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The free energy landscape of short polyproline peptides MAHMOUD MORADI, VOLODYMYR BABIN, CHRISTOPHER ROLAND, CHiPS and Department of Physics, North Carolina State University, THOMAS A. DARDEN, National Institute of Environmental Health Sciences (NIEHS), CELESTE SAGUI, CHiPS and Department of Physics, North Carolina State University — Polyproline is a peptide whose configurations include both left- and right-handed helices. The free energy landscapes of polyproline peptides, as a function of the collective variables of handedness and radius of gyration, were calculated using the recently introduced Adaptively Biased Molecular Dynamics (ABMD) method. The ABMD method, which belongs to the general category of umbrella sampling methods with a time-dependent potential – when combined with replica exchange, multiple walkers and umbrella correction runs – allows for the efficient and accurate determination of the free energy maps. In turn, these free energy maps allow for an estimation of the transition pathways and barriers connecting the different helical structures, which are discussed for polyproline in vacuo, in implicit water, and the organic solvents hexane and propanol.

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