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**Volume 107, Issue 8 , Pages 1736 - 1744**

**Special Issue:** Proceedings from the 3rd Humboldt Conference on Computational Chemistry . Issue Edited by Georgi N. Vayssilov, Tzonka Mineva.

**Published Online:** 3 Jan 2007  
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## Modeling the octanol-water partition coefficient of substituted phenols by the use of structure information

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**Funded by:**

▪ UEFISCSU Romania; Grant Number: ET36/2005

**KEYWORDS**

molecular descriptors family on structure-property relationships (MDF-SPR) • octanol-water partition coefficient • para-substituted phenols

**ABSTRACT**

This work presents the abilities in estimation and prediction of the octanol-water partition coefficient of some para-substituted phenols through the integration of complex structures information by the use of an original molecular descriptors family on the structure-property relationship approach. The proposed approach uses the complex information obtained from para-substituted phenols structure in order to generate and calculate the molecular descriptors family. The structure-property relationship models were built based on the generated descriptors. The obtained multi-varied models (model with two and four descriptors, respectively) were validated through the assessment of the cross-validation leave-one-out score. The comparison between the multi-varied model with two and four descriptors was performed using Steiger's Z-test. The analysis of the statistical characteristics of the obtained models demonstrated that the model with four descriptors has greater ability to estimate and predict compared with the model with two descriptors. This observation was

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also sustained by the results of correlated-correlation analysis. The multi-varied model with four descriptors revealed that the octanol-water partition coefficient of studied para-substituted phenols is likely to be of geometry nature, it is strongly dependent on the partial charges of compounds and group electronegativity, and it is in relation to the elastic force. © 2007 Wiley Periodicals, Inc. Int J Quantum Chem, 2007

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Received: 14 August 2006; Accepted: 29 November 2006

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