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Free energy landscapes of short peptide chains using adaptively biased molecular dynamics VADZIM KARPUSENKA, VOLODYMYR BABIN, CHRISTOPHER ROLAND, CELESTE SAGUI, NCSU, CENTER FOR HIGH PERFORMANCE SIMULATIONS (CHIPS) AND DEPARTMENT OF PHYSICS TEAM — We present the results of a computational study of the free energy landscapes of short polypeptide chains, as a function of several reaction coordinates meant to distinguish between several known types of helices. The free energy landscapes were calculated using the recently developed adaptively biased molecular dynamics method followed up with equilibrium "umbrella correction" runs. Specific polypeptides investigated include small chains of pure and mixed alanine, glutamate, leucine, lysine and methionine (all amino acids with strong helix-forming propensities), as well as glycine, proline(having a low helix forming propensities), tyrosine, serine and arginine. Our results are consistent with the existing experimental and other theoretical evidence.

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