



Second Kazan Summer School on Chemoinformatics

Book of Abstracts
and Scientific Program

July 6-9, 2015
Kazan, Russia

V. Solov'ev¹
M. Glavatskikh^{2,3}
T. Madzhidov^{2,3}
M. Gilles²
D. Horvath²
A. Varnek²

QSPR MODELS FOR HALOGEN BOND STRENGTH

¹ Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Leninskiy prosp., 31, 119071 Moscow, Russia;
² Laboratoire de Chimoinformatique, UMR 7140 CNRS, Université de Strasbourg, 1, rue Blaise Pascal, 67000 Strasbourg, France;
³ Laboratory of Chemoinformatics and Molecular Modeling, Butlerov Institut of Chemistry, Kazan Federal University, Kremlevskaya 18, Kazan, Russia;

solovev-vp@mail.ru

Predicting affinity for halogens of electron-enriched groups in organic molecules – a property related, but not identical to basicity, H-bond acceptor strength and nucleophilicity – represents a complementary approach for better characterization of intermolecular interactions in various contexts, including protein-ligand binding. Here, we report SVM and ensemble MLR models of Halogen bond basicity scale based on the stability constant of halogen bonding ($\log K_{\text{BI2}}$) and the labeled ISIDA fragment descriptors. These models display good predictive performance ($RMSE = 0.39 - 0.47 \log K_{\text{BI2}}$ units) in external cross-validation. Moreover, they are able to reliably estimate stability constants of the complexes of I_2 with polyfunctional molecules ($RMSE = 0.49 - 0.59$). Consensus SVM and ensemble MLR models are available for the users on our websites infochim.u-strasbg.fr/webserv/VSEngine.html (SVM) and <http://vpsolovev.ru/programs/> (eMLR). Details of this work are given in the poster presentation by M. Glavatskikh et al. on this school.