

Supplementary Material

Integration of Fuzzy Matter-Element Method and 3D-QSAR Model for Generation of Environmentally Friendly Quinolone Derivatives

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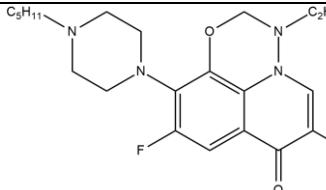
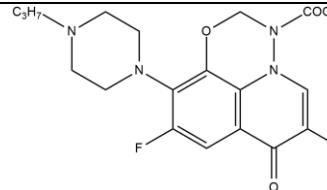
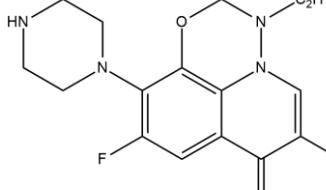
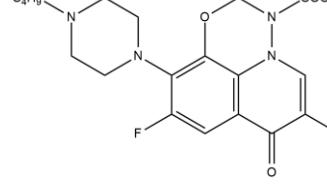
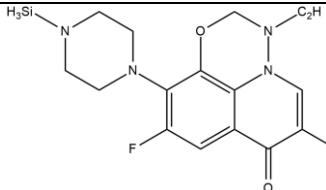
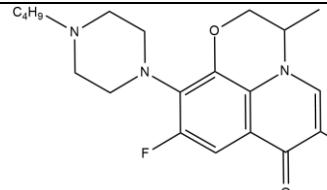
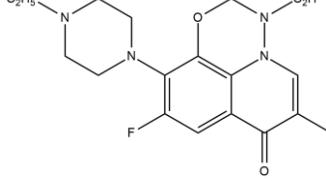
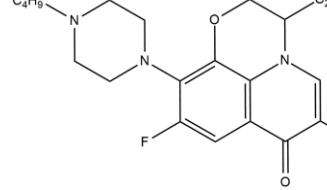
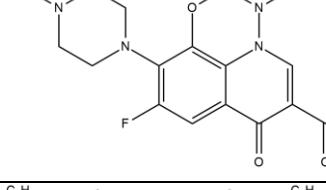
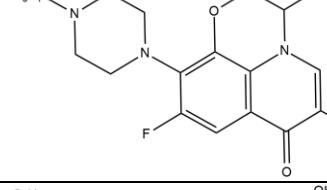
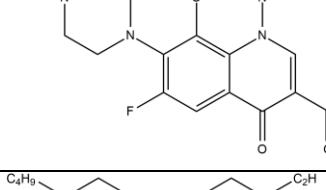
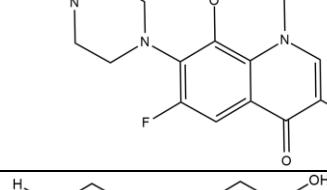
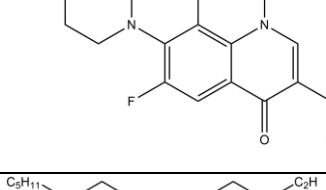
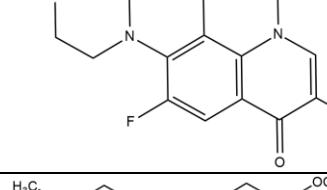
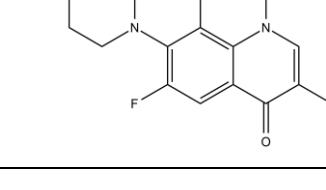
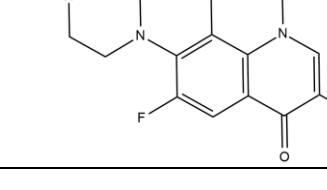
* Corresponding author: bzhang@mun.ca

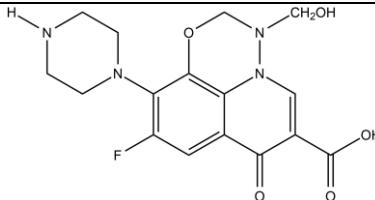
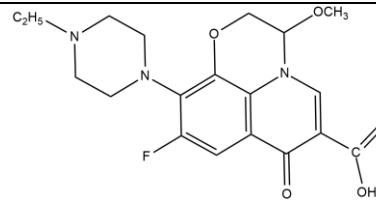
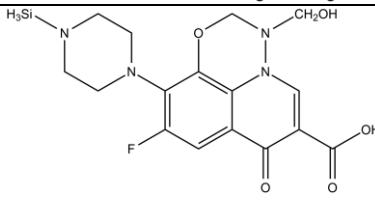
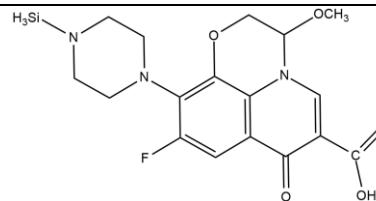
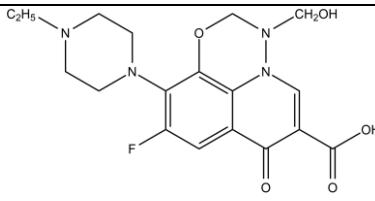
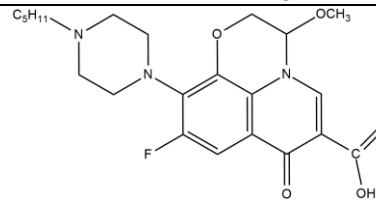
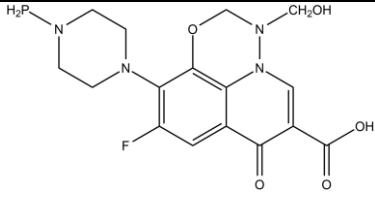
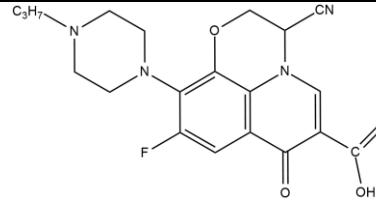
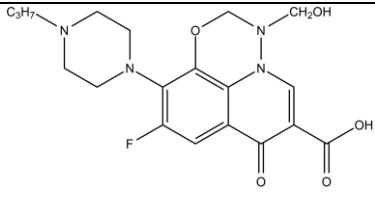
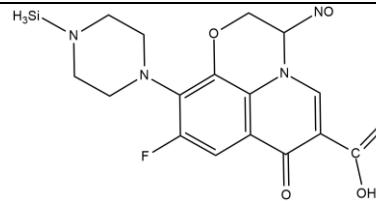
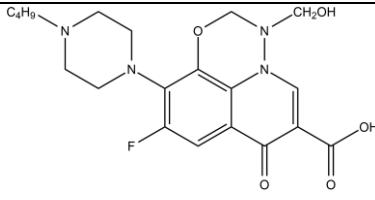
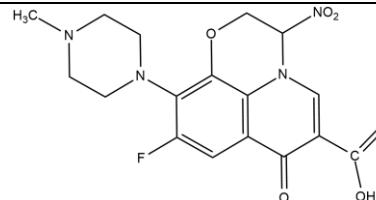
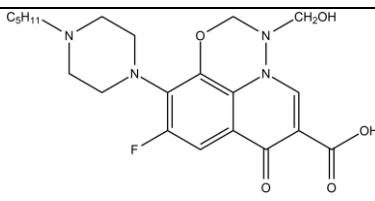
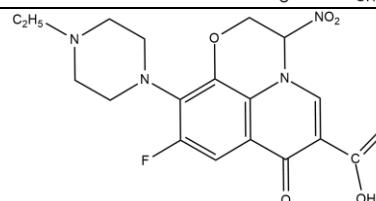
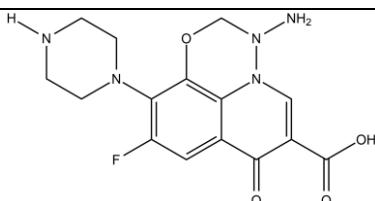
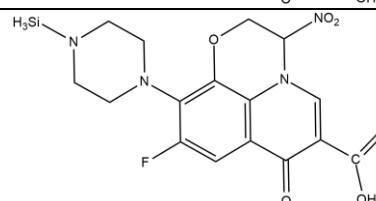
Table S1. Molecular structures of designed QA derivatives

QA derivatives	Molecular structures	QA derivatives	Molecular structures
QA1		QA45	
QA2		QA46	
QA3		QA47	
QA4		QA48	
QA5		QA49	
QA6		QA50	
QA7		QA51	
QA8		QA52	

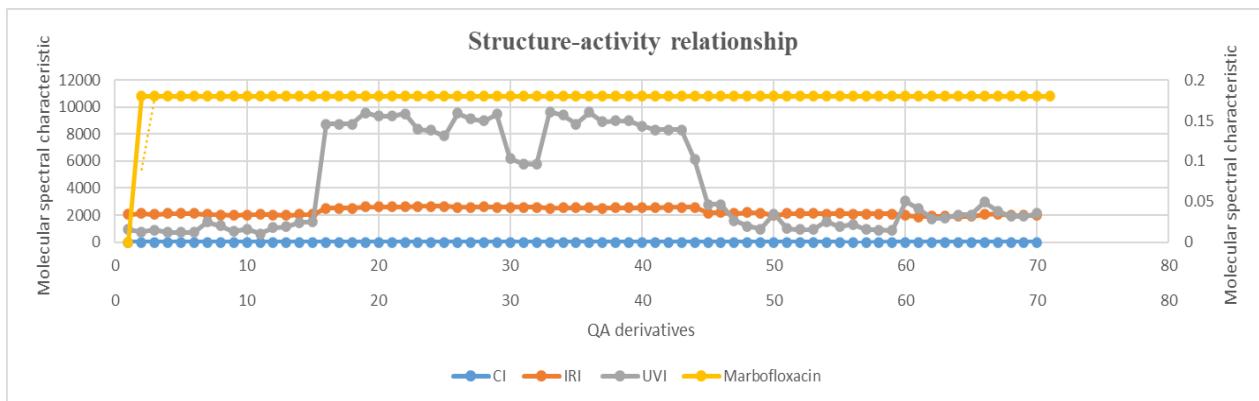
QA9		QA53	
QA10		QA54	
QA11		QA55	
QA12		QA56	
QA13		QA57	
QA14		QA58	
QA15		QA59	
QA16		QA60	

QA17		QA61	
QA18		QA62	
QA19		QA63	
QA20		QA64	
QA21		QA65	
QA22		QA66	
QA23		QA67	
QA24		QA68	

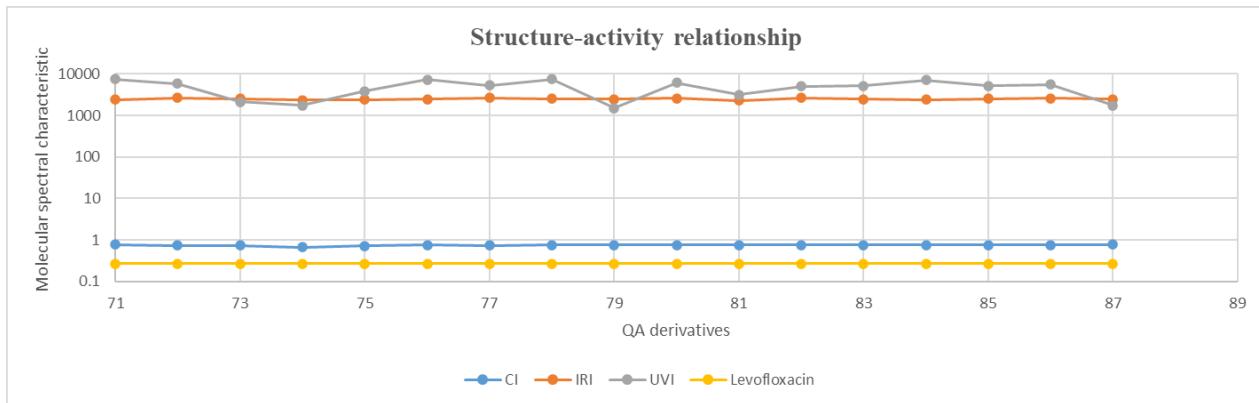
QA25		QA69	
QA26		QA70	
QA27		QA71	
QA28		QA72	
QA29		QA73	
QA30		QA74	
QA31		QA75	
QA32		QA76	

QA33		QA77	
QA34		QA78	
QA35		QA79	
QA36		QA80	
QA37		QA81	
QA38		QA82	
QA39		QA83	
QA40		QA84	

QA41		QA85	
QA42		QA86	
QA43		QA87	
QA44			



(a)



(b)

Figure S1. Relationship between each QA structure and the associated activities (i.e., IRI, UVI and CI) with (a) marbofloxacin and (b) levofloxacin used as the target molecules.