Dr. Antonia Mey

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Edinburgh, August 5th 2020

Dear Prof. Shirts,

Please find attached the manuscript “Best Practices for Alchemical Free Energy Calculations’’ by *Antonia S.J.S. Mey, Bryce K. Allen, Hannah E. BruceMacdonald, John D. Chodera, Maximilian Kuhn, Julien Michel, David L. Mobley, Levi N. Naden, Samarjeet Prasad, Andrea Rizzi, Jenke Scheen, Michael R. Shirts, Gary Tresadern, and Huafeng Xu* that I wish to be considered for publication in the Best Practices section of the Living Journal of Molecular Sciences.

The manuscript gives a broad overview to both new and seasoned practitioners to the field of alchemical free energy calculations. It presents the current best practices to be used for setting up, running, and analyzing alchemical free energy calculations. Furthermore, it provides an overview of the broad range of applicability of alchemical free energy calculations and highlights what can be expected in terms of predictive accuracy as well as highlighting areas in which no best practices are available yet with open research questions remaining. It also discusses the use of alchemical calculations in the pharmaceutical drug discovery process and should be useful to scientists both in industry and academia. Various software programs are highlighted for the use of alchemical calculations as well as a handy checklist for anyone from novice practitioner, to journal article reviewer.

I am looking forward to hearing from you soon with some feedback on the manuscript.

Best wishes,



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