NOVARTIS

Data Science & AI Innovation Postdoctoral Fellow in Machine Learning for Chemical Synthesis and Reactivity Prediction

Job ID
REQ-10082641
июл 01, 2026
Швейцария
Available in: English

Сводка

This postdoctoral fellowship offers a unique opportunity to advance the use of artificial intelligence and machine learning for chemical synthesis and reactivity prediction in drug discovery. The successful candidate will develop and apply state-of-the-art predictive models using large-scale reaction datasets to improve chemical decision-making, reaction optimization, and molecular design, while collaborating with experts across data science, computational chemistry, medicinal chemistry, and synthesis technology. The project aims to accelerate the Design–Make–Test–Analyze cycle and contribute to next-generation AI-powered approaches for discovering new medicines.

Location: Basel, Switzerland
Duration: 3 years
Program start date: October 1, 2026
Application deadline: July 15, 2026 EOB

About the Role

We are excited to invite applications for the Novartis Biomedical Research Postdoctoral Fellowship Program; a unique training opportunity designed for exceptional early-career scientists eager to tackle some of the most challenging problems in biomedical research and drug discovery.

As a Postdoctoral Research Fellow, you will join Global Discovery Chemistry in Basel and pursue an innovative research project at the forefront of biomedical science and drug discovery. You will work alongside leading scientists in a highly collaborative, multidisciplinary environment while gaining exposure to the broader ecosystem that translates scientific discovery into medicines.

Our fellows are empowered to ask bold scientific questions, apply cutting-edge technologies, and develop approaches that have the potential to transform patient care.

Research Opportunity

Join an interdisciplinary research project at the intersection of artificial intelligence, machine learning, and synthetic chemistry. This fellowship aims to develop next-generation machine learning approaches that predict chemical reaction outcomes, reaction conditions, and molecular reactivity using large-scale proprietary and public reaction datasets. By leveraging more than two decades of reaction knowledge generated within Novartis, the fellow will investigate how modern AI methods, including graph neural networks, transformer architectures, and foundation models, can improve the efficiency and success rate of chemical synthesis.

The project will focus on building predictive models that help chemists design more efficient synthetic routes, identify optimal reaction conditions, and expand access to diverse chemical space. The fellow will collaborate closely with experts in data science, computational chemistry, medicinal chemistry, and synthesis technology, with opportunities to integrate predictive chemistry models into generative AI workflows and emerging laboratory automation platforms. The research is expected to result in high-impact publications and contribute to accelerating the Design-Make-Test-Analyze cycle in active drug

discovery projects.

Why Join the Program?

The Novartis Biomedical Research Postdoctoral Fellowship Program is designed to develop the next generation of scientific leaders, powering the future of medicine, through rigorous research, and immersive learning experiences, such as implementation of AI tools in biomedical research.

Postdoctoral Research Fellows benefit from:

- Guidance from accomplished scientific leaders and subject matter experts
- Access to advanced technologies, platforms, and research capabilities
- Collaboration across disciplines and organizational boundaries
- A global and diverse community of postdoctoral fellows
- Dedicated programming designed to help fellows thrive throughout their careers.
- Personalized experiential learning opportunities through a Postdoc Practicum that empower fellows to explore new scientific domains, build cross-functional expertise, and expand their impact beyond their primary research project.
- Opportunities to present research, publish in leading journals, and build an international scientific network

We are entering a new era of biomedical research breakthroughs through the convergence of biology, technology, and artificial intelligence tools, and fellows are also supported in engaging with these emerging approaches. This is a full-time training position of up to three years in duration.

Reimagining Medicine Together

At Novartis, our purpose is to reimagine medicine to improve and extend people’s lives. Through this program, you will grow as a scientist and future leader while contributing to discoveries that may ultimately benefit patients worldwide.

Key Responsibilities

- Analyze large-scale chemical reaction datasets from proprietary and public sources to identify trends, opportunities, and challenges in chemical synthesis.
- Develop, implement, and evaluate machine learning models for predicting reaction success, reaction conditions, yield, regioselectivity, and molecular reactivity.
- Benchmark state-of-the-art AI approaches, including graph neural networks, transformer models, and foundation models, against relevant synthesis prediction tasks.
- Investigate novel pre-training strategies leveraging large-scale chemistry and physics-based datasets to improve predictive performance and generalization.
- Collaborate closely with medicinal chemists, synthetic chemists, and automation experts to address real-world drug discovery challenges.
- Apply predictive models to enable broader substrate scope exploration, reaction optimization, and library synthesis design.
- Explore integration of synthesis prediction models with generative chemistry and AI-driven molecular design workflows.
- Present research findings internally and externally, publish in leading scientific journals, and contribute to the broader scientific community.

Essential Requirements

- PhD in Data Science, Computer Science, Machine Learning, Cheminformatics, Computational Chemistry, Chemistry, Pharmaceutical Sciences, or a related quantitative discipline completed prior to the fellowship start date. The program is intended for scientists immediately following their PhD training (graduated in 2026).
- Demonstrated record of scientific achievement (publications, presentations, patents, or equivalent)

- Demonstrated experience developing and applying deep learning methods to scientific or chemical datasets.
- Strong programming skills in Python and familiarity with modern machine learning frameworks and architectures, such as graph neural networks, transformers, large language models or foundation models for scientific applications.
- Experience with data analysis, statistical modeling, and handling large, complex datasets.
- Strong commitment to learning, innovation, and professional development
- Ability to work effectively in highly collaborative, multidisciplinary research environments.
- Excellent communication skills and ability to present complex scientific concepts to diverse audiences.

Desirable Requirements

- Experience curating, processing, and analyzing large-scale chemical reaction datasets, including reaction encoding, atom mapping, reaction classification, and extraction of chemical knowledge from structured or unstructured data sources.

- Experience designing and querying relational databases or other structured data systems for scientific data management and large-scale analytics.

Important:

Please submit your CV and cover letter by July 15, 2026 end of day.

In your cover letter, please describe your research interests, career aspirations, and how participation in the Novartis Biomedical Research Postdoctoral Fellowship Program will support your long-term development.

The start date for the 2026 Novartis BR Postdoctoral Fellowship Program cohort is October 1, 2026. Please confirm your availability to meet this start date in your cover letter.

Please note that we can only accept applicants who are eligible to work in Switzerland.

Why Novartis: Helping people with disease and their families takes more than innovative science. It takes a community of smart, passionate people like you. Collaborating, supporting and inspiring each other. Combining to achieve breakthroughs that change patients' lives. Ready to create a brighter future together? https://www.novartis.com/about/strategy/people-and-culture

Benefits and Rewards: Learn about all the ways we'll help you thrive personally and professionally.
Read our handbook (PDF 30 MB)

Дивизион
Biomedical Research
Business Unit
Research
Место
Швейцария
Сайт
Basel (City)
Company / Legal Entity
C028 (FCRS = CH028) Novartis Pharma AG
Functional Area
Others
Job Type
Full time
Employment Type
Early Career (Fixed Term)
Shift Work
No
Job ID
REQ-10082641

Data Science & AI Innovation Postdoctoral Fellow in Machine Learning for Chemical Synthesis and Reactivity Prediction

Apply to Job
Job ID
REQ-10082641

Data Science & AI Innovation Postdoctoral Fellow in Machine Learning for Chemical Synthesis and Reactivity Prediction

Apply to Job

Source URL: *https://novartis.ru/careers/career-search/job/details/req-10082641-data-science-ai-innovation-postdoctoral-fellow-machine-learning-chemical-synthesis-and-reactivity-prediction*

List of links present in page

1. https://www.novartis.com/about/strategy/people-and-culture
2. https://www.novartis.com/sites/novartis_com/files/novartis-life-handbook.pdf
3. https://novartis.wd3.myworkdayjobs.com/en-US/Novartis_Careers/job/Basel-City/Data-Science---AI-Innovation-Postdoctoral-Fellow-in-Machine-Learning-for-Chemical-Synthesis-and-Reactivity-Prediction_REQ-10082641
4. https://novartis.wd3.myworkdayjobs.com/en-US/Novartis_Careers/job/Basel-City/Data-Science---AI-Innovation-Postdoctoral-Fellow-in-Machine-Learning-for-Chemical-Synthesis-and-Reactivity-Prediction_REQ-10082641