

QSRR Analysis of 17-Picolyl and 17-Picolinylidene Androstane Derivatives Based on Partial Least Squares and Principal Component Regression

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Abstract : There are several methods for determination of the lipophilicity of biologically active compounds, however chromatography has been shown as a very suitable method for this purpose. Chromatographic (C18-RP-HPLC) analysis of a series of 24 17-picolyl and 17-picolinylidene androstane derivatives was carried out. The obtained retention indices (logk, methanol (90%) / water (10%)) were correlated with calculated physicochemical and lipophilicity descriptors. The QSRR analysis was carried out applying principal component regression (PCR) and partial least squares regression (PLS). The PCR and PLS model were selected on the basis of the highest variance and the lowest root mean square error of cross-validation. The obtained PCR and PLS model successfully correlate the calculated molecular descriptors with logk parameter indicating the significance of the lipophilicity of compounds in chromatographic process. On the basis of the obtained results it can be concluded that the obtained logk parameters of the analyzed androstane derivatives can be considered as their chromatographic lipophilicity. These results are the part of the project No. 114-451-347/2015-02, financially supported by the Provincial Secretariat for Science and Technological Development of Vojvodina and CMST COST Action CM1105.

Keywords : androstane derivatives, chromatography, molecular structure, principal component regression, partial least squares regression

Conference Title : ICBBE 2015 : International Conference on Biochemical and Biomedical Engineering

Conference Location : Madrid, Spain

Conference Dates : November 12-13, 2015