

THE Indicator

MARCH 2012

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Chemistry as a Life Science Symposium XV



Brian Stoltz
California Institute
of Technology



Laura Kiessling
U. of Wisconsin-Madison



Kevan Shokat
U. of California San
Francisco

Paul Robeson
Campus Center
Rutgers, the State University
of New Jersey, Newark
Friday,
March 16, 2012



Jin-Quan Yu
The Scripps
Research
Institute



Marisa Kozlowski
U. of Pennsylvania



Erik Sorensen
Princeton University

<http://www.njacs.org/caals>

See program on page 8.

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Address advertising correspondence to Advertising Manager. Other correspondence to the Editor.

March Calendar

NEW YORK SECTION

Wednesday, March 7, 2012

Hudson-Bergen Chemical Society
See page 14.

Friday, March 16, 2012

Nichols Symposium
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Friday, March 16, 2012

High School Teachers Topical Group
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Tuesday, March 27, 2012

Biochemical Topical Group
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The Indicator is posted to the web on the 15th of the previous month at www.TheIndicator.org

NORTH JERSEY SECTION

Mondays, March 5 and 19, 2012

Careers in Transition Group
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Mondays, March 5 and 19, 2012

Careers in Transition Group
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Wednesday, March 14, 2012

NMR Spectroscopy Discussion Group
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Tuesday, March 20, 2012

NoJ Executive Committee Meeting
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Tuesday, March 20, 2012

Mass Spectrometry Discussion Group
2012 Bruker Daltonics Seminar
See pages 10 and 11.

Wednesday, March 21, 2012

Chromatography Topical Group
See www.njacs.org.

Please Note:

The Deadline Date for Submitting Articles and/or Pictures for Publication in *The Indicator* Has Been Extended to the 20th of the Month, Two Months Prior to the Publication Date, in an Effort to Accommodate More Complete Meeting Information. Deadline for items to be included in the April 2012 issue of *The Indicator* is **February 20, 2012.**



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THIS MONTH IN CHEMICAL HISTORY

By *Harold Goldwhite*, California State University, Los Angeles • hgoldwh@calstatela.edu

I continue the story I began in my last column by discussing the scientific work of Henry Cavendish, 1731- 1810. His first scientific article, published in *Philosophical Transactions* in 1766, was "Three Papers, Containing Experiments on Factitious Air". Some background; the accepted chemical theory of combustion – and many other phenomena- of this time was the phlogiston theory of Stahl, based on phlogiston, the matter of fire. Cavendish accepted this idea, as did most of the chemists of the late 18th. century. By factitious air Cavendish refers to "any kind of air [gas] which is contained in other bodies in an unelastic state, and is produced from thence by art". The first of Cavendish's airs, an inflammable gas, was hydrogen which he produced by reactions between acids (hydrochloric or sulfuric) and metals (zinc, iron, or tin). He showed the identity of the gas from all these precursors and determined its density, a challenging experiment. The second paper is on Black's fixed air, our carbon dioxide, produced from calcium or magnesium carbonates by the action of heat or acids. Determinations of density and solubility and of chemical behavior were included. The third paper on airs produced by fermentation or putrefaction identified these as either pure carbon dioxide from, for example, sugar fermented with yeast; or a mixture of gases including carbon dioxide and hydrogen from putrefying meat broth.

This one publication, with its elegant experimentation, careful observation, and accuracy brought Cavendish to the forefront of pneumatic chemistry. His work on the production of hydrogen from metals and acids indicated to Cavendish that hydrogen, one of his inflammable airs, might be pure phlogiston. Despite the work of Lavoisier and others on the oxygen theory of combustion, Cavendish through most of his career was not convinced that the experimental evidence required abandonment of the phlogiston theory.

Further chemistry followed: the most careful analysis of natural waters to date won Cavendish a Copley Medal from the Royal Society in 1766. Cavendish was also conducting experiments and observations in meteorology and devised an improved hygrometer. In his papers "Experiments on Air" published in 1784 and 1785 Cavendish examined the properties of "phlogisticated air" (nitrogen), the major constituent of ordinary atmospheric air and made one of his most celebrated observations. To use modern terminology by extended sparking of ordinary air with added oxygen the whole of the nitrogen and oxygen of atmospheric air could be removed – but a bubble remained of about 1/120th. part of the whole. In the 1890s Rayleigh and Ramsay recalled this experiment of Cavendish's in their groundbreaking work on the discovery of argon and other noble gases. As referred to in the first of these columns Cavendish also demonstrated that reaction between – again to use modern terminology – oxygen and hydrogen produced water. Others made similar observations at about the same time, including Priestley and Warltire, and James Watt, which led to a controversy about priority. Somewhat later Lavoisier repeated this synthesis of water, and also decomposed water to produce hydrogen, explaining the results in terms of oxygen theory.

While these columns are principally about Cavendish the chemist, it would not be doing justice to this great natural philosopher to omit all reference to his important work in physics. By greatly refining an apparatus devised by Mitchell, which used the torsion of wires to measure small forces, Cavendish directly measured the attractive force between two massive lead spheres which gave him the value of the gravitational constant and, indirectly, a measure of the mass and density of the earth. He published this in 1798. In contrast much of Cavendish's fundamental work on electricity, which included the concept of capacitance and an anticipation of Coulomb's law, remained unpublished until late in the 19th. century when Clark Maxwell, among other, undertook the publication of some of Cavendish's unreported work.

Finally a few words about Cavendish the man. There is only one portrait of Cavendish; a sketched likeness taken without his knowledge it shows him dressed in outdated clothes. Apart from his visits to the meetings of the Royal Society he seems to have had little or no social life, and never married. His cousin, the fifth Duke of Devonshire, warned his wife to stay away from Cavendish's laboratory because "He is not a gentleman – he works!" In his final days Cavendish suffered from a colon inflammation which obstructed the passage of his food; he died at his home in London on February 24, 1810 at the age of 78.

MARCH HISTORICAL EVENTS IN CHEMISTRY

By Leopold May, The Catholic University of America, Washington, DC

March 1, 1862

One hundred and fifty years ago, Edward Franklin was born. He was a researcher in chemistry of nitrogen system of compounds.

March 2, 1848

Phippe A. Barbier, who synthesized the first organomagnesium compound, was born on this date.

March 5, 1637

Three hundred and seventy-five years ago, John van der Heyden, who invented fire extinguisher, was born. He and his brother, Nicolaas, patented it on September 21, 1677.

March 6, 1787

One hundred and twenty-five years ago, Joseph von Fraunhofer, who discovered the dark lines in solar spectrum (Fraunhofer lines), was born.

March 7, 1827

John H. Gladstone, who was born on this date, was a researcher on refractive index of and its relationship with density.

March 9, 1912

One hundred years ago, Stanley G. Thompson was born. He codiscovered berkelium (Bk, 97), californium (Cf, 98) 1950, einsteinium (Es, 99) 1952, fermium (Fm, 100), & mendelevium (Md, 101) 1955.

March 10, 1762

Two hundred and fifty years ago, Jeremias B. Richter, who discovered the law of equivalent proportions, was born. He was the first to establish stoichiometry, the basis of quantitative chemical analysis.

March 11, 1864

Cato M. Guldberg & Peter Waage presented their paper "Studier over Affiniteten" describing the Law of Mass Action to the Norwegian Academy of Sciences and Letters on this date.

March 12, 1790

John F. Daniell, who invented the Daniell electrochemical cell, was born on this date.

March 14, 1931

Ronald C. D. Breslow, who was born on this date, demonstrated antiaromaticity; invented artificial enzymes, and used electrochemical methods to study carbon cation. He also served as President of the ACS.

March 19, 1883

Seventy five years ago in 1937, Walter N. Haworth shared the Nobel Prize in Chemistry for his investigations on carbohydrates and vitamin C with Paul Karrer for his investigations on carotenoids, flavins and vitamins A and B2. He synthesized ascorbic acid (Vitamin C) in 1933, did research on sugars and dextran as blood plasma substitute, and was born on this date.

March 23, 1962

Fifty years ago, Neil Bartlett made the first noble gas compound, XePtF6, on this date.

March 26, 1753

Count Rumford (Benjamin Thompson), who invented a simple photometer, was born on this date. He was a researcher in heat and demonstrated first law of thermodynamics. Also, he improved cooking and heating systems in addition to animal breeding. He married Antoine Lavoisier's widow to improve his position in science.

March 29, 1855

Konrad J. Bredt, who described first correct structure of camphor, Bredt's Rule for bicyclics, was born on this date.

March 31, 1831

Archibald Scott Couper, who was born on this date, developed the organic structural theory at the same time as August Kekule and was first to use bond lines for organic structures.

Additional historical events can be found at Dr. May's website, faculty.cua.edu/may/history.htm.



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Research, **Janssen
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Dr. Tom Sowin,
Senior External
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Wednesday May 9:
Exhibition, Agrichemicals
Panel & Scientific Update
Workshops



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Agenda

Monday May 7 – Wednesday May 9

Monday May 7: 10.45 Start	2nd Scholarship Golf Outing at Manufacturers' Golf & CC in Fort Washington
Tuesday May 8: 9.00am - 5.30pm	Exhibition, Pharma Outsourcing Panel
Wednesday May 9: 9.00am - 5.30pm	Exhibition, Crop Science Panel

More Information

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Chemistry As A Life Science — Symposium XV

The fifteenth in a series of CAALS biennial symposia.

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Laura Kiessling
University of Wisconsin-Madison

Marisa Kozlowski
University of Pennsylvania

Kevan Shokat
University of California
San Francisco

Erik Sorensen
Princeton University

Brian Stoltz
California Institute of Technology

Jin-Quan Yu
The Scripps Research Institute

Program

- 7:30 AM Complimentary Continental Breakfast
8:30 AM Opening Remarks
8:45 AM Brian Stoltz, California Institute of Technology
9:45 AM Kevan Shokat, University of California San Francisco
10:45 AM Welcome, Chancellor Philip Yeagle,
Rutgers University, Newark Campus
11:00 AM Laura Kiessling, University of Wisconsin-Madison
12:00 PM Lunch Break
2:00 PM Erik J. Sorensen, Princeton University
3:00 PM Marisa Kozlowski, University of Pennsylvania
4:00 PM Jin-Quan Yu, The Scripps Research Institute
5:00 PM Closing Remarks
Complimentary Wine and Cheese Reception

Date: Friday, March 16, 2012, 7:30 AM - 5:00 PM

Place: The Paul Robeson Campus Center
Rutgers, The State University of New Jersey
Newark, NJ

Cost: Free and open to the public.

Further information regarding the symposium will be added to the website for the North Jersey Section of the American Chemical Society as it becomes available. Due to limited seating, advance registration is required. <http://www.njacs.org/caals>

Organizing Committee: V. Lombardo (The Chipperson Law Group), Shawn Erickson (Hoffman-La Roche), Stan Hall (Rutgers), Darren Hansen (Rutgers), Dave Hughes (Merck), Joseph Kozlowski (Merck), William Metz (Sanofi), Michael Miller (Bristol-Myers Squibb), Wen Shieh (Novartis)

North Jersey Meetings

<http://www.njacs.org>

NORTH JERSEY EXECUTIVE COMMITTEE MEETING

The March North Jersey ACS Executive Meeting will be held in conjunction with the NoJ Mass Spectrometry Discussion Group Meeting at the Holiday Inn, Somerset, NJ on Tuesday March 20th. Social Hour starts at 5:30 with Dinner at 6:30. The executive committee meeting will begin at 7:00pm.

Executive Committee members must **pre-register** for the meeting if you plan to attend the dinner and that can be done through the Topical Group's website <http://njacs.org/msdg/index.html>.

Date: Tuesday, March 20, 2012

Times: Social Hour 5:30 PM

Dinner 6:30 PM

Executive Committee Meeting
7:00 PM

Place: Holiday Inn
Somerset, NJ

Directions can be found at hotel's website www.ichotelsgroup.com/ihg/hotels/us/en/somerset/pnenj/hoteldetail?requestid=70473



CAREERS IN TRANSITION MEETINGS

Job Hunting??

Are you aware that the North Jersey Section holds bi-monthly meetings at Students 2 Science, Inc. in East Hanover, NJ to help ACS members? Topics covered at these cost-free workshops are:

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- Ways for improving a resume
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- Conducting an effective job search
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Dates: Mondays, March 5 & 19, 2012

Times: Meeting 5:30 - 9:00 PM

Pizza snack and soda 6:30 PM

Place: Students 2 Science, Inc.
66 Deforest Avenue
East Hanover, NJ

Cost: \$5.00

Reservations: at njacs.org/careers.html

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See http://njacs.org/jobs_ifr.html for local jobs and career assistance blogs.



NMR SPECTROSCOPY GROUP

What's New in Stereochemical Determination by NMR

Speaker: Dr. R. Thomas Williamson
Merck & Co.

Date: Wednesday, March 14, 2012

Time: 7:30 PM


Place: Fuji Japanese Sushi & Seafood
1345 US Route 1
North Brunswick, NJ




CHEMISTRY AS A LIFE SCIENCE

Date: Friday, March 16, 2012

(See page 8.)





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Speaker: Dr. Chris Thompson
FTMS Applications Scientist
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As a result of the ongoing expansion in the types of mass spectrometric tools and workflows available to the scientific community, one of the toughest challenges which faces the modern user is to properly outfit themselves with the systems needed to efficiently answer analytical questions. From selection of an appropriate sample cleanup mode to an ionization strategy, to a detection technique, and a variety of post processing options, the parameter space for technique selection is seemingly infinite. The power derived from this flexibility has created a unique opportunity for expansion in mass spectrometry to a variety of application areas that have not been conventionally considered.

Historically, Fourier transform ICR mass spectrometry has been viewed as an “event horizon” platform for the early adaptation or development of many tools used today in conventional mass spectrometry, to include; electron induced dissociation techniques, electrospray ionization, top-down MS, and HDX. Many of these tools developed for the life sciences either had their genesis in, or were refined on FTMS platforms. This tradition is carried on today with the incorporation of MALDI imaging and other advanced or emerging techniques into FTMS instrumentation where these technologies can utilize the unique capabilities and spectral figures-of-merit found in FTMS to answer questions in a fashion that complements other MS strategies. While many types of mass spectrometers can provide access to workflows attributed to FTMS, none can leverage the additional dimension of ultrahigh performance that makes FTMS the most powerful and flexible tool in the mass spec arsenal.

This talk will examine how ultrahigh performance can provide definitive molecular formula determination and identification for a variety of application focus areas.

Specifically, we will look at high resolving power (>250,000 FWHM) mass spectrometry applied to a variety of workflows. In each case, the “extra” chemical information encoded in the isotopic peaks serves as a unique signature to the atomic composition of the target molecule. While methodologies based on analysis of the geometric features of unit-resolved isotopic distributions have become fashionable to overcome the degeneracy associated with mass based elemental assignment, they cannot definitively exclude the possibility of alternative atomic combinations or mixtures. Measuring the individual atomic contribution to each of these peaks can uniquely provide complete confidence formula elucidation, even for complex mass spectra.

Christopher J. Thompson holds a PhD in Physical Chemistry from the University of Massachusetts at Amherst, and a BS in Chemistry and Mathematics from Salve Regina University, Newport, RI. Since October 2003 he has been employed at Bruker Daltonics Inc., Billerica, MA, where he is now Senior Applications Developer, FTMS.

* * * * *

“Characterization of HmqF, a Protein Involved in the Biosynthesis of Unsaturated Quinolones Produced by *Burkholderia thailandensis*”

Speaker: Dr. Darren Hansen
Assistant Professor
Chemistry Department
Rutgers University
Newark, NJ

The opportunistic pathogen *Burkholderia thailandensis* produces a number of structurally similar unsaturated quinolones involved in quorum sensing. However little is known about the biosynthesis of these unsaturated quinolones. In this study we have characterized the starting point in biosynthesis of unsaturated quinolone molecules produced in *Burkholderia thailandensis*. We have shown by using in vitro enzymology and liquid chromatography/mass spectrometry that the protein hmqF is involved in the biosynthesis of unsaturated quinolones produced by *Burkholderia thailandensis*. HmqF consists of three domains; adenylation domain (A domain), dehydrogenase domain (DH domain), and an acyl carrier domain (ACP). The three domains (A, DH and ACP) were cloned and expressed

individually in *E. coli* and their reactivity was studied using HPLC/MS based assays. Our *in vitro* studies show that the A domain catalyzes ATP-dependent activation of medium chain (C6-C14) fatty acids without activation by CoA. Results from competitions assays are consistent with decanoic acid as the preferred substrate. Incubation of the ACP domain with 4'-phosphopantetheine transferase and CoA led to the formation of phosphopantetheinylated-ACP (Ppant-ACP). In Ppant ejection assay using MS/MS a mass was detected consistent with the mass of a cyclic variant of dephosphorylated Ppant. We further demonstrated that Ppant-ACP could be loaded with medium chain fatty acids in the presence of ATP and A domain. MS analysis was consistent with the formation of Ppant-ACP thiol esters of the fatty acids. MS/MS Ppant ejection experiments confirmed the loss of 2H in samples of fatty acids loaded-Ppant-ACP in the presence of DH domain. HPLC analysis of benzyl amide ligation products allowed us to conclude that dehydrogenation produced $\text{trans-}\beta,\gamma$ -unsaturation in the fatty acid chains. Our results are in good agreement with naturally observed quinolone molecules produced by *B. thailandensis*, which predominately pro-

duce 9 carbon $\text{trans-}\beta,\gamma$ -unsaturated alkyl chain quinolone molecules.

Darren B. Hansen received his BA in Chemistry and History from Rutgers College at Rutgers University in New Brunswick, NJ. From 2005-2008 he was postdoctoral fellow at Harvard Medical School. Since 2008 he has been an Assistant Professor of Chemistry at Rutgers University in Newark, NJ.

Date: Tuesday, March 20, 2012

Times: Social and Registration 5:30 PM

Dinner 6:15 PM

Seminar 7:00 PM

Place: Holiday Inn
Somerset, NJ

Cost: Free

For more information, go to:

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CHROMATOGRAPHY TOPICAL GROUP

Date: Wednesday, March 21, 2012

See www.njacs.org for more information.

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Symposium: Mass Spectrometry: New Ways to Probe Molecular Structure and Reactivity

Award Recipient: **PROFESSOR ALAN G. MARSHALL**
 Ion Cyclotron Resonance Program
 National High Magnetic Field Laboratory
 Florida State University, Tallahassee, FL

PROGRAM

- 1:30 PM **Welcome** Professor JaimeLee Iolani Rizzo
 2012 Chair, ACS, New York Section
 Pace University, NYC
- 1:35 PM **Opening of the Distinguished Symposium** Professor Philip H. Mark
 2012 Chair-elect, ACS, New York Section
 Nassau Community College - SUNY
- 1:45 PM **Accelerated Chemical Reactivity Implemented Using Mass Spectrometry** Professor R. Graham Cooks
 Purdue University
- This presentation deals with studies of chemical reactions in solution and at surfaces that are facilitated by the new ambient ionization methods of mass spectrometry. These analytical methods like desorption electrospray ionization (DESI) and paper spray ionization (PS-MS) have facilitated experiments based on reactions occurring outside the mass spectrometer at atmospheric pressure. This talk covers reactions occurring (i) in charged microdroplets generated by spray ionization, (ii) between dry organic ions and reagents on surfaces and (iii) between compounds on paper and surrounding gaseous ions. These unusual media are shown to be effective in driving and accelerating organic reactions. Bimolecular solution phase and heterogeneous reactions are a recent component of the subject, and the possibility of scaling up reactions under these conditions is noteworthy.
- 2:30 PM **Searching for Short-Lived Intermediates in Liquid Chemical Reactions** Professor Richard N. Zare
 Stanford University
- Without measurement we cannot have science, and nothing so much stimulates new measurements as inventing and perfecting new measurement devices. In this presentation I wish to describe some new directions being developed in my laboratory for the use of desorption electrospray ionization (DESI), an ambient ionization technique for mass spectrometry, which was first introduced by Prof. R. Graham Cooks and co-workers, Department of Chemistry, Purdue University. I will stress the use of DESI to record transient intermediates of solution-phase chemical reactions on the millisecond time scale. I will also describe some uses of DESI imaging to examine healthy and diseased tissue. This work has been primarily carried out by Dr. Richard H. Perry and Dr. Ali Ismail under the support of the Air Force Office of Scientific Research.
- 3:15 PM **Coffee Break**
- 3:45 PM **Mass Spectrometry Enables Chemical Footprinting and New Understanding about Proteins** Professor Michael L. Gross
 Washington University
- Our goal is a rapid, sensitive, and specific means of determining protein interactions, folding, and unfolding by using chemical footprinting coupled with MS. Driving this approach is the wide availability of mass spectrometers for analytical proteomics; these should also be applicable to protein footprinting. To this end, we are developing fast photochemical oxidation of proteins (FPOP) and hydrogen/deuterium exchange to interrogate protein interactions, interfaces, and dynamics of folding/unfolding. We will illustrate the potential of H/DX and FPOP with applications to the ApoE family of proteins, a family with important implications in Alzheimers and other diseases.

4:30 PM **Mass: The Universal Chemical Currency** **Professor Alan G. Marshall**
NICHOLS MEDALIST

It is now possible to produce, intact, a gas-phase ion, often under ambient conditions, from almost any molecule, including many not isolable or stable in solution. Ultrahigh resolution and mass accuracy enable determination of elemental composition (CcHhNnOoSs...) for mixtures as complex as petroleum crude oil, peptide amino acid composition and sequence for protein identification, nature and site(s) of protein post-translational modification(s), and mapping of binding surfaces in bio-macromolecular complexes. Recent advances in high-end instrumentation will be described, and applied to problems ranging from the Deepwater Horizon oil spill to identification of drug targets in protein assemblies. Work supported by NSF NIH (R01 GM78359), NSF Division of Materials Research through DMR-06-54118, NSF CHE-10-49753, NSF CHE-1016942, and the State of Florida.

5:45 PM **Social Hour**

6:45 PM **William H. Nichols Medal Award Dinner**

Date: Friday, March 16, 2012

Times: Registration 1:00 PM

Symposium 1:30 PM – 5:30 PM

Reception 5:45 PM

Award Dinner 6:45 PM

Place: Crowne Plaza Hotel, White Plains, NY

More information on the Nichols Medal Events is available on the New York Section's website at <http://www.NewYorkACS.org>.

Tickets may be reserved using the following form or through the New York Section website.

Please reserve _____ places for the symposium & banquet at \$120/person, ACS member
 _____ places for the symposium & banquet at \$150/person, Non-member
 _____ places for the banquet only at \$110/person, ACS member
 _____ places for the banquet only at \$120/person, Non-member
 _____ places for the symposium only at \$40/person, ACS member
 _____ places for the symposium only at \$60/person, Non-member
 _____ places for the symposium only at \$25/person, Students and Unemployed

(For table reservations of 8 or more, use the ACS member \$120/person rate for combination tickets)

Reserve a table in the name of: _____

Names of guests are: _____ Indicate numbers in your group who choose:

_____ Chicken _____

_____ Prime Rib _____

_____ Salmon _____

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BANQUET RESERVATION DEADLINE: MARCH 5, 2012

Please make checks payable to: ACS, NEW YORK SECTION
 Check for \$_____ enclosed

New York Meetings

www.newyorkacs.org

NEW YORK SECTION BOARD MEETING DATES FOR 2012

The dates for the Board Meetings of the ACS New York Section for 2012 were chosen and approved at the September 2011 Board Meeting. The meetings are open meetings – all are welcome. If non board members would like to attend the meeting, please let the New York Section office know by emailing Mrs. Marilyn Jespersen at njesper1@optonline.net or calling the office at (516) 883-7510.

The 2012 Board Meetings will be held on the following Fridays at 6:00 PM at St. Johns University, Writing Center, Jamaica, NY. Dr. JaimeLee lolani Rizzo will chair the meetings.

Friday, April 13
Friday, June 8
Friday September 14
Friday November 16

Also, please mark your calendar with the dates of the following major events.

Friday, March 16, William H. Nichols Medal Award Symposium and Dinner

More information will be posted in future issues of *The Indicator* and on the New York website at <http://www.NewYorkACS.org>.

HUDSON-BERGEN CHEMICAL SOCIETY – JOINT MEETING WITH THE RAMAPO CHAPTER OF SIGMA XI

The Annual Distinguished Lecture

Date: Wednesday, March 7, 2012
Time: 5:00 PM
Place: Ramapo College of New Jersey
Mahwah, NJ

For details and directions or to RSVP for either event please contact Sarah Carberry at sbolton@ramapo.edu.

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HIGH SCHOOL TEACHERS TOPICAL GROUP

Investigating the Evolution of Protein Structures from the Perspective of Structure Motif Building Blocks

Speaker: Mr. Joseph M. Dybas
Dept. of Systems and
Computational Biology
Dept. of Biochemistry
Albert Einstein College of
Medicine
Laboratory of Dr. Andras Fiser

Protein structure, the three dimensional shape of the folded amino acid sequence, dictate important characteristics of the protein such as function. This work explores the evolution of protein structures from the perspective of modularity of structure motif building blocks. The motif building blocks are defined as two consecutive secondary structure elements (helix or strand) that are connected by a loop. A library of motifs was compiled by collecting the constituent motifs from all known proteins and classifying and grouping the motifs by their specific shape. The library is complete and sufficient to build any existing or novel structure. The goal is to ascertain the rules by which these motifs are selected and combined in evolution to produce the repertoire of structures in the protein structure space. The distribution of motifs found in various types of protein structures suggests a continuous structure space and can elucidate evolutionary relationships between protein structures. This knowledge has practical implications in addressing many problems in protein structure biology, including structure classification, computational modeling, protein design and function prediction.

Date: Friday, March 16, 2012
Time: Social and Dinner — 5:45 PM
Place: M&G Pub (Murphy and Gonzales)
21 Waverly Place
(at Green Street, North-east corner)
New York, NY
No reservations required
Time: Meeting 7:15 PM
Place: New York University
Silver Center Room 207
32 Waverly Place (South-east
corner Washington Sq. East)
New York, NY

Security at NYU requires that you show a picture ID to enter the building. In case of unexpected severe weather, call John Roeder, 212-497-6500, between 9 AM and 2

PM to verify that meeting is still on; (516) 385-4698 for other info.

Note: Street parking is free after 6:00 PM. For those who prefer indoor attended parking, it is available at the Melro/Romar Garages. The entrance is on the west side of Broadway just south of 8th Street, directly across from Astor Place. It is a short, easy walk from the garage to the restaurant or meeting room.



BIOCHEMICAL TOPICAL GROUP – JOINT MEETING WITH THE NYAS BIOCHEMICAL PHARMACOLOGY DISCUSSION GROUP



The Pharmacology of Aging: Why Age Matters

Organizers: Seongeun (Julia) Cho, PhD
US Food and Drug Administration

Jennifer Henry, PhD
The New York Academy of Sciences

Speakers: Darrell R. Abernethy, MD, PhD
US Food and Drug Administration

Angela Birnbaum, PhD
University of Minnesota

Jenny Y. Chien, PhD
Eli Lilly

Jeremy D. Walston, MD
Johns Hopkins University School of Medicine

Molly E. Zimmerman, PhD
Albert Einstein College of Medicine

Aging is a complex and multi-dimensional process involving various intrinsic and extrinsic factors. In general, older individuals have high disease burden and are the major users of medications; yet they are often not well-represented in clinical trials studying

investigational drugs, even for those that have high utility in this age group. Considering significant age-dependent changes in physiology, pharmacology and psychiatric functions, we need adequate clinical data in this population to appropriately assess the benefit/risk of medical treatments. In this symposium, the speakers discuss the patho/physiology of aging, key clinical pharmacology considerations for older individuals, and regulatory and industry perspectives on geriatric clinical drug development strategy.

Older individuals are the major users of many medications, yet clinical data to support evidence-based therapy are often lacking. This symposium presents clinical, regulatory and industry considerations in investigating drugs for older patients.

Date: Tuesday, March 27, 2012

Time: 1:00 – 5:00 PM

Place: New York Academy of Sciences
7 World Trade Center
250 Greenwich Street – 40th Floor
New York, NY 10007

Cost: This event is FREE for ACS and NYAS members. Please select the appropriate non-member Registration Category and use the Priority Code ACS. Non-members may attend for a fee of \$30, or \$15 for students and post-docs.

For more information and to register for the event, go to:

www.nyas.org/AgingPharmacology

To become a Member of the Academy, visit www.nyas.org/benefits



EMPLOYMENT AND PROFESSIONAL RELATIONS COMMITTEE OF THE NEW YORK SECTION

To Human Resources Departments in Industry and Academia

The Employment and Professional Relations Committee maintains a roster of candidates who are ACS members seeking a position in the New York metropolitan area. If you have job openings and would like qualified candidates to contact you, please send a brief job description and educational/experience background required to hessytaft@hotmail.com.

Candidates from our roster who meet the requirements you describe will be asked to contact you.

WESTCHESTER CHEMICAL SOCIETY

SPECIAL SEMINAR - The Role of TSG-6 Protein in Extracellular Matrix Remodeling Associated with Inflammation and Fertility

Speaker: Georg Wisniewski
Department of Microbiology
School of Medicine
New York University

TSG-6 protein is a highly conserved protein involved in inflammatory processes, ovulation, and innate immunity. TSG-6 expression is induced by pro-inflammatory cytokines in many cell types, and by certain hormones and growth factors in a tissue-specific manner. Both the spatial and temporal pattern of TSG-6 expression is tightly controlled. TSG-6 interacts with the constitutively expressed plasma protein inter-alpha-inhibitor and with hyaluronan, a ubiquitous glycosaminoglycan in the extracellular matrix of most tissues. TSG-6 transfers a subunit of inter-alpha-inhibitor to hyaluronan, forming covalent hyaluronan-protein complexes. These are the only covalent hyaluronan-protein complexes currently known. These complexes have been associated with stabilization of hyaluronan and protection of the structural integrity of the extracellular matrix during conditions of stress. TSG-6 has shown potent anti-inflammatory and tissue-protective activities in experimental models of acute inflammation and autoimmune arthritis. TSG-6 is produced in large quantities by mesenchymal stem cells and it mediates some of their therapeutic effects.

Dr. Wisniewski is an Associate Professor in the Department of Microbiology at the NYU School of Medicine. His research is focused on the damage to and the remodeling of the extracellular matrix, in particular in cartilage,

during inflammation and related pathologic processes, including rheumatoid arthritis and osteoarthritis, and in the identification of biomarkers that characterize the disease process, predict progression and thereby help to improve medical decision making.

Date: Wednesday, April 11, 2012

Times: Refreshments 5:30 PM

Lecture 6:00 PM

Place: Westchester Community College
75 Grasslands Road
Gateway Building Room 110
Valhalla, NY

Cost: Free and open to the public



For more information, contact Paul Dillon:

E-Mail paul.dillon@siemens.com

Phone 1-914-524-3313



ACS NY SECTION—60TH ANNUAL UNDERGRADUATE RESEARCH SYMPOSIUM (URS)

	60th	ANNUAL UNDERGRADUATE RESEARCH SYMPOSIUM
The New York Chemistry Students' Association Student Affiliate Committee – New York Section American Chemical Society		
Saturday, May 5th, 2012 at SUNY College at Old Westbury		
8:00 am – 3:00 pm (brk kfast, luncheon and award reception included) Sign up as an attendee at http://www.newyorkacs.org/meetings/urs/urs.php		
<i>Keynote Speaker</i>		
Prof. Louis E. Brus Dept. of Chemistry, Columbia University, New York		
The highlight of this year's symposium is the Keynote Address to be delivered by Prof. Louis Brus of Columbia University, New York.		
<small>The Keynote Address will be followed by original research presentations given by students from colleges and universities throughout the tri-state area.</small>		

Nanoscience: Semiconductor Quantum Dots and Carbon Nanotubes

Speaker: Prof. Louis E. Brus
Dept. of Chemistry
Columbia University, NY



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The talk is aimed for a broad audience. I describe the chemistry and physics of semiconductor nanocrystals and carbon nanotubes. Both materials are intermediate between molecules and crystalline solids in their electronic properties. Simple molecular orbital ideas help us to understand the size dependence of their properties. Novel synthesis is the key to scientific progress in both materials. Rigorous understanding and characterization requires that the properties of single nanocrystals and tubes be observed.

The Keynote Address will be followed by original research presentations given by students from colleges and universities throughout the tri-state area.

Date: Saturday, May 5, 2012.

Times: 8:00 AM - 3:00 PM

Place: SUNY College at Old Westbury
Old Westbury, NY

Cost: FREE Registration for student members of the National ACS, faculty mentors who register in advance and sponsors. For non-ACS members and guests, the registration is \$35 in advance. All on-site registration is \$45 for faculty, staff and guests. Breakfast,

luncheon and award reception included.

Checks for the registration fee should be made out to: "NY ACS URS" and sent to:

Prof. Justyna Widera, Adelphi University,
Department of Chemistry, 1 South Avenue,
Garden City, NY 11530

In order to receive the advanced registration benefits, checks need to be **received by April 21, 2012. Early registration fee (Deadline April 11th).**

If you have any questions please contact:
nyacsurs2012@gmail.com or
widera@adelphi.edu (516) 877 4135

2012 URS Committee

**SIGNIFICANT DATES FOR 60TH URS
Deadline for Abstract Submission -
March 7, 2012.**

**Notification of the abstract acceptance
will be announced by April 4, 2012.**

**Deadline for Symposium Advanced
Registration - April 11, 2012**

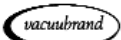
E-mail questions to:
nyacsurs2012@gmail.com

2012 URS Committee

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Call for Nominations

EDWARD J. MERRILL AWARD FOR OUTSTANDING HIGH SCHOOL CHEMISTRY TEACHER FOR 2011

Now is the time to begin thinking about nominations for the Edward J. Merrill Award, North Jersey Section, for Outstanding High School Chemistry Teacher for the year 2012.

Go to the web site, njacs.org under education and obtain your preliminary nomination form and guidelines. The full packet takes time to do a good job!

We all know an outstanding high school chemistry teacher. Perhaps one from your town, your son's or daughter's teacher or just one that you have heard about or worked with at some point. The award carries \$500 for the teacher, \$500 in supplies for the teacher's classroom and a plaque to display at home or in the classroom.

Any questions or help needed contact Bettyann Howson, chemphun@optonline.net.

Call for Volunteers

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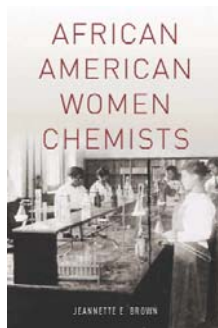


Students 2 Science is a new non-profit organization operating a large, modern analytical chemistry laboratory for the sole purpose of hosting Middle and High School students. Students work with local scientists and operate sophisticated laboratory instruments like spectrophotometers and chromatographs. The students solve real-life business puzzles and acquire an increased excitement and enthusiasm for studying science (STEM). We make science less intimidating, resulting in more students choosing to pursue STEM related careers. We are looking for volunteers to serve as Mentors, Instructors and Teaching Assistants. Hours are 8:30 to 2:30 on days when students are present.

To register, visit our website at www.students2science.org, and click REGISTER, or call (908) 334-8435. Thank you in advance for your support!

Others

Jeannette Brown's Book, African American Women Chemists, to be featured



Jeannette Brown has finally published her first book, *African American Women Chemists*. It is published by Oxford University Press and is available at most book stores now, either on the shelf or by special order. It can be ordered on Amazon.com as well. It is available in print form or kindle or

nook. She is trying to get it on books on tapes because she has two cousins who are legally blind and she would like to have them read it.

The book is about the lives of 25 African American women chemists whose work was hiding in plain sight! Do you know that an African American woman holds the patent on a Nitrate explosive detector which is used by Homeland Security at the air port? Here name is Betty Harris and her life is in the book. Did you know that a young woman developed a medicine for leprosy that scientists with more experience could not do? Her name is Alice Ball and her story is in the book and also in Chem Matters. The life of Allene Johnson, a North Jersey ACS member and award winning high school teacher is also detailed in the book

There will be a book signing on **March 27, 2012**, at the American Chemical Society National Meeting, San Diego California.

She is working on other book signings nationwide to be held at the ACS Regional Meetings.



AMERICAN INSTITUTE OF CHEMICAL ENGINEERS (AIChE)

Chemical Engineers to Gather in Houston in April to Discuss Energy, Safety Developments

Speaker: Michael J. Dolan
Exxon Mobil Corporation

AIChE's Spring Meeting and 8th Global Congress on Process Safety is expected to draw nearly 2,000 chemical engineers with lectures, 9 topical conferences and hundreds of technical sessions. The Spring Meeting

keynote address on **Monday, April 2** will feature Michael J. Dolan, Senior Vice President of ExxonMobil Corporation. Dolan's speech, "Process Safety and Corporate Responsibility" ties together safety and sustainability, two of the major topics of the spring meeting.

The Global Congress on Process Safety covers the critical needs of process safety practitioners more broadly and deeply than any other conference.

A wide range of subjects relevant to the current needs of industry will be featured. In addition to the Global Congress on Process Safety, energy advances will be at the forefront of much of the conference, given Houston's importance to the energy industry. Other highlights of the meeting include:

- § 24th Ethylene Producers' Conference
- § 12th Gas Utilization Topical Conference
- § 15th Topical Conference on Refinery Processing
- § 1st International Conference on Upstream Engineering and Flow Assurance
- § Advances in Sustainability
- § Fossil Energy Utilization
- § More

AIChE will update content on its social media channels throughout the Spring Meeting. News, photos, videos, special event and keynote coverage is available at www.chenected.com/spring. Facebook (www.facebook.com/chenected) and Twitter feeds (@[chenected](https://twitter.com/chenected)) will have regular updates direct from the meeting. The official hashtag for the meeting is #AIChESpring.

Date: Sunday, April 1 – Thursday, April 5, 2012

Place: Hilton-Americas Houston and George Brown Convention Center Houston, TX

For more information about the conference or related workshops and meetings, please go to: <http://www.aiche.org/spring>

Editor's Note: Journalists interested in covering the conference should contact Danielle Gross at dgross@thebravogroup.com



NJIT – DEPARTMENT OF CHEMICAL, BIOLOGICAL AND PHARMACEUTICAL ENGINEERING

Graduate Seminar Series – Spring 2012

Sponsors: Infineum USA L.P. and ConocoPhillips Bayway Refinery

March 5

"The Need for Systems Thinking to Solve 21st Century Challenges"

Professor Sven G. Bilén

Engineering Design, Electrical Engineering and Aerospace Engineering
The Pennsylvania State University, PA

March 26

"Solubility and Thermodynamics of Pharmaceutical Systems"

Professor Yee C. Chiew

Department of Chemical & Biochemical Engineering
Rutgers University
Piscataway, NJ

Times: Refreshments 2:30 PM

Seminars 2:45 PM

Place: NJIT, Room 117, Kupfrian Hall
Newark, NJ

Cost: Free and Open to the Public

Seminar Coordinator: Professor Laurent Simon, (973) 596-5263,

laurent.simon@njit.edu

Education

DREW UNIVERSITY MADISON, NJ

Residential School on Medicinal Chemistry: Biology and Chemistry of Drug Discovery

Date: Monday-Friday, June 4-8, 2012

The Residential School offers an intensive weeklong graduate-level course organized to provide an accelerated program for medicinal chemists, biologists and other industrial and academic scientists who wish to broaden their knowledge of drug discovery and development. The aim of the school is to concentrate on the fundamentals that are useful in drug discovery spanning initial target assay evaluation through clinical development. Several case histories of recent successful drug development programs will also be presented. The five-day program consists of lectures, seminars and case histories.

For more information and application forms visit our website, www.drew.edu/resmed, email resmed@drew.edu, phone (973) 408-3787 or fax (973) 408-3504.

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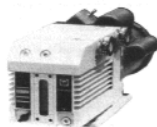
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