

# Computational Chemist or/and Chemoinformatician

Company: NovaMechanics, a leading Cheminformatics & Nanoinformatics company.

Location: Nicosia, Cyprus.

**Overview:** We are seeking a highly motivated scientist specializing in computational chemistry, cheminformatics, statistics, computational biology, or a related discipline to join our drug discovery team. The ideal candidate should be a holder of a Ph.D. with rich experience in developing and applying cheminformatics tools in drug discovery as well as a strong passion for collaborative work across multiple disciplines.

Expected Start Date: January 2024.

### **Roles and Responsibilities:**

- Actively participate and contribute to projects throughout all stages of drug discovery.
- Employ structure-based and ligand-based molecular design techniques for small molecule optimization and structure-based drug discovery.
- Apply computational chemistry methodologies, including homology modelling, molecular docking, molecular dynamics simulations, and more.
- Stay updated and integrate current open-source software and computational tools to enhance drug design.
- Engage in team discussions, present findings, and draft project proposals and reports.

#### **Skills/Qualifications:**

- Ability to work effectively in an interdisciplinary environment.
- Proven skills in hit analyses and clustering, hit expansion methods, scaffold hopping, lead generation, and lead optimization.
- Excellent written and oral communication capabilities, especially in scientific articles, project proposals, grant applications, project reports, and presentations. A strong publication record is a plus.
- Proven competence in computer-aided medicinal chemistry techniques, cheminformatics, and data analysis
- Excellent knowledge of at least one molecular simulation package such GROMACS, AMBER, OPENMM, etc.,
- Familiarity with UNIX/Linux operating systems, scripting and programming languages.
- Proficiency in high-performance computing for large-scale calculations.
- Experience with web-based applications, databases, and automated workflow tools, especially KNIME. Knowledge of Enalos+ KNIME nodes is a strong plus.
- Soft skills: Teamwork, adaptability, problem-solving, and a proactive mindset.

## **Benefits:**

- Comprehensive training and career development opportunities.
- Highly competitive salary package.

## How to Apply: