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In Silico-Driven Identification of Novel Molluscicides Effective Against *Biomphalaria glabrata* (Say, 1818)

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SUPPORT INFORMATION

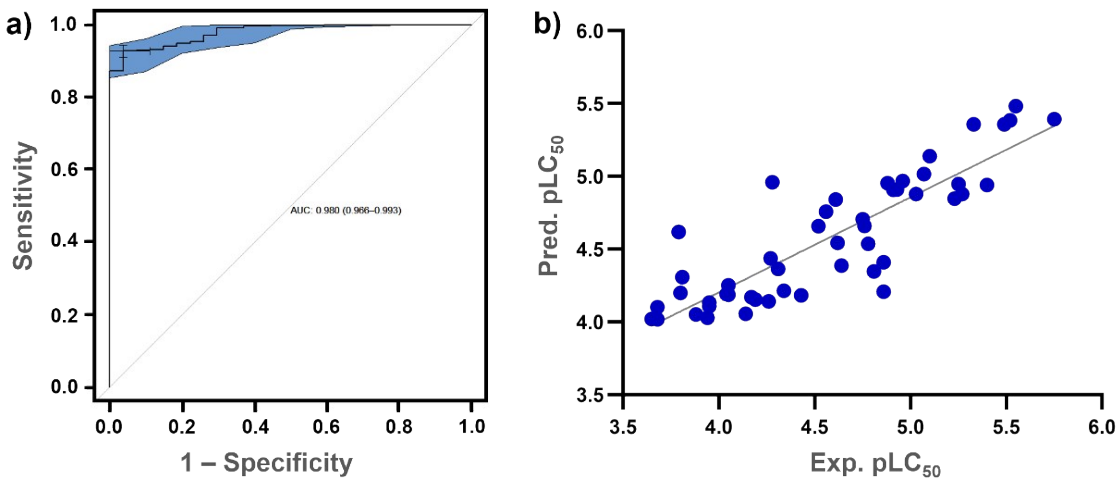
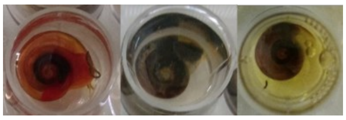
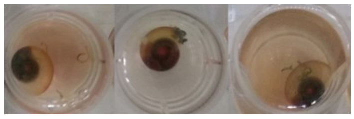


Figure S1. (a) ROC curve of the best shape-based model ranked by the TanimotoCombo scoring function (AUC = 0.98); (b) Scatter plots of observed vs. predicted pLC_{50} values of the best Machine learning model (MACCS+RDKit) generated from 5-fold external cross-validation procedure.

Table S1. Frequency (%) of phenotypic alterations in adult snails of *Biomphalaria glabrata* after exposure to test compounds for 96h. Results are presented as means ± standard deviations.

Compounds concentration (μM)		Morphological alterations		
		Normal (%)	Lethargy and reclusion into the shell (%)	Hemolymph release (%)
				
3	6.25	44.4 ± 19.2	22.2 ± 19.2	33.3 ± 0
	12.5	33.3 ± 0.0	33.3 ± 0	33.3 ± 0
	25	0 ± 0	33.3 ± 0	66.7 ± 0
	50	0 ± 0	22.2 ± 19.2	77.8 ± 19.2
	100	0 ± 0	0 ± 0	100 ± 0
	200	0 ± 0	0 ± 0	100 ± 0
4	6.25	77.8 ± 19.2	0 ± 0	22.2 ± 19.2
	12.5	44.4 ± 19.2	33.3 ± 0	22.2 ± 19.2
	25	22.2 ± 19.2	33.3 ± 0	44.4 ± 19.2
	50	0 ± 0	22.2 ± 19.2	77.8 ± 19.2
	100	0 ± 0	0 ± 0	100 ± 0
	200	0 ± 0	0 ± 0	100 ± 0
5	6.25	88.9 ± 19.2	0 ± 0	11.1 ± 19.2
	12.5	55.6 ± 19.2	33.3 ± 0	11.1 ± 19.2
	25	55.6 ± 19.2	33.3 ± 0	11.1 ± 19.2
	50	44.4 ± 19.2	44.4 ± 19.2	11.1 ± 19.2
	100	0 ± 0	0 ± 0	100 ± 0
	200	0 ± 0	0 ± 0	100 ± 0
6	6.25	77.8 ± 19.2	22.2 ± 19.2	0 ± 0
	12.5	55.6 ± 19.2	33.3 ± 0	11.1 ± 19.2
	25	55.6 ± 19.2	33.3 ± 0	11.1 ± 19.2
	50	33.3 ± 0	55.6 ± 19.2	11.1 ± 19.2
	100	0 ± 0	0 ± 0	100 ± 0
	200	0 ± 0	0 ± 0	100 ± 0
7	6.25	77.8 ± 19.2	22.2 ± 19.2	0 ± 0
	12.5	66.7 ± 0	33.3 ± 0	0 ± 0
	25	55.6 ± 19.2	22.2 ± 19.2	22.2 ± 19.2
	50	22.2 ± 19.2	22.2 ± 19.2	55.6 ± 19.2
	100	0 ± 0	22.2 ± 19.2	77.8 ± 19.2
	200	0 ± 0	11.1 ± 19.2	88.9 ± 19.2
11	6.25	100 ± 0	0 ± 0	0 ± 0
	12.5	55.6 ± 19.2	33.3 ± 0	11.1 ± 19.2
	25	55.6 ± 19.2	33.3 ± 0	11.1 ± 19.2
	50	55.6 ± 19.2	33.3 ± 0	11.1 ± 19.2
	100	0 ± 0	0 ± 0	100 ± 0
	200	0 ± 0	0 ± 0	100 ± 0
12	6.25	100 ± 0	0 ± 0	0 ± 0
	12.5	66.7 ± 0	33.3 ± 0	0 ± 0
	25	66.7 ± 0	33.3 ± 0	0 ± 0
	50	66.7 ± 0	22.2 ± 19.2	11.1 ± 19.2
	100	0 ± 0	22.2 ± 19.2	77.8 ± 19.2
	200	0 ± 0	0 ± 0	100 ± 0