Histogram-free reweighting with grand canonical Monte Carlo: Post-simulation optimization of non-bonded potentials for phase equilibria

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Dear Editor,

We would greatly appreciate you considering the following paper for publication in *Journal of Chemical and Engineering Data*. This manuscript focuses on developing an improved approach for force field parameterization, which is key to obtaining reliable results from molecular simulation. Specifically, we present a novel application of histogram-free reweighting to maximize the information extracted from a single simulation. As this study reports "new property data obtained from molecular modeling and simulations," we believe this manuscript fits the aims and scope of *Journal of Chemical and Engineering Data.* This manuscript was requested as part of a Special Issue following the Fundamentals of Molecular Modeling and Simulation (FOMMS) 2018. We are willing to make any changes that may be required to make the manuscript publishable in *Journal of Chemical and Engineering Data*.

Sincerely,

Richard Messerly