CHEMISTRY PAPER ABSTRACTS

SURVEY OF ACTIVE BIOMOLECULES IN FERTILITY PLANTS. *AMANDA CRUMPTON*, JACKSONVILLE STATE UNIVERSITY. MWEBI NIXON, JACKSONVILLE STATE UNIVERISTY.

The chemical analysis of plants commonly used in African herbal medicine primarily to treat infertile women may provide viable explanations for successful treatment. In African, herbal medicine has been a traditional approach to treating infertility for many years; however the active biomolecules and mechanism of action are still unclear. Polyphenols are organic phytochemicals with antioxidant properties. Because literature suggests polyphenols can act similar to aromatase inhibitors, a form of infertility treatment, it is necessary to analyze these plants for their polyphenolic content. This study employs the Using the Folin-Ciocalteu reagent (F-C reagent) method (Cicco 2009), to quantify the total polyphenols in the plant extracts. Initial screening tests of the herbs indicate presence of polyphenols, steroids, triterpenoids, flavonoids, alkaloids, saponins, glycosides whereas as analysis with the FC reagent indicated presence of polyphenols in the herbal plants.

ENVIRONMENTAL REMEDIATION OF CADMIUM, CHROMIUM AND COPPER USING TEA WASTE. *MICAELA TRUETT*, JACKSONVILLE STATE UNIVERSITY. NICHOLAS HELMS AND MWEBI NIXON, JACKSONVILLE STATE UNIVERISTY.

Heavy metals in the environment pose a serious threat to the health of humans and ecosystems. Once introduced into the environment heavy metals may leach into the soil and local waterways. Industrial activities, such as mining and fracking, can introduce these potentially harmful heavy metals to the environment. As more and more nations become industrialized, it will be necessary to develop a suitable absorbent to remediate heavy metals in the environment. An ideal absorbent will be cheap, readily available, and environmentally friendly. One such candidate is tea waste. Tea is the second most popular beverage in the world, making the tea waste widely available and cheap. Additionally, tea waste is biodegradable and nontoxic making it very safe to use. This study evaluates the potential uptake of various metals by tea waste. Atomic absorption spectroscopy was used to quantify the tea-waste uptake ability of cadmium, chromium, and copper. Our preliminary results show that at optimum conditions tea waste is a viable adsorbent for heavy metals in solution.

CHEMISTRY POSTER ABSTRACTS

SYNTHESIS OF ISOQUINOLINE ANALOGS AS CHEMICAL PROBES FOR SERINE/THREONINE PROTEIN PHOSPHATASE 5. *MADISON TUTTLE*, LARRY YET, WILLIAM SWANN, DAVID GIDDENS, LIA CASTILLO, RICHARD HONKANEN AND MARK SWINGLE, UNIVERSITY OF SOUTH ALABAMA.

Recent studies have shown that the overexpression of serine/threonine protein phosphatase 5 (PP5) is associated with invasive ductal carcinoma of the breast, cancer cell proliferation, and resistance to apoptosis. However, scientists currently lack the molecular equipment with which to further characterize the biological role of PP5 in tumorigenesis. Previous high-throughput screening efforts revealed a potentially selective and potent small molecule chemical probe for PP5C containing a 6,7-dimethoxyisoquinoline core. Several analogs were synthesized and evaluated by means of a homogenous fluorescence intensity-based assay in %inhibition at 50 ŒºM. Based on a structure-activity relationship analysis, the 6,7-dimethoxyisoquinoline series is not potent enough to warrant further study.

SYNTHESIS, STRUCTURE, AND PHOTOLUMINESCENCE OF NOVEL LANTHANIDE COORDINATION COMPLEXES CONTAINING AUROPHILIC INTERACTIONS. *TAYLOR HAMBY*, RICHARD SYKORA AND JEFFREY HENDRICH, UNIVERSITY OF SOUTH ALABAMA.

This work details the synthesis of a series of isostructural lanthanide dicyanoaurates complexes containing the ancillary ligand 2,2'-bipyridine. Syntheses were carried out by reaction of Ln3+ triflate salts and potassium dicyanoaurate with 2,2'-bipyridine (bpy) resulting in the compound, [Ln(C10H8N2)(H2O)4(Au(CN)2)], (Ln=Tb and Gd). X-ray diffraction studies reveal the existence of dimeric aurophilic interactions as well as bipyridine pi-stacking. Photoluminescence studies reveal enhanced lanthanide-based emission due to energy transfer from the dicyanoaurate and 2,2'-bipyridine ligands and is confirmed by the augmented emission spectrum of the Gd analog.

NOVEL PROTEIN SUBSTRATES FOR THIN-LAYER CHROMATOGRAPHY. *NICHOLAS HELMS*, MICAELA TRUETT AND DONNA PERYGIN, JACKSONVILLE STATE UNIVERSITY.

Thin-Layer Chromatography (TLC) is a time-tested method which is used for; separation of substances, monitoring the progress of reactions, and determining whether a substance is present in a solution by comparison to standards. The drug development process involves several stages; discovery and development, preclinical research, clinical research, FDA review, and FDA post-market safety monitoring. The second step, preclinical research, usually involves both in-vitro and in-vivo testing methods. This work proposes to develop a novel in-vitro standard operating procedure, which may be used to validate or invalidate potential candidates before moving further down the drug development pipeline. Through the use of this technology, potential candidates which lack promising activity may be dismissed before animal testing is performed. In this way, animal testing will be greatly reduced. Reduced animal testing results in less suffering for animals, reduced expenditure, and reduced time wasted on

ineffective pharmaceutical products. This technology works through the varying affinity between the stationary phase, affixed to the plate, and the mobile phase (the solvent). We are developing novel technology which involves attaching proteins or enzymes to the TLC plate through a covalent linkage to provide a novel stationary phase. This novel stationary phase will be used to standardize a method of determination of a binding affinity of a substrate for the stationary phase. Standardization will be done by developing the plates, obtaining the native ligand for the respective enzyme, and testing the retention factor to verify the model. (A lower or higher retention factor (Rf), compared to the native ligand, will determine affinity.) This model will be used to compare the Rf value for new potential drug candidates to the standard. If a candidate exhibits a similarly low Rf value, the drug candidate can be pushed forward to an animal trial. If not, the candidate may be eliminated from the trial, leading to reduced suffering.

CHARACTERIZATION OF SUWANNEE RIVER FULVIC ACID BY ALTERNATIVE TOTAL ORGANIC CARBON ANALYSIS AND MASS SPECTROMETRY. *SHAHRZAD BADRI*, ALEXANDRA STENSON AND JIMMIE MCGEHEE, UNIVERSITY OF SOUTH ALABAMA.

Natural organic matter (NOM), a product of decomposing biological matter, has a complex chemical makeup consisting of numerous compounds. To reduce this complexity, NOM is frequently broken into fractions before analysis. NOM consists of fulvic acid (FA), the component soluble in acidic water, and humic acid (HA), the component insoluble in acidic water. NOM is found in all soil and surface water, and it has shown to form carcinogenic disinfection byproducts (DBPs) after water treatment. Samples of chlorinated and unchlorinated Suwannee River fulvic acid (SRFA) were analyzed through Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS), and their chemical compositions were determined from their respective mass spectra. Comparing chlorinated and unchlorinated samples aids in understanding if the chemical composition of humics is altered in the process of chlorination. FTICR-MS is accurate enough to detect the mass difference between formulas that are only one milli-Daltons apart, which is the case for many humic substances. This means that the mass spectra of humic substances reveals thousands of compounds with unique masses. Also, the effects of desalting samples through a ZipTip were observed because chlorinated samples must be desalted for proper function of FTICR-MS. Chlorinated samples were found to contain chlorine and their van Krevelen plots indicate chemical alteration by oxidation. Desalted samples demonstrated an absence of compounds containing higher O/C ratios, likely from removal of compounds containing electronegative O.

A challenge with investigating chlorinated humics is that SRFA concentrations must be consistent for all samples. To determine concentration of carbon, total organic carbon (TOC) analysis is utilized. TOC analysis directly quantifies the concentration of carbon in a sample, often by combustion. Having only a limited amount of sample, the destructive nature of TOC analysis is not feasible. An alternative method of quantifying concentration suggested by Tipping et al. was utilized to translate UV-vis data into concentration by a series of equations that yield the extinction coefficient of a sample. This method is nondestructive and comparable in accuracy to direct TOC analysis. Since humics are highly heterogeneous, Beer's Law cannot be accurately applied to find the extinction coefficient. Tipping's equations for converting UV data into dissolved organic matter (DOC) data using a set of known parameters are:

(1) f_A=(E_1,B-RE_2,B)/ (R*E_2,A-R*E_2,B-E_1,A+E_1,B)

(2)E= f_A*E_A+(a-f_A)*E_B

in which f_A and f_B are fractions of components A and B, E is the extinction coefficient, and R is the ratio of absorbances at two wavelengths. This method treats NOM as if it only consists of two components in order to relate absorbance to TOC. Solving for equation 1 yielded the fraction of A which was used to solve equation 2 at 340 nm, a wavelength SRFA is known to absorb light at. The absorbance and extinction coefficient were then applied to Beer's Law to find the concentration. This method allowed for accurate computation of concentration with relatively low standard deviations.

FRACTIONATION OF HUMIC ACID USING HIGH PERFORMANCE LIQUID CHROMATOGRAPHY. *JIMMIE MCGEHEE*, DOMINIKA HOUSEROVA AND ALEXANDRA STENSON, UNIVERSITY OF SOUTH ALABAMA.

Natural organic matter (NOM) is the material formed by the degradation of organic material in soil; it is present in all drinking water.1 Chlorinating agents added to drinking water react with NOM to form disinfection byproducts (DBPs) linked to increased cancer risk.1 Despite recent study of DBP formation the characteristics and health effects of unaltered NOM are still relatively unexplored. Recent studies have reached contradictory conclusions of NOM being either mutagenic or anti-mutagenic under different circumstances.2,3,4 Because NOM is a complex and variable mixture, it is possible that different compounds are responsible for these competing effects.

Previous experiments by this research team have had success characterizing the acid soluble portion of NOM, fulvic acid (FA), by fractionating the mixture using high performance liquid chromatography (HPLC) before analysis. The portion of NOM that is acid insoluble, humic acid (HA), is more bioactive than FA and has a higher potential to form DBPs during water treatment.1,2 This makes HA a likely source of NOM's health effects; however, fractionating HA is more difficult than fractionating FA. Separating weak acids such as HA with HPLC normally employs an acidic mobile phase. This is to prevent the disassociation of the analyte into polar charged ions that flow freely with the polar mobile phase, preventing separation. Because HA is insoluble in acidic solution, the problem of disassociation must instead be controlled by careful management of pH and a highly tuned mobile phase gradient.

The goal of this paper is to fractionate HA for future characterization of the compounds most responsible for NOM's bioactive effects and DBP formation potential. Utilizing a shallow gradient, HA was successfully fractionated with replicable chromatographic distribution. To fully characterize the fractions, material must be gathered from several HPLC collection cycles. Development is in progress to modify the method for faster cycling and material collection

NOVEL PROTEIN SUBSTRATES FOR THIN-LAYER CHROMATOGRAPHY. *NICHOLAS HELMS*, MICAELA TRUETT AND DONNA PERYGIN, JACKSONVILLE STATE UNIVERSITY.

Thin-Layer Chromatography (TLC) is a time-tested method which is used for; separation of substances, monitoring the progress of reactions, and determining whether a substance is present in a solution by comparison to standards. The drug development process involves several stages; discovery and development, preclinical research, clinical research, FDA review, and FDA post-market safety monitoring. The second step, preclinical research, usually involves both in-vitro and in-vivo testing methods. This work proposes to develop a novel in-vitro standard operating procedure, which may be used to validate or invalidate potential candidates before moving further down the drug development pipeline. Through the use of this technology, potential candidates which lack promising activity may be dismissed before animal testing is performed. In this way, animal testing will be greatly reduced. Reduced animal testing results in less suffering for animals, reduced expenditure, and reduced time wasted on ineffective pharmaceutical products. This technology works through the varying affinity between the stationary phase, affixed to the plate, and the mobile phase (the solvent). We are developing novel technology which involves attaching proteins or enzymes to the TLC plate through a covalent linkage to provide a novel stationary phase. This novel stationary phase will be used to standardize a method of determination of a binding affinity of a substrate for the stationary phase. Standardization will be done by developing the plates, obtaining the native ligand for the respective enzyme, and testing the retention factor to verify the model. (A lower or higher retention factor (Rf), compared to the native ligand, will determine affinity.) This model will be used to compare the Rf value for new potential drug candidates to the standard. If a candidate exhibits a similarly low Rf value, the drug candidate can be pushed forward to an animal trial. If not, the candidate may be eliminated from the trial, leading to reduced suffering.