

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>

Correlation of blood-brain penetration and human serum albumin binding with theoretical descriptors

Karelson, Mati; Dobchev, Dimitar; Tamm, Tarmo; Tulp, Indrek; Jänes, Jaak; Tämm, Kaido; Lomaka, Andre; Savchenko, Deniss; Karelson, Gunnar Arkivoc 2008 / XVI, p. 38-60 : ill <https://www.arkat-usa.org/get-file/26925>

Fragment-based development of HCV protease inhibitors for the treatment of hepatitis C

Karelson, Mati; Dobchev, Dimitar; Karelson, Gunnar; Tamm, Tarmo; Tämm, Kaido; Nikonov, Andrei; Mutso, Margit; Merits, Andres Current computer-aided drug design 2012 / p. 55-61 https://www.researchgate.net/publication/221745366_Fragment-Based_Development_of_HCV_Protease_Inhibitors_for_the_Treatment_of_Hepatitis_C

Have artificial neural networks met expectations in drug discovery as implemented in QSAR framework?

Dobchev, Dimitar; Karelson, Mati Expert Opinion on Drug Discovery 2016 / p. 627 - 639

<https://doi.org/10.1080/17460441.2016.1186876> Journal metrics at Scopus Article at Scopus Journal metrics at WOS Article at WOS

Legitimate utilization of large descriptor pools for QSPR/QSAR models

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

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 study of pharmacological permeabilities

Karelson, Mati; Karelson, Gunnar; Tamm, Tarmo; Tulp, Indrek; Jänes, Jaak; Tämm, Kaido; Lomaka, Andre; Savtšenko, Deniss; Dobchev, Dimitar Arkivoc 2009 / 2, p. 218-238 : ill <https://citeseerx.ist.psu.edu/document?repid=rep1&type=pdf&doi=04010557f978e40f8e33b61f9570340690f7940e>

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 critical micelle concentration of anionic surfactants using computational molecular descriptors

Katritzky, Alan R.; Pacureanu, Liliana; Dobchev, Dimitar; **Karelson, Mati** Journal of chemical information and modeling 2007 / 3, p. 782-793 <https://pubs.acs.org/doi/10.1021/ci600462d>

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/e700607b>

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

Using artificial neural networks to predict cell-penetrating compounds

Karelson, Mati; Dobchev, Dimitar Expert opinion drug discovery 2011 / p. 783-796 : ill

