

# Computational Medicinal Chemist

Job ID  
REQ-10045508  
Mar 26, 2025  
USA

## Summary

Join our vibrant and innovative Computer-Aided Drug Discovery (CADD) team in Cambridge, where we bring together diverse talents to redefine the way Biomedical Research discovery teams validate and develop new targets. We are a driving force behind drug discovery, and we are now eagerly searching for an exceptional computational scientist like you to join our ranks. Imagine the opportunity to unlock hidden knowledge and disruptive insights from the vast and invaluable data collected by one of the world's most renowned pharmaceutical companies. We need your expertise, experience, and unwavering passion to help us extract this wealth of information. Collaborating with a multidisciplinary group of scientists, you will be at the forefront of crafting inventive solutions to the most pressing drug discovery challenges, forging new paths toward groundbreaking medicines.

## About the Role

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

**Position Location:** Cambridge, MA, onsite

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Are you ready to seize this extraordinary chance to make a significant impact in the field of drug discovery? We invite you to embark on this thrilling journey with us, as we push the boundaries of what's possible in scientific exploration. Join our team and be part of a revolution that will shape the future of medicine.

Together, we will transform the landscape of drug discovery, accelerate breakthroughs, and change lives. Apply now and let your expertise shine in our dynamic and forward-thinking environment.

### Your Responsibilities Include:

- Drive the design of medicinal chemistry efforts by applying in-depth knowledge of structure-activity relationships (SAR), 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; familiarity with molecular dynamics, free energy calculations, solvation tools, quantum chemical calculations is a plus.
- Thrive at the intersection of experimental and groundbreaking digital technologies, with a particular emphasis on expertise in machine learning and artificial intelligence (AI) as applied to small molecule/cyclic peptide drug discovery.
- 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 to candidate nomination process. This involves applying and developing predictive models based on project data related to on-target/off-target activity and ADME properties.
- Drive hypothesis generation and molecular compound design to enhance clinical success rates for programs involving small molecules/cyclic peptides.
- 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).

#### **Minimum Requirements:**

- Advanced degree in computational chemistry, chemical physics, physical chemistry, chemical engineering, 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.
- 2+ years of experience (depends on the position level) working with project teams in a drug discovery environment.
- Desirable track record of innovation through analogue design, leading to significant impact on discovery projects.
- Familiarity with drug design tools and high-performance computing environments and strong publication history in peer-reviewed journals.

#### **Skills and Abilities:**

- 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.

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**Novartis Compensation and Benefit Summary:** The pay range for this position at commencement of employment is expected to be between \$119,700 to \$222,300 for Senior Expert I, and \$132,300 to \$245,700/year for Senior Expert II; however, while salary ranges are effective from 1/1/25 through 12/31/25, fluctuations in the job market may necessitate adjustments to pay ranges during this period. Further, final pay determinations will depend on various factors, including, but not limited to geographical location, experience level, knowledge, skills, and abilities. The total compensation package for this position may also include other elements, including a sign-on bonus, restricted stock units, and discretionary awards in addition to a full range of medical, financial, and/or other benefits (including 401(k) eligibility and various paid time off benefits, such as vacation, sick time, and parental leave), dependent on the position offered. Details of participation in these benefit plans will be provided if an employee receives an offer of employment. If hired, employee will be in an "at-will position" and the Company reserves the right to modify base salary (as well as any other discretionary payment or compensation program) at any time, including for reasons related to individual performance, Company or individual department/team performance, and market factors.

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**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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know the nature of your request and your contact information. Please include the job requisition number in your message.

Division

Biomedical Research

Business Unit

Pharma Research

Location

USA

State

Massachusetts

Site

Cambridge (USA)

Company / Legal Entity

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

Functional Area

Data and Digital

Job Type

Full time

Employment Type

Regular

Shift Work

No

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