LIST OF PUBLICATIONS

Mati Karelson

(as of August 6th, 2016)

1. Kumar Das P.; Puusepp, L.; Varghese, F.S.; Utt, A.; Ahola, T.; Kananovich, D.G.; Lopp, M.; Merits, A.; Karelson, M. (2016) Design and validation of novel Chikungunya virus protease inhibitors, Antimicrobial Agents and Chemotherapy (submitted).
2. Dobchev, Dimitar; Karelson, Mati (2016). QSAR of Heterocyclic Compounds in Large Descriptor Spaces, Advances in Heterocyclic Chemistry, 120, 237-274.
3. Tammiku-Taul, J.; Park, R.; Jaanson, K.; Luberg, K.; Dobchev, D. A.; Kananovich, D.; Noole, A.; Mandel, M.; Kaasik, A.; Lopp, M.; Timmusk, T.; Karelson, M. (2016). Indole-like Trk receptor antagonists. European Journal of Medicinal Chemistry, 121, 541−552, 10.1016/j.ejmech.2016.06.003.
4. Dowaidar, M; Regberg, J; • Dobchev, D.A; Lehto, T; Hällbrink, M.; Karelson, M.; Langel, Ü. (2016) Refinement of a Quantitative Structure–Activity Relationship Model for Prediction of Cell-Penetrating Peptide Based Transfection Systems, Int. J. Pept. Res. Ther.

DOI 10.1007/s10989-016-9542-8.

1. Dobchev, Dimitar; Karelson, Mati (2016). Have artificial neural networks met expectations in drug discovery as implemented in QSAR framework? Expert Opinion on Drug Discovery, 11 (7), 627−639, 10.1080/17460441.2016.1186876.
2. Pillai, G.G.; Mederos, L.; Panda, C.S.; Gronski, A.; Burk, P.; Hall, C.D.; Katritzky, A.R.; Tämm, K.; Karelson, M. (2016). Robust Modeling and Scaffold Hopping: Case Study based on HIV Reverse Transcriptase Inhibitors Type-1 Data. Medicinal Chemistry, x−x, 1573406411666151005110141].
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4. 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, 1574886309666141126145756 .
5. Hällbrink, Mattias; Karelson, Mati (2015). Prediction of Cell-Penetrating peptides. In: Methods in molecular biology (Clifton, N.J.) (39−58). Springer.
6. [Kahn, Iiris; Lomaka, Andre; Karelson, Mati (2015). In Silico Approach to Finding New Scaffolds for LRRK2 Inhibition. *In:* https://www.gtcbio.com/europeanpharma/2015/,.](https://www.etis.ee/Research/Publications/Display/8ba26b48-f4c8-4a4d-a917-39d0327cf45c)
7. [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, 10.1039/C4OB00597J.](https://www.etis.ee/Research/Publications/Display/67e89430-cd92-45b8-89aa-2489a5a91b6d)
8. [Dobchev, Dimitar A.; Pillai, Girinath G.; Karelson, M. (2014). Machine-Learning Metods in Drug Development. Current Topics in Medicinal Chemistry, 14 (16), 1913−1922.](https://www.etis.ee/Research/Publications/Display/f2e8fe3b-21e3-448a-bb49-d0eb4d2e896d)
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11. [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. 77.](https://www.etis.ee/Research/Publications/Display/b27636af-f820-49f0-9823-2e75a0329623)
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