

BIOL

Division of Biological Chemistry

L. Hedstrom and S. Kelley, *Program Chairs*

SUNDAY MORNING

Section A

Walter E. Washington Convention Center
Room 145B

Repligen Award for the Chemistry of Biological Processes

W. A. Van Der Donk, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 1. Function and structure of a new class of indole alkaloid cyclases in the Stigonematales cyanobacteria.
D.H. Sherman, S. Li, S.A. Newmister, A.N. Lowell, F. Yu

9:15 2. Diverse evolutionary solutions to β -lactam antibiotic biosynthesis and the partitioning of reactive intermediates by non-ribosomal peptide synthetases. **C.A. Townsend**

9:55 Intermission.

10:10 3. Pathway for production of the bacterial cofactor pyrroloquinoline quinone (PQQ): At the confluence of radical SAM (RS) enzymes and ribosomally synthesized and post-translationally modified peptides (RiPPs). **J. Klinman**

10:50 Award introduction.

10:55 4. Two radical proteins: Hydroxyethylphosphonate dioxygenase and methylphosphonate synthase.
W.A. Van Der Donk

Merck Research Award Symposium

Sponsored by WCC, Cosponsored by BIOL, COMP, MEDI, MPPG, ORGN, PMSE and PROF

Nanotechnology & Single Cell Analysis in Biology & Medicine

Sponsored by ANYL, Cosponsored by BIOL, COLL and PHYS

Experimental & Computational Advances in Understanding Enzyme Specificity & Promiscuity

Catalytic Promiscuity & the Emergence of New Proteins

Sponsored by PHYS, Cosponsored by BIOL and COMP

SUNDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 145B

Mitochondrial Chemical Biology

S. O. Kelley, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 5. Spatiotemporal proteomic analysis of mitochondrial sub-compartments and next-generation enzymatic proximity labeling methods. **T. Branon**, A. Ting

1:40 6. Mitochondrial protein functions elucidated by multi-omic mass spectrometry profiling. **D. Pagliarini**

2:15 7. Mitochondrial nanomedicine. **S. Dhar**

2:50 Intermission.

3:00 8. Targeting mitochondrial DNA. **S.O. Kelley**

3:35 9. Mitochondrial topoisomerases and their repair enzymes. **Y. Pommier**

Section B

Walter E. Washington Convention Center
Room 147B

Gordon Hammes Award Lecture

L. Hedstrom, *Organizer*

A. Schepartz, *Organizer, Presiding*

4:30 Introductory Remarks.

4:35 10. Molecular interactions of lipopolysaccharide with an outer membrane protein from *Pseudomonas aeruginosa* probed by solution NMR. **I. Kucharska**, B. Liang, N. Ursini, L.K. Tamm

4:50 Award Introduction.

4:55 11. Discovery of novel enzymes in novel metabolic pathways. **J.A. Gerlt**

5:40 Concluding Remarks.

Nanotechnology & Single Cell Analysis in Biology & Medicine

Sponsored by ANYL, Cosponsored by BIOL, COLL and PHYS

Science Communications: The Art of Developing a Clear Message

Sponsored by PRES, Cosponsored by BIOL, CARB, CEI, CELL, CEPA, CINF, COLL, CPRC, CTA, DAC, I&EC, INOR, ORGN, PROF, SCHB and YCC

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Computational Tools for Enzyme Evolution & Functional Annotation

Sponsored by PHYS, Cosponsored by BIOL and COMP

MONDAY MORNING

Section A

Walter E. Washington Convention Center
Room 145B

Eli Lilly Award in Biological Chemistry

H. C. Hang, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 12. New bioluminescent tools to spy on cellular communication. **J.A. Prescher**

9:20 13. Understanding the site-specific consequences of O-GlcNAc using synthetic protein chemistry. **M. Pratt**

10:05 Intermission.

10:20 14. Rational strategy to design probes for the chemical genetic analysis of AAA+ proteins. **T. Kapoor**

11:05 Award introduction.

11:10 15. Chemical dissection of host immunity and microbial pathogenesis. **H.C. Hang**

Building a Safety Culture Across the Chemistry Enterprise

Institutional & Enterprise Level Efforts to Developing a Safety Culture

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CCS, CEI, CELL, CEPA, CHAS, CINF, COLL, CPRC, CTA, DAC, ETHX, I&EC, INOR, ORGN, PROF, SCHB and YCC

Nanotechnology & Single Cell Analysis in Biology & Medicine

Sponsored by ANYL, Cosponsored by BIOL, COLL and PHYS

Chemistry in an Evolving Political Climate: Research Priorities & Career Pathways in Public Policy

Sponsored by YCC, Cosponsored by BIOL, CARB, CCPA, CEI, CELL, CEPA, CHED[‡], CINF, COLL, COMSCI, CPRC, DAC, GEOC, IAC, PRES and SCHB

Impact of Carbonyl & Glycative Stress on Diabetic & Aging Related Diseases

Sponsored by AGFD, Cosponsored by BIOL

Many Colors of Copper

Good Cop, Bad Cop

Sponsored by INOR, Cosponsored by BIOL

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Computational Approaches to Enzyme Design

Sponsored by PHYS, Cosponsored by BIOL and COMP

MONDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 145B

Mid-Career Investigators in Biological Chemistry

L. Hedstrom, *Organizer*

A. Sarkar, *Presiding*

1:00 Introductory Remarks.

1:05 16. Volatile nematode sex pheromones. R. Shinya, M. Gronquist, D. Leighton, Y. Hsueh, F. Schroeder, **P.W. Sternberg**

1:25 17. Viewing human DNA polymerase β faithfully and unfaithfully bypass an oxidative lesion by time-dependent crystallography. **Z. Suo**

1:45 18. Dissecting and targeting the dynamic process of BAX activation. **E. Gavathiotis**

2:05 19. High resolution co-crystal structure of the apelin receptor and peptide agonist complex. **W. Zhong**

2:25 20. Proteolytic cleavage of TRIM14 by the VEEV nonstructural protein 2 cysteine protease. E. Morazzani, J. Compton, D.H. Leary, N.E. Zachara, X. Hu, J.J. Marugan, P. Glass, **P.M. Legler**

2:45 Intermission.

3:00 21. Cycloretinal in age-related macular degeneration: Its biosynthesis by the milk protein beta-lactoglobulin and its catabolism as a treatment strategy. **C. Watanabe**

3:20 22. Potent antimicrobial peptide dendrimers against multi-drug resistant *Pseudomonas aeruginosa* and *Acinobacter baumannii*. **T. Darbre**

3:40 23. Toward vancomycin-like antibiotics: Targeting bacterial lipids with synthetic peptides. **J. Gao**

4:00 24. Bioprospecting and the discovery of cationic antimicrobial peptides from American alligator (*Alligator mississippiensis*) and Komodo dragon (*Varanus komodoensis*). **B. Bishop**, M. Juba, P. Russo, M. Devine, S. Barksdale, K. Vliet, J. Schnur, M.L. van Hoek

Section B

Walter E. Washington Convention Center

Room 147B

Early Career Investigators in Biological Chemistry

Cosponsored by PROF

L. Hedstrom, *Organizer*

J. Hougland, *Presiding*

1:00 Introductory Remarks.

1:05 25. Biochemistry of new metal-specific catalytic DNA. **J. Liu**

1:25 26. RNA-biased small molecules and privileged RNA topologies for selective small molecule: RNA recognition. **A.E. Hargrove**, B. Morgan, C.S. Eubanks, N.N. Patwardhan, A. Donlic, J. Forte

1:45 27. Site-specific RNA binding and translation inhibition by transition metal complexes. **S.S. Jain**, C.M. Anderson, M. Breshears, H. Hoang, S. Lundgren

2:05 28. Chemical modification of mRNA: Toward enabling gene therapy. **C. Gampe**

2:25 Intermission.

2:40 29. Targeting structurally and functionally diverse nucleic acids with druglike small molecules. **J.S. Schneekloth, Jr.**

3:00 30. Molecular mechanisms underlying the hijack of host protein-protein interactions by NS1 of the 1918 Spanish influenza A virus. Q. Shen, D. Zeng, J. Shi, B. Zhao, W. Hwang, P. Li, **J. Cho**

3:20 31. Chemical probes to perturb autophagy regulation and Bcl-2 in neurodegenerative disease. **P.C. Trippier**

3:40 32. KaiC is sufficient to reconstitute the evolutionary primitive hourglass type circadian oscillator *in vitro*. Y. Jeong, **Y. Kim**

Building a Safety Culture Across the Chemistry Enterprise

Grassroots Approaches to Developing a Safety Culture

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CCS, CEI, CELL, CEPA, CHAS, CINF, COLL, CPRC, CTA, DAC, ETHX, I&EC, INOR, ORGN, PROF, SCHB and YCC

Nanotechnology & Single Cell Analysis in Biology & Medicine

Sponsored by ANYL, Cosponsored by BIOL, COLL and PHYS

Chemistry in an Evolving Political Climate: Research Priorities & Career Pathways in Public Policy

Sponsored by YCC, Cosponsored by BIOL, CARB, CCPA, CEI, CELL, CEPA, CHED[‡], CINF, COLL, COMSCI, CPRC, DAC, GEOC, IAC, PRES and SCHB

Transformative Research & Excellence in Education Award

Sponsored by COMSCI, Cosponsored by BIOL, COLL, COMP, ENFL, INOR, PHYS and PRES

Impact of Carbonyl & Glycative Stress on Diabetic & Aging Related Diseases

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Many Colors of Copper

Proteins & Models

Sponsored by INOR, Cosponsored by BIOL

Undergraduate Research Posters

Biochemistry

Sponsored by CHED, Cosponsored by BIOL and SOCED

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Discovery & Engineering of Industrially Relevant Enzymes

Sponsored by PHYS, Cosponsored by BIOL and COMP

MONDAY EVENING

Section A

Walter E. Washington Convention Center
Halls D/E

Sci-Mix

L. Hedstrom, *Organizer, Presiding*

8:00 - 10:00

50, 53, 56, 59, 63, 67-68, 84, 86, 89, 94, 98, 109, 114, 124, 129, 131, 160-161, 165. See subsequent listings.

TUESDAY MORNING

Section A

Walter E. Washington Convention Center
Room 145B

Pfizer Award in Enzyme Chemistry

Financially supported by Pfizer
E. P. Balskus, *Organizer*
E. Balskus, *Presiding*

8:30 Introductory Remarks.

8:35 33. Bait-and-switch mechanism in microbial oxalate metabolism. M.I. Gibson, P.Y. Chen, E.J. Brignole, A. Johnson, E. Pierce, M. Can, S.W. Ragsdale, **C.L. Drennan**

9:10 34. Phenotypic screening for molecular messages regulating microbiomes and their hosts. **J. Clardy**

9:45 35. Using host genetics to decipher gut microbial metabolism. **F.E. Rey**

10:20 Award introduction.

10:25 36. Deciphering the human gut microbiota through enzyme discovery. **E.P. Balskus**

Crosslink DNA Repair

Sponsored by TOXI, Cosponsored by BIOL

Understanding the Chemistry of Our Planet

Chemistry's Role in our Earth System

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CEI, CELL, CEPA, CINF, COLL, CPRC, DAC, GEOC, I&EC, INOR, ORGN, SCHB and YCC

Informatics & Chemical Biology: Identifying Targets & Biological Pathways

Sponsored by CINF, Cosponsored by BIOL and MEDI

Trace Organic Contaminants (TrOCs) in Aquatic Systems: Advancements in Monitoring & Remediation

Sponsored by ENVR, Cosponsored by ANYL and BIOL

Many Colors of Copper

Small Molecule Activation

Sponsored by INOR, Cosponsored by BIOL

TUESDAY AFTERNOON

Walter E. Washington Convention Center
Room 145B

Early Career Investigators in Biological Chemistry

Cosponsored by PROF
L. Hedstrom, *Organizer*
A. E. Hargrove, *Presiding*

1:30 Introductory Remarks.

1:35 37. Determining role of protein glutathionylation in muscle. **Y. Ahn**

1:55 38. Multiple microviridin core peptides are processed by an ATP grasp ligase in a distributive and directional manner. **Y. Ding**

2:15 39. Biosynthesis of deep-sea marine natural products: Genes, enzymes and pathways. **G. Wang**

2:35 40. Activity of KS⁰ in *trans*-AT PKS biosynthase: Control of the ACP modification by inhibition of acyltransferase. **Y. You**

2:55 41. Exploring the macromolecular crowding effects on enzyme inhibition. **M.M. Rowland**, T. Legenzoff, A. Payne, A. Anderson, M. Kim, A. Winfrey, A. Waugaman

3:15 Intermission.

3:30 42. Rational redesign of the collagen triple helix interface. **D.M. Chenoweth**

3:50 43. High-throughput discovery of Protein Catalyzed Capture (PCC) agents as antibody alternatives for thermally stable biological assays. **M.B. Coppock**, C. Jones, B.T. Lai, H.D. Agnew, J.R. Heath, D.N. Stratis-Cullum

4:10 44. Cofactor regulation is important for the function of p97/VCP AAA ATPase. **T. Chou**

4:30 45. Protein topography by rapid methylene derivatization during ESI and top-down mass spectrometry. **P.A. Martino**

Section B

Walter E. Washington Convention Center
Room 147B

Graduate Student & Postdoctoral Fellow Symposium

Cosponsored by PROF
L. Hedstrom, *Organizer*
S. S. Jain, *Presiding*

1:30 Introductory Remarks.

1:35 46. Synthesis and evaluation of oxazolidinone-based small molecule libraries for the selective recognition of RNA bulge motifs. **B. Morgan**, R. Culver, C. Eubanks, J. Forte, A.E. Hargrove

- 1:50 47.** Role of HIV-1's highly basic patch and myristoyl group on matrix-tRNA interactions. **C. Gaines**, A. Rivera-Oven, E. Tkacik, P. Somani, A. Yang, A. Achimovich, T. Alabi, M.F. Summers
- 2:05 48.** Targeting folded HIV-1 RRE RNA with unnatural branched peptides: Boosting affinity and selectivity. **A. Peralta**, Y. Dai, J. Wynn, S. Chringma, S.F. Le Grice, W.L. Santos
- 2:20 49.** Novel mechanomagnetic assay to decode the ribosomal frameshifting motion. **H. Yin**, S. Xu, Y. Wang
- 2:35 50.** Study of RNA chemical modifications as crucial epigenetic regulators. **B. Zhao**, X. Wang, A. Beadell, N. Tirumuru, R. Ho, L. Wu, C. He
- 2:50 51.** Spatial regulation of glycolytic and gluconeogenic enzyme compartmentalization by small molecules in human cells. **D. Schmitt**, P. Dranchak, J. Inglese, S. An
- 3:05** Intermission.
- 3:20 52.** Noninvasive imaging of human immune cell infiltration in a human xenograft model of graft-versus-host disease. **M. Rashidian**, C.H. Van Elssen, V. Vrbanac, H. Ploegh
- 3:35 53.** Dynamic multi-color protein labeling in living cells. **C. Li**, M. Plamont, H.L. Sladitschek, V. Rodrigues, I. Aujard, P. Neveu, T. Le Saux, L. Jullien, A. Gautier
- 3:50 54.** Terminal alkynes as Raman probes of α -synuclein aggregation in cellular environments. **J.D. Flynn**, J.C. Lee
- 4:05 55.** Constructing red-shifted fluorescent protein sensors of cellular redox status. **K.J. Trull**, S. Norcross, J. Snaider, S. Doan, K. Tat, L. Huang, M. Tantama
- 4:20 56.** Chemical-proteomic targeting of mitochondrial cysteine residues involved in metabolic and redox regulation. **D. Bak**, M. Pizzagalli, E. Weerapana
- 4:35 57.** Near infrared fluorescence tagged glucosamine for non-invasive *in-vivo* tumor detection. **M. Mathew**, S. Parthasarathy

Understanding the Chemistry of Our Planet

Human Impacts to our Planet

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CEI, CELL, CEPA, CINF, COLL, CPRC, DAC, GEOC, I&EC, INOR, ORGN, SCHB and YCC

Memorial Symposium Honoring Justine Roth: Oxygen & Isotope Effects in Mechanisms, from Enzymes to Small Molecules

Sponsored by INOR, Cosponsored by BIOL

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

Structure-Function Relationships in Enzyme Evolution

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Many Colors of Copper

Catalysis

Sponsored by INOR, Cosponsored by BIOL

TUESDAY EVENING

Section A

Walter E. Washington Convention Center
Hall C

Current Topics in Biochemistry

L. Hedstrom, S. O. Kelley, *Organizers*

7:00 - 9:00

58. Investigating the mechanism of LThDP decarboxylation by DXP synthase. **A. DeColli**, A. Majumdar, N.S. Nemeria, F. Jordan, C. Freel Meyers

59. Developing of plug-and-playable fluorescent cell imaging modular toolkits based on the protein ligation system, SpyTag/SpyCatcher. **Y. Bae**, S. Kang

60. Lead tightly associates with neuronal calcium sensor (NCS) protein DREAM and promotes structural changes analogous to calcium bound DREAM. **S. Azam**, J. Miksovska

61. SMYD2 glutathionylation controls sarcomere stability and myofibril integrity. **D.N. Munkanatta Godage**, K. Samarasinghe, Z. Yang, M. Luo, Y. Ahn

62. Discovery of a small molecule protease inhibitor from an abundant human gut commensal microbe. **B.A. Schneider**, E.P. Balskus

63. Novel anionic conjugated polyelectrolyte lipoplex and its application for apoptosis imaging. **P. Wu, C. Tan**

64. 2-APB and CGP-37157 as neuroprotective agents against the toxicity and uptake of 1-methyl-4-phenylpyridinium in dopaminergic MN9D cell. **V.Q. Le**, M. Mapa, K. Wimalasena

65. Computer-aided analysis of autophagy pathway. **K. Han**, M. Choi, J. Kim

66. Autophagy-induced cellular phase transitions. **K. Han**, J. Kim, M. Choi

- 67.** *Gaussia princeps* luciferase: A bioluminescent substrate for oxidative protein folding. **T. Yu**, J.A. Prescher, C. Thorpe
- 68.** Interactions between human pyruvate dehydrogenase complex (PDC) components and four isoforms of pyruvate dehydrogenase kinases (PDKs). **L. Yang**, N.S. Nemeria, E.L. Guevara, J. Zhou, J. Wang, F. Jordan
- 69.** Impact of carvedilol on the thioredoxin pathway. M. Alharbi, K. Larsen, C. Lynch, **T.M. Seefeldt**
- 70.** Transcriptional regulator of eicosapentaenoic acid synthesis (PfaR): Recombinant expression and evidence of its DNA-binding role. **M.C. Ortiz**, C. Rullán-Lind, Y. Morales-Lozada, M. Pérez-Oquendo, R. González-Méndez, A. Baerga-Ortiz
- 71.** Searching RNA 3D structures for tertiary structural patterns. **M.S. Adams**, K.E. Richardson, C.C. Kirkpatrick, D.W. Gohara, B. Znosko
- 72.** Developing a luciferase based circulating tumor cells detection system using functionally modulated SpyTag/SpyCatcher bacterial clue. **B. Choi**, H. Moon, H. Choi, S. Kang
- 73.** Lipid raft formation: Key role of polyunsaturated phospholipids. **C. Wang**, S.L. Regen
- 74.** Enzymology and drug discovery studies on the L205R mutant of cAMP-dependent Protein Kinase (PKA α). **N. Luzzi**, D. Peterson, K.C. Ellis
- 75.** NagD from *Yersinia pestis*. M. Le, L. Dass, I. Moreno, **S.F. O'Handley**
- 76.** Dissecting the resveratrol-mediated regulation of mitochondria dynamics in replicative senescent yeast cells. Y. Yu, C. Lo, Y. Chen, **C. Chang**
- 77.** Hidden antioxidative functions of NADH coexisting with hemoglobin. **H. Sakai**
- 78.** Progress toward the chemical characterization 3-vinyl-2,3-pyrroline-5-carboxylic acid (VPCA): A bacterial, natural-product synthon. **K.L. Colabroy**, **B. Juliano**, E.R. Gassaway, Z. Zimmerman
- 79.** Fluorescent indicator displacement assay to identify and characterize secondary structure-specific RNA: Small molecule interactions. **S. Wicks**, B. Morgan, A.E. Hargrove
- 80.** Acetyl-group sensing through modulation of conformational dynamics in an arylalkylamine N-acetyltransferase. **A. Aboalroub**
- 81.** Regulatory metabolic complex for glucose metabolism in living cells. **M. Jeon**, C. Kohnhorst, M. Kyoung, D. Schmitt, E.L. Kennedy, S.M. Bracey, J. Ramirez, B.T. Luu, S. Russell, S. An
- 82.** Developing high-field MRI contrast conjugate agents using protein cage nanoparticles. **H. Kim**, S. Jin, H. Choi, H. Cho, S. Kang
- 83.** Understanding the role of TRAF6 in the antiviral activity of Viperin. **A. Patel**, S. Ghosh, A.B. Dumbrepatil, E.G. Marsh
- 84.** Development of chemical probes and high-throughput screening strategies to target an oncogenic RNA triple helix. **A. Donlic**, J. Xu, A. Liu, C. Roble, A.E. Hargrove
- 85.** Elucidating the role of the proximal ligand loop in chloroperoxidase catalysis. **E. Kwong**, X. Wang

- 86.** Biochemical characterization of PRMT5 inhibition by small molecules designed via structure-based design. **W. Zhou**
- 87.** Heterogeneous nucleation of oligomeric superoxide dismutase-1 controlled by glycerolipid head groups. **S. Rasouli**, A. Abdolvahabi, B.F. Shaw, A. Chuprin
- 88.** Study on lipid composition of scalp sebum collected from women in different countries. **K. Nagami**, Y. Nagano
- 89.** Discovery and characterization of notch1 modulating peptides. **D. Schachter**, Y. Li
- 90.** Neutron vibrational spectra of biomolecular building blocks using the high resolution VISION spectrometer and accompanying computed spectra using several computational methods. **A.A. Sedova**, A.C. Fitzsimmons, M.D. Smith, L. Petridis, L. Daemen, A. Ramirez-Cuesta, J. Smith
- 91.** Investigating metastatic potential in colon and prostate cancers using synthetic lectins. **T. Hundal**, J.J. Lavigne
- 92.** *In vitro* kinetics of mutant superoxide dismutase-1 aggregation can predict patient survivability in amyotrophic lateral sclerosis. **A. Abdolvahabi**, S. Rasouli, Y. Shi, C. Croom, B.F. Shaw
- 93.** Investigation of a functionally essential domain within human ghrelin *O*-acyltransferase. **M. Campana**, M. Ashkar, J. Hougland
- 94.** Understanding the alternative activities of DXP synthase. **M. Johnston**, A. Majumdar, C. Freel Meyers
- 95.** New library generation method for metabolic pathway engineering by using CRISPRi system. **J. Lee**, W. Song, S. Seo, B. Kim
- 96.** Probing the mechanism of viral Inhibition by the radical SAM enzyme, Viperin. **S. Ghosh**, C. Makins, G.D. Román-Meléndez, A.B. Dumbrepatil, A. Patel, E.G. Marsh
- 97.** Structure-activity relationships for activation of *Arabidopsis thaliana* cytokinin receptors by analogs of *N*⁶-benzyladenine. **D.I. Osolodkin**, E.M. Saveleva, D.S. Karlov, S.N. Lomin, S.N. Mikhailov, G.A. Romanov
- 98.** Investigation of inhibitor-protein interactions in plants & mammals from EVV 2DIR data. **S. Sim**, H. Sowley, N. Kidley, L. Barter, D. Klug
- 99.** Improved harvesting of potential CAMPs using itaconic acid. **J. D'Onofrio**, M.C. Devine, P. Russo, B. Bishop
- 100.** Curious (unexpected?) behavior of bovine Cu/Zn superoxide dismutase on SDS-PAGE: Formation of multimeric assemblies with discrete mol.wts. that retain enzymatic activity. Similar behavior of Cu/Zn SOD in the hemolymph of mussels. **M.G. Hamilton**
- 101.** Mutational analysis of human ghrelin *O*-acyltransferase. **M. Ashkar**, M. Campana, J. Hougland
- 102.** New insight on polystyrene biodegradation by two different *Tenebrio molitor*s. **B. Peng**
- 103.** Characterization of bifunctional peptides: Porphyrin binding and antimicrobial activity. **D.J. Shirley**, G.A. Caputo

- 104.** Determination of the fatty acid/lipid profiles in a mouse model of Alzheimer's disease. **L.S. Webb, B. Genovese, D. Mitrano, H.J. Grau, R. Quinlan**
- 105.** Effects of Alpha-synuclein uptake on cellular viability, morphology, and localization. **S. Lacy, J.D. Flynn, J.C. Lee**
- 106.** Conserved ion pairs between the barrel and hatch domain of BtuB are required for vitamin B₁₂ transport and/or during transmembrane signaling. **T. Nilaweera, D.S. Cafiso**
- 107.** Influence of ionic liquids on detergent mediated denaturation of myoglobin. **E.M. Kohn, T.D. Vaden, G.A. Caputo**
- 108.** Effect of divalent metal cations on catalytic activity of Rv0045c esterase from *M. tuberculosis*. **I. Bowles, R. Johnson, G.C. Hoops**
- 109.** Global substrate specificity of mycobacterial serine hydrolases. **R. Johnson, B. Bassett, B. Waibel, A. Koelper, G.C. Hoops**
- 110.** Fatty acids analysis of outer membrane vesicles from *Escherichia coli* harboring the *pks island*. **Y. Morales-Lozada, G. Baez Bravo, R. Gómez-Moreno, A. Baerga-Ortiz**
- 111.** Examining the effects of thioamides on proteolysis. **T. Barrett, X. Chen, J. Wang, C. Liu**
- 112.** Photoinduced interaction of ubiquitin binding domains with genetically encoded *p*-Benzoyl-L-phenylalanine monomeric ubiquitin and polyubiquitin chains. **C. Braxton, E. Quartner, T.A. Cropp, D. Fushman**
- 113.** Enzyme function prediction, discovery, and characterization in an undergraduate biochemistry lab. **S.F. O'Handley, J. Mills, K. O'Donovan, A. DiCola, M. Cattalani, A. Fadden, A. Flavin, C. Mcnamara, A. Murphy Shaw, J. Pierce, K. Wilson, T. Wolf, P. Craig**
- 114.** New natural product analog of blasticidin S reveals cellular uptake facilitated by the NorA multidrug efflux pump. **J.R. Davison, K. Lohith, S. Mandadapu, J. Piotrowski, H. Smith, C.A. Bewley**
- 115.** Mechanism of an antimicrobial surface agent and virucidal efficiency. **N. Zhan, Q. Chang, K. Yeung, J. Kwan**
- 116.** Supramolecular organization and function of cartilage extracellular matrix. **F. Horkay, E. Dimitriadis, I. Horkayne-Szakaly, P.J. Basser**
- 117.** Impacts of protein oxidation conditions on structure and function. **G.A. Heinzl, D. Kryndushkin, V. Rao**
- 118.** Lysozyme-Catalyzed polymerization of an ionically conductive polyacetylene. **D. Morris, A.P. Zampino, L. Crandall, A. Tarabozetti, T. Leeper, C.J. Ziegler**
- 119.** Study of the oligomerization process of IAPP using GaNPs derivatives. **A.S. Delgado Carrión, A. Melendez, I. Ramos, R. Oyola**
- 120.** Bioisosteric 5-oxa/aza analogues of ipomoeassin F uncover an H-bonding activity cliff and more. **G. Zong, Z. Hu, X. Sun, R. Bhakta, L. Whisenhunt, W. Shi**

- 121.** Studies on the radical S-adenosylmethionine (SAM) thiazole C-methyltransferase involved in thiomuracin biosynthesis. **N. Mahanta**, Z. Zhang, G.A. Hudson, W.A. Van Der Donk, D.A. Mitchell
- 122.** Computational study of butyrylcholinesterase inhibition by aryl alkyl cholinyl phosphorous derivatives. **N. Humphrey**, M. Sanchez, E.J. Sorin
- 123.** Evaluation of anti-obesity effects based on dynamics of a transcription factor network in the adipogenic differentiation. **K. Choi**, M. Lee
- 124.** DNA methyltransferase DNMT1 activity in the presence of oxidized and extended forms of 5-methylcytosine. **J. Fernandez**, C. Seiler, D. Kotandeniya, Z. Koerperich, M. Andersen, N.Y. Tretyakova
- 125.** Method for the quantification of levels of phosphorylation and phosphorylated sugar moieties in the glycans of recombinant proteins. **S.A. Ketcham**, M. Ashraf, C. Madhavara
- 126.** Oysters from locations in the Elizabeth River show elevated heavy metal concentrations. **B.F. Lasseter**, R.P. Burke, S. Bailey
- 127.** Reversible DNA-protein cross-linking at epigenetic DNA marks. **S. Ji**, N.Y. Tretyakova
- 128.** Discovery of dihydroxy fatty acids as major components of the seed oil of the brassicaceae *Orychophragmus violaceus* suggests a variant mode of elongation. A.M. Teitgen, X. Li, W. Zhang, C. Zhang, E. Cahoon, **R.E. Minto**
- 129.** Investigating the role of cobalamin (vitamin B₁₂) in microbial communities by activity-based protein profiling. **B. Killinger**, J. Rosnow, L. Anderson, P. Nandhikonda, A. Wright
- 130.** Synthesis and screening of a β -amino acid bisintercalator library. **E. Gratton**, B.L. Iverson
- 131.** Developing novel biosensors for the “cross-chiral” detection of structured RNAs. **B. Young**, J. Sczepanski
- 132.** Overexpressing SIT in osteoblasts. **G. Petkov**, T. Owen
- 133.** Phosphoprotein Enriched in Astrocytes 15 (PEA-15) changes confirmation upon phosphorylation & interaction with FADD. **J.P. Marrero**
- 134.** Monooxygenase reaction: revisit of tyrosinase and its application. **B. Kim**
- 135.** *In vitro* evolution of L-ribonucleases capable of cleaving structured D-RNA targets. **N. Kundu**, J. Sczepanski
- 136.** Expression and characterization of straight α - α -helix concatemers for nanosheet formation. **R.A. Bartlett**, V.P. Conticello
- 137.** Interaction of cationic single-chain and gemini surfactants with hen egg white lysozyme: A spectroscopic and computational study. **R. Patel**
- 138.** Sugars and pathogens: Avenues for targeting infections. **A. Sarkar**
- 139.** Atypical split inteins mediated two proteins specific labeling in a mixed system. **X. Li**, Q. Meng

140. Biomimetic spinning of artificial spider silk from a chimeric minispidroin. **Q. Jia**, M. Andersson, Q. Meng, J. Johansson

WEDNESDAY MORNING

Section A

Walter E. Washington Convention Center
Room 145B

ACS Infectious Diseases Young Investigators Award Symposium

Cosponsored by PROF
Financially supported by ACS Infectious Disease (ACS Journal)
C. C. Aldrich, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 141. New Strategies for an old foe. **C. Barry**

9:15 142. A live-attenuated Zika virus vaccine candidate induces sterilizing immunity in mouse models. **C. Shan**

9:50 143. Nature's dirty little secret: Rhizosphere natural products as targeted antibacterial agents. **W.M. Wuest**

10:25 144. Recognition of bacterial peptidoglycans in your beer and guts. **C.L. Grimes**

Section B

Walter E. Washington Convention Center
Room 147B

Mid-Career Investigators in Biological Chemistry

L. Hedstrom, *Organizer*
T. Chou, *Presiding*

8:30 Introductory Remarks.

8:35 145. Expanding the scope of the prenylated proteome: Forbidden C-terminal sequences can be efficiently prenylated by protein farnesyltransferase. **J. Houglund**, M.J. Blanden, K.F. Suazo, W. Schmidt, M.D. Distefano

8:55 146. Metabolic signal transduction via writers and reactivity. **J.L. Meier**

9:15 147. Development of chemical-inducible artificial transcription factors based on sequence-specific DNA binders. **W. Nomura**, D. Matsumoto, T. Hashimoto, T. Sugii, H. Tamamura

9:35 148. Innovative intergrated phyto remediation to remediate not very toxic heavy metals Cu and Zn. **T. Yeh**

9:55 149. Improving prediction of RNA structure from sequence. **B. Znosko**

10:15 Intermission.

10:30 150. Molecular mechanisms in heme protein function: A thermodynamic perspective from fluoride-binding studies. **J. Cerda**, M. Lockwood, K. Frankenfield, T.S. Nagle, K. Wodzanowski, J. Lopez Garriga

10:50 151. Formulation of industrial relevant enzymes. **G. Baier**, Y. Lan, S. Kuebelbeck, F. Runge

11:10 152. Reductive mobilization of iron cations from ferritin by flavins in the presence of oxygen and chaotrope agents. **A. Melman**, F. Bou-Abdallah

11:30 153. Active water transport controls blood pressure: Selenium nutrition prevents thromboses, breast and colon cancers. **M.T. Deans**

Impact of Materials, Surface Chemistry & Modifications on Biofilm Formation in Environmental Remediation & Engineering Applications

Sponsored by ENVR, Cosponsored by BIOL

Experimental & Computational Advances In Understanding Enzyme Specificity & Promiscuity

New Strategies to Expand the Scope of Enzyme Engineering

Sponsored by PHYS, Cosponsored by BIOL and COMP

Many Colors of Copper

Contributed Talks

Sponsored by INOR, Cosponsored by BIOL

WEDNESDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 145B

Chemical Biology of Infectious Disease

E. Derbyshire, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 154. Drug resistance reveals a new family of metabolic regulators in malaria parasites. A. Guggisberg, A. Gandhi, **A.R. Odom**

1:40 155. Target-specific phenotypic screening for rapid and scalable antimalarial drug discovery. **J.C. Niles**, S. Dey, S. Smick

2:15 156. A chemical biology approach reveals ubiquitin signaling in *Plasmodium*. R. Raphemot, A.L. Eubanks, J. Totzke, D. Gurbani, D.A. Carlson, K. Westover, T.A. Haystead, **E. Derbyshire**

2:50 Intermission.

3:05 157. Hit-to-lead studies and pharmacophore identification within a novel class of anti-trypanosomal agents. **L. Ferrins**, R. Diaz, M. Navarro, M.P. Pollastri

3:40 158. Novel antibacterial chemical tools through machine learning. J.S. Patel, X. Wang, A.L. Perryman, S. Kandasamy, S. Ekins, **J.S. Freundlich**

Section B

Walter E. Washington Convention Center
Room 147B

Graduate Student & Postdoctoral Fellow Symposium

Cosponsored by PROF
L. Hedstrom, *Organizer*
C. L. Grimes, *Presiding*

1:00 Introductory Remarks.

1:05 159. Bio-electronic membrane to investigate the gut brain microbiome axis. **P. Ramiah Rajasekaran**, D.N. Quan, A. Chapin, W.E. Bentley, J. Herberholz, R. Ghodssi

1:20 160. Emerging metabolic pathways overcome metabolic blocks. **S. Pontrelli**, S. Teoh, W. Laviña, R.C. Fricke, S. Fitz-Gibbon, S. Prama Putri, A. J Jaeger, C. Chen, P. Lin, M. Chung, G. Saldanha, M. Morselli, M. Pellegrini, E. Fukusaku, J. Liao

1:35 161. Biochemical and structural analysis of a novel toxin-antitoxin module. **F. Piscotta**, A. Link

1:50 162. Metals and acylhomoserine lactone: Disruption of quorum sensing and reduced toxicity of *Chromobacterium violaceum*. **E. McGivney**, K.E. Jones, B. Weber, J.M. Vanbriesen, K.B. Gregory

2:05 Intermission.

2:20 163. Distinctions between bacterial and human thymidylate synthases. **I. Gurevic**, Z. Islam, T. Strutzenberg, A. Ghosh, T. Iqbal, A. Kohen

2:35 164. Dual labeling of bacterial peptidoglycan and tubulin FtsZ to study bacterial cell division. **H. Liang**, C.L. Grimes

2:50 165. Identifying the cellular targets of antibiotics using T7 phage display. **S. Tirunagari**, J. Vo, P. Karuso, A. Piggott

3:05 166. Facile labeling of bacterial pathogens via diazaborine formation of semicarbazide. **S. Cambray**, A. Bandyopadhyay, J. Gao

3:20 167. Self-assembly of trimeric receptor complex for the *Clostridium perfringens* enterotoxin. **F.J. Irudayanathan**, N. Wang, X. Wang, S. Nangia

3:35 168. Investigating distinct structural features that promote flavin transfer in FMN-dependent two-component systems. **D.L. Forbes**, H.R. Ellis

Impact of Materials, Surface Chemistry & Modifications on Biofilm Formation in Environmental Remediation & Engineering Applications

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Many Colors of Copper

Contributed Talks

Sponsored by INOR, Cosponsored by BIOL

WEDNESDAY EVENING

Trace Organic Contaminants (TrOCs) in Aquatic Systems: Advancements in Monitoring & Remediation

Sponsored by ENVR, Cosponsored by ANYL and BIOL

THURSDAY MORNING

Section A

Walter E. Washington Convention Center
Room 145B

Graduate Student & Postdoctoral Fellow Symposium

Cosponsored by PROF
L. Hedstrom, *Organizer*
R. A. Maillard, *Presiding*

8:30 Introductory Remarks.

8:35 169. Computationally-aided revelation of the counteracting forces mediating OmpG loop dynamics.

M.A. Fahie, A. Perez-Rathke, J. Liang, M. Chen

8:50 170. Prodrug-mediated elimination of tumorigenic human pluripotent stem cells using antibody-guided virus-like particles. **S.N. Crooke**, M.K. Preininger, R. Jha, L. Ding, P. Spearman, C. Xu, M. Finn

9:05 171. Ghrelin processing and maturation: Developing a molecular-level framework for hormone activation and biological function. **E. Cleverdon**, J. Hougland

9:20 172. Solid phase synthesis of all hydrocarbon bis-thioether stapled peptides: Application to developing new inhibitors of the master transcriptional regulator EZH2. **G. Zhang**, F. Barragan, K. Wilson, A. Herskovits, G. Gerona-Navarro

9:35 173. Structural effects of thioamide substitution. **D. Szantai-Kis**, E. Petersson

9:50 Intermission.

10:05 174. Immobilization of α amylase in polyelectrolyte complexes. **S. Kübelbeck**, G. Baier, J. Mikhael, A. Brunsen

10:20 175. Design of fibrin-specific targeting peptide: Implication for the new therapeutic target. **M. Yang**, J. Yu, Y. Nam

10:35 176. Effective mineralization of bone cells on nano-designed chitosan surface. **S. Altuntas**, F. Buyukserin

10:50 177. Interrogating the thiol-disulfide redox status of the mammalian cell surface by ratiometric fluorescence imaging. **L. Jiang**, C. Thorpe

11:05 178. Co-opting a bioorthogonal reaction for oncometabolite detection. **T.T. Zengeya**, J.L. Meier

Impact of Materials, Surface Chemistry & Modifications on Biofilm Formation in Environmental Remediation & Engineering Applications

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THURSDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 145B

Graduate Student & Postdoctoral Fellow Symposium

Cosponsored by PROF
L. Hedstrom, *Organizer*
J. L. Meier, *Presiding*

1:00 Introductory Remarks.

1:05 179. Inhibition in the face of thiols: Complexities of protein disulfide isomerase inhibitor evaluation. **C. Foster, C. Thorpe**

1:20 180. Direct observation of ligand-induced domain communication in an allosteric protein complex. **Y. Hao, J.P. England, S.S. Taylor, E. Paci, R.A. Maillard**

1:35 181. Mechanochemistry of peptide thioesters: Uncovering the force-dependency of thioester cleavage and reformation at the single-molecule level. **D. Echelman, J. Rivas-Pardo, F. Julio**

1:50 182. Characterizing the functions of structural genomics proteins through computed chemical properties and biochemical validation. **C.L. Mills, P.J. Beuning, M.J. Ondrechen**

2:05 Intermission.

2:20 183. Pattern recognition classification of RNA secondary structure and topology. **C.S. Eubanks, J. Forte, G.J. Kapral, A.E. Hargrove**

2:35 184. Identification of the molecular origin of disease with single molecule optical tweezers. **J.P. England, Y. Hao, S.S. Taylor, R.A. Maillard**

2:50 185. Membrane remodeling by α -synuclein: Tubules, ribbons, discs, and more. **Z. Jiang, J.C. Lee**

3:05 186. Structural differentiation of α -synuclein fibril strains by fluorescence spectroscopy. **C. Haney, T.S. Mihaila, E. Petersson**

3:20 187. Neutralization of a distributed coulombic switch tunes reflectin assembly and biophotonics. **R. Levenson, C. Bracken, C. Sharma, C. Arata, D.E. Morse**

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