Monthly Meeting
A Medicinal Chemistry Symposium at Sanofi Genzyme, Waltham

Report from Binghamton
By Morton Z. Hoffman

Summer Scholar Report
By Amanda Carey and Michelle Foster

NSYCC Collaborative Symposia
By Catherine Rawlins
At the November meeting Roy Hagen was presented with the 2016 Arno Heyn Memorial Book Prize. The prize honors long-time Nucleus Editor and NESACS Board member, Arno H. A. Heyn, who edited the Nucleus for 16 years and passed away in December 2004.


Roy Hagen graduated in 1968 with a Bachelors Degree in Music Education and Masters Degree in Music Theory and Composition in 1981. He taught in the Salem, Massachusetts, Public Schools for 34 years until he retired in 2003.

During his first seven years in Salem, he taught music. In 1984 he began teaching TV Studio Production at the high school. Many of his TV Studio students went on to pursue careers in television at CNN, Fox, ESPN, and several movie studios, some as producers and others as editors.

Through his work with his TV Studio Production he began incorporating computers into the classroom for graphics and animation. As an early adopter of computers in the classroom, he found his peers looking to him for support in their efforts. For his last seven years in Salem he served as the District Technology Director, bringing computers and networking into all schools and providing staff development. He learned web design as part of his duties, creating and maintaining the school district’s website.

Upon retirement from education in 2003, he continued designing websites. His clients include a South Shore lawyer, a building and remodeling company, a plumbing and heating contractor, a Boston Symphony Orchestra member who sells and repairs basses, and several musicians and musical groups.

He began in July 2007, at the request of Vivian Walworth and under the direction of David Cunningham, working on the NESACS website. The first order of business was to redesign the website. The National ACS Meeting was in Boston that summer in August and the goal was to have the new website live in time for the meeting. Under David’s supervision and with input from Vivian and the Board of Publications, the website was changed from a newspaper-like format to a more graphical design, and was up and running in time for the National Meeting.

David provided guidance the first year. Everything to be posted would go through David, and he or Marilou Cashman would forward it to Roy for posting. In the spring of 2009, a survey was posted on the website at the request of Vince Gale, and some changes were made to the Home Page as a result of the feedback.

In the spring of 2010, David moved to Hawaii, and Roy began to work directly with the new Administrative Coordinator, Anna Singer, and the people who sent him items for posting. He now reported to the BOP, informing them of all the postings, and requesting information from them.

In early 2009, Larry Hardy of Sunovian Pharmaceuticals asked Roy to...
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Cover: Professor Bassam Shakhshiri (University of Wisconsin) with Doris Lewis (Suffolk University and NESACS) and David Sittenfeld (Boston Museum of Science) at the annual Phyllis A. Brauner Memorial Lecture presented by Professor Shakhshiri. (Photo by Morton Z. Hoffman).

March 2017 Issue: January 15, 2017

THE NUCLEUS

The Nucleus is published monthly, except June and August, by the Northeastern Section of the American Chemical Society, Inc. Forms close for advertising on the 1st of the month of the preceding issue. Text must be received by the editor six weeks before the date of issue.

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Report from Binghamton

Morton Z. Hoffman, Chair, NERM Committee, and NESACS Representative to NERACS [hoffman@bu.edu]

NERM 2016
With almost 950 registrants, including high school teachers and students, and more than 640 abstracts, the 41st ACS Northeast Regional Meeting (NERM 2016; Chemistry at the Crossroads of Energy and Life), which was hosted by the Binghamton Local Section in celebration of its 75th anniversary, took place on October 5-8 at the DoubleTree Hotel in downtown Binghamton, NY. The full program of the meeting is available online at <http://nerm2016.sites.acs.org/>.

Among the registrants were approximately 400 undergraduates, graduate students, and postdoctoral research associates. The General Chair for NERM 2016 was Wayne Jones (SUNY Binghamton); Christof Grewer and Nik Dimitrov, also of Binghamton University, were the co-Program Chairs.

In attendance at NERM were members of the ACS Board of Directors (Laura Pence: District I; Ingrid Montes, Dorothy Phillips, and Kathleen Schulz: At-Large) and Allison Campbell, ACS President-Elect.

The meeting started on Wednesday afternoon with a keynote lecture by Susan Band Horwitz of the Albert Einstein College of Medicine, Yeshiva University, on “Taxol, Tubulin and Tumors: A Study in Drug Development,” which was followed by the opening night social mixer, graduate school fair, exhibition with 20 exhibitors, and poster sessions, including those for undergraduate research. The next three days were filled with many symposia, technical sessions, and workshops.

Catherine Rawlins (Northeastern University), Chair of the Northeastern Section Younger Chemists Committee (NSYCC), organized a symposium on “Navigating ACS and Your Career: A Guide for Young Chemists” that featured talks by Jens Breffke (NIST), Glen Labenski (Ortho Clinical Diagnostics), Dan Sykes (Pennsylvania State University), Jennifer Maclachlan (PID Analyzers), and Thomas Gilbert (Northeastern University).

In addition, Jennifer Macalachlan organized a two-session program of oral presentations on “Small Chemical Businesses,” and gave two talks. This reporter spoke in a chemical education session about collaborations in the Middle East facilitated by the Malta Conferences.

Mindy Levine (University of Rhode Island, NESACS Chair-Elect Designate) was the featured speaker at the Women Chemists Committee Luncheon on Thursday; the title of her talk was, “Balancing the Equation of Professorship, Parenting, and Personal Satisfaction as a Female Chemistry Professor.”

At the Awards Banquet on Friday night, Allison Campbell spoke about her personal history that led to her present position as Associate Laboratory Director for Earth and Biological Sciences at the Pacific Northwest National Laboratory. NESACS was then recognized with three honors. The E. Ann Nalley Northeast Region Award for Volunteer Service to the ACS was presented to Jack Driscoll (PID Analyzers); the Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences went to Mindy Levine. The Green Chemistry Commitment: Beyond Benign, Inc., of Wilmington, MA, and the local colleges and universities that collaborate in the program won the Marinda Wu Partners for Progress and Prosperity-Northeast P3 Award. In addition, Tracy Suggs (Vestal, NY, Senior High School) received the ACS Division of Chemical Education Northeast Region Award for Excellence in High School Teaching; the award consisted of a plaque and a check from CHED of $1,000.

NERM 2016 took place in conjunction with the 28th Electronics Packaging Symposium and Workshop.

NERACS Board Meeting
The Board of Directors of the Northeast Region of the ACS, Inc. (NERACS) met on Saturday morning during NERM. Serving on the NERACS Board are representatives of the constituent local sections in the Northeast Region (Binghamton, Central Massachusetts, Central New York, Connecticut Valley, Cornell, Corning, Eastern New York, Green Mountain, Maine, Mid-Hudson, New Haven, Northeastern, Northern New York, Penn-York, Rhode Island, Rochester, Western Connecticut, Western New York) and its officers (Chair: Anthony Noce, Eastern New York; Vice Chair: Willem Leenstra, Green Mountain; Secretary: Alyssa

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2015 NESACS Sponsors

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Meeting Sponsors

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Our editor by calling and saying you appreciate the quality and content of our newsletter. Our editor works hard to maintain a publication of interest to our membership. Oh, and by the way you could also give credit to our advertisers who financially support us.
Monthly Meeting
The 965th Meeting of the Northeastern Section of the American Chemical Society
A Medicinal Chemistry Symposium organized by the Medicinal Chemistry Section of NESACS
Drug Discovery: From Compound to Clinic
Thursday, December 8, 2016
Sanofi Genzyme
153 Second Avenue, Waltham, MA 02451
Northeastern Conference Room
3:00 pm Refreshments
3:15 pm Welcome, Raj Rajur, Med Chem Program Chair, Creagen, Woburn, MA
3:20 pm Introductory Remarks, Daniel Elbaum, Retrophin Inc., Cambridge, MA
3:30 pm Erik Hett, Biogen, Cambridge, MA
Title: What is your MOA? Target Deconvolution of a Phenotypic Screen
4:15 pm Andrew Fensome, Pfizer, Cambridge, MA
Title: Inhibition of Autoimmune Pathways with Dual Inhibition of JAK1 and TYK2: Discovery of PF-06700841
5:00 pm Maria Beconi, Retrophin, Inc., Cambridge, MA
Title: “Beyond Discovery—Identifying and Managing Liabilities”
6:00 pm Social Hour
6:45 pm Dinner
7:45 pm Keynote Presentation: Mark Munson, Sanofi, Waltham, MA
Title: Visualizing Aggregate Data to Support Decisions in Medicinal Chemistry

YOU MUST REGISTER IN ADVANCE TO ATTEND THE SYMPOSIUM; THERE IS NO REGISTRATION FEE. DINNER RESERVATIONS ARE REQUIRED.

THE PUBLIC IS INVITED

NESACS BOARD MEETING: The Board Meeting will be held from 4:30-5:30 PM. at Celtics Conference Room.

• For those who would like to join us for dinner, register by noon, Thursday, December 1, using PayPal: http://acssymposium.com/paypal.html. Select the pay with credit or debit card option and follow the additional instructions on the page. Cost: Members, $30; Non-members, $35; Retirees, $20; Students, $10. Dinner reservations not cancelled at least 24 hours in advance must be paid.

• If you wish to join us for this meeting and not eat dinner, please register by noon, Thursday, December 1, using PayPal: http://acssymposium.com/paypal.html. Select “Seminar only”. The fee is $1.

• New members or those seeking additional information, contact the NESACS administrative coordinator, Anna Singer, at secretary@nesacs.org or at (781) 272-1966 during regular business hours only.

Speaker Biographies and Abstracts:

Erik Hett, Ph.D
Abstract: Cellular phenotypic screens are a powerful way to uncover novel biology and discover druggable targets and chemical matter. One of the main bottlenecks for this approach, as opposed to target-based screening, is determining the mechanism of action of lead hits. Our group is developing approaches to determine the MOA of lead hits. These approaches include using proteomics, RNAi, RNAseq, chemical probes, and in silico studies. We have utilized chemical proteomics and RNAi to unveil the mechanism of a lead series for the project to be inhibition of a kinase that was not previously known to be involved in the pathway. This finding reveals unexpected biology in regards to regulation of this pathway.

Biography: Dr. Erik Hett received his Ph.D. from Harvard University in the lab of Dr. Eric Rubin, studying protein-protein interactions important for mycobacteria. His postdoctoral research was conducted in the lab of Dr. Deborah Hung at Harvard, Broad Institute and Massachusetts General Hospital, where he conducted phenotypic HTS and utilized chemoproteomics for target ID. He previously was a chemical biologist in the MedChem Department at Pfizer and is currently leading a chemical biology team in the mechanisms and pathways group at Biogen.

Andrew Fensome, Ph.D
Abstract: The Janus (JAK) kinases are a family of four non-receptor tyrosine kinases that modulate cytokine signaling through the Signal and Transduction of Transcription (STAT) pathways. The JAK kinases (JAK1, JAK2, JAK3 and TYK2) are important in both the innate and adaptive immune system, in a variety of cell types, for example lymphocytes.
Summer Scholar Report

Replicating Prebiotic Astrochemistry Through the Use of a Silicate Grain Surface Analog

Amanda Carey* and Michelle Foster, Department of Chemistry, College of Science and Mathematics, University of Massachusetts Boston, 100 Morrissey Boulevard, Boston, MA 02125

Through the use of a silicate grain surface analogue, it is possible to replicate the prebiotic astrochemical processes that occur in dark interstellar clouds for terrestrial examination. Silicon dioxide was chosen as a substrate not only due to its abundance in these clouds but also because it is generally inert. SiO₂ nano- and microparticles were subjected to water under controlled conditions, and monitored using diffuse reflectance Fourier transform spectroscopy, allowing for a comparative study of how reactions occur at their surfaces. It was determined that undiluted nanoparticles are a favorable surface analog.

I. Introduction

Astrochemistry is the study of the formation, interaction, and destruction of elements and molecules in space. One main area of astrochemistry is the study of reactions that occur in the interstellar medium where gas clouds are cold, diffuse, and rich in simple gas phase species. When dust grains (mineral in nature such as silicon, carbon, etc.) travel through these clouds, gas molecules attach to the surface of the dust grains and through either radical or thermal activation, react on the surface of the dust grains which are acting as catalytic surfaces. These reactions are theorized to eventually produce the simple sugars or even amino acids that could then attach to passing meteors or asteroids and react further to produce simple but biologically relevant molecules.

Herbst discusses the molecular nature of the interstellar medium and its contribution to observable astrochemical processes as well as the surface assisted formation of molecular hydrogen.¹ Spectroscopic data suggests molecular hydrogen exists in the interstellar medium in concentrations 10⁴ times greater than that of atomic hydrogen. There must be some other plausible pathway of formation for H₂ other than three-body collision given that the densities and temperatures in the interstellar medium are so low. The formation of molecular hydrogen and other small molecules is thought to follow the Langmuir-Hinshelwood surface mechanism where physisorbed hydrogen atoms move from lattice site to lattice site on the grain surface until they collide with another hydrogen atom, reacting to create molecular hydrogen. As chemists, we can mimic and observe these surface processes in an attempt to better understand the chemical transformations that occur in the interstellar medium.

Silicon dioxide has been chosen as a substrate due to not only its inertness but also its abundance in the interstellar medium. Other possible substrates include solid NH₃, solid H₂O, and amorphous carbonaceous compounds.² Exposing SiO₂ micro- and nanoparticles to simple but abundant molecules such as water under controlled conditions allows for the observation of the reactions as they would occur in interstellar space. Particle size (5 nm-250 nm) and shape (amorphous)

has been chosen based on interstellar spectroscopic data outlined by Draine.³ Similar studies using SiO₂ nanoparticles and Fourier transform infrared (FTIR) spectroscopy were performed by Dawley et al. to mimic processes that occur in the atmosphere of Saturn’s largest moon, Titan.¹, ⁴, ⁵

Because it is surfaces that are being studied, it is necessary to choose a surface-sensitive technique for analysis. FTIR spectroscopy, or more specifically, diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), is often used in surface studies because each infrared absorption band is characterized by three independent parameters: frequency, intensity, and width.⁶ Most other commonly used techniques measure average properties but infrared techniques can be used to measure specific functionalities directly. Qualitative changes in intensity correspond to the behavior of physisorbed molecules, which may change the frequency at which a feature appears in the spectrum. The width of a peak corresponds to the homogeneity of surface groups; a narrow band indicates a more homogenous environment and a broad band indicates a wide array of geometric arrangement.

Water was chosen as the main adsorbate in this study given that the hydrogen bonds are largely electrostatic and are therefore driven by Coulombic attractions.⁷ Water is also known to exist in all of its phases in space but largely as an ice mantle, either on its own or at the surface of a grain like the ones mentioned here. This study aims to characterize an acceptable grain analog for DRIFTS studies that replicate prebiotic astrochemical processes that occur in cold interstellar clouds as a result of small gas phase molecules and amorphous dust grains as outlined by Herbst.¹

II. Methods

Two SiO₂ samples were analyzed: microparticles (Acros Organics, 150-420 nm, 50 m²/g) and nanoparticles (Sigma Aldrich, 7 nm-14 nm, 175-420 m²/g). The microparticles were diluted to 0.025% in spectral grade KBr (Sigma Aldrich) and the nanoparticles were diluted to 1% in spectral grade KBr. The nanoparticle and microparticle samples were put into Nicolet iS50 FTIR (Thermo Scientific) equipped with a Praying Mantis DRIFTS accessory and coupled with an in situ high temperature reaction chamber (Herrick). The reaction chamber was connected to a gas-handling manifold and recirculating water bath capable of not only introducing known pressures of gases but also evacuating the chamber to 10⁻³ torr and heating and cooling the sample in situ before and after exposure. The samples were exposed to deionized H₂O that had undergone five freeze-pump-thaw cycles at room temperature, and spectra were collected as a function of exposure. The pressures were monitored.
Summer Scholar Report
Continued from page 6

using baratron pressure gauges coupled to a PR 4000 display (MKS). The spectrometer has a liquid N₂ cooled mercury cadmium telluride (MCT) detector and the system is purged with gaseous N₂ to ensure an inert environment. All spectra reported were collected and analyzed using OMNIC version 7 software with 4 cm⁻¹ resolution and 128 scans per spectrum.

III. Results and Discussion

Figure 1 shows the DRIFTS spectra, using a gold foil background, for the OH bending region of SiO₂ for both the nano- and microparticles after the samples had been evacuated overnight. The broad peak centered at 3150 cm⁻¹ present in both samples indicates that native water is molecularly adsorbed, likely to the KBr that was used to dilute the silica. The nanoparticles show an additional sharp feature at 3745 cm⁻¹, which is indicative of free hydroxyls, or Si-OH bonds. This means that the nanoparticles provide a more advantageous catalytic surface than the microparticles would be able to provide and thereby a more favorable surface for this study.

Figure 2 shows the spectra for both 1% nanoparticles in spectral grade KBr and undiluted nanoparticles. The spectrum of pure SiO₂ nanoparticles shows they are strong absorbers of infrared light below 2250 cm⁻¹ and therefore must be diluted with an ionic salt to examine lower energy transitions such as the bending mode of adsorbed water at ~1630 cm⁻¹. The downside to using an ionic salt diluent is its hygroscopic nature, as shown by the OH stretching feature in the red spectrum, and in all the diluted samples, at 3150 cm⁻¹, indicative of water adsorbed to KBr. This water is on the substrate even after the substrate has been heated to 750°C. The silanol feature in the diluted sample is also much less intense with respect to the low energy Si-O band.

To further prove the adverse effect of the ionic salt diluent, Figure 3 shows the DRIFTS of OH stretching region for diluted SiO₂ nanoparticles as a function of exposure to water. Features grow in at 3444 cm⁻¹, 3230 cm⁻¹, and 3113 cm⁻¹ while the isolated silanol at 3744 cm⁻¹ appears to shrink.

In order to quantify these observations, adsorption isotherms were constructed using the normalized peak heights, which were plotted as a function of water pressure for each of the four features as shown in Figure 4. The isotherms confirm that the Si-OH peak does decrease, which could be due to the physisorbed water masking the silanol groups at the surface. The feature at 3444 cm⁻¹ is due to water adsorbing to the SiO₂ and the peak at 3113 cm⁻¹ is due to water adsorbing to KBr. The feature at 3230 cm⁻¹ follows a similar trend to the 3444 cm⁻¹ (H₂O/SiO₂) feature, indicating it is probably due to water on silica and not KBr.

Figure 1: DRIFTS of the OH stretching region of SiO₂ for both the nano- and microparticles. The spectra show similar broad OH stretching features but the nanoparticles exhibit a sharp Si-OH feature at 3745 cm⁻¹.

Figure 2: DRIFTS of SiO₂ nanoparticles in both pure, undiluted form (black) and diluted in KBr (red). The sample was diluted to examine the water bending features around 1630 cm⁻¹, but the silanol became less intense and adsorbed water is present even after heat treatment, as shown by the bump around 3150 cm⁻¹.

Figure 3: DRIFTS of OH stretching region for diluted nanoparticles as a function of exposure to water. Features grow in at 3444 cm⁻¹, 3230 cm⁻¹, and 3113 cm⁻¹ while the isolated silanol at 3744 cm⁻¹ appears to decrease with increased exposure.

Figure 4: Adsorption isotherms for 1% nanoparticles in KBr as a function of exposure to gas phase water. The isotherms confirm that the peaks at 3444 cm⁻¹, 3230 cm⁻¹, and 3113 cm⁻¹ increase while the isolated silanol at 3744 cm⁻¹ decreases.

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The year 2016 has been busy for the NSYCC; we hosted more events this year than we ever have previously! We had two successful symposia this Fall where we got the chance to collaborate with other committees in NESACS.

On September 28th at Boston University’s Metcalf Science Center, we hosted a symposium entitled, “Science Diplomacy, Policy, and Advocacy: The Impact of Scientists Beyond the Bench.” The idea for this symposium began with a conversation with Mort Hoffman after I saw his presentation about his work with the Malta Conferences Foundation earlier this year.

We decided to make this symposium a Senior Chemists and Younger Chemists Committee collaboration. The goal was to spread the knowledge of what science diplomacy and policy is and, hopefully, invigorate younger “chemists” interest in this subject.

Emily Lewis, NSYCC Chair 2013-14, shared her experience in Washington D.C. with two consecutive fellowships as an ACS Congressional Fellow and an AAAS Science and Technology Policy Fellow. With her Ph.D. focusing on energy science she was able to help form a bill that would help cut methane emissions from oil and gas drilling.

Doris Lewis of the NESACS Government Affairs Committee shared her insights from years of advocating at the State House in Boston and Capitol Hill. She showed how the Act4Chemistry program through ACS is one of the simplest ways to advocate for science funding and policy that affects all of us.

Doris Lewis of the NESACS Government Affairs Committee shared her insights from years of advocating at the State House in Boston and Capitol Hill. She showed how the Act4Chemistry program through ACS is one of the simplest ways to advocate for science funding and policy that affects all of us.

In addition, the NSYCC organized its first symposium at the Northeast Regional Meeting (NERM) in Binghamton, NY, on October 8th. This symposium, entitled “Navigating ACS and Your Career: A Guide for Young Chemists,” was meant to show young chemists in attendance the value of volunteering through ACS and how it can benefit their career. However, many do not know how the ACS structure works and what opportunities are available, which is what we hoped to introduce.

The speakers were organized by the Younger Chemists Committee, Local Section ACS involvement, and National ACS activities to highlight the different ways you can contribute to ACS as a member. Jens Breffke, a Postdoctoral Researcher at NIST, spoke about his experience with the German Chemical Society’s young chemists group (JCF), which is how he became connected to ACS through the German Exchange Program. He served on the National YCC and now the International Affairs Committee. It was inspiring to hear how volunteerism and ACS involvement, have influenced his life along the way.

For Local Section involvement we invited Glen Labenski, Chair of the Rochester Section, and Dan Sykes, Chair of the Central Pennsylvania Section, to share their perspectives. Glen talked about the ways ACS has impacted his career and how the Rochester Section promotes chemistry education and career opportunities to its members.

Dan gave some excellent advice on how to better market your resume for jobs in industry and the need for more support to ACS members who seek careers outside of academia. Representing NESACS and national ACS involvement were Jennifer Maclachlan and Thomas Gilbert; they have both been on many National committees and have a lot of experience. From Jennifer’s talk, we learned how she uses so-
hematopoetic cells and structural cells (keratinocytes and fibroblasts). The current work describes the discovery of a series of selective JAK1/TYK2 inhibitors for a range of inflammatory disorders such as inflammatory bowel disease, systemic lupus erythematosus and psoriasis. Balancing the in-family kinase selectivity is important to optimize the inhibition of pathogenic cytokines while limiting immune suppression, as well as to limit effects driven by JAK2 signaling through EPO and other molecules important in hematopoetic cell differentiation.

An important part of our program has been our understanding of PK:PD developed from our extensive experience with tofacitinib (Xeljanz™) in the clinic and in preclinical animal models. This has been important in setting lab objectives for projecting efficacious target cover and dose; in particular to understand selectivity ratio targets to minimize effects on JAK2 signaling and the hematopoetic system, whilst maximizing efficacy.

We identified a series of ATP competitive pyrimidines from an early library lead, and through a structurally enabled program drove the biological profile and property space to a point where we could advance the lead compound (PF-06700841) into the clinic. The role of primary cell assays has been key to understanding the properties of the lead molecules, corroborated by PK:PD evaluation in-vivo. The lead is a well-behaved molecule with excellent in-vitro potency and a superior off-target poly-pharmacology profile. PF-06700841 is currently in Phase 1 clinical study.

Fensome Biography: Dr. Andrew Fensome obtained his BSc and PhD from the University of Manchester Institute of Science and Technology. He joined Wyeth Research in the UK in 1992 and moved to the Philadelphia PA area in 1995, and transitioned to the Pfizer medicinal chemistry organization in 2009. He has worked across multiple target classes: ion channels, nuclear hormone..}

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16th Annual Sukant Tripathy Symposium

The University of Massachusetts Lowell will hold its 16th Anniversary Symposium on December 2, 2016, to honor the memory of the late Prof. Sukant Tripathy, renowned researcher and former Director of the Center for Advanced Materials, University Provost and Vice Chancellor. This year’s program is also dedicated to the memory of the late Prof. Daniel J. Sandman, former Co-Director of the Center for Advanced Materials, and includes invited talks by former colleagues and students of Dan’s, as well as student poster presentations.

December 2, 2016
8:00 a.m. - 4:00 p.m.
University of Massachusetts Lowell Inn & Conference Center,
50 Warren St., Lowell, MA 01852
Directions at http://www.acc-umlinnandconferencecenter.com/

Speakers

- **Bruce Foxman**, Brandeis University, *Thermal Reactions and Transformations in Crystals*
- **Michael Rubner**, Massachusetts Institute of Technology, *Stimuli-Responsive Polymer Assemblies for Biomedical Applications*
- **D. Venkataraman**, University of Massachusetts, Amherst *Azobenzene-based Polymers for Energy Storage*
- **Dong-Chan Lee**, University of Nevada, Las Vegas, *π-Organogelators Based on Phenazine Derivatives*
- **Virinder S. Parmar**, University of Delhi, Delhi, India, *Development of Novel Polymeric Nanomaterials, Nanocomposites and Dendrons via Biocatalytic Routes*
- **Dionysios Christodoulouas**, University of Massachusetts Lowell, *Paper-based Devices and Paper-like Materials - Fabrication and Applications*
- **Kimberly Hamad-Schifferli**, University of Massachusetts Boston / MIT, *Engineering the Nanoparticle-Biology Interface for Biomedical Applications*

Registration: Pre-registration is required by November 25, 2016. Online registration at: https://www.uml.edu/Research/CAM/Registration-Form.aspx

Parking: Garage gate right of ICC surface lot (student parking) will be open. If no spots are available, proceed to 2nd level entrance of the Lower Locks Municipal Garage. Parking rate is $8/day max. (Shuttle buses from UML campuses are recommended).

Details and Changes: Agenda and all updates about this symposium will be posted on the website http://www.uml.edu/Research/CAM/Tripathy-Memorial/symposium.aspx or you may contact Michele Vercellin@uml.edu or 978-934-3695.

This year’s event sponsored by: Rogers Corporation (http://www.rogerscorp.com/index.aspx) and the University of Massachusetts Lowell, Kennedy College of Sciences and Francis College of Engineering. 

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Monthly Meeting Bios and Abstracts

Continued from page 5

hematopoetic cells and structural cells (keratinocytes and fibroblasts). The current work describes the discovery of a series of selective JAK1/TYK2 inhibitors for a range of inflammatory disorders such as inflammatory bowel disease, systemic lupus erythematosus and psoriasis. Balancing the in-family kinase selectivity is important to optimize the inhibition of pathogenic cytokines while limiting immune suppression, as well as to limit effects driven by JAK2 signaling through EPO and other molecules important in hematopoetic cell differentiation.

An important part of our program has been our understanding of PK:PD developed from our extensive experience with tofacitinib (Xeljanz™) in the clinic and in preclinical animal models. This has been important in setting lab objectives for projecting efficacious target cover and dose; in particular to understand selectivity ratio targets to minimize effects on JAK2 signaling and the hematopoetic system, whilst maximizing efficacy.

We identified a series of ATP competitive pyrimidines from an early library lead, and through a structurally enabled program drove the biological profile and property space to a point where we could advance the lead compound (PF-06700841) into the clinic.

The role of primary cell assays has been key to understanding the properties of the lead molecules, corroborated by PK:PD evaluation in-vivo. The lead is a well-behaved molecule with excellent in-vitro potency and a superior off-target poly-pharmacology profile. PF-06700841 is currently in Phase 1 clinical study.

Fensome Biography: Dr. Andrew Fensome obtained his BSc and PhD from the University of Manchester Institute of Science and Technology. He joined Wyeth Research in the UK in 1992 and moved to the Philadelphia PA area in 1995, and transitioned to the Pfizer medicinal chemistry organization in 2009. He has worked across multiple target classes: ion channels, nuclear hormone..
Solving mysteries through chemistry at the Museum of Science.

Zachary and Sydney and their paper chromatography results.

Professor Shakhashiri with Sydney and Zachary.

In Loving Memory of Dr. Christine Jaworek-Lopes
June 1, 1970 - May 21, 2016

Remembering Christine Jaworek-Lopes (Emmanuel College).

Photographs by Morton Z. Hoffman
Summer Scholar Report

Continued from page 7

The same experiment was repeated for the undiluted nanoparticles and Figure 5 shows the DRIFTS of the OH stretching region as a function of exposure to water. The stretching features for water grow in at 3683 cm⁻¹, 3604 cm⁻¹, and 3497 cm⁻¹. The isolated silanol at 3744 cm⁻¹ appears to decrease with the increase in water pressure, as it had with the diluted particles, but it is much larger with respect to the water stretching features than seen on the dilute sample. An intriguing result is that the features of interest for the undiluted nanoparticles appear at a higher energy in the spectra than the features of the diluted nanoparticles.

In order to quantify the behavior of water on the undiluted nanoparticles, the normalized peak height was again plotted as a function of exposure to water, as shown in Figure 6. The features at 3604 cm⁻¹ and 3497 cm⁻¹ follow near identical trends, indicating that they are due to the same water-SiO₂ interactions. The feature at 3683 cm⁻¹ follows a different trend. This coupled with its high energy suggests it is a different type of Si-OH interaction than the silanol, perhaps reaction between water and a defective SiO₂ surface. It may also be due to the shift in the silanol peak due to H-bonding with adsorbed water molecules.⁶

The shifts of the main features to higher energies in the spectra suggests that interactions are more energetic than they would be in the presence of KBr diluent, which shows that the undiluted nanoparticles are a better model for interstellar reactions using this type of methodology. One possible reason for this shift could be that there are more ways for the silanol groups to stretch or bend at the surface of the sample. As suggested above, it could also be due to hydrogen bonding with molecular water at the surface. Given the spacing of isolated silanols (>30 pm), it is not likely that the groups are hydrogen bonding with each other, but are capable of hydrogen bonding with water to form some sort of water network on the surface of the nanoparticles, which agrees with previous data that suggests that the reactions do not occur on the surface of the particle itself but rather in the icy mantle that likely forms there in the presence of gas phase water at low temperatures.¹

IV. Conclusion

In conclusion, nanoparticles are favorable silicate grain surface analogs to study reactions in the interstellar medium. Using an ionic salt diluent, like KBr, to investigate the surface reactions on SiO₂ can be quite useful when studying the regions of strong absorption below 2750 cm⁻¹. However, KBr can also serve as a substrate for physisorption of polar molecules, and thus must be used with care in those types of investigations. The slight shift and reduction of intensity of the Si-OH stretching features at ~3750 cm⁻¹ indicate that they may interact with the water thin film forming on the substrate as the water vapor pressure increases, probably via hydrogen-bonding. Undiluted nanoparticles are most desirable due to the ability of water and presumably other molecules to physisorb to the surface at even room temperature, thus it is able to serve as a model for space reactions, especially under conditions comparable to those of deep space.

V. Acknowledgements

Funding for this research was provided in part by the Oracle Education Foundation grant to the College of Science and Mathematics. Undergraduate funding for this project was provided by the Norris-Richards Undergraduate Research Scholarship awarded by the Northeastern Section of the American Chemical Society. A special thanks to Professor Michelle Foster and the Foster Lab at UMass Boston for making this project possible.

VI. References


continued on page 14
NESACS Chair Jerry Jasinski presents Joseph Donald Smith with his certificate as a 50-year member of the ACS.

NESACS Chair Jerry Jasinski presents Jack Driscoll with his certificate as a 50-year member of the ACS.

NESACS Secretary Michael Singer (R) presents retiring NESACS Treasurer James Piper with a certificate honoring his many years of service to NESACS.

(L-R) Anthony Cromwell (Tony) Hill, son of Henry A. Hill, with Karen and Jim Piper, 2016 recipients of the Henry A. Hill Award for Outstanding Contributions to NESACS.

Karen and Jim Piper (at center), recipients of the 2016 Henry A. Hill Award for Outstanding Contributions to NESACS, with Jerry Jasinski (at left), NESACS Chair, and Michael Singer, NESACS Secretary.

Malika Jeffries-El (Boston University), at center, speaker on “From Molecules to Materials: Designing Organic Semiconductors for Advanced Applications” with Jerry Jasinski (at right), NESACS Chair, and Lee Johnson, NESACS Chair-Elect.
receptors, kinases and solute transporters, for programs in women’s healthcare, neuroscience, inflammation and auto-immunity. He has served as the team leader on programs from early exploratory target identification, through lead identification and optimization into clinical candidates, and into phase 1 clinical development. He currently holds the position of Associate Research Fellow in the Medicine’s Design department, at the Pfizer Cambridge, MA site.

Maria Beconi, Ph.D

Biography: Maria Beconi is serving as the CSO at Retrophin. Prior to joining Retrophin, Dr. Beconi has served as Founder of KAB DMPK Strategies, LLC, acting as independent consultant for nonclinical sciences to clients including Lundbeck (Ovation), TB Alliance, Boehringer Ingelheim Vet Med and others. Before that, Dr. Beconi held the position of Director DMPK at CHDI Foundation, a virtual not-for-profit biotechnology company aimed at finding therapies for the treatment of Huntington’s disease. Dr. Beconi’s previous positions included Director, Drug Metabolism at Abbott Laboratories; Manager and US-Site Head, rCEDD

Monthly Meeting Bios and Abstracts

Continued from page 9

Abstract: Identifying strategies to increase the probability of success from lead optimization to candidate selection remain a significant challenge within the pharmaceutical field where “fail fast” is an accepted paradigm, there are limited reports of methods quantitatively assessing the progress of lead optimization campaigns. Until very recently, little emphasis has been put into in silico analyses to assess and guide, in real time, the trajectory (positive or negative) of lead optimization. Providing both qualitative and quantitative insights through interactive dashboards could improve cycle times and outcome. We present methodology to analyze and display complex aggregate data through interactive dashboards, employing customizable software to report results to project teams and management.

Biography: Mark Munson received his PhD in 1993 from the University of Minnesota under Professor George Barany. He began his industrial career at Amgen working on peptidomimetics and establishing the early lead generation group. In 1998, he became a founding member of Array Biopharma where his medicinal chemistry work focused on kinase targets in oncology, immunology and fibrosis. During his 14 year career at Array, he led several programs into Phase I and II development. In 2012, he joined the oncology unit at Sanofi in Cambridge. He is presently Director of Medicinal Chemistry, supporting several therapeutic areas including rare diseases, oncology and neuroscience.

Roy Munson

Continued from page 2

readesign the website of the New Drug Metabolism Discussion Group (NEDMDG) and provide regular maintenance for it. He worked with Larry until early 2010, when Vaughn Miller of Agilent Technologies became the contact. In early 2010, Dr. Jerry Jasinski contacted Roy to update the website for the American Institute of Chemists.

In the spring of 2011, Roy began working with Mindy Levine as the representative of the BOP to revise the NE-SACS website to simplify the home page and modernize, streamline, and improve navigation through the site. It was a pleasure working with her. She had a clear vision of the changes that she and the BOP wanted him to make, and the process went very well.

Over the years Roy has had the pleasure of working with many of the members of the Section who regularly send items to post: Mike Filosa with the seminar calendar, Mort Hoffman with many photos from meetings and activities, Harvey Steiner with the PDF of the Nucleus, Ruth Tanner with membership forms, Bobbie Lamont with NEACT conferences, Marietta Schwartz with information about many of the awards, Raj Rajur with Medicinal Chemistry activities, Jack Driscoll with public relations news, and, of course, Anna Singer with information about many other activities.

Recently, Kathy Lee and members of the Board of Publications have expressed a desire for a new design that will bring the ACS branding to the NE-SACS website and at the same time further modernize, streamline, and improve navigation. Roy has begun working with Kathy and Ajay Purohit to come up with a plan and proposal for a new design.

Roy looks forward to making the website continue to meet the needs of the section while aligning even closer to the American Chemical Society’s brand.
Thomas, Central New York; Treasurer: Wayne Jones, Binghamton.

Also in attendance at the meeting were Laura Pence (ACS District I Director) and Dorothy Phillips (ACS Director-at-Large).

The Board reelected Alyssa Thomas as Secretary and Wayne Jones as Treasurer for two-year terms (2017-18).

Treasurer Jones reported that the total net assets of NERACS are now slightly less than $68,000 as a result of the return of the seed loan for NERM 2015 and a return of approximately $9,100 (40% of the surplus) from that meeting last year at Ithaca College.

Wayne Jones reported that NERM 2016 was on track to bring in more than $100,000 in revenue; however, expenses were proving to be higher than budgeted. A surplus of approximately $15,000 is anticipated, from which 40% will return to NERACS.

A special task force presented revisions to the NERACS by-laws for approval by the Board, which was so voted. The new document will be posted on the NERACS website <http://neracs.sites.acs.org/>.

This reporter provided information about the Atlantic Basin Conference on Chemistry (ABCChem, formerly AtlanticChem) from the International Activities Committee meeting in Philadelphia in August. The conference, which will be sponsored by ACS, EuCheMS, Canadian Society for Chemistry, Mexican Chemical Society, and other partners, will take place on January 24-27, 2018, at the Iberostar Resort in Cancun, Mexico, with an overall theme of “Materials and Nanochemistry.” Approximately 500 scientists are expected to attend.

Plans for the Eastern New York Local Section to host NERM 2017 have fallen through, so no meeting will be held that year. Because of ABCChem and the ACS national meeting in Boston in 2018, no NERM will be held that year either. The Rochester Local Section has expressed interest to host the meeting in Fall 2019, and the Green Mountain Local Section is considering holding a meeting in Burlington, VT, in Spring-Summer 2020. Inasmuch as the ACS

Summer Scholar

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Fall 2021 national meeting has been moved from Boston to Atlanta, the question was raised again as to whether NESACS would be interested in hosting NERM that year, possibly in New Hampshire jointly with the Maine Local Section or on or near Cape Cod together with the Rhode Island Local Section.

The next annual meeting of the NERACS Board will take place at noon on Tuesday, August 22, 2017, in Washington, DC, on the occasion of the ACS national meeting. ◇
The Nucleus December 2016 15

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Calendar

Check the NESACS home page for late Calendar additions: http://www.NESACS.org

Note also the Chemistry Department web pages for travel directions and updates. These include:
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http://www.unh.edu/chemistry/events

November 28
Prof. Vincent Meunier (RPI)
Boston University, Life Sciences and Engineering Building, Rm B01 4:00 pm

December 1
Prof. Jing Zhao (Univ. of Connecticut)
Boston College, Merkert 130 4:00 pm

December 2
Prof. Stephen L. Buchwald (MIT)
Boston College, Merkert 127 4:00 pm

December 3
Dr. John Macor (Bristol-Myers Squibb)
Boston College, Merkert 127 4:00 pm
Prof. Stephen L. Buchwald (MIT)
Boston College, Merkert 127 11:15 am

December 4
Prof. Ohyun Kwon (UCLA)
Phosphines and phosphinocatalysis
Brandeis, Gerstenzang 121
4:00 pm
Prof. Joshua Pierce (North Carolina State)
Marine Natural Products Synthesis as a Driving Force for Chemical and Biological Discovery
Boston University, Life Sciences and Engineering Building, Rm B01
4:00 pm

December 5
Dr. Glenn Harris (908 Devices)
Univ. of New Hampshire, Parsons N104
11:10 am
Prof. Ross Berbeco (Brigham and Women’s Hospital)
Nanoparticles for Imaging and Dose Amplification in Radiation Therapy
Tufts, Pearson, Rm. P106
4:30 pm

December 6
Prof. Kim Baines (University of Western Ontario)
Harvard/MIT Inorganic Chem Seminar, MIT Room 4-370
4:15 pm
Prof. Svetlana Lutsenko (Johns Hopkins University)
WPI, GP1002 12:00 Noon
Prof. Irina Bezsonova (University of Connecticut)
“USP7: Structure, function and inhibition.” Northeastern, 129 Hurtig Hall
12:00 pm

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