

### **Computational chemistry approaches for understanding how structure determines properties**

Katritzky, Alan R.; Slavov, Svetoslav H.; Radzvilovits, Maksim; Stoyanova-Slavova, Iva B.; **Karelson, Mati** Zeitschrift für Naturforschung B - a journal of chemical sciences 2009 / 6, p. 773-777

### **Correlation of the photolysis half-lives of polychlorinated dibenzo-p-dioxins and dibenzofurans with molecular structure**

Katritzky, Alan R.; Slavov, Svetoslav H.; Stoyanova-Slavova, Iva B.; **Karelson, Mati** Journal of physical chemistry A 2010 / 7, p. 2684-2688 : ill <https://pubmed.ncbi.nlm.nih.gov/20112909/>

### **Novel computational models for predicting dopamine interactions**

Katritzky, Alan R.; **Dobchev, Dimitar**; Stoyanova-Slavova, Iva B.; Kuanar, Minati; Bespalov, Maxim M.; **Karelson, Mati**; **Saarma, Mart** Experimental neurology 2008 / 1, p. 150-171 <https://www.sciencedirect.com/science/article/pii/S0014488608000368>

### **QSPR modeling of flash points : an update**

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### **Quantitative structure-activity relationship (QSAR) modeling of EC50 of aquatic toxicities for Daphnia magna**

Katritzky, Alan R.; Slavov, Svetoslav H.; Stoyanova-Slavova, Iva B.; **Kahn, Iiris**; **Karelson, Mati** Journal of toxicology and environmental health. Part A, Current issues 2009 / 19, p. 1181-1190 : ill <https://pubmed.ncbi.nlm.nih.gov/20077186/>

### **Quantitative structure-property relationship studies on Ostwald solubility and partition coefficients of organic solutes in ionic liquids**

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