Job Title: Postdoctoral Fellow, Computational Chemistry
Location: United States - Massachusetts – Cambridge

Role Description

The position requires a PhD in computational chemistry or related sciences. Expertise in state of the art molecular dynamics methods will play a key role in this position. Advanced knowledge of computational principles and knowledge of how to apply these techniques to protein-protein interaction is desired. This position will have a key role in expanding the current understanding of the complex dynamic phenomena intrinsic to many potential drug mechanisms, and to make traditionally difficult targets an increasingly fruitful drug discovery area.The candidate should have experienced in computer scripting and programming and significant experience using Linux/UNIX. Experience with commercial softwares especially Schrodinger package is a must. Knowledge of mathematics or statistics is highly desirable. Additionally a demonstrated ability to work in a collaborative environment and work independently, excellent communication skills and being an effective team member, are essential.

Responsibilities

- Understand structural basis for protein-protein interactions
- Molecular dynamics simulations of large protein complexes
- Pocket mining and binding site analysis
- Apply machine learning to develop statistical models
- Develop computational methods to assist druggability assessement
- Pharmacophore modeling

Qualifications

Doctoral level degree in computational chemistry, applied physics and mathematics, or equivalent. Additional research experience in molecular dynamics, scientific programming and/or statistical analysis is a plus.

- Demonstrated computational and scientific expertise
- Broad experience in utilizing molecular dynamics and related techniques to probe protein structure and function, allosteric modulation, and mechanisms of protein function.
- Strong technical skills and knowledge in molecular dynamics techniques and state of the art simulation packages
- Facility with programming languages such as Perl, C++, Python, Java.
- Knowledge of Pipeline Pilot, Spotfire, machine learning tools, MatLab, R, and quantitative methods including statistics and applied mathematics
- Experience with Linux/Windows operating systems
- Familiarity with structure based design

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