Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Can understanding the packing of side chains improve the design of protein-protein interactions?[1] ALICE ZHOU, COREY O'HERN, LYNNE REGAN, Yale University — With the long-term goal to improve the design of protein-protein interactions, we have begun extensive computational studies to understand how side-chains of key residues of binding partners geometrically fit together at protein-peptide interfaces, e.g. the tetratrico-peptide repeat protein and its cognate peptide). We describe simple atomic-scale models of hydrophobic dipeptides, which include hard-core repulsion, bond length and angle constraints, and Van der Waals attraction. By completely enumerating all minimal energy structures in these systems, we are able to reproduce important features of the probability distributions of side chain dihedral angles of hydrophic residues in the protein data bank. These results are the crucial first step in developing computational models that can predict the side chain conformations of residues at protein-peptide interfaces.

[1]CSO acknowledges support from NSF grant no. CMMT-1006527.

Alice Zhou
Yale University

Date submitted: 19 Nov 2010 Electronic form version 1.4