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Authors	Hockstedler, Amy N.;Shah, Anand B.;Edjah, Beatrice A.;Duffek, Glenda M.;Patel, Krishna D.;Mendoza, Hadrian;Arrowood, Hayley B.;Brown, Nicole A.;Azhar, Saajid Z.
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TITLE: ^{13}C NMR Spectroscopy: Transmission Effects in 1-Phenyl-3,5-Diarylpyrazoles

AUTHORS:* Amy N. Hockstedler, Anand B. Shah, Beatrice A. Edjah, Glenda M. Duffek, Krishna D. Patel, Hadrian Mendoza, Hayley B. Arrowood, Nicole A. Brown, Saajid Z. Azhar,
FACULTY SPONSOR: Dr. Alfons L. Baumstark, Professor, Chemistry

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*Note. Authors listed in alphabetical order until completion of the study.

Introduction: A series of 1-phenyl-3,5-diarylpyrazoles will be synthesized from selected chalcones by reaction with phenylhydrazine followed by DDQ oxidation. The compounds to be synthesized will contain aryl groups for which the substituents have been varied from electron-donating to electron-withdrawing. The compounds will be characterized by physical and spectral properties. In particular, ^{13}C NMR spectra will be obtained as part of the structure proof. Previous research of different heterocycles has shown that the structure can be deduced by analysis of the changes in selected chemical shift data in the heterocycle system by substituents on aryl groups (Yu et al., 2015). In the present study, data from the pyrazole ring system will be analyzed to establish trends in chemical data to determine if the approach will allow assignment of structure.

Method: 1-phenyl-3,5-diarylpyrazoles will be synthesized from selected chalcones following published procedures (Barton & Ollis, 1979). ^{13}C NMR, ^{1}H NMR, melting point determination, and mass spectroscopy will be performed on each compound to confirm identity or for unknown compounds as part of the structure proof. ^{13}C NMR spectra will be collected using standard NMR parameters in DMSO-d6.

Results: Current syntheses of approximately ten desired pyrazoles are ongoing. We will collect and purify samples for ^{13}C NMR and carry out additional proofs for unknown compounds.

Conclusion: If data support our hypothesis, substituent effects for the aryl groups transmitted to pyrazole rings will allow this method to be used to determine structure of any pyrazole.

Barton, D., & Ollis, W. D. (Eds.) (1979). *Comprehensive Organic Chemistry* (Vol. 2, p. 389). Oxford, England: Pergamon.

Yu, J., Edjah, B., Argueta-Gonzalez, H., Ross, S., Gaulden, P., Shanderson, R, Dave, J., & Baumstark, A. L. (2015). 13C NMR Spectroscopy of Heterocycles: 3,5-Diaryl-4-bromoisoxazoles. *Heterocyclic Communications, 21*(5). 279-283. doi: 10.1515/hc-2015-0111