

Computational Medicinal Chemist, Computer-Aided Drug Design

Job ID
REQ-10039884
Mar 12, 2025
USA

Summary

Join our vibrant and innovative Computer-Aided Drug Discovery (CADD) team in California, 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 II, Data Science

Position Location: Emeryville, CA, onsite, with the possibility of the position being located onsite in La Jolla, CA.

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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), 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.
- 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).

Minimum Requirements:

- Advanced degree 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.
- 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 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.

Why Novartis: Our purpose is to reimagine medicine to improve and extend people's lives and our vision is to become the most valued and trusted medicines company in the world. How can we achieve this? With our people. It is our associates that drive us each day to reach our ambitions. Be a part of this mission and join us! Learn more here: <https://www.novartis.com/about/strategy/people-and-culture>

You'll receive: You can find everything you need to know about our benefits and rewards in the Novartis Life Handbook: <https://www.novartis.com/careers/benefits-rewards>

Novartis Compensation and Benefit Summary: The pay range for this position at commencement of employment is expected to be between \$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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<https://talentnetwork.novartis.com/network>

You'll receive: You can find everything you need to know about our benefits and rewards in the Novartis Life Handbook: <https://www.novartis.com/careers/benefits-rewards>

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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<https://talentnetwork.novartis.com/network>

Benefits and Rewards: Read our handbook to learn about all the ways we'll help you thrive personally and professionally: <https://www.novartis.com/careers/benefits-rewards>

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Division

Biomedical Research

Business Unit

Pharma Research

Location

USA

State

California

Site

Emeryville

Company / Legal Entity

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

Alternative Location 1

LaJolla/SD, California, USA

Functional Area

Data and Digital

Job Type

Full time

Employment Type

Regular

Shift Work

No

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