NOVARTIS

# Data Science & AI Innovation Postdoctoral Fellow Foundational & Multimodal Proteochemometrics models

Job ID
REQ-10082585

7月 01, 2026

Switzerland

Available in: English

## 摘要

The Novartis Biomedical Research Postdoctoral Fellowship Program offers a 3-year 100% position starting October 1, 2026, in Basel, Switzerland, focusing on foundational multimodal proteochemometrics models in drug discovery. This opportunity enables early-career scientists to work with cutting-edge AI and biomedical research technologies in a collaboration with data and wet-lab scientists. The fellows will train and optimize structure affinity models using high-throughput experimental data and evaluate their predictive performance for drug-target interactions in hit finding and and safety assessments.

## About the Role

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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 Discovery Sciences 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

Foundational structure activity models that can predict small molecule protein interactions from the small molecule structure and protein sequence have attracted scientific attention. However, the practical suitability of such models trained on public structure activity data has been limited as this data is both low in volume and extremely sparse. Industrial large scale screening technologies such as DNA encoded libraries generate larger volumes of dense data. In this project we aim at training a large- proteochemometrics model based on high-throughput experimental data resulting from different read-out modalities and will assess how such models can be predictive for low-volume high quality affinity data with and without fine-tuning on a small number of such quality data points.

## 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 100% 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**

- Train and optimize foundational structure affinity models on high volume experimental data such as DNA encoded library screening data.
- Fine-tune models on high-quality low volume affinity data.
- Evaluate the performance of the models with and without fine-tuning and compare it with the state-of-the-art models.
- Apply and evaluate promising model architectures prospectively in small molecule hit-finding projects.
- Evaluate the performance of the models to predict off-targets for pharmacology safety assessments.

**Essential Requirements**

- PhD (or equivalent doctoral degree) in a relevant scientific 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)
- Strong commitment to learning, innovation, and professional development Hands-on experience with cheminformatic workflows, and familiarity with descriptors and machine learning and deep learning in the context of cheminformatics.
- Expertise working in Linux high performance computing and cloud environments.
- Expertise in Python scientific and deep learning stacks, familiarity with best practices in computational reproducible research (version control, testing, documentation).
- Experience in training foundational models and / or processing huge datasets
- Demonstrated ability to work as part of an interdisciplinary team (i.e., biologists, chemists, data scientists), with proactive and results-oriented communication skills. Dedication to promoting mutual respect, empathy, and positivity in diverse professional settings.

**Desirable Requirements**

- Experience with some of the following: ligand protein docking, ligand protein co-folding, drug-target interaction models
- Experience using synthons and transformations to generate virtual spaces, or to interrogate virtual spaces

**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 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)

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Biomedical Research

Business Unit
Research

地点
Switzerland

站点
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

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