Abstract Submitted
for the SES08 Meeting of
The American Physical Society

**Free energy calculations of short peptide chains using Adaptively Biased Molecular Dynamics** VADZIM KARPUSENKA, VOLODYMYR BABIN, CHRISTOPHER ROLAND, CELESTE SAGUI, North Carolina State University, CENTER FOR HIGH PERFORMANCE SIMULATIONS (CHIPS) AND DEPARTMENT OF PHYSICS TEAM — We performed a computational study of monomer peptides composed of methionine, alanine, leucine, glutamate, lysine (all amino acids with a helix-forming propensities); and proline, glycine tyrosine, serine, arginine (which all have poor helix-forming propensities). The free energy landscapes as a function of the handedness and radius of gyration have been calculated using the recently introduced Adaptively Biased Molecular Dynamics (ABMD) method, combined with replica exchange, multiple walkers, and post-processing Umbrella Correction (UC). Minima that correspond to some of the left- and right-handed $3_{10}$-, $\alpha$- and $\pi$-helixes were identified by secondary structure assignment methods (DSSP, Stride). The resulting free energy surface (FES) and the subsequent steered molecular dynamics (SMD) simulation results are in agreement with the empirical evidence of preferred secondary structures for the peptide chains considered.

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Date submitted: 12 Aug 2008 Electronic form version 1.4