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. $^{13}$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-bromoisoaxazole derivatives will be prepared from the isoxazoles by a reaction with NBS in acetic acid. Compounds were purified and characterized by standard methods. $^{13}$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-bromoisoaxazoles 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° and 35° respectively. $^{13}$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 C$_4$ for 3,5-diarylisoxazoles. Electron donating groups on the 5-aryl group resulted in amplified shifts of the signal for 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 C$_4$ shift signal. Plots of the C$_4$ chemical shifts for the series of 5-aryl substituted isoxazoles vs. those of the 4-bromoisoaxazoles 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.