# CURRICULUM VITAE


## Filip Miljković, MPharm, PhD

Gothenburg, Sweden

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LinkedIn ORCID ResearchGate


**Work Experience**

### Industry

**Associate Principal AI Scientist (*Oct 2024 – Present)***
Medicinal Chemistry, Early Cardiovascular, Renal and Metabolism (CVRM), 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

**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**, *in press.*

**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".