CREATIVE MATH. & INF.
22 (2013), No. 1, 33 - 40

Online version available at http://creative-mathematics.ubm.ro/
Print Edition: ISSN 1584 - 286X Online Edition: ISSN 1843 - 441X

A QSPR study of hydrophobicity of phenols and 2-(aryloxy-α-acetyl)-phenoxathiin derivatives using the topological index ZEP

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ABSTRACT.

The molecular hydrophobicity (R_{MO}) of several newly synthesized phenoxathiin derivatives and of phenols with congeneric structures have been recently correlated with some simple physico-chemical calculated parameters of compounds: the water solubility ($\log S_w$); the partition coefficient ($\log P$); the Gibbs energy of formation (ΔG_f), and the aromaticity index (HOMA) [Beteringhe, A., Radutiu, A. C., Constantinescu, T., Patron, L. and Balaban, A. T., *Quantitative Structure-Property Relationship (QSPR) study of the hydrophobicity of phenols and 2-(aryloxy-α-acetyl)-phenoxathiin derivatives*, Rev. Chim. (Bucureşti) , **59** (2008), No. 11, 1175–1179]. The best correlation was found as a biparametric regression equation in terms of $\log S_w$ and HOMA, which cannot be improved by adding one or two of the parameters aforementioned.
In the present work we describee the weighted electronic distance based topological index (ZEP) and then use it for QSPR studies of R_{MO} in combination with $\log S_w$, $\log P$, ΔG_f and HOMA. Most of the three parameter QSPR correlations of R_{MO} are significantly improved by involving the theoretical parameter ZEP.

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Received: 23.02.2010; In revised form: 19.08.2012; Accepted: 22.09.2012
2010 *Mathematics Subject Classification.* 92E10.
Key words and phrases. *Molecular hydrophobicity, phenoxathiin derivatives, water solubility, HOMA, ZEP topological index, QSPPR.*