

Accessibility of published QSAR models : ecotoxic endpoints

Kahn, Iiris; Ahte, Priit; Sild, Sulev; Maran, Uko ALTEX proceedings. Vol. 4, No. 2 2015 / p. 119

Accessibility of published QSAR models : environmental fate endpoints

Kahn, Iiris; Ahte, Priit; Piir, Geven; Sild, Sulev; Maran, Uko Conferentia Chemometrica 2015 : Budapest, MTA TTK, September 13-16, 2015 / p. P33

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

Karelson, Mati; Dobchev, Dimitar; Karelson, Gunnar; Tamm, Tarmo; Tamm, 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

Fragment-based QSAR approach for novel indole-like TrkA receptor antagonist

Tammiku-Taul, Jaana; Dobchev, Dimitar Atanasov; Karelson, Mati; Timmusk, Tõnis; Park, Rahel; Jaanson, Kaur; Luberg, Kristi; Kananovich, Dzmitry; Noole, Artur; Kanger, Tõnis; Lopp, Margus 8th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2015) : Chios, Greece, June 21-25, 2015 : book of abstracts 2015 / p. 68

Fragment-based QSAR for the prediction of novel TrkA inhibitors

Tammiku-Taul, Jaana; Karelson, Mati; Dobchev, Dimitar Atanasov Scientific programme & book of abstracts : QSAR 2014 2014 / p. 170

Indole-like Trk receptor antagonists

Tammiku-Taul, Jaana; Park, Rahel; Jaanson, Kaur; Luberg, Kristi; Dobchev, Dimitar Atanasov; Kananovich, Dzmitry; Noole, Artur; Mandel, Merle; Kaasik, Allen; Lopp, Margus; Timmusk, Tõnis; Karelson, Mati European journal of medicinal chemistry 2016 / p. 541-552 : ill <https://doi.org/10.1016/j.ejmech.2016.06.003> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Lipoxygenase-catalyzed transformation of epoxy fatty acids to hydroxy-endoperoxides : a potential P450 and lipoxygenase interaction

Teder, Tarvi; Boeglin, William E.; Brash, Alan R. Journal of lipid research 2014 / p. 2587-2596 : ill <https://doi.org/10.1194/jlr.M054072> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

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>

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 prediction of HIV-1 non-nucleoside inhibitor activity based on 3D-molecular descriptors

Pillai, Girinath Gopinathan; Tamm, Kaido; Karelson, Mati TÜ ja TTÜ doktorikool "Funktsionaalsed materjalid ja tehnoloogiad" : 04.-05. märts 2014, Tartu 2014 / [1] p

QSAR study of pharmacological permeabilities

Karelson, Mati; Karelson, Gunnar; Tamm, Tarmo; Tulp, Indrek; Jänes, Jaak; Tamm, 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 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-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>

Rational design of a series of novel amphipathic cell-penetrating peptides

Regberg, Jakob; Srimanee, Artita; Dobchev, Dimitar A.; Karelson, Mati International journal of pharmaceutics 2014 / p. 111-116 : ill <https://doi.org/10.1016/j.ijpharm.2014.01.018> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

The proposal of architecture for chemical splitting to optimize QSAR models for aquatic toxicity

Colombo, Andrea; Benfenati, Emilio; **Karelson, Mati**; Maran, Uko Chemosphere 2008 / 5, p. 772-780 : ill
<https://www.sciencedirect.com/science/article/pii/S0045653508003615>

The quantitative structure activity relationships for predicting HIV protease inhibition by substituted fullerenes

Martin, Dana; **Karelson, Mati** Letters in drug design and discovery 2010 / 8, p.587-595 <https://www.euraselect.com/article/31554>

Topological fingerprints as an aid in finding structural patterns for LRRK2 inhibition

Kahn, Iiris; Lomaka, Andre; Karelson, Mati Molecular informatics 2014 / p. 269-275 : ill <https://doi.org/10.1002/minf.201300057>
[Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)