

THE APPLICATION OF PHENYL COLUMN AS A NEW CHALLENGE IN ANISOTROPIC LIPOPHILICITY DETERMINATION OF 17-PICOLYL AND 17-PICOLINYLIDENE ANDROSTANE DERIVATIVES BY RP-UHPLC METHOD

Strahinja Kovačević¹, Milica Karadžić Banjac¹, Jasmina Anojčić², Jovana Ajduković², Sanja Podunavac-Kuzmanović¹, Slobodan Gadžurić², Lidija Jevrić¹

¹University of Novi Sad, Faculty of Technology Novi Sad, Department of Applied and Engineering Chemistry, Bulevar cara Lazara 1, 21000 Novi Sad, Serbia

²University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
e-mail: strahko@uns.ac.rs

Abstract

Androstane derivatives are highly-potent compounds with anticancer activity. The lipophilicity is one of the most important physicochemical parameters of biologically active compounds. Experimental determination of lipophilicity takes into account numerous approaches among which is chromatography as one of the most reliable analytical methods. Usually, the chromatographic determination of lipophilicity of biologically active compounds is based on application of C₁₈ or C₈ columns. In the case of 17-picolyl and 17-picolinylidene androstane derivatives C₁₈ column has been applied earlier. However, this study presents the challenge in the lipophilicity determination by using phenyl column in reversed-phase ultra-high performance liquid chromatography (RP-UHPLC) system. The method with the phenyl column is specific due to the presence of π - π interactions between the phenyl column and π -electron containing 17-picolyl and 17-picolinylidene androstane derivatives. The mobile phases used were three types of mixtures including methanol/water mixture, acetonitrile/water mixture and methanol/acetonitrile/water mixture. The fraction of water in mobile phases varied from 20 to 30 v/v. The results of the chromatographic analysis showed a good separation of the analyzed androstane derivatives and provided chromatographic parameters (capacity factor – $\log k$) well correlated with *in silico* lipophilicity descriptors (partition coefficient – $\log P$). Therefore, the $\log k$ values, obtained by using phenyl column, of the analyzed androstane derivatives can be considered to be their lipophilicity measures or chromatographic (anisotropic) lipophilicity measures.

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