



Supporting Information

# VenomPred: A Machine Learning Based Platform for Molecular Toxicity Predictions

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**Table S1.** Performance evaluation results, based on test set prediction, obtained with the 5 top-scored models and consensus strategy compared to reference models included in VEGA for the mutagenicity endpoint.

Model	Specificity	Recall	Precision	MCC
RF-PubChem	0.84	0.85	0.87	0.69
SVM-Morgan	0.84	0.85	0.87	0.69
RF-Morgan	0.80	0.88	0.85	0.68
MLP-PubChem	0.80	0.88	0.85	0.68
SVM-PubChem	0.78	0.88	0.84	0.67
Consensus 3	0.84	0.88	0.87	0.72
Consensus 4	0.83	0.89	0.87	0.72
Consensus 5	0.83	0.88	0.87	0.71
VEGA	0.74	0.90	0.81	0.66

**Table S2.** Performance evaluation results, based on test set prediction, obtained with the 5 top-scored models and consensus strategy compared to reference models included in VEGA for the carcinogenicity endpoint.

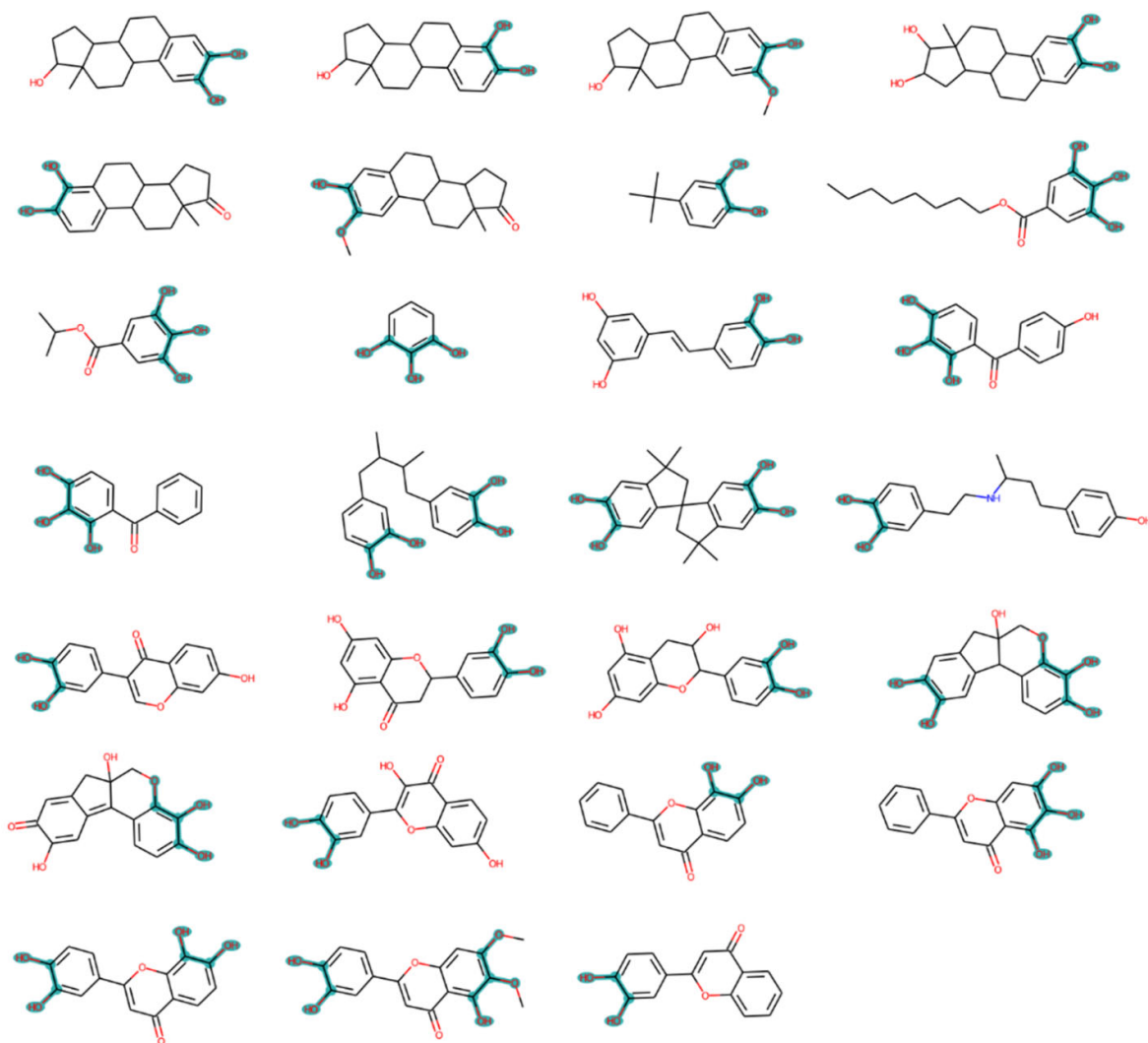
Model	Specificity	Recall	Precision	MCC
RF-PubChem	0.67	0.72	0.73	0.39
RF-RDKit	0.75	0.62	0.75	0.37
SVM-RDKit	0.72	0.63	0.74	0.35
SVM-PubChem	0.72	0.63	0.74	0.35
MLP-RDKit	0.61	0.66	0.68	0.27
Consensus 3	0.69	0.65	0.73	0.34
Consensus 4	0.72	0.69	0.75	0.41
Consensus 5	0.68	0.66	0.72	0.34
VEGA	0.60	0.72	0.69	0.32

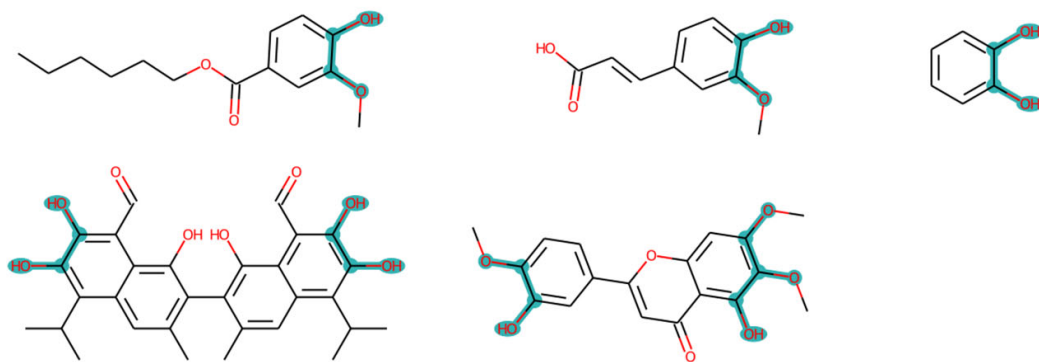
**Table S3.** Performance evaluation results, based on test set prediction, obtained with the 5 top-scored models and consensus strategy compared to reference models included in VEGA for the estrogenicity endpoint.

Model	Specificity	Recall	Precision	MCC
RF-PubChem	0.96	0.85	0.92	0.83
SVM-PubChem	0.91	0.89	0.84	0.79
MLP-PubChem	0.90	0.85	0.82	0.74
SVM-Morgan	0.91	0.78	0.82	0.69
MLP-Morgan	0.89	0.72	0.78	0.62
Consensus 3	0.94	0.91	0.89	0.84
Consensus 4	0.94	0.89	0.89	0.83
Consensus 5	0.95	0.85	0.90	0.81
VEGA	0.88	0.78	0.78	0.65

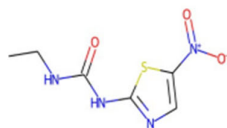
**Table S4.** Performance evaluation results, based on test set prediction, obtained with the 5 top-scored models and consensus strategy compared to reference models included in VEGA for the hepatotoxicity endpoint.

Model	Specificity	Recall	Precision	MCC
SVM-Morgan	0.37	0.86	0.69	0.26
SVM-RDKit	0.40	0.83	0.69	0.25
KNN-RDKit	0.48	0.74	0.70	0.23
MLP-PubChem	0.67	0.55	0.73	0.21
MLP-RDKit	0.63	0.54	0.70	0.17
Consensus 3	0.42	0.85	0.70	0.29
Consensus 4	0.58	0.69	0.73	0.27
Consensus 5	0.63	0.70	0.76	0.33
VEGA	0.37	0.85	0.68	0.24

**Figure S1.** Compounds endowed with estrogenic activity included in the estrogenicity training set showing the potential estrogenic toxicophore (a fragment including two oxygen atoms connected to two vicinal aromatic carbons), highlighted in cyan. In some of the compound, the fragment is observed more than once.



**Figure S2.** Compounds devoid of estrogenic activity included in the estrogenicity training set showing the potential estrogenic toxicophore (a fragment including two oxygen atoms connected to two vicinal aromatic carbons), highlighted in cyan. In some of the compound, the fragment is observed more than once.



<b>Name</b>	Entry_1
<b>SMILES</b>	<chem>CCNC(=O)NC1=NC=C(S1)[N+](=O)[O-]</chem>

Endpoint	Probability
Mutagenicity	89 %
Carcinogenicity	78 %

Endpoint	Probability
Hepatotoxicity	37 %
Estrogenicity	7 %

**Figure S3.** Example of toxicity prediction report produced by VenomPred web tool. The query compound is Nithiazide (CAS# 139-94-6).