

Senior Expert Data Science (Make-on-Demand Cheminformatics & AI)

Job ID
REQ-10048606

4月 22, 2025

Switzerland

摘要

The mission of Novartis is to reimagine medicine, and our team exemplifies that mission by consistently pushing the boundaries of drug discovery technology and data science. We interface with biologists, geneticists, chemists, and computational experts daily, to execute complex collaborations and bring first-in-class and best-in-class drugs to patients with urgent unmet need. We thrive in the earliest phases of drug discovery, partnering with diverse disease areas to nominate the next generation of drug targets and modalities, as well as elucidate complex biological mechanisms and sites of action.

To extend our impact, we're seeking a creative, passionate, and tenacious scientist to join the data science team in Discovery Sciences (DSc) at Novartis Biomedical Research (BR). If you want to make a difference in the field of early drug discovery and want to join our dynamic and collaborative team, we encourage you to apply today.

About the Role

Major accountabilities:

- Champion Make-on-Demand (MoD) workflows and apply and develop computational strategies and workflows that accelerate hit finding activities
- Develop synthon based search strategies to allow teams to leverage ever increasing virtual spaces without having to rely on brute force searches of fully enumerated spaces
- Contribute to the design of internal Low Molecular Weight (LMW) and DNA Encoded libraries in order to fully harness the potential of MoD during hit finding.
- Leverage core expertise in cheminformatics, computational chemistry, and data science, to generate and navigate virtual chemical spaces, build predictive models, collaborate with project teams to accelerate early drug discovery projects.

Minimum Requirements:

- PhD with a cheminformatics, computational chemistry, or physics focus; or alternatively, a degree in a related subject (e.g. chemistry, chemical biology, computer science, or data science) in combination with the equivalent experience applying computational tools in life science / drug discovery setting.
- Hands on experience with cheminformatic workflows, and familiarity with descriptors and machine learning (ML) in the context of cheminformatics.
- Excellent scientific communication, including the ability to present complex data science concepts in digestible terms to diverse scientific audiences while leveraging innovative data visualization.
- 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.
- Expertise working in Linux high performance computing and cloud environments.

- Expertise in Python scientific stacks, familiarity with best practices in computational reproducible research (version control, testing, documentation).

Nice to have:

- Familiarity with structure-based and ligand-based approaches
- Experience with some of the following: ligand protein docking, generative chemistry, deep learning, ligand protein cofolding
- Familiarity with Large Language Models (LLMs)
- Experience or familiarity with organic synthesis
- Experience designing libraries of small molecules
- Experience using synthons and transformations to generate virtual spaces, or to interrogate virtual spaces

Novartis is committed to building an outstanding, inclusive work environment and diverse teams representative of the patients and communities we serve.

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>

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部门
Biomedical Research

Business Unit
Pharma Research

地点
Switzerland

站点
Basel (City)

Company / Legal Entity
C028 (FCRS = CH028) Novartis Pharma AG

Functional Area
Data and Digital

Job Type
Full time

Employment Type
Regular

Shift Work
No

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