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Dear Colleagues,

SAMPL has generally provided data sets that focus on solvation properties and small molecule receptors. For the former, predicting solvation properties of molecules is critical to the accurate prediction of protein-ligand binding, protein-protein interactions, etc. and SAMPL as been the main source of new data to challenge the community to develop better methods in this area. Given that the errors in solvation continue to remain large (thereby affecting the quality of binding affinity predictions) I think it is essential that SAMPL continues to challenge the community to develop newer and more accurate methods. For the latter, small molecule receptors afford a reduced dimensionality problem over dealing with protein systems. Because of this more rigorous methods can be applied like high-level QM methods and methods involving extensive sampling further spurring the development of novel approaches. Overall, SAMPL is an integral part of challenging the community to develop new methodologies in areas of key import. SAMPL affords an alternative set of data over, for example, D3R where protein receptors remain the main challenge. While D3R is important in and of itself, because the systems are larger and more complex many advanced approaches cannot be tested effectively.

In particular, the last SAMPL competition illustrated several issues with our generic set up for movable type (MT) calculations. First, atom typing using standard software packages mis-typed several atoms affecting the outcome of our calculations so this drove us to create a MT specific atom typing protocol. Secondly, we observed some unusual trends in our solvation free energy calculations from the SAMPL competition that stimulated us to refine our solvation model; in particular, the way in which we handle solvent exposed surfaces. From the SAMPL data sets these as well as other

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issues were exposed in our calculations and without SAMPL might of gone long undetected.

Sincerely Yours,

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