Dr. Filip Miljković

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LinkedIn profile https://www.linkedin.com/in/fmiljkovic/

ResearchGate profile https://www.researchgate.net/profile/Filip_Miljkovic

Work experience

February 2020 – Present
Data Scientist, Computational DMPK & Safety
AstraZeneca R&D, Gothenburg, Sweden
Department of Clinical Pharmacology & Safety Sciences

Education

June 2016 – December 2019
Ph.D. (Dr. rer. nat.) in Computational Life Sciences
Rheinische Friedrich-Wilhelms-Universität Bonn, Germany
LIMES Program Unit Chemical Biology and Medicinal Chemistry
Department of Life Science Informatics, b-it
Grade: 0.7 (*Magna cum laude*)
Thesis: Chemoinformatics-Driven Approaches for Kinase Drug Discovery
Supervisor: Prof. Jürgen Bajorath

October 2009 – September 2014
Master degree in Pharmacy (Integrated studies)
University of Niš, Serbia
Faculty of Medicine
Department of Pharmacy
Grade: 9.58/10.00
Thesis: An Overview of Dipeptidyl Peptidase-IV Inhibitors.
Supervisor: Prof. Andrija Šmelcerović

International experience

July 2013 – August 2013
IPSF Student Exchange Programme
Medical University of Gdańsk, Poland
Department of Analytical Chemistry

Description: Quality consistency evaluation of *Melissa officinalis* L. samples using HPLC fingerprints.
Supervisor: Agnieszka Viapiana, PhD

Technical skills

Data extraction/curation (KNIME, RDKit and OpenEye Chemistry Toolkit), SAR analysis, Network analysis (Cytoscape, Gephi, NetworkX Python package), 2D and 3D ligand similarity, Structure- and Ligand-based virtual screening, Molecular modeling suites (MOE), Docking (MOE Dock, AutoDock, PLANTS, DockTite for covalent docking), Protein-ligand interaction fingerprints, Machine learning (SVM, RF, DNN; scikit-learn, TensorFlow).

Computer skills

Windows, Office suite, Chemoffice, Python (advanced knowledge), Bash (basic knowledge), R (basic knowledge), SQL (basic knowledge).

Language skills

Serbian (native)
English (fluent): TOEFL (109/120)
German (good)
Swedish (basic)

Teaching

Master's Program in Pharmacy at the Medical faculty, University of Niš, Serbia

"General Chemistry with Stoichiometry", October 2010 – January 2011.
"Organic Chemistry", March 2011 – June 2011.

Master's Program in Life Science Informatics at the University of Bonn, Germany

"Introduction to Chemistry", September 2016 – October 2016.
"Structural Bioinformatics", October 2016 – January 2018.
"Molecular Modeling and Drug Design", April 2017 – February 2019.
"Programming Lab I" (Python), April 2019 – June 2019.

"Introduction to Machine Learning Tutorial", April 2019 – June 2019.
Supervision of Master Thesis, Mariana González-Medina, 2019.

Visiting Students Coming from Collaborative Projects between University of Bonn, Germany and Kyoto University, Japan or Waseda University, Japan

"Structural Bioinformatics and Molecular Modeling", October 2017 – December 2019.

Publications

1. Rodríguez-Pérez, R.; **Miljković, F.**; Bajorath, J. Assessing the Information Content of Structural and Protein–Ligand Interaction Representations for the Classification of Kinase Inhibitor Binding Modes via Machine Learning and Active Learning. *J. Cheminform.* **2020**, *12*, e36.
2. **Miljković, F.**; Xiong, R.; Sivakumar, D.; Brown, C. A. Members of our Early Career Panel Highlight Key Research Articles on the Theme of Drug Repurposing. *Future Drug Discov.* **2020**, *2*, FDD39.
3. **Miljković, F.**; Rodríguez-Pérez, R.; Bajorath J. Machine Learning Models for Accurate Prediction of Kinase Inhibitors with Different Binding Modes. *J. Med. Chem.* doi: 10.1021/acs.jmedchem.9b00867.
4. Miljković, F.; Bajorath, J. Data structures for computational compound promiscuity analysis and exemplary applications to inhibitors of the human kinome. *J. Comput. Aided Mol. Des.* **2020**, *34*, 1-10.
5. González-Medina, M.; Miljković, F.; Haase, G. S.; Drueckes, P.; Trappe, J; Laufer, S; Bajorath, J. Promiscuity analysis of a kinase panel screen with designated p38 alpha inhibitors. *Eur. J. Med. Chem.* **2020**, *187*, 112004.
6. Feldmann, C.; Miljković, F.; Yonchev, D.; Bajorath, J. Identifying promiscuous compounds with activity against different target classes. *Molecules* **2019**, *24*, e4185.
7. **Miljković, F.**; Bajorath J. Data Structures for Compound Promiscuity Analysis: Cliffs, Pathways, and Hubs Formed by Inhibitors of the Human Kinome. *Future Sci. OA* **2019**, *5*, FSO404.
8. **Miljković, F.**; Vogt, M.; Bajorath, J. Systematic Computational Identification of Promiscuity Cliff Pathways Formed by Inhibitors of the Human Kinome. *J. Comput. Aided Mol. Des.* **2019***, 33*, 559-572.

9. Blaschke, T.; **Miljković, F.**; Bajorath, J. Prediction of Different Classes of Promiscuous and Nonpromiscuous Compounds Using Machine Learning and Nearest Neighbor Analysis. *ACS Omega* **2019**, *4*, 6883-6890.
10. **Miljković, F**.; Bajorath, J. Computational Analysis of Kinase Inhibitors Identifies Promiscuity Cliffs across the Human Kinome. *ACS Omega* **2018**, *3*, 17295–17308.
11. **Miljković, F.**; Bajorath, J. Data-Driven Exploration of Selectivity and Off-Target Activities of Designated Chemical Probes. *Mol.* **2018***, 23,* e2434.
12. **Miljković, F.**; Bajorath, J. Evaluation of Kinase Inhibitor Selectivity Using Cell-Based Profiling Data. *Mol. Inform.* **2018**, *37*, e1800024.
13. **Miljković, F.**; Bajorath, J. Reconciling Selectivity Trends from a Comprehensive Kinase Inhibitor Profiling Campaign with Known Activity Data. *ACS Omega* **2018**, *3*, 3113–3119.
14. **Miljković, F.**; Bajorath, J. Exploring Selectivity of Multikinase Inhibitors across the Human Kinome. *ACS Omega* **2018**, *3*, 1147–1153.
15. **Miljković, F.**; Kunimoto, R.; Bajorath, J. Identifying Relationships between Unrelated Pharmaceutical Target Proteins on the Basis of Shared Active Compounds. *Future Sci. OA* **2017**, *3*, FSO212.
16. Smelcerovic, A.; **Miljkovic, F.**; Kolarevic, A.; Lazarevic, J.; Djordjevic, A.; Kocic, G.; Anderluh, M. An Overview of Recent Dipeptidyl Peptidase-IV Inhibitors: Linking Their Structure and Physico-Chemical Properties with SAR, Pharmacokinetics and Toxicity. *Curr. Top. Med. Chem.* **2015**, *15*, 2342-2372.
17. Toropov, A. A.; Veselinović, J. B.; Veselinović, A. M.; **Miljković, F. N.**; Toropova, A. P. QSAR Models for 1,2,4-Benzotriazines as Src Inhibitors Based on Monte Carlo Method. *Med. Chem. Res.* **2015**, *24*, 283-290.
18. Toropova, A. P.; Toropov, A. A.; Veselinović, J. B.; **Miljković, F. N.**; Veselinović, A. M. QSAR Models for HEPT Derivates as NNRTI Inhibitors Based on Monte Carlo Method. *Eur. J. Med. Chem.* **2014**, *77*, 298-305.

Conferences

1. "Chemoinformatics Strasbourg Summer School", 25 June – 29 June 2018, University of Strasbourg, Strasbourg, France. Poster: **Miljković, F**.; Bajorath, J. "Exploring Selectivity of Multi-kinase Inhibitors across the Human Kinome", awarded as the best poster by public choice.
2. "11th International Conference "Physical Chemistry 2012"", 24 September – 28 September 2012, Society of Physical Chemists of Serbia, Belgrade, Serbia. Conference Paper: Nikolić, G.M.; Veselinović, A. M.; Mitić, Ž. J.; **Miljković F. S.** Application of Multivariate Curve

Resolution-alternating Least Squares (MCRALS) Method for the Study of Cu(II) Ion Influence on the Pyrogallol Autoxidation in Aqueous Solution. *Proceedings of the 11th International Conference on Fundamental and Applied Aspects of Physical Chemistry* **2012**, *1*, 188-190.

3. "4th BBBB International Conference on Pharmaceutical Sciences", 29 September – 1 October 2011, Slovenian Pharmaceutical Society, Bled, Slovenia. Conference Paper: Nikolić, G. M.; Živković, J. V.; Nikolić, M. G; **Miljković, F**. Synergism in the Extraction of Paracetamol from the Aqueous NaCl Solutions by the Diethyl Ether/1-Butanol Binary Solvent Mixtures. *Eur. J. Med. Chem.* **2011**, 44 (S1), 183-184.