***Postdoc** project in computational structural biology:*

Exploiting Water Network Perturbations in Protein Binding Sites

We are recruiting a postdoc for a computational structural biology project that investigates the role of water network at protein ligand interfaces with a view towards ligand discovery. The position is available immediately and NIH funded for 5 years.

We are looking for highly motivated candidates with curiosity and skills to reveal hidden factors that contribute to protein-ligand binding and leverage this information for ligand discovery. As this project integrates experimental and computational data it will require both a solid background in structural biology and significant computational skills for custom data analysis and automation. The project is embedded into a dynamic lab that has strong expertise in modulating protein conformational ensembles with ligands and temperature (see references below).

The project is housed in the Department of Chemical Biology and Therapeutics, and Structural Biology at St. Jude Children's Research Hospital. It builds on strong investments into a world-class infrastructure in structural and chemical biology. This is an exciting time to join us and build a career while living in an affordable city. This postdoc position is NIH funded for 5 years.

Essential requirements:

- PhD in structural biology or related field
- High proficiency in coding incl Python
- Interest in dynamic aspects of structural biology including protein flexibility and hydration

Optional requirements:

- Hands-on molecular biology and crystallography experience

Please direct your questions and application package including a cover letter, current CV, and 3 letters of reference to: Dr. Marcus Fischer (marcus.fischer@stjude.org).

Relevant papers include:
• Bradford et al. (2021). Temperature artifacts in protein structures bias ligand-binding predictions. *Chemical Science*. DOI: 10.1039/D1SC02751D
• Fischer (2021). Macromolecular room temperature crystallography. *Q Rev Biophys* 54. E1
• Darby et al. (2019). Water Networks Can Determine the Affinity of Ligand Binding to Proteins. *JACS* 141, 15818-26.
• Balius et al. (2017). Testing inhomogeneous solvation theory in structure-based ligand discovery. *PNAS* E6839-46.
• Fischer et al. (2015). One crystal, two temperatures: cryocooling penalties alter ligand binding to transient protein sites. *Chembiochem* 1560-64.
• Fischer et al. (2014). Incorporation of protein flexibility & conformational energy penalties in docking screens to improve ligand discovery. *Nature Chemistry* 6, 575-83.

More info at:
https://www.stjude.org/fischer