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Conformational analysis of tripeptides: a molecular dynamics study of rigid and non-rigid tripeptides JOHN SHIBATA, MARK MOCHEL, The University of the South — Molecular dynamics simulations have been performed on different tripeptides classified as structurally rigid and non-rigid (1). The simulations were run using the OPLS-AA force field (2) with and without explicit solvent. Two modeling programs, Tinker (3) and Macromodel (4), were used to simulate the dynamics. The accessible conformations were analyzed using Ramachandran plots of the dihedral angles. The results of this study are compared to the rigidity classification scheme (1), and differences in the results using explicit solvent and a continuum solvent model are noted. (1) Anishetty, S., Pennathur, G., Anishetty, R. BMC Structural Biology **2**:9 (2002). Available from http://www.biomedcentral.com/1472-6807/2/9. (2) Jorgensen, W. L., Maxwell, D. S., Tirado-Rives, J. J. Am. Chem. Soc. **118**, 11225 (1996). (3) Dudek, M. J., Ramnarayan, K., Ponder, J. W. J. Comput. Chem. **19**, 548 (1996). Available from http://dasher.wustl.edu/tinker. (4) Mohamadi, F., Richards, N. G. J., Guida, W. C., Liskamp, R., Lipton, M., Caufield, C., Chang, G., Hendrickson, T., Still, W. C. J. Comput. Chem. **11**, 440 (1990).

John Shibata
The University of the South

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