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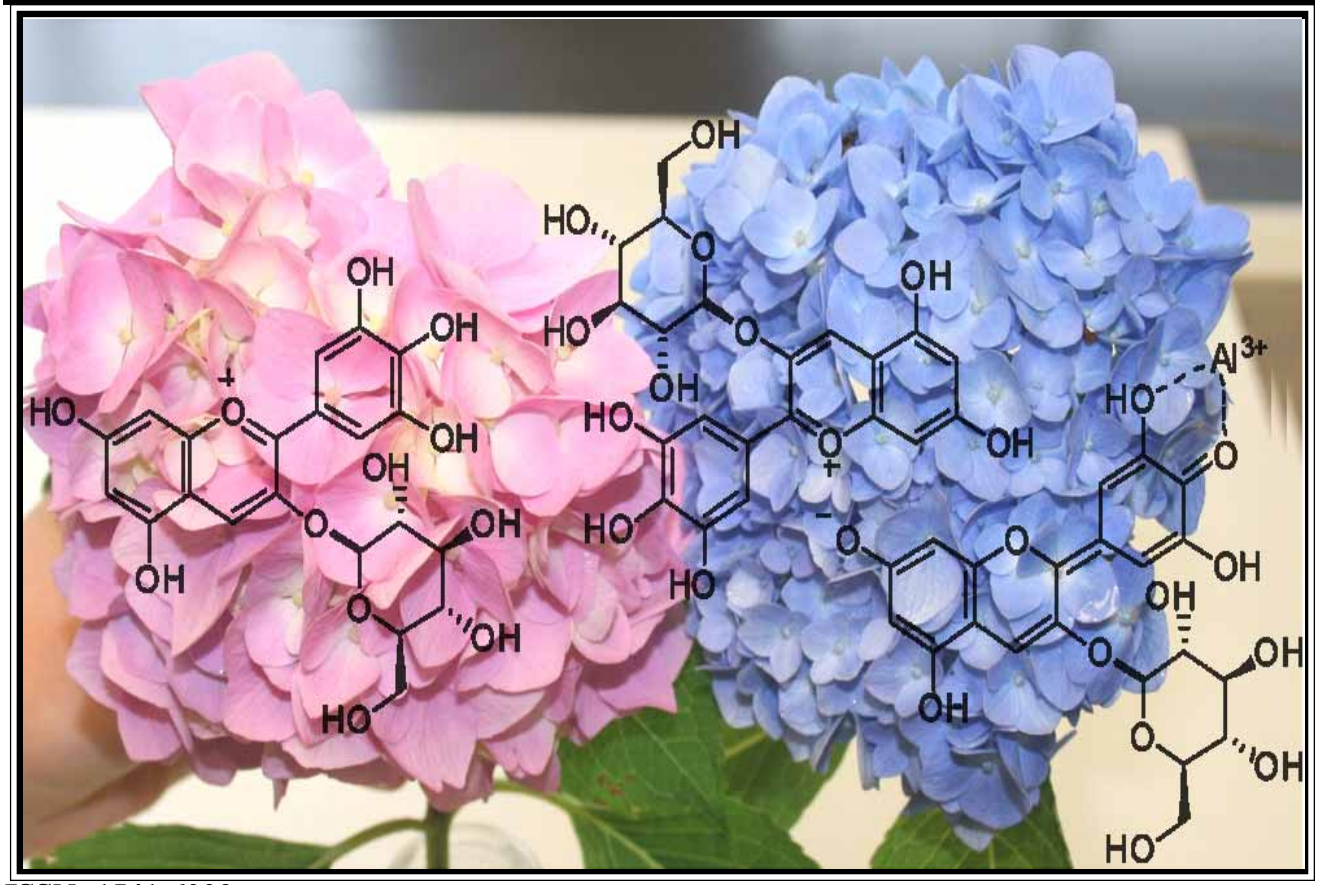

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CONFORMATIONAL ANALYSIS OF DITHIANES AND DIOXANES USING VT-NMR AND EXCEL SIMULATIONS

Heterocyclic six-membered rings undergo a chair to chair ring flip which has been a topic for discussion and research. The present work investigates and estimates the kinetic parameters for this flip of analogues of dioxane and dithiane using VT-NMR and line shape simulations using Microsoft Excel. The values obtained from our experiments and simulations are consistent with values reported for similar heterocyclic six-membered rings.

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DETERMINATION OF OXALATE ION DOPANT LEVEL IN POLYPYRROLE USING FT-IR

A pellet method using standard addition and FT-IR was used to estimate oxalate ion doping levels in electrosynthesized polypyrrole. The method is useful for materials where removal of analyte from an insoluble material is problematic. Here, electrosynthesized oxalate doped polypyrrole is dispersed in potassium bromide. Spikes of sodium oxalate are added and the mixtures pressed into pellets. The oxalate carbonyl absorption peak is then used to quantify the amount of oxalate present in the polypyrrole. The mass fraction of oxalate dopant in polypyrrole was determined to be 0.4 ± 0.1 % and coincides with the original synthesis solution composition.

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SPECTROSCOPIC PH DETERMINATION OF HYDRANGEA SEPALS WITH ACID-BASE INDICATORS

White, red, and blue inflorescences of several cultivars of *Hydrangea macrophylla*, as well as white inflorescences of *Hydrangea quercifolia* and *Hydrangea paniculata*, were infused with an aqueous solution of bromophenol blue. The spectral signature of bromophenol blue in the sepals of these inflorescences was obtained by subtracting post- and pre-infusion spectra of the sepals. This study ascertained that the cellular pH of all hydrangea sepals was about 3.6, independent of the initial sepal coloration. More specifically, cellular pH is the same for both red and blue sepals, with this pH having no role in the unique red-to-blue color changes for hydrangea inflorescences.

Henry D. Schreiber† and Ruthann P. Hodges*
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DESIGN AND SYNTHESIS OF A NOVEL ALPHA-METHYLENE LACTONE CHEMOTHERAPEUTIC AGENT

Goniothalamin, a natural product isolated from the dried stem bark of Malaysian plants of the genus *Goniothalamus*, has been shown to induce apoptosis in cancer cells. The bioactivity of this molecule is thought to be due to its ability to react with thiols. One mechanism involves its reaction with glutathione, a natural antioxidant found in all cells. Using a four step synthetic sequence, a novel gamma-lactone analogue of goniothalamin has been prepared that replaces the endocylic double bond in goniothalamin's lactone core with an exocyclic double bond. It is anticipated that this alteration will allow the compound to react more rapidly with thiols and therefore increase its cytotoxicity towards cancer cells.

Mark F. Mechelke†, Jason T. Brethorst*, Carina Crookston*, Courtney Klinkhammer*, Brittany N. Miller*, Curtis Payne*, Makenzie Pillsbury*, Christina R. Ringsmuth*, and Moriah Traut*
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REACTION OF PENTACYCLOUNDECANE-8,11-DIONE WITH ALCOHOLS AND IMPACT OF ALCOHOL STRUCTURE ON THE FORMATION OF OXA-BIRDCAGE DIKETALS

Generation of novel heterocyclic pentacycloundecane derivatives has potential application in drug design and ion-sensing. Reaction of pentacycloundecane-8,11-dione (PCU-8,11-dione) with alcohols could produce novel heterocyclic derivatives, but product distribution remains unknown. In our hands, reaction of alcohols with pentacycloundecane-8,11-dione in the presence of methanesulfonic acid produced oxa-birdcage diketals as the major products. Alcohol structure had a significant impact on product yield. While phenol did not react, benzyl alcohol produced the oxa-birdcage diketal in 71% (isolated) yield.

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METHANESULFONIC ACID CATALYZED SYNTHESIS OF DINITROCHALCONES AND THEIR CYTOTOXICITIES IN CANCER CELLS.

Substituted chalcones have therapeutic potential which includes anti-cancer properties. Herein four chalcone isomers with nitro-substituents were synthesized by novel methanesulfonic acid catalyzed Claisen-Schmidt condensation. The dinitrochalcone products were characterized and evaluated for cytotoxicity in HEK-293T, MCF7, and MDA-MB-231 cell lines. The 4,4'- and 3,3'-dinitrochalcone exhibited low micromolar efficacies in inducing cellular toxicity in each of the cell lines tested. Interestingly, the 4,3'- and the 3,4'-dinitrochalcone were less potent, with little or no biological activity in the assays tested.

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