K S S CI

2 0 1 7

3rd Kazan Summer School on Chemoinformatics

Book of Abstracts

July 5-7, 2017 Kazan, Russia

V. Solov'ev [1]
A. Varnek [2]

THE ISIDA_QSPR PROGRAM: ENSEMBLE QSPR MODELING ON FRAGMENT DESCRIPTORS

[1] Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Leninskiy prosp., 31, 119071 Moscow, Russia;
[2] Laboratoire de Chémoinformatique, UMR 7140 CNRS, Université de Strasbourg, 1, rue Blaise Pascal, 67000 Strasbourg, France;
solovev-vp@mail.ru

The ISIDA_QSPR program [1, 2] realizes Multiple Linear Regression (MLR) analysis involving ISIDA Substructure Molecular Fragment (SMF) descriptors. The program uses Structure-Data Files as input data for automatic generation of fragment descriptors derived from 2D chemical structures. Ensemble modeling workflow implemented into the program includes (*i*) generation of a great number of individual QSPR models, (*ii*) selection of the most relevant ones and (*iii*) their consensus application to a test set compounds (Fig. 1). The ISIDA_QSPR graphical interface pilotes this workflow and supports analysis of the obtained results. It runs under the Windows operating system. The Consensus Predictor tool realizes property predictions and virtual screening using previously obtained consensus models. It can be used as a convenient tools for design of new compounds with desired properties.

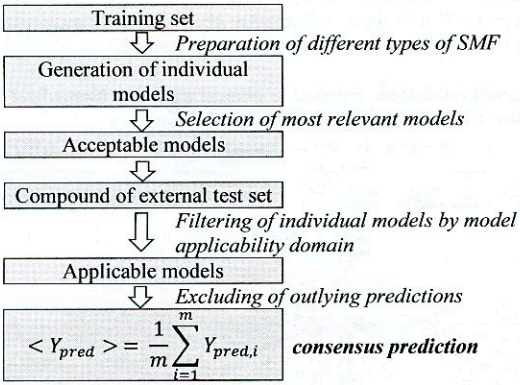

Fig. 1 Ensemble modeling workflow

1. Solov'ev V. et al. *In: Tutorials in Chemoinformatics,* Strasbourg: John Wiley & Sons Ltd, 2017: 135 – 162.
2. Solov'ev V., Varnek A. ISIDA (In Silico Design and Data Analysis) program; version 5.79; 2008–2017. http://vpsolovev.ru/programs/ (accessed 9 April 2017).