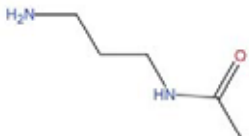
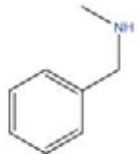
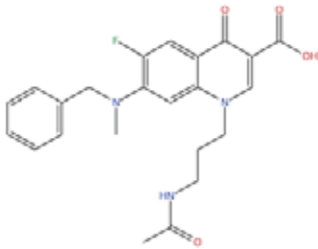
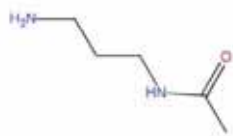
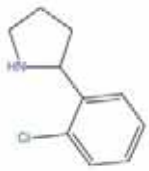
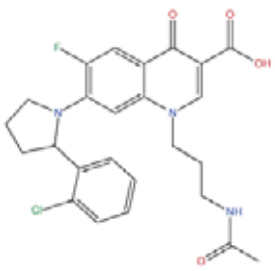
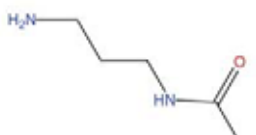
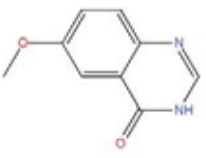
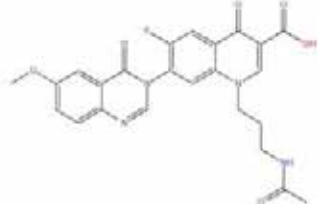
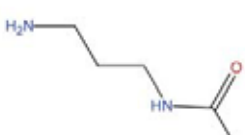
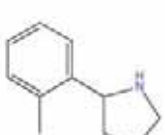
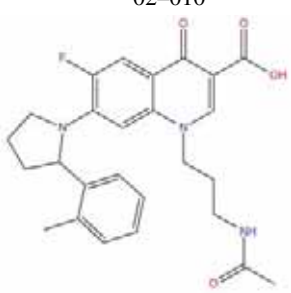
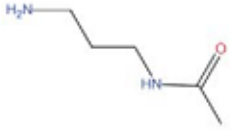
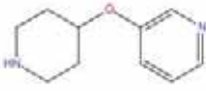
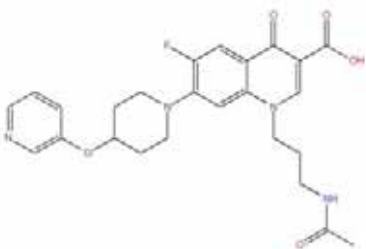
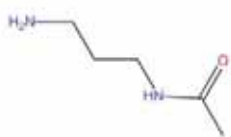
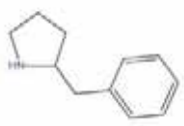
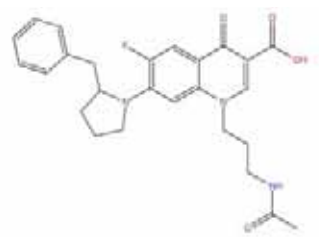
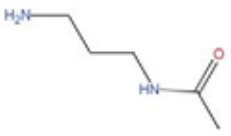
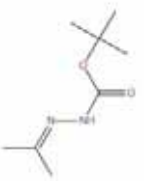
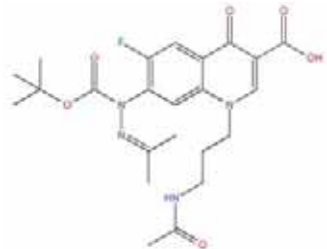
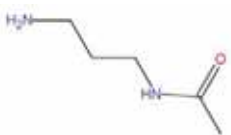
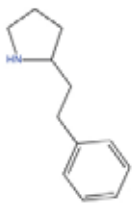
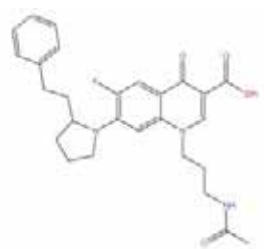
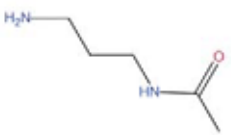
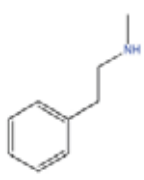
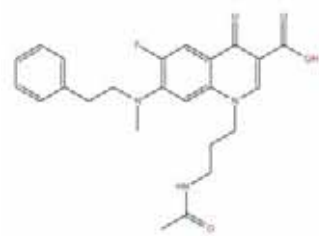
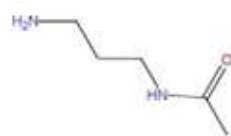
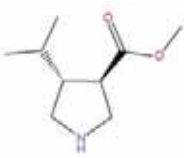
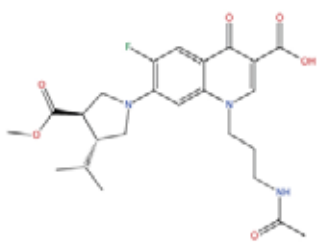
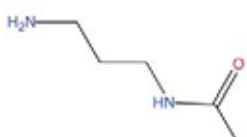
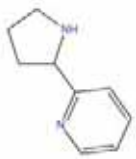
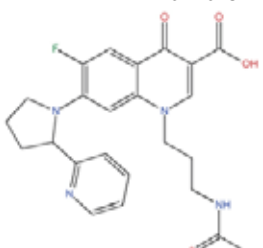
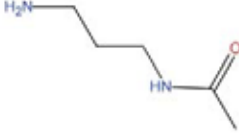
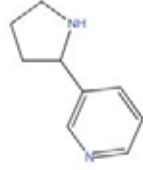
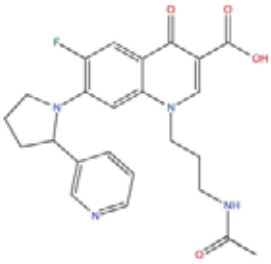
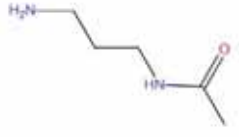
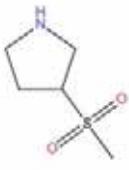
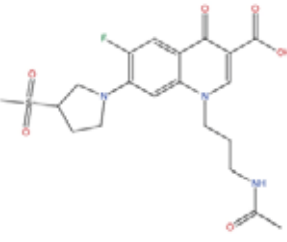
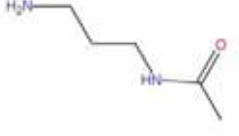
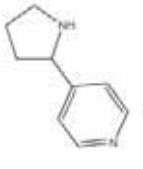
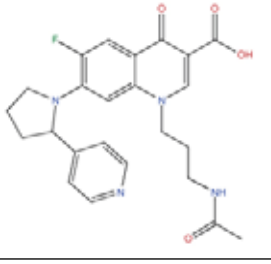
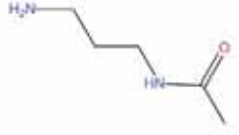
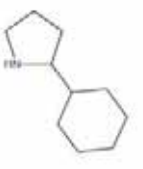
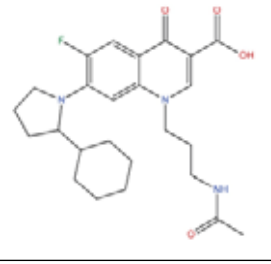
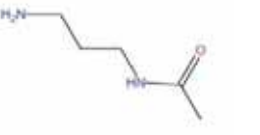
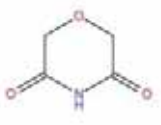
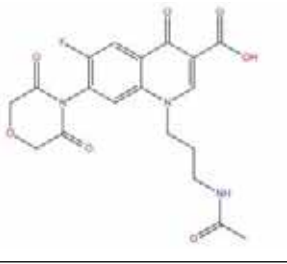
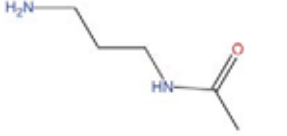
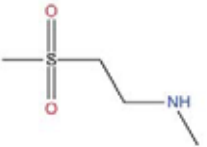
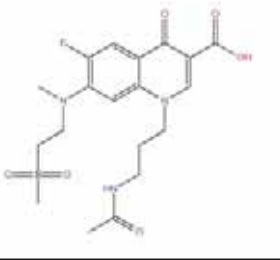


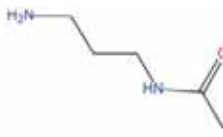
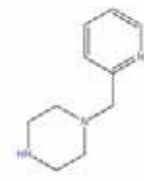
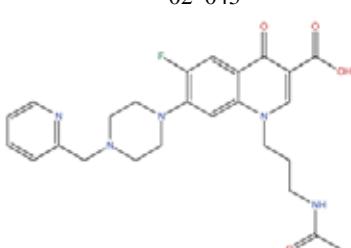
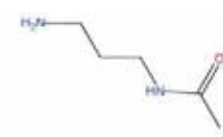
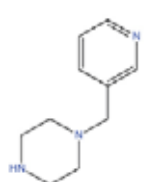
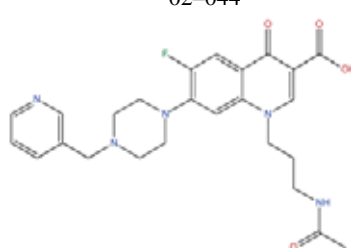
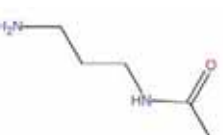
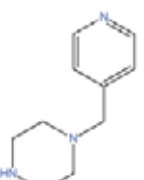
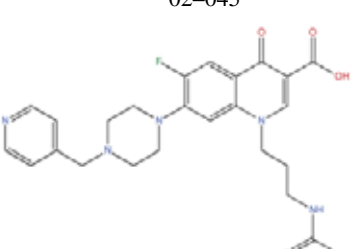
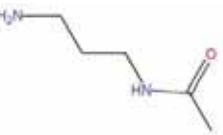
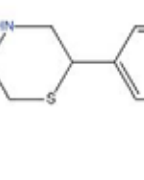
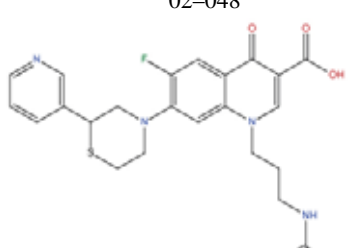
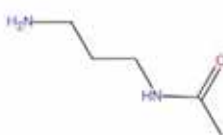
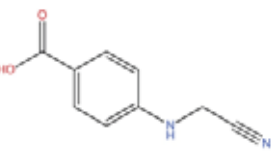
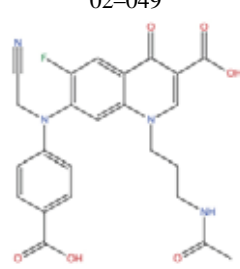
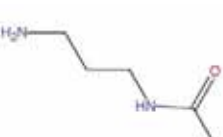
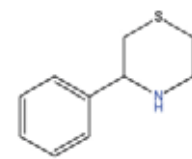
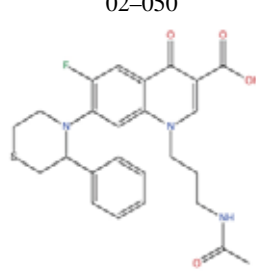
## Supplementary Material Available

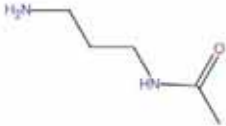
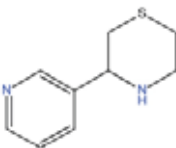
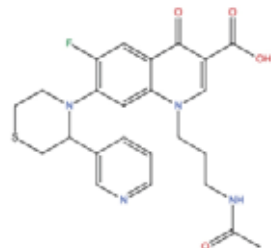
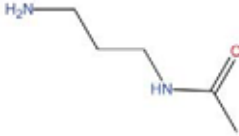
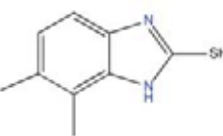
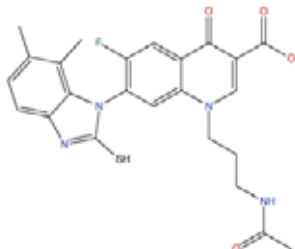
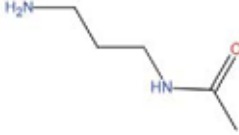
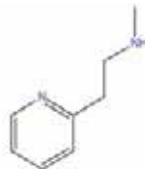
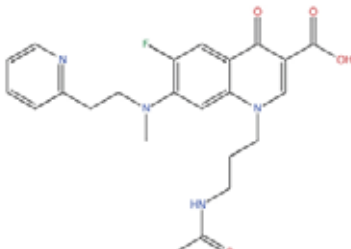
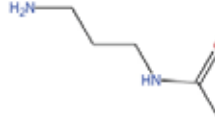
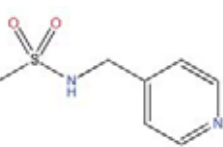
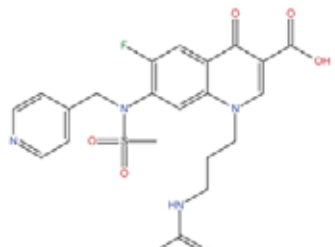
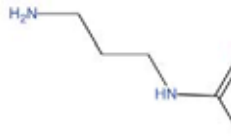
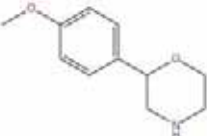
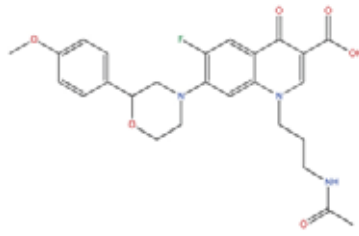
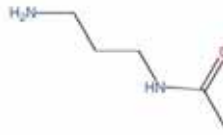
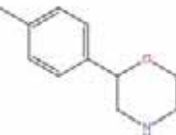
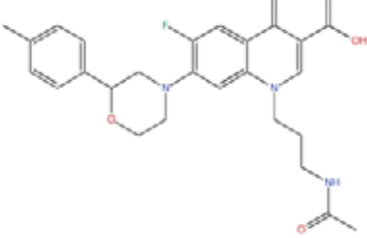
**Table S1.** Chemical structures of the combinatorially obtained, filtered 6-fluoroquinolones (*CombiData*, 304 compounds) as well as the selected *reactant 1* and *reactant 2* substructural fragments. Structures rated in top 5% by activity are highlighted.

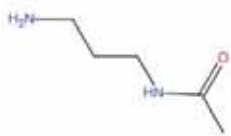
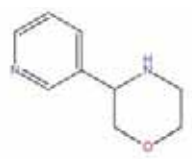
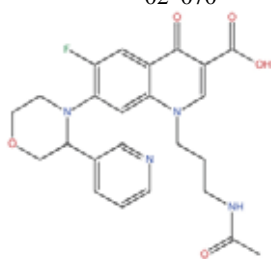
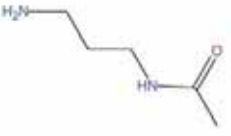
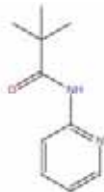
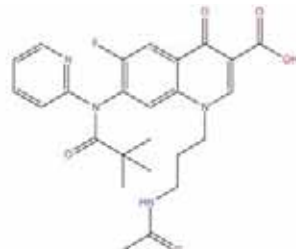
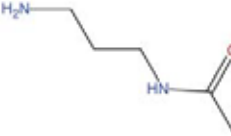
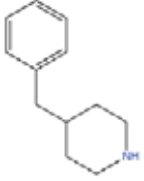
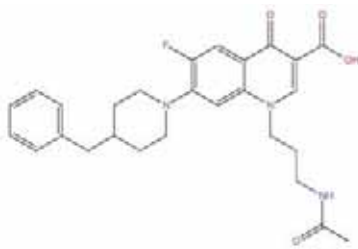
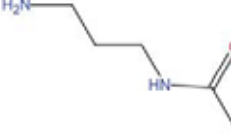
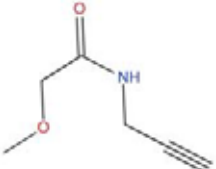
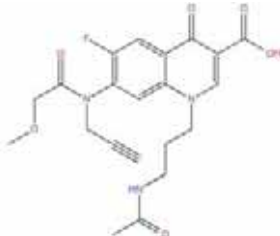
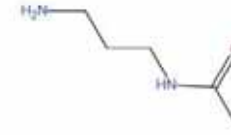
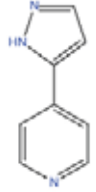
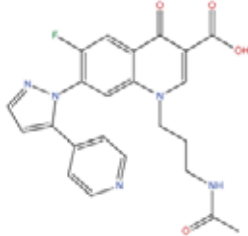
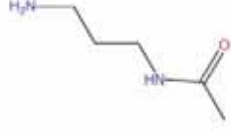
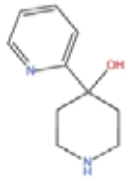
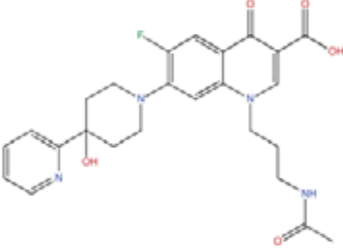
ID	<i>reactant 1</i>	<i>reactant 2</i>	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
1	02 	001 	02-001 	0.4407	0.3625
2	02 	002 	02-002 	0.8841	0.1306
3	02 	009 	02-009 	1.1041	0.0787
4	02 	010 	02-010 	0.8764	0.1329
5	02 	014 	02-014 	-0.3764	2.3790

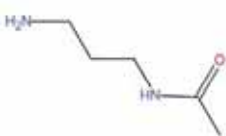
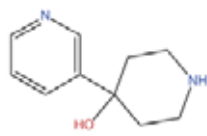
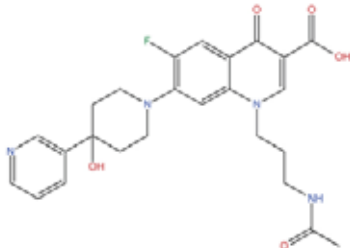
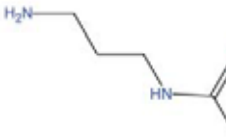
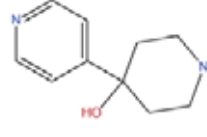
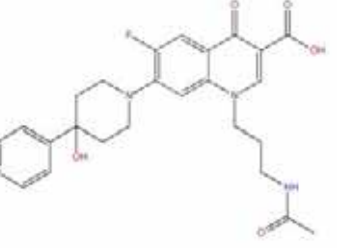
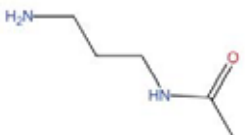
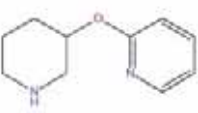
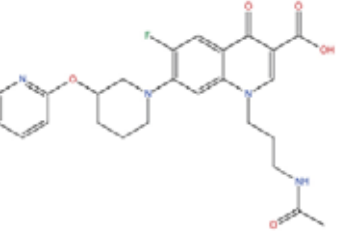
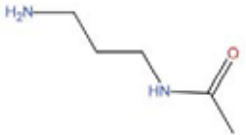
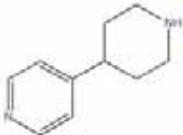
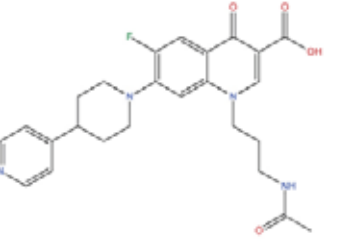
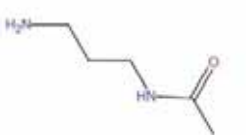
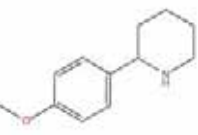
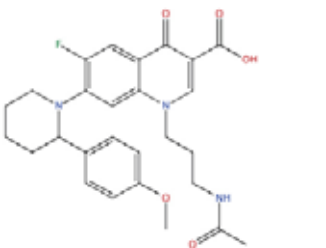
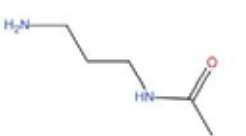
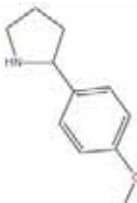
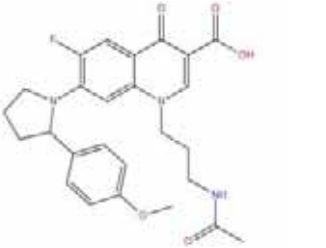
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
6	02	017	02-017	0.2338	0.5837
					
7	02	018	02-018	1.2783	0.0527
					
8	02	020	02-020	-0.0219	1.0517
					
9	02	023	02-023	0.0082	0.9814
					
10	02	024	02-024	0.4778	0.3328
					
11	02	025	02-025	0.6197	0.2400
					

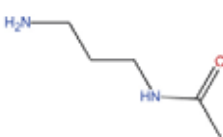
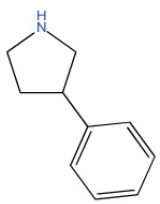
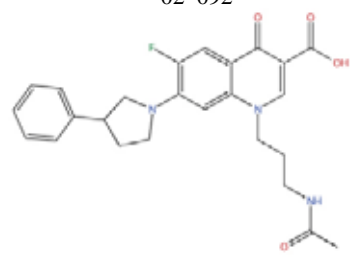
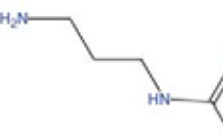
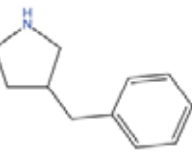
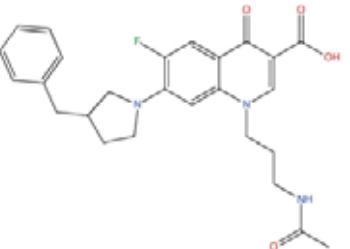
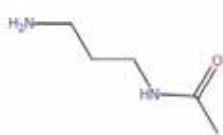
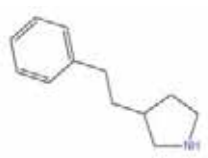
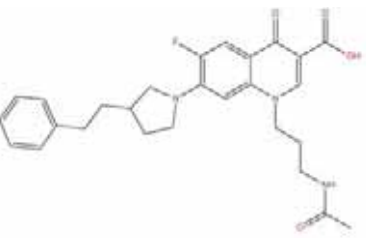
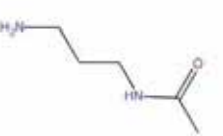
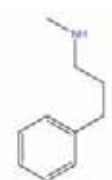
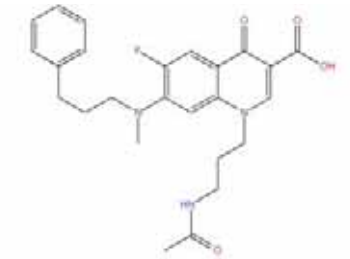
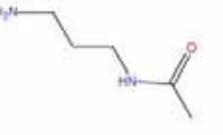
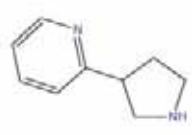
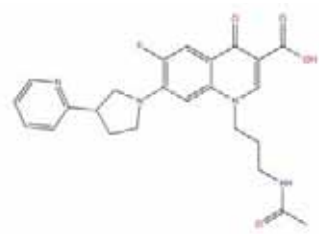
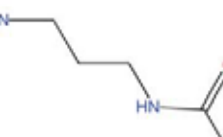
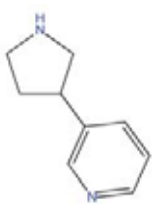
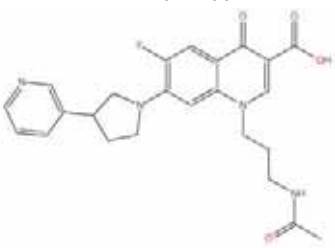
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
12				0.5459	0.2845
13	02	028	02-028	0.2001	0.6308
					
14	02	029	02-029	0.8622	0.1373
					
15	02	032	02-032	0.6956	0.2016
					
16	02	033	02-033	0.7501	0.1778
					
17	02	038	02-038	0.1054	0.7845
					

ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
18	02	043	02-043	-0.1036	1.2694
					
19	02	044	02-044	-0.2901	1.9503
					
20	02	045	02-045	0.0125	0.9716
					
21	02	048	02-048	0.5724	0.2677
					
22	02	049	02-049	0.5100	0.3090
					
23	02	050	02-050	0.7361	0.1836
					

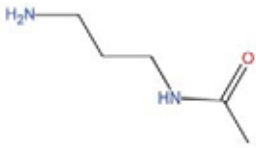
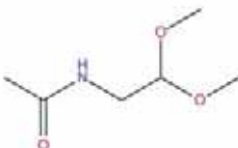
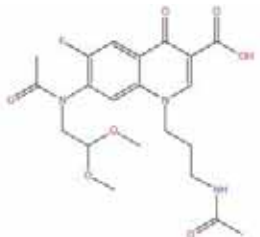
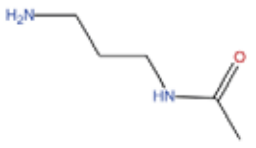
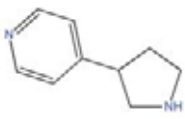
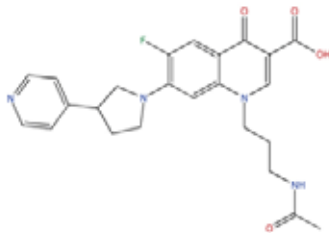
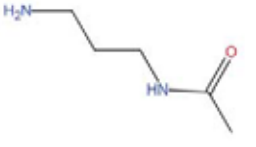
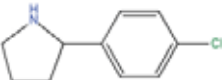
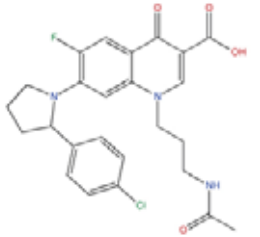
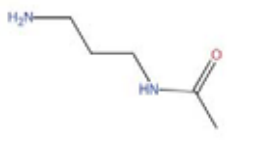
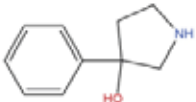
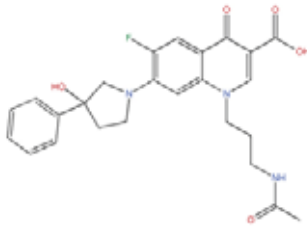
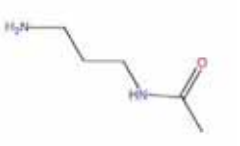
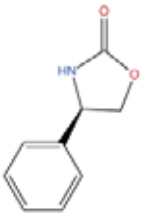
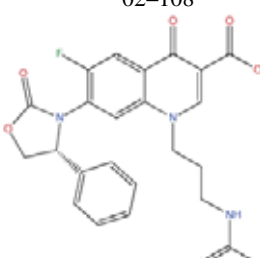
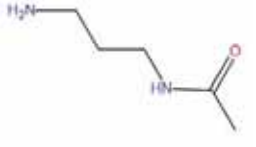
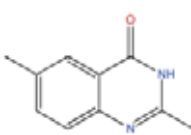
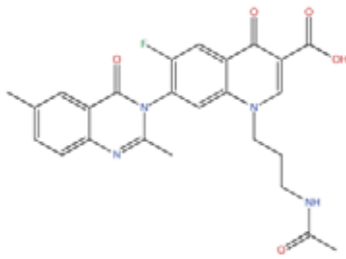
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
24	02	051	02-051	0.6161	0.2420
					
25	02	057	02-057	0.9441	0.1137
					
26	02	059	02-059	-0.1266	1.3384
					
27	02	060	02-060	1.0133	0.0970
					
28	02	063	02-063	0.0875	0.8175
					
29	02	064	02-064	0.2580	0.5521
					

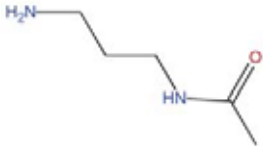
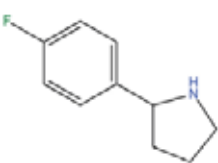
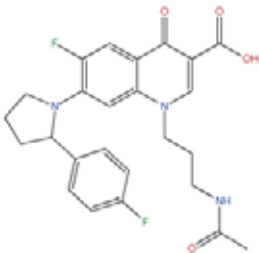
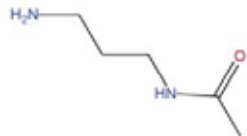
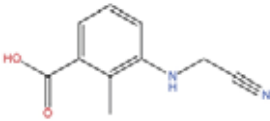

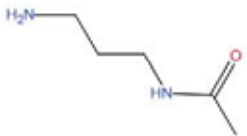
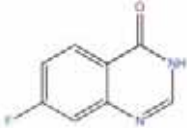
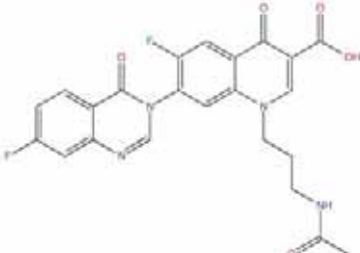
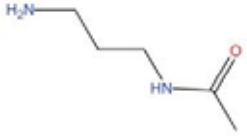
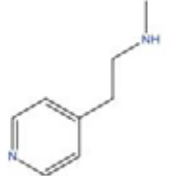
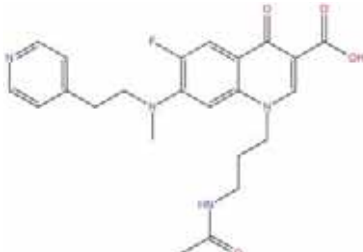
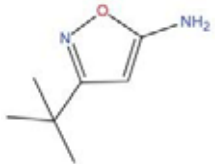
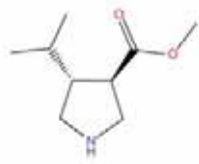
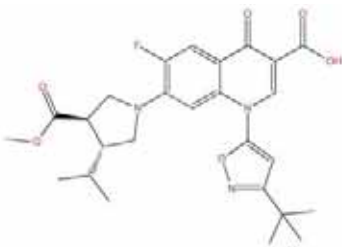
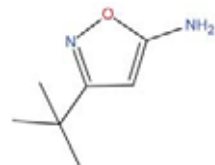
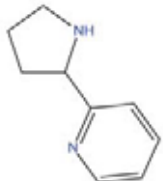
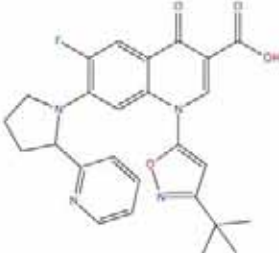
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
30	02	070	02-070	0.5864	0.2592
					
31	02	071	02-071	1.5306	0.0295
					
32	02	072	02-072	-0.0741	1.1860
					
33	02	077	02-077	0.7373	0.1831
					
34	02	079	02-079	0.7718	0.1691
					
35	02	084	02-084	0.2459	0.5677
					

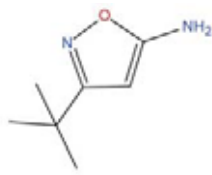
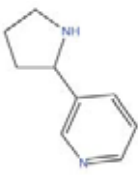
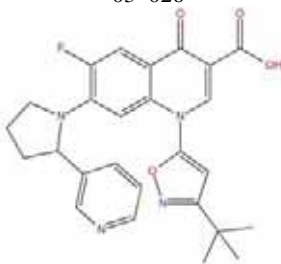
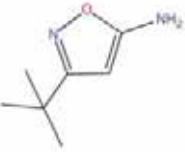
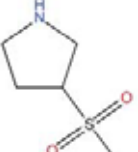
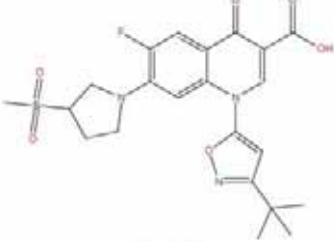
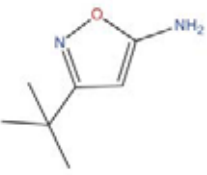
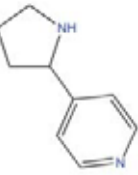
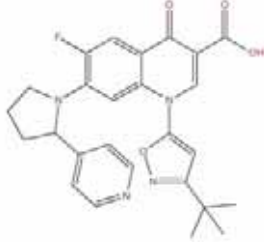
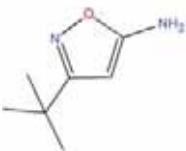
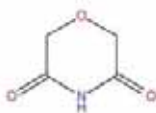
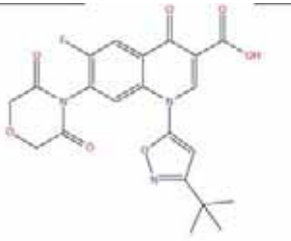
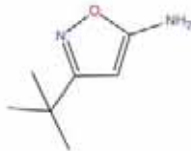
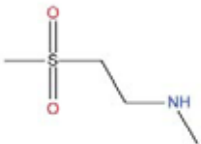
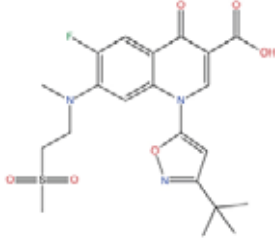
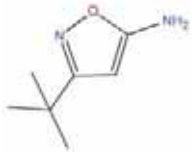
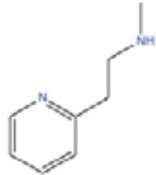
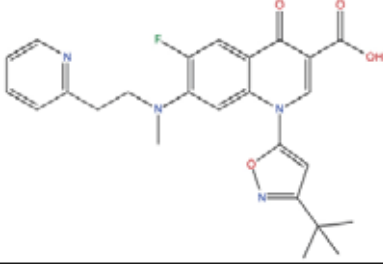
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
36	02	085	02-085	0.1240	0.7516
					
37	02	086	02-086	-0.0435	1.1054
					
38	02	087	02-087	0.2042	0.6249
					
39	02	088	02-088	-0.1360	1.3677
					
40	02	089	02-089	0.8466	0.1424
					
41	02	091	02-091	0.6627	0.2174
					

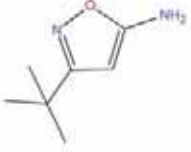
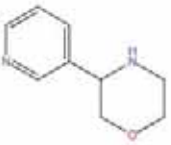
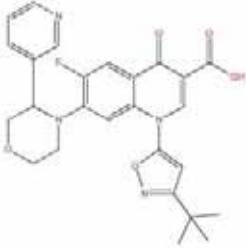
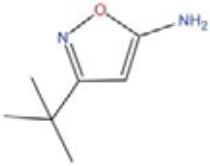
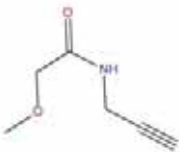
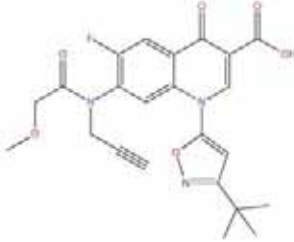
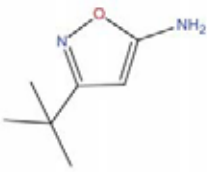
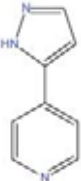
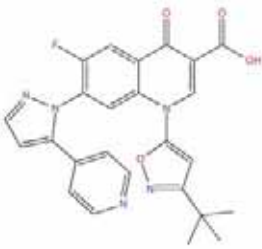
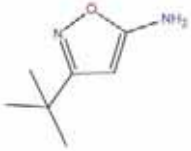
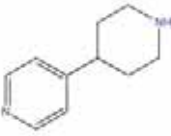
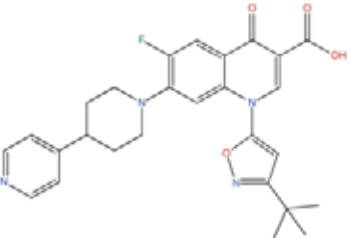
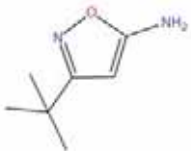
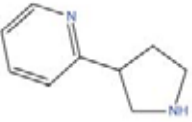
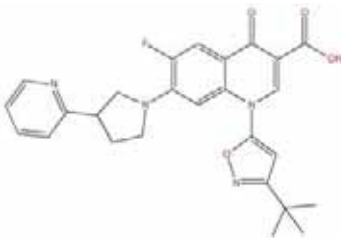
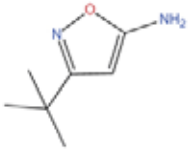
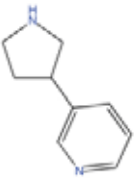
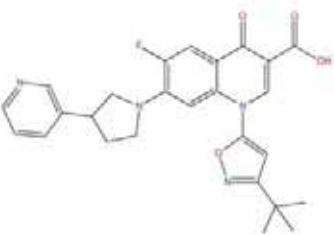
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
42	02	092	02-092	0.2118	0.6140
					
43	02	093	02-093	-0.0585	1.1442
					
44	02	094	02-094	-0.2019	1.5918
					
45	02	096	02-096	-0.2257	1.6815
					
46	02	098	02-098	0.0731	0.8451
					
47	02	100	02-100	0.3865	0.4107
					

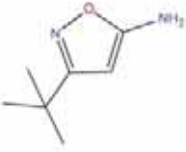
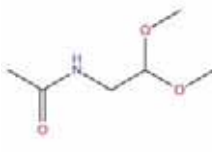
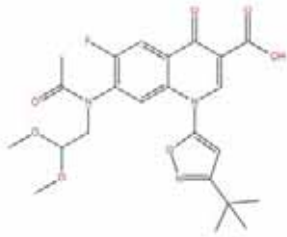
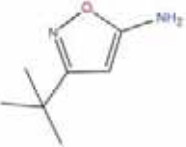
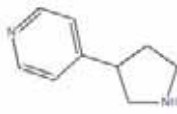
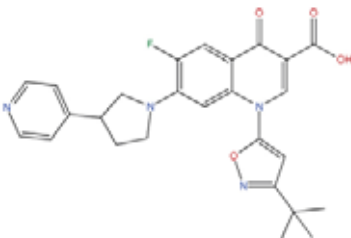
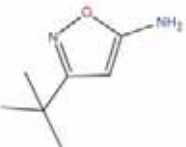
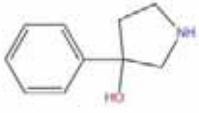
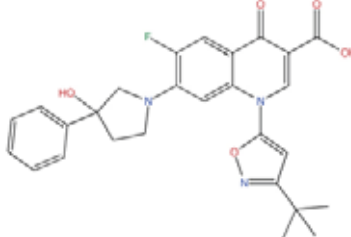
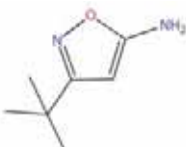
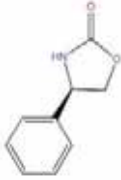
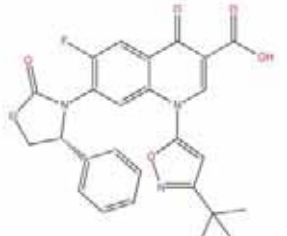
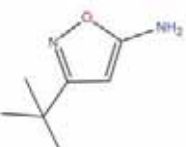
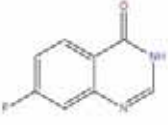
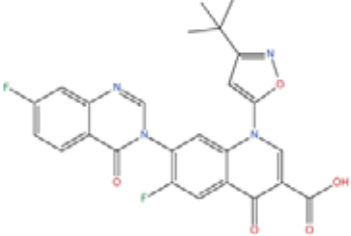
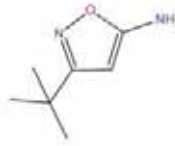
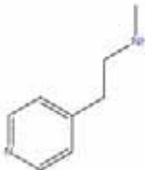
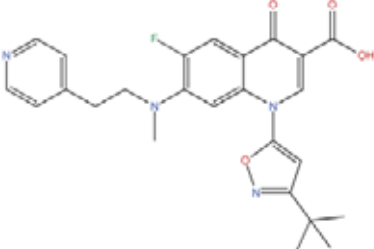


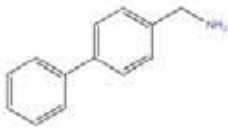
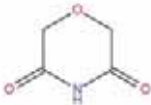
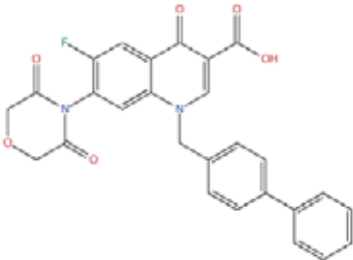
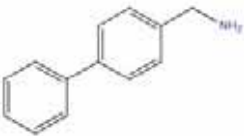
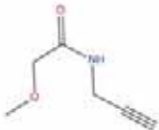
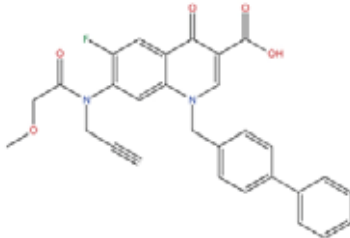
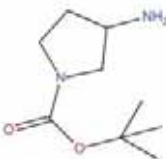
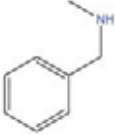
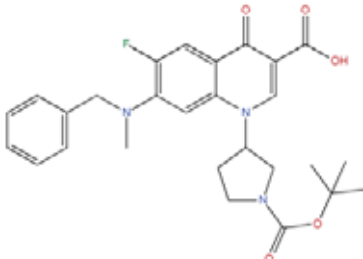
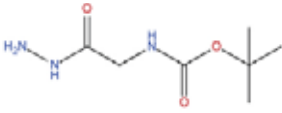
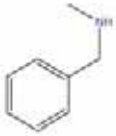
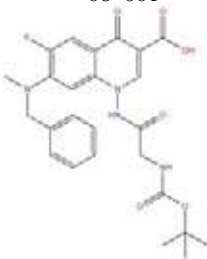
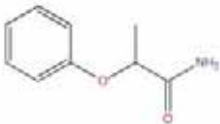
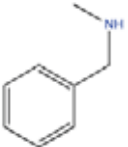
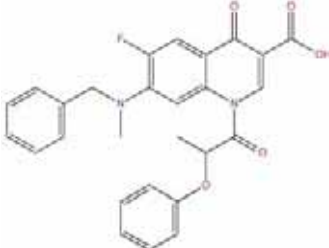
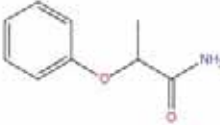
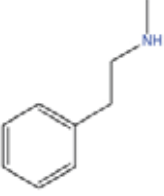
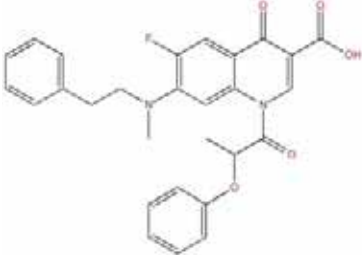
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
48	02	103	02-103	0.7631	0.1725
					
49	02	104	02-104	0.2550	0.5559
					
50	02	106	02-106	0.3072	0.4929
					
51	02	107	02-107	0.2793	0.5257
					
52	02	108	02-108	1.2725	0.0534
					
53	02	113	02-113	1.1009	0.0793
					

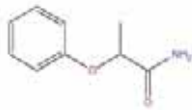
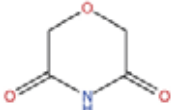
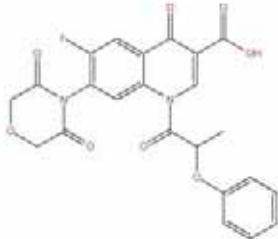
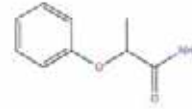
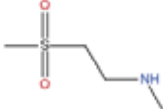
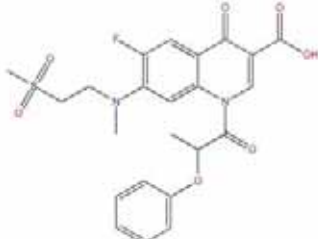
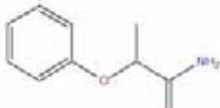
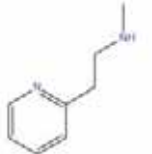
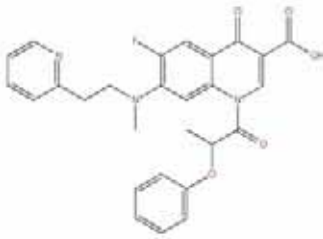
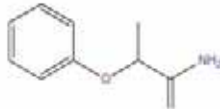
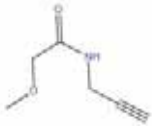
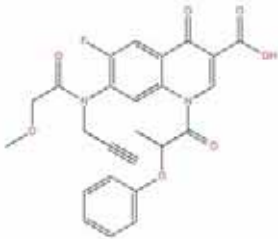
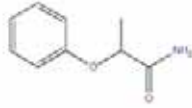
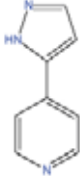
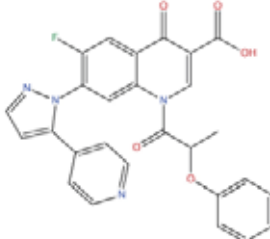
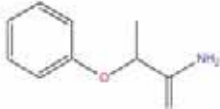
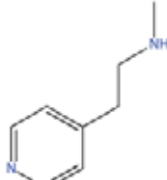
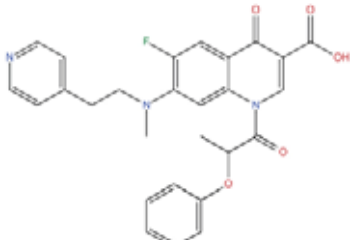
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
54	02	115	02-115	0.7007	0.1992
					
55	02	117	02-117	1.3287	0.0469
					
56	02	118	02-118	0.9732	0.1064
					
57	02	120	02-120	0.1292	0.7427
					
58	03	024	03-024	-0.0310	1.0740
					
59	03	025	03-25	-0.1754	1.4976
					

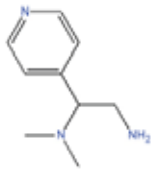
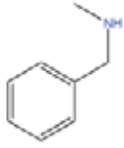
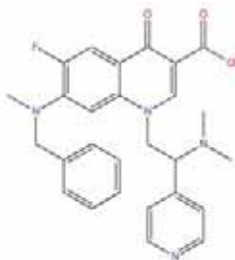
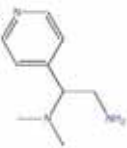
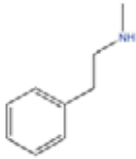
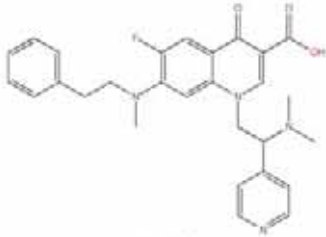
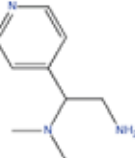
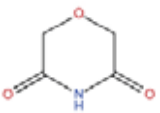
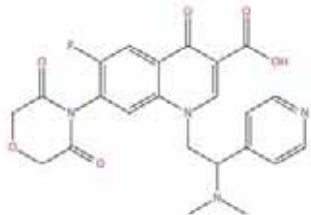
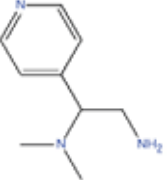
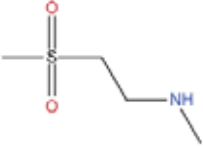
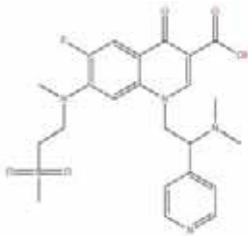
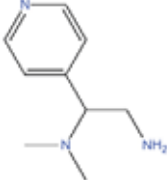
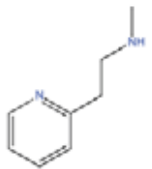
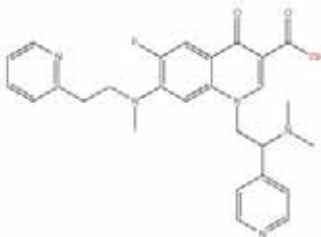
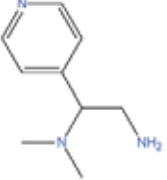
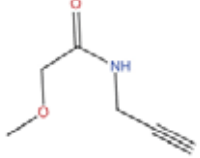
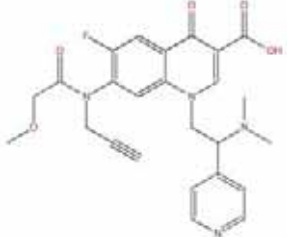
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
60	03	026	03-026	-0.2237	1.6738
					
61	03	028	03-028	-0.0259	1.0615
					
62	03	029	03-029	0.0513	0.8886
					
63	03	033	03-033	0.3897	0.4077
					
64	03	038	03-038	-0.1380	1.3740
					
65	03	059	03-059	-0.6948	4.9522
					

ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
66	03	070	03-070	-0.0819	1.2075
					
67	03	077	03-077	0.1878	0.6489
					
68	03	079	03-079	-0.1494	1.4106
					
69	03	088	03-088	-0.8606	7.2544
					
70	03	098	03-098	-0.6407	4.3722
					
71	03	100	03-100	-0.3588	2.2845
					

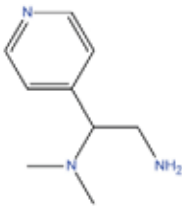
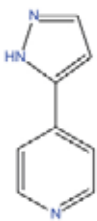
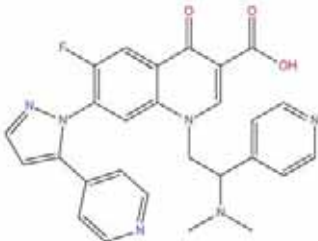
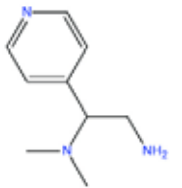
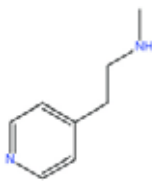
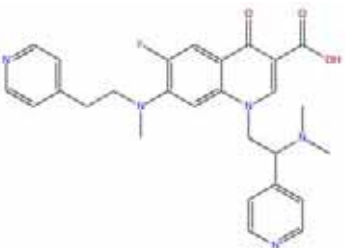
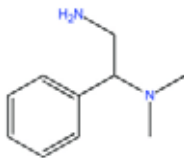
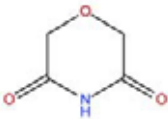
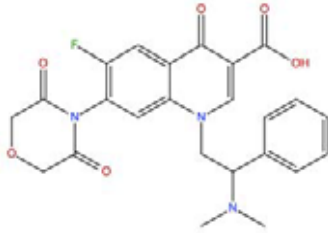
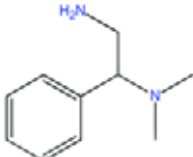
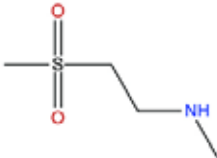
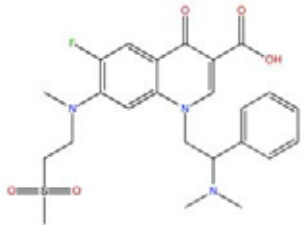
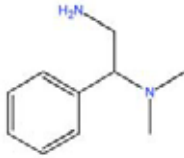
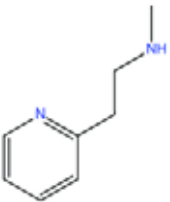
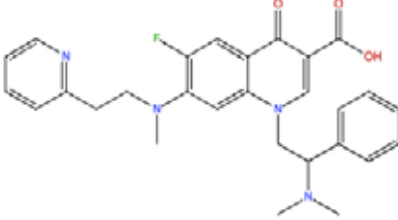
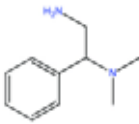
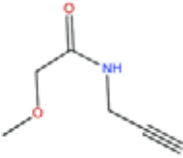
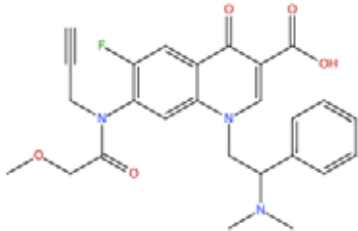
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
72	03	103	03-103	0.2433	0.5711
					
73	03	104	03-104	-0.4718	2.9635
					
74	03	107	03-107	-0.3554	2.2667
					
75	03	108	03-108	0.7265	0.1877
					
76	03	118	03-118	0.5135	0.3065
					
77	03	120	03-120	-0.5547	3.5867
					

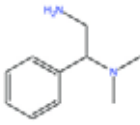
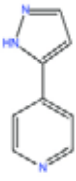
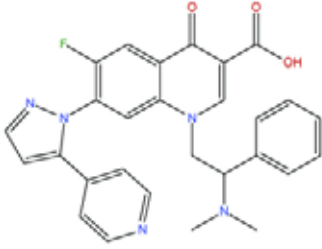
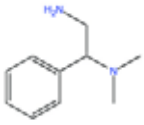
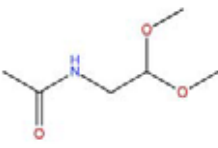
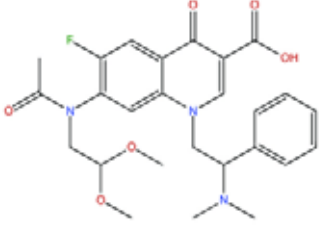
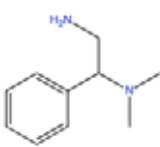
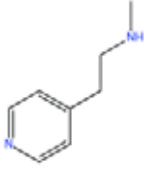
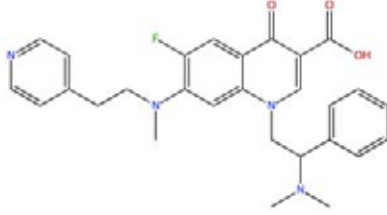
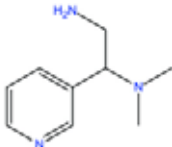
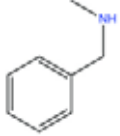
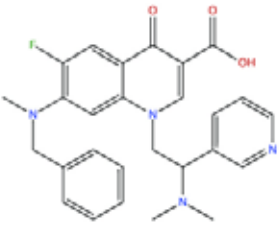
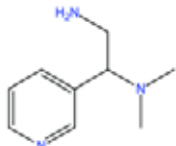
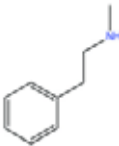
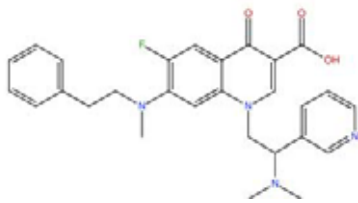
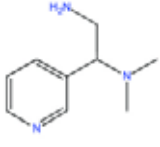
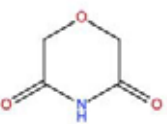
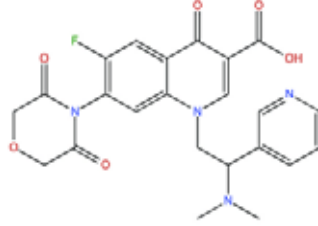
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
78	05	033	05-033	0.2997	0.5015
					
79	05	077	05-077	0.2391	0.5766
					
80	07	001	07-001	0.2380	0.5781
					
81	08	001	08-001	0.0879	0.8168
					
82	09	001	09-001	-0.3623	2.3030
					
83	09	023	09-023	-0.6662	4.6366
					

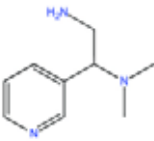
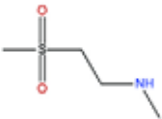
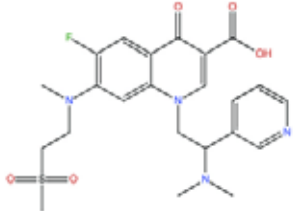
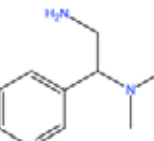
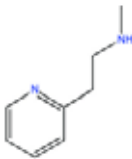
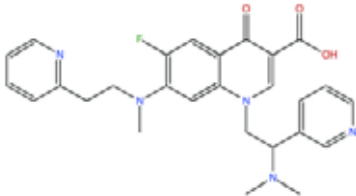
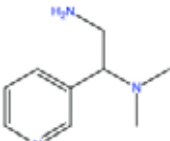
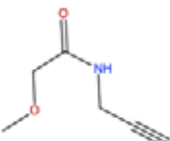
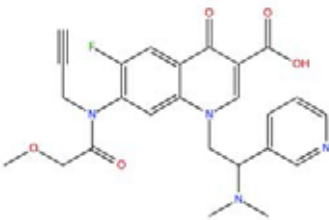
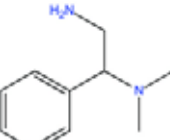
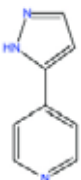
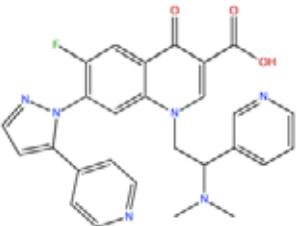
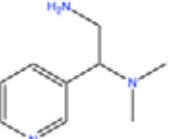
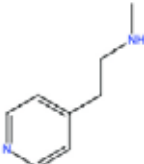
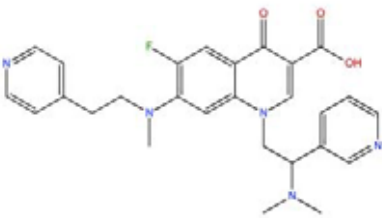
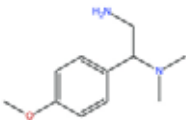
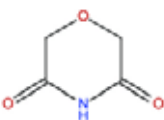
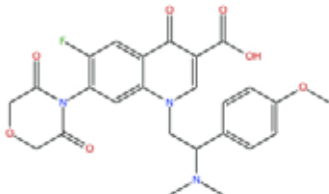
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
84	09	033	09-033	0.2394	0.5762
					
85	09	038	09-038	-0.1041	1.2709
					
86	09	059	09-059	-0.7139	5.1749
					
87	09	077	09-077	0.1876	0.6492
					
88	09	079	09-079	-0.1206	1.3201
					
89	09	120	09-120	-0.5094	3.2315
					

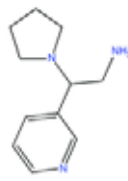
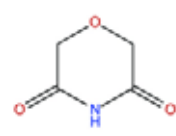
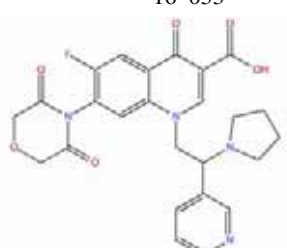
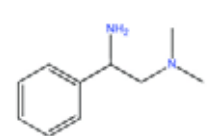
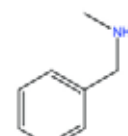
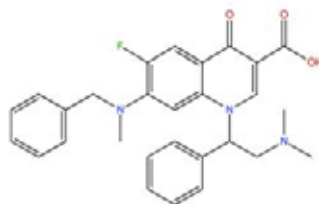
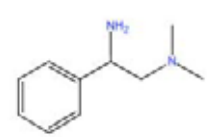
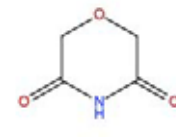
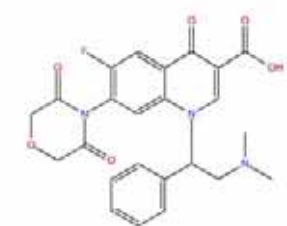
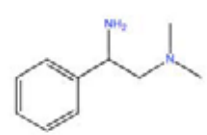
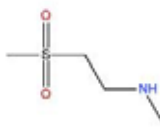
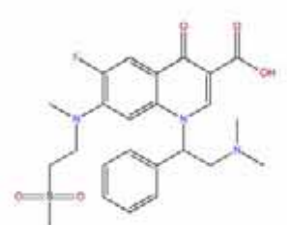
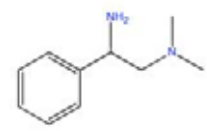
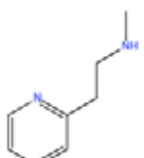
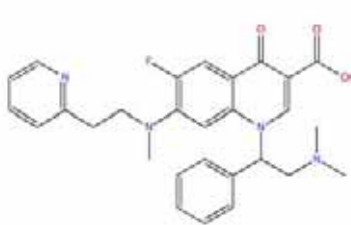
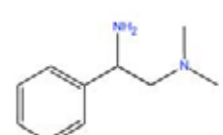
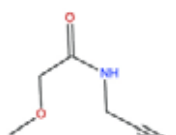
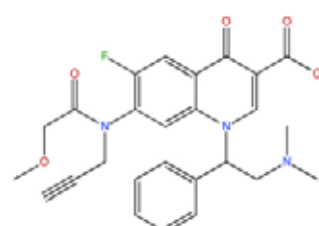
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
90	11	001	11-001	-0.2277	1.6893
					
91	11	023	11-023	-0.5874	3.8672
					
92	11	033	11-033	0.1912	0.6439
					
93	11	038	11-038	-0.0185	1.0435
					
94	11	059	11-059	-0.6834	4.8239
					
95	11	077	11-077	0.3556	0.4410
					

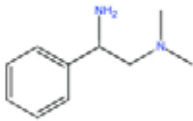
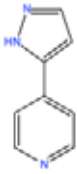
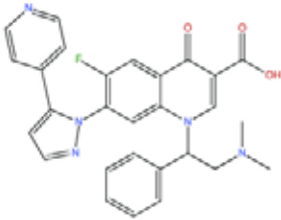
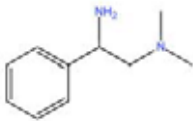
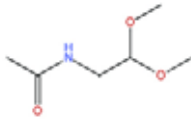
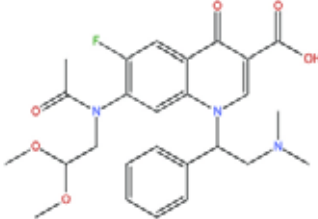
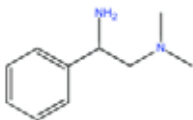
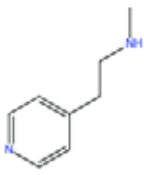
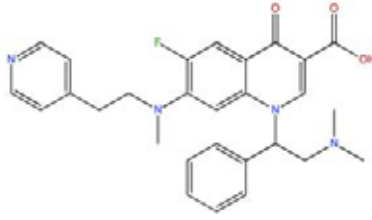
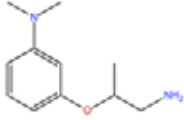
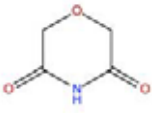
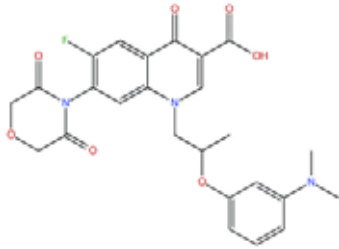
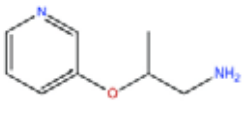
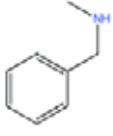
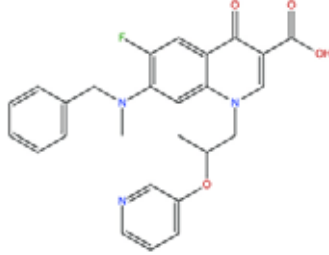
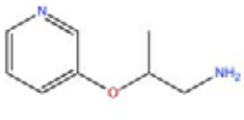
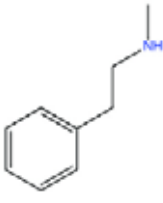
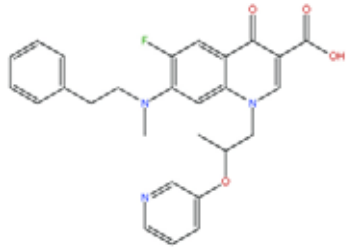


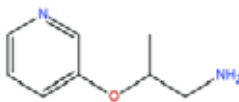
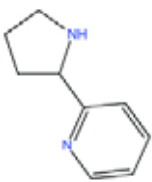
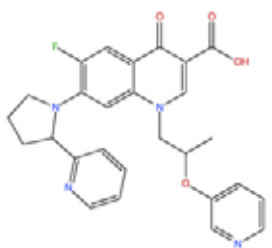
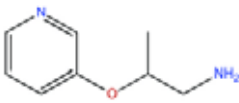
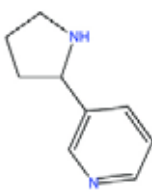
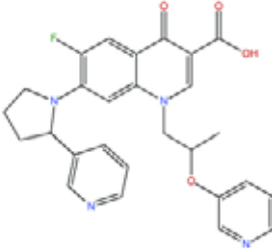
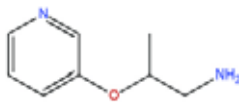
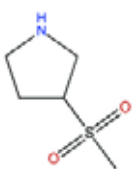
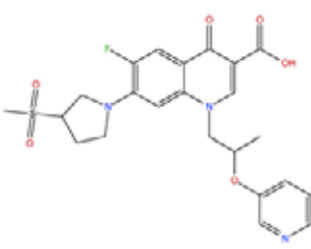
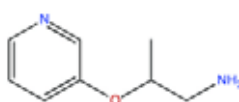
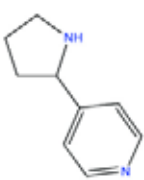
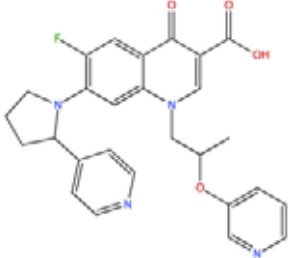
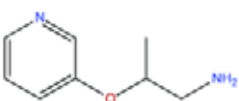
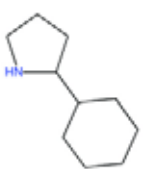
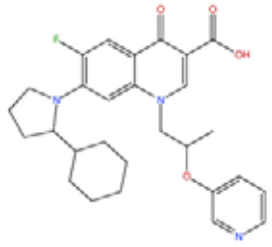
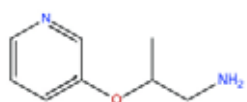
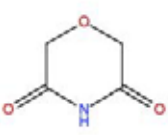
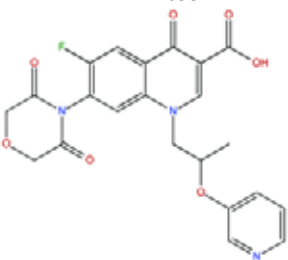
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
96	11	079	11-079	0.1670	0.6808
					
97	11	120	11-120	-0.4611	2.8913
					
98	12	033	12-033	0.1240	0.7516
					
99	12	038	12-038	-0.0881	1.2249
					
100	12	059	12-059	-0.8150	6.5313
					
101	12	077	12-077	0.2746	0.5314
					

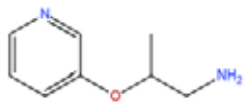
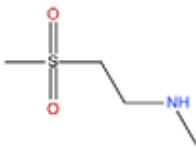
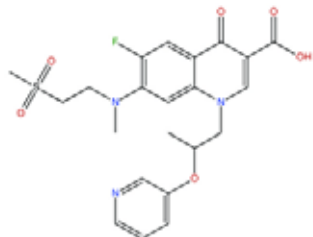
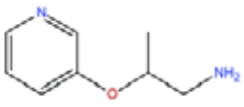
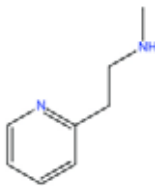
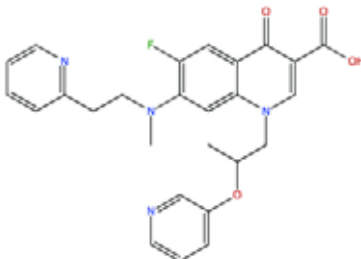
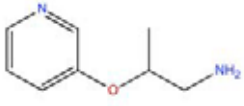
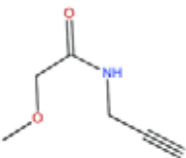
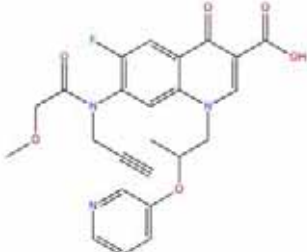
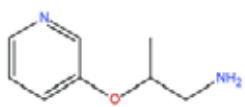
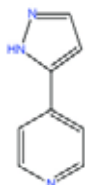
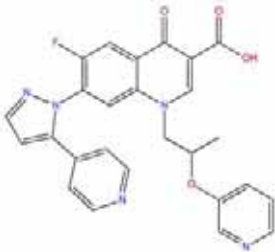
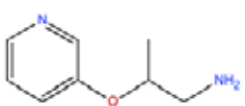
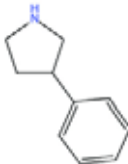
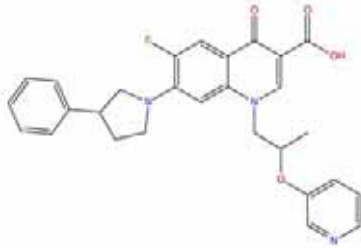
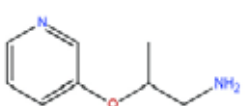
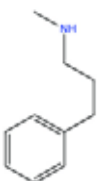
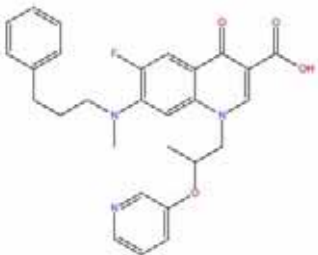
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
102	12	079	12-079	0.0631	0.8648
					
103	12	103	12-103	0.3349	0.4625
					
104	12	120	12-120	-0.5772	3.7775
					
105	13	001	13-001	-0.1876	1.5403
					
106	13	023	13-023	-0.5517	3.5620
					
107	13	033	13-033	0.2378	0.5784
					

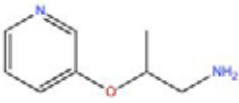
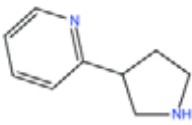
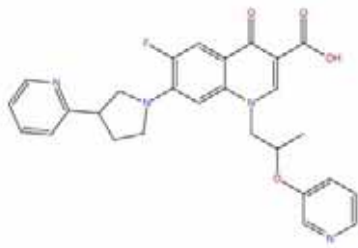
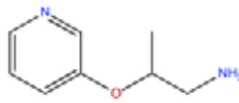
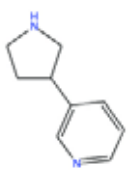
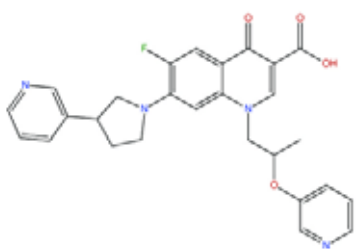
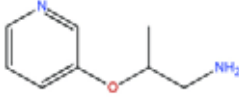
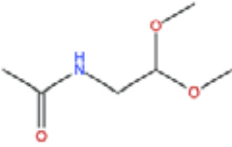
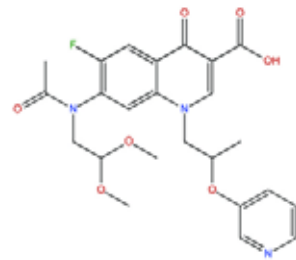
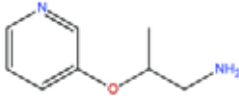
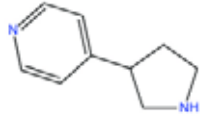
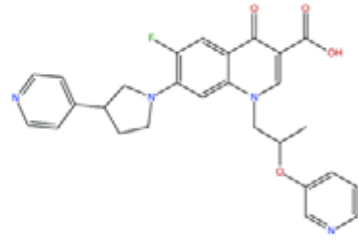
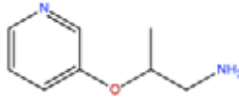
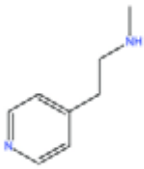
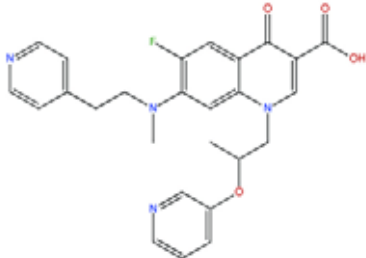
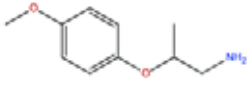
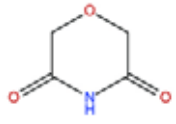
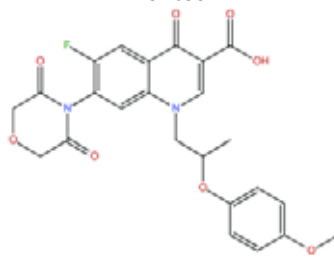
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
108	13	038	13-038	0.0069	0.9843
					
109	13	059	13-059	-0.6466	4.4320
					
110	13	077	13-077	0.3981	0.3999
					
111	13	079	13-079	0.2087	0.6184
					
112	13	120	13-120	-0.4210	2.6363
					
113	14	033	14-033	0.1460	0.7145
					

ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
114	16	033	16-033	0.4185	0.3815
					
115	20	001	20-001	0.0755	0.8404
					
116	20	033	20-033	0.5443	0.2856
					
117	20	038	20-038	0.2745	0.5315
					
118	20	059	20-059	-0.3604	2.2930
					
119	20	077	20-077	0.7081	0.1958
					

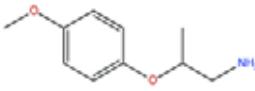
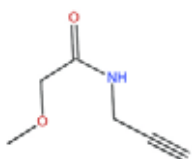
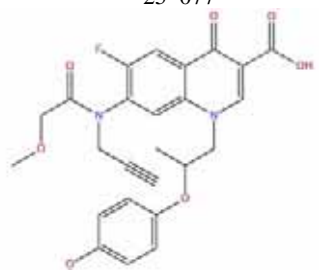
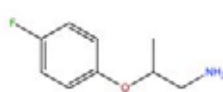
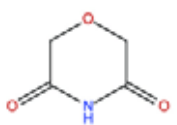
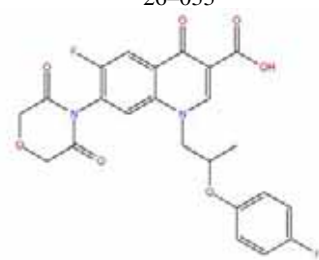
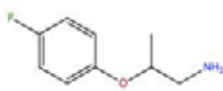
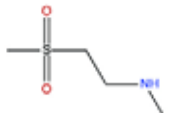
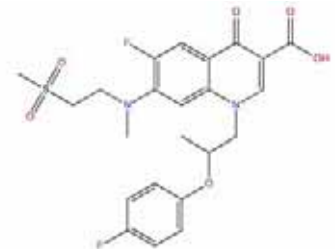
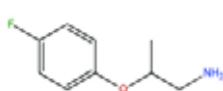
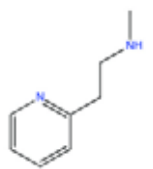
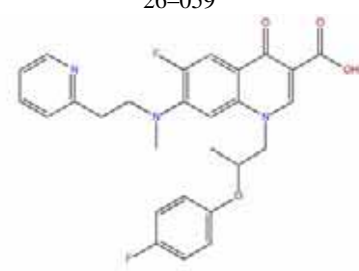
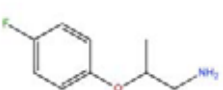
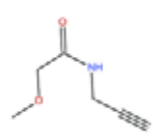
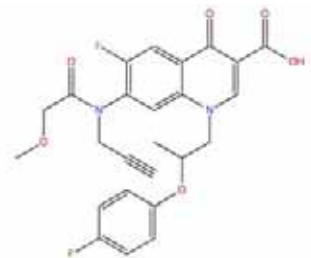
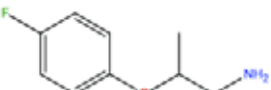
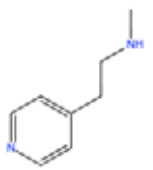
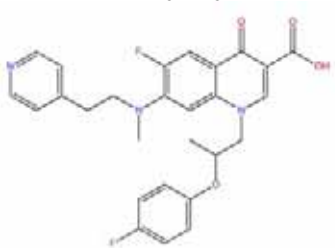
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
120	20	079	20-079	0.5708	0.2687
					
121	20	103	20-103	0.7277	0.1872
					
122	20	120	20-120	-0.1411	1.3839
					
123	23	033	23-033	-0.2464	1.7636
					
124	24	001	24-001	-0.3900	2.4547
					
125	24	023	24-023	-0.7761	5.9717
					

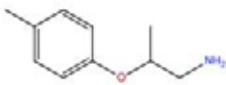
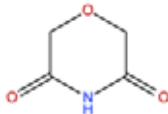
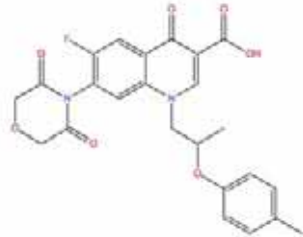
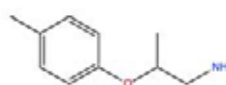
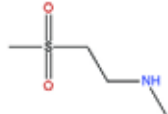
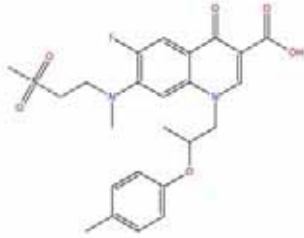
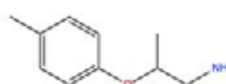
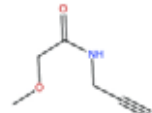
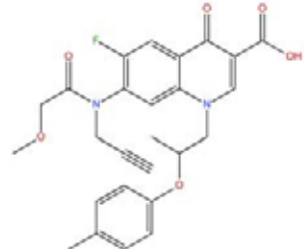
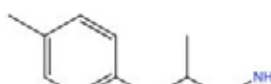
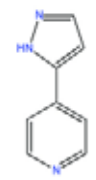
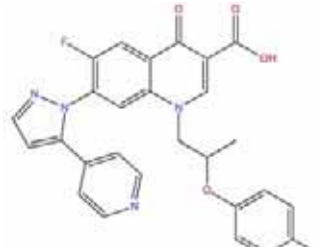
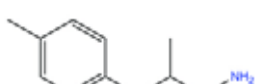
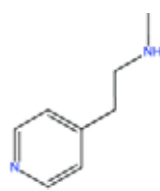
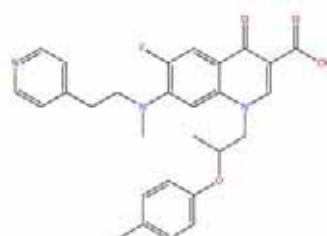
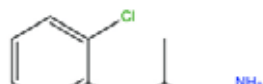
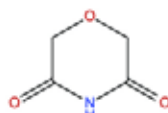
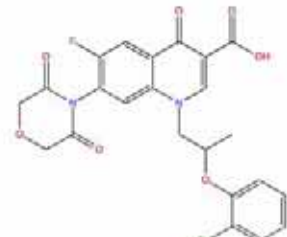
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
126	24	025	24-025	-0.1163	1.3071
					
127	24	026	24-026	-0.1903	1.5499
					
128	24	028	24-028	-0.1668	1.4682
					
129	24	029	24-029	0.0983	0.7974
					
130	24	032	24-032	-0.1050	1.2735
					
131	24	033	24-033	0.0100	0.9772
					

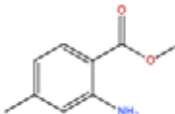
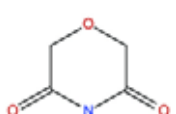
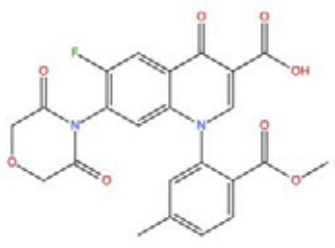
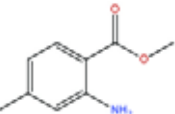
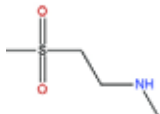
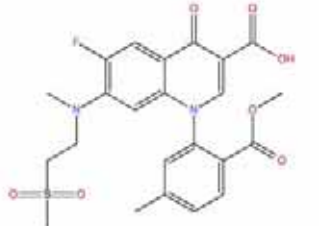
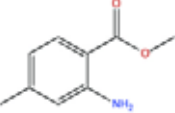
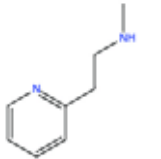
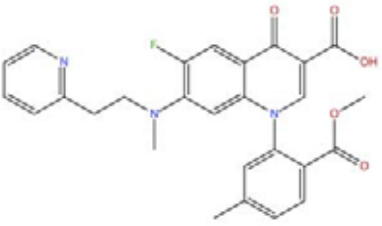
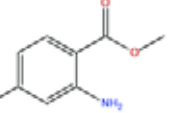
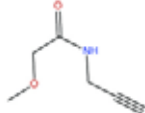
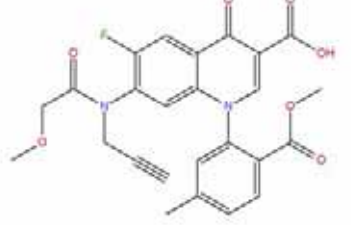
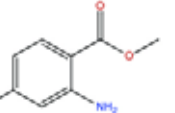
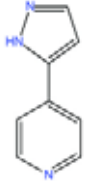
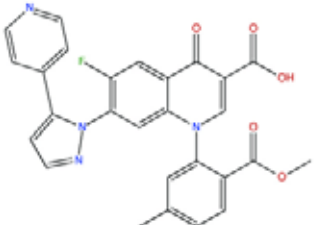
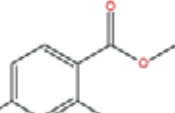
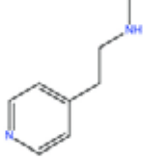
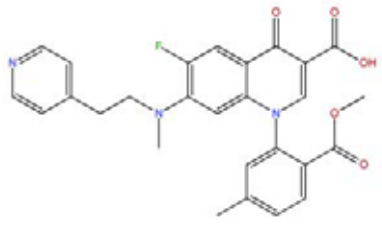
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
132	24	038	24-038	-0.2304	1.6998
					
133	24	059	24-059	-0.8483	7.0518
					
134	24	077	24-077	0.1662	0.6820
					
135	24	079	24-079	0.0943	0.8048
					
136	24	092	24-092	-0.5835	3.8327
					
137	24	096	24-096	-0.9997	9.9931
					

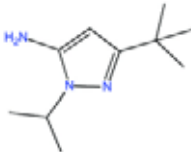
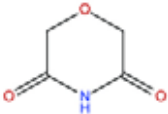
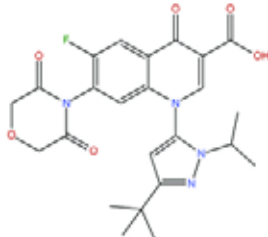
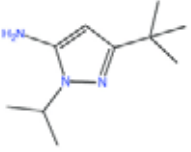
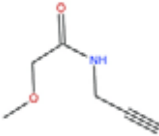
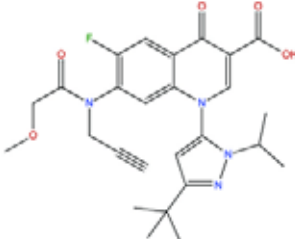
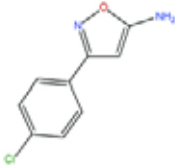
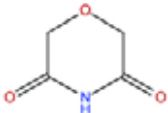
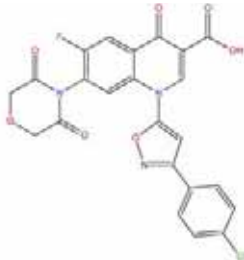
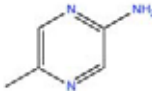
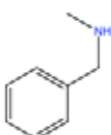
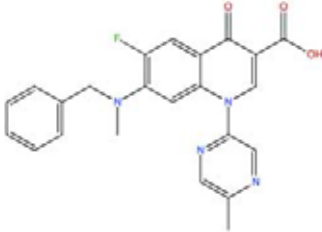
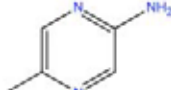
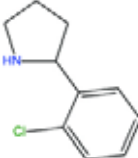
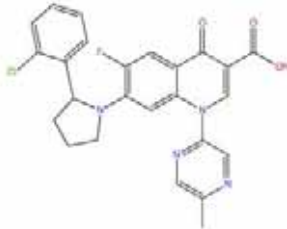
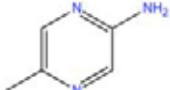
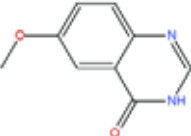
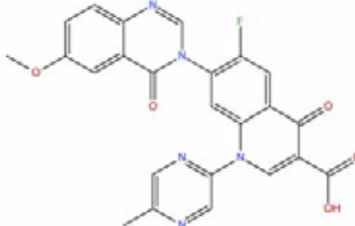
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
138	24	098	24-098	-0.6545	4.5134
					
139	24	100	24-100	-0.3713	2.3513
					
140	24	103	24-103	0.2513	0.5607
					
141	24	104	24-104	-0.4816	3.0311
					
142	24	120	24-120	-0.6127	4.0992
					
143	25	033	25-033	-0.0398	1.0960
					

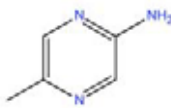
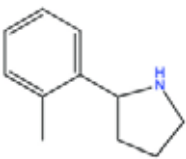
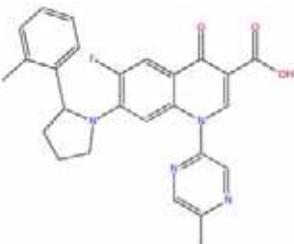
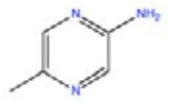
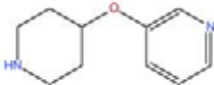
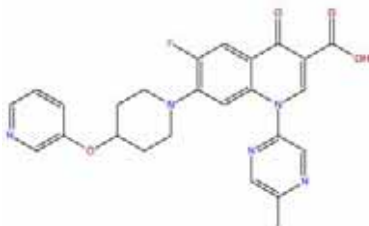
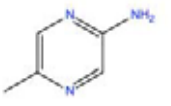
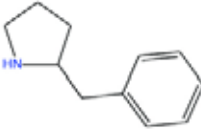
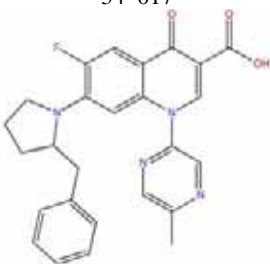
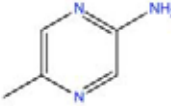
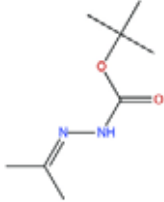
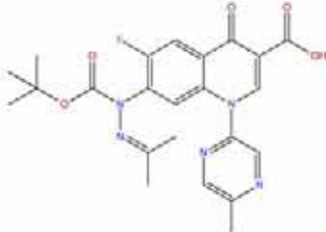
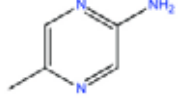
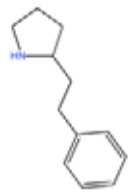
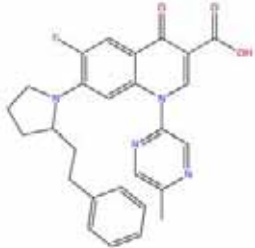
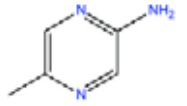
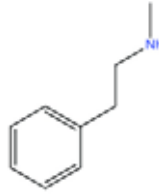
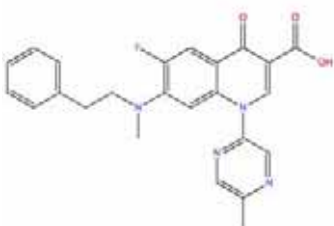


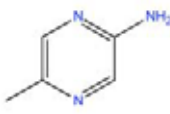
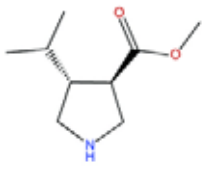
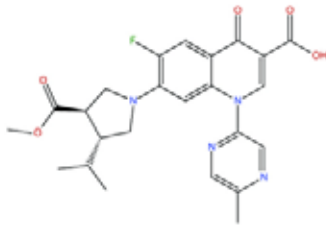
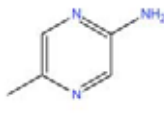
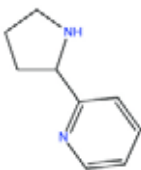
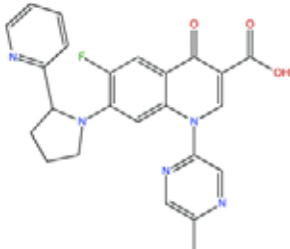
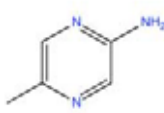
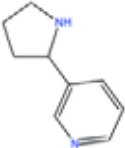
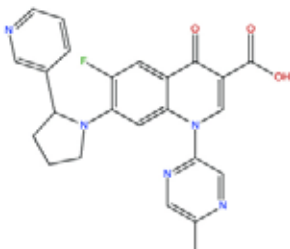
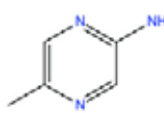
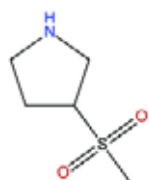
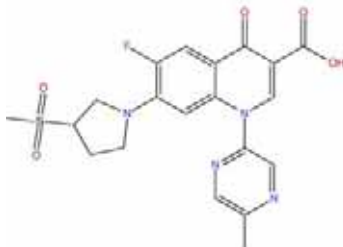
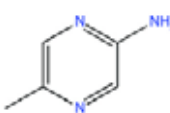
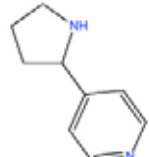
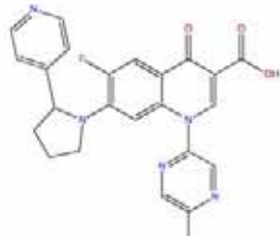
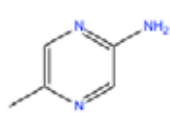
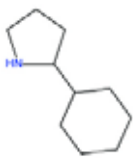
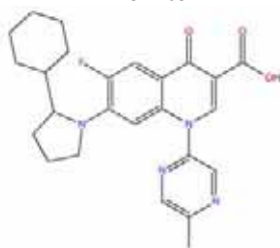
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
144	25	077	25-077	0.0888	0.8151
					
145	26	033	26-033	0.1768	0.6656
					
146	26	038	26-038	-0.0970	1.2503
					
147	26	059	26-059	-0.5433	3.4938
					
148	26	077	26-077	0.2556	0.5551
					
149	26	120	26-120	-0.3401	2.1883
					

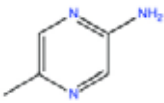
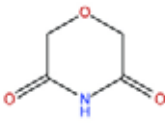
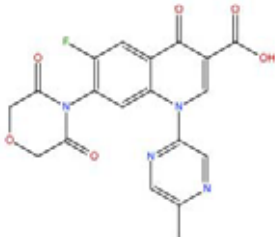
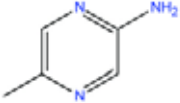
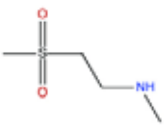
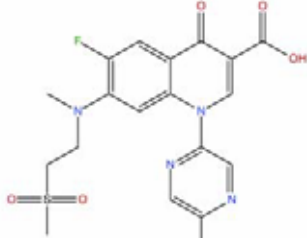
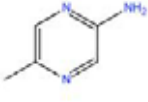
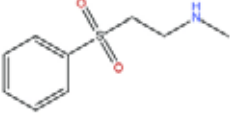
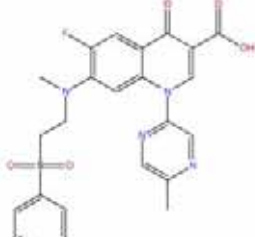
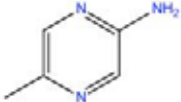
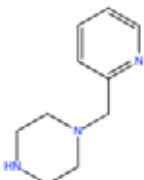
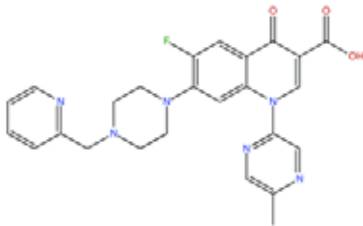
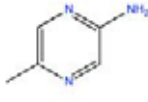
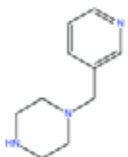
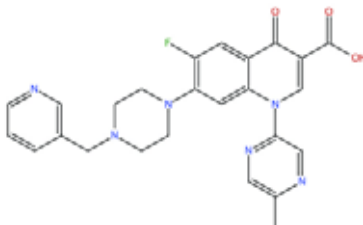
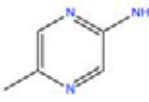
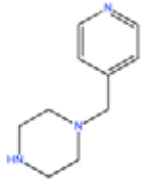
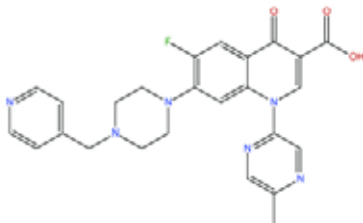
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
150	27	033	27-033	-0.1890	1.5453
					
151	27	038	27-038	-0.4043	2.5369
					
152	27	077	27-077	-0.0311	1.0742
					
153	27	079	27-079	-0.1179	1.3119
					
154	27	120	27-120	-0.8057	6.3929
					
155	28	033	28-033	-0.1193	1.3161
					

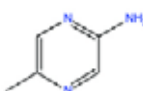
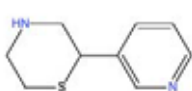
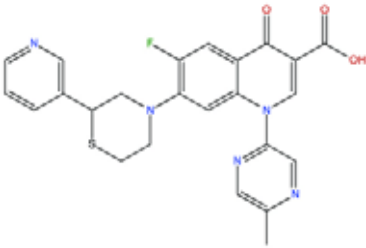
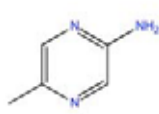
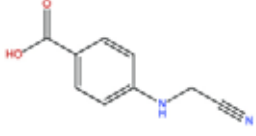

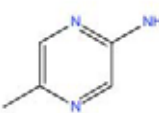
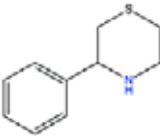
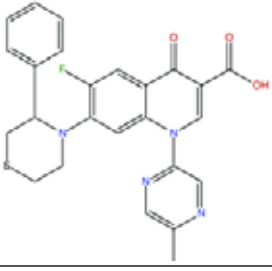
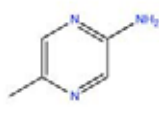
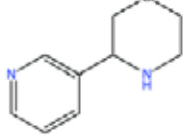
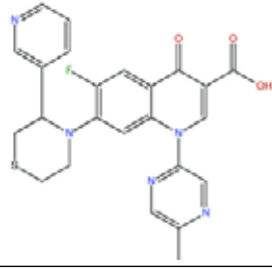
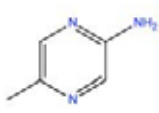
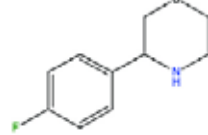
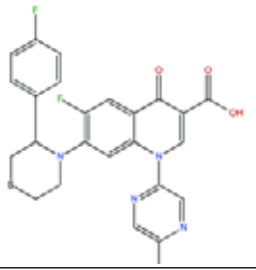
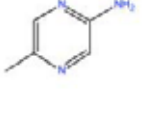
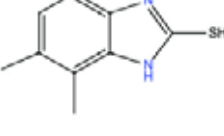
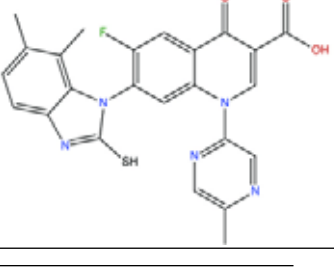
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
156	31	033	31-033	1.7989	0.0159
					
157	31	038	31-038	1.2524	0.0559
					
158	31	059	31-059	1.0813	0.0829
					
159	31	077	31-077	1.7783	0.0167
					
160	31	079	31-079	1.7964	0.0160
					
161	31	120	31-120	1.2556	0.0555
					

ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
162	32	033	32-033	0.6869	0.2056
					
163	32	077	32-077	0.6649	0.2163
					
164	33	033	33-033	0.2440	0.5702
					
165	34	001	34-001	-0.2594	1.8172
					
166	34	002	34-002	0.2809	0.5237
					
167	34	009	34-009	0.6802	0.2088
					

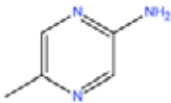
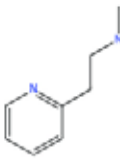
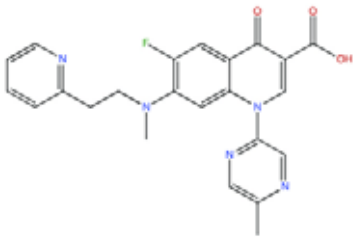
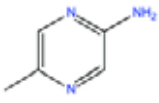
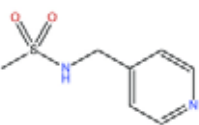
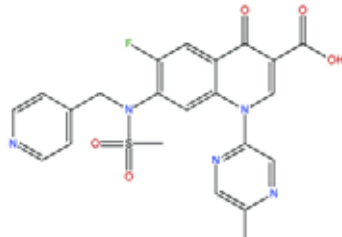
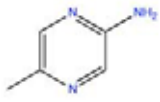
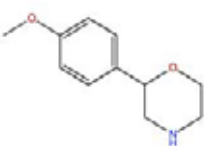
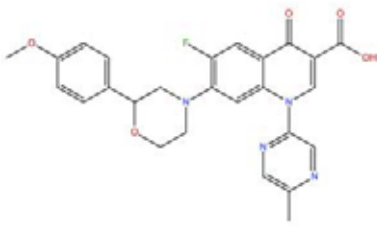
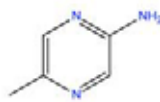
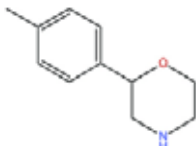
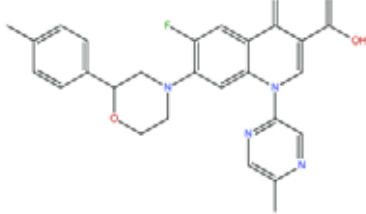
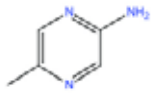
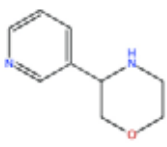
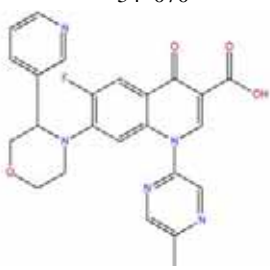
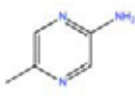
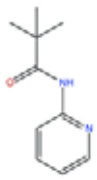
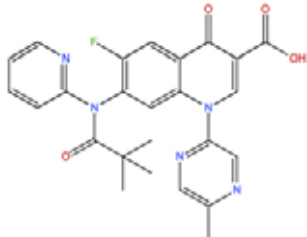
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
168	34	010	34-010	0.2018	0.6283
					
169	34	014	34-014	-0.9724	9.3843
					
170	34	017	34-017	-0.4321	2.7046
					
171	34	018	34-018	0.9241	0.1191
					
172	34	020	34-020	-0.7268	5.3309
					
173	34	023	34-023	-0.7191	5.2372
					

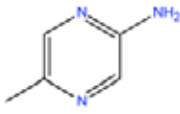
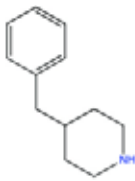
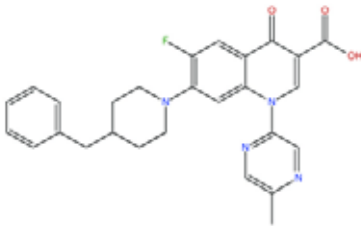
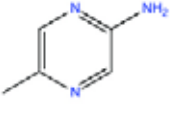
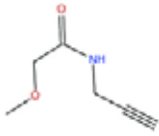
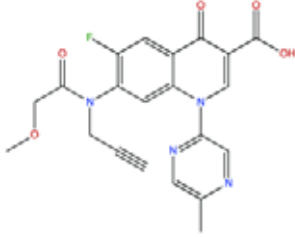
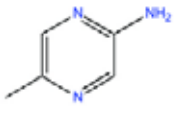
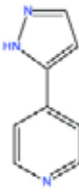
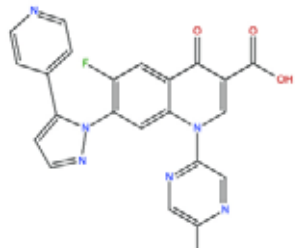
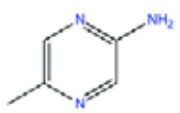
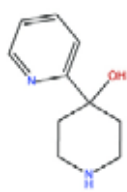
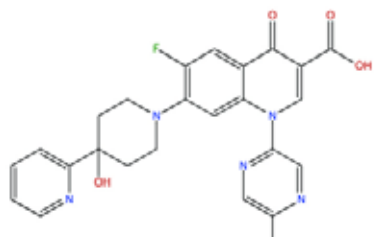
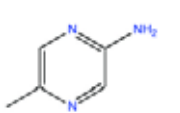
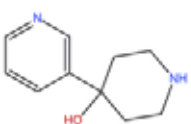
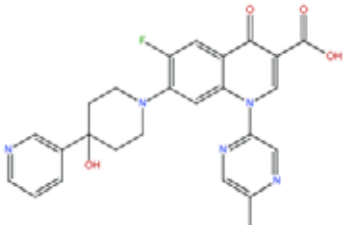
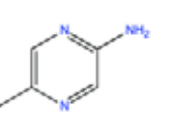
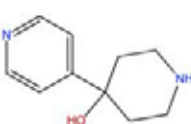
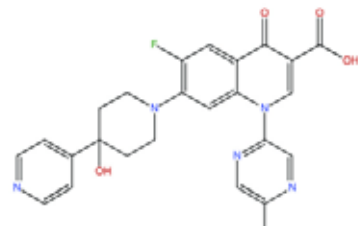
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
174	34	024	34-024	0.0950	0.8035
					
175	34	025	34-025	0.0190	0.9572
					
176	34	026	34-026	-0.0489	1.1192
					
177	34	028	34-028	0.0361	0.9202
					
178	34	029	34-029	0.2728	0.5336
					
179	34	032	34-032	0.0296	0.9341
					

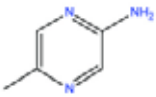
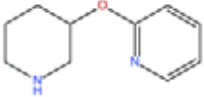
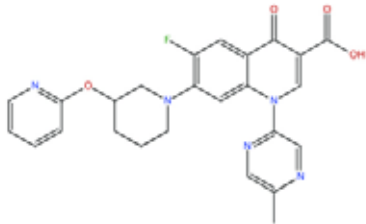
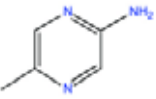
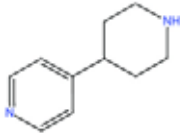
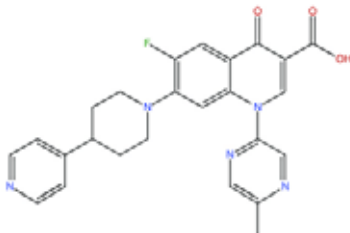
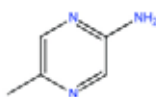
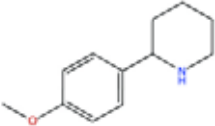
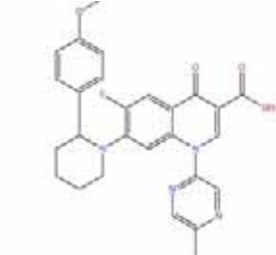
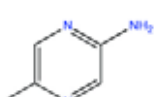
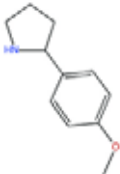
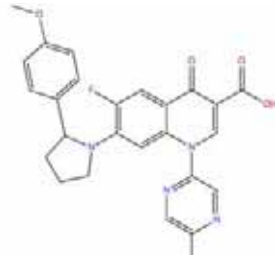
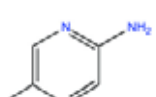
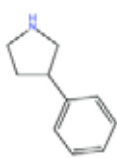
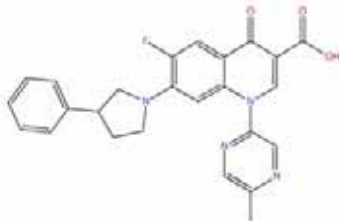
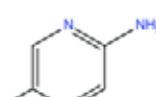
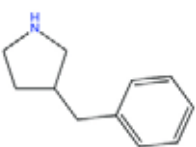
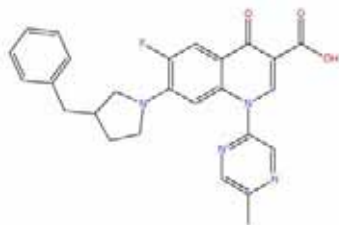
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
180	34	033	34-033	0.3502	0.4465
					
181	34	038	34-038	-0.0649	1.1612
					
182	34	040	34-040	-0.3031	2.0096
					
183	34	043	34-043	-0.7991	6.2965
					
184	34	044	34-044	-0.9787	9.5214
					
185	34	045	34-045	-0.6819	4.8073
					

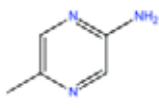
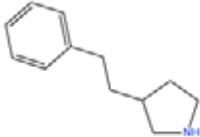
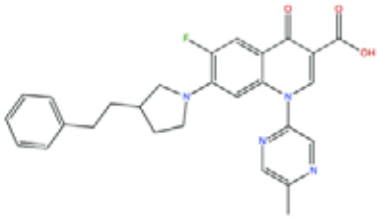
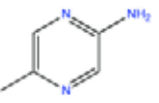
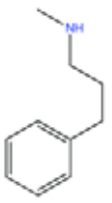
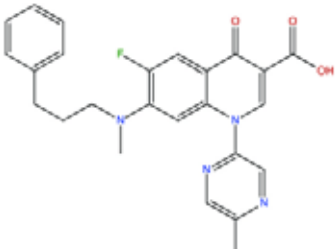
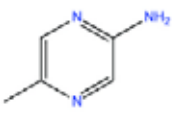
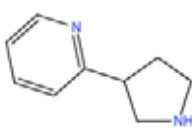
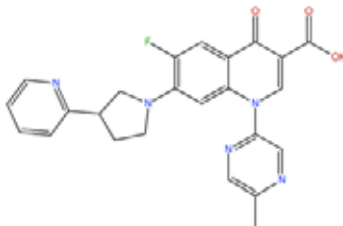
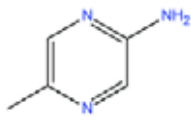
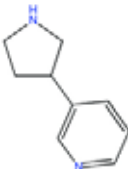
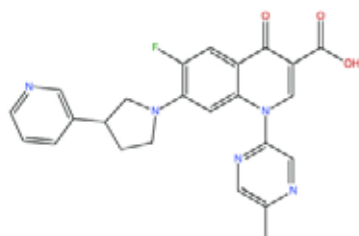
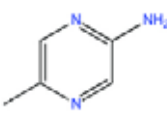
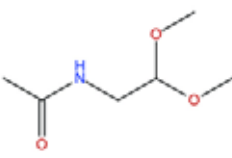
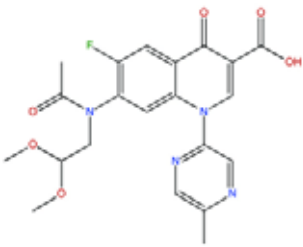
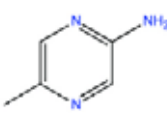
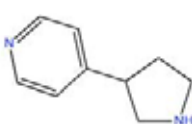
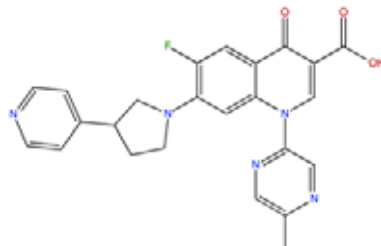
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
186	34	048	34-048	0.1434	0.7188
					
187	34	049	34-049	-0.0510	1.1246
					
188	34	050	34-050	0.2171	0.6066
					
189	34	051	34-051	0.1307	0.7401
					
190	34	053	34-053	0.5700	0.2692
					
191	34	057	34-057	0.6148	0.2428
					

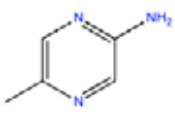
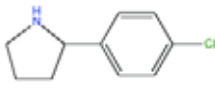
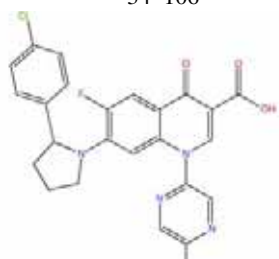
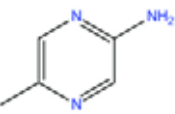
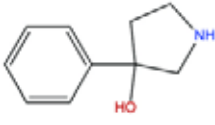
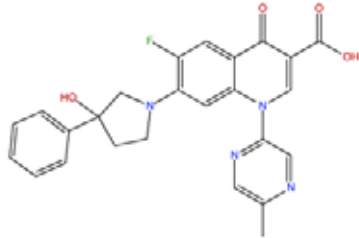
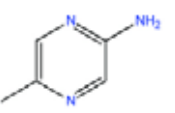
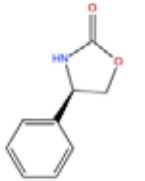
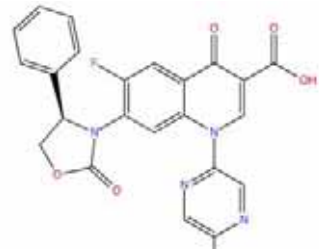
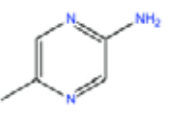
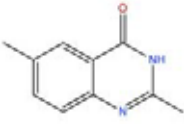
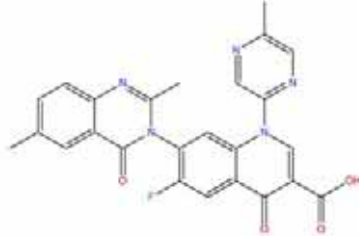
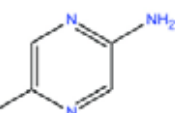
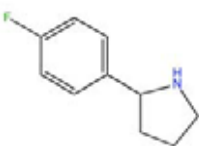
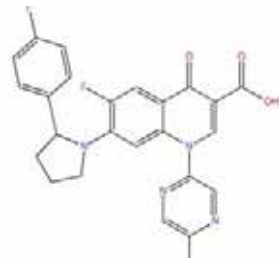
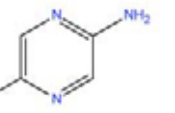
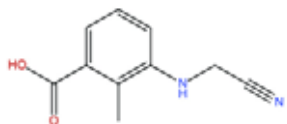
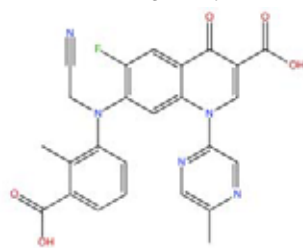


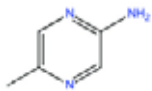
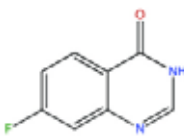
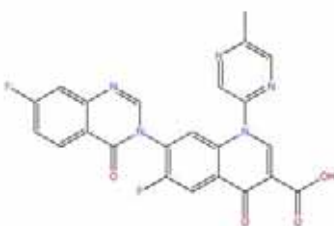
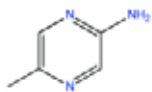
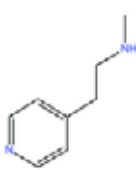
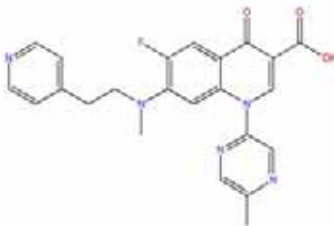
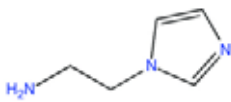
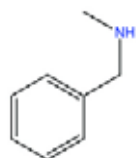
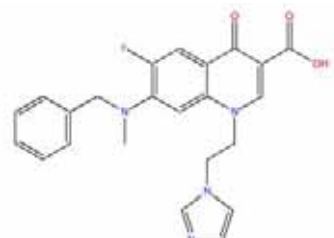
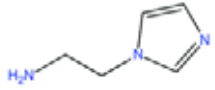
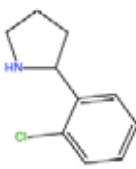
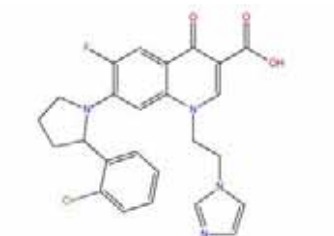
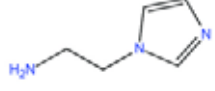
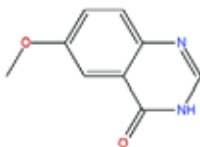
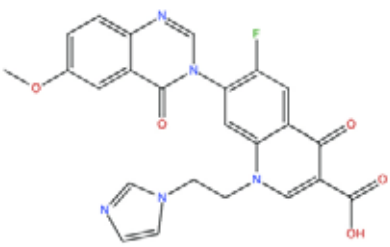
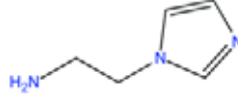
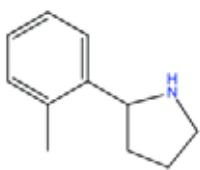
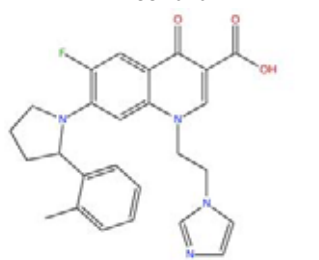
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
192	34	059	34-059	-0.7832	6.0702
					
193	34	060	34-060	0.7961	0.1599
					
194	34	063	34-063	-0.3931	2.4723
					
195	34	064	34-064	-0.3167	2.0735
					
196	34	070	34-070	0.1210	0.7568
					
197	34	071	34-071	1.1392	0.0726
					

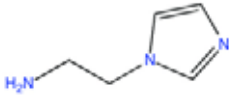
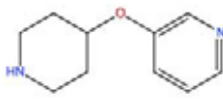
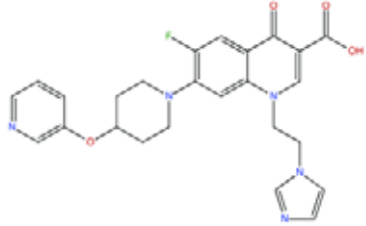
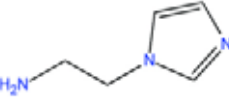
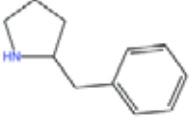
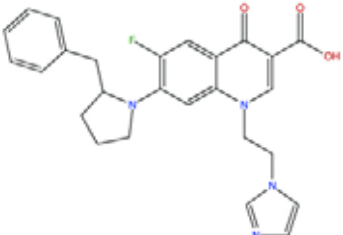
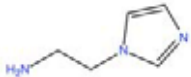
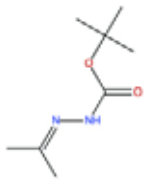
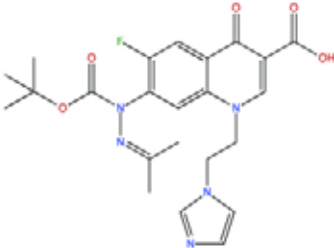
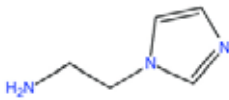
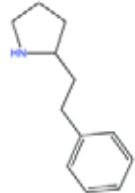
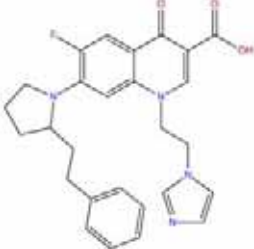
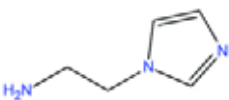
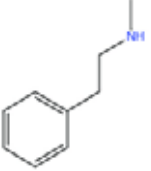
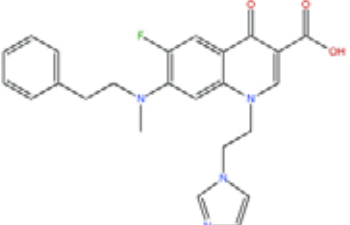
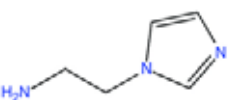
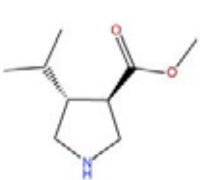
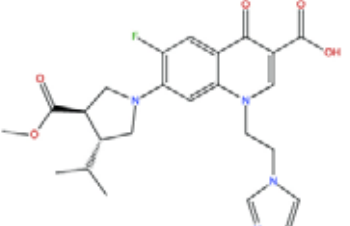
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
198	34	072	34-072	-0.9031	8.0002
					
199	34	077	34-077	0.4017	0.3966
					
200	34	079	34-079	0.1368	0.7298
					
201	34	084	34-084	-0.3148	2.0644
					
202	34	085	34-085	-0.4459	2.7919
					
203	34	086	34-086	-0.6085	4.0598
					

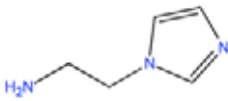
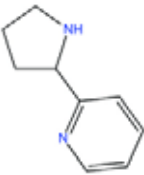
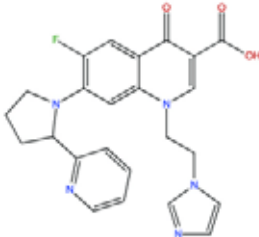
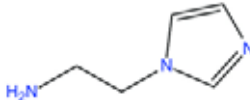
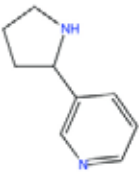
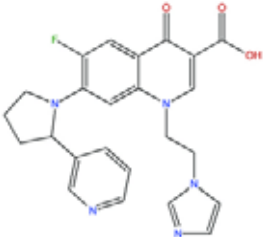
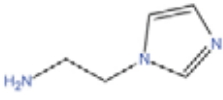
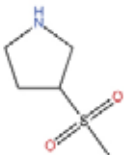
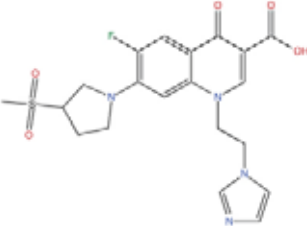
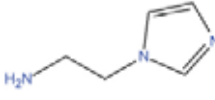
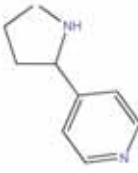
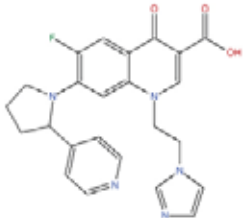
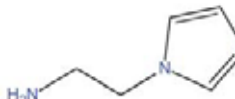
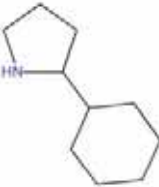
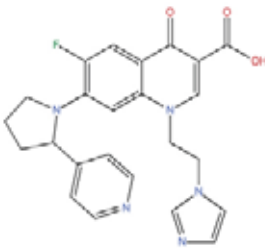
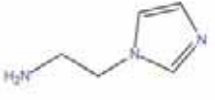
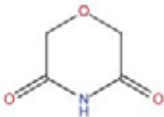
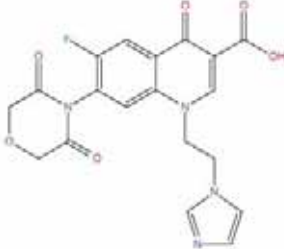
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
204	34	087	34-087	-0.3266	2.1213
					
205	34	088	34-088	-0.8507	7.0909
					
206	34	089	34-089	0.3092	0.4907
					
207	34	091	34-091	0.1703	0.6756
					
208	34	092	34-092	-0.5344	3.4229
					
209	34	093	34-093	-0.8224	6.6435
					

ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
210	34	094	34-094	-1.0344	10.8243
					
211	34	096	34-096	-0.9735	9.4081
					
212	34	098	34-098	-0.6005	3.9857
					
213	34	100	34-100	-0.2804	1.9072
					
214	34	103	34-103	0.4812	0.3302
					
215	34	104	34-104	-0.4167	2.6104
					

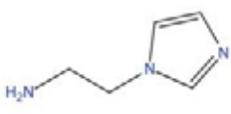
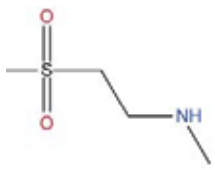
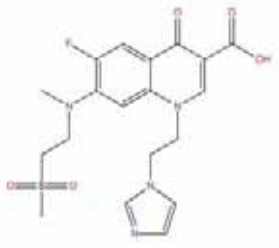
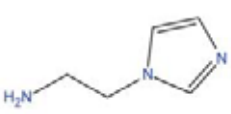
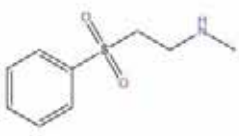
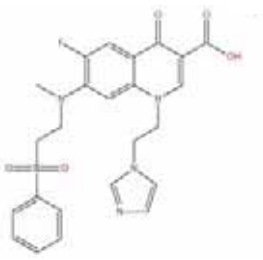
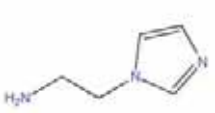
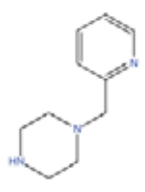
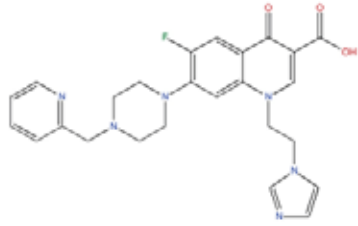
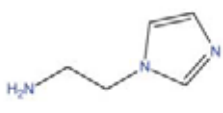
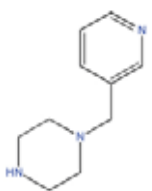
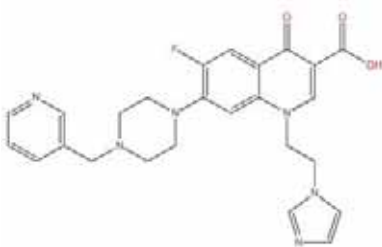
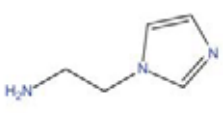
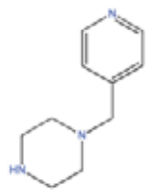
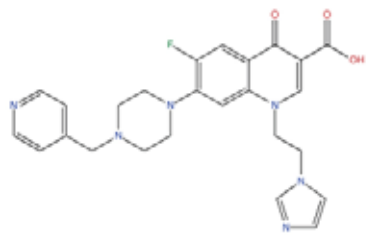
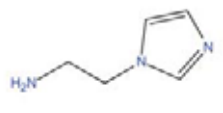
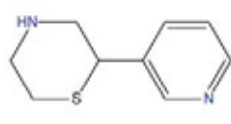
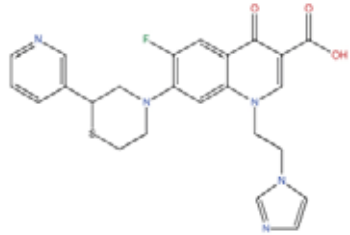
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
216	34	106	34-106	-0.3221	2.0994
					
217	34	107	34-107	-0.2852	1.9284
					
218	34	108	34-108	0.9133	0.1221
					
219	34	113	34-113	0.6467	0.2256
					
220	34	115	34-115	0.2652	0.5430
					
221	34	117	34-117	0.7515	0.1772
					

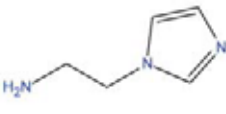
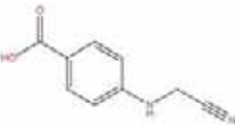

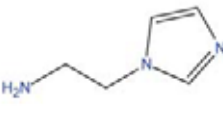
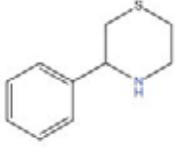
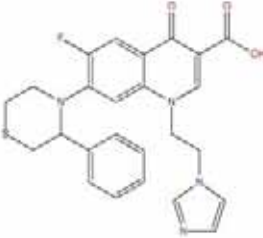
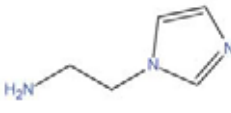
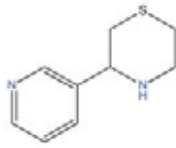
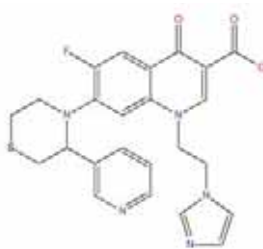
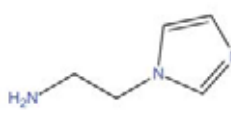
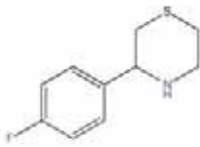
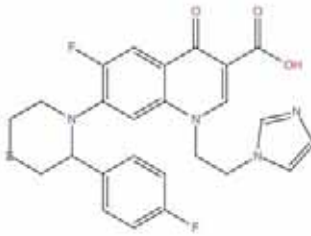
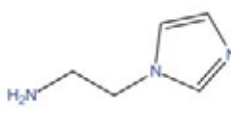
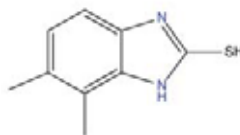
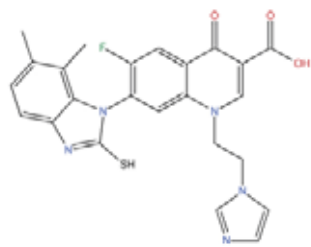
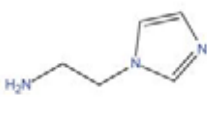
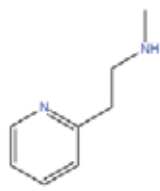
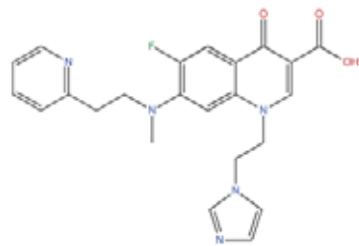
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
222	34	118	34-118	0.5529	0.2800
					
223	34	120	34-120	-0.5295	3.3845
					
224	35	001	35-001	-0.3122	2.0521
					
225	35	002	35-002	0.3777	0.4191
					
226	35	009	35-009	0.5457	0.2846
					
227	35	010	35-010	0.1934	0.6406
					

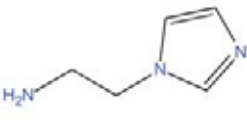
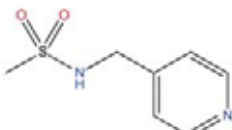
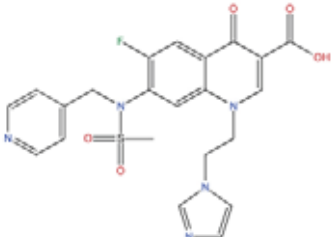
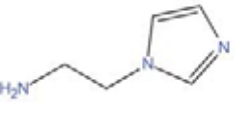
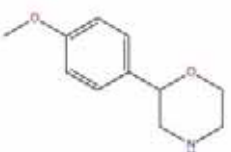
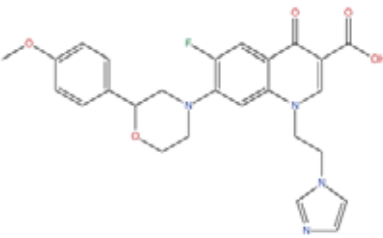
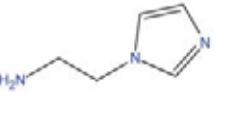
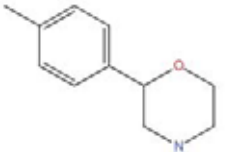
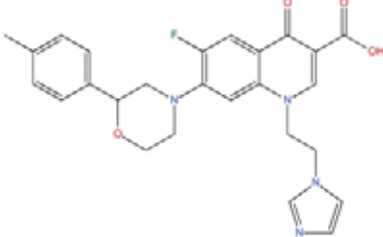
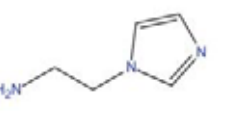
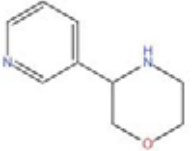
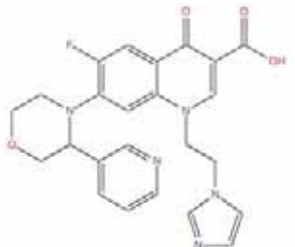
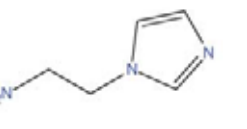
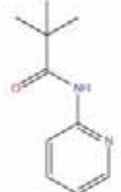
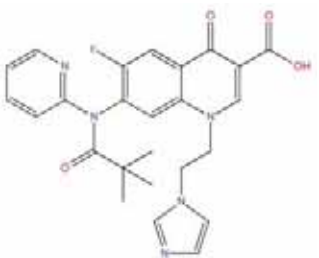
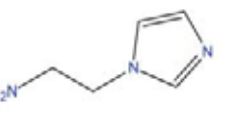
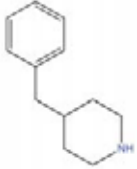
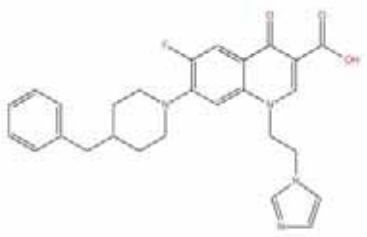
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
228	35	014	35-014	-1.0252	10.5974
					
229	35	017	35-017	-0.3505	2.2413
					
230	35	018	35-018	0.8856	0.1301
					
231	35	020	35-020	-0.6771	4.7544
					
232	35	023	35-023	-0.6804	4.7907
					
233	35	024	35-024	0.0618	0.8674
					

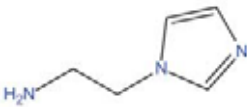
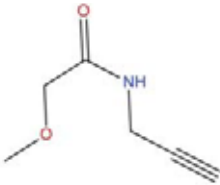
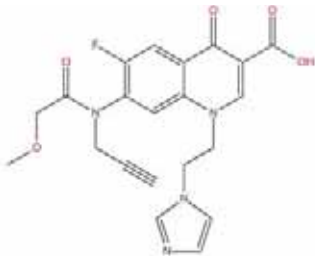
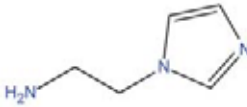
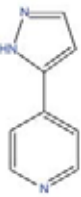
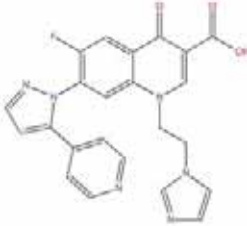
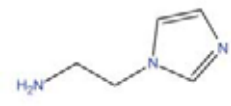
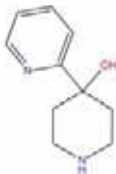
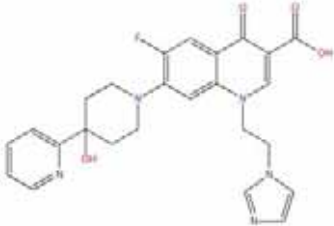
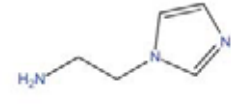
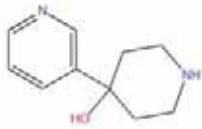
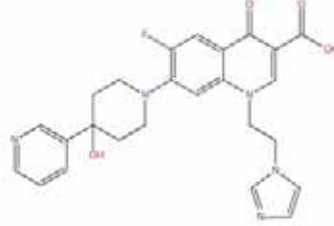
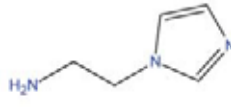
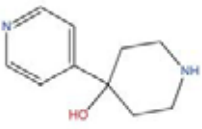
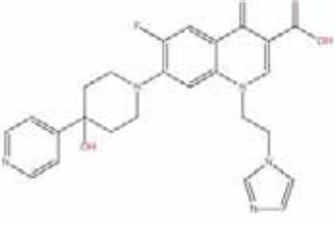
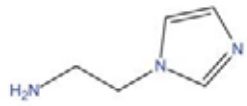
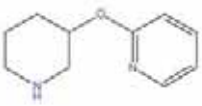
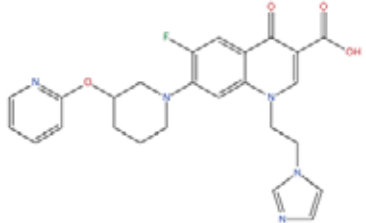
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
234	35	025	35-025	-0.0493	1.1202
					
235	35	026	35-026	-0.0986	1.2549
					
236	35	028	35-028	0.0355	0.9215
					
237	35	029	35-029	0.2194	0.6034
					
238	35	032	35-032	0.0108	0.9754
					
239	35	033	35-033	0.1680	0.6792
					

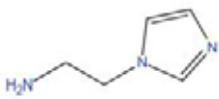
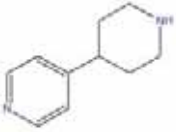
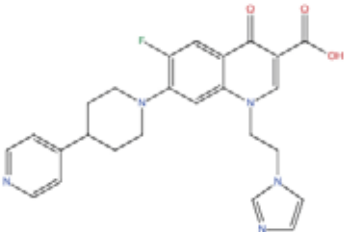
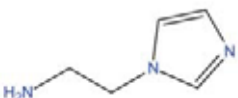
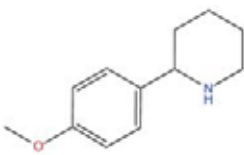
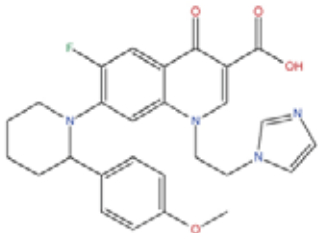
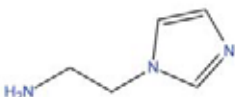
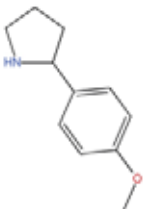
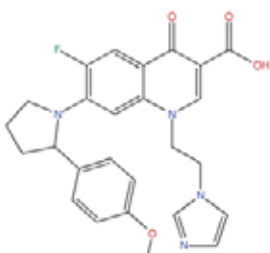
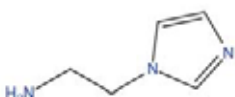
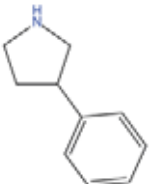
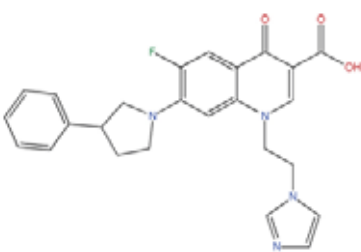

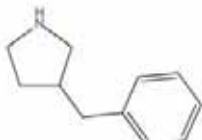
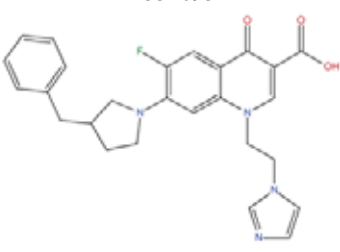
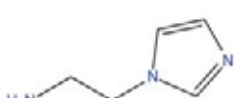
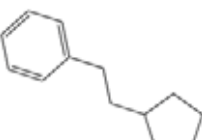
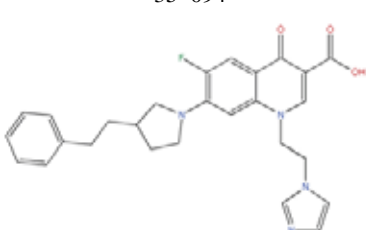


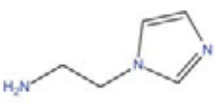
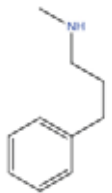
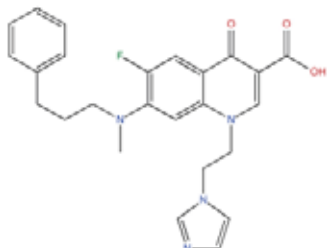
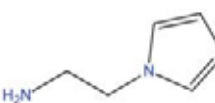
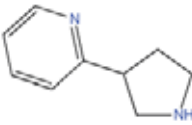
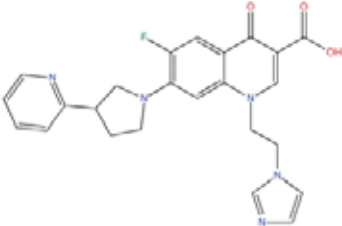
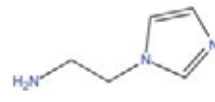
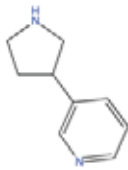
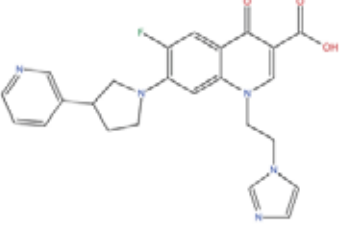

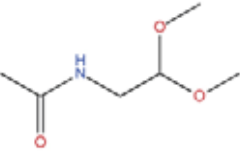
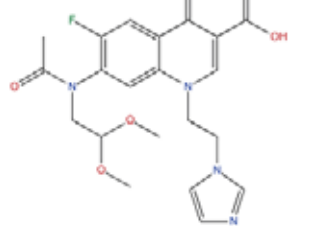
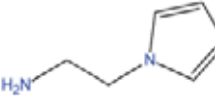
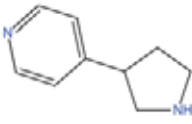
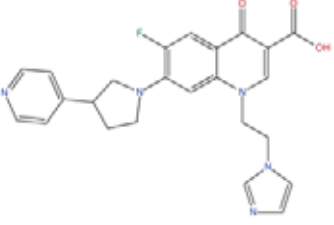
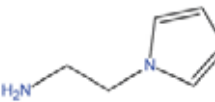
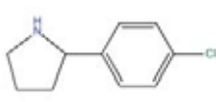
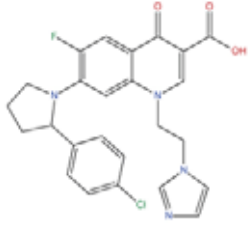
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
240	35	038	35-038	-0.1000	1.2589
					
241	35	040	35-040	-0.3303	2.1394
					
242	35	043	35-043	-0.7569	5.7135
					
243	35	044	35-044	-0.9407	8.7237
					
244	35	045	35-045	-0.6438	4.4035
					
245	35	048	35-048	-0.0153	1.0359
					

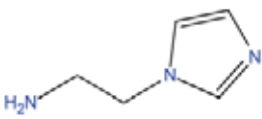
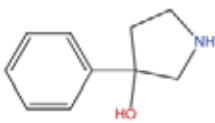
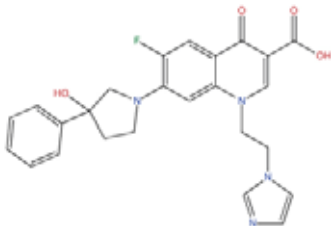
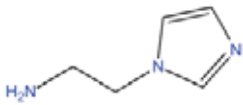
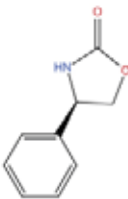
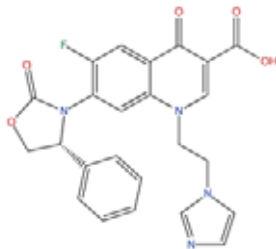
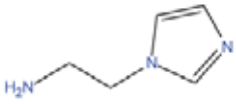
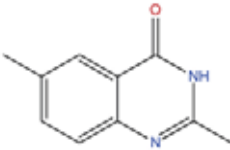
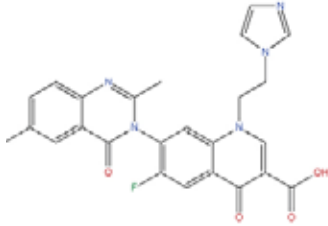
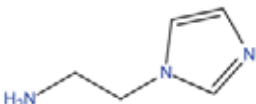
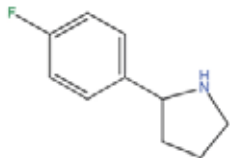
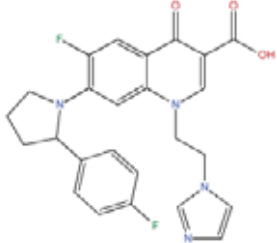
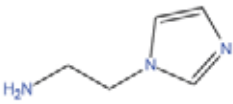
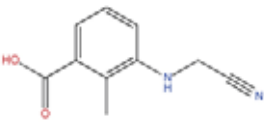
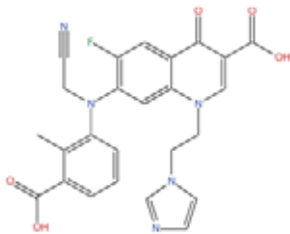
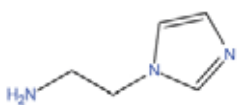
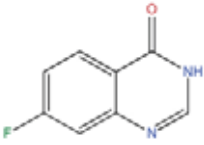
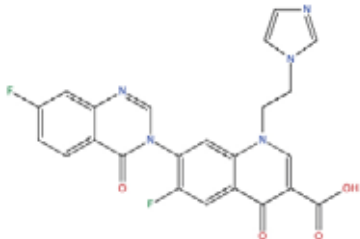
ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
246	35	049	35-049	-0.2775	1.8945
					
247	35	050	35-050	0.2083	0.6190
					
248	35	051	35-051	0.1040	0.7870
					
249	35	053	35-053	0.5874	0.2586
					
250	35	057	35-057	0.3948	0.4029
					
251	35	059	35-059	-0.7907	6.1759
					

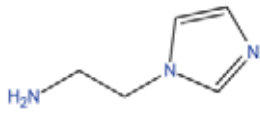
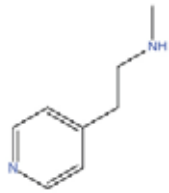
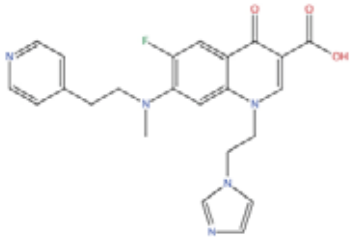
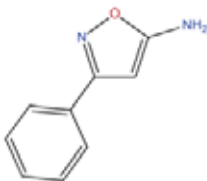
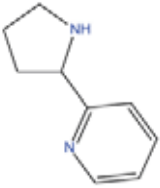
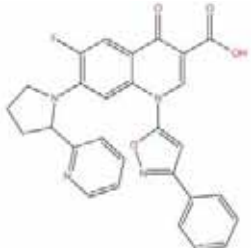
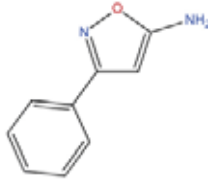
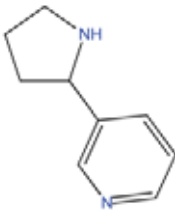
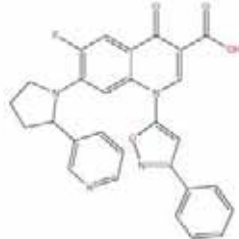
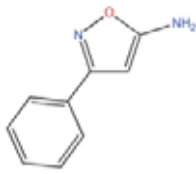
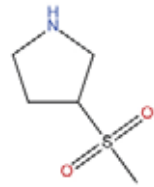
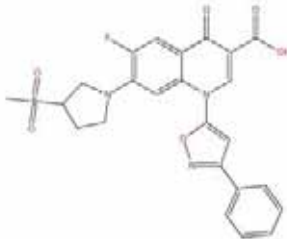
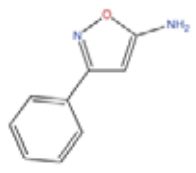
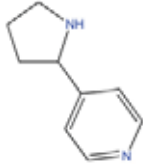
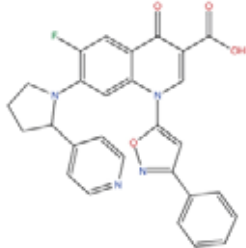
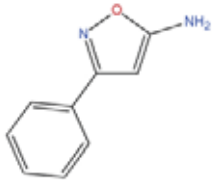
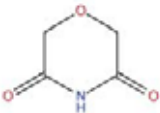
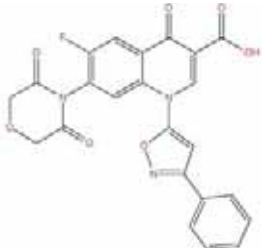
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
252	35	060	35-060	0.6732	0.2122
					
253	35	063	35-063	-0.5797	3.7993
					
254	35	064	35-064	-0.2911	1.9548
					
255	35	070	35-070	0.0732	0.8449
					
256	35	071	35-071	1.0436	0.0904
					
257	35	072	35-072	-0.9182	8.2832
					

ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
258	35	077	35-077	0.2582	0.5518
					
259	35	079	35-079	0.1786	0.6628
					
260	35	084	35-084	-0.2750	1.8836
					
261	35	085	35-085	-0.3986	2.5038
					
262	35	086	35-086	-0.5660	3.6813
					
263	35	087	35-087	-0.3082	2.0333
					

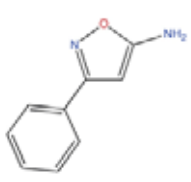
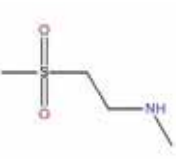
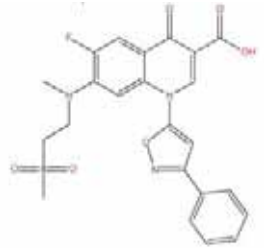
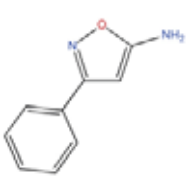
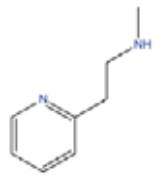
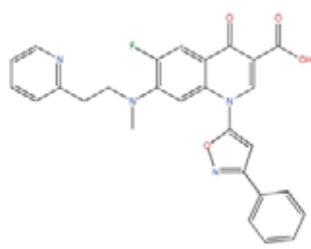
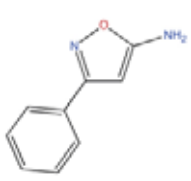
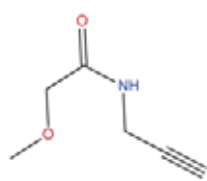
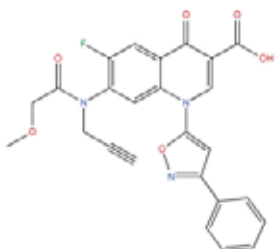
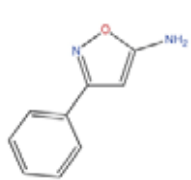
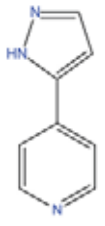
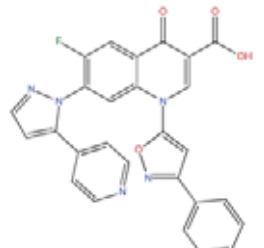
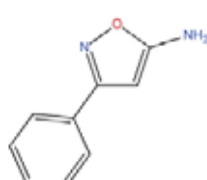
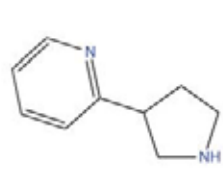
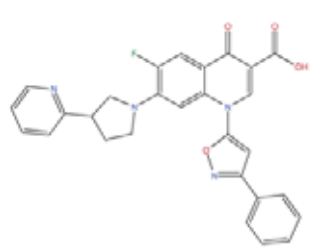
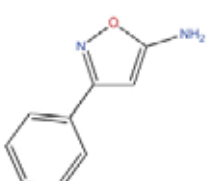
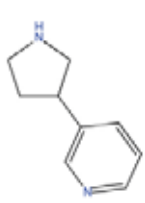
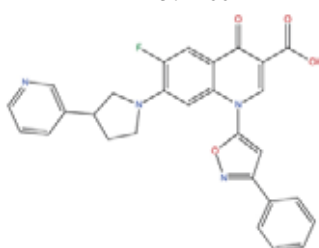
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
264	35	088	35-088	-0.8255	6.6911
					
265	35	089	35-089	0.2447	0.5692
					
266	35	091	35-091	0.0650	0.8610
					
267	35	092	35-092	-0.4958	3.1318
					
268	35	093	35-093	-0.8874	7.7161
					
269	35	094	35-094	-1.1041	12.7087
					

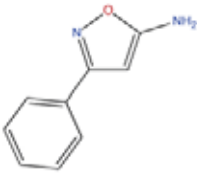
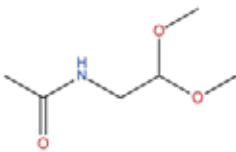
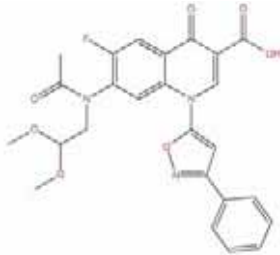
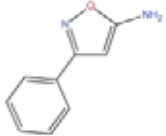
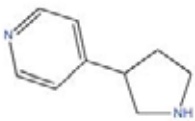
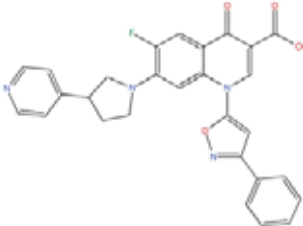
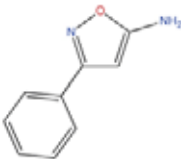
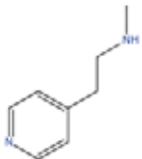
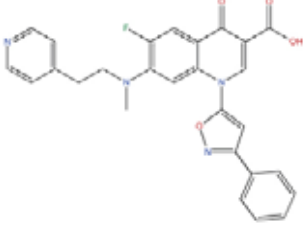
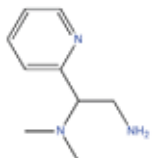
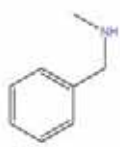
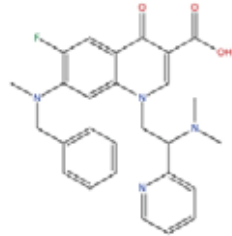
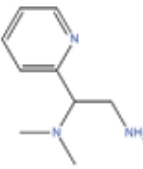
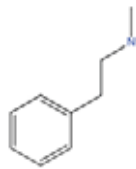
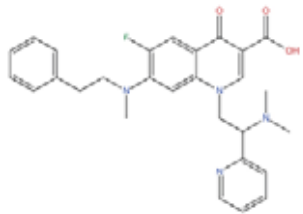
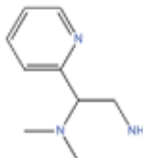
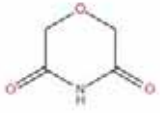
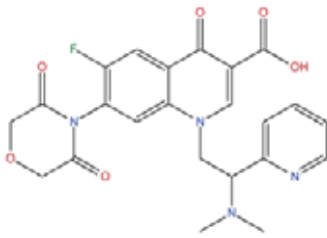
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
270	35	096	35-096	-0.9291	8.4938
					
271	35	098	35-098	-0.6077	4.0523
					
272	35	100	35-100	-0.2758	1.8871
					
273	35	103	35-103	0.0822	0.8276
					
274	35	104	35-104	-0.4075	2.5556
					
275	35	106	35-106	-0.3497	2.2372
					

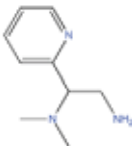
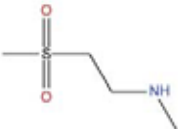
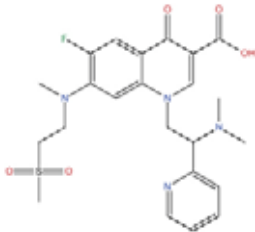
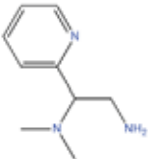
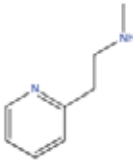
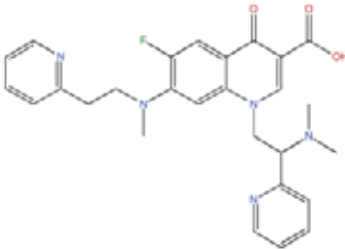
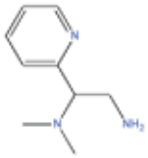
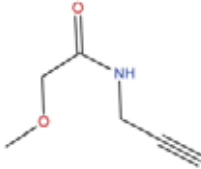
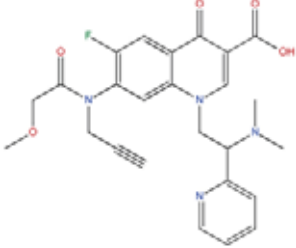
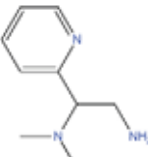
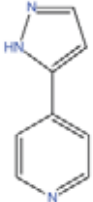
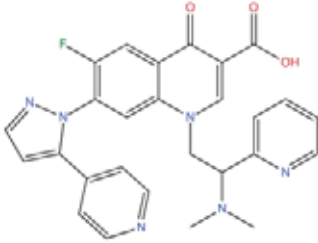
ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
276	35	107	35–107	-0.2473	1.7673
					
277	35	108	35–108	0.6564	0.2206
					
278	35	113	35–113	0.5509	0.2813
					
279	35	115	35–115	0.1786	0.6628
					
280	35	117	35–117	0.6546	0.2215
					
281	35	118	35–118	0.4809	0.3304
					

ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
282	35	120	35-120	-0.5235	3.3381
					
283	37	025	37-025	0.0250	0.9441
					
284	37	026	37-026	-0.0255	1.0605
					
285	37	028	37-028	0.1361	0.7310
					
286	37	029	37-029	0.2520	0.5598
					
287	37	033	37-033	0.3575	0.4390
					



ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
288	37	038	37-038	0.0643	0.8624
					
289	37	059	37-059	-0.5316	3.4009
					
290	37	077	37-077	0.3967	0.4011
					
291	37	079	37-079	0.0463	0.8989
					
292	37	098	37-098	-0.4164	2.6086
					
293	37	100	37-100	-0.1349	1.3643
					

ID	reactant 1	reactant 2	synthID	$pMIC_{pred-combi}$	$MIC_{pred-combi}$
294	37	103	37-103	0.4528	0.3525
					
295	37	104	37-104	-0.2463	1.7632
					
296	37	120	37-120	-0.3044	2.0156
					
297	39	001	39-001	0.0226	0.9493
					
298	39	023	39-023	-0.3394	2.1847
					
299	39	033	39-033	0.4164	0.3834
					

ID	reactant 1	reactant 2	synthID	pMIC <sub>pred-combi</sub>	MIC <sub>pred-combi</sub>
300	39	038	39-038	0.1850	0.6531
					
301	39	059	39-059	-0.4345	2.7196
					
302	39	077	39-077	0.5802	0.2629
					
303	39	079	39-079	0.4067	0.3920
					
304	39	120	39-120	-0.2104	1.6233
	