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Evaluation of Newly Synthesized Steroid Derivatives Using In silico Molecular Descriptors and Chemometric Techniques

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Abstract : This study considered selection of the in silico molecular descriptors and the models for newly synthesized steroid derivatives description and their characterization using chemometric techniques. Multiple linear regression (MLR) models were established and gave the best molecular descriptors for quantitative structure-retention relationship (QSRR) modeling of the retention of the investigated molecules. MLR models were without multicollinearity among the selected molecular descriptors according to the variance inflation factor (VIF) values. Used molecular descriptors were ranked using generalized pair correlation method (GPCM). In this method, the significant difference between independent variables can be noticed regardless almost equal correlation between dependent variable. Generated MLR models were statistically and cross-validated and the best models were kept. Models were ranked using sum of ranking differences (SRD) method. According to this method, the most consistent QSRR model can be found and similarity or dissimilarity between the models could be noticed. In this study, SRD was performed using average values of experimentally observed data as a golden standard. Chemometric analysis was conducted in order to characterize newly synthesized steroid derivatives for further investigation regarding their potential biological activity and further synthesis. This article is based upon work from COST Action (CM1105), supported by COST (European Cooperation in Science and Technology).

Keywords : generalized pair correlation method, molecular descriptors, regression analysis, steroids, sum of ranking differences
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