THE JOURNAL OF PHYSICAL CHEMISTRY B

Expression of Concern

Cite This: J. Phys. Chem. B XXXX, XXX, XXX−XXX

pubs.acs.org/JPCB

Expression of Concern for "Deficiencies in Molecular Dynamics Simulation-Based Prediction of Protein−DNA Binding Free Energy Landscapes"

Morteza Khabiri[†] and Peter L. Freddolino*[,†,‡]

[†]Department of Biological Chemistry, University of Michigan Medical School, Ann Arbor, Michigan, United States

[‡]Department of Computational Medicine and Bioinformatics, University of Michigan Medical School, Ann Arbor, Michigan, United States

J. Phys. Chem. B **2017**, *121* (20), 5151−5161, DOI: 10.1021/acs.jpcb.6b12450

As of May 18, 2018, the authors issue an Expression of Concern to advise readers of potential discrepancies between the results reported in this article and a recent, more successful, report of similar calculations (Gapsys and de Groot, JCTC 13:6275−6289 [DOI: 10.1021/acs.jctc.7b00849]). Based on the more recent publication, the authors now believe that technical shortcomings in the published calculations may underlie the poor agreements that were obtained between computed and experimental binding free energy profiles. The authors are in the process of investigating the likely sources of error, and the status of this article will be updated following the outcome of that investigation.

DOI: 10.1021/acs.jpcb.8b04187
J. Phys. Chem. B XXXX, XXX, XXX−XXX