

Clarification

A statement made in a previous paper published in the 1990 Biophysical Journal (“Molecular dynamics simulation by mass weighting” by Mao and Friedman, 58:803–805) should be clarified. The statement, in the first paragraph on p. 805, “the probability of torsional transitions is increased due to . . .”, would be better as “the probability of torsional transitions in short finite-length simulations is increased . . .”. The ‘probability’ here was intended to be read as the ‘practical opportunity’ for observing such transitions in short finite simulations; the probability of transitions in the statistical mechanical sense, of course, is independent of simulations lengths when sufficiently long simulations are practical. Although the entire work as presented is otherwise sound, we believe this simple, essentially semantic clarification would help prevent any possible misinterpretation.