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Free energy landscapes of short polyproline peptides in vacuo and solvated environments MAHMOUD MORADI, CHRISTOPHER ROLAND, VOLODYMYR BABIN, CELESTE SAGUI, CHiPS and Department of Physics, North Carolina State University — Polyproline peptides are known to occur in two different conformations, including right-handed PPI and left-handed PPII. Depending on the solvated environment and the peptide length, either PPI or PPII is favored. Specifically, we calculated the free energy landscapes of short polyproline peptides (length 6, 9, 13-mers) in vacuo, in implicit water, and in the solvents hexane and propanol as a function of the radius of gyration and handedness. To calculate the free energies, the recently developed Adaptively Biased Molecular Dynamics (ABMD) method, which belongs to the general category of umbrella sampling methods with a time-dependent potential, was used.

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