15 NOTABLE PUBLICATIONS

Mati Karelson

(as of August 6th, 2016)

1. Dobchev, Dimitar; Karelson, Mati (2016). QSAR of Heterocyclic Compounds in Large Descriptor Spaces, Advances in Heterocyclic Chemistry, 120, 237-274.
2. 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.
3. Hällbrink, Mattias; Karelson, Mati (2015). Prediction of Cell-Penetrating peptides. In: Methods in molecular biology (Clifton, N.J.) (39−58). Springer.
4. [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)
5. [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, 10.2174/157340912799218516.](https://www.etis.ee/Research/Publications/Display/5092356e-2317-42eb-b776-bb15f4c79439)
6. [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, 10.1021/cr900238d.](https://www.etis.ee/Research/Publications/Display/2554f935-e3f5-43ec-a81e-9aa1604a8d34)
7. [Katritzky, A.; Dobchev, D.; Slavov, S.; Karelson, M. (2008). The Legitimate Utilization of Large Descriptor pools for QSPR/QSAR Models. Journal of Chemical Information and Modeling, 48 (11), 2207−2213, 10.1021/ci8002073.](https://www.etis.ee/Research/Publications/Display/34e61f63-7791-4639-9914-27fe4e9deec5)
8. [Hétenyi, Csaba; Maran, Uko; García-Sosa, Alfonso T.; Karelson, Mati (2007). Structure-based calculation of drug efficiency indices. Bioinformatics, 23 (20), 2678−2685, bioinformatics/btm431 .](https://www.etis.ee/Research/Publications/Display/06a14ffa-28a3-4071-a102-8a418fcba8f7)
9. [Sild, Sulev; Maran, Uko; Lomaka, Andre; Karelson, Mati (2006). Open Computing Grid for Molecular Science and Engineering. Journal of Chemical Information and Modeling, 46 (3), 953−959, ci050354f.](https://www.etis.ee/Research/Publications/Display/242b4a01-9888-4b2f-9597-055ef8f3d9b0)
10. [Katritzky, AR.; Dobchev, DA.; Karelson, M. (2006). Physical, chemical, and technological property correlation with chemical structure: The potential of QSPR. Zeitschrift für Naturforschung B - a Journal of Chemical Sciences, 61 (4), 373−384.](https://www.etis.ee/Research/Publications/Display/ee039824-c96c-4acc-9f9a-49de04fde113)
11. [Karelson, M. (2000). Molecular Descriptors in QSAR/QSPR. New York: John Wiley & Sons Ltd.](https://www.etis.ee/Research/Publications/Display/6425cad5-7324-49c3-91db-f809f095985e)
12. [Karelson, M. (1997). Quantum chemical treatment of molecules in condensed disordered media. Advances in Quantum Chemistry, 28, 141−157.](https://www.etis.ee/Research/Publications/Display/ee0adb17-43cf-4371-a483-d68943100f2b)
13. [Karelson, M.; Lobanov, VS.; Katritzky, AR. (1996). Quantum-chemical descriptors in QSAR/QSPR studies. Chemical Reviews, 96 (3), 1027−1043.](https://www.etis.ee/Research/Publications/Display/13b148ec-7fa4-4485-819d-78d7424bff78)
14. [Karelson, M.; Tamm, T.; Zerner, MC. (1993). Multicavity reaction field method for the solvent effect description in flexible molecular-systems. Journal of Physical Chemistry, 97 (46), 11901−11907.](https://www.etis.ee/Research/Publications/Display/5a1bade6-30cd-4c5c-b297-47e12b2be728)
15. [Karelson, MM.; Zerner, MC. (1992). Theoretical treatment of solvent effects on electronic spectroscopy. Journal of Physical Chemistry, 96 (17), 6949−6957.](https://www.etis.ee/Research/Publications/Display/55a1a9e0-5da7-4537-9cfa-c0c652aa2a4d)