

Physical, chemical and technological property correlation with chemical structure : the potential of QSPR

Katritzky, Alan R.; Dobchev, Dimitar A.; **Karelson, Mati** Zeitschrift für Naturforschung B 2006 / 4, p. 373-384

<https://www.degruyter.com/document/doi/10.1515/znb-2006-0403/html?lang=en>

Prediction of peptide IMS cross sections from extended molecular connectivity

Oliferenko, Alexander; Tian, Feifei; **Karelson, Mati**; Katritzky, Alan R. International journal of mass spectrometry 2012 / p. 1-5

<https://www.sciencedirect.com/science/article/pii/S1387380611004295>

QSPR modeling of flash points : an update

Katritzky, Alan R.; Stoyanova-Slavova, Iva B.; **Dobchev, Dimitar; Karelson, Mati** Journal of molecular graphics and modelling 2007 /

2, p. 529-536 : ill <https://www.sciencedirect.com/science/article/pii/S1093326307000617>

QSPR modeling of hyperpolarizabilities

Katritzky, Alan R.; Pacureanu, Liliana; **Dobchev, Dimitar; Karelson, Mati** Journal of molecular modeling 2007 / 9, p. 951-963 : ill

https://www.researchgate.net/publication/6267202_QSPR_modeling_of_hyperpolarizabilities

QSPR modeling of UV absorption intensities

Katritzky, Alan R.; Slavov, Svetoslav; **Dobchev, Dimitar; Karelson, Mati** Journal of computer-aided molecular design 2007 / 7, p.

371-377 https://www.researchgate.net/publication/6272883_QSPR_modeling_of_UV_absorption_intensities

QSPR study of the first and second critical micelle concentrations of cationic surfactants

Katritzky, Alan R.; Pacureanu, Liliana M.; Slavov, Svetoslav H.; Dobchev, Dimitar A.; Shah, Dinesh O.; **Karelson, Mati** Computers &

chemical engineering 2009 / 1, p. 321-332 : ill <https://www.sciencedirect.com/science/article/pii/S0098135408001956>

Rapid QSPR model development technique for prediction of vapor pressure of organic compounds

Katritzky, Alan R.; Slavov, Svetoslav; **Dobchev, Dimitar; Karelson, Mati** Computers & chemical engineering 2007 / 9, p. 1123-1130

<https://www.sciencedirect.com/science/article/pii/S0098135406002511>

The classification of solvents by combining classical QSPR methodology with principal component analysis

Katritzky, Alan R.; Fara, Dan C.; Kuanar, Minati; Hür, Evrim; **Karelson, Mati** The journal of physical chemistry. A 2005 / 45, p. 10323-

10341