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Dear SAMPL Organizers,

In response to the recent request for testimonials regarding the SAMPL effort and how it has spurred technological development and my own research efforts, I feel obligated to provide a short account of my own experiences.

My knowledge of and interactions with the SAMPL effort and community actually predate the publication of the SAMPL0 effort. This first effort took the form of a challenge between a small set of researchers in exploring the accuracy of explicit and implicit approaches to hydration free energy predictions. David Mobley, who I overlapped with as a postdoc at UCSF in the Dill research group, asked me to provide feedback on the original J. Med. Chem. manuscript submission. I was developing a hybrid solvent model in the lab at that time, so ***I could see immediately how a larger community prediction effort could benefit the field and how my research efforts could fit into potential future prediction challenges***. As I recall, there was some concern about having a paper on computational predictions properly appeal to the Journal of Medicinal Chemistry. David may not know that I also asked my spouse, who was trained as a Medicinal Organic Chemist, to provide feedback on this formative work and suggest tweaks to broaden the message. I mention this because ***while SAMPL may have started with a small group effort, it has grown and developed from the input and interests of a broad community of scientists***.

The following SAMPL1 effort brought in more involvement beyond the first groups, and while I didn't participate in that round, I did dabble in participating in the broader community SAMPL2 effort. While we weren't published participants, we did testing of our developmental solvent model during the event (which I think was called SAMPL09 at the time) and we gained some insight into our own research obstacles. The ***blind prediction aspect of SAMPL provides extremely valuable perspective***, and ***it forces you to honestly evaluate and reevaluate theoretical assumptions***. When we fully participated in the SAMPL3 event, we had a unique approach that likely provided some value and variety to the field. I have participated in each subsequent SAMPL, trying something new and unique each time in an attempt to maximize the personal research benefit of blind predictions.

The most recent SAMPL5 event was quite interesting in that it refocused the hydration prediction effort to transfer between solvents. This is certainly a more challenging task, but it is one that already aligned with my research interests. If we are to see computational molecular modeling achieve its full promise in biomolecular and medicinal applications, we need the unbiased assessment of blind community efforts. These help us to evaluate what truly works and avoid paths that don't lead in productive directions. The proposed SAMPL future plans look to plot ever more interesting paths, and if implemented, look to present a powerful platform for bridging theoretical developments and practical applications in human health.

Sincerely,

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