NOVARTIS

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

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Сводка

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 integrative 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 an innovative, passionate, and tenacious scientist to join the Data Science team in Discovery Sciences (DSc) at Novartis Biomedical Research, San Diego. As an integral part of our team, you will drive wet/dry lab convergence by leveraging cheminformatics, AI, and data science to accelerate our hit finding efforts in early drug discovery projects in strong collaboration with infrastructure, computational, and experimental teams. If you are passionate about impacting and innovating the field of early drug discovery and excited to join our expert, dynamic, and collaborative team, we encourage you to apply.

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.

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)

EEO Statement:

The Novartis Group of Companies are Equal Opportunity Employers. We do not discriminate in recruitment, hiring, training, promotion or other employment practices for reasons of race, color, religion, sex, national origin, age, sexual orientation, gender identity or expression, marital or veteran status, disability, or any other legally protected status.

Accessibility & Reasonable Accommodations

The Novartis Group of Companies are committed to working with and providing reasonable accommodation to individuals with disabilities. If, because of a medical condition or disability, you need a reasonable accommodation for any part of the application process, or to perform the essential functions of a position, please send an e-mail to us.reasonableaccommodations@novartis.com or call +1(877)395-2339 and let us know the nature of your request and your contact information. Please include the job requisition number in your message.

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