9th Annual Frontiers in Chemistry and Biology Interface Symposium

Johns Hopkins University
Mudd Hall, Homewood Campus
May 14, 2016

Local organizers
Caren Meyers, Dept. of Pharmacology and Molecular Sciences
Steve Rokita, Dept. of Chemistry
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Elsa Garcin, Dept. of Chemistry and Biochemistry, University of Maryland Baltimore County
John Koh, Dept. of Chemistry and Biochemistry, University of Delaware
Ronen Marmorstein, Perelman School of Medicine, University of Pennsylvania
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Millie Sullivan, Dept. of Chemical and Biochemical Engineering, University of Delaware
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ACS Infectious Diseases

VWR We Enable Science
Goals of the Annual Frontiers in Chemistry and Biology Interface Symposium

This day-long symposium is designed to highlight research in the mid-Atlantic region and provide an intimate environment to foster discussion at all levels. The schedule typically includes invited and submitted talks as well as poster sessions. There is no charge to attend this symposium, and everyone – Research Scientists, Faculty, Post-Docs and Graduate Students – involved in research from academic, government and local industrial institutions is encouraged to participate.

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University of Maryland, Baltimore County:
Department of Biological Sciences and Department of Chemistry and Biochemistry

University of Maryland, College Park:
Department of Chemistry and Biochemistry

University of Pennsylvania:
Department of Biochemistry and Biophysics
Saturday, May 14, 2016
Program

8:30-8:55 Registration, Breakfast, Poster setup

8:55-9:00 Introductory Remarks

9:00-10:20 Session I (Chair, Kwaku Dayie, University of MD, College Park, MD)

9:00-9:20 Susana Mourino Lopez (Pharmaceutical Sciences, U. of MD, Baltimore)
“Green is for Go: Biliverdin dependent regulation of the heme assimilation system of P. aeruginosa.”

9:20-9:40 Jordan L. Meier (Chemical Biology Laboratory, NCI, Frederick, MD)
“New insights into protein acetylation from chemoproteomics”

9:40-10:00 Catherine L. Grimes (Chemistry & Biochemistry, Univ. of Delaware, Newark, DE)
“Glycan remodeling of the essential peptidoglycan”

10:00-10:20 Stelios Florinas (MedImmune, Gaithersburg, MD)
“A nanoparticle platform to evaluate bioconjugation and receptor-mediated cell uptake using cross-linked polyion complex micelles bearing antibody fragments”

10:20-11:30 Break/Poster Session 1 (Odd Numbered Posters)

11:30-12:30 Session II (Christian Kaiser, Johns Hopkins University, Baltimore, MD)

11:30-11:50 Brian Chow (Bioengineering, UPenn, Philadelphia, PA)
“Exploring the limits of photosensory protein structure-function to invent new optogenetic tools”

11:50-12:10 Marcos Pires (Chemistry, Lehigh Univ. Bethlehem, PA)
“Remodeling of bacterial cell surfaces using unnatural D-amino acids”

12:10-12:30 Rebecca Schulman (Chem. & Biomol. Eng., Johns Hopkins Univ., Baltimore, MD)
“Programmed self-organization of synthetic biomolecular filaments”

12:30-1:50 Lunch

Career Panel (Jennifer Kavran, Johns Hopkins School of Public Health)
Leighanne Basta (Asst. Prof. Dept. of Chemistry, U.S. Naval Academy, Annapolis, MD)
Greg Feulner (Patent Counsel, Johns Hopkins Technology Ventures, Baltimore, MD)
Greg Gatto (Senior Scientific Investigator, GlaxoSmithKline, King of Prussia, PA)
Adam Kuszak (Health Policy Analyst, Office of Dietary Supplements, NIH, Bethesda, MD)
Amanda McGown (Consulting, Booz Allen Hamilton, Baltimore, MD)
1:50-2:50  Session III (Cynthia Dowd, George Washington University, Washington, DC)

1:50-2:10  Jeffrey G. Gardner (Biology, Univ. of MD, Baltimore County, MD)
“Parsing required versus sufficient enzymes for recalcitrant polysaccharide degradation in bacterial systems”

2:10-2:30  Lai-Xi Wang (Chem. & Biochem. Univ. of MD, College Park, MD)
“Selective enzymatic glycoengineering of therapeutic antibodies. Enzyme substrate specificity is the name of the game”

2:30-2:50  Jim Barrow (Pharmacology and Molecular Sciences, Johns Hopkins, Baltimore, MD)
“Discovery and evaluation of MB-COMT selective inhibitors for treatment of psychiatric conditions”

2:50-4:00  Break/Poster Session 2 (Even Numbered Posters)

4:00-4:45  Session IV (Poster talks) (Rong Huang, VA Commonwealth Univ., Richmond, VA)

4:00-4:15  Nikodimos Gebreselassie (Chem. & Biomol. Engineering, Univ. of Delaware, DE)
“Elucidating the physiology of complex microbial systems through a novel co-culture $^{13}$C-metabolic flux analysis”

4:15-4:30  Danielle Schmitt (Chem. & Biochem., Univ. of MD, Baltimore County, MD)
“Sequestration-mediated downregulation of de novo purine biosynthesis by AMPK”

4:30-4:45  Xue Zhi Zhao (Chem. Biol. Laboratory, National Cancer Institute, Frederick, MD)
“HIV-1 Integrase strand transfer inhibitors that reduce susceptibility to drug resistant mutant integrases”

4:45-5:30  KEYNOTE: Scott Wolkenberg (Merck, Whitehouse Station, NJ)
“Target identification for leads from phenotypic screening: examples from infectious disease”

5:30  Final Remarks and poster awards
**Speaker Abstracts**

**SESSION I**

**Susana Mourino**, postdoctoral fellow, Dept. of Pharmaceutical Sciences, School of Pharmacy, Univ. of Maryland, Baltimore

**Title:** “Green is for Go”: Biliverdin dependent regulation of the heme assimilation system of *P. aeruginosa.***

**Abstract:** The opportunistic pathogen *Pseudomonas aeruginosa* encodes two extracellular heme uptake systems, the *Pseudomonas* heme uptake (phu) and the heme assimilation systems (has) to obtain and use heme as a source of iron from the host. Consistent with recent studies indicating PhuR as the primary heme receptor in clinical infection, our laboratory has shown Phu system is the major heme transporter with the hemophore dependent Has system acting primarily in heme sensing. Employing bacterial genetics and isotopic 13C-heme labeling studies we have shown that replacement of the biliverdin IXβ and IXδ regioselective heme-oxygenase HemO by a BVIX-α selective (hemOα) or a catalytically inactive (hemOin) hemO down regulates expression of the hemophore HasA and its cognate receptor HasR. We propose a new regulatory network where coupling the regioselective metabolic flux of heme through PhuS-HemO with the heme sensing allows *Pseudomonas aeruginosa* to rapidly respond and adapt to fluctuating extracellular heme levels.

**Jordan Meier**, Investigator, Chemical Biology Laboratory (Head), Epigenetics and Metabolism, NIH

**Title:** “New insights into protein acetylation from chemoproteomics”

**Abstract:** A paradox of modern acetylation biology is that the while number of sites of acetylation has climbed rapidly, the number of enzymes thought to catalyze this process has stayed relatively constant. Here we describe the utility of chemical proteomic methods to discover and characterize mechanisms of acetylation in endogenous cellular contexts. Our studies highlight an expanded landscape of lysine acetyltransferases, as well as new strategies to investigate the metabolic regulation and small molecule inhibition of protein acetylation.

**Catherine Grimes**, Assistant Professor, Department of Chemistry, University of Delaware

**Title:** “Glycan Remodeling of the Essential Peptidoglycan”

**Abstract:** Peptidoglycan is an essential component for bacterial cell survival, composed of peptides and two carbohydrates *N*-acetyl-glucosamine (GlcNAc) and *N*-acetyl-muramic acid (MurNAc). We have begun to re-engineer bacterial cell wall biosynthesis. By taking advantage of bacterial cell wall recycling and modifying enzymes, we have found that simple glycans with small modifiable tags can be readily embedded into the bacterial cell wall. Access to bacterial cell wall material in which the carbohydrate is modified will allow us to capture, characterize and visualize bacterial cell wall fragments from a host of bacterial cells, ranging from pathogenic to those found in the human microbiome.

**Stelios Florinas**, Postdoctoral Fellow, Antibody Discovery and Protein Engineering Department, MedImmune

**Title:** “A Nanoparticle Platform To Evaluate Bioconjugation and Receptor-Mediated Cell Uptake Using Cross-Linked Polyon Complex Micelles Bearing Antibody Fragments”

**Abstract:** Targeted nanomedicines are a promising technology for treatment of disease, however, preparation and characterization of well-defined protein-nanoparticle systems remains challenging. Here, we describe a platform technology to prepare antibody binding fragment (Fab) -bearing nanoparticles (NPs) and an accompanying real-time cell-based assay to determine their cellular uptake compared to monoclonal antibodies (mAbs), Fabs, mock-Fab-NPs and non-targeted NPs. Crosslinked polyon complex (PIC) micelles were 30 nm in size and contained approximately 10 polymers per construct. Analysis of Fab-PIC micelle conjugates by FCS, SEC, and UV-Vis absorbance demonstrated that Fab density on micelles (1-3 Fabs per NP) was controlled by simply mixing azide- and methoxy-terminated block copolymers used for micelle formation. Evaluation of cellular uptake in receptor positive cancer cells by *in situ* fluorescence microscopy revealed that targeted Fab-PIC micelles achieved higher cell uptake than mAbs, Fabs, mock-Fab-NPs and non-targeted NPs. Furthermore, time-dependent cell uptake profiles showed that mAb signal plateaued after 3 hrs, whereas nanoparticle signal increased over the entire timeframe of the experiment (12 hrs). Overall, targeted NPs binding the EphA2 receptor showed enhanced cell uptake when compared to Fabs, mAbs, mock-Fab-NPs and non-targeted NPs. The described approach to construct and characterize targeted micelles allowed identification of a NP-based cell-targeting system with unique internalization properties.
SESSION II

Brian Chow, Assistant Professor, Department of Bioengineering, University of Pennsylvania

Title: “Exploring the limits of photosensory protein structure-function to invent new optogenetic tools”

Abstract: Optogenetics permits the light-mediated manipulation and monitoring of cellular physiology, using natural and engineered photosensory proteins that are heterologously expressed in genetically targeted cells. This talk will discuss the development of such molecular tools, and their application in elucidating transcriptional signal processing principles that govern mammalian cellular dynamics. We will emphasize the use of next-generation sequencing and first principles design to push the biochemical and topological boundaries of photosensory proteins.

Marcos Pires, Assistant Professor, Department of Chemistry, Lehigh University

Title: “Remodeling of bacterial cell surfaces using unnatural D-amino acids”

Abstract: Non-traditional routes to combat bacteria may offer an attractive alternative to the ongoing problem of drug discovery in this field. Herein, we describe the development of bacterial D-amino acid Antibody Recruitment Therapy (DART). DART represents a promising antibiotic strategy by exploiting the promiscuity of bacteria to incorporate unnatural D-amino acids and subsequently recruit antibodies to the bacterial surface. The conjugation of 2,4-dinitrophenyl (DNP) to various D-amino acids led to the discovery of an immune stimulant D-amino acid that specifically tags the surface of Bacillus subtilis and Staphylococcus aureus for the recruitment of anti-DNP antibodies (a highly abundant antibody in human serum).

Rebecca Schulman, Assistant Professor, Department of Chemical and Biomolecular Engineering, Johns Hopkins University

Title: “Programmed Self-Organization of Synthetic Biomolecular Filaments”

Abstract: Many biological materials such as the cytoskeleton or the extracellular matrix consist of one-dimensional polymers or fibers whose organization results from complex, programmed interactions with the local environment. I will describe a synthetic toolkit my research group has constructed to study this form of organization and to use this method of assembly to build new materials. We are assembling filaments from synthetic DNA molecules. We can control the nucleation, capping and branching of these structures using engineered nanostructures that can be activated or deactivated by specific DNA sequences. Complex spatiotemporal organization of these structures can be achieved using programmed molecular circuits and in vitro gene networks that control the concentration of these sequences over time. I will show how these elements can be combined to build complex, adaptive nanostructures with new functions.

SESSION III

Jeffrey Gardner, Assistant Professor, Department of Biological Sciences University of Maryland - Baltimore County

Title: “Parsing required versus sufficient enzymes for recalcitrant polysaccharide degradation in bacterial systems”

Abstract: The degradation of recalcitrant polysaccharides is an important ecological process, contributes to human health, and is a major strategy for renewable energy development. In these examples, microbes (bacteria and fungi) are the main drivers of polysaccharide degradation and their genomes often encode for hundreds of enzymes for this process. Currently, it is unclear why these microbes have so many or which enzymes are essential for the degradation of a given polysaccharide. Our laboratory uses a comprehensive systems biology approach to determine, in a physiologically relevant context, what enzymes are essential for recalcitrant polysaccharide degradation, compared to those that are merely sufficient, using the model saprophytic bacterium Cellvibrio japonicus.
Lai-Xi Wang, Professor, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742

**Title:** “Selective Enzymatic Glycoengineering of Therapeutic Antibodies. Enzyme Substrate Specificity Is the Name of the Game”

**Abstract:** Monoclonal antibodies (mAbs) represent an important class of therapeutic proteins widely used for the treatment of cancer, inflammation, and infectious diseases. Compelling evidence has shown that Fc glycosylation can profoundly affect the effector functions of antibodies. This presentation describes a chemoenzymatic method for site-specific glycoengineering of antibody’s Fc and Fab glycans. Our experimental data show that a remarkable site-selectivity in glycosylation remodeling can be achieved by taking advantage of the substrate specificity of a handful of endoglycosidases and glycosidases and their mutants. Examples for glycoengineering of several therapeutic monoclonal antibodies, including rituximab, herceptin, and cetuximab, for improving their effector functions will be provided.

Jim Barrow, Associate Professor, Pharmacology and Molecular Sciences, Johns Hopkins School of Medicine; Associate Director, Drug Discovery, Lieber Institute for Brain Development

**Title:** “Discovery and evaluation of MB-COMT selective inhibitors for treatment of psychiatric conditions”

**Abstract:** Catechol-O-methyltransferase (COMT) plays an important role in the termination of dopamine signaling in brain regions such as the prefrontal cortex and hippocampus, making it an important regulator of a number of cognitive and behavioral processes. Therefore, inhibitors of COMT may be useful in treatment of a variety of conditions associated with dysregulated cortical dopaminergic function like schizophrenia, ADHD, and traumatic brain injury. COMT has two forms encoded from the same gene—a membrane-bound form (MB-COMT) and a soluble form (S-COMT). Genetic and pharmacological studies have demonstrated that the membrane-bound form is especially important in the human brain; however, most known COMT inhibitors such as the nitrocatechol tolcapone have no selectivity between the two forms of the enzyme. Therefore, we sought to determine if a potent and selective MB-COMT inhibitor would be useful for treatment of neurologic disorders. Extensive medicinal chemistry optimization of a quinoline lead from the literature provided a probe molecule with good potency, selectivity, pharmacokinetics, and brain penetration. Examination in rat models of cognition as well as assessment of dopamine metabolism in the brain suggest differences between our selective MB-COMT inhibitors and non-selective nitrocatechols.

**SESSION IV (Poster talks) --** See poster abstracts #78, 31 & 17.

**KEYNOTE**

Scott Wolkenberg: Discovery Chemistry, Merck and Co., Inc., West Point, PA 19486

**Title:** “Target identification for leads from phenotypic screening: examples from infectious disease”

**Abstract:** Improved performance in delivering new medicines depends on the identification of high quality novel therapeutic targets whose modulation translates into robust effects on disease progression. Identification of such targets is challenging, and recent analyses suggest phenotypic approaches may provide equivalent or improved results compared to targeted drug discovery. Three recent experiences with target identification for phenotypic screening leads will be presented: two approaches to HIV treatment focused on host targets, and one aimed at identifying novel antibacterial agents. These studies span a variety of target ID strategies and technologies including chemoproteomics, cellular thermal shift assay, in silico target prediction, and affinity selection/mass spectrometry. Lessons learned from these studies include: the importance of a phenotypic assay with high translation value, the power of cheminformatics for providing readily testable hypotheses, and the value of iterative application of chemoproteomics with structurally distinct probes.
POSTER ABSTRACTS
Ninth Annual Frontiers at the Chemistry-Biology Interface Symposium
May 14, 2016, Johns Hopkins University

Poster # 1  Bioinspired Scanning Ion Conductance Microscopy (Bio-SICM) for Simultaneous Conductance and Specific Molecular Imaging
Florika C. Macazo and Ryan J. White, Ph.D
Department of Chemistry and Biochemistry, University of Maryland Baltimore County

Poster # 2  Interactions of the Hfq RNA binding protein with the PrrF and PrrH sRNAs of Pseudomonas aeruginosa
Louise Djapnje, Subrata Panja, Sarah Woodson, and Amanda Oglesby-Sherrouse
UMB-School of Pharmacy, Pharmaceutical Sciences Department

Poster # 3  Analyzing the successful conjugation of peptide CK2.3 to quantum Dots and its eventually cellular uptake into C2C12 cells.
Vrathasha Vrathasha, Rebecca Noll, Hemanth Akkiraju, Anja Nohe
University of Delaware

Poster # 4  New Tricks for an Old Drug: Inhibition of Glyceraldehyde-3-Phosphate Dehydrogenase by Dithiolethiones to Suppress Cancer Cell Proliferation
Michael R White, Thomas W Miller, Christopher Switzer, John Chavis, Pauline Xu, Erin Oliphant, Patricia Dranchak, Jim Inglese, David Roberts, David Wink, Elsa D Garcia
(1)Chemistry and Biochemistry, University of Maryland, Baltimore County, Baltimore, MD, (2)National Institutes of Health/ National Cancer Institute, Bethesda, MD (3)National Institutes of Health/National Center for Advancing Translational Sciences, Rockville, MD

Poster # 5  Computational Calorimetry
Alexis Webb, Clement Arnarez, Edward Lyman*
Department of Physics and Astronomy University of Delaware, *Department of Chemistry and Biochemistry

Poster # 6  Bone Bioreactor to Maintain Bone Cell Viability ex vivo
Aparna Swarup, Miho Maeda, Jeremy Bonor, Anja Nohe
University of Delaware

Poster # 7  Role of the α2-adrenoceptor in nerve agent-induced status epilepticus
Hilary S. McCarren, Julia Arbutus, Cecelia Jackson, Aymen Alqazzaz, & John H. McDonough
US Army Medical Research Institute of Chemical Defense

Poster # 8  Towards the chemo-enzymatic synthesis of the heptapeptide antibiotic complestatin: investigating the role of the P450 oxygenases ComI and ComJ in aryl linkage formation
Aurelio Mollo, Joshua A. Bulos, A. Nikolai von Kruenstiern, Louise K. Charkoudian
Department of Chemistry, Haverford College, PA

Poster # 9  Near-IR Light-Mediated Cleavage of Antibody-Drug Conjugates Using Cyanine Photocages
Alexander P. Gorka, Roger R. Nani, Tadanobu Nagaya, Hisataka Kobayashi, Martin J. Schnermann
Chemical Biology Laboratory, National Cancer Institute, NIH & Molecular Imaging Program, National Cancer Institute, NIH

Poster # 10  Short-Term Exposure to Soluble Poly(ethylene) Glycol (PEG) Leads to a Reduction in Cellular Metabolic Activity: Time Constraints of PEG Based Material Preparation in Clinical Settings
Rebecca L. McPherson, Marzieh Zamani, and Robert E. Akins
(1)The University of the Sciences, Department of Biological Sciences, Philadelphia, PA: (2) A.I. duPont Children’s Hospital, Department of Biomedical Research, Wilmington, DE

Poster # 11  Specific lipid binding sites identified by coarse-grained simulations
Clement Arnarez*, Xavier Periole*, Sievert-Jan Marrink*, Edward R. Lyman*
*258 Sharp Lab, University of Delaware, Newark, DE 19712, United States; ^Nijhenborg 7, University of Groningen, 9747 AG Groningen, The Netherlands
Poster #12  
Investigation of the Unique Myristylation Signal of the Feline Immunodeficiency Virus Matrix Protein  
University of Maryland, Baltimore County; Howard Hughes Medical Institute

Poster #13  
Remodeling of bacterial cell surfaces using unnatural D-amino acids  
Jon Fura, Sean Pidgeon, Marcos Pires  
Lehigh University

Poster #14  
Developing A Ubiquitin Probe-Based Whole Cell Lysate Assay for the Identification of Small Molecule Deubiquitinase Inhibitors  
Christine A Ott$, Bolormaa Baljinnyam$, Adam Tencer$, Anton Simeonov$, Ajit Jadhav$, Zhihao Zhuang$  
$1Department of Chemistry and Biochemistry, 214A Drake Hall, University of Delaware, Newark, DE, 19716, USA;  
$2National Center for Advancing Translational Sciences, NIH, Bethesda, MD, 20892, USA

Poster #15  
Stirring a Low Reynolds Number MARTINI  
Andrew Zgorski and Dr Edward Lyman  
University of Delaware

Poster #16  
Nod2 directly binds muramyl dipeptide through its leucine rich repeat domains in vitro  
Mackenzie L. Lauro, Brian J. Bahnson, Catherine Leimkuhler Grimes  
Department of Chemistry & Biochemistry, University of Delaware, Newark DE 19716

Poster #17  
HIV-1 Integrase Strand Transfer Inhibitors that Reduce Susceptibility to Drug Resistant Mutant Integrase  
(1) Chemical Biology Laboratory and (2) HIV Dynamics and Replication Program, Center for Cancer Research, National Cancer Institute, National Institutes of Health, Frederick, MD 21702 and (3) Developmental Therapeutics Branch and Laboratory of Molecular Pharmacology, Center for Cancer Research, National Cancer Institute, National Institutes of Health, Bethesda, MD 20892 and (4) Clare Hall Laboratories, The Francis Crick Institute, Blanche Lane, South Mimms, EN6 3LD, UK and (5) Imperial College London, St-Mary’s Campus, Norfolk Place, London, W2 1 PG, UK.

Poster #18  
Synthetic Acyltransferases antagonize Androgen Receptor Activity  
Yuchen Zhang, Pavan K. Mantravadi, John T. Koh  
University of Delaware

Poster #19  
Using molecular simulations to delineate functional conformational transitions in the HCV polymerase  
Ester Sesmero, Ian Thorpe  
UMBC

Poster #20  
Requirements for Innate Immune Receptor Recognition and Response to Bacterial Cell Wall Fragments  
Amy K. Schaefer; James E. Melnyk; Catherine L. Grimes  
Department of Chemistry and Biochemistry, University of Delaware

Poster #21  
Enhancing DNA Crystal Durability Through Chemical Crosslinking  
Diana Zhang, Paul Paukstelis  
University of Maryland College Park

Poster #22  
Autoproteolytic cleavage of membrane enzyme selenoprotein K  
Zhengqi Zhang, Jun Liu, and Sharon Rozovskiy  
Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware 19716, United States

Poster #23  
Bioorganic Investigation of Quaternary Ammonium Compound (QAC) Resistance in Staphylococcus aureus  
Megan C. Jennings, Megan E. Forman, Kevin P.C. Minbiole, William M. Wuest  
Department of Chemistry, Temple University and Department of Chemistry, Villanova University

Poster #24  
Defining and Exploiting APOBEC3A's Cytidine Deaminase Activity on the Extended Epigenome  
Emily K. Schutsky, Jamie E. DeNizio, Christopher S. Nabel, Rahul M. Kohli  
University of Pennsylvania Perelman School of Medicine
Poster # 25 Identification of endogenous ligands for orphan nuclear receptors
Young-Sam Lee, Siizhe Liu, Vivian Jou, and Jenn Seo
Department of Biology, Johns Hopkins University, Baltimore, Maryland 21218, USA

Poster # 26 Nutrient Limitation Enhances Antimicrobial Activity of Alkylacetylphosphonates Targeting DXP synthase
S. Sanders (1), D. Bartee (1), J. Aklinski (2), A. Kopписch (2), C. L. Freel Meyers (1)
(1) Johns Hopkins School of Medicine, Baltimore, MD, USA; (2) Northern Arizona University, Flagstaff, AZ, USA

Poster # 27 Ribosome-templated azide-alkyne cycloadditions: synthesis of potent macrolide antibiotics via in situ click chemistry
Samer Daher, Ian Glassford, Christiana Teijaro, Dr. Rodrigo Andrade
Temple University

Poster # 28 RNA-Targeted Drug Discovery: A Multi-Dimensional Approach is Necessary and Sufficient
Nathan Baird
University of the Sciences

Poster # 29 Modification of Thymine DNA Glycosylase by Small Ubiquitin-Like Modifiers Is Efficient but Not Selective for the Enzyme-Product Complex
Christopher T. Coey(1), Megan E. Fitzgerald(1), Atanu Maiti(1), Dylan McLaughlin(2), Katherine H. Reiter(2), Catherine M. Guzzo(2), Michael J. Matunis(2), and Alexander C. Drohat(1)
(1)Department of Biochemistry and Molecular Biology, University of Maryland School of Medicine, Baltimore, MD 21201; (2) Department of Biochemistry and Molecular Biology, Bloomberg School of Public Health, The Johns Hopkins University, Baltimore, MD 21205

Poster # 30 Crosstalk between Human Mesenchymal Stem Cells and Human Umbilical Vein Endothelial Cells on a Peptide Amphiphile Scaffold
David Chasteen-Boyd, Lily Deng, Dhruv Patel, Jeremy Vines, Amjad Javed, Shawn Gilbert, and Ho-Wook Jun
(1)Dept. of Biomedical Engineering, (2)UAB Institute of Oral Health Research, (3)UAB Dept. of Orthopaedic Surgery

Poster # 31 Sequestration-mediated downregulation of de novo purine biosynthesis by AMPK
Danielle L. Schmitt, Yun-ju Cheng, Junyong Park, and Songon An
Department of Chemistry and Biochemistry, Department of Mathematics and Statistics, University of Maryland Baltimore County

Poster # 32 Remarkable endoplasmic reticulum targeted apoptotic photo-cytotoxicity in visible light of an oxovanadium(IV) vitamin-B6 Schiff base complex
Sanya Banerjee and Akhil R. Chakravarty
Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India.

Poster # 33 Synthesis of β-Substituted FR900098 Organophosphorous Antimicrobials Targeting the Non-Mevalonate Pathway
R. Carl Brothers & Cynthia S. Dowd
The George Washington University

Poster # 34 Phosphatase-stable phosphothreonine analogs that improve the affinity of peptidomimetic ligands of the polo-like kinase 1 polo-box domain
David Hymel and Terrence R. Burke, Jr.
NIH, NCI, Chemical Biology Laboratory

Poster # 35 A new Rosetta refinement algorithm to improve membrane protein structures
Julia Koehler Leman, Drew D'Avino, Jeffrey J. Gray
Department of Chemical and Biomolecular Engineering

Poster # 36 Synthesis and Evaluation of Boronic Acid Analogues of Inhibitors of the Non-mevalonate Isoprenoid Biosynthesis Pathway
James M. Gamrat, Sarah J. Burke, Bryan C. Figula, John W. Tomsho
University of the Sciences in Philadelphia
Poster # 37  Syntheses of (−)-Sungucine, (−)-Isosungucine, and (−)-Strychnogucine B and Progress towards Photoaffinity Analogs
Christian N. Teijaro, Senzhi Zhao, Heng Chen, Rodrigo B. Andrade
Temple University

Poster # 38  Enzyme-catalyzed expressed protein ligation
Samuel Henager, Nam Chu, Zan Chen, Daniel Dempsey, David Bolduc, James Wells, Philip A. Cole
Dept of Pharmacology and Molecular Sciences, Johns Hopkins University; Dept. of Pharmaceutical Chemistry, University of California, San Francisco

Poster # 39  Modulation of p300/CBP acetyltransferase activity by a bromodomain ligand
Johns Hopkins School of Medicine, Fox Chase Cancer Center, Johns Hopkins University

Poster # 40  Differentiation of RAW264.7 monocyte/macrophage cell line to osteoclasts is inhibited by a mimicking peptide, CK2.3
John Nguyen, Anja Nohe
Department of Biological Sciences, University of Delaware

Poster # 41  Mechanism of the pH-dependent activation of the sodium-proton antiporter NhaA
Yandong Huang, Wei Chen, and Jana Shen
Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore

Poster # 42  Diverted Total Synthesis and Biological Investigation of Promysalin and Analogs Thereof
Andrew D. Steele, Colleen E. Keohane, Kyle W. Knouse, Sean E. Rossiter, Sierra J. Williams, and William M. Wuest
Temple University

Poster # 43  Modulating the LexA cleavage rate tunes the SOS response and acquired antibiotic resistance
Charlie Y. Mo, Rahul M. Kohli
University of Pennsylvania

Poster # 44  Diverted Total Synthesis of the Anti-Biofilm Natural Product Carolacton and Analogs Thereof
Temple University

Poster # 45  Bioanalytical Approaches to Measure Iron Speciation in the Plasma of Participants Treated with Iron-Nanoparticle Drug Products
Heather M. Neu, Aaron D. Smith, Joel E. P. Brandis, Anne M. C. Williams, Sameh S. Abdelmalak, Angela Wilks, James Polli, Maureen Kane, Tricia Ting, Sarah L. J. Michel
Department of Pharmaceutical Sciences, University of Maryland, Baltimore, MD, United States

Poster # 46  Design and synthesis of a new class of oligomannose immunogens for recapitulation of the 2G12 HIV epitope
Christian Toonstra, Qiang Yang, and Lai-Xi Wang
University of Maryland-College Park

Poster # 47  Semisynthesis of human selenoenzyme cSeLS through native chemical ligation
Rujin Cheng, Zhengqi Zhang and Sharon Rozovsky
University of Delaware Department of Chemistry and Biochemistry Newark, DE 19716

Poster # 48  Molecular Mechanism of BRAF Activation by Phosphorylation, Dimerization and ATP-Competitive Inhibitors
Christine Candelora§, Nicholas Cope§, Kenneth Wong§, Yana Li*, Philip A. Cole*, Zhihong Wang§¶
§University of the Sciences, Department of Chemistry and Biochemistry,
¶Corresponding author, *Johns Hopkins University School of Medicine

Poster # 49  Mutations at a single active site residue in TET2 stall oxidation at 5hmC and reveal requirements for catalysis
Monica Yun Liu*, Hedieh Torabifard**, Daniel J. Crawford*, Jamie E. DeNizio*, G. Andres Cisneros**, Rahul M. Kohli*
*Dept. of Medicine and Dept. of Biochemistry & Biophysics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA; **Department of Chemistry, Wayne State University, Detroit, MI
Poster # 50  **Inhibiting P. aeruginosa Heme Oxygenase Via Allosteric Binding Shows Activity in Clinical Isolates**
Geoffrey A. Heinzl, Bennett J. Giardina, Wenbo Yu, Alexander D. MacKerell, Jr., Angela Wilks, Fengtian Xue
Pharmaceutical Sciences, School of Pharmacy, University of Maryland, Baltimore

Poster # 51  **Functionalized 3D DNA Crystals Through Layer-by-Layer Assembly**
Ronald W. McNeil and Paul J. Paukstelis
University of Maryland College Park

Poster # 52  **Synthesis of Theranostic Gold Nanoparticles for Drug Delivery**
Arunendra Saha Ray, Marie-Christine Onuta
UMBC

Poster # 53  **Selenoprotein S**
Zhengqi Zhang, Vicki Wallace, Jun Liu, and Sharon Rozovsky
University of Delaware, Department of Chemistry and Biochemistry

Poster # 54  **Development of prodrug approaches for long-acting nanoformulations of emtricitabine-based regimens**
Amer Al-khouja, Melanie Johnston, David Meyers, Caren Freel Meyers
Johns Hopkins University School of Medicine,

Poster # 55  **The Importance of the P. aeruginosa Has System in Extracellular Heme Sensing and Acquisition**
Alecia T. Thomas, Susana Mourino, Aaron D. Smith, and Angela Wilks
Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland, Baltimore

Poster # 56  **Role of TET processivity in shaping the extended epigenome**
Jamie E. DeNizio, Sajid Marhon, Kyoung Jae Won, Rahul M. Kohli
University of Pennsylvania

Poster # 57  **Collagen Mimetic Peptides for Integration of Growth Factor Gene Delivery with Tissue Repair**
Morgan A. Urello, Kristi L. Kiick, and Millicent O. Sullivan
University of Delaware

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Johns Hopkins Drug Discovery Program, Johns Hopkins University, Baltimore, Maryland 21205, United States; Department of Neurology, Johns Hopkins University, Baltimore, Maryland 21205, United States; Department of Pathology, Johns Hopkins University, Baltimore, Maryland 21231, United States; Department of Molecular and Comparative Pathobiology, Johns Hopkins University, Baltimore, Maryland 21205, United States

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Angela T. Nguyen(1), Jace W. Jones1, Stephanie J. Shiffka(1), Miguel Camara(2), Paul Williams(2), Maureen A. Kane(1), and Amanda G. Oglesby-Sherrouse(1,3)
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Pharmaceutical Sciences, University of Maryland Baltimore, Baltimore, MD, United States.
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(a) Department of Chemistry and Biochemistry, University of Maryland College Park; (b) Department of Anesthesia, Critical Care and Pain Medicine, Massachusetts General Hospital, and Harvard Medical School, Boston

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Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland at Baltimore, Baltimore, Maryland; Bioreclamation IVT, Baltimore, Maryland; Department of Radiation Oncology, School of Medicine, CaseWestern Reserve University, Cleveland, Ohio; Department of Medicine, University of Maryland School of Medicine and Stewart Greenebaum Cancer Center, Baltimore, Maryland.

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(1) Department of Chemistry, Johns Hopkins University, Baltimore, MD; (2) Department of Biology, Johns Hopkins University, Baltimore, MD

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Chemistry-Biology Interface Program, Department of Chemistry, Johns Hopkins University

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(1) Department of Physics and Astronomy, University of Delaware, Newark, DE, United States. (2) Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN, United States. (3) Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN, United States. (4) Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

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Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland, Baltimore
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Department of Biomedical Engineering, School of Medicine, Division of Cardiology, University of Alabama at Birmingham, Birmingham, AL; Department of Radiology, Mayo Clinic, Rochester MN

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University of Delaware Department of Biology and Department of Chemistry and Biochemistry

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