Pacific Northwest National Laboratory (PNNL) is a world-class research institution powered by a highly educated, diverse workforce committed to the values of Integrity, Creativity, Collaboration, Impact, and Courage. Every year, scores of dynamic, driven people come to PNNL to work with renowned researchers on meaningful science, innovations and outcomes for the U.S. Department of Energy and other sponsors; here is your chance to be one of them!

At PNNL, you will find an exciting research environment and excellent benefits including health insurance, flexible work schedules and telework options. PNNL is located in eastern Washington State—the dry side of Washington known for its stellar outdoor recreation and affordable cost of living. The Lab’s campus is only a 45-minute flight (or ~3 hour drive) from Seattle or Portland, and is serviced by the convenient PSC airport, connected to 8 major hubs.

The Computational Biology Group at the Pacific Northwest National Laboratory (PNNL) is seeking a Senior Data Scientist for Computational Biophysics to join our team as well as lead in the development of new research proposals with strong expertise in computational chemistry, biophysics and predictive biology, protein/metabolite function prediction, Artificial Intelligence (AI)/Machine Learning (ML), and software development.

The Senior Data Scientist for Computational Biophysics will contribute to diverse fundamental science research programs studying DOE relevant systems for biofuels/bioproducts organism/microbial and human health problems such as cancer and infectious diseases. The candidate will be responsible for computational and data science tool development for fully autonomous design/build, work directly in interdisciplinary teams including chemists, bioinformaticians, computer scientists, data scientists and software developers. The position involves working with high-performance computing platforms, statistical analysis, and data integration methods that will be used to develop AI and robotic systems for high throughput molecule/protein design. The incumbent will define and carry out the application of existing methodologies, as well as perform original research in the field of computational chemistry, biophysics and cheminformatics as needed to predict phenotypic function from complex biological data. In addition to technical research, this position expects participation in publishing, project leadership, and business development.

The candidate will help in developing new capabilities for the study of protein and compound chemistry in conjunction with the computational infrastructure for cell/pathway/gene-level mechanistic studies by using advanced data science tools for rapid prioritization of chemical structures with pre-defined functional properties. The ideal candidate should have a strong applied mathematics, AI/ML, and object-oriented coding skills with domain knowledge in computational chemistry, structural proteomics, and structural biology. The successful candidate must be able to collaborate, identify scientific problems and opportunities, and leverage concepts and tools including recent advances in deep learning, to develop data driven computational solutions. The candidate should also have an interest in applying new approaches and knowledge to science problems associated with human health, bioenergy, biofuels design, and carbon cycling. The candidate should have effective communication skills with a demonstrated capability to perform multi-disciplinary, collaborative research.
Minimum Qualifications:

- BS/BA with 5 years of experience
- MS/MA with 3 years of experience
- PhD with 1 year of experience

Preferred Qualifications:

- Ph.D. in computational chemistry/biology, computer science, structural biology, medicinal chemistry, bioinformatics or a closely related field with some post-doctoral experience in the areas outlined above.
- Develop software stack for automating a computational pipeline. Experience with Unix/Linux, HPC environments, and experience with a scripting and programming language (e.g. Python, R, C/C++ etc).
- Expertise in the design, execution of algorithmic solutions for curation, analysis, mining, and modeling of chemical and biological data.
- Experience with deep learning framework such as TensorFlow, Keras, or PyTorch, including parallelism, Boltzmann Machines, Auto Encoders and Transfer Learning.
- Solid foundation in computational chemistry/biology, physics-based modeling (Quantum/Molecular Mechanics and Molecular Dynamics) and computer science with AI/ML expertise for data integration to predict patterns/features that are useful for new experiment design.
- Strong organizational skills with the ability collaborate with internal/external researchers.

For more information and/or to apply, please visit: https://careers.pnnl.gov/jobs/4073?lang=en-us

Questions? Please contact Kim Willer at kimberly.willer@pnnl.gov