

A comparative QSAR study of SVM and PPR in the correlation of lithium cation basicities

Katritzky, Alan R.; Ren, Yueying; Slavov, Svetoslav H.; **Karelson, Mati** Collection of Czechoslovak chemical communications 2009 / p. 217-241 <https://doi.org/10.1135/cccc2008191>

Comparison between 2D and 3D-QSAR approaches to correlate inhibitor activity for a series of indole amide hydroxamic acid

Katritzky, Alan R.; Slavov, Svetoslav; **Dobchev, Dimitar; Karelson, Mati** QSAR & combinatorial science 2007 / 3, p. 333-345 <https://onlinelibrary.wiley.com/doi/abs/10.1002/qsar.200630021>

Computational chemistry approaches for understanding how structure determines properties

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

Correlation of blood-brain penetration using structural descriptors

Katritzky, Alan R.; Kuanar, Minati; Slavov, Svetoslav; Dobchev, Dimitar A.; Fara, Dan C.; **Karelson, Mati**; Acree, William E.; Solov'ev, Vitaly P.; Varnek, Alexandre Bioorganic & medicinal chemistry 2006 / 14, p. 4888-4917 : ill

Correlation of the melting points of potential ionic liquids (Imidazolium Bromides and Benzimidazolium Bromides) using CODESSA program [J.Chem.Inf.Comput.Sci. 42, 225-231 (2002)]

Katritzky, Alan R.; Jain, Ritu; **Lomaka, Andre**; Petrukhin, Ruslan; **Karelson, Mati**; Visser, Ann E.; Rodgers, Robin D. Journal of chemical information and modeling 2005 / 2, p. 533-534 <https://pubs.acs.org/doi/10.1021/ci049691z>

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/>

Estimating the toxicities of organic chemicals in activated sludge process

Katritzky, Alan R.; Kasemets, Kalev; Slavov, Svetoslav; Radzivilovits, Maksim; Tamm, Kaido; **Karelson, Mati** Water research 2010 / 8, p. 2451-2460 : ill

A general treatment of solubility 4. Description and analysis of a PCA model for Ostwald solubility coefficients

Tulp, Indrek; Dobchev, Dimitar A.; Katritzky, Alan R.; Acree, William jr; Maran, Uko Journal of chemical information and modeling 2010 / 7, p. 1275-1283 : ill <https://pubs.acs.org/doi/10.1021/ci1000828>

Legitimate utilization of large descriptor pools for QSPR/QSAR models

Katritzky, Alan R.; **Dobchev, Dimitar**; Slavov, Svetoslav; **Karelson, Mati** Journal of chemical information and modeling 2008 / 11, p. 2207-2213 : ill <https://pubs.acs.org/doi/10.1021/ci8002073>

Novel computational models for predicting dopamine interactions

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

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>

QSAR modeling of blood : air and tissue : air partition coefficients using theoretical descriptors

Katritzky, Alan R.; Kuanar, Minati; Fara, Dan C.; **Karelson, Mati**; Acree, William E.; Solov'ev, Vitaly P.; Varnek, Alexandre Bioorganic & medicinal chemistry 2005 / 23, p. 6450-6463 <https://pubmed.ncbi.nlm.nih.gov/16202613/>

QSAR modeling of the antifungal activity against Candida albicans for a diverse set of organic compounds

Katritzky, Alan R.; Slavov, Svetoslav; **Dobchev, Dimitar; Karelson, Mati** Bioorganic & medicinal chemistry 2008 / 14, p. 7055-7069 : ill <https://www.sciencedirect.com/science/article/pii/S0968089608004446>

QSAR modeling of the inhibition of glycogen synthase kinase-3

Katritzky, Alan R.; Pacureanu, Liliana M.; Dobchev, Dimitar A.; Fara, Dan C.; Duchowicz, Pablo R.; **Karelson, Mati** Bioorganic & medicinal chemistry 2006 / 14, p. 4987-5002 : ill <https://www.sciencedirect.com/science/article/pii/S0968089606002069>

QSAR studies on 1-phenylbenzimidazoles as inhibitors of the platelet-derived growth factor

Katritzky, Alan R.; Dobchev, Dimitar A.; Fara, Dan C.; **Karelson, Mati** Bioorganic & medicinal chemistry 2005 / 24, p. 6598-6608 <https://pubmed.ncbi.nlm.nih.gov/16230017/>

QSAR treatment of drugs transfer into human breast milk

Katritzky, Alan R.; Dobchev, Dimitar A.; Hür, Evrim; Fara, Dan C.; **Karelson, Mati** Bioorganic & medicinal chemistry 2005 / 5, p. 1623-1632 <https://pubmed.ncbi.nlm.nih.gov/15698780/>

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>

Quantitative structure-activity relationship modeling of bioconcentration factors of polychlorinated biphenyls

Katritzky, Alan R.; Radzivilovits, Maksim; Slavov, Svetoslav; Kasemets, Kalev; Tamm, Kaido; **Karelson, Mati** Toxicological & environmental chemistry 2010 / 7, p. 1233-1247 : ill <https://www.tandfonline.com/doi/full/10.1080/02772240903306417>

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

Katritzky, Alan R.; Kuanar, Minati; Stoyanova-Slavova, Iva B.; Slavov, Svetoslav H.; **Dobchev, Dimitar; Karelson, Mati**; Acree, William jr Journal of chemical and engineering data 2008 / 5, p. 1085-1092 <https://pubs.acs.org/doi/full/10.1021/jc700607b>

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>

Synthesis and bioassay of improved mosquito repellents predicted from chemical structure

Katritzky, Alan R.; Wang, Zuoquan; Slavov, Svetoslav; Tsikolia, Maia; **Dobchev, Dimitar** Proceedings of the National Academy of Sciences of the United States of America 2008 / 21, p. 7359-7364

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