

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.
- Balias 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>