

vega-toolkit QSAR Models

No.	Section	Endpoint	Model
1	Human Toxicity	Mutagenicity (Ames test)	Mutagenicity (Ames test) model (CAESAR)
2	Human Toxicity	Mutagenicity (Ames test)	Mutagenicity (Ames test) model (ISS)
3	Human Toxicity	Mutagenicity (Ames test)	Mutagenicity (Ames test) model (SarPy-IRFMN)
4	Human Toxicity	Mutagenicity (Ames test)	Mutagenicity (Ames test) model (KNN-Read-Across)
5	Human Toxicity	Mutagenicity (Ames test)	Mutagenicity (Ames test) CONSENSUS model
6	Human Toxicity	Developmental toxicity	Developmental Toxicity model (CAESAR)
7	Human Toxicity	Developmental toxicity	Developmental/Reproductive Toxicity library (PG)
8	Human Toxicity	Carcinogenicity	Carcinogenicity model (CAESAR)
9	Human Toxicity	Carcinogenicity	Carcinogenicity model (ISS)
10	Human Toxicity	Carcinogenicity	Carcinogenicity model (IRFMN-ISSCAN-CGX)
11	Human Toxicity	Carcinogenicity	Carcinogenicity model (IRFMN-Antares)
12	Human Toxicity	Carcinogenicity	Carcinogenicity oral classification model (IRFMN)
13	Human Toxicity	Carcinogenicity	Carcinogenicity oral Slope Factor model (IRFMN)
14	Human Toxicity	Carcinogenicity	Carcinogenicity inhalation classification model (IRFMN)
15	Human Toxicity	Carcinogenicity	Carcinogenicity inhalation Slope Factor model (IRFMN)
16	Human Toxicity	Carcinogenicity	 Carcinogenicity in male rat (CORAL)
17	Human Toxicity	Carcinogenicity	 Carcinogenicity in female Rat (CORAL)
18	Human Toxicity	Acute Toxicity (LD50)	 Acute Toxicity (LD50) model (KNN)
19	Human Toxicity	Skin Sensitization	Skin Sensitization model (CAESAR)
20	Human Toxicity	Skin Sensitization	Skin Sensitization model (IRFMN-JRC)
21	Human Toxicity	Skin Sensitization	Skin Sensitization model (NCSTOX)
22	Human Toxicity	Skin Sensitization	 Skin Sensitization model (TOXTREE)
23	Human Toxicity	Chromosomal aberration	Chromosomal aberration model (CORAL)
24	Human Toxicity	Micronucleus assay	In vitro Micronucleus activity (IRFMN-VERMEER)
25	Human Toxicity	Micronucleus assay	In vivo Micronucleus activity (IRFMN)
26	Human Toxicity	Estrogen receptor effect	Estrogen Receptor-mediated effect (IRFMN-CERAPP)
27	Human Toxicity	Estrogen receptor effect	Estrogen Receptor Relative Binding Affinity model (IRFMN)
28	Human Toxicity	Androgen receptor effect	Androgen Receptor-mediated effect (IRFMN-COMPARA)
29	Human Toxicity	Thyroid receptor effect	Thyroid Receptor Alpha effect (NRMEA)
30	Human Toxicity	Thyroid receptor effect	Thyroid Receptor Beta effect (NRMEA)
31	Human Toxicity	Endocrine Disruptor activity	 Endocrine Disruptor activity screening (IRFMN)
32	Human Toxicity	NOAEL	NOAEL (IRFMN-CORAL)
33	Human Toxicity	NOAEL	Liver NOAEL (CORAL)
34	Human Toxicity	LOAEL	Liver LOAEL (CORAL)
35	Human Toxicity	Cramer classification	Cramer classification (TOXTREE)
36	Human Toxicity	Hepatotoxicity	Hepatotoxicity model (IRFMN)
37	EcoToxicity	BCF	BCF model (CAESAR)
38	EcoToxicity	BCF	BCF model (Meylan)
39	EcoToxicity	BCF	BCF model (Arnot-Gobas)
40	EcoToxicity	BCF	BCF model (KNN-Read-Across)
41	EcoToxicity	Aquatic Acute Toxicity	Fish Acute (LC50) Toxicity model (IRFMN)
42	EcoToxicity	Aquatic Acute Toxicity	Fish Acute (LC50) Toxicity model (NIC)
43	EcoToxicity	Aquatic Acute Toxicity	Fish Acute (LC50) Toxicity model (KNN-Read-Across)
44	EcoToxicity	Aquatic Acute Toxicity	Fish Acute (LC50) Toxicity classification (SarPy-IRFMN)

45	EcoToxicity	Aquatic Acute Toxicity	Fish Acute (LC50) Toxicity model (IRFMN-Combase)
46	EcoToxicity	Aquatic Acute Toxicity	Fathead Minnow LC50 96h (EPA)
47	EcoToxicity	Aquatic Acute Toxicity	Fathead Minnow LC50 model (KNN-IRFMN)
48	EcoToxicity	Aquatic Acute Toxicity	Daphnia Magna Acute (EC50) Toxicity model (IRFMN)
49	EcoToxicity	Aquatic Acute Toxicity	Daphnia Magna LC50 48h (EPA)
50	EcoToxicity	Aquatic Acute Toxicity	Daphnia Magna LC50 48h (DEMETRA)
51	EcoToxicity	Aquatic Acute Toxicity	Daphnia Magna Acute (EC50) Toxicity model (IRFMN-Combase)
52	EcoToxicity	Aquatic Acute Toxicity	Guppy LC50 model (KNN-IRFMN)
53	EcoToxicity	Aquatic Acute Toxicity	Algae Acute (EC50) Toxicity model (IRFMN)
54	EcoToxicity	Aquatic Acute Toxicity	Algae Classification Toxicity model (ProtoQSAR-Combase)
55	EcoToxicity	Aquatic Acute Toxicity	Algae Acute (EC50) Toxicity model (ProtoQSAR-Combase)
56	EcoToxicity	Aquatic Chronic Toxicity	Fish Chronic (NOEC) Toxicity model (IRFMN)
57	EcoToxicity	Aquatic Chronic Toxicity	Daphnia Magna Chronic (NOEC) Toxicity model (IRFMN)
58	EcoToxicity	Aquatic Chronic Toxicity	Algae Chronic (NOEC) Toxicity model (IRFMN)
59	EcoToxicity	Mode of Action	Verhaar classification (TOXTREE)
60	EcoToxicity	Mode of Action	MOA fish toxicity classification (EPA T.E.S.T.)
61	EcoToxicity	Mode of Action	MOA pesticide classification (IRFMN)
62	EcoToxicity	Terrestrial Acute Toxicity	Bee acute toxicity model (KNN-IRFMN)
63	EcoToxicity	Sludge Toxicity	Sludge Classification Toxicity model (ProtoQSAR-Combase)
64	EcoToxicity	Sludge Toxicity	Sludge (EC50) Toxicity model (ProtoQSAR-Combase)
65	EcoToxicity	Zebrafish embryo activity	Zebrafish embryo AC50 (IRFMN-CORAL)
66	Fate & Distribution	Ready biodegradability	Ready Biodegradability model (IRFMN)
67	Fate & Distribution	Persistence (sediment)	Persistence (sediment) model (IRFMN)
68	Fate & Distribution	Persistence (sediment)	Persistence (sediment) quantitative model (IRFMN)
69	Fate & Distribution	Persistence (soil)	Persistence (soil) model (IRFMN)
70	Fate & Distribution	Persistence (soil)	Persistence (soil) quantitative model (IRFMN)
71	Fate & Distribution	Persistence (water)	Persistence (water) model (IRFMN)
72	Fate & Distribution	Persistence (water)	Persistence (water) quantitative model (IRFMN)
73	Fate & Distribution	Persistence (air)	Air Half-Life (IRFMN-CORAL)
74	Physical-Chemical properties	Octanol/Water partition coefficient (logP)	LogP model (Meylan-Kowwin)
75	Physical-Chemical properties	Octanol/Water partition coefficient (logP)	LogP model (MLogP)
76	Physical-Chemical properties	Octanol/Water partition coefficient (logP)	LogP model (ALogP)
77	Physical-Chemical properties	Water solubility	Water solubility model (IRFMN)
78	Physical-Chemical properties	Hydrolysis	Hydrolysis (IRFMN-CORAL)
79	Physical-Chemical properties	Henry's law constant	Henry's Law model (OPERA)
80	Physical-Chemical properties	Octanol/air partition coefficient (KOA)	KOA model (OPERA)
81	Physical-Chemical properties	Soil adsorption coefficient of organic compounds (KOC)	KOC model (OPERA)
82	Human PBPK	Plasma Protein Binding	 Plasma Protein Binding – LogK (IRFMN)
83	Human PBPK	Plasma Protein Binding	 Plasma Protein Binding – sqFU (CORAL)
84	Human PBPK	Aromatase activity	Aromatase activity model (IRFMN)
85	Human PBPK	Aromatase activity	 Aromatase activity model (TOX21)
86	Human PBPK	P-Glycoprotein activity	P-Glycoprotein activity model (NIC)
87	Human PBPK	Hepatic Steatosis MIE	 Hepatic Steatosis MIE assay for PXR up (TOXCAST)
88	Human PBPK	Hepatic Steatosis MIE	 Hepatic Steatosis MIE assay for PPARγ up (TOXCAST)
89	Human PBPK	Hepatic Steatosis MIE	 Hepatic Steatosis MIE assay for PPARα up (TOXCAST)
90	Human PBPK	Hepatic Steatosis MIE	 Hepatic Steatosis MIE assay for NRF2 (TOXCAST)

91	Human PBPK	Skin permeation (LogKp)	Skin Permeation (LogKp) model (Potts and Guy)
92	Human PBPK	Skin permeation (LogKp)	Skin Permeation (LogKp) model (Ten Berge)
93	Human PBPK	Adipose tissue-blood partition	Adipose tissue – blood model (INERIS)
94	Human PBPK	Body elimination half-life	Total body elimination half-life (QSARINS)
95	Ecological PBPK	kM/Half Life	kM/Half-Life model (Arnot-EpiSuite)