T14. QSAR/QSPR: the universal approach to the prediction of properties of chemical compounds and materials

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QSAR/QSPR (Quantitative structure-activity/property relationships) approaches can be considered as universal techniques for the modeling and prediction of nearly any properties of chemical compounds and many properties of materials. These approaches are based on the automatic analysis of structures and property values for a series of known chemical compounds with known properties, the chemical structures being described numerically with a series of parameters (descriptors). The structure-property relationships are usually evaluated using artificial neural networks. After creation of structure-property model it can be used for the prediction of properties for new chemical compounds for which these properties were never studied or compounds themselves were never synthesized. Some properties of materials can be predicted as dependent on the structure of small molecules used as additives (e.g. antioxidants, etc.). We have correlated successfully, e.g. the properties of tire rubbers with the structure of accelerators of vulcanization. Good results of modeling had been obtained for the diffusion coefficients of small molecules in some polymers. A number of properties of polymers had been modeled as dependent on the chemical structure of a monomeric unit (e.g. glass transition temperature, molar heat capacity).

A large number of properties were modeled for various organic compounds basing on their structural formulas, e.g. density, boiling points, viscosity, surface tension, magnetic susceptibility, lipophilicity (octanol-water distribution coefficient), critical temperature, flash points, polarizability, enthalpy of evaporation, etc.

Prediction of toxicity is a challenging problem which until now is not completely solved. However the toxicity for many industrially important compounds can be predicted basing on the computation of lipophilicity, taking into account the presence of toxophores and using fragmental descriptors.