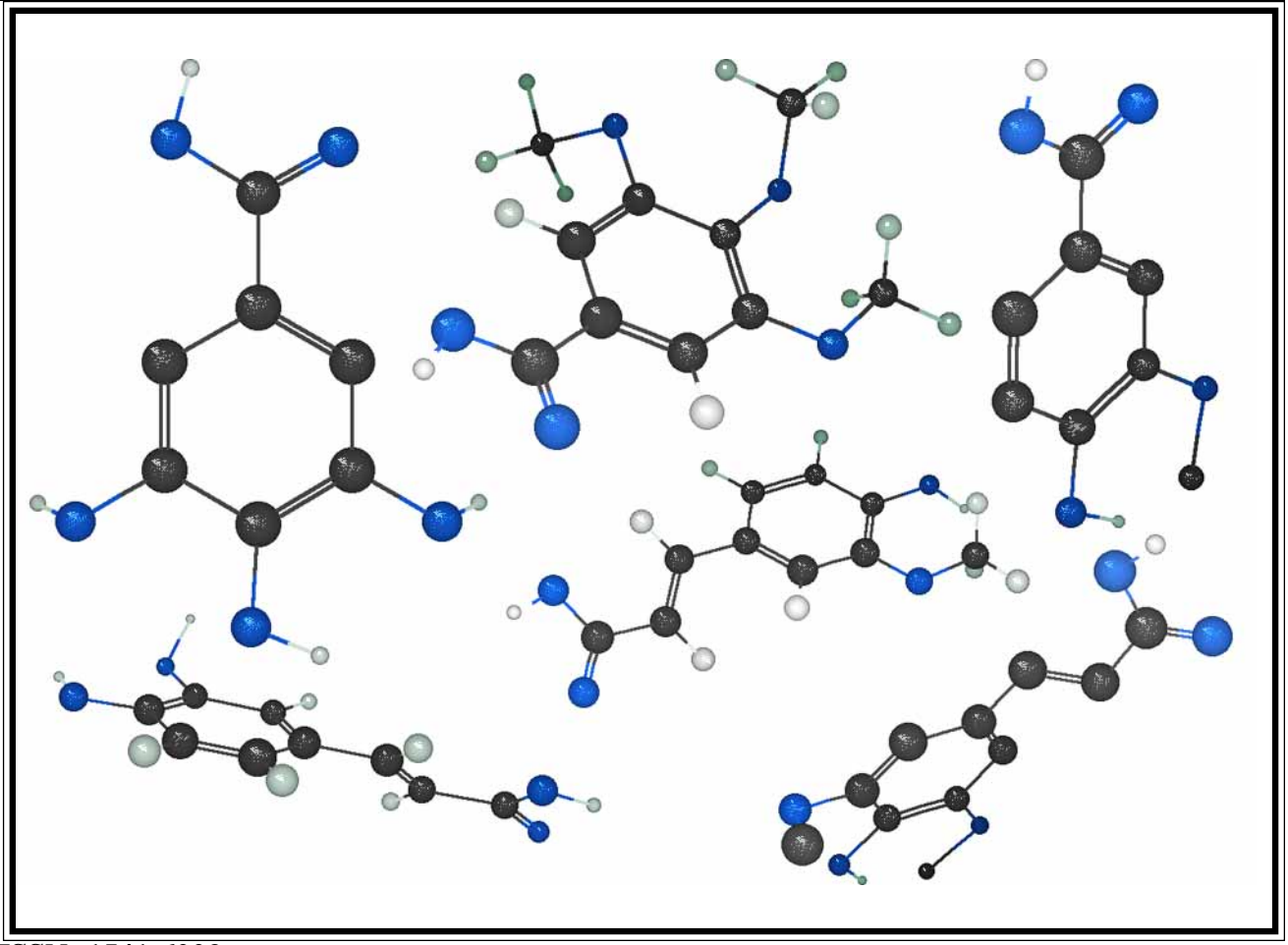
Winter 2010 Volume 9, Number 1

Journal of Undergraduate Chemistry Research



ISSN: 1541-6003

Volume 9, Number 1 **Winter 2010**

Journal of Undergraduate Chemistry Research

ISSN: 1541-6003

CONTENTS

ELECTROCHEMISTRY OF PROTEIN AND REDOX POLYMER S TRAPPED IN POLYETHYLENE GLYCOL DIACRYLATE GEL
Amos Mugweru† and Zuliang Shen* 1

REMOVAL OF CARBAMAZEPINE IN WATER SAMPLES USING NANOPARTICLES, MICROBEADS AND POWDERED ACTIVATED CARBON
Chris Wang*, Stephen E. Gibbons, Yinfa Ma† 6

TWO-DIMENSIONAL HOMONUCLEAR J-RESOLVED NMR SPECTROSCOPY OF A COBALT(III) COMPLEX CONTAINING TRIS(2-AMINOETHYL)AMINE AND 1,10-PHENANTHROLINE
Mark R. McClure† and Mary E. McMillan* 11

STABILIZATION OF ACYCLIC N_4 BY CHAIN-TERMINAL BONDING GROUPS
Hasan Carmichael* and Douglas L. Strout† 15

EVALUATION OF GALLIC ACID AND RELATED COMPOUNDS AS ANTIOXIDATIVE AGENTS
Fulgentius N. Lugemwa†, Adam Shoemaker* 18

DEVELOPMENT OF A NOVEL METHOD FOR MAGNETIC BEAD EXTRACTION OF TAXANES FROM SERUM FOLLOWED BY SEPARATION AND DETECTION BY LIQUID CHROMATOGRAPHY
Abidemi Olayinka*, Aaron Hernandez-Santana, Shane Bermingham, Gillian McMahon† 22

DETERMINATION OF THE ETHANOL LEVEL IN COMMERCIAL GASOLINES BY GAS CHROMATOGRAPHY
Terrence P. Sherlock† and Elliot Taylor* 27

The *Journal of Undergraduate Chemistry Research* publishes papers of original research performed by undergraduates on all aspects of chemistry including analytical, organic, inorganic, physical, polymers and biochemistry. Articles about laboratory experiments to be used in the teaching of chemistry are not applicable. The *Journal of Undergraduate Chemistry Research* is issued quarterly and indexed once per year by Dr. Daniel Y. Pharr Editor, Chemistry Department, Virginia Military Institute, Lexington, VA 24450. Subscriptions price per year U.S.A.: institutional $ 120.00, individual $ 50.00 all other countries US $ 150.00. Claims for missing issues will not be honored after four months of issue date. Duplicate copies may not be sent due to the change of address when the publisher was not notified in a timely manner. The *Journal of Undergraduate Chemistry Research* can be contacted via phone (540-464-7244), fax (540-464-7261) or e-mail (PharrDY@vmi.edu) through Dr. Daniel Y. Pharr Editor. No responsibility is assumed by this journal, editor, reviewers or sponsors for any injury and/or damage from products, negligence, experiments, instructions or ideas contained in this journal that result in damage to persons or property. **POSTMASTER**: Send change of address to: Journal of Undergraduate Chemistry Research, Dr. Daniel Y. Pharr Editor, Chemistry Department, Virginia Military Institute, Lexington VA 24450.

ELECTROCHEMISTRY OF PROTEIN AND REDOX POLYMERS TRAPPED IN POLYETHYLENE GLYCOL DIACRYLATE GEL

Assembly of multi-analyte electrochemical sensors was achieved by immobilization of redox polymers and heme proteins on pyrolytic graphite (PG)electrode. Hemoglobin, poly[4-vinylpyridine Os(bipyridine)$_2$Cl]-co-ethylamine (POs-EA) and Ru[bipy(PVP)$_{10}$Cl]Cl$^-$ were physically trapped using a photo-polymerization reaction involving polyethylene glycol diacrylate (PEG-DA) molecule and using a photo-initiator, 1-phenyl-2-hydroxy-2-methyl-1-propanone. Electrochemistry of these redox species was observed on pyrolytic graphite electrode after gel hydration. Three independent redox centers were observed corresponding to Os^{II}/Os^{III}, Ru^{II}/Ru^{III} and $HbFe^{III}/HbFe^{II}$ at 0.32 V, 0.78V and -0.25V versus Ag/AgCl respectively. The electroactive centers were found to catalytically respond to presence of acetaminophen and hydrogen peroxide both individually and in a mixture without interference.

Amos Mugweru† and Zuliang Shen*
Department of Chemistry and Biochemistry, 201 Mullica Hill Road, Glassboro, NJ 08028, Rowan University, mugweru@rowan.edu

REMOVAL OF CARBAMAZEPINE IN WATER SAMPLES USING NANOPARTICLES, MICROBEADS AND POWDERED ACTIVATED CARBON

Pharmaceuticals and personal care products (PPCPs) are common chemicals used by people for reasons pertaining to health, cosmetics, and agribusiness. However, PPCPs are often detected as contaminants in many water sources such as river water, wastewater, and drinking water, although in trace amounts. Since it is possible that PPCPs may adversely affect human health, its removal is of critical importance. Wastewater treatment plants can successfully remove most PPCPs from wastewater, but trace amounts that remain in drinking water can potentially impose health impact on humans. One commonly detected PPCP in surface water resources is carbamazepine. In this paper, the removal of carbamazepine in spiked standard solutions and lake water samples was studied by using silica nanoparticles and five different hydroxyapatite (HA) beads. The results were compared with those by using powdered activated carbon (PAC). The results demonstrated that even though every type of material was capable of removing some carbamazepine from water, PAC was the most effective in carbamazepine removal. The information from this study is valuable for water treatment facilities.

Chris Wang*, Stephen E. Gibbons, Yinfa Ma†
Department of Chemistry and Environmental Research Center, Missouri University of Science and Technology, Rolla, MO 65409, yinfa@mst.edu

TWO-DIMENSIONAL HOMONUCLEAR J-RESOLVED NMR SPECTROSCOPY OF A COBALT(III) COMPLEX CONTAINING TRIS(2-AMINOETHYL)AMINE AND 1,10-PHENANTHROLINE

Two-dimensional homonuclear J-resolved NMR spectroscopy was used to study the complex [Co(tren)(phen)]Cl_3. Using the homonuclear J-resolved experiment, the chemical shifts and multiplicities of the aliphatic and aromatic protons were obtained. To our knowledge this paper describes the first application of the homonuclear J-resolved experiment to the study of cobalt(III) complexes, and the first reported synthesis of [Co(tren)(phen)]Cl_3.

Mark R. McClure† and Mary E. McMillan*
University of North Carolina at Pembroke, Department of Chemistry and Physics, P.O. 1510, Pembroke, North Carolina 28372

STABILIZATION OF ACYCLIC N_4 BY CHAIN-TERMINAL BONDING GROUPS

Complex nitrogen molecules have been the subject of much research study for their potential as high-energy materials. However, many such molecules are insufficiently stable to serve in energetic applications. For example, the open-chain molecule N_4 dissociates into a pair of N_2 molecules with essentially a zero barrier. In the current study, theoretical calculations are carried out on N_4 chains that have been modified by chain-terminal CH_2 bonding groups. Halogen substitutions are also calculated to determine their impact on stability. Moller-Plesset (MP2) theory is used for geometry optimizations and transition state searches. Stability trends are calculated and discussed.

Hasan Carmichael* and Douglas L. Strout†
Department of Physical Sciences, Alabama State University, Montgomery, AL 3610, dstrout@alasu.edu

EVALUATION OF GALLIC ACID AND RELATED COMPOUNDS AS ANTIOXIDATIVE AGENTS

Gallic acid is a potent antioxidant and a scavenger of hydroxyl and superoxide anion radicals. Esters of gallic acid inhibit lipid peroxidation and are used as food preservatives. In order to evaluate the relationship of structure to radical scavenging activity, methyl 3,4,5-trihydroxybenzoate and 3,4,5-trimethoxybenzoic acid were synthesized, and their radical scavenging activity measured together with that of gallic acid, 3,4,5-trihydroxybenzamide, syringic acid, vanillic acid, sinapic acid, ferulic acid and caffeic acid using 2,2-diphenyl-1-picryhydrazyl (DPPH) assay. Gallic acid, methyl-3,4,5-trihydroxybenzoate and 3,4,5-trihydroxybenzamide showed the highest activity. Caffeic and syringic acid showed about half the activity of gallic acid. Sinapic acid and ferulic acid were less active than caffeic acid and syringic acid. Vanillic acid and 3,4,5-trimethoxybenzoic acid showed the lowest antioxidative activity. Blocking of the hydroxyl group with methyl groups reduced the radical scavenging activity significantly. These results indicate that, one, methylation or amidation of the carboxylic acid does not result in decreased antioxidative activity; two, the presence of hydroxyl groups is critical for the radical scavenging activity; and three, extending the conjugation of the aromatic system increases activity.

Fulgentius N. Lugemwa†, Adam Shoemaker*
Pennsylvania State University, York, PA 17403-3398, ful4@psu.edu

DEVELOPMENT OF A NOVEL METHOD FOR MAGNETIC BEAD EXTRACTION OF TAXANES FROM SERUM FOLLOWED BY SEPARATION AND DETECTION BY LIQUID CHROMATOGRAPHY

Magnetic beads have been used for the first time to extract taxanes from serum prior to separation and detection by liquid chromatography with UV detection. The taxanes, docetaxel and paclitaxel, were successfully captured from blood serum with good recoveries of 71-75% for both drugs at 10 µg/mL concentration and 95-120% for paclitaxel at 1 µg/mL concentration, which compare well with recoveries obtained in current offline liquid-liquid extraction (LLE) and solid-phase extraction (SPE) procedures. In comparison to the more traditional LLE and SPE methods, the magnetic bead extraction method is simple and fast (1 hr) and requires only very small volumes of biological fluid (20 µL) and beads (25 µL, 0.25 mg). With further optimisation, this method offers a safe, reliable, simple, sensitive and fast way of monitoring levels of taxanes in patients during chemotherapy.

Abidemi Olayinka*, Aaron Hernandez-Santana, Shane Bermingham, Gillian McMahon†
Bioanalytical Chemistry & Diagnostics Group, School of Chemical Sciences, Dublin City University, Dublin 9, Ireland, gillian.mcmahon@dcu.ie

DETERMINATION OF THE ETHANOL LEVEL IN COMMERCIAL GASOLINES BY GAS CHROMATOGRAPHY

The ethanol that is blended into gasolines to reduce pollution and boost octane ratings can reduce a car's fuel economy and lead to corrosion of engine parts if the ethanol levels exceed the nominal 10% level and approach 15% (1,2). This research describes the development of a method, using an academic grade gas chromatograph, which accurately quantifies the ethanol level in gasoline in 5 minutes. Samples of three commercial 87 octane regular gasolines and a sample of premium 93 octane gasoline were analyzed. Results indicate that all gasolines tested contained between 9% and 10% ethanol by volume.

Terrence P. Sherlock† and Elliot Taylor*
Burlington County College, Department of Chemistry, 3331 Route 38, Mount Laurel, NJ 08054, Tsherlock@bcc.edu

Journal of Undergraduate Chemistry Research JUCR@vmi.edu

Dr. Daniel Y. Pharr Editor
Chemistry Department
Virginia Military Institute
Lexington VA 24450
phone (540-464-7244)
fax (540-464-7261)
email (PharrDY@vmi.edu)

Editoral Board

Dr. Eugene M. Gregory
Associate Professor Biochemistry Virginia Tech. University, gregorye@vt.edu

Dr. John T. Gupton III
Chairman of Chemistry Department at Richmond University, jgupton@richmond.edu

Dr. Christine K. F. Hermann
Professor Radford University, chermann@runet.edu

Dr. Willie L. Hinze
Professor Wake Forest University, hinze@wfu.edu

Dr. Benjamin P. Huddle
Professor Roanoke College, huddle@roanoke.edu

Dr. Frank A. Settle Jr.
Professor Washington and Lee University, settlef@wlu.edu

Dr. Henry D. Schreiber
Chemistry Department at Virginia Military Institute, SchreiberHD@vmi.edu

Dr. Stanton Q. Smith
Chemistry Department at Virginia Military Institute, SmithSQ@vmi.edu

Dr. James E. Turner Sr.
Chairman Biology Department at Virginia Military Institute,TurnerJE@vmi.edu

ACKNOWLEDGMENT
The *Journal of Undergraduate Chemistry Research* wishes to acknowledge the generous support of the VMI Chemistry Department and the Virginia Military Institute for their support of this journal.

The ***Journal of Undergraduate Chemistry Research,*** **ISSN: 1541-6003,** is issued quarterly and indexed once per year.Subscriptions price per year U.S.A.: institutional $ 120.00, individual $ 50.00 all other countries US $ 150.00. Claims for missing issues will not be honored after four months of issue date. Duplicate copies may not be sent due to the change of address when the publisher was not notified in a timely manner. The ***Journal of Undergraduate Chemistry Research*** can be contacted via phone (540-464-7244), fax (540-464-7261) or e-mail (JUCR@vmi.edu) through Dr. Daniel Y. Pharr Editor. No responsibility is assumed by this journal, editor, reviewers or sponsors for any injury and/or damage from products, negligence, experiments, instructions or ideas contained in this journal that result in damage to persons or property.