

Data Science, Cheminformatics & AI: Lab-in-the-Loop Hit Finding

Job ID

REQ-10079266

Jun 22, 2026

LOC_US

About the Role

Internal Job Title: Senior Expert II, Data Science

Position Location: onsite, San Diego, CA #LI-onsite

Role responsibilities:

- Locally lead and execute the data science strategy for Lab-in-the-Loop (LitL) workflows to accelerate low-molecular-weight therapeutic discovery in close collaboration with experimental and computational partners from different departments. Champion best practices for model development and deployment within LiTL workflows, including model monitoring and prediction telemetry, in alignment with enterprise model initiatives.
- Develop and execute in silico hit finding strategies in synergy with project teams, leveraging internally available as well as external compounds from ultra large virtual (Make-on-Demand) chemical spaces. Ensure best-practice computational tools are applied to accelerate/diversify hit finding in a rapidly evolving field.
- Apply in silico hit finding approaches (e.g., cheminformatics, generative AI, Make-on-Demand chemistry) with internal multi-modal data (e.g., structure, chemogenomics, gene expression, imaging) to drive impact in early hit finding projects. Internalize, develop and apply cutting-edge in silico methods (e.g., agentic workflows, drug-target interaction modeling) translating methodological innovation into tangible impact on discovery projects.
- Drive the design and implementation of scalable, robust data pipelines for high-throughput assay data in partnership with informatics and data excellence teams, enabling automated and reproducible hit-finding workflows.

Essential Requirements:

- PhD in cheminformatics or chemistry; or a degree in a related field (e.g., chemical biology, physics, or computer science) with demonstrated applicable experience.
- 4+ years of post-graduate experience applying cheminformatics, data science, and machine learning approaches to hit finding in an early drug discovery setting.
- Experience with hit-finding technologies such as high-throughput screening and/or advanced phenotypic screening
- 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, automation engineers), with proactive and results-oriented communication skills. Dedication to promoting mutual respect, empathy, and positivity in diverse professional settings.
- Strong experience working in Linux-based high-performance computing and/or cloud environments.
- Proficiency in the Python scientific ecosystem, along with experience in agent-based/agentic coding approaches and reproducible research best practices (version control, testing, documentation), databases, and SQL.
- Experience with implementing AI in Lab-in-the-Loop, iterative, or self-driving lab workflows.
- Experience with Make-on-Demand and virtual spaces like Enamine REAL for hit finding.

Desirable Requirements:

- Experience with orchestrating agents, computational tools, and physical automated screening workflows.
- Experience building or integrating workflows into agentic systems for drug discovery.
- Track record of turning project-specific in silico approaches into reproducible, generalizable workflows that impact hit

finding.

- Familiarity with some of the following: ligand protein docking, generative chemistry, active learning, drug-target interaction modeling, free energy perturbation.
- Track record of publication in peer-reviewed journals and/or scientific conferences.

The salary for this position is expected to range between \$138,600 and \$257,400 USD per year. The final salary offered is determined based on factors like, but not limited to, relevant skills and experience, and upon joining Novartis will be reviewed periodically. Novartis may change the published salary range based on company and market factors.

Your compensation will include a performance-based cash incentive and, depending on the level of the role, eligibility to be considered for annual equity awards.

US-based eligible employees will receive a comprehensive benefits package that includes health, life and disability benefits, a 401(k) with company contribution and match, and a variety of other benefits. In addition, employees are eligible for a generous time off package including vacation, personal days, holidays and other leaves.

To learn more about the culture, rewards and benefits we offer our people click [here](#).

Role Requirements

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 \(PDF 30 MB\)](#)

Division

DIV_RE

Business Unit

Research

Location

LOC_US

Site

San Diego

Company / Legal Entity

U175 (FCRS = US175) Novartis Institutes for BioMedical Research, Inc.

Functional Area

FCT_DD

Job Type

Full time

Employment Type

Regular

Shift Work

No

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