CURRICULUM VITAE

Dr. Filip Miljković

Gothenburg, Sweden

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LinkedIn ORCID ResearchGate

Work Experience

January 2021 – Present

Affiliate Scientist
Department of Life Science Informatics, b-it, LIMES Program Unit Chemical Biology and Medicinal Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn, Germany

February 2020 – Present

Senior Data Scientist
Imaging and Data Analytics, Clinical Pharmacology & Safety Sciences, AstraZeneca R&D, Gothenburg, Sweden

Education

June 2016 – December 2019

Ph.D. (Dr. rer. nat.) in Computational Life Sciences
Department of Life Science Informatics, b-it, LIMES Program Unit Chemical Biology and Medicinal Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn, Germany

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)
Department of Pharmacy, Faculty of Medicine, University of Niš, Serbia

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
Department of Analytical Chemistry, Medical University of Gdańsk, Poland

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/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, XGB, DNN, GCNN; scikit-learn, TensorFlow)

Computer Skills Python (advanced knowledge), Bash (basic knowledge), R (basic knowledge), SQL (basic knowledge), ChemOffice, Biovia, KNIME/Pipeline Pilot, Office suite, Windows/Linux

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

Teaching Experience

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

25. Rodríguez-Pérez, R.; **Miljković, F.**; Bajorath, J. Machine Learning in Chemoinformatics and Medicinal Chemistry. *Ann. Rev. Biomed. Data Sci.* **2022**, *in press*.
24. Laufkötter, O.; Hu, H.; **Miljković, F.**; Bajorath, J. Structure- and Similarity-Based Survey of Allosteric Kinase Inhibitors, Activators, and Closely Related Compounds. *J. Med. Chem.* **2022**, *in press*.
23. Miljković, F.; Rodríguez-Pérez, R.; Bajorath, J. Impact of Artificial Intelligence on Compound Discovery, Design, and Synthesis. *ACS Omega* **2021**, *6*, 33293-33299.
22. Miljković, F.; Martinsson, A.; Obrezanova, O.; Williamson, B.; Johnson, M.; Sykes, A.; Bender, A.; Greene, N. Machine Learning Models for Human *In Vivo* Pharmacokinetic Parameters with In-House Validation. *Mol. Pharmaceutics* **2021**, *18*, 4520-4530.
21. Hu, H.; Laufkötter, O.; **Miljković, F.**; Bajorath, J. Data Set of Competitive and Allosteric Protein Kinase Inhibitors Confirmed by X-ray Crystallography. *Data in Brief* **2021**, *35*, e106816.

20. Hu, H.; Laufkötter, O.; **Miljković, F.**; Bajorath, J. Systematic Comparison of Competitive and Allosteric Kinase Inhibitors Reveals Common Structural Characteristics. *Eur. J. Med. Chem.* **2021**, *214*, e113206.
19. Miljković, F.; Chaudhari, R. Members of our Early Career Panel Highlight Key Research Articles on the Theme of Computer-Aided Drug Design. *Future Drug Discov.* **2020**, *2*, FDD52.
18. 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.
17. 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.
16. Miljković, F.; Rodríguez-Pérez, R.; Bajorath J. Machine Learning Models for Accurate Prediction of Kinase Inhibitors with Different Binding Modes. *J. Med. Chem.* **2020**, *63*, 8738-8748.
15. 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.
14. 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.
13. Feldmann, C.; **Miljković, F.**; Yonchev, D.; Bajorath, J. Identifying Promiscuous Compounds with Activity Against Different Target Classes. *Molecules* **2019**, *24*, e4185.
12. 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.
11. 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.
10. 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.
9. Miljković, F.; Bajorath, J. Computational Analysis of Kinase Inhibitors Identifies Promiscuity Cliffs across the Human Kinome. *ACS Omega* **2018**, *3*, 17295–17308.
8. Miljković, F.; Bajorath, J. Data-Driven Exploration of Selectivity and Off-Target Activities of Designated Chemical Probes. *Mol.* **2018**, *23*, e2434.
7. Miljković, F.; Bajorath, J. Evaluation of Kinase Inhibitor Selectivity Using Cell-Based Profiling Data. *Mol. Inform.* **2018**, *37*, e1800024.
6. Miljković, F.; Bajorath, J. Reconciling Selectivity Trends from a Comprehensive Kinase Inhibitor Profiling Campaign with Known Activity Data. *ACS Omega* **2018**, *3*, 3113–3119.
5. Miljković, F.; Bajorath, J. Exploring Selectivity of Multikinase Inhibitors across the Human Kinome. *ACS Omega* **2018**, *3*, 1147–1153.
4. 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.
3. 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.
2. 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.
1. 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.

Selected Abstracts and Conference Publications

3. "Proceedings of IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2021). IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2021)", December 9-12, 2021, Institute of Electrical and Electronics Engineers (IEEE), Virtual. Conference Paper: Bai, P.; **Miljković, F.**; Ge, Y.; Greene, N.; John B.; Lu. H. "Hierarchical Clustering Split for Low-Bias Evaluation of Drug-Target Interaction Prediction".
2. "19th International Workshop on (Q)SAR in Environmental and Health Sciences – QSAR 2021 From QSAR to New Approach Methodologies (NAMs)", June 7-9, 2021, American Society for Cellular and Computational Toxicology (ASCCT), Virtual. Oral Presentation: **Miljković, F.**; Martinsson, A.; Obrezanova, O.; Williamson, B.; Johnson, M.; Oprisiu, I.; Bender, A.; Greene N. "Machine Learning Models for Predicting Human *In Vivo* PK Parameters Using Chemical Structure and Dose".
1. "Chemoinformatics Strasbourg Summer School", June 25-29 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.