I. I. Baskin[1,2,3]
N. I. Zhokhova[1]
G. V. Sitnikov[3,4]
A. Varnek[2,3]

3D QSAR: achievments and perspectives

[1] Chair of Polymer and Crystal Physics, Faculty of Physics, M.V.Lomonosov Moscow State University, Leninskie Gory, Moscow, Russia;
[2] A.M. Butlerov Institute of Chemistry, Kazan Federal University, Kremlyovskaya St. 18, Kazan, Russia;
[3] Laboratoire de Chémoinformatique, UMR 7140 CNRS, Université de Strasbourg, 1 rue Blaise Pascal, Strasbourg, France;
[4] A.N.Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, Vavilova St. 28, Moscow, Russia;

The lecture reviews the state of the art in 3D QSAR methods combining both alignment-based and alignment-free approaches. Three types of molecular fields are considered: molecular interection fields, atomic property fields, and the fields based on the electron density function. The main problems and challengies for 3D QSAR analysis are outlined. The perspectives of 4D QSAR modeling will be discussed.

The second part of the lecture is devoted to the theory and applications of the continuous molecular field approach [1-2] to building 3D QSAR regression and one-class classification models. Particular attention is paid to continuous indicator fields [3], which combine the 3D QSAR methodology and the substructural approach. Continuous indicator fields (CIF) can be considered as 3D analogues of topological substructural fragments. CIF models can be interpreted in terms of preferable and undesirable positions of certain types of atoms in space. This helps to understand which changes in chemical structure should be made in order to design a compound possessing desirable properties. The applications concidered in the lecture concern 3D QSAR models for protein-ligand interaction, metal complexation and absorption of coloring dyes.

The last part of the lecture describes the perspectives of 3D QSAR. The possibilities of using machine learning for solving 3D QSAR problems will be discussed.

1. Baskin I.I., Zhokhova N.I. *J. Comput.-Aided Mol. Des.*, 2013, **27(5)**: 427-442.
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3. Sitnikov G.V., Zhokhova N.I., Ustynyuk Yu.A., Varnek A., Baskin I.I. *J. Comput.-Aided Mol. Des.*, 2015, **29(3)**: 233-247.

Most of this work was supported by Russian Foundation for Basic Research (Grant 13-07-00511). A part of this study was supported by Russian Scientific Foundation (Agreement No 14-43-00024, dated by October 1, 2014).