allied academies

4th International Congress on

DRUG DISCOVERY, DESIGNING AND DEVELOPMENT &

International Conference and Exhibition on

BIOCHEMISTRY, MOLECULAR BIOLOGY: R&D

November 02-03, 2017   Chicago, USA

The dependence of the kNN-QSAR models on the initial descriptors set generation

Fatima T Adilova, Rifkat R Davronov and **Uygun U Jamilov**
Institute of Mathematics, Academy of Sciences, Uzbekistan

Statement of the Problem: QSAR model development and validation has led to establish a complex strategy that can be used to prioritize the selection of chemicals for the experimental validation. The high accuracy of the training set model characterized with leave-one-out cross validated R2 (q2).However, the dependence of this method on the descriptors initial set has not been previously studied.

Methodology & Theoretical Orientation: In this study, following the kNN-QSAR principle, we to study the dependence of the kNN-QSAR on the initial set of descriptors, using of two other packages -rcdk , Dragon, and all calculations were carried out in the system R.

Findings: The first data set was a well-known group of ligands of corticosteroid binding globulin. From all 320 models from two training sets the best predictive model was characterized by $q2 = 0.74$, $R2 = 0.86$, $R0 2 = 0.82$, $RMSE = 0.04$, $F = 49.3$, $k = 0.98$ and $P = 1.1 \times 10-4$. The second data set was the alkaloids of harmala ordinary quinazoline structure and derivatives. The original sample was randomly broken up three times divided into a training, test samples, while laying down an external sample. Three series of simulation running were conducted, in each of which 242, 99 and 10 QSAR models were built; the best predictive model produced from the first training set: $q2 = 0.72$, $R2 = 0.92$, $R02 = 0.87$, $RMSE = 0.005$, $F = 318.88$, $k = 1.02$ and $P = 6.9 \times 10-7$.

Conclusion & Significance: The required dependence exists, so it is necessary to determine the criteria for the robustness of the models. In addition, it would be promising to study other methods for determining the proximity and similarity of compounds.

Speaker Biography

Adilova Fatima has completed her PhD at the age of 30 years Institute of Cybernetics, Academy of Sciences, Uzbekistan and postdoctoral studies from the Institute of Control Science, Russian Academy of Sciences. She is the Head of Biomedical Lab., Institute of Mathematics , Academy of Sciences, Uzbekistan. She has published more than 60 papers in reputed journals and has been serving as an expert of State Committee of Science &Technology.

e: fatima _adilova@rambler.ru

Notes: