

COMPUTATIONAL MEDICINAL CHEMIST

AccelBio is looking for one Computational Medicinal Chemist to join AccelBio, in the scope of the project <Pacto de Inovação “HfPT – Health from Portugal”>, with the funding support of «Agendas/Alianças mobilizadoras para a Inovação Empresarial» Component 5 of Resilience and Recuporation Plan (PRR) under the call n.º 02/C05-i01/2022.

Job summary

We are seeking a talented and motivated Computational Medicinal Chemist with a strong background in the biotech/pharma industry. As a key member of the drug discovery group, you will play a crucial role in advancing our pipeline by applying computational techniques to validate new targets and design and optimize new therapeutics.

Responsibilities

- Lead the computational medicinal chemistry efforts by applying in-depth knowledge of structure-activity relationships (SAR) and target biology for assessing the on- and off-target activity, physical properties, pharmacokinetics/pharmacodynamics (PK/PD), toxicity and synthetic feasibility of therapeutic compounds, based on computational and molecular modelling methodologies;
- Work 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 drug discovery;
- Develop and implement cutting-edge algorithms and software for molecular simulation, docking, virtual screening, and AI-driven *de novo* drug design;
- Utilize digital tools and AI technologies to hasten the drug discovery process and forecast pre-clinical testing;
- Be tightly integrated in a multidisciplinary drug discovery team making substantial intellectual contributions to program direction, molecular design, and synthetic priority;
- Collaborate with translational scientists to maximize savvy usage of predictive modeling;
- Maintain an active role in pertinent national, EU, and global networks and initiatives centered around computational chemistry and drug discovery;

- Contribute effectively to grant writing, publications, and presentations in the realm of computational chemistry and medicinal research;
- Stay abreast of the latest advancements in computational medicinal chemistry, especially AI technologies, and integrate these breakthroughs into our research framework.
- Administer and manage Linux-based systems, ensuring robust performance and security for high-performance computing environments.
- Demonstrate proficiency in Linux system administration, including configuration, troubleshooting, and optimization for computational workflows.

Required skills and qualifications

Education

- PhD in Computational Chemistry, Medicinal Chemistry, or a related discipline. Applicant should be fluent in chemistry to influence compound design and productively engage with medicinal chemists and other scientists;

Professional experience

- Proven experience in the biotech/pharma industry, especially in computational drug design, is preferred;
- Demonstrable achievements in leveraging computational methodologies to fuel drug discovery projects;

Linux System Administration

- Hands-on administration of Linux-based systems (Ubuntu/Debian), including user/group management, permissions, SSH hardening, and systemd services;
- Installation, configuration, and troubleshooting of NVIDIA GPU drivers, CUDA, and acceleration libraries for compute workloads;
- Experience with job schedulers (preferably SLURM): queue configuration, resource partitions, accounting, and fairshare policies;
- Configuration management & automation (e.g., Bash/Python scripting) for repeatable environment setup and cluster maintenance;
- Containerization and reproducible environments (Docker and/or Singularity, Conda/mamba, Environment Modules);

- Systems monitoring & logging, patching, firewalling, and basic security hardening in multiuser HPC contexts;
- Working knowledge of storage & filesystems (NFS/SMB), backup/restore, and quota management;
- Familiarity with networking basics (TCP/IP, DNS, load balancing) and troubleshooting distributed compute issues;

Computational Drug Discovery, Chemoinformatics and AI/ML

- Proficiency with common computational chemistry software suites and a keen understanding of AI technologies for *de novo* drug design;
- Proficiency with molecular modeling & simulation (e.g., GROMACS, AMBER, OpenMM), docking/virtual screening (e.g., Glide, AutoDock, GOLD), and freeenergy methods (FEP/TI/MBAR);
- Experience in ligand and structurebased design, pharmacophore modeling, selectivity/ADMET predictions, and SAR interpretation;
- Practical cheminformatics skills (e.g., RDKit, data curation, library design), including handling large compound sets;
- Strong Git and GitHub workflow habits and documentation;

Programming and Software Engineering

- Strong Python (scientific stack: NumPy/Pandas); Bash and awk scripting;

Collaboration and Communication

- Good communication skills and proficiency in English, both in written and spoken;
- Proven ability to operate in multidisciplinary teams.

Preferred skills and qualifications

- Ability to work in a startup environment and with government, academia or industry;
- Team player, capacity to train other scientists;
- Proven leadership and management skills;

Ability to navigate, problem-solve, execute, and lead in a dynamic, fast-paced and evolving environment.

About AccelBio | Collaborative Laboratory to Foster Translation and Drug Discovery

AccelBio is a collaborative laboratory that aims to be the bridge that brings biomedical science closer to the market. With a set of partners that cover all the necessary capacities and expertise to drive drug discovery, AccelBio selects fundamental research discoveries and cutting-edge technology platforms and tools and guides the transformation of breakthrough science into validated and investment-worthy assets. AccelBio complements academic research groups and start-ups with industry-standard drug discovery capabilities - target validation, assay development, high-throughput screening, in silico modelling, medicinal chemistry, in vitro and in vivo testing, IP support and business development. Innovative platforms are also being developed within a well-defined R&I agenda that will further boost drug discovery. By providing these capacities and specialized expertise, AccelBio will de-risk drug discovery assets until they are ready to be out-licensed to industry or established as the foundation of new spin-off companies.

AccelBio consists of the following **associate members**

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|---|---------------------|
| - Instituto Gulbenkian de
Medicina Molecular | - BSIM Therapeutics |
| - Instituto Superior Técnico | - Valvian |
| - Universidade de Coimbra | - TargTex |
| - Biocant Park | - Basinnov |
| - Roche Portugal | - Vertical Sentinel |
| | - Biovance Capital |

Monthly remuneration

Gross monthly remuneration is 3.209,67€.

Start Date and workplace

The contract is expected to start in December 2025 with a duration aligned with project execution; the activities will be developed in a hybrid mode at Gulbenkian Institute of Molecular Medicine in Lisbon and/or other necessary locations to their execution.

Evaluation criteria

The admitted applications will be evaluated based on the quality and relevance of their professional path and their adequacy to the proposed plan, through the analysis of the

Curriculum Vitae (90%) and Interview (10%). Only the candidates with a score above 80% in the CV assessment will proceed to the interview stage.

Members of the jury and Deliberations

The jury is composed by Bruno Victor (PhD, President of the Jury), Bárbara Gomes (PhD) and Silvia Almeida (PhD). The panel shall deliberate by means of roll-call voting based on the adopted and disclosed selection criteria, with no abstentions allowed. Minutes of panel meetings shall be taken. These shall contain a summary of events, as well as details of the votes cast by each of the members and their respective reasoning. After all selection criteria have been applied, the panel shall prepare a ranked list of approved candidates and their respective classification. Results will be publicly available at AccelBio website for a period of ten days following results publication. Candidates will be notified by email once this list has been made available. After notification of the results, candidates have ten days to respond. In the following five days (counting from the end of the candidates' response period), the panel's final decision is issued.

Application process

Submission of the CV, motivation letter and Degree(s) Certificates at AccelBio's website, from October 29th to November 22nd.

Note: The non-compliance with these requirements will result in the rejection of the application.