

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>

Complexes of oligopyrrole dications with inorganic anions : a comparative theoretical HF/post-HF study

Tamm, Tarmo; Tamm, Jüri; **Karelson, Mati** Synthetic metals 2005 / 1, p. 47-52 <https://www.sciencedirect.com/science/article/abs/pii/S037967790400503X>

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 and human serum albumin binding with theoretical descriptors

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

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/>

Energiaallikat vaid 80 aastaks : [võimalikest muutustest energiatootmises lähtudes nafta lõppemisest : Mati Karelsoni jt. arvamustega]

Karelson, Mati Eesti Päevaleht 2004 / 13. nov., lk. 22 <https://epl.delfi.ee/artikkel/50997248/energiaallikat-vaid-80-aastaks>

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, 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; 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 for the prediction of novel Trk inhibitors

Tammiku-Taul, Jaana; Karelson, Mati; Dobchev, Dimitar Atanasov XIV European Symposium of Organic Reactivity (ESOR XIV) : book of abstracts 2013 / p. 181

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

GDNF receptors as a drug target for neural repair

Bespalov, Maxim M.; Hetenyi, C.; **Karelson, Mati; Saarma, Mart** Cell transplantation 2007 / 3, p. 313-314 https://www.researchgate.net/publication/295730047_GDNF_receptors_as_a_drug_target_for_neural_repair

A general approach to the synthesis of 5-S-functionalized pyrimidine nucleosides and their analogues

Kananovich, Dzmitry; Reino, Aili; Ilmarinen, Kaja; Rõõmusoks, Marko; Karelson, Mati; Lopp, Margus 8th Biennial International Conference on Organic Synthesis : Balticum Organicum Syntheticum : July 6-9, 2014, Vilnius : program and abstract book 2014 / p. 77 <https://pubs.rsc.org/en/content/articlelanding/2014/ob/c4ob00597j>

A general approach to the synthesis of 5-S-functionalized pyrimidine nucleosides and their analogues

Kananovich, Dzmitry; Reino, Aili; Ilmarinen, Kaja; Rõõmusoks, Marko; Karelson, Mati; Lopp, Margus Organic & biomolecular

chemistry 2014 / p. 5634-5644 : ill <https://pubs.rsc.org/en/content/articlelanding/2014/ob/c4ob00597j> <https://doi.org/10.1039/c4ob00597j>
[Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Human tropomyosin-related kinase A and B : from transcript diversity to novel inhibitors = Inimese tropomüosiin-seoselised kinaasid A ja B : transkriptide mitmekesisusest uudsete inhibiitoriteni
Luberg, Kristi 2017 <https://digi.lib.ttu.ee/i/?7373> https://www.ester.ee/record=b4665007*est

In silico machine learning methods in drug development

Dobchev, Dimitar Atanasov; Pillai, Girinath Gopinathan; Karelson, Mati Current topics in medicinal chemistry 2014 / p. 1913-1922
<https://doi.org/10.2174/1568026614666140929124203> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Keemia : orgaaniline keemia gümnaasiumile

Karelson, Mati; Töldsepp, Aarne 2007 https://www.ester.ee/record=b2272821*est

Keemia : üldine ja anorgaaniline keemia gümnaasiumile

Karelson, Mati; Töldsepp, Aarne 2011 https://www.ester.ee/record=b2676529*est

Kiletükk töötab läbimurret kadunuks jäänute otsinguil : [ettevõtja Neinar Seli ja teadlase Mati Karelsoni koostöös loodud kilemarkerist]

Niitra, Nils; Karelson, Mati; Seli, Neinar Tartu Postimees 2007 / 12. märts, lk. 1 <https://majandus.postimees.ee/1639075/kiletukk-tootab-labimurret-kadunuks-jaanute-otsinguil>

Kvantitatiivsed struktuur-omadus sõltuvused kondenseeritud ringsüsteemide polariseeritavuse modelleerimiseks

Martin, Dana; Sild, Sulev; Maran, Uko; Karelson, Mati XXX Eesti keemiapäevad : teaduskonverentsi teesid = 30th Estonian Chemistry Days : abstracts of scientific conference 2007 / lk. 94-95 : ill

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>

Mati Karelson : teadusguru naftagigandi teenistuses : [intervjuu Mati Karelsoniga]

Laurisaar, Riho; Karelson, Mati Eesti Päevaleht 2004 / 18. sept., lk. 17 : portr <https://epl.delfi.ee/artikkel/50993119/mati-karelson-teadusguru-naftagigandi-teenistuses>

Mati Karelson loob tarkvara, mis teeks temast miljardäri

Salu, Mikk; Karelson, Mati Eesti Päevaleht 2006 / 23. aug., Ärielt, lk. 6 : portr <https://arileht.delfi.ee/artikkel/51053339/mati-karelson-loob-tarkvara-mis-teeks-temast-miljardari>

Mati Karelson loob tehnoloogiasirde firmade gruppi

Karelson, Mati; Sarv, Mikk Eesti Päevaleht 2007 / 6. juuni, Ärielt, lk. 4-5 : portr <https://arileht.delfi.ee/artikkel/51089754/mati-karelson-loob-tehnoloogiasirde-firmade-gruppi>

Molekulaartehnoloogia õppetool [Tartu Ülikoolis]

Karelson, Mati Tartu Ülikooli keemiaosakond 1947 - 2007 2007 / lk. 59-68 : fot https://artiklid.elnet.ee/record=b2384906*est

Novel computational models for predicting dopamine interactions

Katritzky, Alan R.; Dobchev, Dimitar; Stoyanova-Slavova, Iva B.; Kuanar, Minati; Bepalov, 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 cell-penetrating peptides using artificial neural networks

Dobchev, Dimitar A.; Mäger, Imre; Tulp, Indrek; Karelson, Gunnar; Tamm, Tarmo; Tamm, 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>

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>

QRSP modeling of the polarizability of polyaromatic hydrocarbons and fullerenes

Martin, Dana; Sild, Sulev; Maran, Uko; Karelson, Mati Journal of physical chemistry C 2008 / 13, p. 4785-4790
https://www.researchgate.net/publication/231648921_QSPR_Modeling_of_the_Polarizability_of_Polyaromatic_Hydrocarbons_and_Fullerenes

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 of heterocyclic compounds in large descriptor spaces

Karelson, Mati; Dobchev, Dimitar Atanasov Advances in Heterocyclic Chemistry ; Vol. 120 2016 / p. 237 - 273
<https://doi.org/10.1016/bs.aihch.2016.03.006> Article collection metrics at Scopus Article at Scopus Article collection metrics at WOS Article at WOS

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 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 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>

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 modelling of solubility of polyaromatic hydrocarbons and fullerene in 1-octanol and n-heptane

Martin, Dana; Maran, Uko; Sild, Sulev; **Karelson, Mati** Journal of physical chemistry B 2007 / 33, p. 9853-9857
<https://pubs.acs.org/doi/10.1021/jp071679x>

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>

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>

QSPR treatment of the soil sorption coefficients of organic pollutants

Kahn, Iiris; Fara, Dan; **Karelson, Mati**; Maran, Uko; Andersson, Patrik L. Journal of chemical information and modeling 2005 / 1, p. 94-105 <https://pubs.acs.org/doi/10.1021/ci0498766>

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

Katritzky, Alan R.; Radzvilovits, 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-activity relationships of environmentally relevant properties
Kahn, Iiris 2007

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>

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

Refinement of a quantitative structure-activity relationship model for prediction of cell-penetrating peptide based transfection systems

Dowaidar, Moataz; Regberg, Jakob; Dobchev, Dimitar Atanasov; Lehto, Tõnis; Hällbrink, Mattias; Karelson, Mati; Langel, Ülo International journal of peptide research and therapeutics 2017 / p. 91-100 : ill <https://doi.org/10.1007/s10989-016-9542-8> Journal metrics at Scopus Article at Scopus Journal metrics at WOS Article at WOS

Small molecular weight ARTN mimetic for the treatment of neuropathic pain

Sidorova, Y.A.; Bepalov, Maxim M.; Karelson, Mati; Saarma, Mart Cell transplantation 2012 / p. 792 <https://researchportal.helsinki.fi/en/publications/small-molecular-weight-artn-mimetic-for-the-treatment-of-neuropat>

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

Dobchev, Dimitar A.; Tulp, Indrek; Karelson, Gunnar; Tamm, Tarmo; Tamm, Kaiko; 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

Teoreetilised keemiast molekulaartehnoloogiani

Karelson, Mati; Maran, Uko Teadusmõtte Eestis : täppisteadused : [artiklikogumik] 2006 / lk. 169-172 https://www.ester.ee/record=b2230239*est

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

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.eurekaselect.com/article/31554>

Theoretical chemistry and molecular design

Karelson, Mati Research in Estonia : present and future 2011 / p. 336-338

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

Using artificial neural networks to predict cell-penetrating compounds

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

Химия : неорганические и органические вещества : учебник для IX класса

Karelson, Mati; Lukason, Anneli; Töldsepp, Aarne; Härsing, Irina 2009 https://www.ester.ee/record=b2504157*est

Химия : органическая химия. Учебник для гимназии

Karelson, Mati; Töldsepp, Aarne 2008 https://www.ester.ee/record=b2385031*est