COMPUTATIONAL MODELING OF DISTRIBUTION COEFFICIENT OF TRIAZINE DERIVATIVES AND ITS INFLUENCE ON THEIR CHROMATOGRAPHIC BEHAVIOR IN RP-UHPLC SYSTEM

Benjamin Salaković[1], Strahinja Kovačević[1], Milica Karadžić Banjac[1], Jasmina Anojčić[2], Lidija Jevrić[1], Sanja Podunavac-Kuzmanović[1], Slobodan Gadžurić[2], Dušan Antonović[3]

[1]University of Novi Sad, Faculty of Technology Novi Sad, Department of Applied and Engineering Chemistry, Bulevar cara Lazara 1, 21000 Novi Sad, Serbia
[2]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
[3]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia
e-mail: benjamin.salakovic@uns.ac.rs

Abstract

In the present study, the distribution coefficient (log*D*) of a series of *s*-triazine derivatives with acyclic and cyclic substituents was modelled by using MarvinSketch software. The calculation of log*D* was done by Viswanadhan and Ghose (VG), Klopman's (KLOP) and PHYSPROP© (PHYS) methods. During the calculations, the tautomerization and resonance were taken into account. The pH-log*D* dependences were obtained for each molecule. The log*D* data determined at various pH values were further correlated with retention parameter (log*k*) of studied compounds. The log*k* values were determined by using revered-phase ultra-high performance liquid chromatography (RP-UHPLC) with C_{18} stationary phase and mobile phase as a mixture of methanol and water. The volume fraction of methanol in the mobile phase varied from 50 to 85 (v/v). Based on the retention time and dead time, log*k* parameters were determined and further correlated with log*D* values. The outstanding linear correlations were obtained. Considering the fact that log*D* parameter is in most cases a better descriptor of the lipophilicity of a compound than partition coefficient (log*P*), it can better describe the retention behavior in reversed-phase liquid chromatography that strongly depends on the compound's lipophilicity.

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