Summary of doctoral dissertation

„Influence of the method of describing the chemical structure of ionic liquids on the quality of prediction in structure-properties models”

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The quantitative structure-activity/property relationship (QSAR/QSPR) method allows to estimate the physicochemical properties as well as the biological activity of different groups of chemical compounds, including the ionic liquids. It is based on the assumption that it is possible to link the chemical structure (expressed with the molecular descriptors) with the modeled property by determining the appropriate mathematical function. However, in the case of the ionic liquids, it is possible to use various strategies for describing the chemical structure of these compounds during the model development, e.g. the calculated descriptors can describe individual ions or the entire ionic pair. Therefore, the main goal of my dissertation is to verify the research hypothesis, according to which the method of describing the structure of ionic liquids affects the quality of prediction in structure-activity/property models (QSAR/QSPR).

The development and analysis of a number of QSAR/QSPR models differing in the method of describing the ionic liquid allowed for the verification of the hypothesis. Based on the results of the research presented in the cycle of three papers, which are part of the doctoral dissertation, it can be concluded that:

- method of describing the structure of ionic liquids influences the quality of prediction in the structure-activity/property models (QSAR/QSPR);
- the semi-empirical method (PM7) is sufficient to build a reliable QSPR model for ionic liquids, assuming that the ions are described separately;
- taking into account the interaction between the ions (optimization of the geometry of the ionic pair structure) is not necessary to develop a reliable QSPR model;
- the strategy assuming the description of the compound structure by 2D descriptors calculated for the ionic pair is the most advantageous, both in terms of the value of measures describing the quality of the model and the possibility of its reuse.

The results presented in the doctoral dissertation are the next step towards the development of computational methods for the risk assessment of ionic liquids. The presented

dissertation summarizes the impact of the method of describing the structure of ionic liquids on the quality of QSAR/QSPR models and provides guidelines for the optimal selection of molecular descriptors calculation methods for ionic liquids in QSAR/QSPR modeling.