

Computational Medicinal Chemist

Job ID

REQ-10084143

Jul 22, 2026

LOC_US

About the Role

Internal Job Title: Senior Expert I/II, Data Science

Position Location: San Diego, CA, hybrid

Your Responsibilities Include:

- Drive the design of medicinal chemistry efforts by applying in-depth knowledge of structure-activity relationships (SAR), structure-based and ligand-based drug design, a profound understanding of target biology, and predictive methods for assessing on- and off-target activity, physical properties, pharmacokinetics/pharmacodynamics (PK/PD), and synthetic feasibility.
- Thrive at the intersection of experimental and groundbreaking digital technologies, with a particular emphasis on expertise in machine learning, active learning and physics-based CADD methodologies as applied to small molecule drug discovery as well as in the induced proximity space.
- Stay abreast of scientific literature and engage with internal and external scientists to incorporate biological insights into lead characterization and screening initiatives.
- Collaborate with interdisciplinary project teams to facilitate effective decision-making throughout the target identification, lead optimization and drug candidate nomination process. This involves applying and developing predictive models based on high-content and time-resolved screening data, including imaging techniques.
- Drive hypothesis generation to enhance clinical success rates for programs involving small molecules, peptides, RNAs, protein degradation, molecular glues, transient covalent inhibitors, and kinetic stabilization of drug-target complexes.
- Take a leading role in cross-disciplinary mechanistic studies using physics-based modeling and simulation, biophysical characterization, and cellular validation. These studies will inform the strategic targeting strategies of discovery projects, aiming for optimal mechanisms of action (MoAs).

Essential Requirements:

- PhD in medicinal chemistry, computational chemistry, computational biology, computational chemical biology, or a related field. Candidates with a laboratory-based background in chemistry and biology, supplemented with strong computational experience, are also encouraged to apply. We will also consider MS applicants with 6+ years of relevant Pharma/biotech experience.
- 3+ years of experience working with project teams in a drug discovery environment.
- Proven track record of innovation through analogue design, leading to significant impact on discovery projects.
- Familiarity with computational drug design tools (e.g. Schrödinger, CCG, OpenEye, etc.), high-performance computing environments, and strong publication history in peer-reviewed journals.
- Proactively anticipates project needs with a clinical focus.
- Demonstrates rigor and diligence in idea substantiation, analogue design, and experimentation.
- Strong team orientation with multitasking and adaptability in support and leadership roles.
- Effective listener with excellent written and oral communication skills.
- Proficient in data visualization to effectively communicate insights.

Compensation & Benefits:

The salary for this position is expected to range between \$126,000 and \$234,000 USD annually for Senior Expert I, Data

Science, and \$138,600 and \$257,400 USD annually for Senior Expert II, Data Science. 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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