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QSPR FOR PREDCTING SENSOR CHARACTERISTICS OF CALIXARENES FOR DETERMINATION OF VOLATILE ORGANIC COMPOUNDS

Ashina Yu.S. (ITMO University), **Boichenko E.S.** (ITMO University), Surkova A.A. (ITMO University)

Supervisor – D.Sc. (Chemistry), researcher Kirsanov D.O. (ITMO University)

Introduction. QSPR (quantitative structure-property relationship) modeling is a computational method for predicting the chemical properties of compounds based on their molecular structure. QSPR is widely used in the drug design because it reduces the number of empirical experiments by replacing them with theoretical calculations. Moreover, in this field large sample sizes of known compounds with described therapeutic properties are available to researchers. Nevertheless, it has been shown recently that QSPR works also in the case of small samples, for example, to predict the analytical performance (sensitivity and selectivity) of potentiometric sensors based on the chemical structure of ionophores in their membranes [1].

Main part. Application of QSPR modeling makes it possible to reduce the cost of development of new analytical devices, especially multisensor systems, which often require the synthesis of various sensitive membranes. The development of such devices is relevant for rapid analysis of biological samples in gas and liquid phase for diagnostics and monitoring of treatment of various diseases, cancer in particular [2]. To build a regression model relating the molecular structure of a material to its properties, the structure is represented as a set of descriptors: for example, the presence of certain functional groups, dielectric constant, etc. In this work, a descriptor selection procedure for a set of calixarenes potentially suitable for a nanophotonic sensor system for rapid detection of volatile organic compounds in gaseous biosamples is presented. Within this experiment, ΔG values of interaction with propanol-1 molecules in the gas phase were theoretically calculated for different calixarenes.

Conclusion. A satisfactory correlation was shown for the regression model trained on the optimized set of descriptors and calculated ΔG values, sufficient for semi-quantitative evaluation.

References:

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