Supplementary Material (SM)

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Virtual chemical analysis and machine learning-based prediction of polyethylene terephthalate nanoplastics toxicity on aquatic organisms as influenced by particle size and properties

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- **Tables S1 and S2**
- **References from 41R-55R**

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Table S1. SVM training output for the Tc AChE

Show	Method	Kernel Function	Cost	Gamma	# SV	Training RASE	Best
[ ]	Model 1	Radial Basis Function	3.37672	0.18732	5	0.13275	
[ ]	Model 2	Radial Basis Function	4.51948	0.23859	5	0.10908	
[ ]	Model 3	Radial Basis Function	3.17072	0.03026	4	0.76519	
[ ]	Model 4	Radial Basis Function	4.75716	0.01584	4	0.85201	
[ ]	Model 5	Radial Basis Function	3.94507	0.10586	5	0.26179	
[ ]	Model 6	Radial Basis Function	2.44329	0.14979	5	0.3744	
[ ]	Model 7	Radial Basis Function	0.10312	0.01009	4	1.0334	
[ ]	Model 8	Radial Basis Function	0.58043	0.09079	4	0.86356	
[ ]	Model 9	Radial Basis Function	2.07709	0.05255	5	0.70446	
[ ]	Model 10	Radial Basis Function	0.88454	0.33193	4	0.61806	
[ ]	Model 11	Radial Basis Function	1.37366	0.39858	4	0.39096	
[ ]	Model 12	Radial Basis Function	0.19173	0.47808	4	0.89397	
[ ]	Model 13	Radial Basis Function	1.70465	0.20981	5	0.44003	
[ ]	Model 14	Radial Basis Function	0.40487	0.24775	5	0.81678	
[ ]	Model 15	Radial Basis Function	2.25157	0.29769	5	0.1908	
[ ]	Model 16	Radial Basis Function	2.95083	0.43345	4	0.10288	
[x]	Model 17	Radial Basis Function	2.49247	0.49978	4	0.09741	Smallest RASE
[ ]	Model 18	Radial Basis Function	4.37551	0.46078	4	0.09894	
[ ]	Model 19	Radial Basis Function	4.95611	0.38486	5	0.10916	
[ ]	Model 20	Radial Basis Function	3.67731	0.36429	5	0.10918	

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Table S2. SVM training output for the Zf CYP450

Show	Method	Kernel Function	Cost	Gamma	# SV	Training RASE	Best
[ ]	Model 1	Radial Basis Function	3.34595	0.28001	5	0.12246	
[ ]	Model 2	Radial Basis Function	4.49687	0.23651	5	0.12248	
[ ]	Model 3	Radial Basis Function	2.79785	0.16683	5	0.33749	
[x]	Model 4	Radial Basis Function	3.71729	0.19253	4	0.11033	Smallest RASE
[ ]	Model 5	Radial Basis Function	4.02318	0.00538	4	1.18516	
[ ]	Model 6	Radial Basis Function	4.92471	0.12673	5	0.20215	
[ ]	Model 7	Radial Basis Function	0.64441	0.15186	5	0.96752	
[ ]	Model 8	Radial Basis Function	0.23326	0.25538	5	1.0937	
[ ]	Model 9	Radial Basis Function	1.23388	0.02136	4	1.165	
[ ]	Model 10	Radial Basis Function	0.02829	0.06238	4	1.2187	
[ ]	Model 11	Radial Basis Function	1.91165	0.09835	5	0.85228	
[ ]	Model 12	Radial Basis Function	3.05518	0.04884	5	0.92632	
[ ]	Model 13	Radial Basis Function	0.53571	0.48436	5	0.84824	
[ ]	Model 14	Radial Basis Function	1.39501	0.42868	5	0.33586	
[ ]	Model 15	Radial Basis Function	2.19444	0.2182	5	0.33487	
[ ]	Model 16	Radial Basis Function	1.04508	0.30485	5	0.64818	
[ ]	Model 17	Radial Basis Function	1.73037	0.3514	5	0.24177	
[ ]	Model 18	Radial Basis Function	3.85506	0.39807	5	0.12253	
[ ]	Model 19	Radial Basis Function	3.22307	0.49968	5	0.12247	
[ ]	Model 20	Radial Basis Function	4.74514	0.44231	5	0.1223	

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