QSAR and Toxicity Prediction Software

cQSAR: A regression program that has dual databases of over 21,000 QSAR models. Distributed by BioByte.
SeeSAR: Program for interactive, visual compound promotion and optimization. It include PD and PK parameters and can be linked to other modules for physicochemical and ADME. Distributed by Bio
clogP: Program for calculating log $P_{oct/water}$ from structure. Distributed by BioByte.
ClogP/CMR: Estimates Molar Refractivity and logP. Distributed by Tripos
QikProp: Provides rapid ADME predictions of drug candidates. Distributed by Schrodinger.
VolSurf: Calculate ADME Properties and Create Predictive ADME Models. Distributed by Tripos.
GastroPlus: Simulates the oral absorption, pharmacokinetics, and pharmacodynamics for drugs in human and preclinical species. The underlying model is the Advanced Compartmental Absorption and Transit (ACAT) model. Distributed plu Simulation Plus, Inc.
MedChem Studio: Cheminformatics platform for computational and medicinal chemists supporting lead identification and optimization, in silico ligand based design, and clustering/classifying of compound libraries. It is integrated with MedChem Designer and ADMET Predictor. Distributed by Simulation Plus, Inc.
ADMET Predictor: Software for advanced predictive modeling of ADMET properties. ADMET Predictor estimates a number of ADMET properties from molecular structures, and is also capable of building predictive models of new properties from user's data via its integrated ADMET Modeler module. Distributed by Simulations Plus, Inc.
DDDPlus: Models and simulates the in vitro dissolution of active pharmaceutical ingredients (API) and formulation excipients dosed as powders, tablets, capsules, and swellable or non-swellable polymer matrices under various experimental conditions. Distributed by Simulations Plus, Inc.
ADMEWORKS ModelBuilder: Builds QSAR/QSPR models that can later be used for predicting various chemical and biological properties of compounds. Models are based on values of physicochemical, topological, geometrical, and electronic properties derived from the molecular structure, and can be imported into ADMEWORKS Predictor.
ADMEWORKS Predictor: QSAR based Virtual (in silico) screening system intended for simultaneous evaluation of the properties of compounds.
MedChem Designer: Tool that combines molecule drawing features with a few free ADMET property predictions from ADMET Predictor. Distributed by Simulations Plus, IncMedChem Designer 3.0 is a *free* chemical structure drawing program. MedChem Designer can open SMILES, SDF, MOL, CSK, and RXN file types.
IMPACT-F: Expert system to estimate oral bioavailability of drug-candidates in humans. IMPACT-F is composed of several QSAR models to predict oral bioavailability in humans. Developed by PharmaInformatic, Germany.
MolScore-Drugs: Expert system to identify and prioritise drug candidates. Developed by PharmaInformatic, Germany.
Natural product likeness calculator: Calculates Natural Product(NP)-likeness of a molecule, i.e. the similarity of the molecule to the structure space covered by known natural products. NP-likeness is a useful criterion to screen compound libraries and to design new lead compounds.
ADMET Modeler:ADMET Predictor as an additional predicted property. Distributed by Simulations Plus, Integrated module of ADMET Predictor that automates the process of making high quality predictive structure-property models from sets of experimental data. It works seamlessly with ADMET Predictor structural descriptors as its inputs, and appends the selected final model back to Inc.

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Metabolizer: Enumerates all the possible metabolites of a given substrate, predicts the major metabolites and estimates metabolic stability. It can be used for the identification of metabolites by MS mass values, discovery of metabolically sensitive functionalities and toxicity prediction, and provide information related to the environmental effects of chemicals by bacterial degradation. Provided by ChemAxon.
ACD/PhysChem Suite: predicts basic physicochemical properties like pka, logp, logD, aqueous solubility and other molecular properties in seconds, user a fragment-based models. Distributed by ACD/Labs.
ACD/ADME Suite: Predicts of ADME properties from chemical structure, like Predict P-gp specificity, oral bioavailability, passive absorption, blood brain barrier permeation, distribution, P450 inhibitors, substrates and inhibitors, maximum recommended daily dose, Abraham-type (Absolv) solvation parameters. Distributed by ACD/Labs.
ACD/Tox Suite: Collection of software modules that predict probabilities for basic toxicity endpoints. Several modules including hERG Inhibition, CYP3A4 Inhibition, Genotoxicity, Acute Toxicity, Aquatic Toxicity, Eye/Skin Irritation, Endocrine System Disruption, and Health Effects. Distributed by ACD/Labs.
ACD/DMSO Solubility: Predictssolubility in DMSO solution. Distributed by ACD/Labs.
Filter-it: Command-line program for filtering molecules with unwanted properties out of a set of molecules. The program comes with a number of pre-programmed molecular properties that can be used for filtering. Open source software distributed by Silicos.
Virtual LogP: Bernard Testa's Virtual logP calculator. Provided by the Drug Design Laboratory of the University of Milano.
FAF-Drugs2: Free package for in silico ADMET filtering. Distributed by the university of Paris Diderot.
Discovery Studio TOPKAT Software: Cross-validated models for the assessments of chemical toxicity from chemical's molecular structure. Distributed by Accelrys.
Discovery Studio ADMET Software: The ADMET Collection provides components that calculate predicted absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties for collections of molecules. Distributed by Accelrys.
PreADME. Calculates molecular descriptors. Predicts Drug-likeness. ADME predictions.
Molcode Toolbox. Molcode Toolbox allows prediction of medicinal and toxicological endpoints for a large variety of chemical structures, using proprietary QSAR models.
KOWWIN - EPI Suite. Estimates the log octanol-water partition coefficient of chemicals using an atom/fragment contribution method. Distributed by the EPA~s Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC) as part of the EPI Suite. For Windows.
ADRIANA.Code: Program to calculate physico-chemical properties of small molecules: number of H-bonds donor and acceptors, logP, logS, TPSA, dipole moment, polarizability, etc. Distributed by Molecular Networks.
Derek Nexus: Gives accurate toxicity predictions quickly. Derek Nexus is a knowledge-based expert systems that predicts the toxicity and metabolism of a chemical, respectively. It offers an effective mechanism for the sharing of data and knowledge on chemical toxicity and metabolism.
Predicts toxicity properties using QSAR and other expert knowledge rules. Distributed by Lhasa Limited.
Meteor: Predicts metabolic fate of chemicals using other expert knowledge rules in metabolism. Distributed by Lhasa Limited.
OncoLogic: Evaluates the likelihood that a chemical may cause cancer, using SAR analysis, experts decision mimicking and knowledge of how chemicals cause cancer in animals and humans.

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Distributed for free by the US Environmental Protection Agency (EPA).
HazardExpert Pro. Predicts the toxicity of organic compounds based on toxic fragments. Distributed by CompuDrug.
MetabolExpert. Predicts the most common metabolic pathways in animals, plants or through photodegradation. Distributed by CompuDrug.
MEXAlert. Identifies compounds that have a high probability of being eliminated from the body in a first pass through the liver and kidney. Distributed by CompuDrug.
PrologP/PrologD. Predicts the logP/logD values using a combination of linear and neural network methods. Distributed by CompuDrug.
pKalc. Program for predicting acidic and basic pKa. Distributed by CompuDrug.
Leadscope. Estimates toxiticy using QSAR. Distributed by Leadscope.
COMPACT. Identifies potential carcinogenicity or toxicities mediated by CYP450s.
CASETOX. Uses MCASE to predict toxicity. Distributed by MultiCASE.
META. Predicts metabolic paths of molecules. Distributed by MultiCASE.
PK-Sim. Predicts ADMET properties. Distributed by Bayer technology Services.
SimCYP. The SimCYP Population-based ADME Simulator is a platform for the prediction of drug-drug interactions and pharmacokinetic outcomes in clinical populations. Distributed by SimCYP.
Cloe Predict. Pharmacokinetic prediction using phisiologically based pharmacokinetic modeling (PBPK), and prediction of human intestinal absorption using solubility, pKa and Caco-2 permeability data. Distributed by Cyprotex Discovery.
KnowItAll - ADME | Tox Edition. Prediction of ADME Tox properties using consensus modeling. Distributed by Bio-Rad Laboratories.
PASS. Identificationof probable targets and mechanisms of toxicity.
MetaDrug. Predicts toxicity and metabolism of compounds using >70 QSAR models for ADME/Tox properties. Distributed by Thomson ReutersLC.
MetaSite. Computational procedure that predicts metabolic transformations related to cytochrome-mediated reactions in phase I metabolism. Distributed by Moldiscovery.
IMPACTS. In-silico Metabolism Prediction by Activated Cytochromes and Transition States (IMPACTS) predicts site of metabolism on small molecules by CYP450. It is included in the Forecaser suite and provided by Molecular Forecaster Inc.
FAME2. Program to predict site of metabolism and regioselectivity of CYP450 oxidation. Machine learnin approach relying on randomized trees and simple 2D descriptors. Software package free of charge from the Department of Computer Science, Center for Bioinformatics, Universität Hamburg, Germany.
StarDrop. Allows the identification of the region of a molecule that are the most vulnerable to metabolism by the major drug metabolising isoforms of cytochrome P450. Distributed by optibrium.
isoCYP. Software for the prediction of the predominant human cytochrome P450 isoform by which a given chemical compound is metabolized in phase I. Distributed by Molecular Networks
QSAR Toolbox.The Toolbox is a free software application that supports reproducible and transparent chemical hazard assessment. It offers functionalities for retrieving experimental data, simulating metabolism and profiling properties of chemicals.
Tox-CNN: Predicts toxicity state of cells under different treatments from microscopy images of fluorescently labeled nuclei by using convolutional neural networks (CNNs). Tox-CNN is based on a deep-learning approach for in vitro cell-based toxicity assessment.

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ECOSAR: Estimates aquatic toxicity. ECOSAR is a computerized version of the ecotoxicity analysis procedures as practiced by the Office of Pollution Prevention and Toxics (OPPT) when data are lacking for risk assessment development. The software, using computerized Structure Activity Relationships (SARs), allows to predict both short-term and long-term toxicity to aquatic organism.
TOPKAT: Calculates the compound performance in experimental assays and animal models. TOPKAT exploits the molecular structure to measure and approve assessments of the toxic and environmental effects of chemicals.
TopTox:Allows quantitative toxicity investigation and determination of small molecules. TopTox is based on the element specific topological descriptor (ESTD) method.
LTMap:A web server for evaluating the potential liver toxicity based on genome-wide transcriptomics data.
ProTox :A web server for the prediction of rodent oral toxicity. The prediction method is based on the analysisof the similarity of compounds with known median lethal doses (LD50) and incorporates the identification of toxic fragments, therefore representing a novel approach in toxicity prediction.
ProTox II: A virtual lab for the prediction of toxicities of small molecules. The prediction of compound toxicities is an important part of the drug design development process.
PreADMET:Predicts ADME data and builds drug-like library using *insilico*method. PreADMET is a web-based application and can be accessed by browsers such as Netscape or Internet Explorer.
HazardExpert:Considers the bioavailability of the compounds by a simple but powerful model. HazardExpert is an ideal tool for quick prediction of compound's toxicity in the drug discovery process or during the dispositional research phase.
Metatox:Allows to predictxenobiotic's metabolism and calculates toxicity of metabolites based on the structural formula of chemicals products. The Metatox method uses dictionaries of biotransformation and is based on preliminary prediction of possible classes of biotransformation reactions.
Lazar: Helps for the prediction of complex toxicological endpoints, like carcinogenicity, long-term, and reproductive toxicity. Lazar is a generic prediction algorithm for any biological endpoint with sufficient experimental data.
Percepta Predictors: Predicts properties from simple structure input. Percepta Predictors is an in-depth understanding of structure-property relationships with ACD/Labs' fully powered predictive models for physiochemical and absorption, Distribution, Metabolism, and Excretion (ADME) properties, and toxicity endpoints.
MetaCore: Accelerates discovery research with systems biology content, analytics, and expertise. MetaCore is an integrated software suite for functional analysis of Next Generation Sequencing (NGS), gene expression, copy number variation (CNV), metabolic, proteomics, microRNA, and screening data.

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CarcinoPred-EL: Classifies compounds as Carcinogens and Non-Carcinogens using only their two-dimensional structures. CarcinoPred-EL is a free carcinogenicity prediction online server. endpoints or other pathological drug properties of chemicals.
DeepTox: Performs toxicity prediction based on Deep Learning. DeepTox consists of: (1) cleaning and quality control of the data containing the chemical description of the compounds, (2) creation of chemical descriptors as input features for the models, (3) model selection including feature selection if required by the model class, (4) evaluation of the quality of models to choose the best ones, and (5) combination of models and ensemble predictors.
Tox-RCNN: Provides a convolutional neural networks (CNNs) for cytotoxicity datasets. Tox-RCNN is based on a deep-learning approach for in vitro cell-based toxicity assessment.
MuDRA:Serves as a Chembench module for quantitative structure-activity relationship QSAR toxicity predictions. MuDRA is able to develop accurate and interpretable models and its approach is related to the k-nearest neighbor (kNN) approach.
EPI Suite:A Windows-based suite of physical/chemical property and environmental fate estimation programs developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC).
Toxtree:A full-featured and flexible user-friendly open source application, which is able to estimate toxic hazard by applying a decision tree approach.
FAF-Drugs:Allows users to detect small molecules. FAF-Drugs is a web application which allows users to filter large compound libraries or determine some ADME-Tox properties (Adsorption, Distribution, Metabolism, Excretion and Toxicity).
Auto QSAR:Identifying Quantitative Structure-Activity Relationships (QSAR) has been a powerful technique in researchers' computational arsenal for decades. It's widely used in lead optimization, ADME/Toxmodeling, genotypic and phenotypic screening analysis, and many other applications.