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CONTENTS

β-CATENIN COMPLEXED WITH TCF-4 AND SOME OF THE PROCESSES INVOLVED WITH COMPUTER-AIDED DRUG DESIGN AND PROTEIN ANALYSIS	
Travis Unger*, Raelene Lawrence and David Soriano†	39
CONVERSION OF ANILINE IN AQUEOUS WASTE WITH THE FENTON REACTION	
Shardell Hawkins* , Yan Waguespack†	51
DETERMINATION OF VOLATILE ORGANIC COMPOUNDS ADSORBED ON AIRBORNE FINE PARTICULATE MATTER (PM_{2.5}) USING GC/MS	
John E. Spencer* and Michael J. Baird†	55
ON DIASTEREOSELECTIVITY OF LEWIS ACID MEDIATED COUPLING OF <i>p</i>-TolSCl, TWO MOLECULES OF <i>tert</i>-BUTYL VINYL ETHER, AND SILICON-CAPPED π-DONORS	
Darren Wakefield*, Margarita Lazereva†, and Ron Caple.....	61
RELATING STRUCTURE AND FUNCTION IN A SERIES OF INSECT PHEROMONES BY USING MOLECULAR MECHANICS	
Krayton Keith* and Maureen K. Murphy†	67
STRUCTURAL DETERMINATION OF A SERIES OF ORTHO-QUINONE THIOSEMICARBAZONE COMPOUNDS USING NMR SPECTROSCOPY	
James W. Carter*, Richard Mayes, Kristin A. Pierce*, Richard Lawson*, and Edward C. Lisic†.....	73
ANALYSIS OF THE MASS SPECTRAL FRAGMENTATION PATTERNS OF ESSENTIAL OIL COMPONENTS FROM OREGANO (<i>ORIGANUM VULGARE</i> SSP. <i>HIRTUM</i>)	
Stacy E. Price* and George W. Mushrush†.....	79

CHEMISTRY



DEPARTMENT

Abstracts

β -Catenin Complexed with TCF-4 and Some of the Processes Involved with Computer-Aided Drug Design and Protein Analysis

Molecular informatics is a fairly new area of research that encompasses both biological and chemical aspects of protein and drug research. β -Catenin is a protein that has major implications in cancer research. A potential active site was found and several drugs active against β -catenin were explored.

Travis Unger, Raelene Lawrence and David Soriano[†]

[†]Chemistry Department, University of Pittsburgh Bradford PA. 16701

Conversion of Aniline in Aqueous Waste with the Fenton Reaction

Aniline has a high acute toxicity to aquatic life and moderate acute toxicity to birds. The chronic toxic effects include shortened lifespan, infertility, and changes in appearance or behavior. The death of animals and plants can also result from overexposure to aniline. It is clear that aniline waste is a serious threat to the health and prosperity of our ecological resources. Our goal was to convert this energy or coal related waste into useful materials with the greatest efficiency. The Fenton reaction was used to convert aqueous aniline solutions into polymers that could then be extracted. In the Fenton reaction the hydroxyl radical is formed by the catalytic decomposition of H₂O₂ with ferrous iron. The hydroxyl radical has strong oxidizing potential and high reactivity towards undesirable organics such as aniline. The products of the Fenton reaction are very useful polymers. The efficiency of the removal of aniline from the solution was measured by using GPC, FT-IR and GC/MS.

Shardell Hawkins*, Yan Waguespack[†]

[†] Department of Natural Sciences, University of Maryland Eastern Shore, Princess Anne, MD 21853, ywaguespack@mail.umes.edu

Determination of Volatile Organic Compounds Adsorbed on Airborne Fine Particulate Matter (PM_{2.5}) Using GC/MS

The objective of this research was to identify the volatile organic compounds (VOC's) that deposit on airborne fine particulate matter having a diameter less than 2.5 micron. VOC's are precursors to the formation of ozone, which cause atmospheric and climate changes and also may be harmful to our health. Samples of particulate matter were obtained from the U.S. Department of Energy's National Energy Technology Laboratory site in Pittsburgh that were collected on quartz filter paper in a gas sampler over a three-day period. Analysis of the filter material by GC/MS revealed mass fragments that were identified by the on-line NIST Mass Spectral Library as anthracene or phenanthrene, 1,8-naphthalic anhydride, fluoranthrene, pyrene, benz[*a*]anthracene, and di-*n*-octyl phthalate. Standards of the above compounds were added to a blank filter and analyzed to confirm the retention times and mass spectra of the various hydrocarbons. The possible sources of these adsorbed VOC's are coal-fired power plants located along the Ohio River west of Pittsburgh, PA.

John E. Spencer* and Michael J. Baird[†]

Department of Chemistry, Wheeling Jesuit University, Wheeling, WV 26003, Baird@wju.edu

On Diastereoselectivity of Lewis Acid Mediated Coupling of *p*-TolSCI, Two Molecules of *tert*-Butyl Vinyl Ether, and Silicon-Capped π -Donors.

A one-pot Et₂AlCl induced assemblage of polyfunctional compounds via a sequential coupling of *p*-TolSCI, two molecules of *t*-butyl vinyl ether, and Si-capped carbon nucleophiles is shown to proceed with moderate diastereoselectivity at two newly created chiral centers. Variation in the nature of the Lewis acid was found to have little effect on the diastereomeric ratio of the products

Darren Wakefield*, Margarita Lazereva[†], and Ron Caple

[†]Department of Chemistry, University of Minnesota Duluth, Duluth, MN 55812, lazereva@d.umn.edu

Relating Structure and Function in a Series of Insect Pheromones by Using Molecular Mechanics

We have studied a series of alarm and trail ant pheromones and have used molecular mechanics to calculate overall energies for the molecules, charge densities, and values for the LUMO (lowest unoccupied molecular orbital) of each carbon present in the pheromones. Ant pheromones with higher overall energies were found to be associated with more complex structures and functions. Assessment of the reactive binding center for each pheromone was accomplished by mapping the electron density and calculating LUMO values to give qualitative and quantitative data for each carbon in the structure of the pheromones. Our results show that the pheromone carbon atoms with larger LUMO values are more susceptible to nucleophilic attack or bonding at a receptor site. From this data, atomic models of the recognition sites for trail and alarm pheromones have been generated. In addition, we have found that pheromone functional groups and number of carbons in insect mandibular and cephalic glands appear to have been conserved over time from the Order Odonata (Devonian Period) to the Order Isoptera (Upper Cretaceous).

Krayton Keith* and Maureen K. Murphy

Department of Biology and Chemistry, Huntingdon College,
Montgomery, AL 36106-2148, maureenm@huntingdon.edu

STRUCTURAL DETERMINATION OF A SERIES OF ORTHO-QUINONE THIOSEMICARBAZONE COMPOUNDS USING NMR SPECTROSCOPY

Thiosemicarbazone compounds are an important class of multidentate ligands that contain potential binding sites for a wide variety of metal ions. This work will present the successful synthesis of three series of ortho-quinone based monothiosemicarbazone compounds. The first series is based on acenaphthenequinone, the second series is based on 1,2-naphthoquinone-4-sulfonic acid, and the third series is based on phenanthrenequinone. These three different quinones were each reacted with thiosemicarbazide, 4-methyl-3-thiosemicarbazide, and 4-phenyl-3-thiosemicarbazide to give three sets of three monothiosemicarbazones. Of the nine compounds synthesized for this study, five are new compounds. These compounds have been characterized by ¹H NMR, ¹³C NMR, and infrared spectroscopy, and this data supports an assignment for the structure of the monothiosemicarbazones to include a stable and strongly hydrogen-bonded hydrazinic proton that forms a portion of a uniquely characteristic six-membered ring. The far-downfield

resonance (12-15 ppm) in the proton NMR spectrum for this unique hydrogen-bonded proton makes it very easy to identify. These ortho-quinone based monothiosemicarbazone compounds are special in that they can potentially form a tridentate chelate with metal ions by utilizing three different ligating atoms: S, O, and N.

James W. Carter*, Richard Mayes, Kristin A. Pierce*, Richard Lawson*, and Edward C. Lisic†

Chemistry Department, Tennessee Technological University, Cookeville,
TN 38505, edlisic@tntech.edu

Analysis of the Mass Spectral Fragmentation Patterns of Essential Oil Components from *Oregano (Origanum vulgare ssp. hirtum)*

The mass spectral fragmentation patterns of eight major essential oil components, *p*-cymene, *α*-thujene, thymol, carvacrol, carvacrol methyl ether, *γ*-terpinene, *α*-terpinene, and myrcene have been analyzed in detail. All the spectra contained peaks at *m/z* 39, 51, 65, 77, and 91. These are typical aromatic fragments, resulting from loss of acetylene from the tropylium and phenyl cations. Myrcene, *γ*-terpinene, and *α*-thujene are not aromatic, but are unsaturated hydrocarbons that lose hydrogen radicals to produce aromatic fragments. Most the compounds had prominent molecular ion peaks and a *M*-15 base peak.

Stacy E. Price* and George W. Mushrush†, Department of Chemistry,
3E2, George Mason University, Fairfax, VA 22030