CURRICULUM VITAE

Filip Miljković, MPharm, PhD

Gothenburg, Sweden

E-mail: filipm90@yahoo.com, *Website*: filipm90.github.io

LinkedIn ORCID ResearchGate

Work Experience

Industry

Associate Principal AI Scientist (*Oct 2024 – Present)*
Medicinal Chemistry, Cardiovascular, Renal and Metabolism (CVRM), Discovery Sciences, AstraZeneca R&D, Gothenburg, Sweden

AI Scientist (*July 2022 – Sep 2024*)
Medicinal Chemistry, Early Cardiovascular, Renal and Metabolism (CVRM), AstraZeneca R&D, Gothenburg, Sweden

Senior Data Scientist (*Feb 2020 – June 2022)*
Imaging and Data Analytics, Clinical Pharmacology & Safety Sciences, AstraZeneca R&D, Gothenburg, Sweden

Academia

Visiting Researcher (*Jan 2025 – Present)*
Pharmaceutical Bioinformatics, Department of Pharmaceutical Biosciences, Uppsala University, Uppsala, Sweden

Affiliate Scientist (*Jan 2021 – Present)*
Department of Life Science Informatics, b-it, LIMES Program Unit Chemical Biology and Medicinal Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn, Germany

Other

Pharmacy Apprentice (Professional Pharmaceutical Practice) (*Oct 2014 – Oct 2015*)
ZUA Farmakop, Niš, Serbia
Prerequisite for the state exam: Licensed Pharmacist (Nov 2015)

Education

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

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

International Research Visits

IPSF Student Exchange Program (*July 2013 – Aug 2013*)
Department of Analytical Chemistry, Medical University of Gdańsk, Poland
Description: Quality consistency evaluation of *Melissa officinalis* L. samples using HPLC fingerprints
Supervisor: dr hab. n. farm. Agnieszka Viapiana

Teaching Experience

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

- "General Chemistry with Stoichiometry", Oct 2010 – Jan 2011.
- "Organic Chemistry", Mar 2011 – June 2011.

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

- "Introduction to Chemistry", Sept 2016 – Oct 2016.
- "Structural Bioinformatics", Oct 2016 – Jan 2018.
- "Molecular Modeling and Drug Design", Apr 2017 – Feb 2019.
- "Programming Lab I" (Python), Apr 2019 – June 2019.
- "Introduction to Machine Learning Tutorial", Apr 2019 – June 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", Oct 2017 – Dec 2019.

Upsala University, Sweden

- Involved in different Master programs, 2025 - *Present*

Mentorship Experience

Rheinische Friedrich-Wilhelms-Universität Bonn, Germany

- Supervision of two Master theses, 2019; 2023.
- Supervision of a visiting PhD student, 2023.

AstraZeneca R&D, Sweden

- Supervision of a graduate scientist coming from the Data Science & AI Graduate Program, September 2021 – May 2022.
- Career development discussion with two graduate scientists coming from the Data Science & AI Graduate Program, 2021 – 2024.
- Supervision of a visiting postdoctoral researcher coming from a collaboration with the University of Vienna, Austria, October 2023 – November 2023.
- Supervision of a Master thesis in collaboration with the Chalmers University of Technology, Sweden, January 2024 – June 2024 (two students).
- Supervision of a Master thesis in collaboration with the Chalmers University of Technology, Sweden, January 2025 – June 2025 (two students).

Languages

Serbian (Native)
English (Full professional proficiency): TOEFL (109/120)
Swedish (Advanced working proficiency)
German (Elementary proficiency)

Research

Publications

(* indicates the corresponding author)

45. Larsson, S.; Carlsson, M.; Beckmann, R.; **Miljković, F.***; Mercado, R. LAGOM: A Transformer-Based Chemical Language Model for Drug Metabolite Prediction. *Artif. Intell. Life Sci.* **2025**, 8, 100142.

44. Chen, Y.; Winiwarter, S.; Jacob, R. A.; Ahlqvist, M.; Mazzolari, A.; **Miljković, F.***; Kirchmair, J. Metabolite Identification Data in Drug Discovery, Part 2: Site-of-Metabolism Annotation, Analysis, and Exploration for Machine Learning. *Mol. Pharmaceutics* **2025**, *22*, 6772-6787.

43. Ahlqvist, M.; Bonner Karlsson, I.; Ekdahl, A.; Ericsson, C.; Jurva, U.; **Miljković, F.***; Chen, Y.; Winiwarter, S. Metabolite Identification Data in Drug Discovery, Part 1: Data Generation and Trend Analysis. *Mol. Pharmaceutics* **2025**, *22*, 6788-6802.

42. Liu, J.; Peter, B.; Rhodes, L.; Ormö, M.; Peng, B.; Hansson P.; Gunnarsson, A.; Knerr, L.; **Miljković, F.**; Ölwegård-Halvarsson, M.; Dezfouli, M.; Dekker, N.; Lindmark, H.; Andersson, S. Development of Novel High-Throughput Biochemical Competition Assays to Identify Ligands of Human Asialoglycoprotein Receptor 1. *SLAS Discov.* **2025**, *35*, 100265.

41. Bai, P.; **Miljković, F.**; Liu, X.; De Maria, L.; Croasdale-Wood, R.; Rackham, O.; Lu, H. Mask-Prior-Guided Denoising Diffusion Improves Inverse Protein Folding. *Nat. Mach. Intell.* **2025**, 7, 876-888.

40. Santisteban Valencia, Z.; Kingston, J. **Miljković, F.**; Rowbottom, H.; Mann, N.; Davies, S.; Ekblad, M.; Di Castro, S.; Kwapień, K.; Malmerberg, E.; Friis, S. D.; Lundbäck, T.; Leek, T.; Wernevik, J. Closing the Design–Make–Test–Analyze Loop: Interplay between Experiments and Predictions Drives PROTACs Bioavailability. *J. Med. Chem.* **2024**, *67*, 20242-20257.

39. Miljković, F.*; Bajorath, J. Kinase Drug Discovery: Impact of Open Science and Artificial Intelligence. *Mol. Pharmaceutics* **2024**, *21*, 4849-4859.

38. Gawehn, E.; Greene, N.; **Miljković, F.;** Obrezanova, O.; Subramanian, V.; Trapotsi, M.-A.; Winiwarter, S. Perspectives on the Use of Machine Learning for ADME Prediction at AstraZeneca. *Xenobiotica* **2024**, *54*, 368-378.

37. Miljković, F.*; Medina-Franco, J. L. Artificial Intelligence-Open Science Symbiosis in Chemoinformatics. *Artif. Intell. Life Sci.* **2024**, *5*, 100096.

36. Chen, Y.; Seidel, T.; Jacob, R. A.; Hirte, S.; Mazzolari, A.; Pedretti, A.; Vistoli, G.; Langer, T.; **Miljković, F.**; Kirchmair, J. Active Learning Approach for Guiding Site-of-Metabolism Measurement and Annotation. *J. Chem. Inf. Model.* **2024**, *64*, 348–358.

35. Bajorath, J.; Gardner, S.; Grisoni, F.; Horta Andrade, C.; Kirchmair, J.; Landon, M.; Medina-Franco, J.-L.; **Miljković, F.**; Montanari, F.; Rodríguez-Pérez, R. First-generation Themed Article Collections. *Artif. Intell. Life Sci.* **2023**, *4*, e100088.

34. Xerxa, E.; **Miljković.**; Bajorath, J. Data-Driven Global Assessment of Protein Kinase Inhibitors with Emphasis on Covalent Compounds. *J. Med. Chem.* **2023**, *66*, 7657-7665.

33. Bai, P.; **Miljković, F.**; John, B.; Lu, H. Interpretable Bilinear Attention Network with Domain Adaptation Improves Drug–Target Prediction. *Nat. Mach. Intell.* **2023**, *5*, 126-136.

32. Gill, G.; Moullet, M.; Martinsson, A.; **Miljković, F.**; Williamson, B.; Arends, R. H.; Pilla Reddy, V. Evaluating the Performance of Machine-Learning Regression Models for Pharmacokinetic Drug–Drug Interactions. *CPT: Pharmacomet. Syst. Pharmacol.* **2023**, *1*, 122-134.

31. Gill, G.; Moullet, M.; Martinsson, A.; **Miljković, F.**; Williamson, B.; Arends, R. H.; Pilla Reddy, V. Comparing the Applications of Machine Learning, PBPK, and Population Pharmacokinetic Models in Pharmacokinetic Drug–Drug Interaction Prediction. *CPT: Pharmacomet. Syst. Pharmacol.* **2022**, *11*, 1560-1568.

30. Martínez Mora, A.; Mogemark, M.; Subramanian, V.; **Miljković, F.*** Interpretation of Multi-Task Clearance Models from Molecular Images Supported by Experimental Design. *Artif. Intell. Life Sci.* **2022**, *2*, e100048.

29. Trapotsi, M.-A.; Mouchet, E.; Williams, G.; Monteverde, T.; Juhani, K.; Turkki, R.; **Miljković, F.**; Martinsson, A.; Mervin, L; Pryde, K. R.; Müllers, E.; Barrett, I.; Engkvist, O.; Bender, A; Moreau, K. Cell Morphological Profiling Enables High-Throughput Screening for PROteolysis TArgeting Chimera (PROTAC) Phenotypic Signature. *ACS Chem. Biol.* **2022**, *17*, 1733-1744.

28. Martínez Mora, A.; Subramanian, V.; **Miljković, F.*** Multi-Task Convolutional Neural Networks for Predicting *In Vitro* Clearance Endpoints from Molecular Images. *J. Comput. Aided Mol. Des.* **2022**, *36*, 443-457.

27. Obrezanova, O.; Martinsson, A.; Whitehead, T.; Mahmoud, S.; Bender, A.; **Miljković, F.;** Grabowski, P.; Irwin, B.; Oprisiu, I.; Conduit, G.; Segall, M.; Smith, G. F.; Williamson, B.; Winiwarter, S.; Greene, N. Prediction of *In Vivo* Pharmacokinetic Parameters and Time-Exposure Curves in Rats Using Machine Learning from the Chemical Structure. *Mol. Pharmaceutics* **2022**, *19*, 1488-1504.

26. Rodríguez-Pérez, R.; **Miljković, F.**; Bajorath, J. Machine Learning in Chemoinformatics and Medicinal Chemistry. *Ann. Rev. Biomed. Data Sci.* **2022**, *5*, 43-65.

25. 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**, *65*, 922-934.

24. Yoshimori, A.; **Miljković, F.**; Bajorath, J. Approach for the Design of Covalent Protein Kinase Inhibitors via Focused Deep Generative Modeling. *Molecules* **2022**, *27*, e570.

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.

Patents

2. WO2025104699A1
1. WO2025104697A1

Selected Abstracts and Conference Publications

2. "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".
1. "Chemoinformatics Strasbourg Summer School", June 25-29, 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 (no designated certificate received).

Selected Oral Presentations

5. ACS Spring 2025, Division of Chemical Information, Chemoinformatics in the Open Science Era: From Data Science to Artificial Intelligence, March 23-27, 2025, American Chemical Society (ACS), In Person, Oral Presentation: **Miljković, F.** "Closing the Design–Make–Test–Analyze Loop: Interplay between Experiments and Predictions Drives PROTACs Bioavailability".
4. b-it Alumni Lecture Series Winter Semester 2023/2024, October 24, 2023, Bonn-Aachen International Center for Information Technology (B-IT), University of Bonn, Bonn, Germany, Virtual, Oral Presentation: **Miljković, F.** "On Career and Beyond".
3. ACS Fall 2023, Division of Chemical Information, Chemical Informatics (R)evolution: Towards Democratization and Open Science, August 13-17, 2023, American Chemical Society (ACS), In Person, Oral Presentation: **Miljković, F.** "Machine Learning Models for Predicting Human *In Vivo* PK Parameters Using Chemical Structure and Dose".
2. Industry Symposium on "AI in the Life Sciences", June 26-27, 2023, Bonn-Aachen International Center for Information Technology (B-IT), University of Bonn, Bonn, Germany, In Person, Oral Presentation: **Miljković, F.** "Machine Learning Models for Predicting Human *In Vivo* PK Parameters Using Chemical Structure and Dose".
1. "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".