

Non-Parametric Ranking of Triazine Derivatives based on Chromatographic Parameters

Authors : Sanja Podunavac-Kuzmanović, Strahinja Kovačević, Milica Karadžić Banjac, Lidija Jevrić, Jasmina Anojčić

Abstract : The two groups of symmetrical triazine derivatives were analyzed applying sum of ranking differences (SRD) approach in terms of their chromatographic lipophilicity parameters determined in reversed-phase ultra-high performance liquid chromatography (RP-UHPLC) system. The first group of compounds (1-4) contained the triazines with two acyclic substituents, while the second group (5-8) included the compounds with two cyclic substituents (cyclopentyl, cyclohexyl, cycloheptyl and cyclooctyl). The compounds were analyzed applying two stationary phases (C18 and phenyl) and three mobile phases (methanol/water, methanol/acetonitrile/water and acetonitrile/water). The retention parameters considered in the ranking analysis are the following: capacity factors ($\log k$ and $\log k_0$), alternative lipophilicity parameter (C_0) and the slope (S) of the dependence between the fraction of modifier in mobile phase (φ) and $\log k$. SRD analysis was applied on the retention data normalized by min-max normalization method. The ranking was based on row average as a reference ranking. The SRD results were validated by 7-fold cross-validation approach. The results indicate that the compounds 1, 4 and 5 are the closest to the reference ranking, while the compounds 6, 2, 7 and 8 are far from the reference. The compound 3 is placed between these two groups. The compounds that are placed furthest from the average ranking have several retention parameters that significantly deviate from others, particularly compounds 7 and 8 that are the biggest molecules in the analyzed groups. The SRD analysis did not discriminate the compounds based on their substituents. Acknowledgement: The present research is supported by the project of Provincial Secretariat for Higher Education and Scientific Research of AP Vojvodina (Molecular engineering and chemometric tools: Towards safer and greener future, No. 002902513 2024 09418 003 000 000 001 04 002).

Keywords : chromatography, lipophilicity, pesticides, triazines

Conference Title : ICCCM 2025 : International Conference on Computational Chemistry and Modelling

Conference Location : Malaga, Spain

Conference Dates : September 06-07, 2025