIP-049-096 CombiLibHits sdf 35 dock3	0.0329	84.23	T	T	4	T
CIP-049-101	CIP-049-101 CombiLibHits sdf 36 dock2	0.0401	84.44	T	F	0	F
	CIP-049-101 CombiLibHits sdf 36 dock1	0.0401	83.40	T	F	2	F
	CIP-049-101 CombiLibHits sdf 36 dock4	0.0401	81.98	T	F	1	F
CIP-059-096	CIP-059-096 CombiLibHits sdf 37 dock3	0.0250	84.82	F	F	1	F
	CIP-059-096 CombiLibHits sdf 37 dock8	0.0250	83.82	F	F	1	F
	CIP-059-096 CombiLibHits sdf 37 dock6	0.0250	83.34	T	T	4	T
CIP-059-102	CIP-059-102 CombiLibHits sdf 38 dock3	0.0250	83.05	F	F	0	F
	CIP-059-102 CombiLibHits sdf 38 dock10	0.0250	82.15	T	T	4	T
	CIP-059-102 CombiLibHits sdf 38 dock2	0.0250	81.92	T	F	1	F
CIP-060-090	CIP-060-090 CombiLibHits sdf 39 dock5	0.0499	88.76	F	F	2	F
	CIP-060-090 CombiLibHits sdf 39 dock7	0.0499	88.54	F	F	2	F
	CIP-060-090 CombiLibHits sdf 39 dock8	0.0499	80.44	F	F	0	F
CIP-096-098	CIP-096-098 CombiLibHits sdf 40 dock3	0.0401	84.59	T	T	4	T
	CIP-096-098 CombiLibHits sdf 40 dock8	0.0401	84.38	T	T	4	T
	CIP-096-098 CombiLibHits sdf 40 dock6	0.0401	84.26	T	T	4	T
CIP-101-101	CIP-101-101 CombiLibHits sdf 41 dock1	0.0401	86.29	T	F	1	F
	CIP-101-101 CombiLibHits sdf 41 dock2	0.0401	86.04	T	F	2	F
	CIP-101-101 CombiLibHits sdf 41 dock3	0.0401	83.56	T	F	2	F
MOX'-016-005	MOX'-016-005 CombiLibHits sdf 42 dock1	0.0499	83.28	T	T	4	T

	MOX'-016-005 CombiLibHits sdf 42 dock3	0.0499	83.12	T	T	4	T
	MOX'-016-005 CombiLibHits sdf 42 dock4	0.0499	82.51	T	T	4	T
MOX'-016-116	MOX'-016-116 CombiLibHits sdf 43 dock3	0.0499	84.90	T	F	2	F
	MOX'-016-116 CombiLibHits sdf 43 dock4	0.0499	84.02	T	F	3	F
	MOX'-016-116 CombiLibHits sdf 43 dock1	0.0499	81.46	T	F	3	F
MOX'-016-137	MOX'-016-137 CombiLibHits sdf 44 dock3	0.0300	90.14	T	T	4	T
	MOX'-016-137 CombiLibHits sdf 44 dock2	0.0300	89.66	T	T	4	T
	MOX'-016-137 CombiLibHits sdf 44 dock6	0.0300	89.24	T	T	4	T
MOX'-028-116	MOX'-028-116 CombiLibHits sdf 45 dock4	0.0130	85.85	T	F	4	F
	MOX'-028-116 CombiLibHits sdf 45 dock6	0.0130	84.96	T	F	3	F
	MOX'-028-116 CombiLibHits sdf 45 dock3	0.0130	81.45	T	F	2	F
MOX'-039-005	MOX'-039-005 CombiLibHits sdf 46 dock8	0.0499	86.03	F	F	0	F
	MOX'-039-005 CombiLibHits sdf 46 dock1	0.0499	83.95	T	T	4	T
	MOX'-039-005 CombiLibHits sdf 46 dock6	0.0499	82.89	T	F	2	F
MOX'-060-033	MOX'-060-033 CombiLibHits sdf 47 dock5	0.0401	83.12	T	F	2	F
	MOX'-060-033 CombiLibHits sdf 47 dock2	0.0401	81.62	T	F	2	F
	MOX'-060-033 CombiLibHits sdf 47 dock3	0.0401	80.32	T	T	4	T
MOX'-065-050	MOX'-065-050 CombiLibHits sdf 48 dock6	0.0401	87.99	T	F	2	F
	MOX'-065-050 CombiLibHits sdf 48 dock7	0.0401	85.89	T	F	2	F
	MOX'-065-050 CombiLibHits sdf 48 dock5	0.0401	84.78	T	F	2	F

Legend	
GSF	GOLDScore Fitness Function
VO	Visual Orientation
VF	Visual Fitness
NMPF	Number of Matching Pharmacophoric Features

Table S3. The results obtained after the Level 2 Boolean-based (T/F (true/false)) clustering (Score-based clustering) of the (T)-signed combinatorially-generated drug-like 6-FQ binding poses from Level 1 for the constructed *gyrB* mutant models: a) N473T_{mod}, b) T474P_{mod}, and c) E475V_{mod}.

a) N473T_{mod}.

Cluster ID	DOCK POSE (Level 1)	MICpred_combi	GSF	GSF ≥ 80 (T/F)	HGSF (T/F)	Result (T/F)
CIP'-028-002	CIP'-028-002_CombiLibHits_sdf_2_dock7	0.0499	86.52	T	T	T
	CIP'-028-002_CombiLibHits_sdf_2_dock10	0.0499	85.67	T	F	F
CIP'-028-055	CIP'-028-055_CombiLibHits_sdf_4_dock2	0.0234	94.05	T	T	T
	CIP'-028-055_CombiLibHits_sdf_4_dock3	0.0234	93.57	T	F	F
	CIP'-028-055_CombiLibHits_sdf_4_dock1	0.0234	93.44	T	F	F
CIP'-028-073	CIP'-028-073_CombiLibHits_sdf_6_dock3	0.0021	88.03	T	T	T
CIP'-028-113	CIP'-028-113_CombiLibHits_sdf_7_dock3	0.0499	90.60	T	T	T
	CIP'-028-113_CombiLibHits_sdf_7_dock2	0.0499	90.34	T	F	F
	CIP'-028-113_CombiLibHits_sdf_7_dock1	0.0499	89.81	T	F	F
CIP'-028-128	CIP'-028-128_CombiLibHits_sdf_8_dock4	0.0021	90.64	T	T	T
	CIP'-028-128_CombiLibHits_sdf_8_dock1	0.0021	89.83	T	F	F
	CIP'-028-128_CombiLibHits_sdf_8_dock2	0.0021	89.63	T	F	F
CIP'-028-148	CIP'-028-148_CombiLibHits_sdf_9_dock3	0.0499	84.72	T	T	T
CIP'-028-149	CIP'-028-149_CombiLibHits_sdf_10_dock3	0.0021	86.71	T	T	T
CIP'-028-154	CIP'-028-154_CombiLibHits_sdf_11_dock2	0.0021	89.93	T	T	T
	CIP'-028-154_CombiLibHits_sdf_11_dock5	0.0021	89.33	T	F	F
CIP'-036-057	CIP'-036-057_CombiLibHits_sdf_12_dock1	0.0021	86.09	T	T	T
CIP'-059-176	CIP'-059-176_CombiLibHits_sdf_19_dock3	0.0329	81.20	T	T	T
	CIP'-059-176_CombiLibHits_sdf_19_dock1	0.0329	80.60	T	F	F
	CIP'-059-176_CombiLibHits_sdf_19_dock6	0.0329	80.57	T	F	F
CIP'-095-057	CIP'-095-057_CombiLibHits_sdf_21_dock2	0.0021	91.83	T	T	T
	CIP'-095-057_CombiLibHits_sdf_21_dock3	0.0021	91.11	T	F	F
	CIP'-095-057_CombiLibHits_sdf_21_dock4	0.0021	90.45	T	F	F
CIP'-095-073	CIP'-095-073_CombiLibHits_sdf_23_dock5	0.0401	93.43	T	T	T

	CIP'-095-073_CombiLibHits_sdf_23_dock3	0.0401	93.06	T	F	F
CIP'-095-183	CIP'-095-183_CombiLibHits_sdf_25_dock6	0.0401	93.24	T	T	T
CIP'-100-073	CIP'-100-073_CombiLibHits_sdf_26_dock1	0.0329	87.91	T	T	T
	CIP'-100-073_CombiLibHits_sdf_26_dock2	0.0329	87.81	T	F	F
CIP-028-066	CIP-028-066_CombiLibHits_sdf_28_dock8	0.0300	86.79	T	T	T
CIP-028-082	CIP-028-082_CombiLibHits_sdf_29_dock1	0.0300	97.48	T	T	T
	CIP-028-082_CombiLibHits_sdf_29_dock2	0.0300	97.41	T	F	F
	CIP-028-082_CombiLibHits_sdf_29_dock3	0.0300	90.80	T	F	F
CIP-049-096	CIP-049-096_CombiLibHits_sdf_35_dock2	0.0329	84.44	T	T	T
	CIP-049-096_CombiLibHits_sdf_35_dock5	0.0329	83.90	T	F	F
	CIP-049-096_CombiLibHits_sdf_35_dock6	0.0329	83.86	T	F	F
CIP-049-101	CIP-049-101_CombiLibHits_sdf_36_dock2	0.0401	84.41	T	T	T
CIP-096-098	CIP-096-098_CombiLibHits_sdf_40_dock1	0.0401	86.61	T	T	T
	CIP-096-098_CombiLibHits_sdf_40_dock3	0.0401	85.35	T	F	F
	CIP-096-098_CombiLibHits_sdf_40_dock2	0.0401	84.97	T	F	F
MOX'-016-137	MOX'-016-137_CombiLibHits_sdf_44_dock3	0.0300	89.24	T	T	T
	MOX'-016-137_CombiLibHits_sdf_44_dock1	0.0300	88.71	T	F	F
MOX'-028-116	MOX'-028-116_CombiLibHits_sdf_45_dock1	0.0130	86.34	T	T	T
	MOX'-028-116_CombiLibHits_sdf_45_dock7	0.0130	82.94	T	F	F
MOX'-039-005	MOX'-039-005_CombiLibHits_sdf_46_dock5	0.0499	82.47	T	T	T
	MOX'-039-005_CombiLibHits_sdf_46_dock1	0.0499	82.32	T	F	F
	MOX'-039-005_CombiLibHits_sdf_46_dock3	0.0499	82.12	T	F	F
MOX'-060-033	MOX'-060-033_CombiLibHits_sdf_47_dock5	0.0401	80.08	T	T	T
	MOX'-060-033_CombiLibHits_sdf_47_dock2	0.0401	76.41	F	F	F
	MOX'-060-033_CombiLibHits_sdf_47_dock3	0.0401	76.18	F	F	F

Legend	
GSF	GOLDScore Fitness Function
HGSF	Highest GOLDScore Fitness
compounds with score >= 80	
selected highly scored compounds	

b) T474P_{mod}.

Cluster ID	DOCK POSE (Level 1)	MICpred_combi	GSF	GSF ≥ 80 (T/F)	HGSF (T/F)	Result (T/F)
CIP'-024-176	CIP'-024-176_CombiLibHits_sdf_1_dock2	0.0250	79.98	F	T	F
CIP'-028-002	CIP'-028-002_CombiLibHits_sdf_2_dock2	0.0499	89.04	T	T	T
	CIP'-028-002_CombiLibHits_sdf_2_dock1	0.0499	88.35	T	F	F
	CIP'-028-002_CombiLibHits_sdf_2_dock4	0.0499	86.02	T	F	F
CIP'-028-055	CIP'-028-055_CombiLibHits_sdf_4_dock3	0.0234	94.07	T	T	T
CIP'-028-059	CIP'-028-059_CombiLibHits_sdf_5_dock6	0.0499	85.09	T	T	T
CIP'-028-073	CIP'-028-073_CombiLibHits_sdf_6_dock1	0.0021	87.33	T	T	T
	CIP'-028-073_CombiLibHits_sdf_6_dock2	0.0021	86.74	T	F	F
	CIP'-028-073_CombiLibHits_sdf_6_dock4	0.0021	86.26	T	F	F
CIP'-028-128	CIP'-028-128_CombiLibHits_sdf_8_dock9	0.0021	88.10	T	T	T
CIP'-028-148	CIP'-028-148_CombiLibHits_sdf_9_dock2	0.0499	85.89	T	T	T
CIP'-036-057	CIP'-036-057_CombiLibHits_sdf_12_dock1	0.0021	84.48	T	T	T
	CIP'-036-057_CombiLibHits_sdf_12_dock3	0.0021	83.65	T	F	F
	CIP'-036-057_CombiLibHits_sdf_12_dock2	0.0021	83.16	T	F	F
CIP'-036-092	CIP'-036-092_CombiLibHits_sdf_14_dock6	0.0250	85.96	T	T	T
CIP'-046-149	CIP'-046-149_CombiLibHits_sdf_17_dock2	0.0311	85.94	T	T	T
	CIP'-046-149_CombiLibHits_sdf_17_dock1	0.0311	85.27	T	F	F
CIP'-046-156	CIP'-046-156_CombiLibHits_sdf_18_dock7	0.0311	80.78	T	T	T
CIP'-059-176	CIP'-059-176_CombiLibHits_sdf_19_dock10	0.0329	81.38	T	T	T
CIP'-095-057	CIP'-095-057_CombiLibHits_sdf_21_dock1	0.0021	86.99	T	T	T
CIP'-095-073	CIP'-095-073_CombiLibHits_sdf_23_dock4	0.0401	92.04	T	T	T
	CIP'-095-073_CombiLibHits_sdf_23_dock5	0.0401	91.98	T	F	F
	CIP'-095-073_CombiLibHits_sdf_23_dock2	0.0401	90.13	T	F	F
CIP'-095-177	CIP'-095-177_CombiLibHits_sdf_24_dock9	0.0401	91.01	T	T	T
	CIP'-095-177_CombiLibHits_sdf_24_dock4	0.0401	90.85	T	F	F
CIP'-095-183	CIP'-095-183_CombiLibHits_sdf_25_dock2	0.0401	91.65	T	T	T
	CIP'-095-183_CombiLibHits_sdf_25_dock3	0.0401	87.40	T	F	F
CIP'-100-073	CIP'-100-073_CombiLibHits_sdf_26_dock10	0.0329	89.48	T	T	T
	CIP'-100-073_CombiLibHits_sdf_26_dock6	0.0329	89.01	T	F	F

	CIP'-100-073_CombiLibHits_sdf_26_dock9	0.0329	88.62	T	F	F
CIP-028-082	CIP-028-082_CombiLibHits_sdf_29_dock4	0.0300	97.90	T	T	T
	CIP-028-082_CombiLibHits_sdf_29_dock2	0.0300	96.85	T	F	F
CIP-028-083	CIP-028-083_CombiLibHits_sdf_30_dock1	0.0499	84.10	T	T	T
CIP-028-102	CIP-028-102_CombiLibHits_sdf_31_dock8	0.0130	80.32	T	T	T
CIP-036-096	CIP-036-096_CombiLibHits_sdf_32_dock1	0.0250	80.86	T	T	T
	CIP-036-096_CombiLibHits_sdf_32_dock8	0.0250	80.45	T	F	F
	CIP-036-096_CombiLibHits_sdf_32_dock6	0.0250	80.35	T	F	F
CIP-049-096	CIP-049-096_CombiLibHits_sdf_35_dock2	0.0329	85.58	T	T	T
	CIP-049-096_CombiLibHits_sdf_35_dock1	0.0329	85.09	T	F	F
	CIP-049-096_CombiLibHits_sdf_35_dock6	0.0329	84.85	T	F	F
CIP-096-098	CIP-096-098_CombiLibHits_sdf_40_dock2	0.0401	84.49	T	T	T
	CIP-096-098_CombiLibHits_sdf_40_dock5	0.0401	83.63	T	F	F
CIP-101-101	CIP-101-101_CombiLibHits_sdf_41_dock3	0.0401	87.07	T	T	T
MOX'-016-005	MOX'-016-005_CombiLibHits_sdf_42_dock1	0.0499	84.12	T	T	T
MOX'-016-116	MOX'-016-116_CombiLibHits_sdf_43_dock1	0.0499	84.96	T	T	T
MOX'-016-137	MOX'-016-137_CombiLibHits_sdf_44_dock2	0.0300	90.86	T	T	T
	MOX'-016-137_CombiLibHits_sdf_44_dock5	0.0300	87.49	T	F	F
	MOX'-016-137_CombiLibHits_sdf_44_dock1	0.0300	84.24	T	F	F
MOX'-028-116	MOX'-028-116_CombiLibHits_sdf_45_dock3	0.0130	87.27	T	T	T
	MOX'-028-116_CombiLibHits_sdf_45_dock4	0.0130	86.69	T	F	F
	MOX'-028-116_CombiLibHits_sdf_45_dock10	0.0130	85.68	T	F	F
MOX'-039-005	MOX'-039-005_CombiLibHits_sdf_46_dock2	0.0499	84.48	T	T	T
MOX'-060-033	MOX'-060-033_CombiLibHits_sdf_47_dock9	0.0401	83.72	T	T	T
	MOX'-060-033_CombiLibHits_sdf_47_dock4	0.0401	82.52	T	F	F
	MOX'-060-033_CombiLibHits_sdf_47_dock7	0.0401	79.88	F	F	F
MOX'-065-050	MOX'-065-050_CombiLibHits_sdf_48_dock7	0.0401	85.92	T	T	T

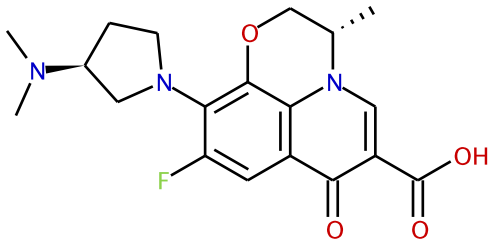
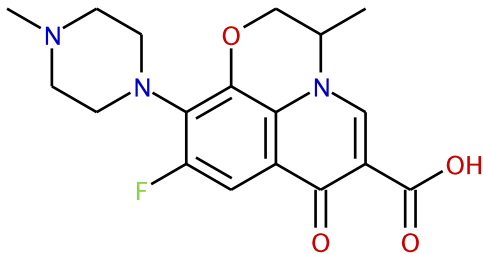
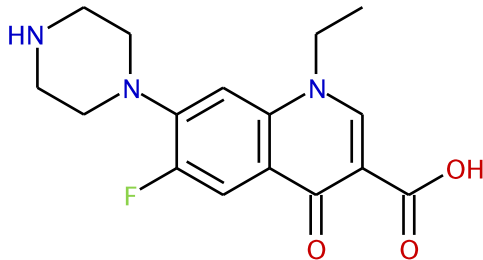
Legend	
GSF	GOLDScore Fitness Function
HGSF	Highest GOLDScore Fitness
compounds with score >= 80	
selected highly scored compounds	

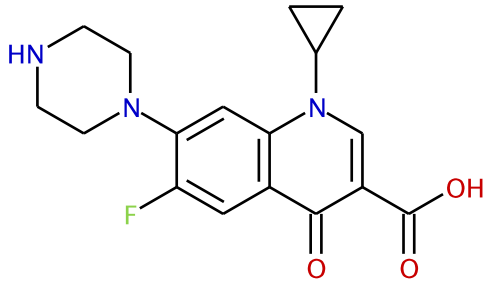
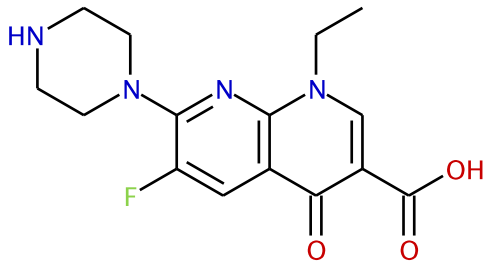
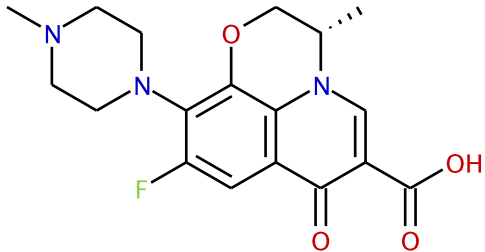
c) E475V_{mod}.

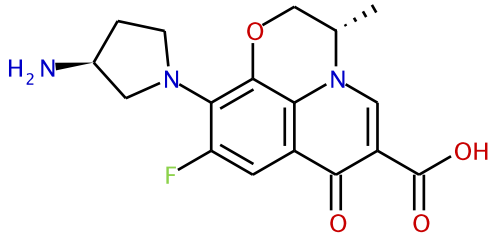
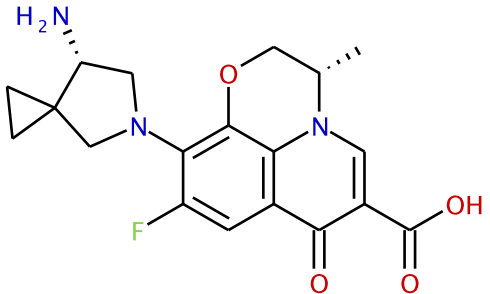
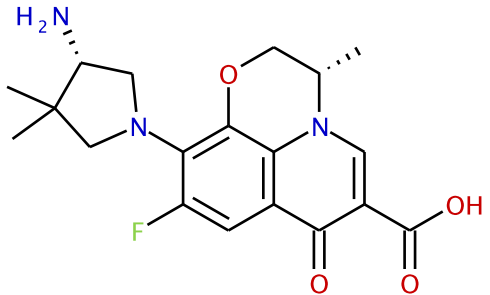
Cluster ID	DOCK POSE (Level 1)	MICpred_combi	GSF	GSF ≥ 80 (T/F)	HGSF (T/F)	Result (T/F)
CIP'-024-176	CIP'-024-176_CombiLibHits_sdf_1_dock1	0.0250	80.53	T	T	T
CIP'-028-002	CIP'-028-002_CombiLibHits_sdf_2_dock2	0.0499	86.78	T	T	T
	CIP'-028-002_CombiLibHits_sdf_2_dock1	0.0499	86.67	T	F	F
CIP'-028-018	CIP'-028-018_CombiLibHits_sdf_3_dock7	0.0300	84.54	T	T	T
CIP'-028-055	CIP'-028-055_CombiLibHits_sdf_4_dock2	0.0234	90.09	T	T	T
CIP'-028-073	CIP'-028-073_CombiLibHits_sdf_6_dock2	0.0021	88.26	T	T	T
	CIP'-028-073_CombiLibHits_sdf_6_dock3	0.0021	86.72	T	F	F
CIP'-028-113	CIP'-028-113_CombiLibHits_sdf_7_dock1	0.0499	89.75	T	T	T
	CIP'-028-113_CombiLibHits_sdf_7_dock3	0.0499	88.37	T	F	F
	CIP'-028-113_CombiLibHits_sdf_7_dock2	0.0499	87.46	T	F	F
CIP'-028-128	CIP'-028-128_CombiLibHits_sdf_8_dock6	0.0021	87.56	T	T	T
CIP'-028-148	CIP'-028-148_CombiLibHits_sdf_9_dock2	0.0499	84.33	T	T	T
CIP'-028-149	CIP'-028-149_CombiLibHits_sdf_10_dock9	0.0021	87.04	T	T	T
CIP'-028-154	CIP'-028-154_CombiLibHits_sdf_11_dock1	0.0021	88.91	T	T	T
	CIP'-028-154_CombiLibHits_sdf_11_dock2	0.0021	87.93	T	F	F
	CIP'-028-154_CombiLibHits_sdf_11_dock4	0.0021	87.88	T	F	F
CIP'-036-057	CIP'-036-057_CombiLibHits_sdf_12_dock1	0.0021	83.37	T	T	T
CIP'-036-092	CIP'-036-092_CombiLibHits_sdf_14_dock3	0.0250	85.04	T	T	T
CIP'-046-018	CIP'-046-018_CombiLibHits_sdf_15_dock7	0.0300	89.03	T	T	T
CIP'-059-176	CIP'-059-176_CombiLibHits_sdf_19_dock1	0.0329	80.19	T	T	T
	CIP'-059-176_CombiLibHits_sdf_19_dock4	0.0329	79.99	F	F	F
CIP'-095-057	CIP'-095-057_CombiLibHits_sdf_21_dock2	0.0021	87.21	T	T	T
	CIP'-095-057_CombiLibHits_sdf_21_dock6	0.0021	86.85	T	F	F
CIP'-095-059	CIP'-095-059_CombiLibHits_sdf_22_dock2	0.0021	90.32	T	T	T
	CIP'-095-059_CombiLibHits_sdf_22_dock4	0.0021	90.30	T	F	F
CIP'-095-073	CIP'-095-073_CombiLibHits_sdf_23_dock1	0.0401	93.04	T	T	T
	CIP'-095-073_CombiLibHits_sdf_23_dock4	0.0401	92.80	T	F	F
CIP'-095-177	CIP'-095-177_CombiLibHits_sdf_24_dock6	0.0401	91.01	T	T	T
	CIP'-095-177_CombiLibHits_sdf_24_dock3	0.0401	90.75	T	F	F

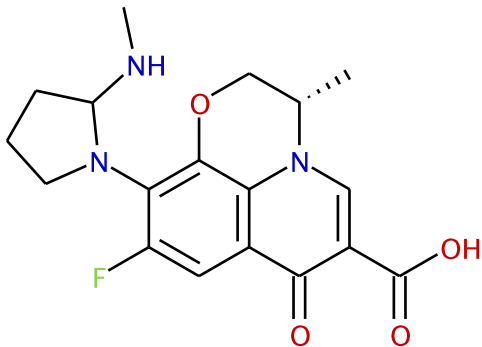
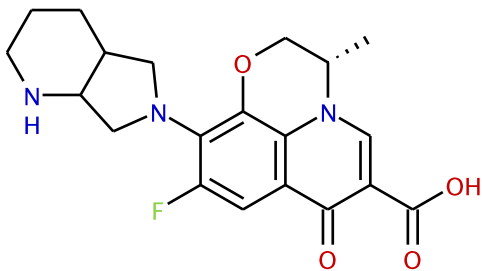
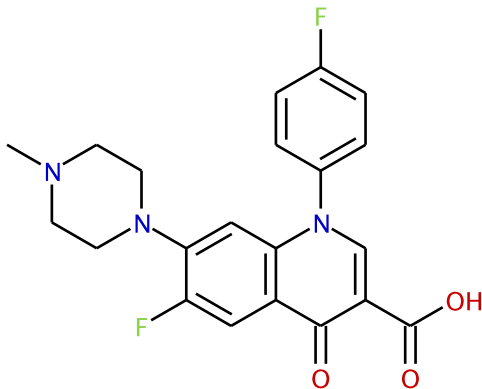
CIP'-095-183	CIP'-095-183_CombiLibHits_sdf_25_dock1	0.0401	95.69	T	T	T
	CIP'-095-183_CombiLibHits_sdf_25_dock5	0.0401	94.35	T	F	F
CIP'-100-073	CIP'-100-073_CombiLibHits_sdf_26_dock1	0.0329	89.43	T	T	T
	CIP'-100-073_CombiLibHits_sdf_26_dock3	0.0329	87.49	T	F	F
	CIP'-100-073_CombiLibHits_sdf_26_dock4	0.0329	87.18	T	F	F
CIP-028-082	CIP-028-082_CombiLibHits_sdf_29_dock2	0.0300	92.24	T	T	T
CIP-028-102	CIP-028-102_CombiLibHits_sdf_31_dock2	0.0130	80.22	T	T	T
CIP-036-096	CIP-036-096_CombiLibHits_sdf_32_dock1	0.0250	80.68	T	T	T
	CIP-036-096_CombiLibHits_sdf_32_dock2	0.0250	80.01	T	F	F
CIP-049-083	CIP-049-083_CombiLibHits_sdf_34_dock3	0.0130	88.62	T	T	T
CIP-049-096	CIP-049-096_CombiLibHits_sdf_35_dock4	0.0329	85.23	T	T	T
	CIP-049-096_CombiLibHits_sdf_35_dock3	0.0329	84.23	T	F	F
CIP-059-096	CIP-059-096_CombiLibHits_sdf_37_dock6	0.0250	83.34	T	T	T
CIP-059-102	CIP-059-102_CombiLibHits_sdf_38_dock10	0.0250	82.15	T	T	T
CIP-096-098	CIP-096-098_CombiLibHits_sdf_40_dock3	0.0401	84.59	T	T	T
	CIP-096-098_CombiLibHits_sdf_40_dock8	0.0401	84.38	T	F	F
	CIP-096-098_CombiLibHits_sdf_40_dock6	0.0401	84.26	T	F	F
MOX'-016-005	MOX'-016-005_CombiLibHits_sdf_42_dock1	0.0499	83.28	T	T	T
	MOX'-016-005_CombiLibHits_sdf_42_dock3	0.0499	83.12	T	F	F
	MOX'-016-005_CombiLibHits_sdf_42_dock4	0.0499	82.51	T	F	F
MOX'-016-137	MOX'-016-137_CombiLibHits_sdf_44_dock3	0.0300	90.14	T	T	T
	MOX'-016-137_CombiLibHits_sdf_44_dock2	0.0300	89.66	T	F	F
	MOX'-016-137_CombiLibHits_sdf_44_dock6	0.0300	89.24	T	F	F
MOX'-039-005	MOX'-039-005_CombiLibHits_sdf_46_dock1	0.0499	83.95	T	T	T
MOX'-060-033	MOX'-060-033_CombiLibHits_sdf_47_dock3	0.0401	80.32	T	T	T

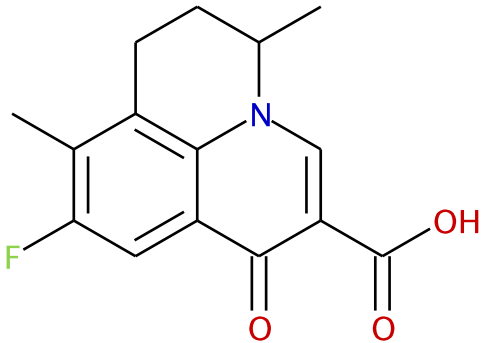
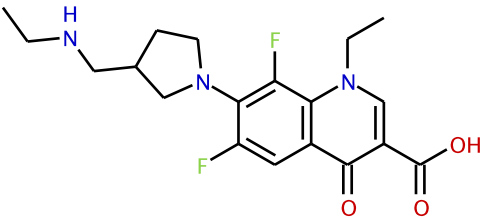
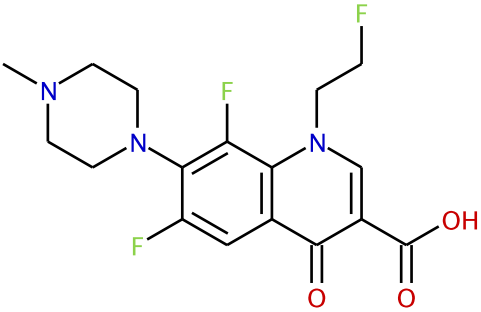
Legend	
GSF	GOLDScore Fitness Function
HGSF	Highest GOLDScore Fitness
compounds with score >= 80	
selected highly scored compounds	

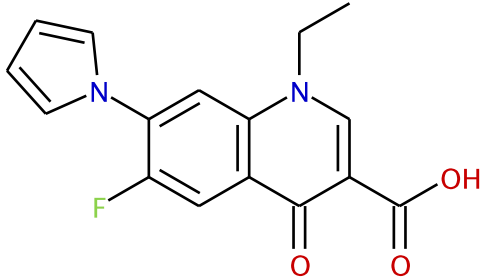
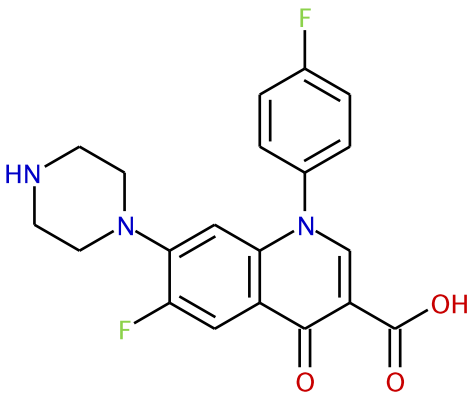
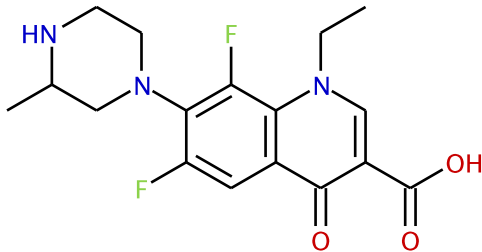
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
1.	 Structure001	3.0000	-0.4771
2.	 Structure002	0.0115	1.9393
3.	 Structure003	0.3000	0.5229

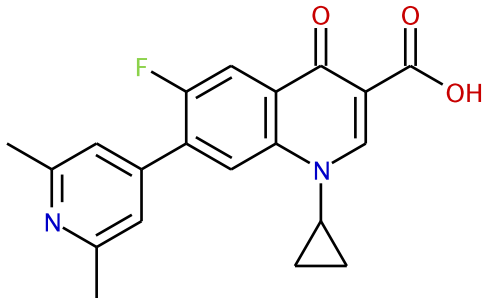
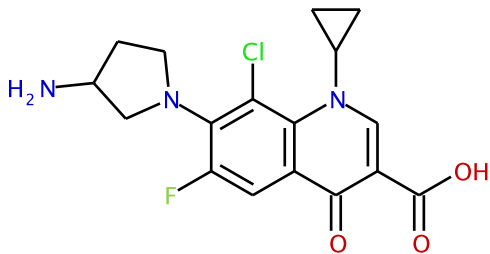
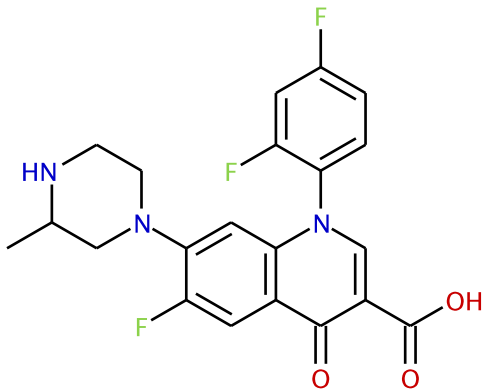
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
4.	 Structure004	0.0100	2.0000
5.	 Structure005	0.3000	0.5229
6.	 Structure006	0.1200	0.9208

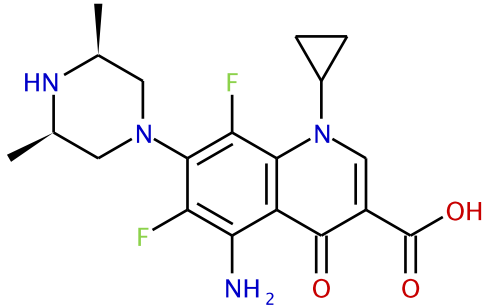
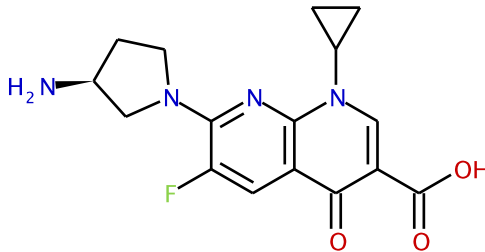
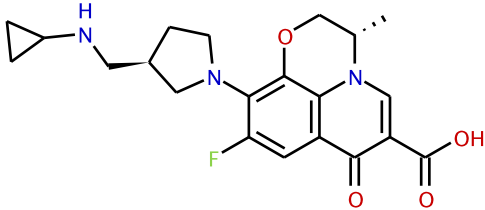
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
7.	 Structure007	3.5000	-0.5441
8.	 Structure008	0.1000	1.0000
9.	 Structure009	1.4000	-0.1461

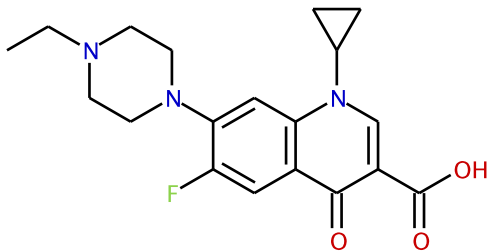
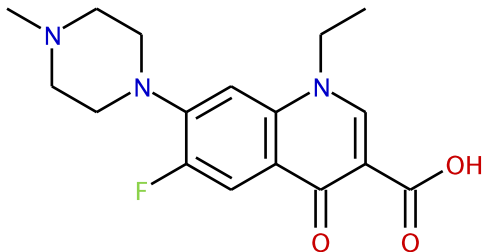
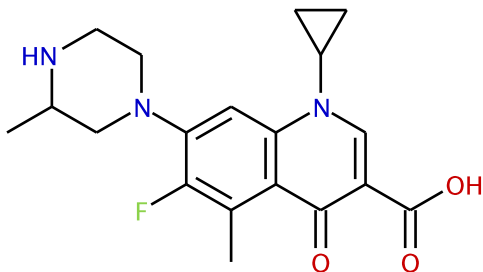
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
10.	 Structure010	3.2000	-0.5051
11.	 Structure011	0.0500	1.3010
12.	 Structure012	0.5000	0.3010

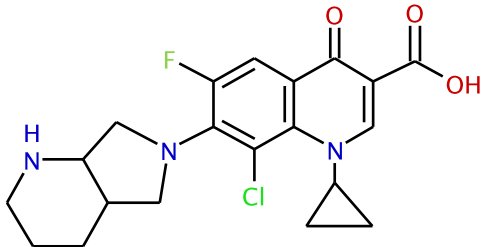
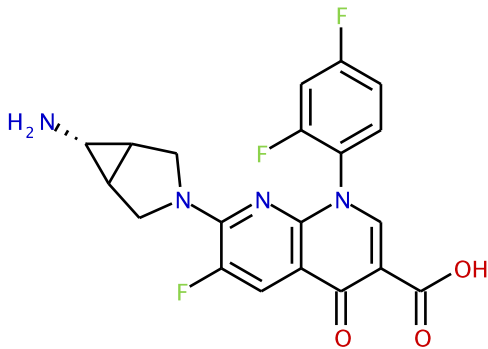
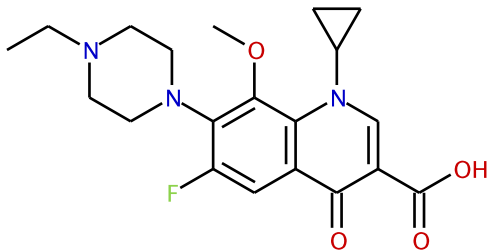
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
13.	 Structure013	1.6000	-0.2041
14.	 Structure014	0.5000	0.3010
15.	 Structure015	0.5000	0.3010

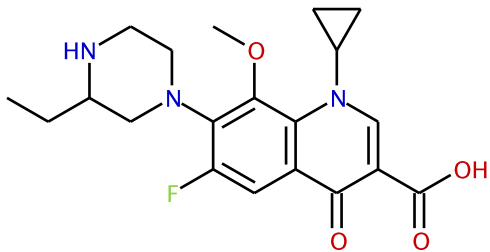
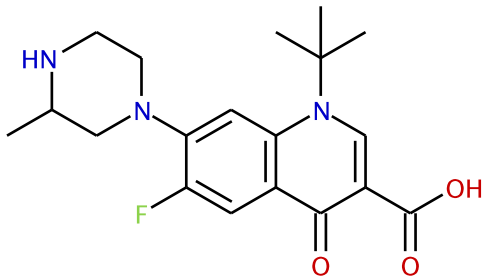
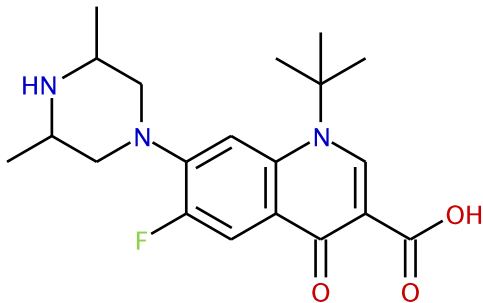
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
16.	 Structure016	2.0000	-0.3010
17.	 Structure017	0.5000	0.3010
18.	 Structure018	0.5000	0.3010

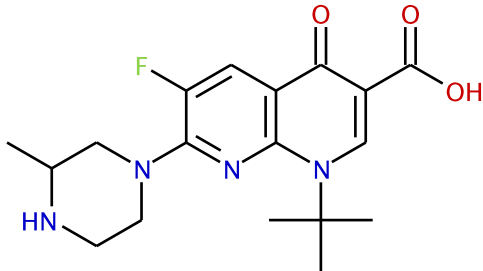
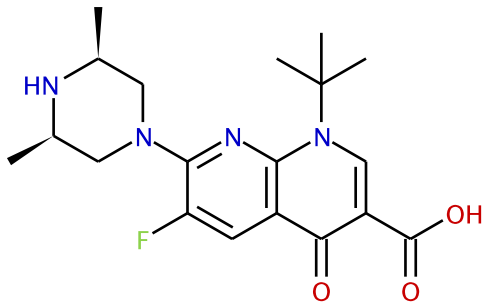
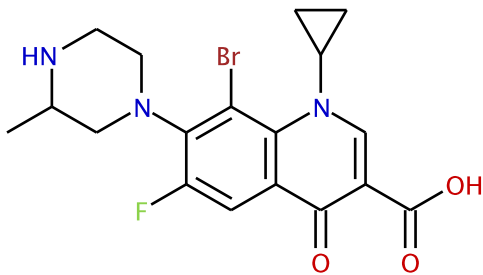
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
19.	 Structure019	0.2500	0.6021
20.	 Structure020	0.0100	2.0000
21.	 Structure021	0.0310	1.5086

ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
22.	 Structure022	0.0100	2.0000
23.	 Structure023	0.0100	2.0000
24.	 Structure024	0.9000	0.0458

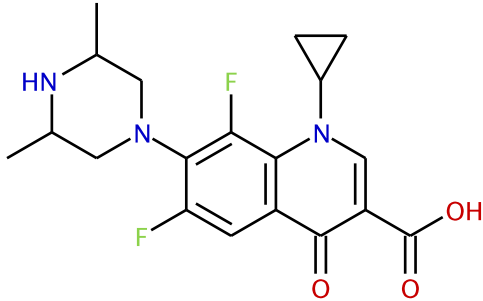
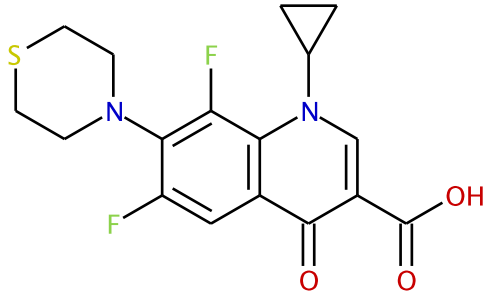
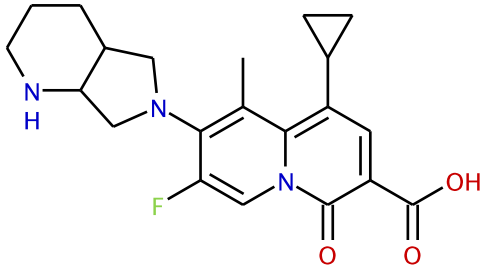
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
25.	 Structure025	0.1250	0.9031
26.	 Structure026	0.3000	0.5229
27.	 Structure027	0.1200	0.9208

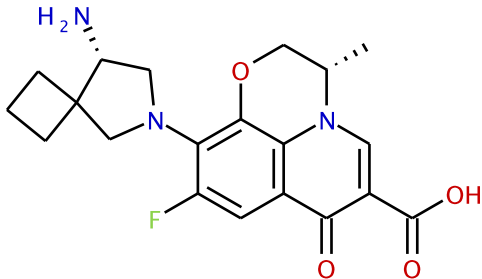
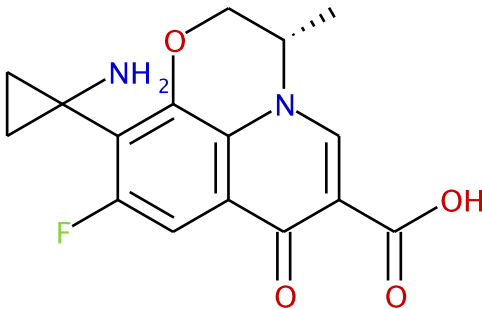
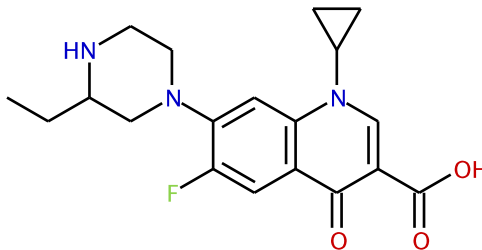
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
28.	 Structure028	0.0040	2.3979
29.	 Structure029	2.0000	-0.3010
30.	 Structure030	0.3900	0.4089

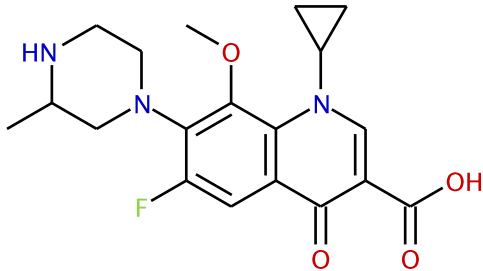
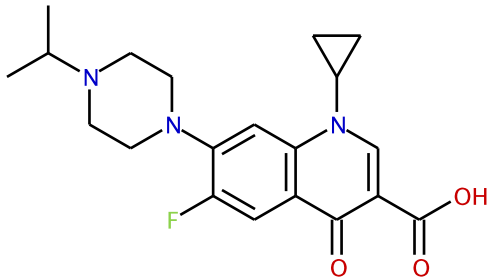
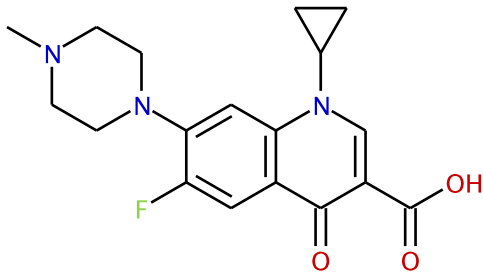
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
31.	 Structure031	0.0600	1.2218
32.	 Structure032	0.3900	0.4089
33.	 Structure033	0.3900	0.4089

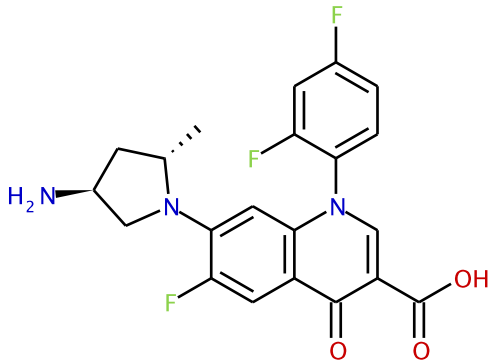
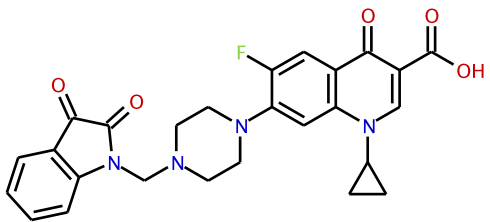
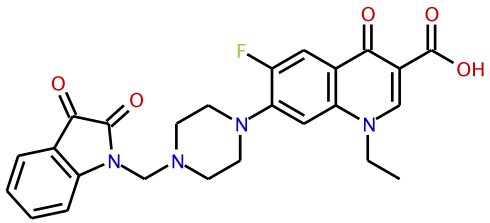
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
34.	 Structure034	0.7800	0.1079
35.	 Structure035	0.7800	0.1079
36.	 Structure036	0.7800	0.1079

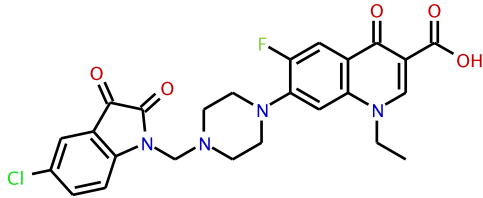
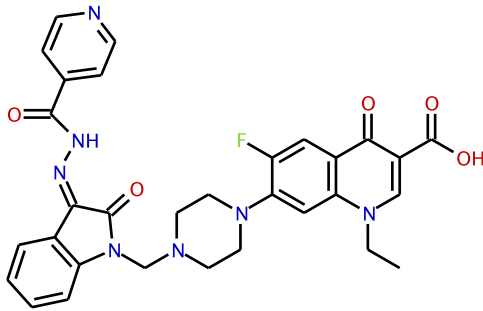
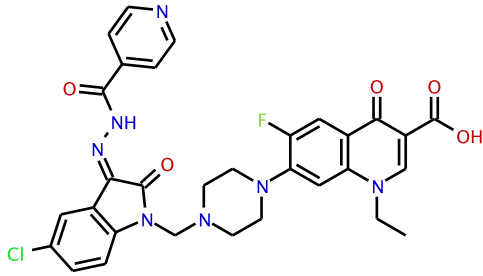
ID	Chemical Structure	MIC (ug/mL)	pMIC
37.	Structure037	0.1250	0.9031
38.	Structure038	0.0020	2.6990
39.	Structure039	0.1100	0.9586

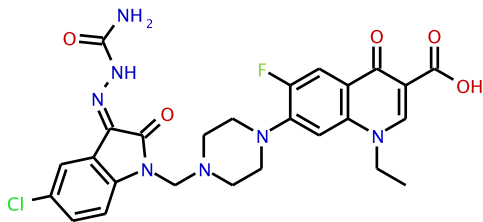
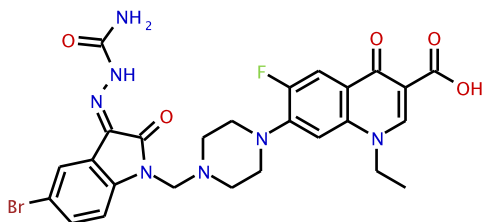
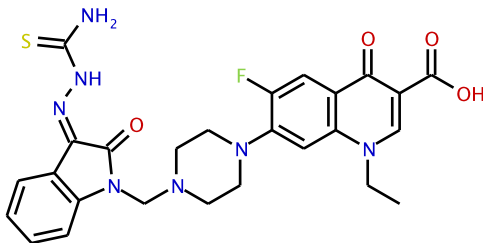
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
40.	 Structure040	0.0120	1.9208
41.	 Structure041	0.2500	0.6021
42.	 Structure042	0.0160	1.7959

ID	Chemical Structure	MIC (ug/mL)	pMIC
43.	 Structure043	0.6000	0.2218
44.	 Structure044	0.3900	0.4089
45.	 Structure045	0.3000	0.5229

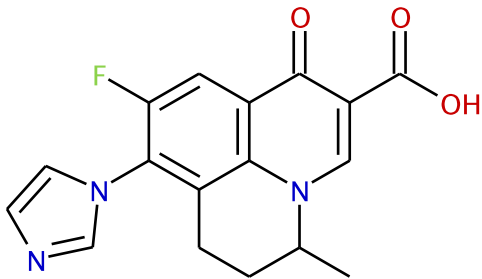
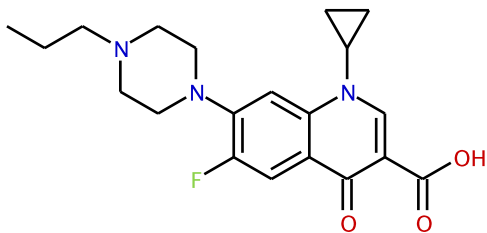
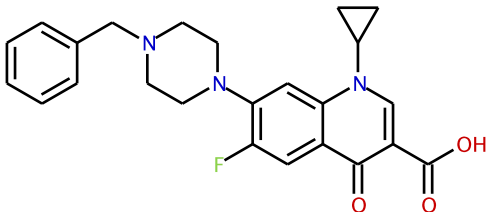
ID	Chemical Structure	MIC (ug/mL)	pMIC
46.	 Structure046	0.0300	1.5229
47.	 Structure047	0.1250	0.9031
48.	 Structure048	0.1250	0.9031

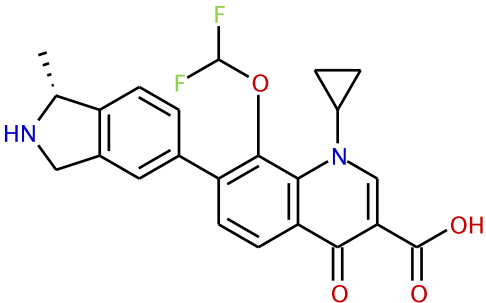
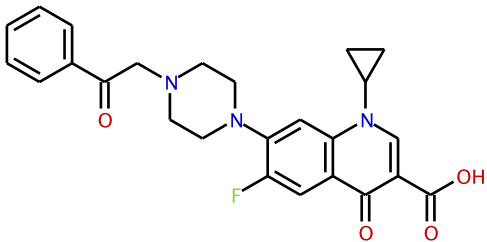
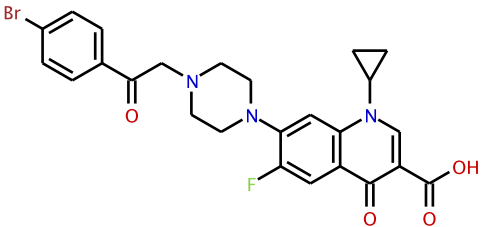
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
49.	 Structure049	0.5000	0.3010
50.	 Structure050	0.0016	2.7986
51.	 Structure051	6.3000	-0.7993

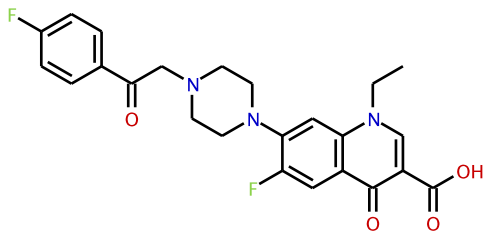
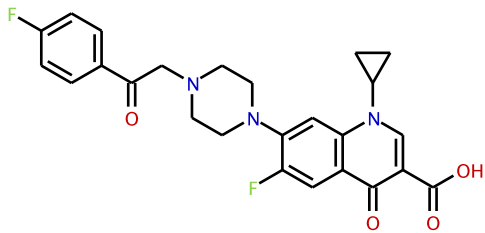
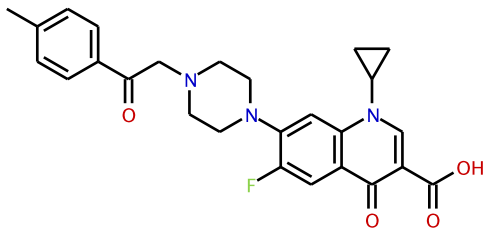
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
52.	 Structure052	6.5700	-0.8176
53.	 Structure053	5.2000	-0.7160
54.	 Structure054	6.9000	-0.8388

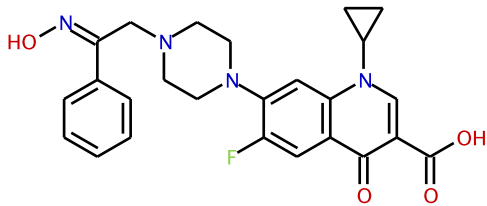
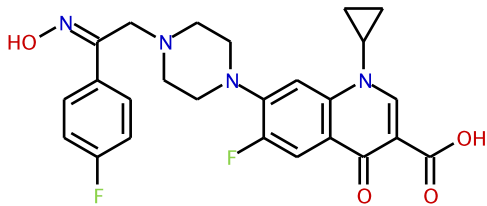
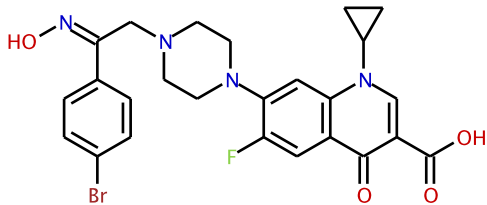
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
55.	 Structure055	6.4500	-0.8096
56.	 Structure056	6.7000	-0.8261
57.	 Structure057	6.3000	-0.7993

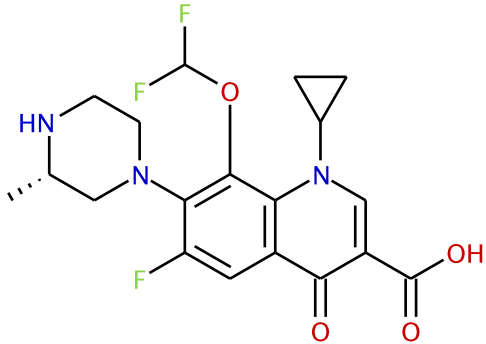
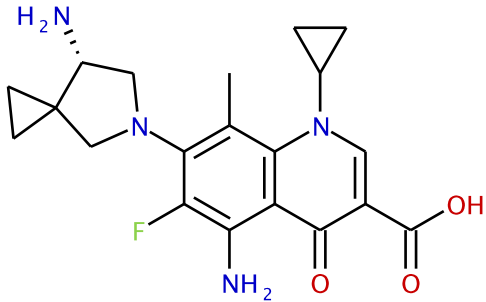
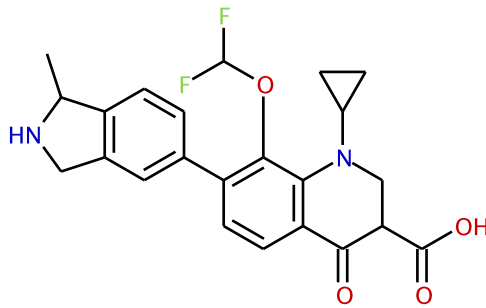
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
58.	Structure058	6.2600	-0.7966
59.	Structure059	6.9200	-0.8401
60.	Structure060	0.0300	1.5229

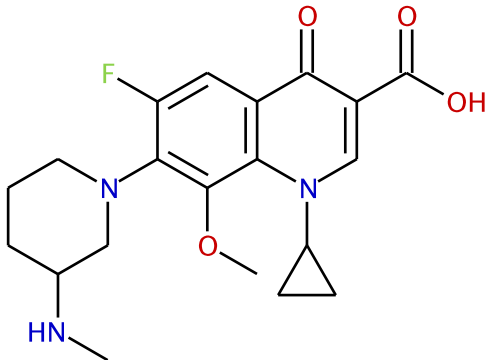
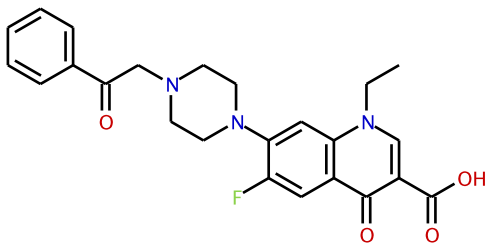
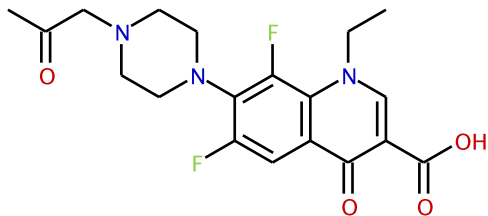
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
61.	 Structure061	3.2000	-0.5051
62.	 Structure062	0.1250	0.9031
63.	 Structure063	0.5000	0.3010

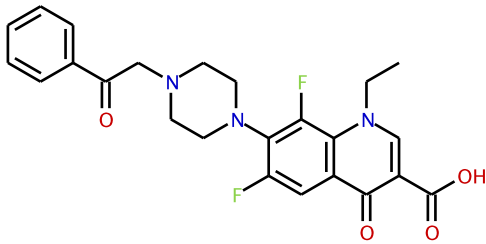
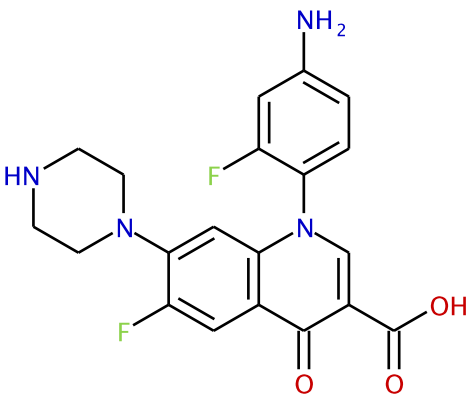
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
64.	 Structure064	0.0300	1.5229
65.	 Structure065	0.7800	0.1079
66.	 Structure066	0.7800	0.1079

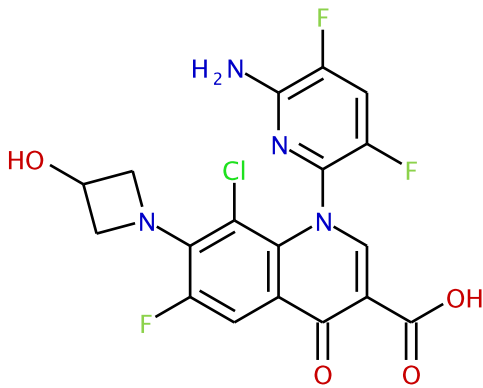
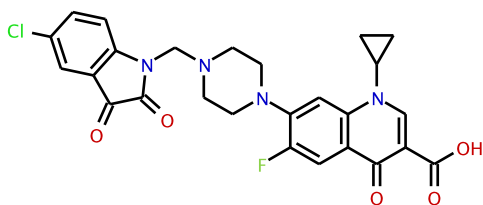
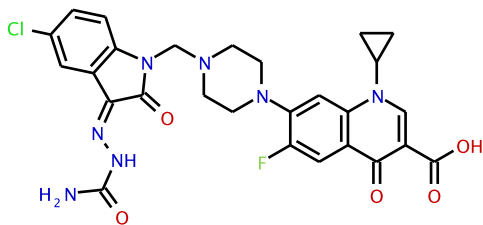
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
67.	 Structure067	6.2500	-0.7959
68.	 Structure068	0.7800	0.1079
69.	 Structure069	1.5600	-0.1931

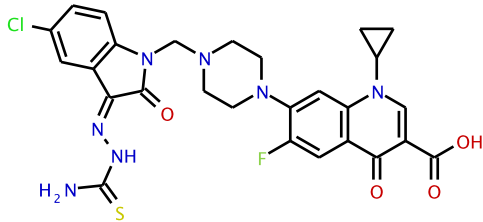
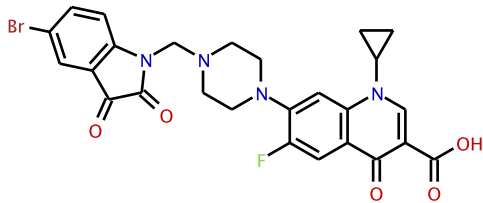
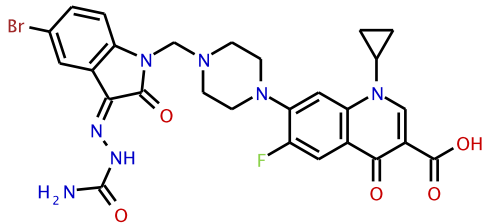
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
70.	 Structure070	1.5600	-0.1931
71.	 Structure071	3.1300	-0.4955
72.	 Structure072	7.1200	-0.8525

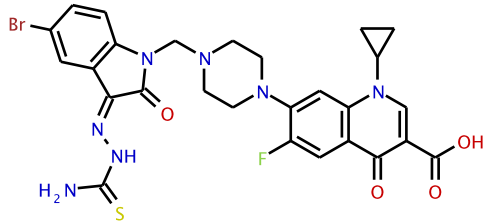
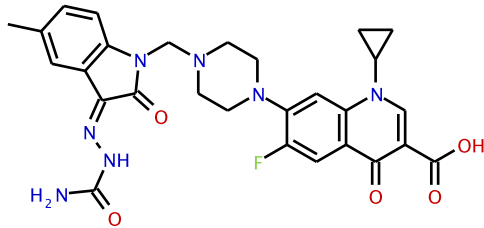
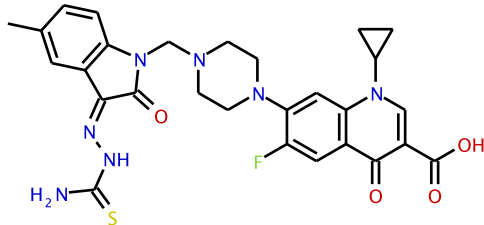
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
73.	 Structure073	0.0600	1.2218
74.	 Structure074	0.7800	0.1079
75.	 Structure075	0.0625	1.2041

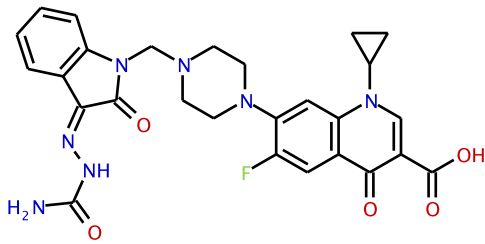
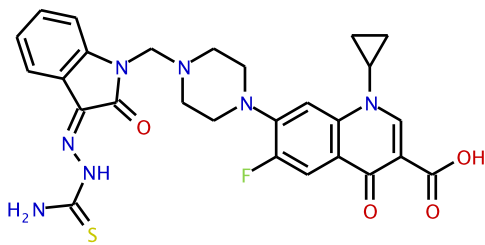
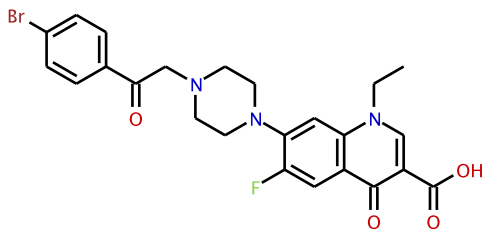
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
76.	 Structure076	0.1250	0.9031
77.	 Structure077	6.2500	-0.7959
78.	 Structure078	3.1300	-0.4955

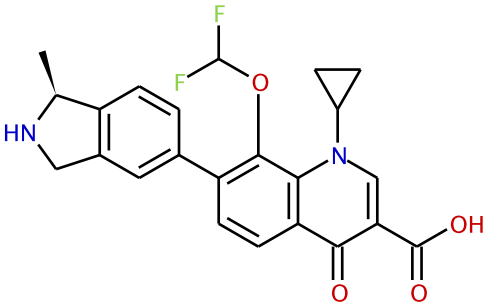
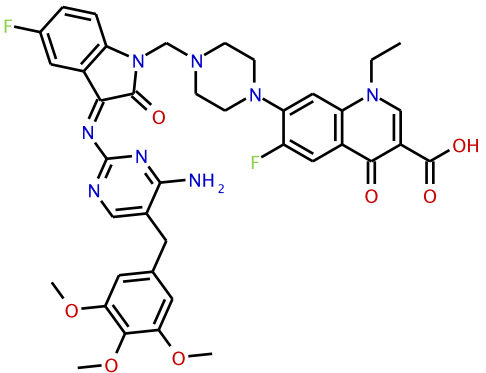
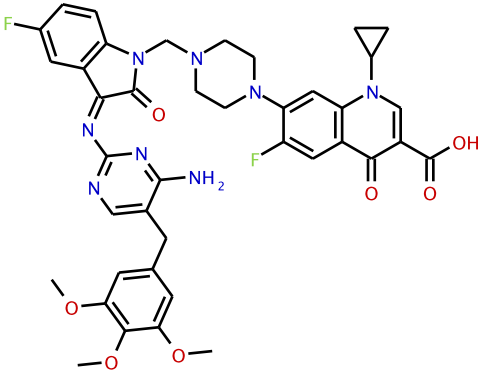
ID	Chemical Structure	MIC (ug/mL)	pMIC
79.	 Structure079	3.1300	-0.4955
80.	 Structure080	1.5600	-0.1931
81.		0.3900	0.4089

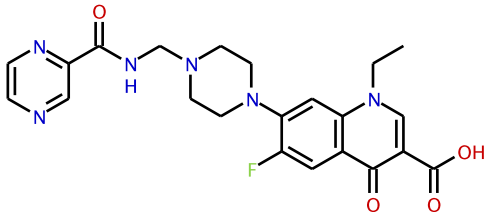
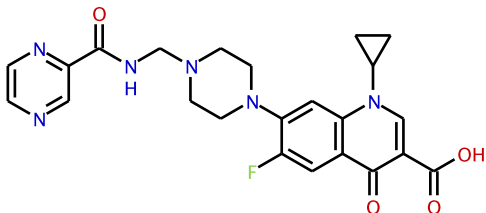
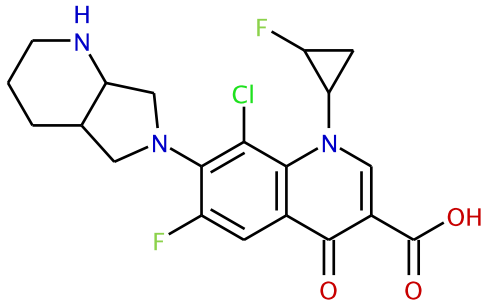
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
	 Structure081		
82.	 Structure082	0.0030	2.5272
83.	 Structure083	0.0027	2.5719

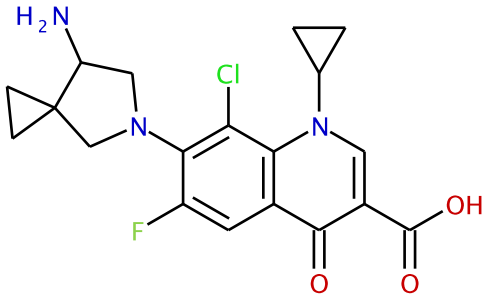
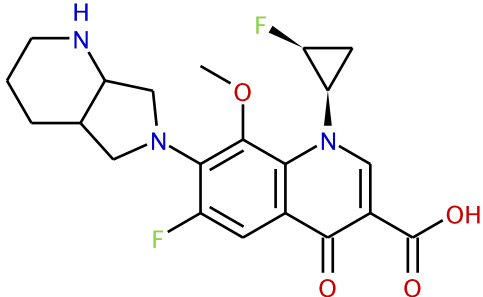
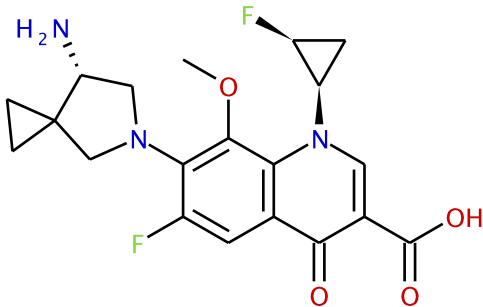
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
84.	 Structure084	0.0026	2.5834
85.	 Structure085	0.0027	2.5622
86.	 Structure086	0.0012	2.9066

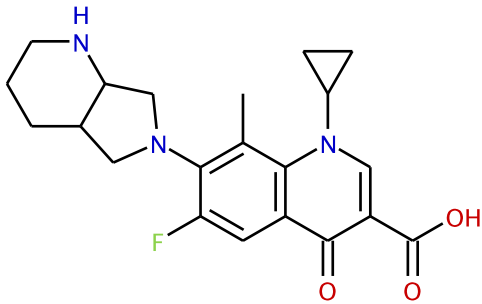
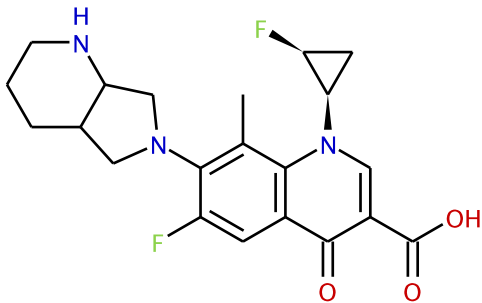
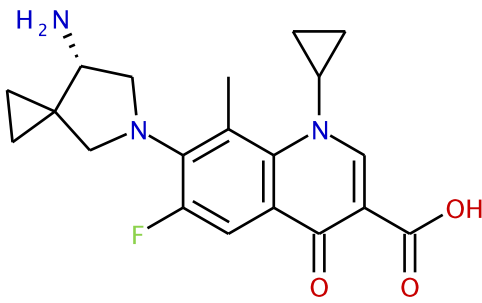
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
87.	 Structure087	0.0012	2.9172
88.	 Structure088	0.0014	2.8570
89.	 Structure089	0.0108	1.9658

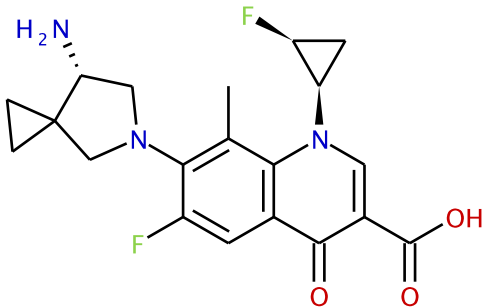
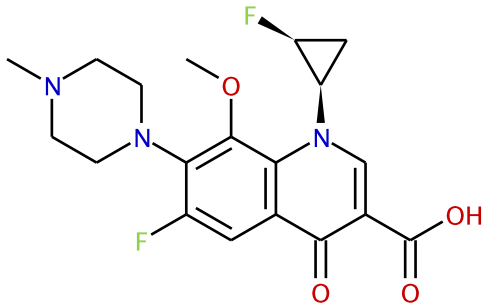
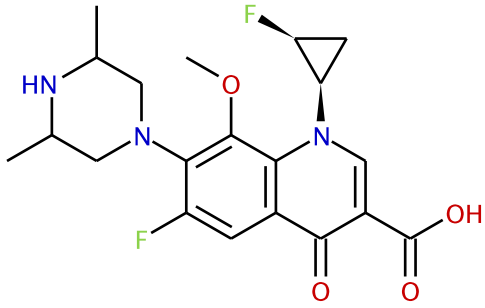
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
90.	 Structure090	0.0029	2.5452
91.	 Structure091	0.0014	2.8601
92.	 Structure092	6.2500	-0.7959

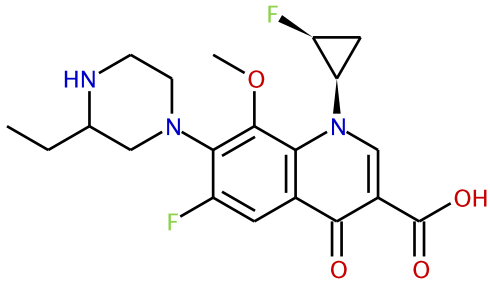
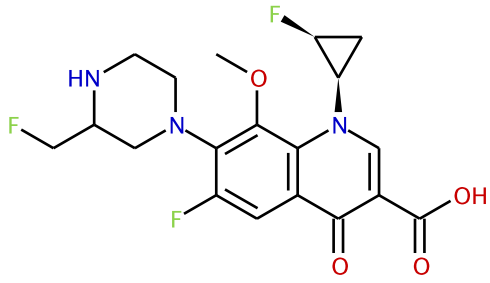
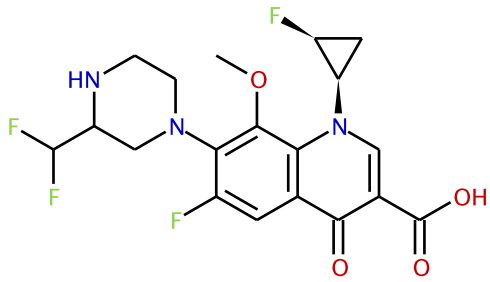
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
93.	 Structure093	0.1250	0.9031
94.	 Structure094	3.1300	-0.4955
95.	 Structure095	0.7800	0.1079

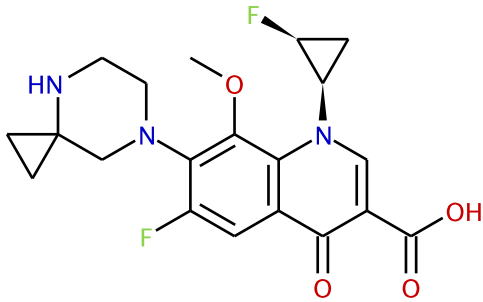
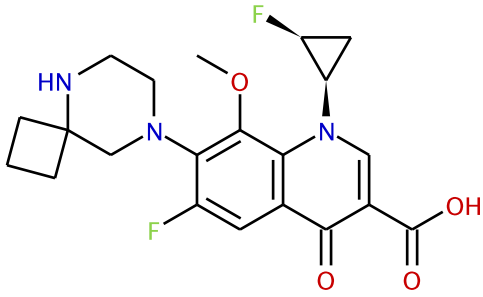
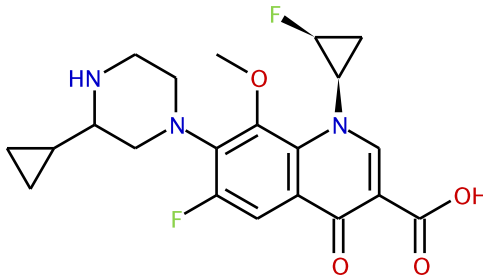
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
96.	 Structure096	0.7800	0.1079
97.	 Structure097	0.7800	0.1079
98.	 Structure098	0.0060	2.2218

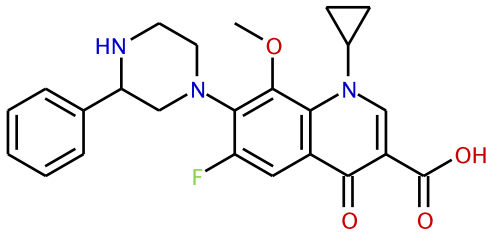
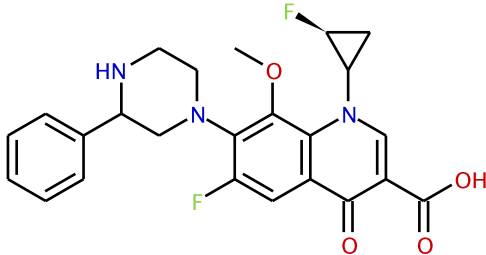
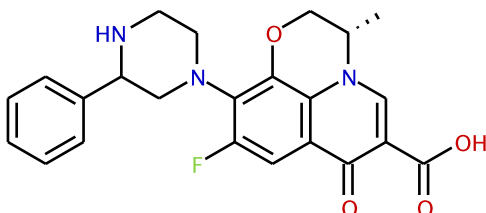
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
99.	 Structure099	0.0060	2.2218
100.	 Structure100	0.0130	1.8861
101.	 Structure101	0.0060	2.2218

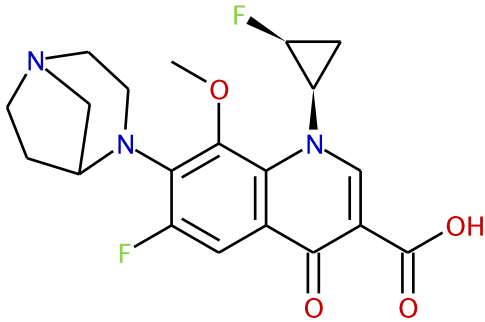
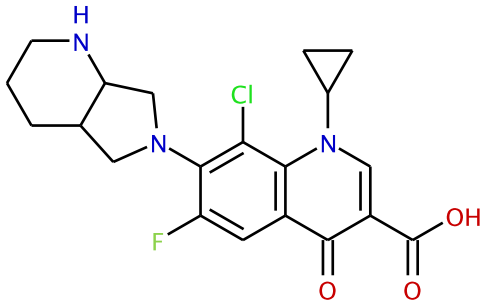
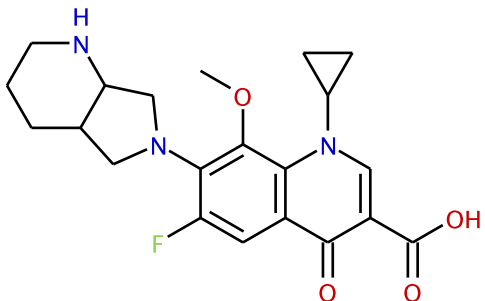
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
102.	 Structure102	0.0010	3.0000
103.	 Structure103	0.0020	2.6990
104.	 Structure104	0.0130	1.8861

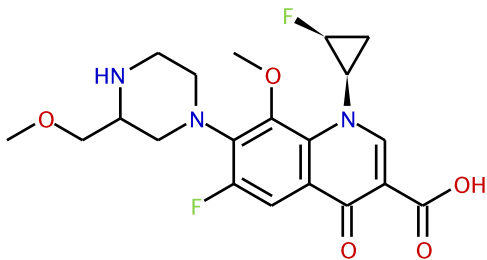
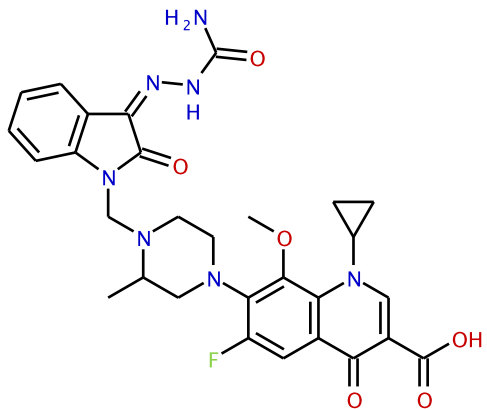
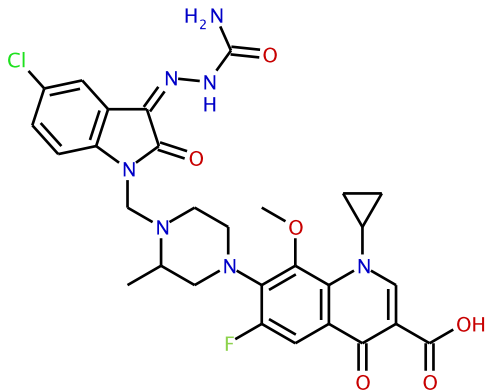
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
105.	 Structure105	0.0060	2.2218
106.	 Structure106	0.0250	1.6021
107.	 Structure107	0.0300	1.5229

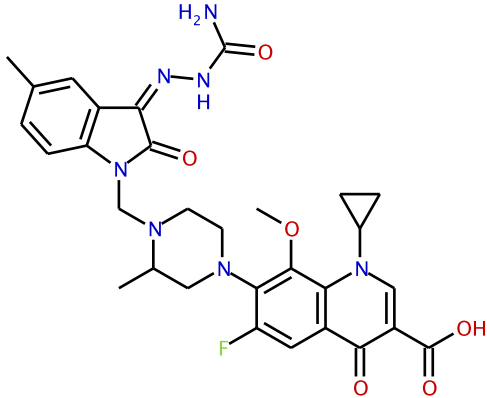
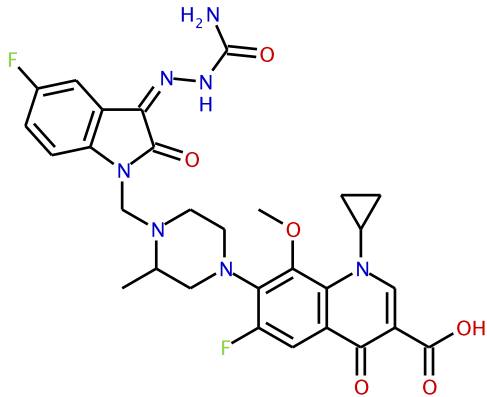
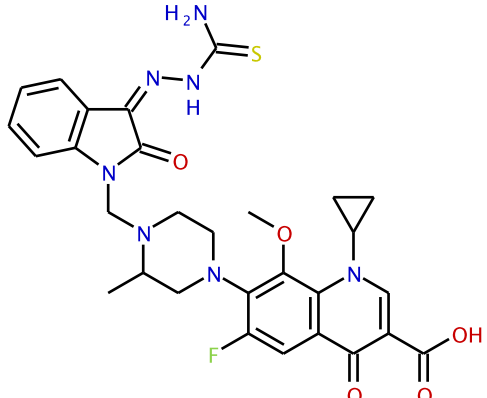
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
108.	 Structure108	0.0600	1.2218
109.	 Structure109	0.2000	0.6990
110.	 Structure110	0.3900	0.4089

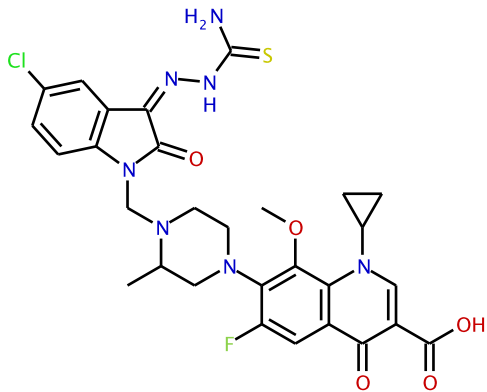
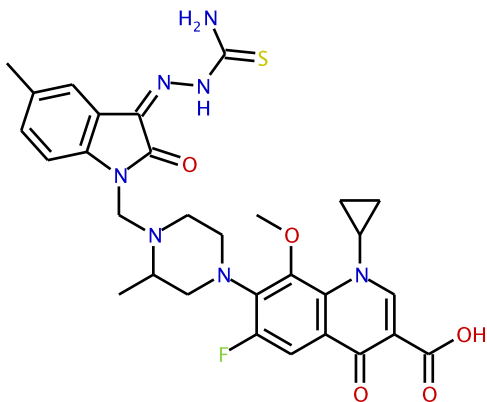
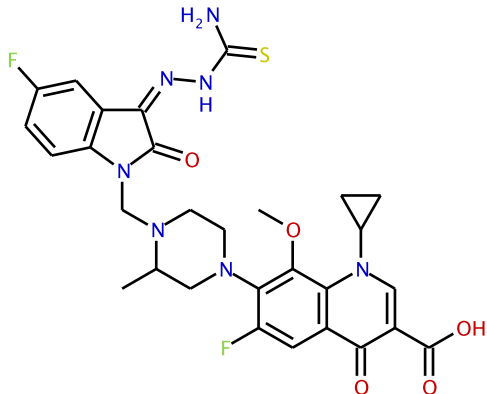
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
111.	 Structure111	0.7800	0.1079
112.	 Structure112	1.5600	-0.1931
113.	 Structure113	0.3900	0.4089

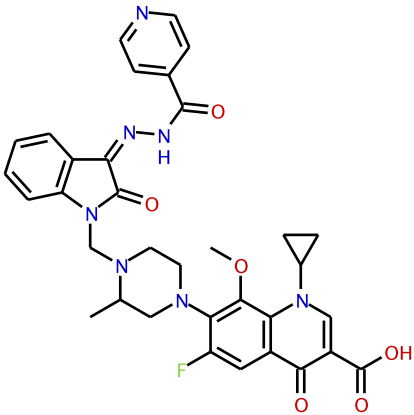
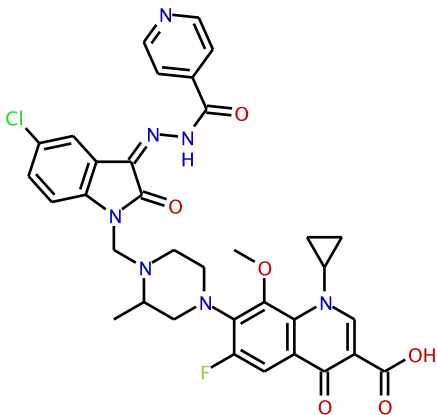
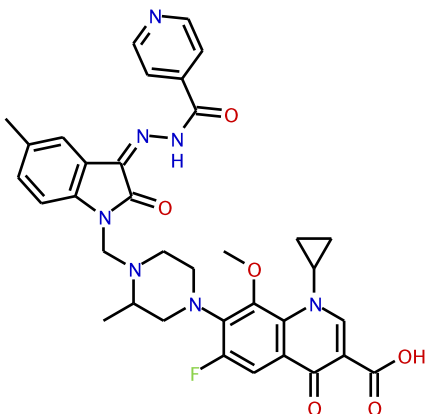
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
114.	 Structure114	0.1000	1.0000
115.	 Structure115	0.1000	1.0000
116.	 Structure116	0.1000	1.0000

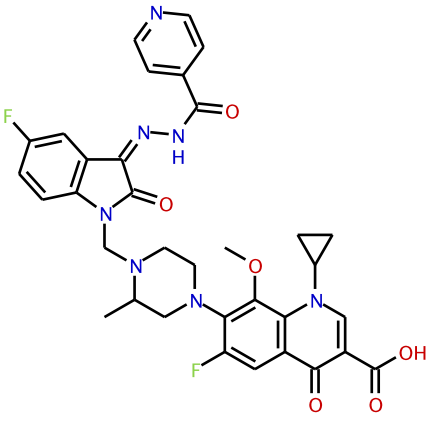
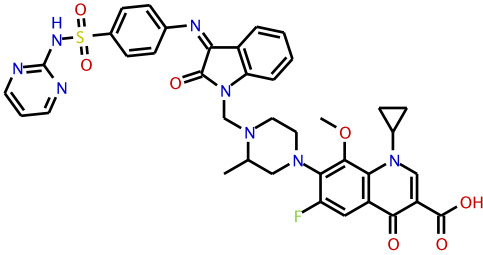
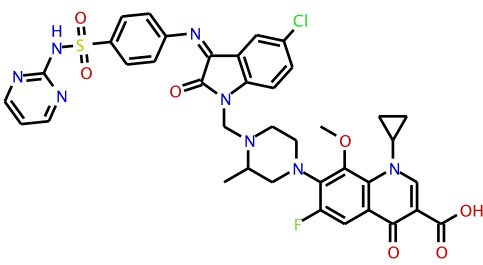
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
117.	 Structure117	0.2000	0.6990
118.	 Structure118	0.0015	2.8239
119.	 Structure119	0.0250	1.6021

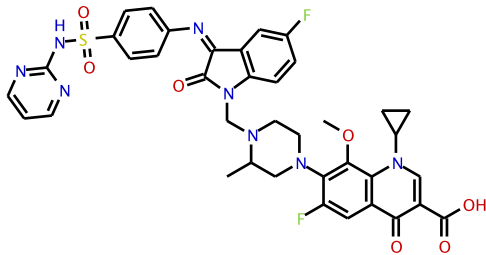
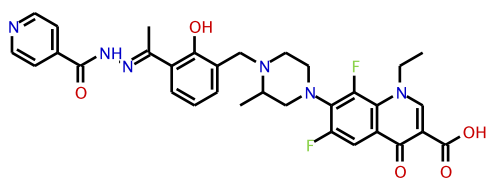
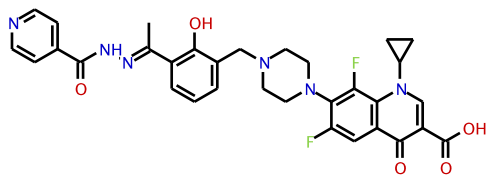
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
120.	 Structure120	0.3900	0.4089
121.	 Structure121	0.0125	1.9031
122.	 Structure122	0.3900	0.4089

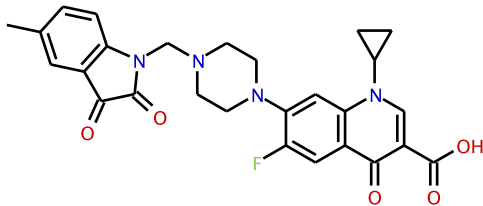
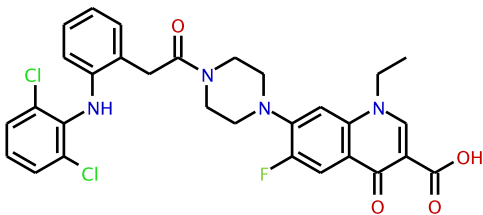
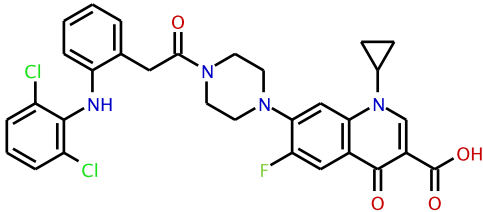
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
123.	 Structure123	0.3900	0.4089
124.	 Structure124	0.2000	0.6990
125.	 Structure125	0.2000	0.6990

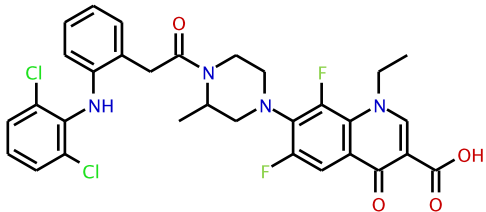
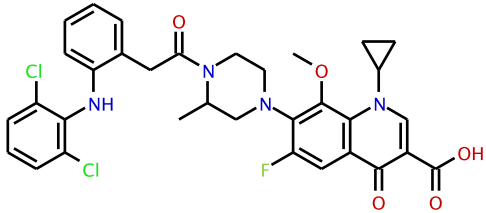
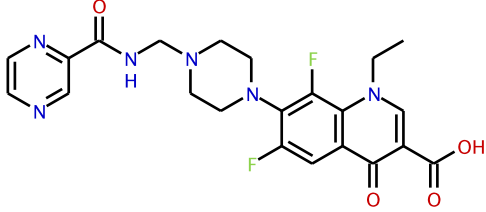
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
126.	 Structure126	0.3900	0.4089
127.	 Structure127	0.7800	0.1079
128.	 Structure128	0.1000	1.0000

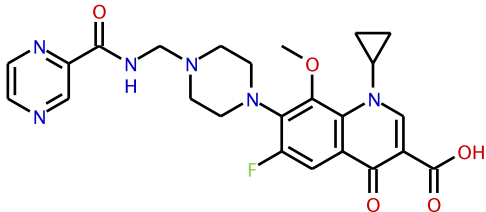
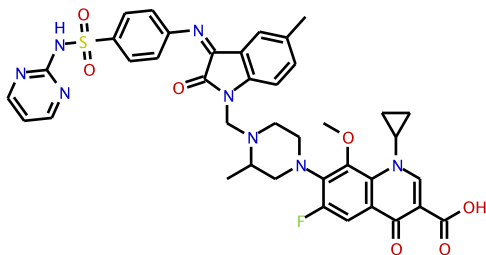
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
129.	 Structure129	0.2000	0.6990
130.	 Structure130	0.3900	0.4089
131.	 Structure131	0.7800	0.1079

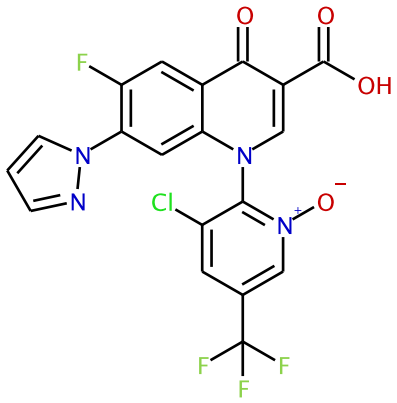
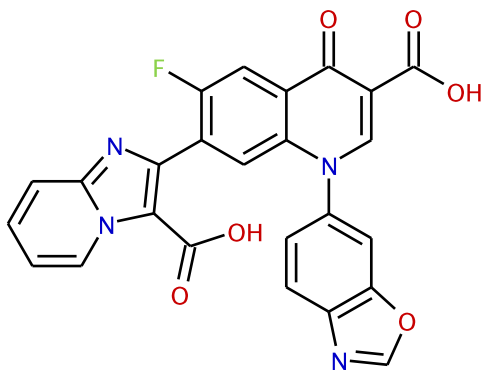
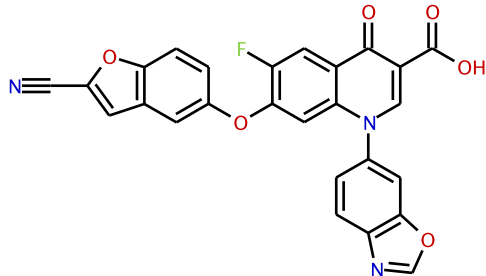
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
132.	 Structure132	0.7800	0.1079
133.	 Structure133	0.1000	1.0000
134.	 Structure134	0.1000	1.0000

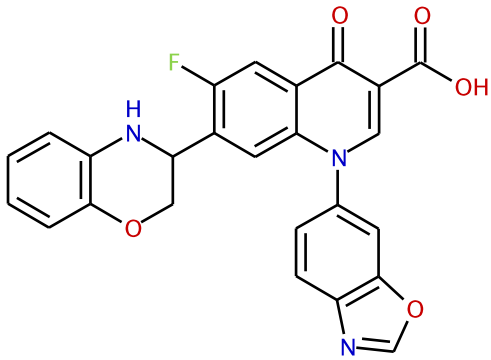
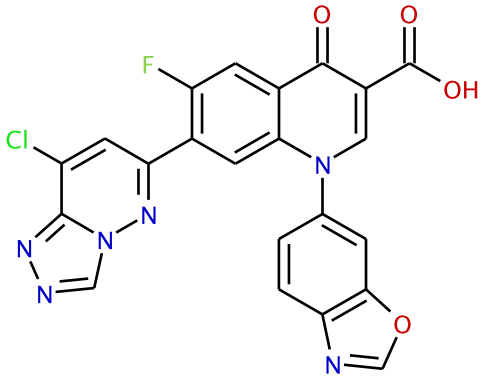
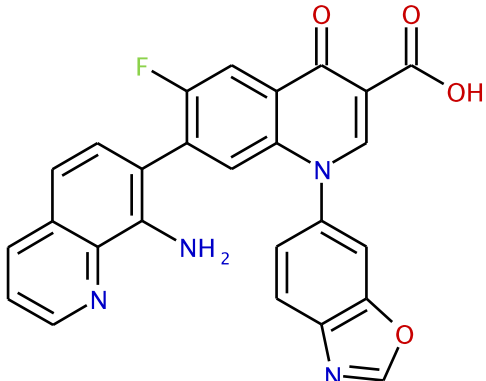
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
135.	 Structure135	0.1000	1.0000
136.	 Structure136	1.2600	-0.1004
137.	 Structure137	1.3000	-0.1139

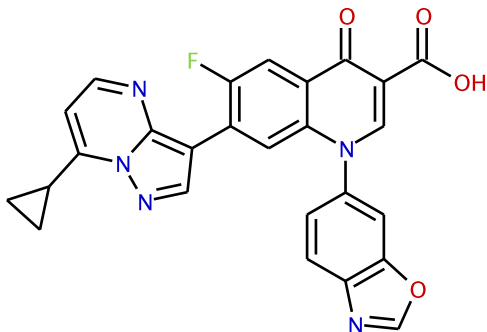
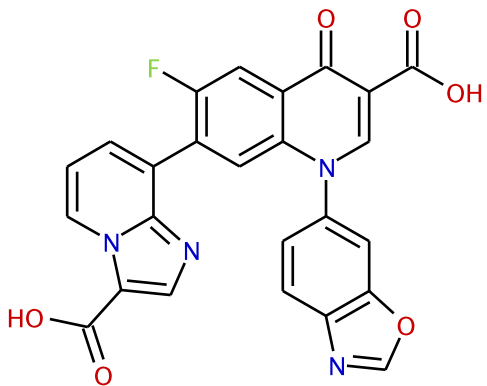
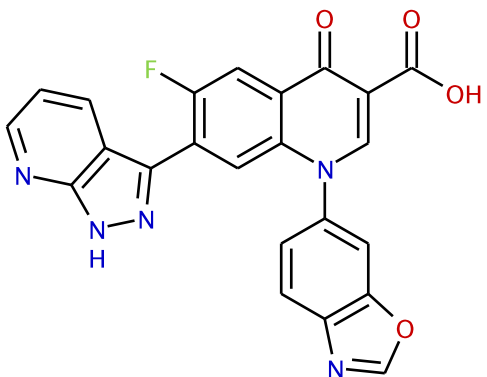
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
138.	 Structure138	0.0031	2.5100
139.	 Structure139	0.3300	0.4815
140.	 Structure140	0.1600	0.7959

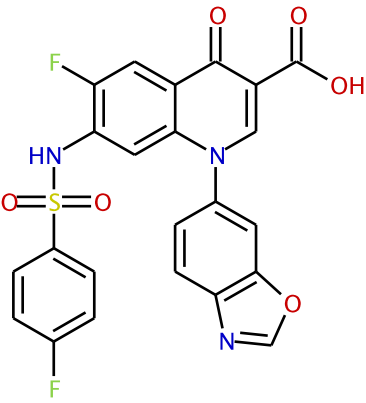
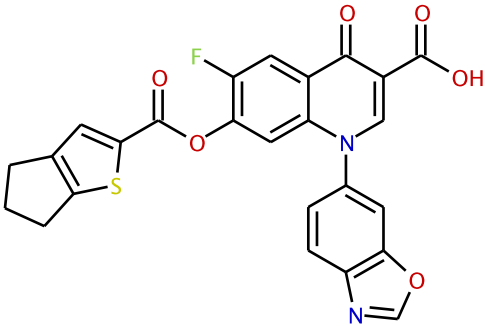
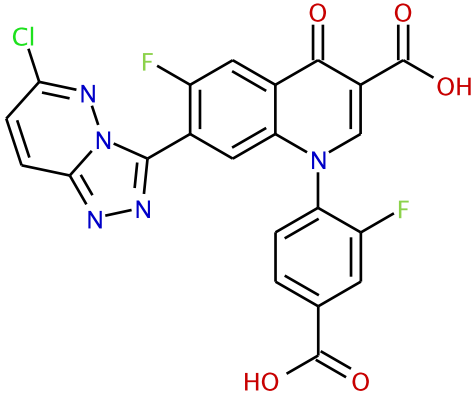
ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
141.	 Structure141	0.3200	0.4949
142.	 Structure142	0.0400	1.3979
143.	 Structure143	0.7800	0.1079

ExpLib			
ID	Chemical Structure	MIC (ug/mL)	pMIC
144.	 Structure144	0.2000	0.6990
145.	 Structure145	0.1000	1.0000

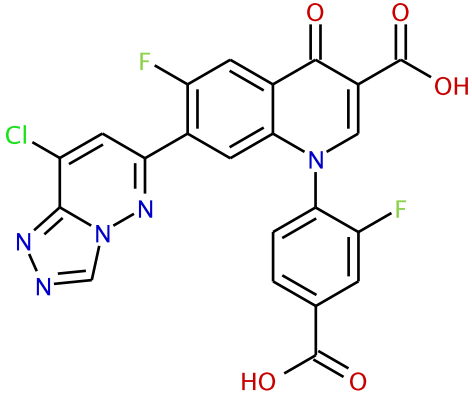
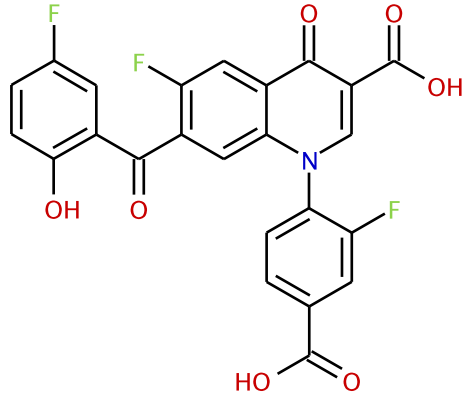
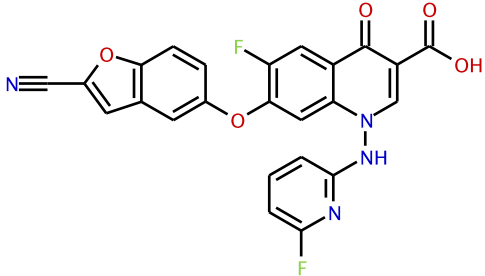
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
1.	 CIP'-024-176	0.0250	1.6016
2.	 CIP'-028-002	0.0499	1.3022
3.	 CIP'-028-018	0.0300	1.5230

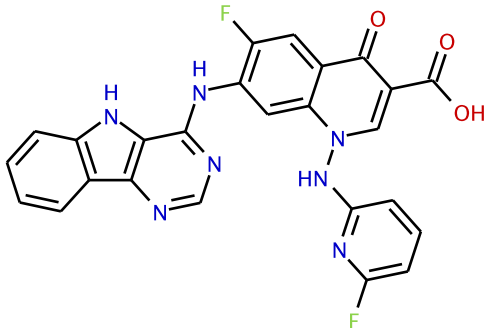
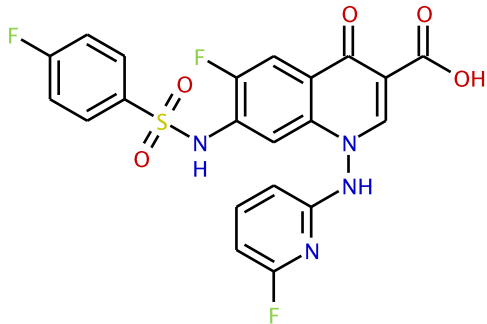
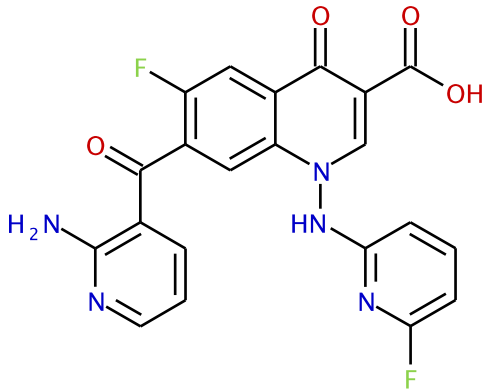
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
4.	 CIP'-028-055	0.0234	1.6304
5.	 CIP'-028-059	0.0499	1.3022
6.	 CIP'-028-073	0.0021	2.6818

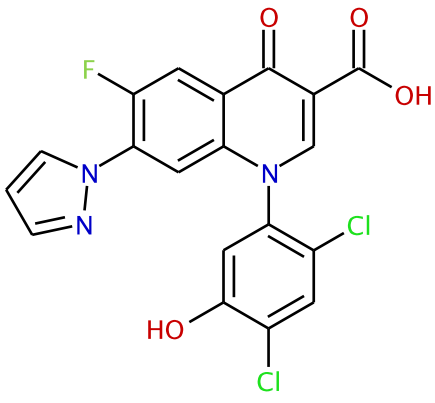
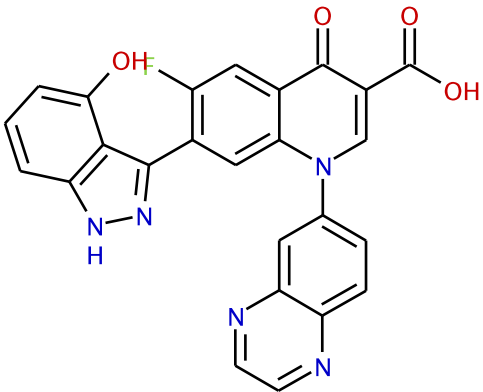
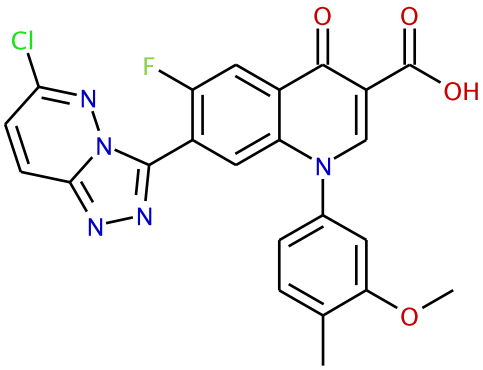
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
7.	 CIP'-028-113	0.0499	1.3022
8.	 CIP'-028-128	0.0021	2.6818
9.	 CIP'-028-148	0.0499	1.3022

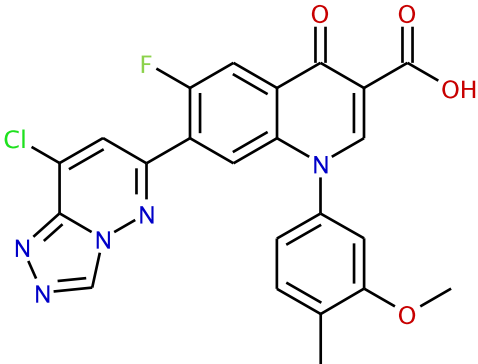
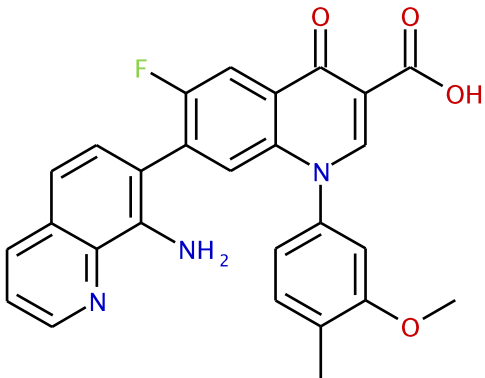
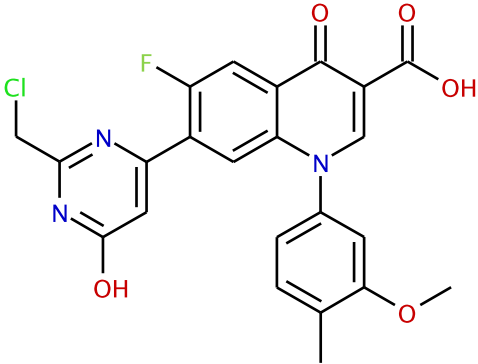
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
10.	 CIP'-028-149	0.0021	2.6818
11.	 CIP'-028-154	0.0021	2.6818
12.	 CIP'-036-057	0.0021	2.6818

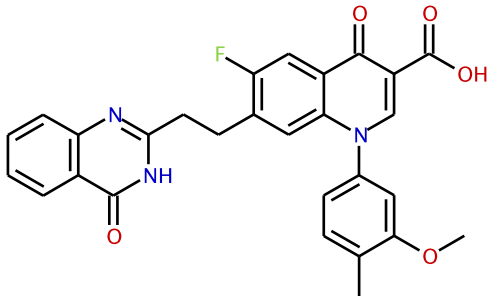
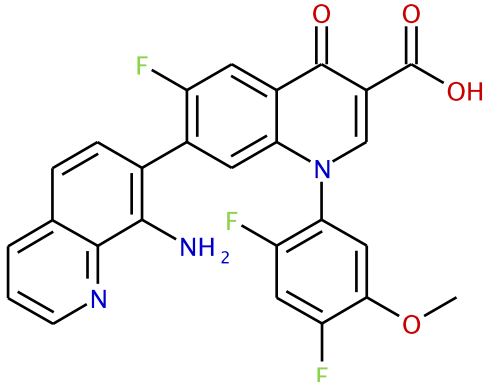
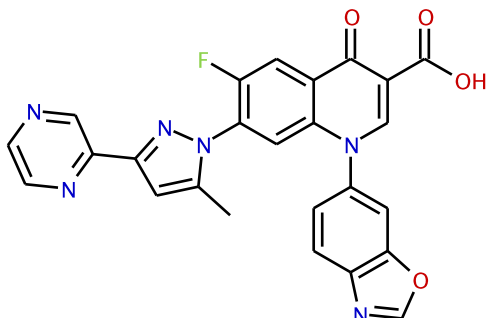
CombiLibHits

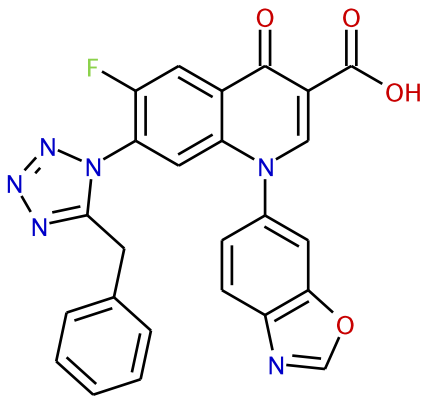
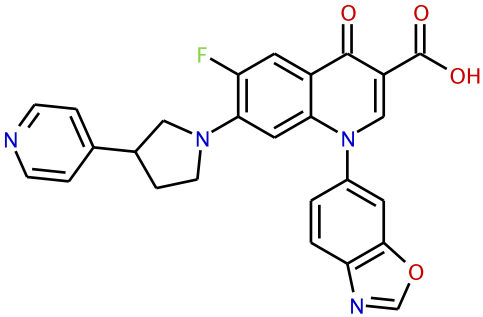
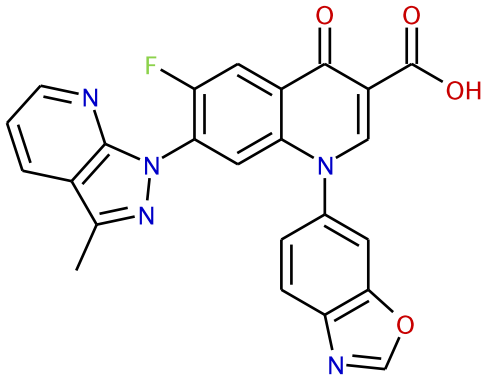
ID	Chemical Structure	MIC (ug/mL)	pMIC
13.	 CIP'-036-059	0.0021	2.6818
14.	 CIP'-036-092	0.0250	1.6016
15.	 CIP'-046-018	0.0300	1.5230

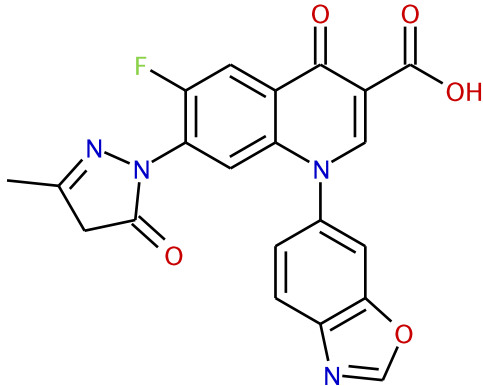
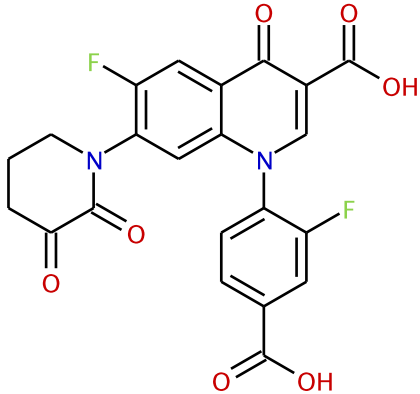
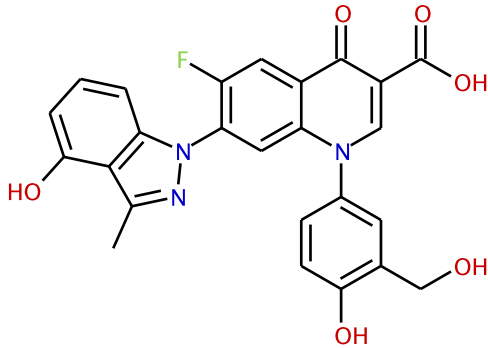
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
16.	 CIP'-046-069	0.0300	1.5230
17.	 CIP'-046-149	0.0311	1.5079
18.	 CIP'-046-156	0.0311	1.5079

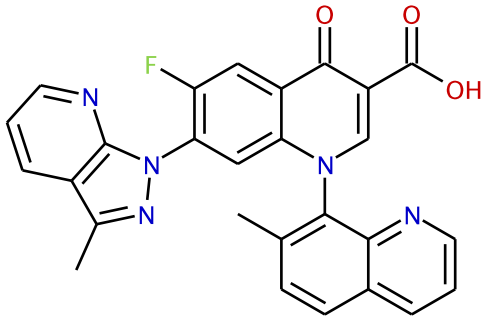
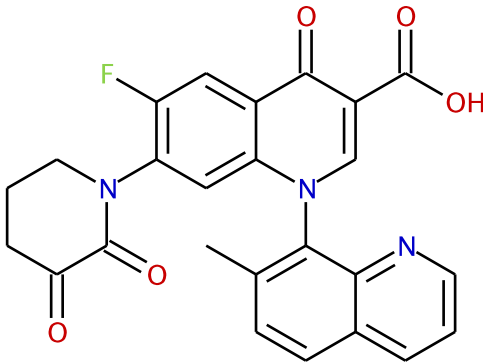
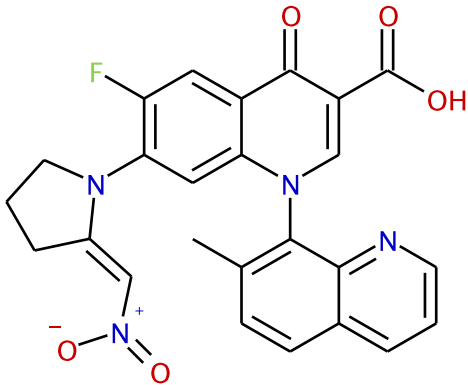
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
19.	 CIP'-059-176	0.0329	1.4825
20.	 CIP'-060-169	0.0499	1.3022
21.	 CIP'-095-057	0.0021	2.6818

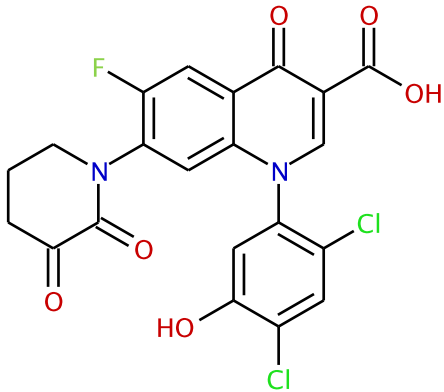
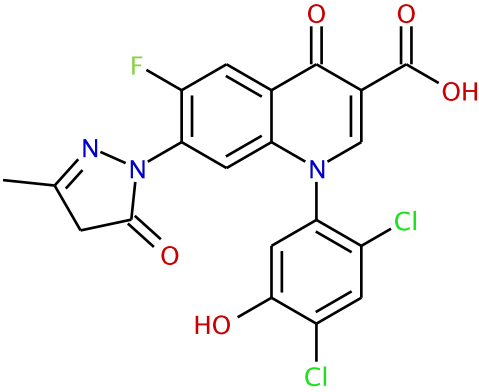
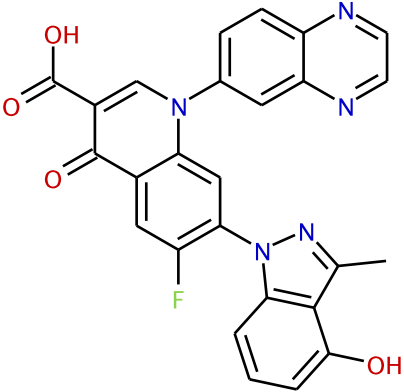
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
22.	 CIP'-095-059	0.0021	2.6818
23.	 CIP'-095-073	0.0401	1.3970
24.	 CIP'-095-177	0.0401	1.3970

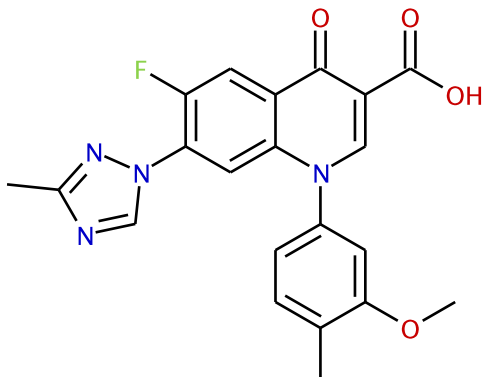
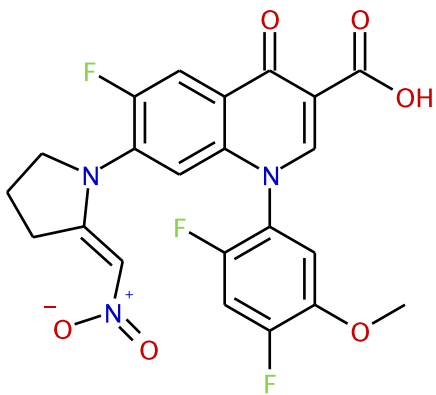
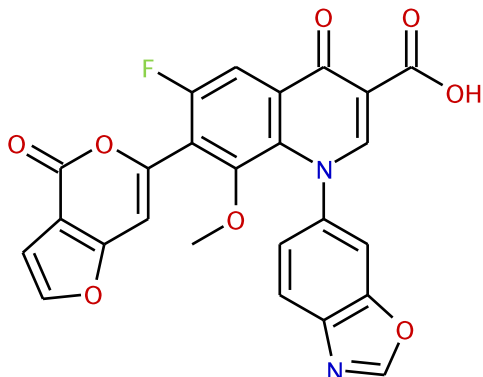
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
25.	 CIP'-095-183	0.0401	1.3970
26.	 CIP'-100-073	0.0329	1.4825
27.	 CIP-028-056	0.0021	2.6818

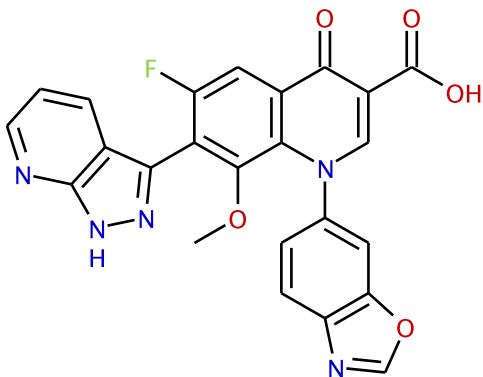
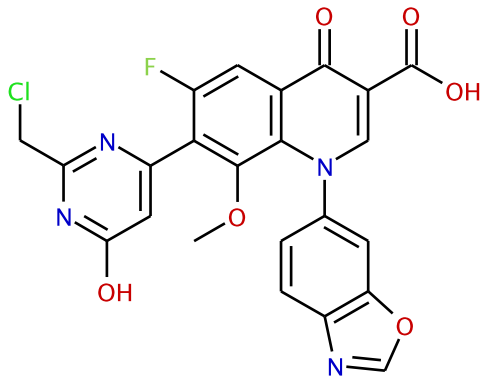
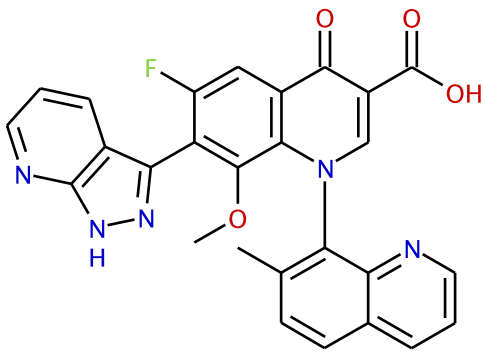
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
28.	 CIP-028-066	0.0300	1.5230
29.	 CIP-028-082	0.0300	1.5230
30.	 CIP-028-083	0.0499	1.3022

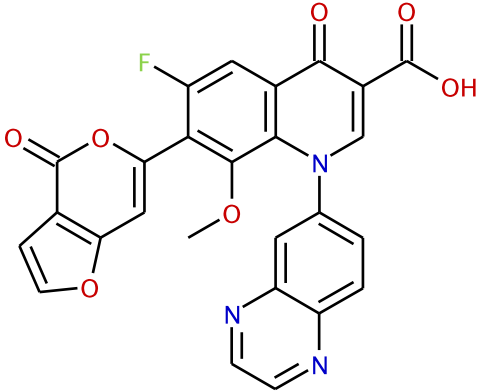
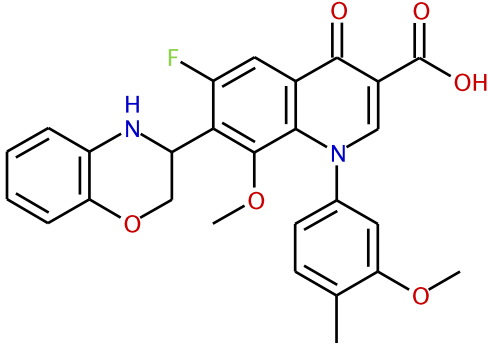
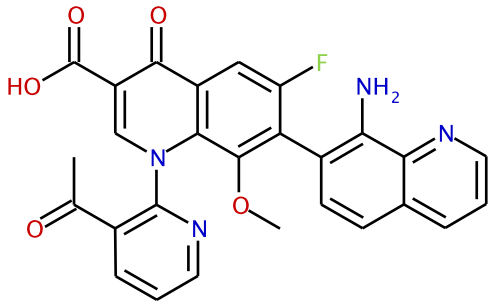
CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
31.	 CIP-028-102	0.0130	1.8851
32.	 CIP-036-096	0.0250	1.6016
33.	 CIP-037-090	0.0130	1.8851

CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
34.	 CIP-049-083	0.0130	1.8851
35.	 CIP-049-096	0.0329	1.4825
36.	 CIP-049-101	0.0401	1.3970

CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
37.	 CIP-059-096	0.0250	1.6016
38.	 CIP-059-102	0.0250	1.6016
39.	 CIP-060-090	0.0499	1.3022

CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
40.	 CIP-096-098	0.0401	1.3970
41.	 CIP-101-101	0.0401	1.3970
42.	 MOX'-016-005	0.0499	1.3022

CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
43.	 MOX'-016-116	0.0499	1.3022
44.	 MOX'-016-137	0.0300	1.5230
45.	 MOX'-028-116	0.0130	1.8851

CombiLibHits			
ID	Chemical Structure	MIC (ug/mL)	pMIC
46.	 MOX'-039-005	0.0499	1.3022
47.	 MOX'-060-033	0.0401	1.3970
48.	 MOX'-065-050	0.0401	1.3970