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Non-Linear Assessment of Chromatographic Lipophilicity and Model Ranking of Newly Synthesized Steroid Derivatives

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Abstract : The present paper deals with chromatographic lipophilicity prediction of newly synthesized steroid derivatives. The prediction was achieved using in silico generated molecular descriptors and quantitative structure-retention relationship (QSRR) methodology with the artificial neural networks (ANN) approach. Chromatographic lipophilicity of the investigated compounds was expressed as retention factor value logk. For QSRR modeling, a feedforward back-propagation ANN with gradient descent learning algorithm was applied. Using the novel sum of ranking differences (SRD) method generated ANN models were ranked. The aim was to distinguish the most consistent QSRR model that can be found, and similarity or dissimilarity between the models that could be noticed. In this study, SRD was performed with average values of retention factor value logk as reference values. An excellent correlation between experimentally observed retention factor value logk and values predicted by the ANN was obtained with a correlation coefficient higher than 0.9890. Statistical results show that the established ANN models can be applied for required purpose. This article is based upon work from COST Action (TD1305), supported by COST (European Cooperation in Science and Technology).

Keywords : artificial neural networks, liquid chromatography, molecular descriptors, steroids, sum of ranking differences
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