Monthly Meeting
Catherine Costello to speak at the University of New Hampshire, Durham, NH

Summer Scholar Report
By Francesca Barucci, Taylor Bullock and Christine A. Caputo, University of New Hampshire

Medicinal Chemistry Symposium
Contemporary Approaches to Targeting Cancer at Bristol-Myers Squibb, Cambridge, MA

Photos from January and February Meetings
By Brian D’Amico and Joel Laino
Photos from the January Meeting

Photos by Brian D’Amico

Anna Sromek (NESACS Chair) presiding at the NESACS monthly meeting on January 21, 2020, at Alnylam Pharmaceuticals (Cambridge, MA).

Luis Echegoyen presenting his talk, “Buckyball Maracas: Fullerene Nanocontainers that Stabilize Unusual Atoms and Clusters Inside.”

Luis Echegoyen (ACS President) speaking about his plans and initiatives during his term as ACS President.

Attentive attendees

Anna Sromek with Luis Echegoyen (ACS President).
Contents

Photos from the January Meeting ........................................... 2
By Brian D’Amico

Career Perspective ............................................................. 4
By Elina N. Khachiyan, Esq.

Monthly Meeting ............................................................. 5
Catherine Costello to speak on “Mass Spectrometric Investigations of Molecular Details that Impact Biological Functions.” At the University of New Hampshire, Durham, NH. Thursday, March 12, 2020.

Catalyst ............................................................................. 6

A Medicinal Chemistry Symposium .................................... 7
Contemporary Approaches in Targeting Cancer, Wednesday, March 4, 2020 at Bristol-Myers Squibb Research and Development, Cambridge, MA

Summer Scholar Report ..................................................... 8
Grignard vs. Mother Nature by Francesca Barucci, Taylir Bullock and Christine Caputo, University of New Hampshire.

Northeast Student Chemistry Research Conference ............. 10
Saturday, April 4, 2020 at Boston University

NESACS 2020 Candidates for Election ................................. 11
By Joel Laino

Photos from the February Meeting ..................................... 12
By Joel Laino

Seminar Calendar .............................................................. 15


The Nucleus

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Career Perspective

What Do I Want To Be When I Grow Up?

By Elina N. Khachiyan, Esq., RAC

There I was, over 15 years ago now, at the Suffolk University Registrar’s Office, trying to decide on my major. Like all other college freshman, I was about to make a decision that would send me on a particular career path, a decision which would certainly affect the rest of my life in one way or another.

I narrowed my choices down to a science discipline and finally settled on the Chemistry and Secondary Education program.

Truthfully, I had no idea what I wanted to do after college, but there were three major reasons behind this decision. I knew a science degree would always be in demand, and there would likely always be a job available for me. I also knew that if I picked one of the more challenging programs, which science programs tend to be known for, then I would be able to train and discipline myself to take on most other programs should I decide to in the future. And finally, I just simply loved the idea of learning about chemicals and performing experiments in the lab!

After college I went on to work in hospital and pharmaceutical settings, in all of which my chemistry education came in handy. Then I decided to change things up a bit and went on to law school. After law school, I worked in the pharmaceutical and chemical industries primarily in the area of Regulatory Affairs, and then went on to open a law practice focused on assisting businesses in navigating the complexities of regulatory compliance. Elina N. Khachiyan, Esq., RAC, is a Massachusetts based practicing attorney, focused on pharmaceutical, chemical, and nutritional regulatory matters. Elina has been working in regulatory for five years and in various roles within the pharmaceutical industry for over 10 years. Khachiyan holds a Juris Doctorate, a Bachelor’s in Chemistry and Secondary Education, as well as various industry certifications, including three RAC Credentials. She is the founder of Elina Khachiyan Consulting, LLC, a law practice focused on assisting businesses in navigating the complexities of regulatory compliance. ♢

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Monthly Meeting

The 995th Meeting of the Northeastern Section of the American Chemical Society

Thursday, March 12, 2020

University of New Hampshire
Huddleston Hall Ballroom
73 Main Street, Durham, NH 03824

4:30 pm NESACS Board Meeting (Lamprey Board Room, Holloway Commons Building: Map I16)
5:30 pm Social Hour (Huddleston Hall Ballroom, Map: I17)
6:30 pm Dinner (Huddleston Hall Ballroom)
7:30 pm Anna Sromek, NESACS Chair, Presiding

Keynote Presentation
Professor Catherine Costello, Boston University School of Medicine, Boston, MA
Title: Mass Spectrometric Investigations of Molecular Details That Impact Biological Functions

YOU MUST REGISTER IN ADVANCE TO ATTEND THE MEETING: THERE IS NO REGISTRATION FEE TO ATTEND THE MEETING; DINNER RESERVATIONS ARE REQUIRED. THE PUBLIC IS INVITED

• For those who would like to join us for dinner, register by 5pm, Thursday, March 5th, at https://NESACSmarchmeeting.eventbrite.com.

• Cost: Members, $30; Non-members, $35; Retirees, $20; Students, $10. Dinner reservations not cancelled at least 24 hours in advance will not be refunded. Reservations for new members and for additional information contact the Administrative Coordinator, Anna Singer, via e-mail at secretary@nesacs.org.

• If you wish to join us for this meeting and not eat dinner, please register by 5pm, Thursday, March 5th, at https://NESACSmarchmeeting.eventbrite.com. Select “Seminar only”.

• Directions to UNH: use GPS to the following address 73 Main Street, Durham, NH 03824. Parking is available in the Campus Crossing lot (6 Mill Road, Durham NH 03824) or there are a limited number of spots along Main Street in front of Huddleston Hall - both are pay by the hour. A campus map is available here:

  https://www.unh.edu/sites/default/files/departments/facilities/Maps/s_uu_dwg_map_camp_sm_map_2018_campus_map_with_index.pdf

If you have any questions or require additional information, contact the Administrative Coordinator, Anna Singer, via email at secretary@nesacs.org.

If you have any questions or require additional onsite information, contact Christine Caputo via email at christine.caputo@unh.edu

Abstract:

Mass Spectrometric Investigations of Molecular Details That Impact Biological Functions

Development of new drugs and diagnostic tools requires increased understanding of infection, cancer, and the immune system. Infectious agents usually gain entrance to their hosts through the interactions of surface molecules. The immune system is responsible for and exploits the interactions of proteins with one another and with glycans (and other classes). In order to explore these phenomena, to investigate how the body can combat challenges (even with sometimes deleterious consequences), and to utilize this knowledge to control disease, we now rely heavily on insight provided by mass spectrometry. This lecture will focus on mass spectrometry approaches that we are developing and using to elucidate critical pathways in the inter- and intra-molecular interactions that are important in infection, carcinogenesis, and neurodegeneration.

Biography:

Catherine E. Costello is a William Fairfield Warren Distinguished Professor at Boston University, with appointments in the Depts. of Biochemistry, Biophysics and Chemistry. She earned her AB at Emmanuel College, Boston, and PhD at Georgetown University, Washington, DC. She was a postdoctoral fellow and Senior Research Scientist at MIT, where she served as Associate Director of the NIH Mass Spectrometry Resource for more than 20 years. She founded the BU School of Medicine Center for Biomedical Mass Spectrometry in 1994. Her research centers on development of mass spectrometry-based instrumentation and methods for biopolymers and their application to study glycobiology, protein post-translational modifications, protein misfolding disorders, cardiovascular and infectious diseases, and bioactive lipids. She has authored >375 scientific papers. She serves on multiple editorial
Our third event…

In 2016, the Gordon Research Conference (GRC) initiated The Power Hour™, an informal session giving scientists an opportunity to discuss issues of diversity and inclusion.

Catalyst, a networking series featuring women in chemistry, sponsored by Blueprint Medicines and the Northeastern Section of the American Chemical Society, is partnering with GRC to host a local Power Hour™ for the community.

<table>
<thead>
<tr>
<th>When</th>
<th>Where</th>
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<tbody>
<tr>
<td>Tuesday</td>
<td>Blueprint Medicines</td>
</tr>
<tr>
<td>March 17, 2020</td>
<td>45 Sidney Street</td>
</tr>
<tr>
<td>8:30 – 10:30 AM</td>
<td>Cambridge, MA 02139</td>
</tr>
</tbody>
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### Agenda:

- **8:30 - 9:00 AM** – Breakfast and networking
- **9:00 -10:00 AM** – **GRC Power Hour™** featuring Nancy Ryan Gray, PhD

This GRC Power Hour™ will highlight how the Gordon Research Conferences have created new forums for conversations about inclusivity within its 400+ communities and discuss the culture change that is needed to support women throughout their scientific careers.

Nancy Ryan Gray, PhD
President and CEO of Gordon Research Conferences

catalyst@blueprintmedicines.com

For more information: www.grc.org/the-power-hour

To register: https://catalyst-iii-grc-power-hour.eventbrite.com

Questions?
A Medicinal Chemistry Symposium
Organized by Bristol-Myers Squibb Discovery Chemistry, Cambridge and the Medicinal Chemistry Section of the North-eastern Section, American Chemical Society

“Contemporary Approaches in Targeting Cancer”
Wednesday, March 4, 2020
Bristol-Myers Squibb Research and Development
100 Binney Street, Cambridge, MA 02142

Meeting Agenda
3:00 pm Arrival and Check-in
3:15 pm Welcome
Gregory Vite, Ph.D., SVP, Small Molecule Drug Discovery, Bristol-Myers Squibb
3:20 pm Introductory Remarks
Raj Rajur, Ph.D., NESACS Medicinal Chemistry Section Chair, CreaGen, Woburn, MA

Moderator: Daniel Elbaum, Ph.D. CSO, QurAlis, Cambridge, MA

3:30 pm Dylan England, Ph.D., Senior Scientist, Takeda, Cambridge, MA
Title: Discovery of TAK-981, a First in Class Inhibitor of Sumo Activating Enzyme (SAE)

4:15 pm Li Peng, Ph.D., CSO, Palleon Pharmaceuticals, Waltham, MA
Title: A Novel Therapeutic Modality of Inhibiting the Glyco-Immune Checkpoint

5:00 pm Philip Chamberlain, Ph.D., Executive Director, Protein Homeostasis and Structural Biology, Bristol-Myers Squibb, San Diego, CA
Tentative Title: Protein Degradation via Cereblon Modulators

5:45 pm Social Hour and Dinner

7:00 pm Michelle Lamb, Ph.D., Team Leader, Chemistry, AstraZeneca, Waltham, MA
Title: A2aR Antagonists: Targeting the Adenosine Pathway to Reverse Immune Suppression in the Tumor Microenvironment

NESACS Med Chem Organizing Committee: Scott Edmondson, Daniel Elbaum, Brian Aquila, Paul Greenspan, Mark Ashwell, Jeremy Green, Adrian Hobson, Blaise Lippa, Min Lu, Lisa Marcaurelle, Andrew Scholte, Kap-Sun Yeung, Raj (SB) Rajur

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

• Dinner reservations should be made no later than 11:30 PM, Tuesday, February 25, 2020. Reservations are to be made using Eventbrite https://nesacs-bms-oncology.eventbrite.com Members, $30; Non-members, $35; Retirees, $20; Students, $10.

• If you wish to join us for this meeting and not dinner, please register by 11:30 PM, Tuesday, February 25, 2020 at https://nesacs-bms-oncology.eventbrite.com Select “Seminar only”.

• New members or those seeking additional information, please contact the NESACS administrative coordinator, Anna Singer at secretary@nesacs.org.

• For questions about the symposium, please contact Kap-Sun Yeung at kapsun.yeung@bms.com or Raj Rajur at rrajur@creagenbio.com

Bristol-Myers Squibb Cambridge Research Site
The Bristol-Myers Squibb Cambridge research site is located at 100 Binney Street, Cambridge, MA 02142, between Second Street and Third Street. It is within walking distance of the MBTA Kendall station on the Red Line (about 0.3 miles) or the Lechmere station on the Green Line (about 0.5 miles).

Parking Garage: There are several parking garages within walking distance from BMS. Pilgrim Parking is behind the BMS building on Linskey Way, between East Kendall Street and Second Street. Kendall Square South Garage and Kendall Center Green Garage are respectively about 0.2 and 0.5 miles from BMS. ♦
The proposed plan for the Summer of 2019 was originally a synthetic route to produce my desired N-Heterocyclic carbene (NHC) (Figure 1), a project that I had already been working on for about 5 months, inconsistently, by the time summer started. During the spring semester, I was able to form the \(N,N\)-dibenzyl-4-bromoaniline (Figure 1) species with ease during the first week spent researching under my scholarship. The next step required the generation of bismesityl-boronfluoride (Mes\(_2\)BF) using a Grignard reaction.

Victor Grignard shared The Nobel Prize in Chemistry with Paul Sabatier in 1912 for the discovery of the Grignard Reagent, one of the most widely used organic chemistry methods for the formation of carbon-carbon bonds. The simplicity of the Grignard reaction is probably the main reason behind its widespread popularity over the past 100+ years. However, as chemists, we know that nothing is ever quite as simple as mixing two starting materials together.

Upon being taught how to perform this reaction by my coworkers, following a literature procedure, it seemed doable, but it slowly became clear that no amount of expertise in making Mes\(_2\)BF would make up for one single factor: the humidity. I underwent a total of 13 attempts to make bismesityl-boronfluoride (Mes\(_2\)BF) using the Grignard reaction, with 2-bromomesitylene as starting material. Last 2 steps expected to form the desired product (N,N dibenzyl-4-(bismesityl)borylaniline) in project’s synthetic route. b) Desired NHC product, from originally proposed synthetic route, for the Summer Undergraduate Research Scholarship 2019.

I understood that what was holding me back from successfully generating Mes\(_2\)BF was the fact that it was summer. If you didn’t already know, summer in New Hampshire typically consists of sweltering hot and humid days. Tententimes, a very good dose of warm summer rain helps keeps the humidity around. Lucky for us, this weather pattern usually lasts until the end of August.

Below I have included a climograph (Figure 2) plotting the average rainfall and temperature recorded each month in Durham, NH. It is clear that the peak rainfall did indeed occur during the 3 months I was employed at the University of New Hampshire. If you don’t understand what I am trying to get at here, it became abundantly clear to me that Grignard reactions will not work when it is humid outside and that this particular project may have been better suited for a winter research fellowship or, alternatively, carried out somewhere New Mexico, rather than New Hampshire! I don’t know how Floridians ever use Grignard reactions for anything!

Finally, my patience paid off and (with the generous help from one of my lab colleagues) I successfully obtained my intermediate Mes\(_2\)BF material and I was able to push one step further into the synthetic route towards my target NHC ligand.

continued on page 9
and. Even though I was not able to isolate the desired product from the second step, trying and learning a new reaction was a much-needed change, which, in itself felt like a reward.

Reflections
Many would agree that most of the actual learning a young research chemist experiences — especially during one’s first summer working at an academic institution — comes from these very types of trials and failures. I believe most chemists, especially the more experienced, would find this type of thing exciting; like a detective figuring out a cold case. For a young chemist, still unsure of what she wants out of life, I can assure you this was not the easiest or more enjoyable part of the chemistry game to accept. It’s a steep learning curve and one that doesn’t get the attention it deserves!

This is not an essay on why synthetic chemistry is sometimes painstakingly difficult, or about how 99% of the time you will fail; it is simply a reflection that I hope highlights the beauty of repeatedly trying, and failing, getting up and trying again as you work towards a goal. In striving to create your synthetic target (it is what you are being paid to do every day as a student after all), but more than that, it is okay to fail, because each trial, and each error is a learning experience. In what other profession is this experimentation possible? Everyone’s chemistry career is a different story of success, perhaps (as mine was) rooted in initial failure(s).

What do you think keeps chemists coming to work every morning? I think perseverance and the joy of knowing that today might be the day you get it right, keeps us going. This past summer, I am proud to have learned the basis of what might be the day you get it right, keeps us going. This past summer, I am proud to have learned the basis of what many Eastern religions would call, ‘embracing your suffering’. What I mean by this is; as chemists, we are all encouraged to become best friends with our worst enemy, our failed reactions.

I know that even without completing my synthetic target, in fact not even getting a third of the way there, I was still able to walk away from this summer research experience with valuable knowledge gained and an unflappable perseverance that will allow me to always push further, in whatever career I choose.

Despite my synthetic struggles, I would like to express my gratitude in receiving this award. To have had the opportunity to continue working with my professor, along with the graduate and undergraduate students in the lab all summer, was not only a major learning opportunity in my experience as an undergraduate chemistry major and new researcher, but also provided me with valuable insight into the challenges of research, that has helped shape my future career goals.

Experimental
Grignard reactions were performed under a nitrogen atmosphere, and all glassware was oven-dried prior to use. DMF and THF were obtained from solvent purification system, and THF was stored over 4Å molecular sieves. Pentane was dried over calcium hydride. Hexanes and ethyl acetate were used as obtained. All NMR spectra were gathered either on a Varian Mercury 400 MHz or Bruker 500 MHz spectrometer.

N,N-dibenzy1-4-bromoaniline: The following procedure was adapted from the literature.1 4-bromoaniline (2 g, 11 mmol, 1 eq.), DMF (10 mL), K2CO3 (4.29 g, 31.0 mmol, 3 eq.), and benzyl bromide (3 mL, 25 mmol, 2.2 eq) were added to a 50 mL round bottom flask, and heated to reflux at 120°C for 30 h. Upon cooling to room temperature, a precipitate formed. Additional DMF was added until this precipitate re-dissolved. The excess K2CO3 was removed by vacuum filtration. The product was extracted with 1:1 hexanes/ethyl acetate (130 mL), and washed with saturated LiCl (30 mL), water and brine. The organic layer was dried (Na2SO4) and concentrated by rotary evaporation, yielding a yellow oil (2.77 g). The crude product was then recrystallized in boiling EtO (95%, 150 mL), and cooled slowly to room temperature, then to -20°C. Upon cooling the product formed as a white precipitate, which was isolated by gravity filtration (1.56 g, 4.7 mmol, 39% yield). 1H NMR (400 MHz, CDCl3) δ 7.33 (dd, J = 8.2, 6.6 Hz, 4H), 7.28 (s, 2H), 7.24 – 7.18 (m, 6H), 6.62 – 6.56 (m, 2H), 4.63 (s, 4H).

Dimesityl-boronfluoride: Magnesium turnings (1.057 g, 30.77 mmol) were added to 3-neck round bottom flask. THF (45 mL) was cannula transferred into the flask and heated to 50°C prior to slow addition of bromomesitylene (5 mL). The contents of the flask were then heated to reflux, until an opaque, charcoal-colored suspension was observed. BF3-OEt2 (2 mL, 16.57 mmol, 48% solution in hexanes) was added to a separate 200 mL Schlenk flask and cooled to -78°C. The Grignard suspension was then added dropwise to the BF3-OEt2. Halfway through addition, the contents were allowed to warm to room temperature. After complete addition of Grignard, THF was removed by dynamic vacuum on a Schlenk line, and pentane (15 mL) was added via cannula. Mg salts were removed by filtration through Celite, and pentane was removed in vacuo, yielding a yellow solid. The crude product was recrystallized from pentane (30 mL) at –78°C. Pentane was removed in vacuo, yielding a light-yellow solid (1.63 g, 6.1 mmol, 75% yield). 11B{1H} NMR (160 MHz, CDCl3): δ 53.29 ppm. 19F NMR (470 MHz, CDCl3): δ –14.43 ppm. 1H NMR (500 MHz, CDCl3) δ 6.81 (d, J = 10.0 Hz, 4H), 2.31 – 2.23 (m, 23H).

References
1) Barraza, S. J.; Denmark, S. E.; Synlett. 2017, 28, 2891-2895.
22nd Annual Northeast Student Chemistry Research Conference
Saturday, April 4, 2020

Boston University, CILSE Building
610 Commonwealth Avenue, Boston,
MA 02215

Featured Keynote Speaker
Crystal Shih, PhD
Investigator III
Novartis Pharmaceuticals

Abstract Deadlines
Oral Presentation: Saturday, March 7, 2020
Poster Presentation: Saturday, March 14, 2020

For updates and registration, visit www.nsycc.org/nscrc
BIography

Continued from page 5

and advisory boards. She is Immediate Past President of the International Mass Spectrometry Foundation; she was President of ASMS in 2002-04 and International HUPO in 2011-12. She has been a Councilor for the NESACS since 1989 and was Chair of the section in 2014. She is a Board Member of the Malta Conferences Foundation. She has received several major awards in the fields of mass spectrometry, proteomics and chemistry and is a Fellow of the ACS and the AAAS. ♦

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Photos from the February Meeting

Photos by Joel Laino

The meeting was graciously hosted by Pfizer at their Kendall Square Research center.

Cato T. Laurencin presenting his fascinating talk on “Regenerative Tissue Engineering.”

Tom Gilbert (R) presents the Henry A. Hill Award of James Phillips (posthumously) to his family (L-R) Elizabeth Mayo, Logan Mayo, Anthony Phillips, Crystal Mayo and Dorothy Phillips.

Dorothy Phillips (L) with Catherine Costello

(L-R) Anna Sromek, Dorothy Phillips, Lendsey Thicklin, Eman Akam

February speaker, Cato Laurencin (L) with Patrick Gordon (R)

Photos continued on page 13
February Meeting Photos
Continued from page 12


Guest mingle during the cocktail hour

Hicham Fenniri (L) and Craig Sergeant (R).

(L-R) Michael Filosa, J. Donald Smith, Doris Lewis, Tom Gilbert

(L-R) Tom Gilbert, Malika Jeffries-EL, and Hicham Fenniri.

Pfizer Head of Medicine Design, and host of the meeting, Charlotte Allerton, with Katherine Lee, Pfizer and ACS Board of Directors.
What’s Yours?
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http://www.NESACS.org

Note also the Chemistry Department web pages for travel directions and updates.
These include:
http://www.bc.edu/schools/cas/chemistry/seminars.html
http://www.bu.edu/chemistry/seminars/
http://www.brandeis.edu/departments/chemistry/events/index.html
http://chemistry.harvard.edu/calendar/upcoming
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http://www.chem.umb.edu/
http://www.umassd.edu/cas/chemistry/
http://www.wpi.edu/academics/departments/chemistry-biochemistry

March 2
Prof. Christian Whitman (Univ. Texas Austin)
Boston University, Rafik B Hariri Building, Rm 208 11:00 am

March 3
Prof. Adam Cohen (Harvard)
Membrane voltage and membrane tension: physical forces that shape cell physiology
MIT, Building 6-120 4:00 pm
Dr. Peter Senter (Seattle Genetics)
Tufts, Pearson P-106 4:30 pm
Dr. Kathleen Jeffrey (UNH)
U. New Hampshire, Parsons N104 11:10 am

March 4
Prof. John Anderson (Harvard)
MIT, Building 4-370 4:15 pm
Prof. Paul J. Bracher (Saint Louis Univ.)
Tufts, Pearson P-106 12:00 pm

March 5
Prof. Omar Yaghi (UCal-Berkeley)
Harvard, Pfizer Lecture Hall 4:15 pm

March 6
Prof. Thomas E. Mallouk (Penn)
Boston College, Merkert 130 4:00 pm
Prof. Chumphak Chatterjee (Univ. Washington)
MIT, Building 4-270 4:00 pm

March 10
Prof. Thomas E. Mallouk (Univ. Pennsylvania)
Boston College, Merkert 130 4:00 pm
Prof. Jaqueline K. Barton (Caltech)
Tufts, Pearson, P-106 4:30 pm

March 11
Prof. Thomas E. Mallouk (Penn)
Boston College, Merkert 130 4:00 pm
Prof. Jacqueline K. Barton (Caltech)
Harvard, Pfizer Lecture Hall 4:15 pm
Dr. Hanna Moon (MIT)
MIT, Building 4-370 4:15 pm

March 12
Prof. Alison Narayan (Univ. Michigan)
MIT, Building 6-120 4:00 pm

March 16
Prof. Ellen Matson (Univ. Rochester)
Boston University, Rafik B Hariri Building, Rm 208 11:00 am
Prof. Linda Hsies-Wilson (Caltech)
Broad Inst., Rm 1154 4:00 pm

March 17
Prof. Guy Bertrand (UCal-San Diego)
Boston College, Merkert 130 4:00 pm

March 18
Prof. Tara Meyer (Univ. Pittsburgh)
Boston College, Merkert 130 4:00 pm
Dr. Connor Gihula (MIT)
MIT, Building 4-370 4:15 pm

March 25
Prof. Jennifer Prescher (UCal-Irvine)
Tufts, Pearson, P-106 12:00 pm

March 26
Prof. Greg Liu (Virginia Tech)
Boston College, Merkert 130 4:00 pm
Prof. Jefferson Chan (Univ. Illinois)
Harvard, Pfizer Lecture Hall 4:15 pm

March 27
Prof. Mark Grinstaff (BU)
Polymers for Cartilage Tissue Supplementation and Lubrication
UMass-Lowell, Olsen 102 3:30 pm

March 30
Prof. Xin Zhang (Penn State Univ.)
Boston University, Rafik B Hariri Building, Rm 208 11:00 am
Prof. Xiaowei Zhuang (Harvard)
MIT, Building 4-270 4:00 pm

March 31
Prof. Keary Engle (Scripps)
Boston College, Merkert 130 4:00 pm

Notices for The Nucleus Calendar of Seminars should be sent to: Samurdhi Wijesundera,
Email: samu.amameth@gmail.com

For late breaking news, job postings and the latest meeting and event information please visit us at
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