

## Organic Solvents Influence on Electronic Absorption Spectra of 4-R-phenyl-5-carboxyethyl-6-methyl-3,4-dihydropyrimidine-2-tione Derivatives. Ionization Constants Determination

Nada U. Perišić-Janjić<sup>1</sup>, Gy.Gy. Vastag<sup>1</sup>, J.D. Janjić<sup>1</sup>, B.Ž. Jovanović<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Sciences, Trg D. Obradovića 3, 21000 Novi Sad, Serbia

<sup>2</sup>Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Beograd, Serbia

Derivatives of 4-R-phenyl-carboxyethyl-6-methyl-3,4-dihydropyrimidine-2-tione known as “Biginelli compounds” [1] are widely investigated due to their biological activity [2]. For the further application of these biologically active compounds, it is necessary to investigate their physicochemical characteristics. The aim of this work was to study solvents polarity effect and proton-donor ability on electronic absorption spectra of some “Biginelli compounds” and determination of their ionization constants by spectrophotometric method.

Absorption spectra of 4-R-phenyl-carboxyethyl-6-methyl-3, 4-dihydropyrimidine-2-tione derivatives show characteristic absorption maximum at about 302-310 nm in aqueous solutions. A bathochromic shift of absorption maximum and increase of absorption intensity, with decrease of solvent polarity were registered. Absorption spectra recorded in aqueous and alcoholic solution pass through isobestic point at about 290 nm. Changes of absorption maximum position with change of solvent polarity indicate that hydrogen bonds were formed between solvent and investigated compounds. In order to explain the effect of solvent polarity and hydrogen bonding on the absorption spectra, linear solvation energy relationship (LSER) concept developed by Kamlet and Taft [3] was performed.

Ionization constants of “Biginelli compounds” were determined by spectrophotometric method. Effects of chemical structure on ionization constants were investigated. Good correlation was obtained between ionization constants and Hammett substituents constants,  $\sigma$ . Since “Biginelli compounds” are biologically active, correlations between ionization constants, as electronic descriptors, and measure of lipophilicity (log P) of investigated compounds were established. Using computer program “Chemsilico” [4], the biological activity of investigated compounds were determined and correlated with calculated ionization constants. Satisfactory correlation was obtained.

[1] P. Biginelli, Gazz. Chim. Ital. 23, (1993) 360.

[2] C.O. Kappe, Tetrahedron 49 (1993) 6937.

[3] M.J. Kamlet, J.L.M. Abboud, M.H. Abraham, R.W. Taft, J. Org. Chem. 48 (1983) 2877.

[4] <http://www.chemsilico.com/>