SUM OF RANKING DIFFERENCES AND GENERALIZED PAIR CORRELATION METHOD IN SELECTION OF OPTIMAL LIPOPHILICITY PARAMETERS OF NOVEL ANTICANCER STEROIDAL DERIVATIVES

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Abstract

Lipophilicity occurs as one of the most experimentally exploited feature of novel potential drug candidates. A novel set of 30 investigated steroids expressed affinity toward different cancer cell lines. In order to additionally characterize these compounds their chromatographic lipophilicity was determined. This study covers chromatographic lipophilicity (log*k*) determination using reversed-phase ultra-high performance liquid chromatography (RP-UHPLC) with polar aprotic and protic solvents and C18 column. As mobile phases mixtures methanol-water (60:40 v/v), methanol-acetonitrile-water (30:30:40 v/v) and acetonitrile-water (60:40 v/v) were used. Also, a set of different *in silico* lipophilicity descriptors (log*P*) and water solubility descriptors (log*S*) were calculated based on 2D and 3D molecular structures, as well as the average log*P* and average log*S* values were estimated. Two non-parametric methods, sum of ranking differences (SRD) and generalized pair correlation method (GPCM) were used for the optimal lipophilicity parameters selection. The experimentally obtained log*k* values and *in silico* log*P* and log*S* values were taken into calculations for SRD and GPCM analysis. Results showed that majority of *in silico* descriptors are placed nearby the experimentally obtained log*k* values and can be used as optimal parameters for lipophilicity estimation.

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