

Curriculum Vitae

Name	Mati Karelson
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Career

Institution and position held	2005 - ... University of Tartu, Faculty of Science and Technology, Institute of Chemistry, Tartu University, Chair of Molecular Technology; Professor (1.00) 2004 - 2014 Tallinn University of Technology , Faculty of Science, Department of Chemistry, Chair of Molecular Technology; Professor (0.20) 1999 - 2002 Centre of Strategic Competence, University of Tartu, Director 1996 - 2014 University of Florida, Adjunct Professor 1992 - 2004 Professor of Theoretical Chemistry, University of Tartu 1988 - 1992 Laboratory of Chemical Kinetics and Catalysis, University of Tartu, Head 1985 - 1988 Tartu State University, Laboratory of Chemical Kinetics and Catalysis, Head of sector 1975 - 1985 Laboratory of Chemical Kinetics and Catalysis, Tartu State University, Senior research fellow 1972 - 1975 Junior & senior research fellow, Tartu State University
Education	1967 - 1972 Tartu State University
Administrative responsibilities	2007 - ... Estonian Academy of Sciences, Member 2006 - ... Member, International Academy of Mathematical Chemistry 1999 - ... Member, American Chemical Society 1990 - ... Member, International Society of Quantum Biology and Pharmacology 2007 - 2012 Advisory Board, The President of Estonia 2005 - 2014 Advisor on R&D, Prime Minister of Estonia

Research activity

Degree information	Mati Karelson, Doctor's Degree, 1975, (sup) Viktor Palm, Proverka primenimosti elektrostatičeskikh modelei v organičeskoj himii (Applicability of electrostatic models in organic chemistry), University of Tartu
Honours & Awards	2014, Mati Karelson; Ostwald Medal 2008, Mati Karelson; Honorary Citizen, City of Tartu 2006, Mati Karelson; White Star order of Republic of Estonia (III class) 2002, Mati Karelson; Medal of Tartu

	2001, Yearly Award, Natural Sciences and Engineering - Mati Karelson; National Science Prize
	1996, Mati Karelson; Honorary Fellow, Florida Center of Hetrocyclic Compounds
Field of research	4. Natural Sciences and Engineering, 4.11. Chemistry and Chemical Technology(theoretical chemistry and molecular engineering)
Dissertations under supervision	Deniss Savtšenko, PhD Student, (sup) Mati Karelson, Andre Lomaka, Orbital-related descriptors in QSAR/QSPR, Tallinn University of Technology , Faculty of Science, Department of Chemistry Girinath Gopinathan Pillai, PhD Student, (sup) Mati Karelson, Applications of Computational Chemistry to the prediction of Physical, Chemical and Biological Properties of Novel Insecticides and Insect Repellents, University of Tartu Kristi Luberg, PhD Student, (sup) Tõnis Timmusk, Mati Karelson, TrkB receptor structure, signaling and low molecular weight agonists, Tallinn University of Technology , Faculty of Science, Department of Gene Technology
Dissertations supervised	Iva Stoyanova-Slavova, Doctor's Degree, 2013, (sup) Mati Karelson, Validation of QSAR/QSPR for regulatory purposes, University of Tartu, Faculty of Science and Technology, Institute of Chemistry, Tartu University Dana Martin, Doctor's Degree, 2011, (sup) Mati Karelson, The QSPR/QSAR approach for the prediction of properties of fullerene derivatives, University of Tartu, Faculty of Science and Technology Iiris Kahn, Doctor's Degree, 2007, (sup) Mati Karelson, Uko Maran, Quantitative Structure-Activity Relationships of Environmentally Relevant Properties, University of Tartu, Faculty of Science and Technology, Institute of Chemistry, Tartu University Svetoslav Hristov Slavov, Doctor's Degree, 2007, (sup) Mati Karelson, Biomedical applications of the QSAR approach, University of Tartu Dimitar Atanasov Dobchev, Doctor's Degree, 2006, (sup) Mati Karelson, Robust QSAR Methods for the Prediction of Properties from Molecular Structure, University of Tartu, Faculty of Physics and Chemistry Dan Cornel Fara, Doctor's Degree, 2004, (sup) Mati Karelson, QSPR Modeling of Complexation and Distribution of Organic Compounds, University of Tartu, Faculty of Physics and Chemistry Andre Lomaka, Doctor's Degree, 2003, (sup) Mati Karelson, Biomedical Applications of Predictive Computational Chemistry, University of Tartu, Faculty of Physics and Chemistry Tarmo Tamm, Doctor's Degree, 2003, (sup) Jüri Tamm, Mati Karelson, Quantum chemical modelling of polypyrrole, University of Tartu, Faculty of Physics and Chemistry Kostyantyn Kirichenko, Doctor's Degree, 2003, (sup) Mati Karelson, Benzotriazole - Mediated Carbon-Carbon Bond Formation, University of Tartu, Faculty of Physics and Chemistry Anti Perkson, Doctor's Degree, 2002, (sup) Mati Karelson, Synthesis and Characterisation of Nanostructured Carbon, University of Tartu, Faculty of Physics and Chemistry Sulev Sild, Doctor's Degree, 2001, (sup) Mati Karelson, QSPR/QSAR Approaches for Complex Molecular Systems, University of Tartu, Faculty of Physics and Chemistry, Institute of Chemical Physics

Ruslan Petrukhin, Doctor's Degree, 2001, (sup) Mati Karelson, Industrial Applications of the Quantitative Structure-Property Relationships, University of Tartu, Faculty of Physics and Chemistry

Jaan Leis, Doctor's Degree, 1998, (sup) Mati Karelson, Conformational Dynamics and Equilibria in Amides (Conformational Dynamics and Equilibria in Amides), University of Tartu, Faculty of Physics and Chemistry

Uko Maran, Doctor's Degree, 1997, (sup) Mati Karelson, Quantum-Mechanical Study of Potential Energy Surfaces in Different Environments, University of Tartu, Faculty of Physics and Chemistry

Mu Lan, Doctor's Degree, 1996, (sup) Mati Karelson, QSPR Treatment of Solvent Effects on Physical Properties in Liquids and Solutions, University of Florida

Victor Lobanov, Doctor's Degree, 1995, (sup) Mati Karelson, Quantitative Structure-Property Relationships in Large Descriptor Spaces, University of Tartu, Faculty of Physics and Chemistry

Toomas Tamm, Doctor's Degree, 1993, (sup) Mati Karelson, Quantum-Chemical Simulation of Solvent Effects, University of Tartu, Faculty of Physics and Chemistry

Maike Käär, Master's Degree, 2008, (sup) Mati Karelson, Jaan Leis, Katalüsaatorite toime karbiidset päritolu süsinikmaterjalide poorusele ja mikrostruktuurile (The influence of catalyst on the porosity and the microstructure of carbide-derived carbon), University of Tartu, Faculty of Science and Technology, Institute of Chemistry, Tartu University

Deniss Savtšenko, Master's Degree, 2007, (sup) Mati Karelson, Tarmo Tamm, QSAR Modeling of Toxicities Using Quantum-Chemical Orbital Descriptors, University of Tartu, Faculty of Physics and Chemistry

Tarmo Tamm, Master's Degree, 1998, (sup) Jüri Tamm, Mati Karelson, Oksüdeeritud oligopürroolide ja polüpürrooli teoreetiline uurimine (A Theoretical Study Oxidized Oligopyrroles and Polypyrrole), University of Tartu, Faculty of Physics and Chemistry

Jaan Leis, Master's Degree, 1994, (sup) Mati Karelson, Isomerism in Hindered N-Arylamides: Structure and Stereodynamics (Isomerism in Hindered N-Arylamides: Structure and Stereodynamics), University of Tartu, Faculty of Physics and Chemistry

Kalju Kahn, Master's Degree, 1994, (sup) Mati Karelson, Poly-(N-ethyl-4-vinylpyridine): synthesis and complexes with DNA, University of Tartu, Faculty of Physics and Chemistry, Institute of Chemical Physics

Uko Maran, Master's Degree, 1993, (sup) Mati Karelson, Ab Initio and semiempirical study of the Menshutkin reaction, University of Tartu, Faculty of Physics and Chemistry

Oleksandr Kulshyn, Master's Degree, 2006, (sup) Mati Karelson, Chemical Database of Optimized Molecular Geometries, University of Tartu, Faculty of Physics and Chemistry

Ruslan Svetlitski, Master's Degree, 2004, (sup) Mati Karelson, QSPR Modelling of Lanthanide-Organic Complex Stability Constants, University of Tartu, Faculty of Physics and Chemistry

Iiris Kahn, Master's Degree, 2003, (sup) Mati Karelson, Electrostatic Molecular Descriptors in Quantitative Structure-Property Analysis, University of Tartu, Faculty of Physics and Chemistry

Andre Lomaka, Master's Degree, 2000, (sup) Mati Karelson, The Modified Lowest Energy Pivot Algorithm as a Method for Generating a Set of Low Energy Structures of Organic Molecules, University of Tartu, Faculty of Physics and Chemistry

Sulev Sild, Master's Degree, 1998, (sup) Mati Karelson, QSPR Approach for Theoretical Modeling of Polymers, University of Tartu, Faculty of Physics and Chemistry

Marek Strandberg, Master's Degree, 1988, (sup) Mati Karelson, Квантово-химическое определение ароматичности гетероциклических соединений методом самосогласованного реакционного поля (Quantum chemical description of aromaticity of heterocyclic compounds by self constant reaction field method), Tartu State University

Publications

Hällbrink, Mattias; Karelson, Mati (2015). Prediction of Cell-Penetrating peptides. *Methods in molecular biology* (Clifton, N.J.) (39 - 58). Springer

Kahn, Iiris; Lomaka, Andre; Karelson, Mati (2015). In Silico Approach to Finding New Scaffolds for LRRK2 Inhibition. In: Abstracts: European Pharma Summit, Berlin (Germany), May 5-8, 2015. <https://www.gtcbio.com/europeanpharma/2015/>.

Mutso, M.; Nikonov, A.; Pihlak, A.; Žusinaite, E.; Viru, L.; Selyutina, A.; Reintamm, T.; Kelve, M.; Saarma, M.; Karelson, M.; Merits, A. (2015). RNA interference-guided targeting of hepatitis C virus replication with antisense locked nucleic acid-based oligonucleotides containing 8-oxo-dG modifications. *PLoS ONE*, 10 (6), xUNSP e0128686

Pillai, Girinath G.; Sikk, Lauri; Tamm, Tarmo; Karelson, Mati; Burk, Peeter; Tamm, Kaido. (2015). Theoretical Modeling of HPV: QSAR and Novodesign with Fragment Approach. *Current Computer Aided-Drug Design*, 10(4), 303 - 314.

Dobchev, Dimitar A.; Pillai, Girinath G.; Karelson, M. (2014). Machine-Learning Methods in Drug Development. *Current Topics in Medicinal Chemistry*, 14(16), 1913 - 1922.

Kahn, I.; Lomaka, A.; Karelson, M. (2014). Topological Fingerprints as an Aid in Finding Structural Patterns for LRRK2 Inhibition. *Molecular Informatics*, 33(4), 269 - 275.

Kananovich, D.G.; Reino, A.; Ilmarinen, K.; Rõõmusoks, M.; Karelson, M.; Lopp, M. (2014). A General Approach to the Synthesis of 5-S-functionalized Pyrimidine Nucleosides and their Analogues. *Organic and Biomolecular Chemistry*, 12, 5634 - 5644.

Kananovich, D.G.; Reino, A.; Ilmarinen, K.; Rõõmusoks, M.; Karelson, M.; Lopp, M. (2014). A general approach to the synthesis of 5-S-functionalized pyrimidine nucleosides. *BOS 2014 - International Conference on Organic Synthesis*, 77.

Regberg, J.; Srimanee, A.; Erlandsson, M.; Sillard, R.; Dobchev, D.A.; Karelson, M.; Langel, Æ. (2014). Rational design of a series of novel amphipathic cell-penetrating peptides (*International Journal of Pharmaceutics*). *International Journal of Pharmaceutics*, 464(1-2), 111 - 116.

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Tammiku-Taul, J.; Karelson, M.; Dobchev, D. A. (2014). Fragment-based QSAR for the Prediction of Novel TrkA Inhibitors. 16th International Workshop on Quantitative Structure-Activity Relationship in Environmental and Health Sciences (QSAR 2014), Milan, Italy, 16-20 June. , 170.

Dobchev, D. A.; Tulp, I.; Karelson, G.; Tamm, T.; Tämm, K.; Karelson, M. (2013). Subchronic Oral and Inhalation Toxicities: a Challenging Attempt for Modeling and Prediction . Molecular Informatics, 32(9-10), 793 - 801.

Tammiku-Taul, J.; Karelson, M.; Dobchev, D. A. (2013). Fragment-based QSAR for the Prediction of Novel Trk Inhibitors. XIV European Symposium of Organic Reactivity (ESOR XIV), Prague, Czech Republic, September 1-6. , in Book of Abstracts: p. 181.

Karelson, M.; Dobchev, D.A.; Karelson, G.; Tamm, T.; Tämm, K.; Nikonov, A.; Mutso, M.; Merits, A. (2012). Fragment-based development of HCV protease inhibitors for the treatment of hepatitis C. Current Computer-Aided Drug Design, 8(1), 55 - 61.

Oliferenko, A.A.; Tian, F.F.; Karelson, M. ; Katritzky, A.R. (2012). Prediction of peptide IMS cross sections from extended molecular connectivity. International Journal of Mass Spectrometry, 314, 1 - 5.

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Karelson, M.; Dobchev, D. (2011). Using artificial neural networks to predict cell-penetrating compounds . Expert Opinion on Drug Discovery, 6(8), 783 - 796.

Karelson, M.; Koppel, I.A.; Leito, I.; Kaljurand, M.; Samel, N.; Lopp, M.; Pehk, T. (2011). Chemistry in Estonia-Review and Outlook. Engelbrecht, J. (Eds.). Research in Estonia. Present and Future (319 - 345). Tallinn: Estonian Academy of Sciences

Katritzky, A.R.; Stoyanova-Slavova, I.B.; Tämm, K.; Tamm, T.; Karelson, M. (2011). Application of the QSPR Approach to the Boiling Points of Azeotropes. Journal of Physical Chemistry A, 115 (15), 3475 - 3479.

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Katritzky, A.; Kuanar, M.; Slavov, S.; Hall, C.; Karelson, M.; Kahn, I.; Dobchev, D. (2010). Quantitative Correlations of Physical and Chemical Properties with Chemical Structure; Utility for Prediction. Chemical Reviews, 110(10), 5714 - 5789.

Katritzky, A.R.; Kasemets, K.; Slavov, S.; Radzvilovits, M.; Tämm, K.; Karelson, M. (2010). Estimating the toxicities of organic chemicals in activated sludge process . Water Research, 44(8), 2451 - 2460.

Katritzky, A.R.; Radzvilovits, M.; Slavov, S.; Kasemets, K.; Tamm, K.; Karelson, M. (2010). Quantitative structure-activity relationship modeling of bioconcentration factors of polychlorinated biphenyls . Toxicological and Environmental Chemistry, 92(7), 1233 - 1247.

Katritzky, Alan R.; Slavov, Svetoslav H.; Stoyanova-Slavova, Iva B.; Karelson, Mati (2010). Correlation of the Photolysis Half-Lives of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans with Molecular Structure. Journal of Physical Chemistry A, 114(7), 2684 - 2688.

Martin, D.; Karelson, M. (2010). The Quantitative Structure Activity Relationships for Predicting HIV Protease Inhibition by Substituted Fullerenes. *Letters in Drug Design and Discovery*, 7(8), 587 - 595.

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Katritzky, A. R.; Ren, Yueying; S., Svetoslav H.; Karelson, M. (2009). A comparative QSAR study of SVM and PPR in the correlation of lithium cation basicities. *Collection of Czechoslovak Chemical Communications*, 74(1), 217 - 241.

Katritzky, A. R.; Slavov, S. H.; Stoyanova-Slavova, I. S.; Kahn, I.; Karelson, M. (2009). Quantitative Structure–Activity Relationship (QSAR) Modeling of EC50 of Aquatic Toxicities for *Daphnia magna*. *Journal of Toxicology and Environmental Health Part A: Current Issues*, 72(19), 1181 - 1190.

Katritzky, A. R.; Slavov, S.; Radzvilovits, M.; Stoyanova-Slavova, I.; Karelson, M. (2009). Computational Chemistry Approaches for Understanding how Structure Determines Properties. *Zeitschrift für Naturforschung B - a Journal of Chemical Sciences*, 64(6), 773 - 777.

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Karelson, M.; Dobchev, D.; Tamm, T.; Tulp, I.; Jänes, J.; Tamm, K.; Lomaka, A.; Savchenko, D.; Karelson, G. (2008). Correlation of Blood-Brain Penetration and Human Serum Albumin Binding with Theoretical Descriptors. *Arkivoc*, xvi, 38 - 60.

Katritzky, A. R.; Slavov, S. H.; Dobchev, D.A.; Karelson, M. (2008). QSAR modeling of the antifungal activity against *Candida albicans* for a diverse set of organic compounds. *Bioorganic & Medicinal Chemistry*, 16(14), 7055 - 7069.

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Katritzky, A.R.; Kuanar, M.; Stoyanova-Slavova, I.B.; Slavov, S. H.; Dobchev, D.A.; Karelson, M.; Acree, W.E., Jr. (2008). Quantitative structure-property relationship studies on Ostwald solubility and partition coefficients of organic solutes in ionic liquids. *Journal of Chemical and Engineering Data*, 53(5), 1085 - 1092.

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Katritzky, A. R.; Stoyanova-Slavova, I. B.; Dobchev, D. A.; Karelson, M. (2007). QSPR modeling of flash points: An update. *Journal of Molecular Graphics and Modelling*, 26, 529 - 536.

Katritzky, A.R.; Pacureanu, L.; Dobchev, D.; Karelson, M. (2007). QSPR Study of Critical Micelle Concentration of Anionic Surfactants Using Computational Molecular Descriptors. *Journal of Chemical Information and Modeling*, 47(3), 782 - 793.

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Inventions

Invention: Method and apparatus for the design of chemical compounds with predetermined properties; Owner: Mati Karelson, Mehis Pilv, MolCode; Authors: Mati Karelson, Mehis Pilv; Priority number: WO2007EP52856; Priority date: 26.03.2007

Invention: Composite materials for infrared sensing markers; Owner: Raidenil OÜ; Authors: Mati Karelson, Neinar Seli; Priority number: EE20060000004; Priority date: 03.03.2006

Invention: Use of oligonucleotides with modified bases as antiviral agents; Owner: Baltic Technology Development Ltd.; Authors: Mati Karelson, Mart Saarma, Andres Merits; Priority number: US60/985,548; Priority date: 05.11.2007

Invention: A method for manufacturing of a smart packing material; Owner: Raidenil OÜ; Authors: Mati Karelson, Kaupo Karelson, Jaan Leis, Neinar Seli; Priority number: US20070917541P; Priority date: 11.05.2007

Invention: Antisense Agents Combining Strongly Bound Base-Modified Oligonucleotide and Artificial Nuclease; Owner: Baltic Technology Development Ltd.; Authors: Mati Karelson, Mart Saarma, Mehis Pilv; Priority number: US20060797448P; Priority date: 03.05.2006

Invention: Use of oligonucleotides with modified bases in hybridization of nucleic acids; Owner: Baltic Technology Development Ltd.; Authors: Mati Karelson, Erkki Truve, Allan Olspert, Maria Cecilia Sarmiento Guerin, Mart Saarma; Priority number: US60/985,552; Priority date: 05.11.2007

Invention: Methods of Facilitating Neural Cell Survival Using GDNF Family Ligand (GFL) Mimetics or RET Signaling Pathway Activators ; Owner: Genecode Ltd.; Authors: Mati Karelson, Mart Saarma, Mehis Pilv, Maxim Beshpalov; Priority number: US61/285,858; Priority date: 11.12.2009