INDIANA BIOSCIENCES RESEARCH INSTITUTE

Computational Chemistry Staff position in Integrated Data Sciences Innovation

We are the Indiana Biosciences Research Institute (IBRI). We are a leading translational research institute that advances academic and industry science through collaboration to improve patient health outcomes. Building your career at the IBRI in Indianapolis' 16 Tech Innovation District, means being part of a team of renowned scientists, creative thinkers and innovative leaders.

Today's research is being driven by significant advances in our abilities to study complex disease processes and propose new ways to improve patients' lives. To reflect the evolving nature of life sciences research and encourage synergies through collaboration, we're enhancing our integrated capabilities, adding depth to how we approach patient-informed translational science and pursuing four foundational areas of scientific focus. These four areas will provide us the core talent and capability to pursue translational science in this new patient-centric framework:

- **Disease, Systems, Pathways –** We're working to better understand diabetes and identify new ways to combat the disease. We're applying this learning to other diseases that share common systems and pathways.
- **Molecular Innovation** – We're developing new capabilities for molecular design and drug discovery to investigate disease processes and pursue new therapeutic approaches.
- **Integrated Data Sciences** – We're pursuing advanced data sciences to create novel end-user inspired solutions that address complex analysis, simulation and prediction across the translational sciences.
- **Enabling Technologies** – We're building a rich platform of enabling technologies that give our scientists, partners and collaborators access to the best tools to solve complex scientific problems.

The IBRI's vision is to build a world-class organization of researchers, innovators and business professionals that catalyze activities across the Indiana (and beyond) life sciences community. To achieve that vision, we look for curious and collaborative team members who are energized by innovation, guided by integrity and inspired by diversity.

The Opportunity:

The Molecular Innovation and Integrated Data Sciences Innovation areas have a staff position available for a talented individual with training and experience in computational chemistry and specifically molecular modeling techniques, including docking and simulation supporting data analysis and design of molecules supporting drug discovery. This position will be an integral part of the team as it empowers science and the IBRI strategy through data access, cheminformatics analysis, molecular modeling, molecular docking/simulation and applying an in-silico driven approach to assist target enablement and drug discovery teams.

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The individual in this role will have familiarity with both commercial and open-source tools supporting molecular modeling, docking and simulation. The ideal candidate for this role is one who can collaborate directly with medicinal chemists to understand their scientific goals and work to access the appropriate internal and external data, perform the necessary analyses, and interpret these analyses to the team to drive selection and design of new compounds for the therapeutic target.

Success in this role will be measured by the ability to drive scientific excellence in a team setting through participation in applied research projects leading to publications, grants, patents, tools and innovation. This position will directly assist the IBRI's applied research mission to deliver innovation in target enablement, hit identification and lead development.

This position is ideal for you if you want to work in an innovative institute in the middle of a technology district with opportunities to interact with other life sciences organizations in the region.

Responsibilities:

- Provide computational chemistry and molecular modeling support to multi-disciplinary research teams comprised of biologists, chemists and/or clinicians.
- Leverage the appropriate open-source, or commercially licensed tools to access data, perform virtual screens, understand the fit of a ligand to a protein through docking or free energy perturbation methods, and compute properties for target compounds to acquire/synthesize, driven by the team's requirements. Developing novel hypotheses for ligand-protein interactions will be appreciated!
- Continue to grow your knowledge of the state-of-the-art techniques in computational chemistry and molecular modeling and apply this to the IBRI's strategy and projects/targets.
- Effectively communicate to collaborating researchers in other centers so that they understand their data, analysis workflow and the results of the analysis.
- Participate in the IBRI's collaborative efforts with colleagues at research universities and in the life sciences industry.

Qualifications:

- PhD in cheminformatics, computational chemistry, computer science or related scientific discipline with at least two (2) years of research experience in drug discovery or chemistry-related synthesis/design efforts.
- Proficiency accessing, mining and applying statistical analyses of public structural data sets such as Pubchem, ChEMBL, PDB, DrugBank and Patent Literature.
- Knowledge and proficiency in computational chemistry, cheminformatics and molecular modeling tools – either custom, open-source or commercial.
- Understanding of machine learning techniques and generation of chemistry or structural features to use in model building.
- Demonstrated ability working in a multi-disciplinary team to drive the identification of new molecular entities to drive target enablement and new screening efforts in drug discovery.

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- Proven skills in communication of complex analytic approaches, results and visualizations to peers and scientists in other disciplines.
- Experience in scripting/programming in languages such as Python, Perl, C/C++, R, BASH.
- Knowledge of general biology, molecular modeling and chemistry techniques.
- Ability and desire to rapidly learn new science and develop/use computational techniques to drive applied research leading to innovation.

Additional preferred qualifications:

- Knowledge of medicinal chemistry and/or drug discovery process.
- Exemplified application of chemical analyses to identify new molecular entities as applied to problems in diabetes, oncology or related diseases.
- Demonstrated technical skills across multiple operating systems including PC/Windows, MacOS and variants of Linux in a cluster-computing and/or cloud-based environment.
- Experience working in a team setting using open-source tools, source version control repositories and test-driven development.
- Experience with modeling and cheminformatics software packages (e.g., Schrödinger Maestro, MOE, ChemAxon, StarDrop).
- Experience working with APIs (WebServices, REST, XML, JSON).
- Experience with cheminformatics workflow or open-source tools (e.g., Pipeline Pilot, KNIME, RDKit).
- Experience with cloud computing environments (e.g., AWS, Azure or GCP).
- Desire to work in a fast-paced, growing, entrepreneurial-style organization in the heart of an innovation district.

Compensation:
Competitive salary and comprehensive benefits offered, commensurate with experience.

Equal Employment Opportunity:
The IBRI provides equal employment opportunities to all employees and applicants and does not discriminate on the basis of age, race, color, religion, gender, sexual orientation, gender identity, gender expression, national origin, protected veteran status, disability or any other legally protected status.

Apply:
Please visit us at https://www.indianabiosciences.org/careers/ to learn more and/or apply for this opportunity. Interested individuals are encouraged to provide their CV/resume and a brief cover letter with their application.