

# **Advancing Informatics and Computation for Drug Discovery**

**Michael K. Gilson**

*University of California, San Diego*

I will present recent advances in the capabilities and data collection of BindingDB, the first publicly accessible medicinal chemistry database; and an early-stage project, the Drug Design Data Resource, which is working with industry to move protein-ligand interaction datasets into the public domain for use in testing and improving computational drug design methods. I will also present recent work connecting detailed molecular simulations with experimental calorimetric studies of binding, in order to gain mechanistic insight and improve computational accuracy.