Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Predictive binary mixture toxicity modeling of fluoroquinolones (FQ) and the projection of toxicity of hypothetical binary FQ mixtures: A combination of 2D-QSAR and machine-learning approaches

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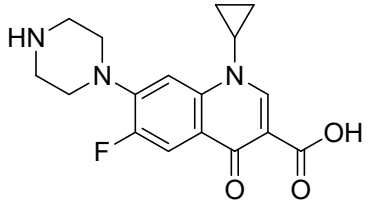
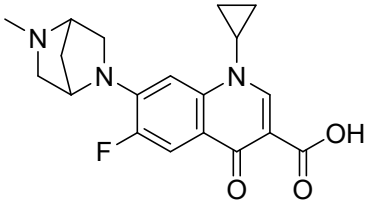
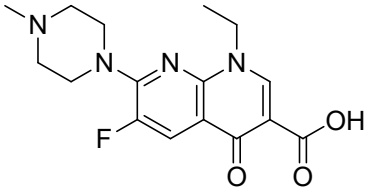
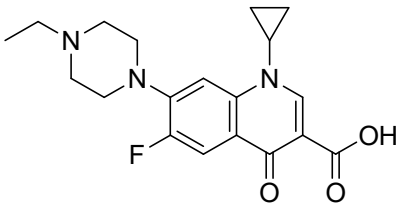
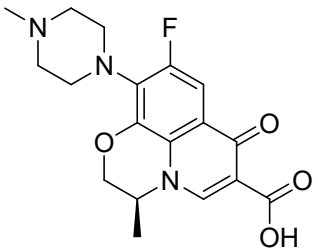
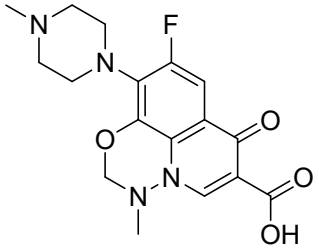
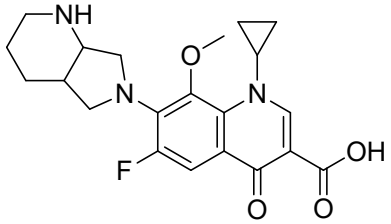
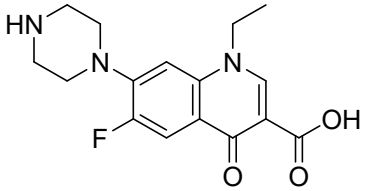
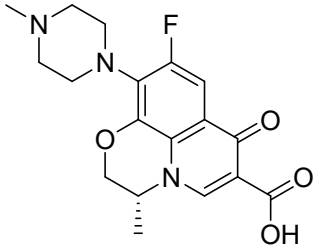
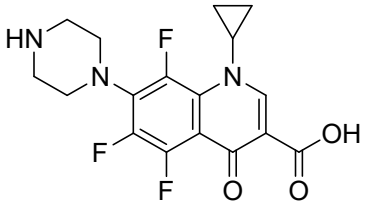
Supplementary Materials (Tables and Figures)

Table S1. Toxicity data [Log (1/IC50) in molar scale] of mixture components (fluoroquinolones) along with their 2D structures

Serial No.	Name (Abbreviation)	CS No.	2D Structure	Experimental toxicity [Log (1/IC50)]
C1	Ciprofloxacin (CIP)	85721-33-1		7.30
C2	Danofloxacin (DAN)	112398-08-0		6.90
C3	Enoxacin (ENO)	74011-58-8		6.13
C4	Enrofloxacin (ENR)	93106-60-6		6.98
C5	Levofloxacin (LEV)	100986-85-4		6.42

C6	Marbofloxacin (MAR)	115550-35-1		7.27
C7	Moxifloxacin (MOX)	151096-09-2		6.71
C8	Norfloxacin (NOR)	70458-96-7		6.18
C9	Ofloxacin (OFL)	82419-36-1		6.74
C10	Orbifloxacin (ORB)	113617-63-3		6.96

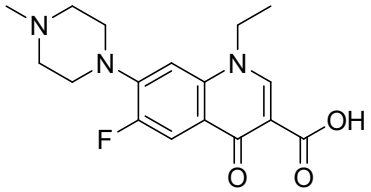
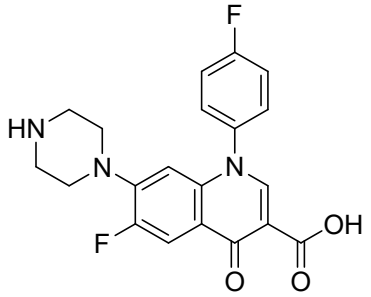
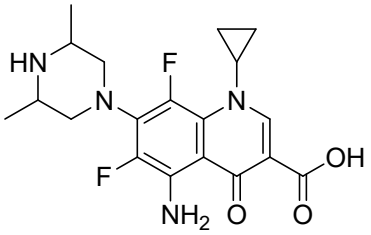
C11	Pefloxacin (PEF)	70458-92-3		6.25
C12	Sarafloxacin (SAR)	98105-99-8		7.10
C13	Sparfloxacin (SPA)	110871-86-8		7.32

Table S2. Composition and experimental toxicity data [Log (1/IC50) in molar scale] of studied mixtures

Mixture No.	Comp. A	Mole Fraction	Comp. B	Mole Fraction	Experimental toxicity [Log (1/IC50)]
M1	C1	0.28	C2	0.72	7.05
M2	C1	0.06	C3	0.94	6.43
M3	C1	0.32	C4	0.68	7.27

M4	C1	0.12	C5	0.88	6.71
M5	C1	0.48	C6	0.52	7.28
M6	C1	0.2	C7	0.8	6.84
M7	C1	0.07	C8	0.93	6.34
M8	C1	0.22	C9	0.78	6.99
M9	C1	0.31	C10	0.69	7.27
M10	C1	0.08	C11	0.92	6.56
M11	C1	0.39	C12	0.61	7.2
M12	C1	0.51	C13	0.49	7.4
M13	C2	0.15	C3	0.85	6.51
M14	C2	0.55	C4	0.45	7
M15	C2	0.25	C5	0.75	6.64
M16	C2	0.7	C6	0.3	7.02
M17	C2	0.39	C7	0.61	6.96
M18	C2	0.16	C8	0.84	6.48
M19	C2	0.41	C9	0.59	6.78
M20	C2	0.53	C10	0.47	7.18

M21	C2	0.18	C11	0.82	6.52
M22	C2	0.61	C12	0.39	7.27
M23	C2	0.72	C13	0.28	7
M24	C3	0.88	C4	0.12	6.5
M25	C3	0.66	C5	0.34	6.47
M26	C3	0.93	C6	0.07	6.42
M27	C3	0.79	C7	0.21	6.25
M28	C3	0.53	C8	0.47	6.16
M29	C3	0.8	C9	0.2	6.37
M30	C3	0.87	C10	0.13	6.39
M31	C3	0.57	C11	0.43	6.39
M32	C3	0.9	C12	0.1	6.47
M33	C3	0.94	C13	0.06	6.41
M34	C4	0.22	C5	0.78	6.82
M35	C4	0.66	C6	0.34	7.05
M36	C4	0.35	C7	0.65	6.87
M37	C4	0.14	C8	0.86	6.54

M38	C4	0.37	C9	0.63	6.98
M39	C4	0.49	C10	0.51	6.93
M40	C4	0.16	C11	0.84	6.8
M41	C4	0.57	C12	0.43	7.2
M42	C4	0.69	C13	0.31	7.21
M43	C5	0.88	C6	0.12	6.52
M44	C5	0.66	C7	0.34	6.78
M45	C5	0.37	C8	0.63	6.24
M46	C5	0.68	C9	0.32	6.46
M47	C5	0.78	C10	0.22	6.77
M48	C5	0.4	C11	0.6	6.39
M49	C5	0.83	C12	0.17	6.49
M50	C5	0.89	C13	0.11	6.54
M51	C6	0.22	C7	0.78	6.94
M52	C6	0.08	C8	0.92	6.36
M53	C6	0.23	C9	0.77	6.98
M54	C6	0.33	C10	0.67	7.06

M55	C6	0.09	C11	0.91	6.86
M56	C6	0.4	C12	0.6	7.17
M57	C6	0.53	C13	0.47	7.24
M58	C7	0.23	C8	0.77	6.43
M59	C7	0.52	C9	0.48	6.69
M60	C7	0.64	C10	0.36	6.94
M61	C7	0.26	C11	0.74	6.62
M62	C7	0.71	C12	0.29	6.71
M63	C7	0.8	C13	0.2	6.7
M64	C8	0.78	C9	0.22	6.43
M65	C8	0.86	C10	0.14	6.48
M66	C8	0.54	C11	0.46	6.4
M67	C8	0.89	C12	0.11	6.44
M68	C8	0.93	C13	0.07	6.39
M69	C9	0.62	C10	0.38	6.78
M70	C9	0.24	C11	0.76	6.57
M71	C9	0.7	C12	0.3	6.85

M72	C9	0.79	C13	0.21	6.98
M73	C10	0.16	C11	0.84	6.6
M74	C10	0.58	C12	0.42	7.01
M75	C10	0.7	C13	0.3	7.09
M76	C11	0.88	C12	0.12	6.5
M77	C11	0.92	C13	0.08	6.63
M78	C12	0.62	C13	0.38	7.07

Table S3. Computed validation metrics of preliminary GA-MLR models (Number of descriptors in each model = 6)

Mixing rule 1 (Linear combination of molecular contributions)					
Division	R^2	Q^2_{LOO}	$ME_{Train95\%}$	Q^2_{F1}	$ME_{Test95\%}$
4-1ABD	0.897	0.870	0.081	0.809	0.097
4-1DBD	0.886	0.856	0.082	0.817	0.106
4-2ABD	**0.874**	**0.842**	**0.087**	**0.837**	**0.088**
4-2DBD	0.863	0.828	0.089	0.889	0.084
4-3ABD	0.880	0.850	0.088	0.833	0.092
4-3DBD	0.874	0.844	0.092	0.863	0.072
4-4ABD	0.884	0.857	0.085	0.833	0.086
4-4DBD	0.887	0.858	0.084	0.827	0.092

75-25KS	0.901	0.875	0.082	0.733	0.102
Average	**0.883**	**0.853**	**0.085**	**0.827**	**0.091**

Mixing rule 2 (Square molecular contributions)

Division	R^2	Q^2_{LOO}	$ME_{Train95\%}$	Q^2_{F1}	$ME_{Test95\%}$
4-1ABD	0.890	0.861	0.079	0.774	0.103
4-1DBD	0.858	0.822	0.092	0.840	0.085
4-2ABD	0.863	0.827	0.088	0.825	0.090
4-2DBD	0.872	0.838	0.090	0.751	0.092
4-3ABD	0.877	0.846	0.084	0.810	0.091
4-3DBD	0.878	0.847	0.081	0.734	0.117
4-4ABD	0.865	0.829	0.088	0.815	0.091
4-4DBD	0.869	0.835	0.083	0.801	0.107
75-25KS	0.882	0.852	0.087	0.762	0.091
Average	0.873	0.840	0.086	0.790	0.096

Mixing rule 3 (Norm of molecular contributions)

Division	R^2	Q^2_{LOO}	$ME_{Train95\%}$	Q^2_{F1}	$ME_{Test95\%}$
4-1ABD	0.865	0.829	0.088	0.767	0.099
4-1DBD	0.829	0.778	0.099	0.773	0.098
4-2ABD	0.829	0.783	0.100	0.765	0.102
4-2DBD	0.862	0.823	0.083	0.737	0.141
4-3ABD	0.835	0.782	0.097	0.817	0.095

4-3DBD	0.888	0.858	0.083	0.644	0.121
4-4ABD	0.887	0.857	0.076	0.576	0.130
4-4DBD	0.849	0.806	0.096	0.764	0.089
75-25KS	0.864	0.820	0.089	0.744	0.100
Average	0.856	0.815	0.090	0.732	0.108

Table S4. Composition of the hypothetical mixtures designed from the FQs and their corresponding degradation products

Hypothetical Mixture No.	COMP. 1	FRACTION 1	COMP. 2	FRACTION 2
HM1	CIP	0.5	CIP1	0.5
HM2	CIP	0.5	CIP2	0.5
HM3	CIP	0.5	CIP3	0.5
HM4	CIP	0.5	CIP4	0.5
HM5	CIP	0.5	CIP5	0.5
HM6	CIP	0.5	CIP6	0.5
HM7	CIP	0.5	CIP7	0.5
HM8	CIP	0.5	CIP8	0.5
HM9	CIP	0.5	CIP9	0.5
HM10	CIP1	0.5	CIP2	0.5
HM11	CIP1	0.5	CIP3	0.5

HM12	CIP1	0.5	CIP4	0.5
HM13	CIP1	0.5	CIP5	0.5
HM14	CIP1	0.5	CIP6	0.5
HM15	CIP1	0.5	CIP7	0.5
HM16	CIP1	0.5	CIP8	0.5
HM17	CIP1	0.5	CIP9	0.5
HM18	CIP2	0.5	CIP3	0.5
HM19	CIP2	0.5	CIP4	0.5
HM20	CIP2	0.5	CIP5	0.5
HM21	CIP2	0.5	CIP6	0.5
HM22	CIP2	0.5	CIP7	0.5
HM23	CIP2	0.5	CIP8	0.5
HM24	CIP2	0.5	CIP9	0.5
HM25	CIP3	0.5	CIP4	0.5
HM26	CIP3	0.5	CIP5	0.5
HM27	CIP3	0.5	CIP6	0.5
HM28	CIP3	0.5	CIP7	0.5
HM29	CIP3	0.5	CIP8	0.5
HM30	CIP3	0.5	CIP9	0.5

HM31	CIP4	0.5	CIP5	0.5
HM32	CIP4	0.5	CIP6	0.5
HM33	CIP4	0.5	CIP7	0.5
HM34	CIP4	0.5	CIP8	0.5
HM35	CIP4	0.5	CIP9	0.5
HM36	CIP5	0.5	CIP6	0.5
HM37	CIP5	0.5	CIP7	0.5
HM38	CIP5	0.5	CIP8	0.5
HM39	CIP5	0.5	CIP9	0.5
HM40	CIP6	0.5	CIP7	0.5
HM41	CIP6	0.5	CIP8	0.5
HM42	CIP6	0.5	CIP9	0.5
HM43	CIP7	0.5	CIP8	0.5
HM44	CIP7	0.5	CIP9	0.5
HM45	CIP8	0.5	CIP9	0.5
HM46	DAN	0.5	DAN1	0.5
HM47	DAN	0.5	DAN2	0.5
HM48	DAN	0.5	DAN3	0.5
HM49	DAN	0.5	DAN4	0.5

HM50	DAN	0.5	DAN5	0.5
HM51	DAN	0.5	DAN6	0.5
HM52	DAN	0.5	DAN7	0.5
HM53	DAN	0.5	DAN8	0.5
HM54	DAN	0.5	DAN9	0.5
HM55	DAN1	0.5	DAN2	0.5
HM56	DAN1	0.5	DAN3	0.5
HM57	DAN1	0.5	DAN4	0.5
HM58	DAN1	0.5	DAN5	0.5
HM59	DAN1	0.5	DAN6	0.5
HM60	DAN1	0.5	DAN7	0.5
HM61	DAN1	0.5	DAN8	0.5
HM62	DAN1	0.5	DAN9	0.5
HM63	DAN2	0.5	DAN3	0.5
HM64	DAN2	0.5	DAN4	0.5
HM65	DAN2	0.5	DAN5	0.5
HM66	DAN2	0.5	DAN6	0.5
HM67	DAN2	0.5	DAN7	0.5
HM68	DAN2	0.5	DAN8	0.5

HM69	DAN2	0.5	DAN9	0.5
HM70	DAN3	0.5	DAN4	0.5
HM71	DAN3	0.5	DAN5	0.5
HM72	DAN3	0.5	DAN6	0.5
HM73	DAN3	0.5	DAN7	0.5
HM74	DAN3	0.5	DAN8	0.5
HM75	DAN3	0.5	DAN9	0.5
HM76	DAN4	0.5	DAN5	0.5
HM77	DAN4	0.5	DAN6	0.5
HM78	DAN4	0.5	DAN7	0.5
HM79	DAN4	0.5	DAN8	0.5
HM80	DAN4	0.5	DAN9	0.5
HM81	DAN5	0.5	DAN6	0.5
HM82	DAN5	0.5	DAN7	0.5
HM83	DAN5	0.5	DAN8	0.5
HM84	DAN5	0.5	DAN9	0.5
HM85	DAN6	0.5	DAN7	0.5
HM86	DAN6	0.5	DAN8	0.5
HM87	DAN6	0.5	DAN9	0.5

HM88	DAN7	0.5	DAN8	0.5
HM89	DAN7	0.5	DAN9	0.5
HM90	DAN8	0.5	DAN9	0.5
HM91	ENO	0.5	ENO1	0.5
HM92	ENO	0.5	ENO2	0.5
HM93	ENO	0.5	ENO3	0.5
HM94	ENO	0.5	ENO4	0.5
HM95	ENO	0.5	ENO5	0.5
HM96	ENO	0.5	ENO6	0.5
HM97	ENO	0.5	ENO7	0.5
HM98	ENO	0.5	ENO8	0.5
HM99	ENO	0.5	ENO9	0.5
HM100	ENO1	0.5	ENO2	0.5
HM101	ENO1	0.5	ENO3	0.5
HM102	ENO1	0.5	ENO4	0.5
HM103	ENO1	0.5	ENO5	0.5
HM104	ENO1	0.5	ENO6	0.5
HM105	ENO1	0.5	ENO7	0.5
HM106	ENO1	0.5	ENO8	0.5

HM107	ENO1	0.5	ENO9	0.5
HM108	ENO2	0.5	ENO3	0.5
HM109	ENO2	0.5	ENO4	0.5
HM110	ENO2	0.5	ENO5	0.5
HM111	ENO2	0.5	ENO6	0.5
HM112	ENO2	0.5	ENO7	0.5
HM113	ENO2	0.5	ENO8	0.5
HM114	ENO2	0.5	ENO9	0.5
HM115	ENO3	0.5	ENO4	0.5
HM116	ENO3	0.5	ENO5	0.5
HM117	ENO3	0.5	ENO6	0.5
HM118	ENO3	0.5	ENO7	0.5
HM119	ENO3	0.5	ENO8	0.5
HM120	ENO3	0.5	ENO9	0.5
HM121	ENO4	0.5	ENO5	0.5
HM122	ENO4	0.5	ENO6	0.5
HM123	ENO4	0.5	ENO7	0.5
HM124	ENO4	0.5	ENO8	0.5
HM125	ENO4	0.5	ENO9	0.5

HM126	ENO5	0.5	ENO6	0.5
HM127	ENO5	0.5	ENO7	0.5
HM128	ENO5	0.5	ENO8	0.5
HM129	ENO5	0.5	ENO9	0.5
HM130	ENO6	0.5	ENO7	0.5
HM131	ENO6	0.5	ENO8	0.5
HM132	ENO6	0.5	ENO9	0.5
HM133	ENO7	0.5	ENO8	0.5
HM134	ENO7	0.5	ENO9	0.5
HM135	ENO8	0.5	ENO9	0.5
HM136	ENR	0.5	ENR1	0.5
HM137	ENR	0.5	ENR2	0.5
HM138	ENR	0.5	ENR3	0.5
HM139	ENR	0.5	ENR4	0.5
HM140	ENR	0.5	ENR5	0.5
HM141	ENR	0.5	ENR6	0.5
HM142	ENR	0.5	ENR7	0.5
HM143	ENR	0.5	ENR8	0.5
HM144	ENR	0.5	ENR9	0.5

HM145	ENR1	0.5	ENR2	0.5
HM146	ENR1	0.5	ENR3	0.5
HM147	ENR1	0.5	ENR4	0.5
HM148	ENR1	0.5	ENR5	0.5
HM149	ENR1	0.5	ENR6	0.5
HM150	ENR1	0.5	ENR7	0.5
HM151	ENR1	0.5	ENR8	0.5
HM152	ENR1	0.5	ENR9	0.5
HM153	ENR2	0.5	ENR3	0.5
HM154	ENR2	0.5	ENR4	0.5
HM155	ENR2	0.5	ENR5	0.5
HM156	ENR2	0.5	ENR6	0.5
HM157	ENR2	0.5	ENR7	0.5
HM158	ENR2	0.5	ENR8	0.5
HM159	ENR2	0.5	ENR9	0.5
HM160	ENR3	0.5	ENR4	0.5
HM161	ENR3	0.5	ENR5	0.5
HM162	ENR3	0.5	ENR6	0.5
HM163	ENR3	0.5	ENR7	0.5

HM164	ENR3	0.5	ENR8	0.5
HM165	ENR3	0.5	ENR9	0.5
HM166	ENR4	0.5	ENR5	0.5
HM167	ENR4	0.5	ENR6	0.5
HM168	ENR4	0.5	ENR7	0.5
HM169	ENR4	0.5	ENR8	0.5
HM170	ENR4	0.5	ENR9	0.5
HM171	ENR5	0.5	ENR6	0.5
HM172	ENR5	0.5	ENR7	0.5
HM173	ENR5	0.5	ENR8	0.5
HM174	ENR5	0.5	ENR9	0.5
HM175	ENR6	0.5	ENR7	0.5
HM176	ENR6	0.5	ENR8	0.5
HM177	ENR6	0.5	ENR9	0.5
HM178	ENR7	0.5	ENR8	0.5
HM179	ENR7	0.5	ENR9	0.5
HM180	ENR8	0.5	ENR9	0.5
HM181	LEV	0.5	LEV1	0.5
HM182	LEV	0.5	LEV2	0.5

HM183	LEV	0.5	LEV3	0.5
HM184	LEV	0.5	LEV4	0.5
HM185	LEV	0.5	LEV5	0.5
HM186	LEV	0.5	LEV6	0.5
HM187	LEV	0.5	LEV7	0.5
HM188	LEV	0.5	LEV8	0.5
HM189	LEV	0.5	LEV9	0.5
HM190	LEV1	0.5	LEV2	0.5
HM191	LEV1	0.5	LEV3	0.5
HM192	LEV1	0.5	LEV4	0.5
HM193	LEV1	0.5	LEV5	0.5
HM194	LEV1	0.5	LEV6	0.5
HM195	LEV1	0.5	LEV7	0.5
HM196	LEV1	0.5	LEV8	0.5
HM197	LEV1	0.5	LEV9	0.5
HM198	LEV2	0.5	LEV3	0.5
HM199	LEV2	0.5	LEV4	0.5
HM200	LEV2	0.5	LEV5	0.5
HM201	LEV2	0.5	LEV6	0.5

HM202	LEV2	0.5	LEV7	0.5
HM203	LEV2	0.5	LEV8	0.5
HM204	LEV2	0.5	LEV9	0.5
HM205	LEV3	0.5	LEV4	0.5
HM206	LEV3	0.5	LEV5	0.5
HM207	LEV3	0.5	LEV6	0.5
HM208	LEV3	0.5	LEV7	0.5
HM209	LEV3	0.5	LEV8	0.5
HM210	LEV3	0.5	LEV9	0.5
HM211	LEV4	0.5	LEV5	0.5
HM212	LEV4	0.5	LEV6	0.5
HM213	LEV4	0.5	LEV7	0.5
HM214	LEV4	0.5	LEV8	0.5
HM215	LEV4	0.5	LEV9	0.5
HM216	LEV5	0.5	LEV6	0.5
HM217	LEV5	0.5	LEV7	0.5
HM218	LEV5	0.5	LEV8	0.5
HM219	LEV5	0.5	LEV9	0.5
HM220	LEV6	0.5	LEV7	0.5

HM221	LEV6	0.5	LEV8	0.5
HM222	LEV6	0.5	LEV9	0.5
HM223	LEV7	0.5	LEV8	0.5
HM224	LEV7	0.5	LEV9	0.5
HM225	LEV8	0.5	LEV9	0.5
HM226	MAR	0.5	MAR1	0.5
HM227	MAR	0.5	MAR2	0.5
HM228	MAR	0.5	MAR3	0.5
HM229	MAR	0.5	MAR4	0.5
HM230	MAR	0.5	MAR5	0.5
HM231	MAR	0.5	MAR6	0.5
HM232	MAR	0.5	MAR7	0.5
HM233	MAR	0.5	MAR8	0.5
HM234	MAR	0.5	MAR9	0.5
HM235	MAR1	0.5	MAR2	0.5
HM236	MAR1	0.5	MAR3	0.5
HM237	MAR1	0.5	MAR4	0.5
HM238	MAR1	0.5	MAR5	0.5
HM239	MAR1	0.5	MAR6	0.5

HM240	MAR1	0.5	MAR7	0.5
HM241	MAR1	0.5	MAR8	0.5
HM242	MAR1	0.5	MAR9	0.5
HM243	MAR2	0.5	MAR3	0.5
HM244	MAR2	0.5	MAR4	0.5
HM245	MAR2	0.5	MAR5	0.5
HM246	MAR2	0.5	MAR6	0.5
HM247	MAR2	0.5	MAR7	0.5
HM248	MAR2	0.5	MAR8	0.5
HM249	MAR2	0.5	MAR9	0.5
HM250	MAR3	0.5	MAR4	0.5
HM251	MAR3	0.5	MAR5	0.5
HM252	MAR3	0.5	MAR6	0.5
HM253	MAR3	0.5	MAR7	0.5
HM254	MAR3	0.5	MAR8	0.5
HM255	MAR3	0.5	MAR9	0.5
HM256	MAR4	0.5	MAR5	0.5
HM257	MAR4	0.5	MAR6	0.5
HM258	MAR4	0.5	MAR7	0.5

HM259	MAR4	0.5	MAR8	0.5
HM260	MAR4	0.5	MAR9	0.5
HM261	MAR5	0.5	MAR6	0.5
HM262	MAR5	0.5	MAR7	0.5
HM263	MAR5	0.5	MAR8	0.5
HM264	MAR5	0.5	MAR9	0.5
HM265	MAR6	0.5	MAR7	0.5
HM266	MAR6	0.5	MAR8	0.5
HM267	MAR6	0.5	MAR9	0.5
HM268	MAR7	0.5	MAR8	0.5
HM269	MAR7	0.5	MAR9	0.5
HM270	MAR8	0.5	MAR9	0.5
HM271	NOR	0.5	NOR1	0.5
HM272	NOR	0.5	NOR2	0.5
HM273	NOR	0.5	NOR3	0.5
HM274	NOR	0.5	NOR4	0.5
HM275	NOR	0.5	NOR5	0.5
HM276	NOR	0.5	NOR6	0.5
HM277	NOR	0.5	NOR7	0.5

HM278	NOR	0.5	NOR8	0.5
HM279	NOR	0.5	NOR9	0.5
HM280	NOR1	0.5	NOR2	0.5
HM281	NOR1	0.5	NOR3	0.5
HM282	NOR1	0.5	NOR4	0.5
HM283	NOR1	0.5	NOR5	0.5
HM284	NOR1	0.5	NOR6	0.5
HM285	NOR1	0.5	NOR7	0.5
HM286	NOR1	0.5	NOR8	0.5
HM287	NOR1	0.5	NOR9	0.5
HM288	NOR2	0.5	NOR3	0.5
HM289	NOR2	0.5	NOR4	0.5
HM290	NOR2	0.5	NOR5	0.5
HM291	NOR2	0.5	NOR6	0.5
HM292	NOR2	0.5	NOR7	0.5
HM293	NOR2	0.5	NOR8	0.5
HM294	NOR2	0.5	NOR9	0.5
HM295	NOR3	0.5	NOR4	0.5
HM296	NOR3	0.5	NOR5	0.5

HM297	NOR3	0.5	NOR6	0.5
HM298	NOR3	0.5	NOR7	0.5
HM299	NOR3	0.5	NOR8	0.5
HM300	NOR3	0.5	NOR9	0.5
HM301	NOR4	0.5	NOR5	0.5
HM302	NOR4	0.5	NOR6	0.5
HM303	NOR4	0.5	NOR7	0.5
HM304	NOR4	0.5	NOR8	0.5
HM305	NOR4	0.5	NOR9	0.5
HM306	NOR5	0.5	NOR6	0.5
HM307	NOR5	0.5	NOR7	0.5
HM308	NOR5	0.5	NOR8	0.5
HM309	NOR5	0.5	NOR9	0.5
HM310	NOR6	0.5	NOR7	0.5
HM311	NOR6	0.5	NOR8	0.5
HM312	NOR6	0.5	NOR9	0.5
HM313	NOR7	0.5	NOR8	0.5
HM314	NOR7	0.5	NOR9	0.5
HM315	NOR8	0.5	NOR9	0.5

HM316	PEF	0.5	PEF1	0.5
HM317	PEF	0.5	PEF2	0.5
HM318	PEF	0.5	PEF3	0.5
HM319	PEF	0.5	PEF4	0.5
HM320	PEF	0.5	PEF5	0.5
HM321	PEF	0.5	PEF6	0.5
HM322	PEF	0.5	PEF7	0.5
HM323	PEF	0.5	PEF8	0.5
HM324	PEF	0.5	PEF9	0.5
HM325	PEF1	0.5	PEF2	0.5
HM326	PEF1	0.5	PEF3	0.5
HM327	PEF1	0.5	PEF4	0.5
HM328	PEF1	0.5	PEF5	0.5
HM329	PEF1	0.5	PEF6	0.5
HM330	PEF1	0.5	PEF7	0.5
HM331	PEF1	0.5	PEF8	0.5
HM332	PEF1	0.5	PEF9	0.5
HM333	PEF2	0.5	PEF3	0.5
HM334	PEF2	0.5	PEF4	0.5

HM335	PEF2	0.5	PEF5	0.5
HM336	PEF2	0.5	PEF6	0.5
HM337	PEF2	0.5	PEF7	0.5
HM338	PEF2	0.5	PEF8	0.5
HM339	PEF2	0.5	PEF9	0.5
HM340	PEF3	0.5	PEF4	0.5
HM341	PEF3	0.5	PEF5	0.5
HM342	PEF3	0.5	PEF6	0.5
HM343	PEF3	0.5	PEF7	0.5
HM344	PEF3	0.5	PEF8	0.5
HM345	PEF3	0.5	PEF9	0.5
HM346	PEF4	0.5	PEF5	0.5
HM347	PEF4	0.5	PEF6	0.5
HM348	PEF4	0.5	PEF7	0.5
HM349	PEF4	0.5	PEF8	0.5
HM350	PEF4	0.5	PEF9	0.5
HM351	PEF5	0.5	PEF6	0.5
HM352	PEF5	0.5	PEF7	0.5
HM353	PEF5	0.5	PEF8	0.5

HM354	PEF5	0.5	PEF9	0.5
HM355	PEF6	0.5	PEF7	0.5
HM356	PEF6	0.5	PEF8	0.5
HM357	PEF6	0.5	PEF9	0.5
HM358	PEF7	0.5	PEF8	0.5
HM359	PEF7	0.5	PEF9	0.5
HM360	PEF8	0.5	PEF9	0.5
HM361	SAR	0.5	SAR1	0.5
HM362	SAR	0.5	SAR2	0.5
HM363	SAR	0.5	SAR3	0.5
HM364	SAR	0.5	SAR4	0.5
HM365	SAR	0.5	SAR5	0.5
HM366	SAR	0.5	SAR6	0.5
HM367	SAR	0.5	SAR7	0.5
HM368	SAR	0.5	SAR8	0.5
HM369	SAR	0.5	SAR9	0.5
HM370	SAR1	0.5	SAR2	0.5
HM371	SAR1	0.5	SAR3	0.5
HM372	SAR1	0.5	SAR4	0.5

HM373	SAR1	0.5	SAR5	0.5
HM374	SAR1	0.5	SAR6	0.5
HM375	SAR1	0.5	SAR7	0.5
HM376	SAR1	0.5	SAR8	0.5
HM377	SAR1	0.5	SAR9	0.5
HM378	SAR2	0.5	SAR3	0.5
HM379	SAR2	0.5	SAR4	0.5
HM380	SAR2	0.5	SAR5	0.5
HM381	SAR2	0.5	SAR6	0.5
HM382	SAR2	0.5	SAR7	0.5
HM383	SAR2	0.5	SAR8	0.5
HM384	SAR2	0.5	SAR9	0.5
HM385	SAR3	0.5	SAR4	0.5
HM386	SAR3	0.5	SAR5	0.5
HM387	SAR3	0.5	SAR6	0.5
HM388	SAR3	0.5	SAR7	0.5
HM389	SAR3	0.5	SAR8	0.5
HM390	SAR3	0.5	SAR9	0.5
HM391	SAR4	0.5	SAR5	0.5

HM392	SAR4	0.5	SAR6	0.5
HM393	SAR4	0.5	SAR7	0.5
HM394	SAR4	0.5	SAR8	0.5
HM395	SAR4	0.5	SAR9	0.5
HM396	SAR5	0.5	SAR6	0.5
HM397	SAR5	0.5	SAR7	0.5
HM398	SAR5	0.5	SAR8	0.5
HM399	SAR5	0.5	SAR9	0.5
HM400	SAR6	0.5	SAR7	0.5
HM401	SAR6	0.5	SAR8	0.5
HM402	SAR6	0.5	SAR9	0.5
HM403	SAR7	0.5	SAR8	0.5
HM404	SAR7	0.5	SAR9	0.5
HM405	SAR8	0.5	SAR9	0.5

*N.B. HM = hypothetical mixtures, CIP =ciprofloxacin, DAN = danofloxacin, ENO = enoxacin, ENR = enrofloxacin, LEV = levofloxacin, MAR = marbofloxacin, NOR = norfloxacin, PEF = pefloxacin, and SAR = sarafloxacin

Table S5. Computed X-variances, R^2, and Q^2_{LOO} values after incorporating each LVs

Number of LVs	X-Variance	R^2	Q^2_{LOO}	Inference
1	0.316	0.599	0.544	-

2	0.623	0.671	0.612	-
3	0.732	0.766	0.657	-
4	0.833	0.864	0.801	-
5	**0.948**	**0.882**	**0.849**	Mximum possible X-variance accounted. Thus, the optimum number of **LVs = 5**
6	1.000	0.885	0.858	In PLS, the number of LVs < number of descriptors

Table S6. Optimized hyperparameters of the ML algorithm used in this study

ML algorithm	Optimized setting
RF	*Max-depth = 2, max_leaf_nodes = none, min_impurity_decrease = 0.0, min_sample_split = 2, min_sample_leaf = 3, n_estimator = 200, min_weight_fraction_leaf =0.0*
AdaBoost	*n-Estimator =70 , loss =square*
GB	*Max-depth = 4, min_sample_split = 2, min_sample_leaf = 1, n_estimator = 50, criterion = friedman_msc, min_weight_fraction_leaf = 0.0, min_impurity_decrease = 0.0, subsample = 1.0, learning_rate = 0.1, loss = squared_error*
XGB	*n_estimator = 200, max_depth = none, booster = gblinear, learning_rate =1.0*
SVM	*C = 5, degree = 2, gamma =auto*
LSVM	*C =1*
RR	*Alpha (α) =0.5*

Table S7. Toxicity prediction of hypothetical binary mixtures along with their reliability of prediction and AD status

Hypothetical Mixtures	Predicted response	PredictionQuality	AD status	Toxic class
1	7.277	Good	In	Less toxic
2	7.342	Good	In	Highly toxic
3	7.313	Good	In	Highly toxic
4	7.280	Good	In	Less toxic
5	7.288	Good	In	Less toxic
6	7.219	Good	In	Less toxic
7	7.500	Moderate	In	Highly toxic
8	7.250	Good	In	Less toxic
9	7.443	Moderate	In	Highly toxic
10	7.308	Good	In	Highly toxic
11	7.278	Good	In	Less toxic
12	7.246	Good	In	Less toxic
13	7.254	Good	In	Less toxic
14	7.185	Good	In	Less toxic
15	7.466	Moderate	In	Highly toxic
16	7.216	Good	In	Less toxic
17	7.409	Moderate	In	Highly toxic

18	7.343	Good	In	Highly toxic
19	7.310	Good	In	Highly toxic
20	7.319	Good	In	Highly toxic
21	7.249	Good	In	Less toxic
22	7.530	Moderate	In	Highly toxic
23	7.280	Good	In	Less toxic
24	7.474	Moderate	In	Highly toxic
25	7.281	Good	In	Less toxic
26	7.289	Good	In	Less toxic
27	7.220	Good	In	Less toxic
28	7.501	Moderate	In	Highly toxic
29	7.251	Good	In	Less toxic
30	7.444	Moderate	In	Highly toxic
31	7.257	Good	In	Less toxic
32	7.188	Good	In	Less toxic
33	7.469	Moderate	In	Highly toxic
34	7.219	Good	In	Less toxic
35	7.412	Moderate	In	Highly toxic
36	7.196	Good	In	Less toxic
37	7.477	Moderate	In	Highly toxic
38	7.227	Good	In	Less toxic
39	7.420	Moderate	In	Highly toxic

40	7.408	Moderate	In	Highly toxic
41	7.158	Good	In	Less toxic
42	7.351	Good	In	Highly toxic
43	7.439	Moderate	In	Highly toxic
44	7.632	Moderate	In	Highly toxic
45	7.382	Good	In	Highly toxic
46	7.012	Good	In	Less toxic
47	7.051	Good	In	Less toxic
48	7.008	Good	In	Less toxic
49	7.302	Good	In	Highly toxic
50	7.289	Good	In	Less toxic
51	7.281	Good	In	Less toxic
52	7.525	Moderate	In	Highly toxic
53	7.264	Good	In	Less toxic
54	7.482	Moderate	In	Highly toxic
55	7.042	Good	In	Less toxic
56	7.000	Good	In	Less toxic
57	7.293	Good	In	Less toxic
58	7.280	Good	In	Less toxic
59	7.273	Good	In	Less toxic
60	7.516	Moderate	In	Highly toxic
61	7.255	Good	In	Less toxic

62	7.474	Moderate	In	Highly toxic
63	7.038	Good	In	Less toxic
64	7.332	Good	In	Highly toxic
65	7.318	Good	In	Highly toxic
66	7.311	Good	In	Highly toxic
67	7.555	Moderate	In	Highly toxic
68	7.294	Good	In	Less toxic
69	7.512	Moderate	In	Highly toxic
70	7.289	Good	In	Less toxic
71	7.276	Good	In	Less toxic
72	7.268	Good	In	Less toxic
73	7.512	Moderate	In	Highly toxic
74	7.251	Good	In	Less toxic
75	7.469	Moderate	In	Highly toxic
76	7.570	Moderate	In	Highly toxic
77	7.562	Moderate	In	Highly toxic
78	7.806	Bad/Unreliable	In	Highly toxic
79	7.545	Moderate	In	Highly toxic
80	7.763	Bad/Unreliable	In	Highly toxic
81	7.549	Moderate	In	Highly toxic
82	7.792	Bad/Unreliable	In	Highly toxic
83	7.531	Moderate	In	Highly toxic

84	7.750	Bad/Unreliable	In	Highly toxic
85	7.785	Bad/Unreliable	In	Highly toxic
86	7.524	Moderate	In	Highly toxic
87	7.742	Bad/Unreliable	In	Highly toxic
88	7.768	Bad/Unreliable	In	Highly toxic
89	7.986	Bad/Unreliable	In	Highly toxic
90	7.725	Bad/Unreliable	In	Highly toxic
91	6.319	Good	In	Less toxic
92	6.409	Good	In	Less toxic
93	6.319	Good	In	Less toxic
94	6.348	Good	In	Less toxic
95	6.316	Good	In	Less toxic
96	6.309	Good	In	Less toxic
97	6.600	Good	In	Less toxic
98	6.300	Good	In	Less toxic
99	6.754	Good	In	Less toxic
100	6.397	Good	In	Less toxic
101	6.307	Good	In	Less toxic
102	6.336	Good	In	Less toxic
103	6.304	Good	In	Less toxic
104	6.296	Good	In	Less toxic
105	6.588	Good	In	Less toxic

106	6.287	Good	In	Less toxic
107	6.742	Good	In	Less toxic
108	6.397	Good	In	Less toxic
109	6.426	Good	In	Less toxic
110	6.394	Good	In	Less toxic
111	6.387	Good	In	Less toxic
112	6.678	Good	In	Less toxic
113	6.378	Good	In	Less toxic
114	6.832	Good	In	Less toxic
115	6.337	Good	In	Less toxic
116	6.304	Good	In	Less toxic
117	6.297	Good	In	Less toxic
118	6.588	Good	In	Less toxic
119	6.288	Good	In	Less toxic
120	6.742	Good	In	Less toxic
121	6.333	Good	In	Less toxic
122	6.326	Good	In	Less toxic
123	6.617	Good	In	Less toxic
124	6.317	Good	In	Less toxic
125	6.771	Good	In	Less toxic
126	6.294	Good	In	Less toxic
127	6.585	Good	In	Less toxic

128	6.285	Good	In	Less toxic
129	6.739	Good	In	Less toxic
130	6.578	Good	In	Less toxic
131	6.277	Good	In	Less toxic
132	6.732	Good	In	Less toxic
133	6.569	Good	In	Less toxic
134	7.023	Good	In	Less toxic
135	6.723	Good	In	Less toxic
136	7.115	Good	In	Less toxic
137	7.211	Good	In	Less toxic
138	7.111	Good	In	Less toxic
139	7.066	Good	In	Less toxic
140	7.117	Good	In	Less toxic
141	7.032	Good	In	Less toxic
142	7.370	Good	In	Highly toxic
143	7.104	Good	In	Less toxic
144	7.340	Good	In	Highly toxic
145	7.203	Good	In	Less toxic
146	7.102	Good	In	Less toxic
147	7.057	Good	In	Less toxic
148	7.108	Good	In	Less toxic
149	7.023	Good	In	Less toxic

150	7.361	Good	In	Highly toxic
151	7.096	Good	In	Less toxic
152	7.331	Good	In	Highly toxic
153	7.199	Good	In	Less toxic
154	7.153	Good	In	Less toxic
155	7.204	Good	In	Less toxic
156	7.119	Good	In	Less toxic
157	7.457	Moderate	In	Highly toxic
158	7.192	Good	In	Less toxic
159	7.427	Moderate	In	Highly toxic
160	7.053	Good	In	Less toxic
161	7.104	Good	In	Less toxic
162	7.019	Good	In	Less toxic
163	7.357	Good	In	Highly toxic
164	7.092	Good	In	Less toxic
165	7.327	Good	In	Highly toxic
166	7.059	Good	In	Less toxic
167	6.974	Good	In	Less toxic
168	7.312	Good	In	Highly toxic
169	7.046	Good	In	Less toxic
170	7.282	Good	In	Less toxic
171	7.025	Good	In	Less toxic

172	7.363	Good	In	Highly toxic
173	7.097	Good	In	Less toxic
174	7.333	Good	In	Highly toxic
175	7.278	Good	In	Less toxic
176	7.012	Good	In	Less toxic
177	7.248	Good	In	Less toxic
178	7.350	Good	In	Highly toxic
179	7.586	Moderate	In	Highly toxic
180	7.321	Good	In	Highly toxic
181	6.539	Good	In	Less toxic
182	6.541	Good	In	Less toxic
183	6.641	Good	In	Less toxic
184	6.581	Good	In	Less toxic
185	6.613	Good	In	Less toxic
186	6.477	Good	In	Less toxic
187	6.806	Good	In	Less toxic
188	6.516	Good	In	Less toxic
189	6.705	Good	In	Less toxic
190	6.445	Good	Outside AD	Less toxic
191	6.544	Good	In	Less toxic
192	6.484	Good	In	Less toxic
193	6.517	Good	In	Less toxic

194	6.380	Good	In	Less toxic
195	6.710	Good	In	Less toxic
196	6.420	Good	In	Less toxic
197	6.608	Good	In	Less toxic
198	6.547	Good	Outside AD	Less toxic
199	6.487	Good	In	Less toxic
200	6.519	Good	In	Less toxic
201	6.383	Good	In	Less toxic
202	6.712	Good	Outside AD	Less toxic
203	6.422	Good	In	Less toxic
204	6.610	Good	Outside AD	Less toxic
205	6.586	Good	In	Less toxic
206	6.619	Good	In	Less toxic
207	6.482	Good	In	Less toxic
208	6.811	Good	Outside AD	Less toxic
209	6.521	Good	In	Less toxic
210	6.710	Good	In	Less toxic
211	6.559	Good	In	Less toxic
212	6.422	Good	In	Less toxic
213	6.751	Good	In	Less toxic
214	6.461	Good	In	Less toxic
215	6.650	Good	In	Less toxic

216	6.455	Good	In	Less toxic
217	6.784	Good	In	Less toxic
218	6.494	Good	In	Less toxic
219	6.682	Good	In	Less toxic
220	6.647	Good	In	Less toxic
221	6.357	Good	In	Less toxic
222	6.546	Good	In	Less toxic
223	6.687	Good	In	Less toxic
224	6.875	Good	Outside AD	Less toxic
225	6.585	Good	In	Less toxic
226	7.129	Good	In	Less toxic
227	7.153	Good	In	Less toxic
228	7.218	Good	In	Less toxic
229	7.187	Good	In	Less toxic
230	7.197	Good	In	Less toxic
231	7.089	Good	In	Less toxic
232	7.397	Moderate	In	Highly toxic
233	7.106	Good	In	Less toxic
234	7.302	Good	In	Highly toxic
235	7.063	Good	In	Less toxic
236	7.128	Good	In	Less toxic
237	7.097	Good	In	Less toxic

238	7.107	Good	In	Less toxic
239	6.999	Good	In	Less toxic
240	7.307	Good	In	Highly toxic
241	7.016	Good	In	Less toxic
242	7.211	Good	In	Less toxic
243	7.152	Good	In	Less toxic
244	7.121	Good	In	Less toxic
245	7.131	Good	In	Less toxic
246	7.023	Good	In	Less toxic
247	7.331	Good	Outside AD	Highly toxic
248	7.040	Good	In	Less toxic
249	7.235	Good	In	Less toxic
250	7.186	Good	In	Less toxic
251	7.196	Good	In	Less toxic
252	7.088	Good	In	Less toxic
253	7.396	Moderate	In	Highly toxic
254	7.105	Good	In	Less toxic
255	7.300	Good	In	Highly toxic
256	7.165	Good	In	Less toxic
257	7.057	Good	In	Less toxic
258	7.365	Good	In	Highly toxic
259	7.074	Good	In	Less toxic

260	7.269	Good	In	Less toxic
261	7.068	Good	In	Less toxic
262	7.375	Good	Outside AD	Highly toxic
263	7.084	Good	In	Less toxic
264	7.280	Good	In	Less toxic
265	7.267	Good	In	Less toxic
266	6.977	Good	In	Less toxic
267	7.172	Good	In	Less toxic
268	7.284	Good	In	Less toxic
269	7.480	Moderate	Outside AD	Highly toxic
270	7.189	Good	In	Less toxic
271	6.240	Good	In	Less toxic
272	6.289	Good	In	Less toxic
273	6.294	Good	In	Less toxic
274	6.194	Good	In	Less toxic
275	6.267	Good	In	Less toxic
276	6.141	Good	In	Less toxic
277	6.466	Good	In	Less toxic
278	6.216	Good	In	Less toxic
279	6.396	Good	In	Less toxic
280	6.242	Good	In	Less toxic
281	6.246	Good	In	Less toxic

282	6.146	Good	In	Less toxic
283	6.220	Good	In	Less toxic
284	6.094	Moderate	In	Less toxic
285	6.418	Good	In	Less toxic
286	6.169	Good	In	Less toxic
287	6.348	Good	In	Less toxic
288	6.295	Good	In	Less toxic
289	6.195	Good	In	Less toxic
290	6.269	Good	In	Less toxic
291	6.143	Good	In	Less toxic
292	6.467	Good	In	Less toxic
293	6.217	Good	In	Less toxic
294	6.397	Good	In	Less toxic
295	6.200	Good	In	Less toxic
296	6.273	Good	In	Less toxic
297	6.147	Good	In	Less toxic
298	6.472	Good	In	Less toxic
299	6.222	Good	In	Less toxic
300	6.402	Good	In	Less toxic
301	6.173	Good	In	Less toxic
302	6.047	Moderate	In	Less toxic
303	6.371	Good	In	Less toxic

304	6.122	Good	In	Less toxic
305	6.301	Good	In	Less toxic
306	6.121	Good	In	Less toxic
307	6.445	Good	In	Less toxic
308	6.196	Good	In	Less toxic
309	6.375	Good	In	Less toxic
310	6.319	Good	In	Less toxic
311	6.069	Moderate	In	Less toxic
312	6.249	Good	In	Less toxic
313	6.394	Good	In	Less toxic
314	6.573	Good	In	Less toxic
315	6.324	Good	In	Less toxic
316	6.530	Good	In	Less toxic
317	6.595	Good	In	Less toxic
318	6.562	Good	In	Less toxic
319	6.418	Good	In	Less toxic
320	6.554	Good	In	Less toxic
321	6.380	Good	In	Less toxic
322	6.777	Good	In	Less toxic
323	6.516	Good	In	Less toxic
324	6.722	Good	In	Less toxic
325	6.561	Good	In	Less toxic

326	6.528	Good	In	Less toxic
327	6.384	Good	In	Less toxic
328	6.520	Good	In	Less toxic
329	6.346	Good	In	Less toxic
330	6.743	Good	In	Less toxic
331	6.482	Good	In	Less toxic
332	6.688	Good	In	Less toxic
333	6.593	Good	In	Less toxic
334	6.449	Good	In	Less toxic
335	6.585	Good	In	Less toxic
336	6.411	Good	In	Less toxic
337	6.809	Good	In	Less toxic
338	6.547	Good	In	Less toxic
339	6.753	Good	In	Less toxic
340	6.416	Good	In	Less toxic
341	6.552	Good	In	Less toxic
342	6.378	Good	In	Less toxic
343	6.775	Good	In	Less toxic
344	6.514	Good	In	Less toxic
345	6.720	Good	In	Less toxic
346	6.407	Good	In	Less toxic
347	6.234	Good	In	Less toxic

348	6.631	Good	In	Less toxic
349	6.370	Good	In	Less toxic
350	6.576	Good	In	Less toxic
351	6.369	Good	In	Less toxic
352	6.767	Good	In	Less toxic
353	6.505	Good	In	Less toxic
354	6.711	Good	In	Less toxic
355	6.593	Good	In	Less toxic
356	6.332	Good	In	Less toxic
357	6.538	Good	In	Less toxic
358	6.729	Good	In	Less toxic
359	6.935	Good	In	Less toxic
360	6.674	Good	In	Less toxic
361	7.113	Good	Outside AD	Less toxic
362	7.268	Good	Outside AD	Less toxic
363	7.048	Good	Outside AD	Less toxic
364	7.075	Good	Outside AD	Less toxic
365	7.134	Good	Outside AD	Less toxic
366	7.017	Good	Outside AD	Less toxic
367	7.390	Moderate	Outside AD	Highly toxic
368	7.071	Good	Outside AD	Less toxic
369	7.320	Good	Outside AD	Highly toxic

370	7.208	Good	Outside AD	Less toxic
371	6.987	Good	Outside AD	Less toxic
372	7.014	Good	Outside AD	Less toxic
373	7.073	Good	Outside AD	Less toxic
374	6.956	Good	Outside AD	Less toxic
375	7.329	Good	Outside AD	Highly toxic
376	7.011	Good	Outside AD	Less toxic
377	7.259	Good	Outside AD	Less toxic
378	7.142	Good	Outside AD	Less toxic
379	7.170	Good	Outside AD	Less toxic
380	7.229	Good	Outside AD	Less toxic
381	7.112	Good	Outside AD	Less toxic
382	7.485	Moderate	Outside AD	Highly toxic
383	7.166	Good	Outside AD	Less toxic
384	7.414	Moderate	Outside AD	Highly toxic
385	6.949	Good	Outside AD	Less toxic
386	7.008	Good	Outside AD	Less toxic
387	6.891	Good	Outside AD	Less toxic
388	7.264	Good	Outside AD	Less toxic
389	6.945	Good	Outside AD	Less toxic
390	7.193	Good	Outside AD	Less toxic
391	7.036	Good	Outside AD	Less toxic

392	6.918	Good	Outside AD	Less toxic
393	7.292	Good	Outside AD	Less toxic
394	6.973	Good	Outside AD	Less toxic
395	7.221	Good	Outside AD	Less toxic
396	6.977	Good	Outside AD	Less toxic
397	7.350	Good	Outside AD	Highly toxic
398	7.032	Good	Outside AD	Less toxic
399	7.280	Good	Outside AD	Less toxic
400	7.233	Good	Outside AD	Less toxic
401	6.915	Good	Outside AD	Less toxic
402	7.163	Good	Outside AD	Less toxic
403	7.288	Good	Outside AD	Less toxic
404	7.536	Moderate	Outside AD	Highly toxic
405	7.217	Good	Outside AD	Less toxic

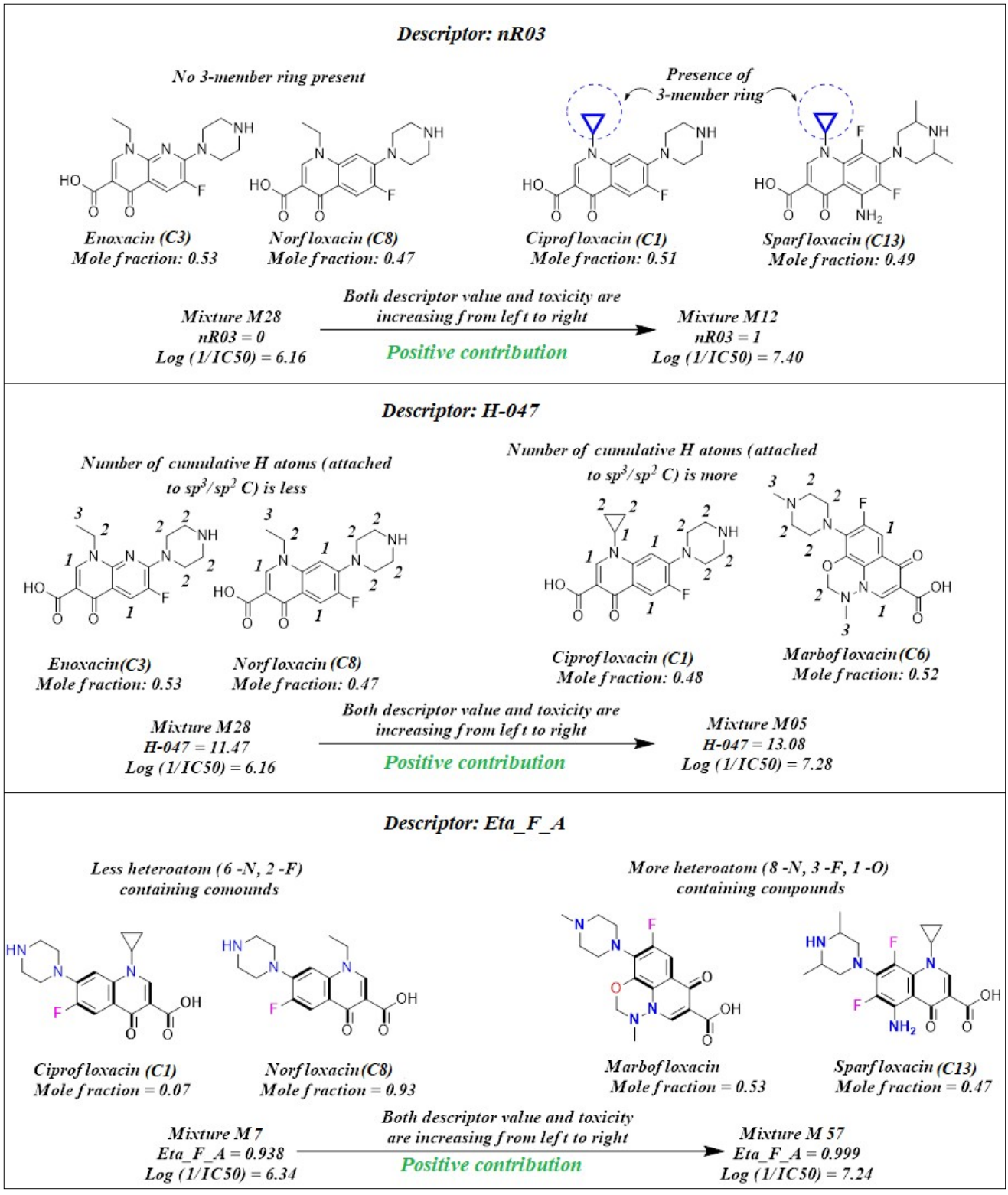


Figure S1. Significance of positive contributory descriptors towards toxicity

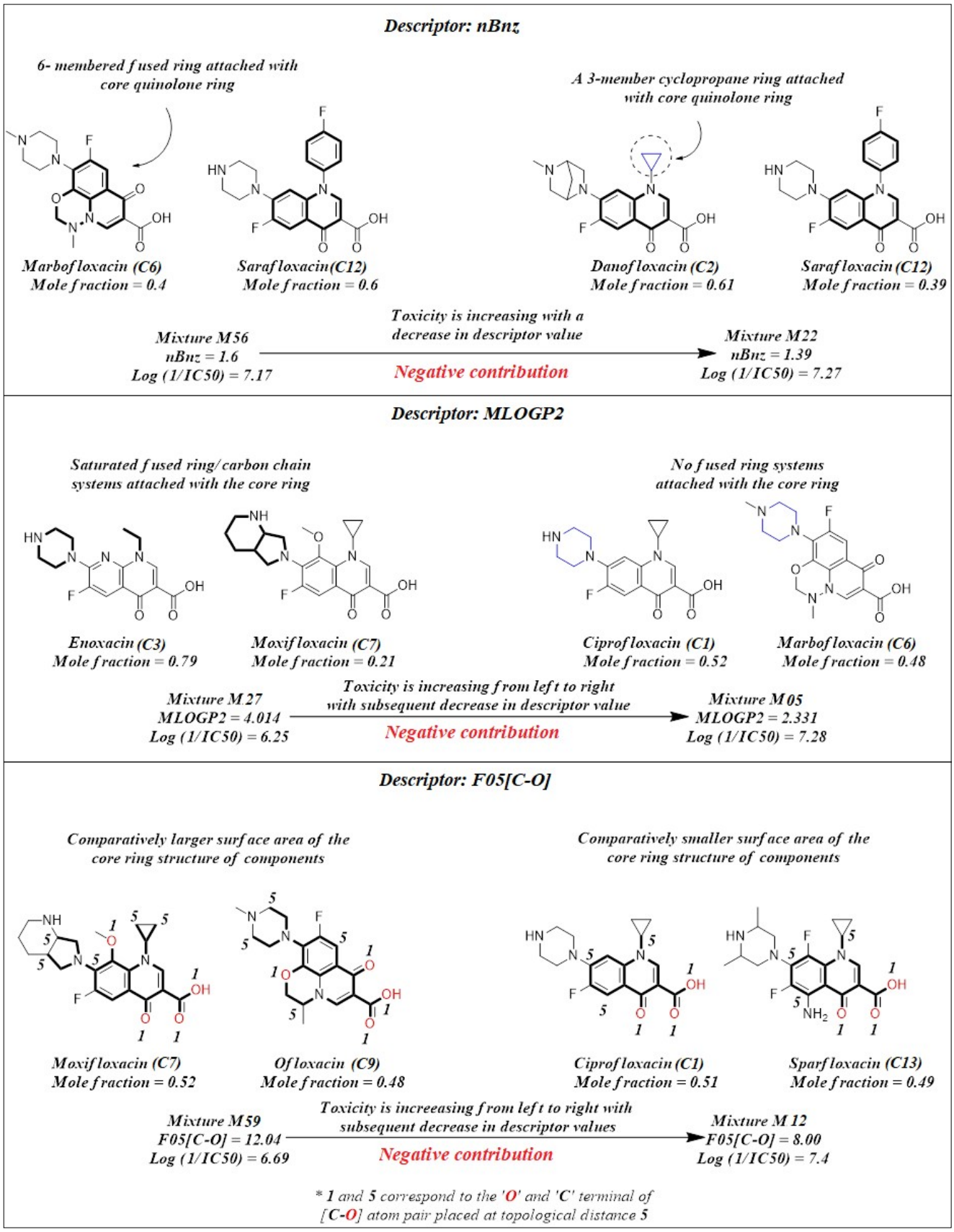


Figure S2. Significance of negative contributory descriptors towards toxicity

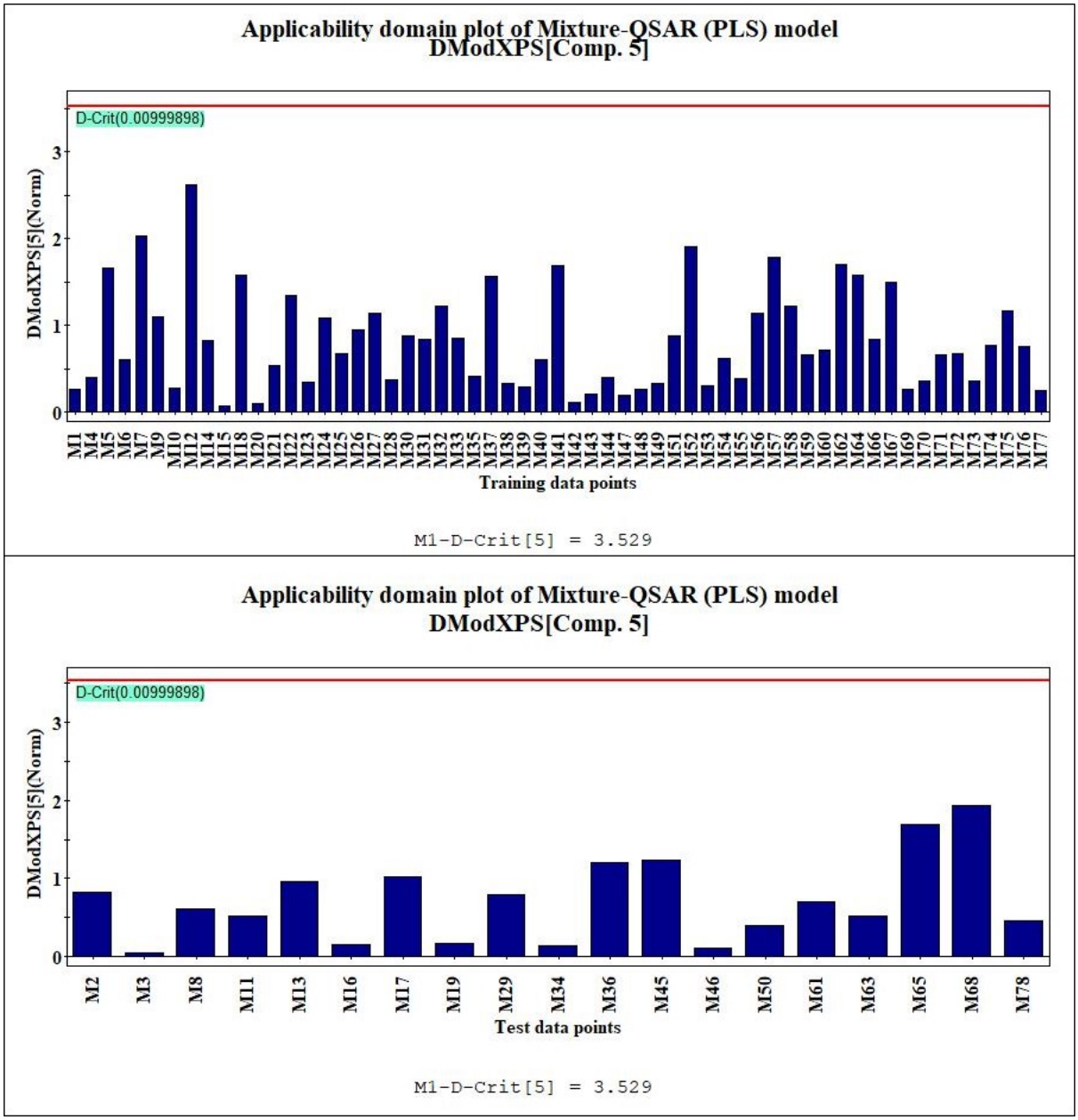


Figure S3. Applicability domain plot of the developed Mixture-QSAR (PLS) model