Bridging the gap between thermodynamic integration and umbrella sampling provides a novel analysis method: "Umbrella integration"

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(Received 21 July 2005; accepted 11 August 2005; published online 7 October 2005)

We present a method to analyze biased molecular-dynamics and Monte Carlo simulations, also known as umbrella sampling. In the limiting case of a strong bias, this method is equivalent to thermodynamic integration. It employs only quantities with easily controllable equilibration and greatly reduces the statistical errors compared to the standard weighted histogram analysis method. We show the success of our approach for two examples, one analytic function, and one biological system.

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