

Predicting molecular properties of environmental contaminants

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Risk assessment of chemicals is an important step in chemical regulation. The information for risk assessment has two parts. The first part is the information on exposure routes, i.e., on the contact probability and the intake of a chemical. The second part is the hazard assessment of a chemical. The hazard is described with series of toxicological data, which are traditionally obtained by expensive, time consuming and highly restricted animal experiments. For estimation of physico-chemical, toxicological and eco-toxicological parameters, which are important for risk assessment the in silico methods, which includes different mechanistic and statistical modelling, became an important alternative method. This section is focused to all key-tasks of modelling: to the data collection and selection, to the modelling techniques, to the testing and validation of models, and to the application of existing models on compounds and data sets of interest. The data, which are used to build and to test the models, must be obtained under the same laboratory conditions. An emerging and important class of data are the information about receptors (proteins), which may play a role in different toxicities. For the modelling different mathematical (computational) techniques are available, from the standard statistical tools including the tools for classification to the physico-chemical (quantum chemical) methods for description of molecules' activity or molecule-receptor interactions. The application of existing models (free or commercial) on particular data sets is one of the focuses of this section.

Keywords: QSAR models, mechanistic models, classification of chemicals, receptors.

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