

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/>

Estimating the toxicities of organic chemicals in activated sludge process

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

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

Prediction of cell-penetrating peptides using artificial neural networks

Dobchev, Dimitar A.; Mäger, Imre; Tulp, Indrek; **Karelson, Gunnar; Tamm, Tarmo;** Tämm, Kaido; Jänes, Jaak; Langel, Ülo; **Karelson, Mati** Current computer-aided drug design 2010 / 2, p. 79-89
<https://www.ingentaconnect.com/contentone/ben/cad/2010/00000006/00000002/art00001?crawler=true>

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

Pillai, Girinath Gopinathan; Tämm, 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; 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>

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

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

Subchronic oral and inhalation toxicities : a challenging attempt for modeling and prediction

Dobchev, Dimitar A.; Tulp, Indrek; **Karelson, Gunnar;** Tamm, Tarmo; Tämm, Kaido; **Karelson, Mati** Molecular informatics 2013 / p. 793-801 : ill <https://doi.org/10.1002/minf.201300033> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)