



NEOMORPH

Share:



## Senior Scientist, Computational Chemistry

San Diego, CA

\$149,000 – \$184,000 Annually

[Apply for this position](#)

[Back to Jobs](#)

### Position overview:

Neomorph is looking for a curious, creative, and driven Senior Scientist to join our growing Computational Chemistry team. This is a unique opportunity to work at the forefront of small molecule drug discovery and targeted protein degradation in a fast-paced, collaborative startup environment.

In this role, you'll actively contribute to every stage of the discovery process — from target selection to advancing chemical series from hits to leads, optimizing leads, and selecting drug candidates. You'll apply both structure- and ligand-based design approaches to drive innovation across programs and play a key role in evolving Neomorph's computational chemistry platform.

This individual will have the opportunity to work at a company with a robust biophysics platform that is fully committed to leveraging computational chemistry to advance drug discovery projects from target identification to lead optimization and beyond. With access to cutting-edge CADD software and hardware, the Senior Scientist will make a direct and meaningful impact on the drug discovery process, ultimately improving patient outcomes.

### Job responsibilities:

- Work as a key member of the multidisciplinary team of medicinal chemistry, structure biology, biochemistry, and biology and guide the team by providing computational expertise in structure-based drug design and other methods.

- Building and applying suitable hypotheses to design compounds aimed at improving potency, target selectivity, physicochemical and/or pharmacokinetic properties, as evidenced by project impact
- Develop, optimize and deploy novel computational methods and workflows to improve productivity
- Apply molecular dynamics to simulate protein flexibility to allow high-accuracy prediction of binding site, binding mode, and binding kinetics of small molecules.
- Design compounds and predict their potency and ADMET using cutting-edge computational chemistry methods, including physics/ML based activity prediction.
- Drive structure/ligand virtual screening and generative AI methodologies for effective hit identification and hit-to-lead.
- Investigate, explore, and implement state-of-the-art computational chemistry methods that potentially accelerate discovery of molecular glue.

### **Required qualifications:**

- PhD in Computational Chemistry, or related field with 5+ years, MS with 8+ years or BS with 11+ years of relevant experience
- At least 5 years of experience working as a computational chemist in the pharmaceutical/biotech industry (will consider relevant post-doctoral work).
- Expertise in structure-based design, and ligand-based design with a solid background in physical chemistry, and knowledge of medicinal chemistry principles
- Proven track record of drug design with significant impact on drug discovery projects.
- Team oriented and highly collaborative with a hands-on approach; take ownership of projects and advance them with a strong sense of urgency in a fast-paced environment
- Strong interpersonal, communication, influencing and problem-solving skills and presentation skills at all levels both internally and externally
- Experience in physics-based activity prediction methods, including MM-GB/PBSA, FEP, and TI.
- Familiarity with commercial computational chemistry suites. The Schrodinger and OpenEye suites are preferred.
- Proficiency in scientific programming skills (e.g. Python, R) is essential.

### **Preferred qualifications:**

- Knowledge and experience of Cloud Computing is plus.
- Expertise in protein-protein docking tools is plus.
- Knowledge and experience working with Protein-Protein Interaction targets
- Familiarity with quantum mechanics, cheminformatics, bioinformatics
- Experience in application of MD packages (AMBER, GROMACS, OPENMM) to analyze protein-ligand or protein-protein interaction and to estimate ligand affinity is preferred.

### **What we offer:**

- Industry competitive compensation
- Annual target bonus
- Stock options
- 401K plan

- Career advancement opportunities
- Monthly town halls to share business and scientific updates

## **Work Hard, Stay Well**

- Comprehensive medical, dental, and vision plans for employees and their dependents
- Health and Dependent Care FSA and HSA Plan with monthly Neomorph contribution
- Employee Assistance Program
- 10 holidays + Winter Shutdown + 3 weeks of vacation time with additional accruals after 2nd year of employment, separate sick leave.
- Supplemental pay for Pregnancy Disability Leave
- Paid Parental Leave for employees with a newborn child or a child placed with them for adoption or foster care

## **Lifestyle**

- Casual work environment
- Volunteer days off each year to spend time contributing to causes you care about
- Flexible work schedule
- Access to onsite gym
- Onsite space to store your bicycle (or surfboard)

## **Have Fun!**

We believe in work/life balance and Fun is at the core of our Core Values. In addition to department and company happy hours, we have regular company-wide and department lunches and social events (ie Padres games, summer picnic, holiday party, bring your kids to work day).

## **About Us:**

Neomorph is a venture backed biotechnology company solving critical problems in human health through the discovery and development of innovative new medicines against ‘undruggable targets’. Our team is comprised of industry leading experts in protein degradation and molecular glues who have a track record of ground-breaking discoveries in the field. We are committed to leadership in advancing the science and technology of molecular glue drug discovery, while prosecuting a pipeline of projects through clinical development. Our patient-first, science-driven approach is complemented by our dedication to a supportive and collaborative work environment.

Neomorph is headquartered in San Diego, California.

Neomorph is committed to pursuing and hiring a diverse workforce and is proud to be an equal opportunity employer. All qualified applicants will receive consideration for employment and will not be discriminated against on the basis of any characteristic protected by applicable federal, state or local law.

***Notice to agencies:*** Neomorph will not accept unsolicited assistance from recruiting/search agencies for this employment opportunity. Please, no phone calls or emails. All resumes submitted by recruiting or search

*agencies to any employee at Neomorph via email, the Internet or in any form and/or method without a valid written search/recruitment agreement in place for this position will be deemed the sole property of Neomorph. No fee will be paid in the event the candidate is hired by Neomorph as a result of the referral or through other means.*

Apply for this position

## Get Updates

Are you interested in hearing about new opportunities at Neomorph, Inc. in real time? Enter your email address to be notified automatically when new positions are posted.

Enter your email address

SEI

Powered by [AlphaStaff Hiring](#) © 2025 | [Privacy Policy](#)

[Admin Login](#) | [Subscribe via RSS](#)

We use cookies to improve your user experience while on our website and to analyze our website traffic. For more information please see our Cookie Policy. You may update your cookie preferences at any time in your browser. [Learn More](#)

Accept