Associated Director, Computational Chemistry

Humanwell Pharmaceuticals US, St Louis, MO

Interested candidate, please submit resumes to email: hr@humanwellus.com

Summary

Humanwell Pharmaceutical US, Inc. is a St Louis, MO-based pharmaceutical research and development company which focuses on research and development of novel therapeutics to address unmet medical needs. At Humanwell, we work towards improving patients' quality of life and are committed to creating a happier and healthier world.

We are seeking an experienced computational chemist at Associate Director level with advanced knowledge of computational chemistry/artificial intelligence-assisted drug discovery concepts, principles, and practices to lead our computational group. The candidate will design, build, and manage computational chemistry/artificial intelligence-assisted drug design infrastructure to meet the needs of drug discovery and development in Humanwell Pharmaceutical US.

The Drug Innovation Center of Humanwell Pharmaceutical US consists of medicinal chemists, biologists, computational chemists, formulation scientists and analytical chemists who employ state of the art technologies to drive drug discovery and development. The successful candidate will be the one who is able to effectively communicate the results of modeling studies to non-experts and to work effectively in a multidisciplinary team environment.

Primary Duties and Responsibilities

Proactively providing computational chemistry/AI-assisted drug discovery guidance to drug discovery team to solve problems and drive progress, including but not limited to:

1. Build a computational chemistry/artificial intelligence-assisted drug innovation team.
2. Identify, implement, and promote cut-edge computational chemistry and artificial intelligence (AI) technologies which can speed up lead identification and optimization in drug discovery.
3. Carry out protein construct via Homology Modeling or Machine Learning.

4. Guide the drug discovery teams by providing Structure Based Drug Design (SBDD), Ligand Based Drug Design or QSAR predictions.
5. Build and maintain computational chemistry/AI drug discovery infrastructures including chemo-informatics and data management to support drug discovery and development.
6. Effectively communicates new project proposals, computational chemistry/AI-assisted drug discovery strategies, innovative ideas and results at the meetings with colleagues or management

Required Qualifications and Skills:

1. Ph.D. in computational chemistry, biophysics, chemical engineering, or related disciplines.
2. 10+ years of post-graduate experience in the pharmaceutical industry or academia.
3. A strong track record of delivering significant contribution to drug discovery project entering preclinical studies by using computational chemistry/AI drug discovery tools.
4. Skilled in applying computational chemistry methods and tools for structure-based drug design, in silico screening, QSAR, molecular dynamics, and pharmacophore development.
5. Strong oral and written communication skills.
6. Strong track record of recent publications and/or presentations.
7. Managing and supervisory experience.
8. Qualified candidate must be authorized to work in the USA

PREFERRED QUALIFICATIONS

1. Experience with Linux.
2. Experience with artificial intelligence.
3. Proficiency with modeling software packages (e.g. Schrodinger, MOE, Rosetta, LAMMPS, GROMACS, CHARMM).
4. Proficiency in general molecular modeling techniques (docking, molecular dynamics simulation, homology modeling, quantum mechanics, Free energy perturbation, ligand- and structure-based design).
5. Experience with QSAR, machine learning, deep learning is a plus
6. Experience with scripting and programming languages (e.g. Python, shell, Perl, C^{++}) that are used in scientific application and data analytics (e.g. Spotfire, SQL) is a big plus
7. Demonstrated leadership in an industrial drug discovery environment is a plus.

Job Type: Full-time

Job Location: Ballwin, MO

At Humanwell, all of our employees are part of a team that cares about them. We all share the purpose of making the world a healthier place. We hope that you seek to join us on our journey as we develop medicine and improve global human well-being.