

**TITLE:**  $^{13}\text{C}$  NMR Spectroscopy: Transmission Effects in 3,5-Diaryl-4-Bromoisoxazoles**AUTHORS:** Beatrice Edjah, Stephanie Ross, Julia Dave, Patrick Gaulden, Hector Argueta-Gonzalez, Joseph Akinoso, Ronald Shanderson, Jiyao Yu, Gayle Miller, Shanyne Douglas, Shian McLeish**FACULTY SPONSOR:** Dr. A.L. Baumstark, Professor, Chemistry Department**Keywords:** *Molecular Modeling, Transmission,  $^{13}\text{C}$  NMR, Substituent Effects, 4-Bromoisoxazole***Introduction:**

Transmission effects have been studied in 3,5-diarylisoxazoles. The present study seeks to investigate if transmission is altered in isoxazoles when a bulky group has been added to the central position of the ring to force the 3,5-diaryl groups to twist.  $^{13}\text{C}$  NMR spectral data will be plotted against that of the parent system to determine the effect.

**Methods:**

3,5-Diarylisoxazoles were prepared by published procedures. The 4-bromoisoxazole derivatives will be prepared from the isoxazoles by a reaction with NBS in acetic acid. Compounds were purified and characterized by standard methods.  $^{13}\text{C}$  NMR spectra will be collected using standard NMR parameters in DMSO- $d_6$ . Collected data for known compounds were in agreement with those previously published. Molecular modeling studies were conducted using the Spartan' 14 program. X-ray analysis will be obtained commercially to verify the three-dimensional geometry (dihedral angles between the aromatic rings) of the heterocyclic system.

**Results:**

Molecular modeling results for 3,5-diarylisoxazoles and the corresponding 4-bromoisoxazoles showed the former to be flat and the latter to be twisted with dihedral angles between the two aryl groups and the central isoxazole ring of about  $15^\circ$  and  $35^\circ$  respectively.  $^{13}\text{C}$  spectra data of both series of compounds were obtained and assigned. In agreement with published work, transmission of substituent effects were observed on the chemical shift of  $\text{C}_4$  for 3,5-diarylisoxazoles. Electron donating groups on the 5-aryl group resulted in amplified shifts of the signal for  $\text{C}_4$  of the isoxazoles while electron withdrawing groups showed the opposite. Substituents on the 3-aryl groups had little to no effect of the  $\text{C}_4$  shift signal. Plots of the  $\text{C}_4$  chemical shifts for the series of 5-aryl substituted isoxazoles vs. those of the 4-bromoisoxazoles should be linear, and the slope of which should allow determination of any changes in transmission efficiency.

**Discussion:**

Molecular modeling is valuable in predicting three-dimensional structures of molecules including the distortions created as a result of adding bulky groups. Comprehending transmission of substituent effects in heterocyclic compounds will lead to a better understanding of the properties of these molecules and their reactivity in chemical reactions.