Article

Ciprofloxacin and clinafloxacin antibodies for an immunoassay of quinolones: quantitative structure-activity analysis of cross-reactivities

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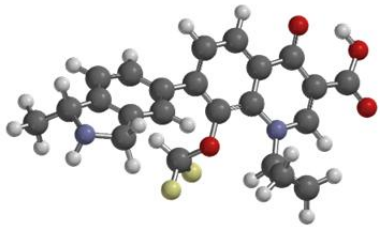
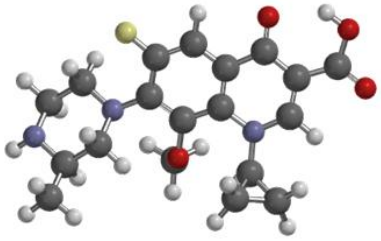
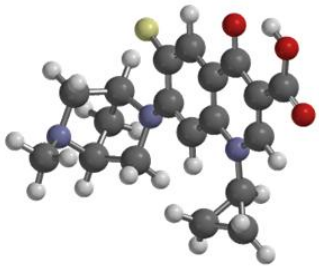
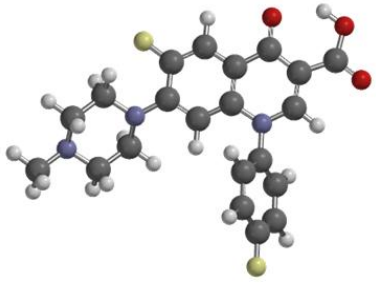
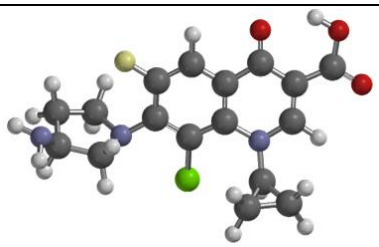
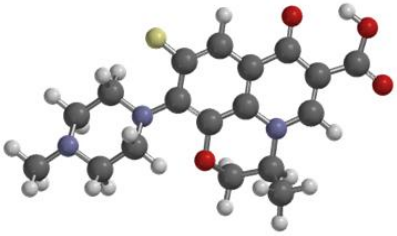
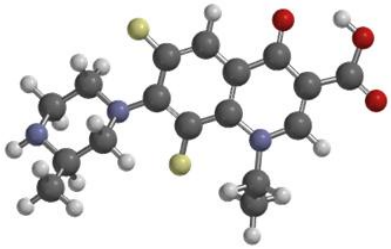
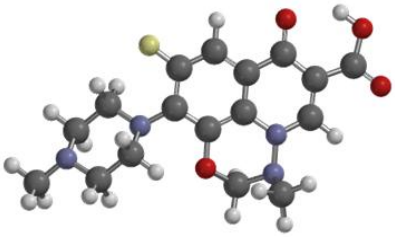
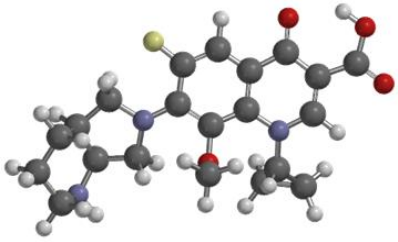
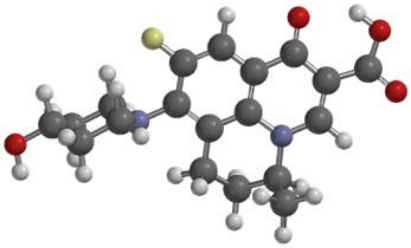
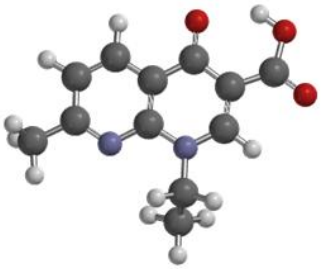
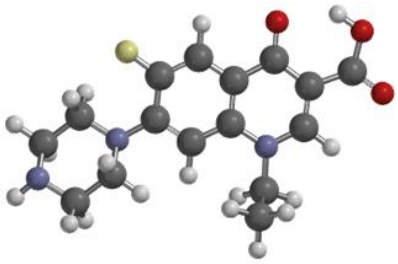
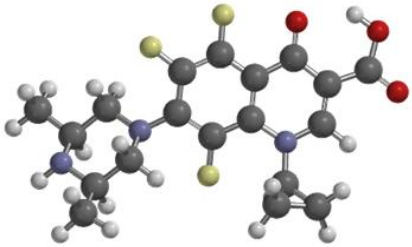
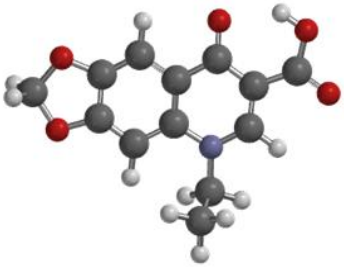
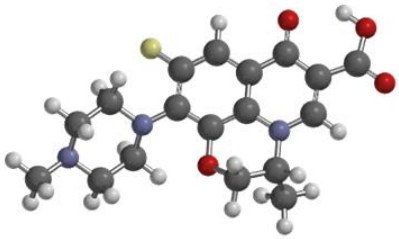
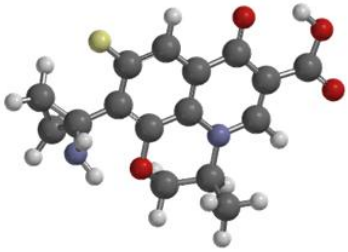
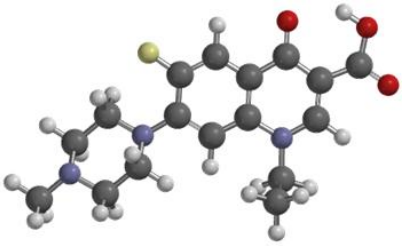
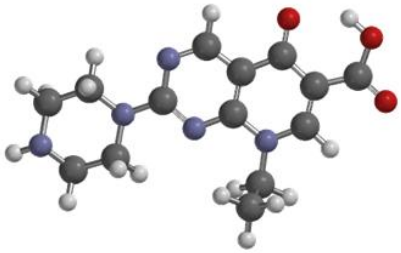
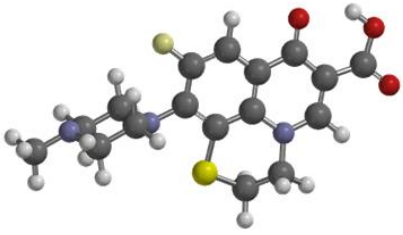
Supplementary Information

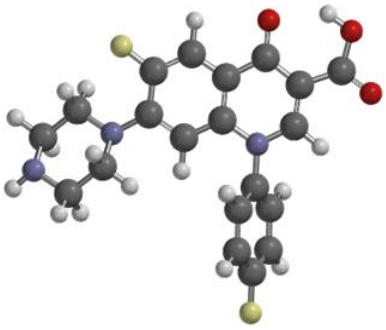
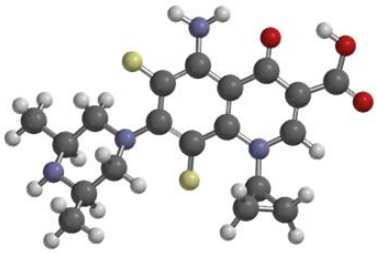
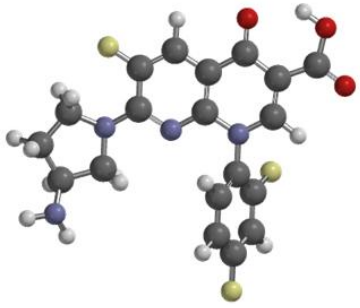
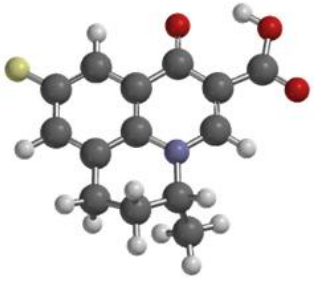
Table S1. 3D geometry of the most favorable low-energy conformer for each molecule optimized with AM1 method (carbon atoms are colored in grey, nitrogens – blue, oxygens – red, fluorines – yellow, hydrogens - white); experimental and predicted cross-reactivity values.

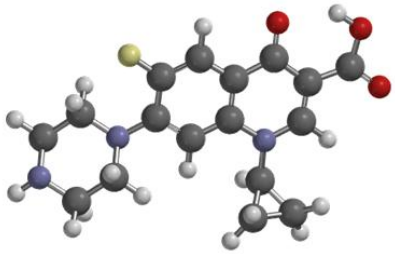
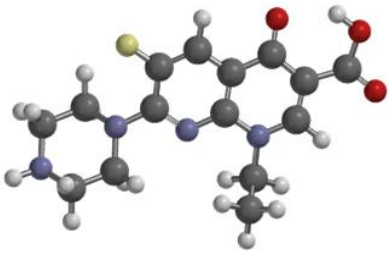
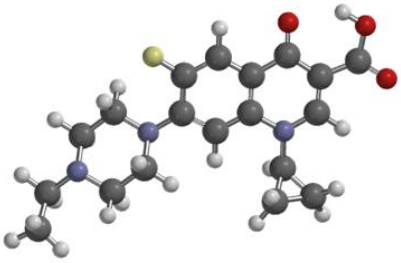
№	Compound	CIP-113 / PAZ-FITC		CLI-132 / CLI-C5-OVA, ELISA	
		Exp.	Pred.	Exp.	Pred.
1	Garenoxacin 	1.75	1.69	1.96	2.04
2	Gatifloxacin [T1] 	1.72	1.41	1.18	1.38
3	Danofloxacin 	1.88	1.71	1.80	1.45
4	Difloxacin [T1] 	0	0.18	-0.30	-0.22
5	Clinafloxacin	1.72	1.60	2.0	1.30

					
6	Levofloxacin 	-	-	-0.30	-0.39
7	Lomefloxacin 	1.40	1.37	-0.30	-0.32
8	Marbofloxacin 	1.28	1.10	-0.30	-0.22
9	Moxifloxacin 	1.40	1.76	0.90	1.45

10	Nadifloxacin [T2] 	1.69	1.62	1.95	1.19
11	Nalidixic acid [T2] 	1.89	1.89	-0.30	-0.22
12	Norfloxacin 	1.45	1.41	-0.30	-0.22
13	Orbifloxacin 	1.76	1.81	1.0	1.06
14	Oxolinic acid 	1.56	1.90	-0.30	-0.22

15	R-Ofloxacin 	-	-	-0.30	-0.39
16	Pazufloxacin 	1.38	1.49	-0.30	-0.39
17	Pefloxacin [T1, T2] 	1.41	1.34	-0.22	-0.30
18	Pipemidic_acid 	1.64	1.56	-0.30	-0.22
19	Rufloxacin [T2] 	1.11	1.23	-0.22	-0.30

20	Sarafloxacin 	0	0.22	-0.30	-0.22
21	Sparfloxacin 	1.63	1.74	1.0	1.14
22	Tosufloxacin [T1] 	0.78	0.65	-0.30	-0.39
23	Flumequine 	1.86	1.99	-0.30	-0.32

24	Ciprofloxacin 	2.0	1.61	1.86	1.47
25	Enoxacin [T1, T2] 	1.59	1.45	0.70	-0.22
26	Enrofloxacin 	1.76	1.46	1.52	1.46

[T] – Compounds presented in the test set