Pfizer Worldwide Research and Development
Internal Medicine Medicinal Chemistry
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**Worldwide Research & Development**

May 25, 2017

David Mobley
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Dear Dr. Mobley and Dr. Chodera,

We are very excited to be involved in your proposal, "Advancing predictive physical modeling through focused development of model systems to drive new modeling innovations." As you may be aware, we believe physical modeling is poised to have a real impact on the pharmaceutical drug discovery process, but we also believe there are key challenges remaining to be resolved before it can have the impact it might.

This letter is to confirm that we would like to be involved with facilitating the collection of experimental data to facilitate new SAMPL physical property prediction challenges to drive the improvement of these methods. We expect our involvement will at least involve providing access to equipment you need to measure physical properties, such as our multiplexed capillary electrophoresis measurement of pKa (Shalaeva, J Pharm Sci. 2008;97(7):2581), our RP-HPLC method for measuring partition coefficients (J Med Chem. 2000 Jul 27;43(15):2922-8.), or our method for measuring membrane permeabilities (J Pharm Sci. 2011 Nov;100(11):4974-85) for SAMPL challenges along with help on how to perform these measurements effectively. It is also possible we will be able to facilitate an internship to provide someone who could actually perform the measurements. Otherwise, you would need to provide personnel who would come here and work with us to perform the measurements.

We have seen this model work previously at Genentech for measurement of water-cyclohexane log D values for the SAMPL5 challenge, and we believe a similar model will work well here as well, so we are confident we will be able to support your proposal and future SAMPL challenges in this way.

Very truly yours,

Dr. Xinjun Hou
Director, Internal Medicine Computational Chemistry