Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Sterically allowed configuration space for amino acid dipeptides
DIEGO CABALLERO, Yale Univ, JUKKA MAATTA, MARIA SAMMALKORPI, Aalto Univ, COREY O'HERN, LYNNE REGAN, Yale Univ — Despite recent improvements in computational methods for protein design, we still lack a quantitative, predictive understanding of the intrinsic propensities for amino acids to be in particular backbone or side-chain conformations. This question has remained unsettled for years because of the discrepancies between different experimental approaches. To address it, I performed all-atom hard-sphere simulations of hydrophobic residues with stereo-chemical constraints and non-attractive steric interactions between non-bonded atoms for ALA, ILE, LEU and VAL dipeptide mimetics. For these hard-sphere MD simulations, I show that transitions between α-helix and β-sheet structures only occur when the bond angle $\tau(N - C_\alpha - C) > 110^\circ$, and the probability distribution of bond angles for structures in the 'bridge' region of ϕ-ψ space is shifted to larger angles compared to that in other regions. In contrast, the relevant bond-angle distributions obtained from most molecular dynamics packages are broader and shifter to larger values. I encounter similar correlations between bond angles and side-chain dihedral angles. The success of these studies is an argument for re-incorporating local stereochemical constraints into computational protein design methodology.

Diego Caballero
Yale Univ

Date submitted: 15 Nov 2013 Electronic form version 1.4