

# Journal of Undergraduate Chemistry Research

ISSN: 1541-6003  
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## ALLELOCHEMICAL PHENOLIC ACIDS FROM *GYPSOPHILA PANICULATA*

Bioassay-guided fractionation of *Gypsophila paniculata* L. (Caryophyllaceae) resulted in the isolation of the phenolics *p*-coumaric acid [1], dihydroferulic acid [2], and syringic acid [3]. In addition to their noted weak antimicrobial activity, compounds [1] and [3] are known to be potent exuded allelochemicals. Compound [2] has been reported to undergo microbial degradation to vanillic acid [4], which is also known to be an exuded allelochemical. This is the first report of these phenolics from *G. paniculata*.

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## FLUORESCENCE DETECTION AND INTERACTIONS OF SINGLET OXYGEN

The indirect detection of photosensitized singlet oxygen was investigated by fluorescence spectroscopy. Rose Bengal was employed as the photosensitizing agent in 100 mM Tris buffer at pH 7.5. In the absence of the photosensitizer, singlet oxygen sensor green produced an emission band at 530 nm when excited at 504 nm. The addition of Rose Bengal resulted in a hypsochromic shift of this band with a maximum centered at 525 nm. The intensity of the emission band increased after illuminating Rose Bengal for 2 minutes at 525 nm. Titration of L-Trp with Rose Bengal results in quenching the amino acid's emission band around 350 nm. Stern-Volmer analysis suggests that the mechanism of quenching was neither static nor dynamic. Results indicate the formation of a Rose Bengal-Albumin complex that may not appreciably affect the location of Trp<sup>214</sup> in Human Serum Albumin, and that Trp<sup>214</sup> quenching is caused by singlet oxygen.

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## DEVELOPMENT OF PRESSED CRYSTAL MEMBRANE PHOSPHATE ION-SELECTIVE ELECTRODES

Ion-selective electrodes for many analytes are readily available and widely used in a variety of applications. Despite the relative importance of phosphate analysis in many diverse fields, ion-selective electrodes for this analyte are not commercially available and have received little attention in recent publications. In this work, a pressed crystal membrane phosphate ion-selective electrode is prepared using a mixture of Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> and CaF<sub>2</sub>. An important factor affecting the

sensitivity of the pressed crystal membrane ion-selective electrode is its conductivity, which is adjusted by varying the percentage of CaF<sub>2</sub> during membrane preparation. Crystal membrane ion-selective electrodes containing 5%(w/w) F are capable of detecting phosphate at concentrations as low as 0.27ppm PO<sub>4</sub><sup>3-</sup>. For a series of measurements using a pressed crystal membrane ISE containing 5%(w/w) F in solutions containing 0.01 M PO<sub>4</sub><sup>3-</sup>, an average potential of 3.08 ± 0.11mV vs. Ag/AgCl corresponding to a 5% relative standard deviation is achieved.

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## ASSESSMENT OF GAS-PHASE STABILITY OF A NEURO-PEPTIDE: SUBSTANCE P-SALT COMPLEX BY MATRIX-ASSISTED LASER DESORPTION / IONIZATION (MALDI) TIME-OF-FLIGHT (TOF) MASS SPECTROMETRY

The neuropeptide substance P, (SP) was used as a model peptide in its characterisation under matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometry conditions. Specifically, four parameters were assessed: (i) The intensity of the parent peak,  $([M + H]^+)_{\text{pseudo-molecular ion}}$  (where X represent the cations H<sup>+</sup>, Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup> and M represents the peptide substance P); (ii) the potential gas-phase binding affinity (Kd) of the cations to substance P under MALDI-TOF conditions, (iii) the intensity of the isolated parent peak from a mixture (containing seven other peptides)  $([M + H]^+)_{\text{LIFT}}$  (where LIFT represents fragmentation due to laser induced fragmentation time-of-flight); and (iv) its corresponding fragmentations, from which the sequence coverage was assessed. It was noted that the most intense peak followed the order: H<sup>+</sup> > Li<sup>+</sup> > Na<sup>+</sup> ~ K<sup>+</sup>, for the parent (whole mass) peak and a three-way comparison was determined to be statistically significant (P < 0.05). For an estimation of the affinity, the peak intensities were re-plotted. For the binding calculation the ratio of the alkali cation to proton peak (X/H) versus the normalizing difference ratio (1-(H/X)) was used. An estimation of the binding affinity for lithium was calculated at 86 μM, however, due to the large variation in the measurements (between successive runs) it was deemed unreliable and concluded that Electrospray ionization or use of an internal isotopic label may provide affinity data with greater precision and reliability. For the cationized peak in parent-isolation mode (prior to peptide fragmentation) the most intense form was the lithiated form and the least intense was the potassiumated form  $([M + Li]^+ > [M + K]^+)_{\text{LIFT}}$ , which was also statistically

significant ( $P < 0.05$ ). The resulting peptide fragmentation gave greater sequence coverage and (ten amino acids identified out of total of twelve amino acids) with lithium than with potassium (which only identified seven). This was speculated to be due to the difference in the internal energy of the complex, or greater energy resulting in more fragmentation from which the entire peptide sequence could be assembled.

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### **SYNTHESIS AND $^1\text{H}$ NMR STRUCTURAL CHARACTERIZATION OF A SERIES OF 5-SUBSTITUTED ISATIN THIOSEMI-CARBAZONE AND SEMICARBAZONE COMPOUNDS**

This work will present the synthesis and  $^1\text{H}$  NMR characterization of three series of 5-substituted isatin thiosemicarbazone compounds. The 5-nitroisatin, 5-fluoroisatin and 5-sulfonic acid isatin substrates were reacted with thiosemicarbazide, 4-methyl-3-thiosemicarbazide, 4-ethyl-3-thiosemicarbazone, 4-benzyl-3-thiosemicarbazone, 4-phenyl-3-thiosemicarbazide, 4,4-dimethyl-3-thiosemicarbazide, semicarbazide, and 4-phenyl-3-semicarbazide to give three series of thiosemicarbazone and semicarbazone compounds. Studies using  $^1\text{H}$  NMR show the presence of intramolecular hydrogen bonding in solution for all of the 5-substituted isatin thiosemicarbazone compounds.

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### **FACILE ROUTE TO PREPARE SILVER NANOPARTICLES**

We fabricated and characterized silver (Ag) particles as catalyst and characterize Ag microstructure. In this phase, the primary construction of the catalytic component was investigated. The novelty of our approach was that nanostructured silver particles were prepared by a facile and cost-efficient method. The advantages of our method are: simplicity of aqueous matrix, low temperature, and controllable acidity. The characterization techniques used were: X-ray Powder Diffraction (XRD), Electron and Optical Microscopy, UV-Visible and Raman Spectroscopy to determine the microstructure of nanostructured silver. XRD spectra indicated a formation of body centered cubic phase of silver. The UV-Visible absorbance of Ag nanostructure displayed well-defined plasmon band at 413 nm, which indicated presence of silver-silver metal interactions also consistent with XRD results. Electron and Optical

Microscope images indicated spherical silver particle were in the size range from 10 to 60 nm and spiral topography of growth respectively.

**Daniel Clancy\*** and **Jingbo Louise Liu†**

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### **HETEROLOGOUS EXPRESSION OF A MOSS BIFUNCTIONAL KAURENE SYNTHASE IN *E. COLI***

The cyclization of geranylgeranyl diphosphate (GGPP) to *ent*-kaurene is the first committed step in gibberellin biosynthesis. In flowering plants, *ent*-kaurene is formed via two enzymes: copalyl diphosphate synthase and *ent*-kaurene synthase, while in fungi, only a single bifunctional enzyme is utilized. A diterpene cyclase gene was identified in the genome of the moss *Physcomitrella patens* and heterologously expressed in *Escherichia coli*. Bacterial lysates incubated with GGPP were analyzed by gas chromatography-mass spectrometry (GC-MS). The results revealed *de novo* formation of both *ent*-kaurene and 16 $\alpha$ -hydroxykaurane, the major secondary metabolite of *P. patens*. This suggests that the diterpene cyclase gene identified in *P. patens* is a bifunctional diterpene cyclase, having both copalyl diphosphate synthase and *ent*-kaurene synthase activities, and is intriguingly also a potential hydratase.

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