Cheminformatician, Drug Discovery Platform

Atomwise 🗗

San Francisco Bay Area, CA

$160,000 - $230,000 a year

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Profile insights

Here's how the job qualifications align with your profile 🗗.

💡 **Skills**

| ✓ Software development ⌄ | ✓ Scripting ⌄ | ✓ Python ⌄ | ✓ Machine learning ⌄ | ✓ Linux ⌄ |

| ✓ Jupyter ⌄ | ✓ Git ⌄ | ✓ Data science ⌄ | ✓ Data analysis skills ⌄ | ✓ Analysis skills ⌄ |

| ✓ Algorithms ⌄ | ✓ AI ⌄ | - show less

📖 **Education**

| ✓ Master's degree ⌄ | ✓ Doctoral degree ⌄ |

Job details

Here's how the job details align with your profile 🗗.

💳 **Pay**

| 💚 $160,000 - $230,000 a year ⌄ |

Benefits

Pulled from the full job description

- 401(k) matching
- Commuter assistance
- Dental insurance
- Employee assistance program
- Flexible schedule
- Flexible spending account
- Paid holidays

Show more ⌄

Full job description

Atomwise is a TechBio company leveraging AI/ML to revolutionize small molecule drug discovery. The Atomwise team invented the use of deep learning for structure-based drug design; a core technology of Atomwise's best-in-class AI discovery and optimization engine, which is differentiated by its ability to find and optimize novel chemical matter. The company's belief is that structurally novel chemical matter increases the likelihood of developing first-in-class and best-in-class medicines that have the potential to transform patient care.

Atomwise has extensively tested its discovery and optimization engine, delivering hit ID success in over 230 academic and collaboration projects-to-date that cover a wide breadth of protein classes and numerous "hard-to-drug" targets. Atomwise is building a pipeline of small-molecule drug candidates with first-in-class and best-in-class potential in immunology.

The Role:

We are seeking a talented and passionate cheminformatics scientist to join our growing team. "Cheminformatics" at Atomwise is a broad tent and encompasses a diverse range of computational biology and chemistry research areas to further our drug discovery goals. This role is focused on applying machine learning methods to chemistry and structural biology data at large scale to fulfill our goal of drugging challenging targets. You will be developing models applicable to these problems, designing benchmarks to measure and track model performance, and conducting innovative drug discovery research. You will play a crucial role in developing and maintaining our cheminformatics infrastructure, supporting our machine learning and drug discovery efforts. Your expertise will be essential in managing, analyzing, and interpreting chemical data, enabling our scientists to make informed decisions and accelerate the discovery of novel therapeutics.

Responsibilities:

- Develop, maintain, and curate cheminformatics databases and tools, particularly for ultra-large chemical libraries
- Train and validate machine learning models on chemistry and biology datasets
- Design and refine benchmark datasets and analyses to track model performance on drug discovery problems such as potency and property prediction

- Design effective data visualizations to communicate data analysis and results to audiences with a wide range of scientific backgrounds
- Collaborate with machine learning researchers and software engineers to develop, release, and maintain new tools
- Contribute cheminformatics expertise to project teams, including data analysis, visualization, and interpretation.

Qualifications:

- M.S. or Ph.D. in Biochemistry, Computational Chemistry, Computer Science, Mathematics, Physics, Structural Biology, or a related field.
- 3+ years of industry experience or post-graduate work.
- Biomolecular modeling experience in one or more of the following: molecular docking, structure-based virtual screening, molecular dynamics simulations, homology modeling
- Hands-on experience working with protein structure data and common software in molecular modeling (e.g. RDKit, Biopython, Rosetta, molecular simulation packages, or similar)
- Hands-on experience with common data science software stacks (e.g., Python, Jupyter notebooks, git, etc) and with using software development best practices
- Strong knowledge of cheminformatics principles and techniques such as molecular property prediction, similarity searching, molecular diversity, QSAR analysis, protein-ligand interaction analysis; experience with ADMET data is a plus
- Strong programming skills in Python and/or other scripting languages, and familiarity with the Linux command-line environment.
- Experience working with scalable algorithms using large datasets is a plus.
- Experience with cloud-based computing is a plus.

Compensation & Benefits

- Competitive salary, commensurate with experience
- Stock compensation plan – you'll be an Atomwise co-owner
- Platinum health, dental, and vision benefits for you and your dependents
- 401(k) retirement plan with generous company match (up to 4%)
- Flexible paid time off (PTO), 13 paid holidays, and wellness breaks for employees to spend time with their loved ones and recharge
- Health Savings and Flexible Spending Account options to help save money on healthcare, daycare, and commuting
- Employee Assistance Program (EAP) and Pet Insurance
- Funding for professional development and conference attendance
- Flexible work schedule
- Generous paid parental leave

Atomwise is an equal opportunity employer and strives to foster an inclusive workplace. We are a TechBio company leveraging AI/ML to revolutionize small-molecule drug discovery, and we know that we need a diverse team to develop medicines that serve diverse populations. Accordingly, Atomwise does not make any employment decisions (including but not limited to, hiring, compensation, and

promotions) on the basis of race, religion, color, national origin, gender, gender identity, sexual orientation, age, veteran status, disability status, or any other characteristics protected by applicable federal, state, and local law.

We strongly encourage people of diverse backgrounds and perspectives to apply.

The base salary for this position is $160,000 - $230,000. Pay is determined by multiple factors including, but not limited to, a candidate's geographical location, experience and skills. We're considering all levels of experience for this position.

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