Abstract

The generation of free energy landscapes corresponding to conformational equilibria in complex molecular systems remains a significant computational challenge. Adding to this challenge is the need to represent, store, and manipulate the often high-dimensional surfaces that result from rare-event sampling approaches employed to compute them. In this Letter, we propose the use of artificial neural networks as a solution to these issues. Using specific examples, we discuss network training using enhanced-sampling methods and the use of the networks in the calculation of ensemble averages.