

Abstract Submitted
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Multi-field C-13 NMR Relaxation Study of the Tripeptide Glycine-Proline-Glycine-NH₂ JOHN SHIBATA, MARY FORRESTER, University of the South — T₁ and T₂ C-13 NMR relaxation measurements were performed on the tripeptide Gly-Pro-Gly-NH₂ on 300 MHz, 500 MHz, and 800 MHz NMR instruments (1). T₁ and T₂ data at different field strengths were analyzed to reveal the internal dynamics of this tripeptide. The results are compared to the classification scheme of rigidity by Anishetty, et al. (2). The dynamics of the tripeptide at different carbons in the molecule probe the site-specificity of the motions. We compare the dynamics revealed at the glycines with the dynamics in the proline ring. These motions are also being studied by molecular dynamics using the molecular modeling program Tinker (3). (1) Measurements at 500 MHz and 800 MHz were performed at the Alabama High Field NMR Center, University of Alabama at Huntsville, Huntsville, AL. (2) Anishetty, S., Pennathur, G., Anishetty, R. *BMC Structural Biology* **2**:9 (2002). <http://www.biomedcentral.com/1472-6807/2/9>. (3) Dudek, M. J., Ramnarayan, K., Ponder, J. W. *J. Comput. Chem.* **19**, 548 (1996). <http://dasher.wustl.edu/tinker>.

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