Computational Quantum Chemist/Biochemist – Technical Leader

Qunova Computing, Inc. (www.qunovacomputing.com) is a quantum application startup with a focus in quantum chemistry and quantum algorithm development. Our goal is to accelerate new drug and material discovery by developing quantum computing software solutions that will deliver accurate electronic structures of large molecular and solid state systems.

Qunova is looking for a computational quantum chemist or biochemist with experience in drug discovery. He/she will be responsible for leading a team that develops and applies computational methods integrating quantum computing, AI and quantum chemistry software, and managing the corresponding workflow to support all aspects of small molecule drug discovery ranging from hit to lead optimization. Suitable candidates will plan and manage structure and fragment-based drug design projects through high-quality computation, including hit to lead optimization, virtual screening, and library design.

This position is open at Qunova's research centers in South Korea, either in Daejeon or Seoul. The Technical Leader will work hand-in-hand with Qunova's multinational research team and collaborate with the world-renowned scientists in the Qunova-KAIST team, as well as drug development companies.

Responsibilities

- Develop and apply quantum molecule modeling, molecular dynamics, conformational analysis, homology modeling and pharmacophore hypothesis generation to ligand-protein complex design.
- Research and develop *ab initio* and machine learning based molecule modeling and screening.
- Develop and maintain a deep knowledge of machine learning and computational approaches for drug discovery.
- Supervise team members, including computer scientists, quantum modeling scientists, and quantum chemists in drug design tool development projects.

Qualifications

- Ph.D. with min 5 years of experience in computational chemistry/biochemistry or a related discipline, or equivalent experience; experience related to computer-aided drug design or material science will be highly considered; knowledge about quantum computing is a plus.
- Advanced knowledge of computational chemistry principles and modeling techniques for pharmaceutical research projects is desirable.
- Fragment based molecule orbital (FMO) modeling as well as variational quantum eigensolver (VQE) experience is a plus.
- Experience in computer scripting and programming, and significant experience in using Linux/UNIX.
- Ability to work in a collaborative environment and a strong publication record.
- Demonstrated supervisory skills including managing teams and leading research projects in industry and/or academia.

Related Skills

- Expertise in computational chemistry concepts and techniques, such as structure-based and ligand-based drug design; protein-ligand docking and scoring; virtual screening; bioinformatics; QSAR and predictive modeling.
- Experience using standard computational chemistry software (e.g. Schrödinger, Gaussian, GAMESS, AMBER, qiskit/VQE).
- Knowledge of data science and machine learning algorithms and tools (e.g. Random Forest, Deep Neural Networks, Generative Adversary Network).
- Programming skills (e.g. Python and C/C++); familiarity with debugging and profiling tools; experience in using scientific, numeric, and chemistry libraries.
- Networking for technical exchanges in academia and pharma industry.

Salary and Benefits

- Competitive salary depending on level of experience (median salary: US$100,000 per annum)
- Company stock options
- Fringe benefits including health insurance and retirement plan contributions
- Annual personal holiday plus national holidays, with flexibility to carry over
- Relocation allowance if applicable

Location: Daejeon or Seoul, South Korea

Contact: recruit@qunovacomputing.com