Dear Dr. Mobley and Dr. Chodera,

We are at GlaxoSmithKline, a large pharmaceutical company with interests in a wide range of disease areas. Eric Manas leads in our computational chemistry group, and person B specializes in measuring ABC.

We are enthusiastic about the prospects of physical modeling to help guide pharmaceutical drug discovery, and have been very interested in the progress of SAMPL challenges over the years. Thus, we are delighted to help support your proposed, “Advancing predictive physical modeling through focused development of model systems to drive new modeling innovations.” While free energy calculations recently have shown some real promise for guiding pharmaceutical design, challenges like this are vital to help them continue to make progress.

Because of our enthusiasm about SAMPL and blind prediction challenges, we want to confirm our willingness to host a student to help collect experimental data for SAMPL physical property challenges. We can provide access to equipment necessary for measuring physical properties that is not typically available to academic laboratories, such as the Sirius T3 (for measurement of pKa, logD, and logS), high-throughput automated shake-flask measurements of logD and logP, and automated membrane permeability assays for compounds available from commercial vendors. We have multiple mechanisms available through which these measurements can be performed. In addition to sending students from your laboratories to visit our group to perform measurements, we also have an internship program that provides a stipend for focused measurement projects like these.

We have seen the model of hosting an academic student to conduct SAMPL physical property measurements work previously at Genentech for measurement of water-cyclohexane log D values for the SAMPL5 challenge. Thus, we believe we will be able to use a similar approach here as well to collect the data needed for new SAMPL challenges..

Sincerely,