Senior computational chemist - Drug hunter

AQEMIA is a next-gen techbio generating one of the world's fastest-growing drug discovery pipelines. Our mission is to design fast many innovative drug candidates for critical diseases. Our differentiation lies in our unique quantum and statistical mechanics algorithms to power a generative artificial intelligence designing novel drug candidates, without the need to train on experimental data. We already delivered several drug discovery successes in the internal pipeline as well as in collaboration with Pharma companies - most advanced programs being currently in vivo optimization.

About the team you'll join

As a Drug Hunter at Aqemia, you will play a pivotal role in our mission. You will be responsible for selecting and optimizing molecules for synthesis in various Drug Discovery programs, guided by clear, data-driven hypotheses. Your involvement will span the entire project lifecycle, from initial stages to the nomination of pre-clinical candidates.

You will be a key member of a dynamic team, contributing to both internal Drug Discovery initiatives and collaborative projects with external partners. You will work closely with a diverse group of professionals, including machine learning engineers, project managers, medicinal chemists, and physicists, bringing your expertise to the forefront of our innovative efforts.

You will be an essential part of a highly dynamic team, contributing to internal Drug Discovery initiatives and collaborative projects with external partners. Each Drug Discovery program team typically consists of a Program Lead, one Senior Medicinal Chemist, two Drug Hunters (each dedicating 50% of their time), and support from a Biologist as needed. Our team structure is flexible, frequently evolving to adapt to the specific needs and stages of our programs, ensuring that we leverage the right expertise at the right time to drive our innovative efforts forward. You'll work closely with talented colleagues of diverse backgrounds and expertise including but not limited to machine learning engineers, project managers, medicinal chemists and physicists.

Your role as a Senior Drug Hunter at Aqemia

As a Drug Hunter at Aqemia, you will embark on a journey of scientific innovation and discovery. Your role will encompass several critical areas:

- **Molecule Design:** You will design and generate small molecules targeting specific therapeutic areas, focusing on affinity and selectivity of validated drug targets, leveraging Aqemia's platform technology.
- **Optimization:** You will be leveraging Aqemia's platform technology to enhance the efficacy and safety of drug candidates.

- **Communication:** Your ability to clearly present and communicate your findings to stakeholders at all levels will be essential. You will ensure that your conclusions are robust and data-driven, fostering trust and collaboration within the team.
- **Technology Application:** You will apply and validate Aqemia's baseline technologies, which include generative AI algorithms, property prediction models, molecular dynamics, and chemoinformatics tools. Your expertise will ensure that these technologies are used effectively to accelerate drug discovery.
- **Feedback and Improvement:** Your project experience and experimental results will provide valuable insights. You will offer systematic feedback on Aqemia's platform, driving continuous improvement and enhancing our technological capabilities.
- **Innovation and Advocacy:** You will proactively propose and implement new approaches to advance our Drug Discovery programs. Your innovative mindset will help improve Aqemia's technology for greater accuracy, speed, and scalability, keeping us at the forefront of scientific discovery.
- **Interdisciplinary Collaboration:** Your collaboration with machine learning engineers, project managers, medicinal chemists, and physicists will be pivotal in pushing the boundaries of what is possible in drug discovery.

Senior-level responsibilities:

- **Mentorship:** Guide and support junior drug hunters, helping them unlock their potential and grow within the organization.
- **Leadership:** Champion the Aqemia Way by influencing strategic direction, advising stakeholders on feasibility, and identifying solutions.
- **Ownership:** Actively participate in multiple drug discovery programs, demonstrating initiative and proposing optimizations in processes and documentation.
- **Expertise Recognition:** Serve as a subject matter expert, providing strategic insights and being a key resource within the organization.

Expected milestones:

- **First Month:** Familiarize yourself with Aqemia’s processes and pipelines, and provide feedback through a “discovery report.”
- **Within Three Months:** Operate independently on drug discovery programs and present project outcomes to stakeholders.
- **Within Six Months:** Mentor new team members, contribute to technology development, and advance drug discovery programs to the lead optimization phase.

Skills we are looking for

- **Industry Experience:** At least 3 years of experience in pharmaceutical, biotech, or CRO companies, with a focus on computational chemistry for small molecule drug discovery.
- **Technical Expertise:** Proficiency in computational chemistry, utilizing structure-based and ligand-based methods.

- **Educational Background:** Ph.D. and/or postdoctoral experience, with a proven track record of technical excellence as evidenced by peer-reviewed publications.
- **Drug Discovery Contributions:** Proven success in advancing compounds from hit identification to pre-clinical candidates.
- **Diverse Target Experience:** Experience with various targets, including kinases, GPCRs, phosphatases, ion channels, and bromodomains.
- **Data Proficiency:** Skilled in handling experimental data, including biochemical assays and ADME-Tox data.

Technical Skills:

- Proficiency in object-oriented programming in Linux/UNIX environments.
- Mandatory experience in Python programming.
- Familiarity with standard computational chemistry packages (e.g., RDKIT, OpenMM, Ambertools, GROMACs, parmed, Open Babel).
- Extensive knowledge of protein structures and interactions.
- Experience in structure-based drug design and chemoinformatics techniques such as:
    - Protein homology modeling
    - Small molecule docking and pharmacophore hypothesis generation
    - Virtual (*in silico*) screening
    - Structure-activity relationship (SAR) analysis
    - QSAR and ADMEt property modeling
    - Multi-property optimization-based compound design
    - Combinatorial library design
    - Free energy based affinity prediction
    - Molecular dynamics simulations
- Broad understanding of medicinal chemistry principles and computational methods for optimizing drug properties.
- Ability to analyze chemical data and identify trends using statistical methods to ensure reproducibility and data-driven decision-making.

Our recruitment process:

- 1 - Hiring manager interview: you'll meet your future manager (1h, visio call)
- 2 - Technical assessment of your skills: questions on molecular modeling, medicinal chemistry, molecular docking and cheminformatics, with an expert from the team (1h, visio call)
- 3 - Culture-fit interview with our co-founder and COO Emmanuelle (45min, visio call)
- 4 - Final interview with our co-founder and CEO Maximilien (45min, visio call)

About us

We work for a mission: joining us means having your own impact on changing the way drugs are discovered, and helping to shape the direction of our fast-growing company and team.

- **Mission-Driven:** We want to find many drugs and change drug discovery paradigm
- **Fast-growing drug discovery pipe and proofs:**
    - **Internal pipeline** with multiple programs against cancer for now, most advanced ones currently in vivo proof of concept/ patent stage
    - **Collaborations** with several top Pharma companies such as Sanofi, J&J, Servier, incl. 140M$ deal with Sanofi
- **Interdisciplinary world-Class team:** built a team of 60 top tier people at the crossroads of tech and life sciences
- **Experienced Founders:** 15+ years experience including resp. leading research at ENS, Oxford, Cambridge and career in strategy consulting at BCG.
- **DeepTech Innovators:** Part of the French Tech 120 and France 2030, spinoff of Ecole Normale Superieure and CNRS
- **Prime Location:** Paris (1 Bd Pasteur) with 2 days of remote per week.
- **International environment:** Our working language is English. We offer a relocation package for those who wish to join us in France, which includes assistance in finding an apartment, help with all administrative tasks, and optional French lessons.
- **Fundraising:** $60M with European tech/deeptech funds - Elaia Partners (French leader deeptech VC), Eurazeo (largest European investment fund), Bpifrance Large Venture (largest French fund and fund of funds) and Wendel (PE tech fund).

To apply

Send your CV at career@aqemia.com