# BUDGET JUSTIFICATION – CHODERA LABORATORY

**Senior/Key Personnel**

**John D. Chodera, Ph.D., Co-Investigator (1.0 calendar months effort)** will direct the protein-ligand model systems work for this project, support the execution of SAMPL blind challenge exercises, and co-supervise graduate student work in industry laboratories for the collection of data for blind challenges. He is an Assistant Member (Assistant Professor equivalent rank) at the Sloan Kettering Institute---the basic science arm of the Memorial Sloan Kettering Cancer Center---with extensive experience in biomolecular simulation, molecular simulation algorithm development, alchemical free energy calculations for ligand binding, and the use and interpretation of automated biophysical experiments. He has a publication track record spanning over 15 years of highly regarded work in these fields. He has a decade of experience with the Folding@home worldwide distributed computing project, wrote the GPU-accelerated alchemical free energy calculation code that will be used to compute small molecule binding affinities, has contributed to the development of the GPU-accelerated OpenMM simulation code that will be used for constant-pH simulations, and designed the automated biophysical wetlab in his laboratory at MSKCC that will be used for experimentally measuring binding affinities and other physical properties. He also has extensive experience with computing biophysical observables---including NMR data---from biomolecular simulations.

**Other Personnel**

**Mehtap Isik, Graduate Student in the Tri-Institutional PhD Program in Chemical Biology (12.0 calendar months effort)** BSc degrees in Chemistry and Molecular Biology & Genetics, ranked top of her graduating class from Bogazici University in Instanbul, Turkey. Ms. Isik will both develop the informatics platform for the identification of useful model systems for experimental development and will perform the experiments to collect new data in the Chodera laboratory at MSKCC. Ms. Isik is a third-year graduate student in the Chodera laboratory with extensive experience in biophysical experiments, computational biophysics, and structural and chemical bioinformatics.

**OTHER DIRECT COSTS**

**Travel:** We ask for $3,000/year in travel support to allow the PI and PhD student to attend the SAMPL blind challenge meetings and other conferences to present the results of this project.

**Publication fees:** We request $2,500/year to defer publication fees.

**Materials and Supplies:** We request $30,000/year for experimental laboratory supplies and instrument usage fees to cover the costs of cloning new protein constructs, engineering protein mutants, expressing proteins, performing binding assays, and other physical property measurements to develop data for blind challenges and subsequent public dataset release.