Computational Quantum Chemist/Biochemist – Technical Manager

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 developing and applying computational methods integrating quantum computing, AI and quantum chemistry software to support all aspects of small molecule drug discovery ranging from hit to lead optimization. Suitable candidates will participate in structure and fragment-based drug design projects through high-quality computation, including hit to lead optimization, virtual screening, and library design.

Qunova's research centers are located in Daejeon and Seoul, South Korea. Qualified candidates will be allowed to work remotely but must be flexible about working with colleagues and clients in different time zones worldwide. The Technical Manager 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 ligand-based learning and computational approaches in drug discovery.
- Interact with drug discovery and material science customers.

Qualifications

- Ph.D. in computational chemistry/biochemistry or a related discipline, or a M.S. with min 4 years of experience; experience related to computer-aided drug design will be highly considered.
- Advanced knowledge of computational chemistry principles and modeling techniques for pharmaceutical research projects is desirable.
- Experience in computer scripting and programming and significant experience on high performance computing on Linux/UNIX.
- Ability to work in a collaborative environment as exemplified by a strong publication record with collaborators.

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 with using scientific, numeric, and chemistry libraries.
- Drug design, medicinal chemistry, or/and biochemistry.

Salary and Benefits

- Competitive salary depending on level of experience (median salary: US$90,000 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; global remote for qualified candidates

Contact: recruit@qunovacomputing.com