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Non-Linear Assessment of Chromatographic Lipophilicity of Selected Steroid Derivatives

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Abstract : Using chemometric approach, the relationships between the chromatographic lipophilicity and in silico molecular descriptors for twenty-nine selected steroid derivatives were studied. The chromatographic lipophilicity was predicted using artificial neural networks (ANNs) method. The most important in silico molecular descriptors were selected applying stepwise selection (SS) paired with partial least squares (PLS) method. Molecular descriptors with satisfactory variable importance in projection (VIP) values were selected for ANN modeling. The usefulness of generated models was confirmed by detailed statistical validation. High agreement between experimental and predicted values indicated that obtained models have good quality and high predictive ability. Global sensitivity analysis (GSA) confirmed the importance of each molecular descriptor used as an input variable. High-quality networks indicate a strong non-linear relationship between chromatographic lipophilicity and used in silico molecular descriptors. Applying selected molecular descriptors and generated ANNs the good prediction of chromatographic lipophilicity of the studied steroid derivatives can be obtained. This article is based upon work from COST Actions (CM1306 and CA15222), supported by COST (European Cooperation and Science and Technology).

Keywords : artificial neural networks, chemometrics, global sensitivity analysis, liquid chromatography, steroids
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