XVIII МЕНДЕЛЕЕВСКИЙ СЪЕЗД ПО ОБЩЕЙ И ПРИКЛАДНОЙ ХИМИИ

Москва, 23–28 сентября 2007 г.

ТЕЗИСЫ ДОКЛАДОВ

В пяти томах

Том 5

IV Российско-французский симпозиум «Супрамолекулярные системы в химии и биологии»

II Российско-индийский симпозиум по органической химии

Международный симпозиум по современной радиохимии «Радиохимия: достижения и перспективы»

Международный симпозиум «Зеленая химия, устойчивое развитие и социальная ответственность химиков»

Симпозиум «Нуклеофильное замещение водорода в ароматических системах и родственные реакции»

Москва – 2007

THE USE OF MODERN MACHINE LEARNING APPROACHES TO MODEL PROPERTIES DEPENDING ON INTERMOLECULAR INTERACTIONS. THE MELTING POINTS OF ION LIQUIDS AND STABILITY CONSTANTS OF SUPRAMOLECULAR COMPLEXES

Baskin I.I.,[a] Zhokhova N.I.,[a] Varnek A.,[b] Kireeva N.,[b] Tetko I.V.,[c] Solov'yov V.P.[d]

[a]Department of Chemistry, Moscow State University, Leninskie Gory 1/3, 119992 Moscow, Russia
[b]Laboratoire d'Infochimie, UMR 7551 CNRS, Université Louis Pasteur, 4, rue B. Pascal, Strasbourg 67000, France
[c]Institute of Bioorganic Chemistry and Petrochemistry, Kiev, Ukraine
[d]Institute of Physical Chemistry, Russian Academy of Sciences, Leninskiy prospect 31a, 119991 Moscow, Russia

The need of creating new materials based on supramolecular complexes and nanomolecular structures necessitates the development of computational approaches capable of predicting various properties depending on the stability of intermolecular interactions and molecular recognition. Along with the molecular modeling approaches, the methods of chemoinformatics based on statistical processing of databases containing relevant experimental data start to play an important role in this field nowadays.

In this study, a big battery of modern machine learning approaches, ranging from traditional multiple linear regression up to advanced types of artificial neural networks and kernel-based support vector machines, in conjunction with the use of various types of molecular descriptors, ranging from easy-to-compute graph-topology based fragmental descriptors and topological indices up to 3D descriptors, was applied to study the ability of these methods to predict properties depending on intermolecular interactions. The case studies included predicting the melting points of ion liquids and the stability constants of crown ether complexes with several metals as well as the stability constants of host-guest inclusion complexes of organic ligands with beta-cyclodextrines. For the case of the melting points of ion liquids, which play an important role in modern "green chemistry" technologies and for which this property is an important technical parameter, several tested approaches have demonstrated comparable performance limited by the reproducibility and the complexity of the solid-liquid phase transition phenomenon. Machine learning methods have also shown good performance in predicting stability constants of crown-ether and beta-cyclodextrine complexes.

This works was carried out in the framework of ARCUS "Alsace – Russia/Ukraine" project.

References

1. A. Varnek, N. Kireeva, I. V. Tetko, I. I. Baskin, V. P. Solov'ev, *J. Chem. Inf. Mod.* 2007, **47**, ASAP article.