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MOLCODE TOOLBOX: Software tool for property prediction of chemicals

Molcode Toolbox 2.4

The unique computational expert system **Molcode Toolbox** is designated for the fast and robust prediction of biomedically and environmentally important properties of chemical compounds and materials. It is based on proprietary methods that are mapping the properties of compounds on large pools of molecular descriptors. These pools include thousands of descriptors developed by using quantum chemical theory and accounting for the subtle details in the spatial and electronic structure of molecules. Prior to these calculations, molecular mechanics is applied for the conformational search of large compounds.

Molcode Toolbox presents proprietary QSAR (Quantitative Structure-Activity Relationship) models developed by Molcode. Within the Molcode Toolbox, the user can load the structures of his own compounds, modify the encoded compounds or create/optimize completely new ones, and predict/analyze their specific properties, as well as create statistical reports for the later analysis. The intuitive and clear user interface allows the user to predict the desired properties of compounds in four easy steps/clicks.

Molcode Toolbox features:

Data set information // experimental and predicted values of properties // descriptor calculation and respective values // statistical validation // structure editor // structure optimization // structure or structure folder upload // prediction reports

Molcode Toolbox is a powerful tool for the prediction of medicinal and toxicological endpoints for a large variety of chemical structures. Molcode Toolbox includes the feature for Molecular engineering which helps to design novel chemicals or drug candidates. With the help of Molcode Toolbox, the medicinal properties and possible side effects, including toxicological parameters of novel drug candidates which can be estimated in very early

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stage of drug delivery process.

Custom modeling upon request: the Toolbox can be fitted with models provided by the client and/or models custom-built for the client using the source data provided by the client (Cost: negotiable).

Endpoints

Molcode Toolboxes are custom-fitted with models from a unique and industry-leading list of diverse medicinal, toxicology, ADME etc. endpoints.

We also develop custom Toolboxes based on client's data if there is a need unmet by standard Toolboxes.

See Appendix 1 for the full list of the Molcode Toolbox predictive models.

Validation

Unlike most of the other prediction software around, Molcode Toolbox is not a “black box” program, where the users have no idea what the obtained prediction was based on.
For the sake of transparency, Molcode Toolbox comes with the full data of the background of each model, including optimized molecular structures, experimental and predicted values for the endpoint, descriptor values and results of the statistical analysis. Each model has been validated and cross-validated, to meet strict statistical criteria. Both internal and external validation is used.
The procedure and model documentation is designed to meet the OECD guidelines for QSAR.

Applicability domain

Whenever you consider a model or model system, each of them has an applicability domain where the particular model can be used. The same is true for any QSAR model. Based on the chemical range of the training set, each model is applicable to only these compounds that are reasonably similar to the training set comounds. Unfirtunately, the applicability domain is commonly overlooked when making predictions. In Molcode Toolbox, the applicability domain control is performed automatically.
If the chemical structure of interest falls out or is on the limit of chemical space of the model, a color-coded warning will be displayed.

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Technical information:
Molcode Toolbox includes:A total number of 61 validated QSAR models with full information of the numerical, statistical, and chemical (structural) data, structure import, modification and optimization tools for the end user structures,
molecular descriptor calculator, property prediction module, statistical validation module, analysis report.

Working platforms

Microsoft Windows XP or later.

Training

The user interface of Molcode Toolbox is designed to be simple and user-friendly. In addition, Molcode offers an on-site training course and workshop by their representatives

The workshop also includes an informal lecture with practical examples of the capacities of Molcode Toolbox and modern computational chemistry in the field of molecular design and drug delivery.

Molcode expertise

Molcode, Ltd. operates in the rapidly developing field of molecular engineering and design. One of the main activities for the company is developing of computational solutions for molecular design and property prediction.
The company's roots lie in various research groups' work on molecular engineering.

Molcode, Ltd. delivers highly expert consultations and research on the computational modeling of chemical reactivity and molecular properties, and on the molecular design of new chemical compounds, drugs and materials.

The expertise is based on the long-time leading scientific research and software development in quantum chemistry, especially in the quantum chemistry of molecular systems in condensed disordered media (liquids, solutions, polymers) and in quantitative structure activity/property relationships (QSAR/QSPR).

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Publications

For the list of publications of Molcode team members please visit:

www.molcode.com > Publications

Direct link: www.molcode.com/?mid=20&lang=en

Appendix 1: Endpoints encoded to Molcode Toolbox, full module (08.12.2009)

	Name	R^2	Domain
1	Adenosine A3 receptor inhibition	0.850	diverse hA3AR antagonist candidates
2	Alzheimer CDK (cyclin-dependent kinase 5) /p25 inhibition	0.801	thiazoles
3	Anti HIV activity	0.769	2-amino-6-arylsulfonylbenzonitriles and derivates
4	Antimalarial activity for Dd2 strain of Plasmodium falciparum	0.708	2,5-diaminobenzophenone deriv
5	Antimalaria activity #1 (Plasmodium falciparum)	0.694	bisbenzamidines
6	Antitumor activity (cytotoxicity) (human lung) (EC50)	0.744	tylophorine derivatives
7	Antitumor activity (cytotoxicity) (human lung) (IC50)	0.721	bioisostere of benzophenanthridine alkaloids
8	Aryl HydroCarbon Receptor binding	0.747	halogenoaromatics
9	Blood - brain barrier	0.810	drugs
10	Brain serotonin-1A (5-HT1A) receptor inhibition	0.780	3,4 -Dhydro-2h-benzoxazinones, thienopyrimidinone derivatives, arylpiperazine compounds
11	Ca channel blockers IC50	0.855	1,4-Dihydropyridines
12	Caco-2 cell monolayer permeability	0.724	drugs

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13	Carbonic anhydrase transmembrane isozyme XIV inhibition	0.854	sulfonamides
14	cardio hERG IC50 -logM	0.750	drugs
15	Caspace-3 inhibition	0.700	Isoquinoline-1,3,4-trione derivatives
16	CDK2 (cyclin-dependent kinase 2) inhibition #1	0.757	Pyrazolo[1,5-a]pyrimidines
17	Central Benzodiazepine Receptor (BzR) inhibition	0.860	2-aryl (heteroaryl)-2, 5-dihydropyrazolo [4, 3-c] quinolin-3-(3H)-ones
18	CXCR3 (chemokine receptor) inhibition	0.802	sulfonamides
19	Gamma-secretase inhibition #2 (wca)	0.832	Thiazole-diamides
20	Human blood - air partition	0.874	div org
21	Human brain - air partition	0.899	div org
22	Human fat - air partition	0.860	div org
23	Human kidney - air partition	0.950	div org
24	Human liver - air partition	0.894	non H-bond organics
25	Human muscle - air partition	0.914	div org
26	Human Serum Albumin binding	0.812	drugs
27	Human Serum Albumin binding	0.845	drugs
28	Inhibition of Caspase-3 (IC50) MMFFs-W	0.750	Dipeptidyl aspartyl fluoromethylketones
29	Inhibition of Glycogen Synthase Kinase-3 Class I	0.873	maleimide derivates
30	Inhibition of Glycogen Synthase Kinase-3 Class III	0.797	2 sets of derivates
31	Inhibition of proteasome pKi (MMFFs_w)	0.817	tripeptide aldehydes
32	Norepinephrine reuptake inhibition	0.752	3-(1H-indol-1-yl)-3-arylpropan-1-amines
33	Inhibition of Platelet Derived Growth Factor	0.711	1-phenylbenzimidazoles
34	Permeability (PAMPA) (logPapp(pH5.5)) MMFFs	0.665	drugs

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35	Permeability (PAMPA) (logPapp(pH7.4)) MMFFS	0.759	drugs
36	Rat blood-brain penetration	0.684	drugs
37	Rat fat - air partition	0.941	div org
38	Rat liver - air partition	0.928	div org
39	Rat muscle - air partition	0.947	div org
40	Serotonin reuptake inhibition	0.772	3-(1H-indol-1-yl)-3-arylpropan-1-amines
41	Toxicity to Porphyromonas gingivalis	0.895	phenol derivatives
42	Toxicity to Selenomonas artemidis	0.779	phenol derivatives
43	Toxicity to Streptococeus sorbrinius	0.909	phenol derivatives
44	Acute oral toxicity - acute toxicity LD50	0.805	div org
45	Acute Oral Toxicity- *in vitro* (cytotoxicity)	0.850	div org
46	Acute toxicity: eye irritation/corrosion	0.893	org liquids
47	Mutagenicity: Reverse mutation test using bacteria #2 (TA98)	0.722	aromatic amines
48	Chronic toxicity LOAEL (rat) #1	0.733	div org
49	Carcinogenicity test (Female rat)	0.730	nitro compounds
50	Acute toxicity for fish (Danio rerio) LC50, 96h #1	0.804	div org
51	Acute toxicity for fish (Fathead minnow), LC50 #1	0.764	div org
52	Acute toxicity for fish (Rainbow trout) #1	0.860	div org
53	Toxicity to Daphnia magna EC50, 96h	0.749	pesticides
54	Activated sludge respiration inhibition #1	0.790	div org
55	Bioconcentration factor: flow - through fish test #1	0.946	polychlorinated biphenyls
56	Bioconcentration factor: flow - through fish test #2	0.83	pesticides
57	Honeybees - acute contact toxicity test	0.82-	amides, ethers, esters, amines (separate

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		0.84	models)
58	Organic carbon-sorption partition coefficient Koc	0.756	pesticides
59	Estrogen receptor binding affinity	0.800	div org
60	Human Serum Albumin Binding #1	0.835	drugs
61	Toxicity to Tetrahymena pyriformis IGC50	0.871	non H-bond aromatics

Notes:

1) For the endpoint # 57 four models available according to classification
2) Documentation and background for the endpoints: www.molcode.com, CD

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