



Humanwell Pharmaceutical US, Inc.  
421 Sovereign Court, Ballwin, MO 63011  
Phone (636)-220-3636  
[www.humanwellus.com](http://www.humanwellus.com)

## Senior Scientist, Computational Chemistry

Humanwell Pharmaceuticals US, St Louis, MO

Interested candidate, please submit resumes to email: [hr@humanwellus.com](mailto: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 a computational chemist at the Scientist/Senior Scientist level with advanced knowledge of computational chemistry principles, concepts, and practices to join our research group. The candidate will guide medicinal chemistry projects in a pharmaceutical industry with the ability to work effectively both independently and as part of a New Drug Discovery Team.

New Drug Discovery team of Humanwell Pharmaceutical US consists of medicinal chemists, biologists, and computational chemist, who employ state of the art capabilities to drive a drug design. The successful candidate will be the one who is able to effectively communicate the results of modeling studies to non-experts and to work in a multidisciplinary team environment.

### Primary Duties and Responsibilities

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

1. Assist the medicinal chemistry teams with compound design based on both physics-based and knowledge-based computational chemistry methods.
2. Protein construct via Homology Modeling or Machine Learning.
3. Guide the drug discovery teams by providing Structure Based Drug Design (SBDD) or QSAR predictions to prioritize the compounds.
4. Promote and evaluate new computational techniques and up to date informatics for drug discovery.



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5. Provide informative data with appropriate visualizations.

### **Basic Qualifications:**

1. Ph.D. in computational chemistry, biophysics, computational chemical engineering, or related discipline
2. 3+ years of post-graduate experience in the pharmaceutical industry or academia applying various methods of computer modeling to biological system
3. Skilled in applying state-of-the-art methods and tools for structure-based drug design, in silico screening, QSAR, and pharmacophore development
4. Strong oral and written communication skills
5. Strong track record of recent publications and/or presentations
6. Qualified candidate must be eligible to work in USA.

### **Preferred Qualifications:**

1. Experience with Linux
2. Proficiency with modeling software packages (e.g. Schrodinger, MOE, Rosetta, LAMMPS, GROMACS, CHARMM)
3. Proficiency in general molecular modeling techniques (docking, molecular dynamics simulation, homology modeling, quantum mechanics, Free energy perturbation, ligand- and structure-based design)
4. Experience with QSAR, machine learning, deep learning is a plus
5. 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

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.*