Dear Dr. Mobley and Dr. Chodera,

We write to confirm our support of your proposal, “Advancing predictive physical modeling through focused development of model systems to drive new modeling innovations,” and to express our enthusiasm for collaborating on the blind challenges you propose, including on meetings and on challenge logistics, as we detail below.

As PIs of the NIH-funded Drug Design Data Resource (D3R), we work with the pharmaceutical industry to obtain protein-ligand binding data from inside pharma and use it to feed a series of blind prediction challenges (D3R Grand Challenges) for the community. These focus on predicting properties which are important to drug discovery, such as protein-ligand bound structures, binding affinities, or which molecules from a set of possible ligands will in fact bind to the target. In addition to these blind challenges, D3R hosts regular workshops on the results of the challenges.

D3R focuses on existing protein-ligand datasets, and its mandate does not cover generating new data such as on physical properties or even on simpler protein-ligand systems such as those focused on in your proposal. However, given the complexity of typical pharmaceutical datasets, so far we have seen relatively limited success of computational methods on D3R Grand Challenges. This means that your effort – focused on obtaining new datasets of somewhat less complexity – is particularly critical for helping to advance computational techniques to where they can have more success at pharmaceutical problems and at the D3R Grand Challenges.

As you are well aware, in 2015-2016, D3R helped organized the SAMPL5 challenge by coordinating submission of blind predictions and by providing funding/support for the D3R workshop to also cover SAMPL5; the first day of the workshop covered components of both D3R and SAMPL, and the second day had two break-out sessions, one focused on D3R and one on SAMPL. This meeting was a tremendous success, and we believe that the SAMPL challenge played an important role in what was learned from the workshop. Unfortunately, D3R cannot provide financial support to generate new data for SAMPL – but we are enthusiastic to continue co-hosting workshops.

Thus, this letter is to confirm our plan to continue the link between SAMPL (as covered by your proposal) and D3R by:

1. Co-hosting yearly workshops, where D3R would continue to cover the workshop cost
2. Continuing to handle submissions for the proposed blind challenges
3. Helping with advertising of the challenges by coordinating our mailing lists

and in general continuing to work together to have the SAMPL and D3R efforts dovetail to improve modeling work in this general space.

Sincerely,