

# BIOL

## DIVISION OF BIOLOGICAL CHEMISTRY

L. Hedstrom, *Program Chair*

### SUNDAY MORNING

Section B

Venue  
Placeholder

#### Graduate Student & Postdoctoral Fellow Symposium-Oral

L. Hedstrom, *Organizer*

**8:30** Introductory Remarks.

**8:35** . RNA labeling induced by oxidation with high spacial resolution. **Y. Li**, R. Spitale

**8:50** . CRISPR-Cas9: Computational insights toward improved genome editing. **G. Palermo**, Y. Miao, R. Walker, M. Jinek, J. McCammon

**9:05** . Luminescence probes of deaminated nucleotide surveillance enzymes DUT and ITPA. **d. ji**, Y. Pavlov, E.T. Kool

**9:20** . Monitoring the phenotypic response of FoxO1 at the single cell level in patient samples. **J. Simpson**

**9:35** . Identification of novel allosteric HSP72 inhibitors. **H. Traynor**, R. Burke, Y. Le Bihan, I. Collins, R.L. van Montfort

**9:50** . Polymerase-mediated synthesis of TNA polymers containing a fluorescent base that can read through G-repeats in a DNA template. **H. Mei**, C. Shi, J. Chaput

**10:05** Intermission.

**10:20** . Antibiotic resistance evolved via inactivation of a ribosomal RNA methylating enzyme. **V. Stojkovic**, L. Noda-Garcia, D.G. Fujimori

**10:35** . Comparative analysis of translesion DNA synthesis by a high fidelity DNA polymerase. **a. dasari**

**10:50** . Ultra-photostable, genetically directed fluoromodule enables STED nanoscopy and long time scale single protein tracks in live bacteria. **S. Saurabh**, A.M. Perez, C.J. Comerchi, L. Shapiro, W.E. Moerner

**11:05** . Infrared spectroscopy reveals a base stacking limit in DNA G-quadruplexes. **D.A. Price**, Z.J. Kartje, T.D. Hill, G. Cairo-Baza, K.T. Gagnon, S.D. Moran

**11:20** . Synthesis, spectroscopic investigation, biological screening, interaction with SS-DNA and DFT study of aliphatic ferrocenyl ureas. **F. Asghar**, A. Badshah, I.S. Butler

Section B

Venue  
Placeholder

**Ronald Breslow Award for Achievement in Biomimetic Chemistry: Symposium in honor of Benjamin G. Davis-Invited, Oral**

B. G. Davis, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05** . Chemical Immunology - New approaches to study killer T-cell activation. **S. van Kasteren**

**8:25** . Immunomodulation by targeted delivery of carbon monoxide using artificial metalloproteins. **G. Bernardes**

**8:45** . Sulfur chemistry for biology and human health. **J.M. Chalker**

**9:05** . Chemical biology tools for studying the O-GlcNAc modification of proteins. **D.J. Vocadlo**

**9:40** Introduction of Awardee.

**9:50** . Controlling biological machines with synthetic photoswitches. **D. Trauner**

**10:25** . Mass spectrometry of membrane proteins - the lipid connection. **C. Robinson**

**11:00** . Homogeneous glycoproteins for structural and functional study. **C. Wong**

**11:35** Intermission.

**11:40 . Sugars & proteins: Towards a synthetic biology. B.G. Davis**

**LGBT Graduate & Postdoctoral Student Chemistry Research Symposium-Oral**

**Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis, & Spectroscopy**

Sponsored by PROF, Cosponsored by ANYL<sup>‡</sup>, BIOL<sup>‡</sup>, CHED, CMA, COLL, COMP, CWD, ENVR, INOR<sup>‡</sup>, MEDI, MPPG, ORGN, PHYS, PMSE<sup>‡</sup>, POLY, PRES<sup>‡</sup> and WCC

**National Fresenius Award: Symposium in honor of Neal K. Devaraj**

Sponsored by ORGN, Cosponsored by BIOL

**Cellulose Structure & Biosynthesis-Oral**

**Cellulose in the Plant Cell Wall**

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

**SUNDAY AFTERNOON**

Section A

Venue

Placeholder

**Goodman Award: Symposium in honor of Jennifer Doudna-Invited, Oral**

J. Doudna, *Organizer*

**2:00** Introductory Remarks.

**2:05 .** CRISPR immune response to viruses that infect bacteria. **B. Wiedenheft**

**2:50 .** Retooling CRISPR to turn genes on and off. **L. Gilbert**

**3:35 .** CRISPRi/dCas9 for complex genome regulation and disease research. **L. Qi**

**4:20** Introduction of Awardee.

**4:25** . CRISPR biology: Expanding nature's toolkit for genome engineering. **J. Doudna**

Section B

Venue

Placeholder

**ACS Award in Pure Chemistry: Symposium in honor of Neal K. Devaraj-Invited, Oral**

N. K. Devaraj, *Organizer, Presiding*

**2:00** Introductory Remarks.

**2:05** . Measuring and modulating the repair of DNA damage. **E.T. Kool**

**2:35** . TBA. **V.W. Cornish**

**3:05** . Transition metal signaling in the brain and beyond. **C.J. Chang**

**3:35** Intermission.

**3:55** . Evolving click chemistry → SuFEx. **K.B. Sharpless**

**4:25** Introduction of Awardee.

**4:30** . In Situ Synthesis and Modification of Lipid Membranes. **N.K. Devaraj**

**5:05** Closing remarks.

**LGBT Graduate & Postdoctoral Student Chemistry Research Symposium-Oral**

**Novel Reactions, Methodologies & Syntheses in Organic Chemistry**

Sponsored by PROF, Cosponsored by ANYL<sup>‡</sup>, BIOL<sup>‡</sup>, CCA, CHED, COLL, COMP, CWD, ENVR, INOR<sup>‡</sup>, MEDI, MPPG, ORGN, PHYS, PMSE<sup>‡</sup>, POLY, PRES<sup>‡</sup> and WCC

**Cellulose Structure & Biosynthesis-Oral**

**Evolution of Cellulose Synthases & Fine Structure of Cellulose Microfibrils**

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

**Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges-Invited, Oral**

Sponsored by INOR, Cosponsored by BIOL

**SUNDAY EVENING**

Section A

Venue  
Placeholder

**Current Topics in Biochemistry-Poster**

L. Hedstrom, *Organizer*

**7:00 - 9:00**

- . Clarification by flocculation: A promising solution for high cell density. **C. Decarnin**
- . Exploration of the N-terminal extension's role in human gamma-S crystallin function. **K. Roskamp**, A. Chenault, R. Martin
- . Chemical biology approach for dimethyllysine incorporation into proteins. **Z.A. Wang**, W. Liu
- . New tools for controlling the supramolecular assembly of proteins in living cells. **G.R. Casey**, X. Zhou, B. Xu, C.I. Stains
- . Structural analysis of heme *c* motifs for the template-based design of heme *c* proteins. **J. Kleingardner**
- . Unnatural lysine analogues to mimic the catalytic pocket of human DNA polymerase  $\beta$ . **C. Bhattacharya**, S.M. Daskalova, S. Hecht
- . Efficient method to study engineering temperature shift strategies for Chinese hamster ovary cell culture via mechanistic macroscopic kinetic modeling. **y. wang**, J. Xu, p. tang, s. liu, z. li
- . Investigating the specificity of methylated DNA binding by MBD1 and mutant peptides for transcriptional regulation. **S. Scherer**, A. Stewart
- . Synthesis and evaluation of a norbornene containing substrate for protein farnesyltransferase. **J. Wollack**, J. Rowe, C. Sutton, L. Crepeau, K. Caron, M.D. Distefano

- . Developing a pipeline for generating TNA-phosphoramidite and TNA-triphosphate monomers for the *in vitro* evaluation of the properties of the polymers. **S. Bala**, J. Liao, J. Chaput
- . Exploring the role of Tat-SF1 as an HIV-1 host factor. **M. Warrick**, H.B. Miller
- . Mutational studies of a deoxyribozyme by high-throughput sequencing. **D. Venugopal**, S. Kobori, Y. Yokobayashi
- . Transcriptome-wide mapping of RNA-RNA interactions. **M. Oumais**, A. Luptak
- . Possible prebiotic fabrication of ribonucleotides using microdroplets. **I. Nam**, J. Lee, H. Nam, R.N. Zare
- . Tat-specific factor 1's role in HIV RNA stability. **A.P. Goodwin**, H.B. Miller
- . Theoretical characterization of the H-bonding and stacking potential of two nonstandard nucleobases expanding the genetic alphabet. **M. Chawla**, **R. Oliva**, **L. Cavallo**
- . Live cell imaging of RNA using endogenous fluorophore protoporphyrin IX. **D. Zhang**
- . ADARs and RNA; Structural basis for site selectivity of ADAR2. **J. Thomas**, M. Matthews, Y. Zheng, P.A. Beal, A.J. Fisher
- . Nucleobase analogs as probes for substrate recognition and repair by DNA glycosylase MutY. **C. Majumdar**, S.S. David, A. Manlove
- . Bioorthogonal near-infrared fluorogenic probe for mRNA detection. H. Wu, S.C. Alexander, **S. Jin**, N.K. Devaraj
- . Bioluminescent detection of HIV persistency via a stem-loop probe. **B. Cherif**, A. Moutsopoulos
- . Optimizing the production of FOXA2 to unravel the interaction between homeodomain and Forkhead transcription factors. **S. Ramirez**
- . Investigation into the broad substrate specificity of the DNA glycosylase hNEIL1. **B. Anderson**, J. Ashby, A.M. Fleming, C.J. Burrows, S.S. David
- . Influence of loop mutations on G-quadruplex unfolding. **B.A. Tucker**, J.S. Hudson, D.E. Graves
- . Oncostatin M mediated regulation of microRNA-21 function in HeLa cells. **N. Jain**, S. Ahmed, **M.J. Sever**
- . 5' Start site heterogeneity of the HIV-1 RNA and its effect on structure and function. **D. Francis**, M. Orellana, J. Brown, M. Summers

- . Parallel stranded G-quadruplex composed of threose nucleic acid (TNA). **J. Liao**, I. Anosova, S. Bala, W.D. Van Horn, J. Chaput
- . Structural stability analysis of a *S. cerevisiae* DEAD-box protein. **Z. Iezzi**, C. Bardine, H. Englert, I. Garcia
- . High-throughput mutational analysis and engineering of self-cleaving ribozymes by sequencing. **S. Kobori**, Y. Yokobayashi
- . Elucidation of the role of adenine DNA glycosylase mutyh in MNNG-mediated cell cytotoxicity. **D.M. Banda**, A.G. Raetz, G. Xu, X. Ma, P.L. McKibbin, A. Rajavel, C.B. Lebrilla, S.S. David
- . Synthesis and screening of a naphthalene diimide bisintercalator library. **E. Gratton**, B.L. Iverson
- . High-yield syntheses of DNA duplexes containing interstrand cross-links at a single well-defined location via a reductive amination reaction between 2-aminopurine and an abasic site. **M. Imani Nejad**, N.E. Price, Y. Wang, K.S. Gates
- . Engineering the N-terminal domain of pyrrolysyl-tRNA synthetase: Optimizing genetic incorporation of non-canonical amino acids. **V. Sharma**, W. Liu
- . Complete Zn<sup>2+</sup> linchpin coordination sphere of the DNA repair glycosylase MUTYH. **N. Nunez**, S.S. David, J.B. Siegel, C. Lim
- . Enzymatic site-specific labeling with RNA-TAG for affinity purification of RNA-protein complexes. **K.N. Busby**, N.K. Devaraj
- . 5-Hydroxymethylcytosine impacts Holliday junction structure to promote recombination via recognition by Endonuclease G. **C. Vander Zanden**, R.K. Rowe, A.J. Broad, A.B. Robertson, P.S. Ho
- . Ligand selectivity in a pathogenic preQ<sub>1</sub> riboswitch aptamer domain. **K.M. Yamakawa**, M. Doan, J.M. Davison, M.N. Pahl, I.T. Suydam
- . E2F1 and p27 regulation in non-neuronal cells by isoxazole 9. **M. McCabe**, **M.J. Sever**
- . Structural and energetic characterization of the emissive RNA alphabet based on the isothiazolo[4,3-d]pyrimidine heterocycle core. M. Chawla, R. Oliva, **L. Cavallo**
- . Interaction of Menaquinone (MK) analogs (MK-1 and MK-2) with phospholipids. **G. Cardiff**, B.J. Peters, J.T. Koehn, J.B. Hough, A. Groninger, D.C. Crick, D.C. Crans, F. Fontes
- . Ca<sup>2+</sup> induced conformational changes of calmodulin and troponin C chimera. **C. Wei**, D. Jensen, K. Schafer, E.A. Fabry

- . Selective detection of protein homologues by outer membrane protein G nanopore. **B. Yang**, M.A. Fahie, H. Wang, P. Limpikirati, R.W. Vachet, S. Thayumanavan, M. Chen
- . How Host Gender Affects the Polysaccharide Capsule of *Cryptococcus neoformans*. **P. Doski**, E. McClelland
- . Structure of the pro-apoptotic BCL-2 family protein BAD and insight into BAD-calcineurin interactions. **S.N. Blakeney**, E.C. Cook, T.P. Creamer
- . Aquaporin inspired water purification membrane based on graphene oxide membrane. **C. LEE**, D. KIM, G. LEE, Y. Lee, Y. Lee
- . Amyloid Forming Sequences in *Trichomonas vaginalis*. **A. Asakawa**, C. Chan
- . Exploration of the interactions of hen egg white lysozyme with deoxyribonucleic acids. **E.A. Fabry**, C. Wei, T. Shields
- . Proteomics-based screening and identification method for redox sensitivities of global cellular cysteine residues. **K. Araki**, K. Fukui, T. Natsume
- . Light-Induced disassembly of  $\beta$ -amyloid aggregates by ruthenium complex. **G. SON**, C. Park, B. Lee, Y. Chung
- . Functionalization of polydopamine via the Aza-Michael reaction for antimicrobial interfaces. **P.T. Ha**, C. Huang, C. Liu, Y. Huang
- . Utilization of extracts of garlic, oregano, neem and a commercial insecticide on endophyte bacteria on orange leaves infected by *citrus greening*. **J. Becerra Lopez**, **A. Perez Matos**
- . Structural insight into the inactivation mechanism of Ldt<sub>M2</sub>, a non-classical *Mycobacterium tuberculosis* transpeptidase, by carbapenem antibiotics. M.A. Bianchet, Y. Pan, **L. Basta**, H. Saavedra, E. Lloyd, P. Kumar, R. Mattoo, C.A. Townsend, G. Lamichhane
- . Characterization of the huntingtin aggregation pathway via single-molecule and super-resolution fluorescence microscopy. **C. Becker**, **R. Harman**, **A. Khan**, R. Levy, W.C. Duim
- . Is it a biological response or chemical process? Chemical and transcriptional regulation experiments probe the cause for the increased accumulation of chlorogenic acid (CGA) in carrot root slices exposed to UV-B light. G.E. Bartley, R.J. Avena-Bustillos, W. Du, M. Hidalgo, B. Cain, **A.P. Breksa**
- . N acetyl cysteine as an inducer of retina regeneration. **J. Landers**, K. Del Rio-Tsonis, N. Echeverri
- . 5-azidomethyl-2'-deoxyuridine triphosphate can be efficiently incorporated by a repair DNA polymerase. **C. Garcia**, Y. Ren, Z. Wen, S.F. Wnuk, Y. Liu



- . Comparison of synthetases in the incorporation of the non-natural amino acid p-azidophenylalanine in the oncogenic protein kRas. **M. Wheeler**, T. Andresson, R.E. Connor
- . Precise delivery of a chemotherapeutic Prodrug to mitochondria of prostate cancer cells to bypass repair induced resistance. **U. Basu**
- . Visualizing the chain-flipping mechanism to study inhibition and protein-protein interaction in fatty acid biosynthesis. **K. Charov**, J. Beld, M.D. Burkart
- . Assessing cysteine residue thiol status in T-Darpp, a protein involved in chemoresistance. **J.A. Aldana-Mendoza**, **P. Farias**, J. Momand
- . Nanomaterials toxicological evaluation: Natural product shielded magnetite nanoparticles. **H. Huang**, J.L. Liu, S. Bashir
- . Analogs of methyl 4-(4-chlorophenyl)-4-oxobut-2-enoate that inhibit MenB in the bacterial menaquinone biosynthesis pathway. **Y. Si**, J. Matarlo, F. Daryaei, P.J. Tonge
- . Characterization of a robust serine protease from *P. intermedia*. **S. Spradlin**, C.M. Evilia
- . Reverse transcription past major guanine oxidation products in RNA. **A. Alenko**, A.M. Fleming, C.J. Burrows
- . Importance of F365 in the binding of inhibitors in *Escherichia coli* beta-glucuronidase. **S. Van Shufflin**
- . Ratiometric fluorescent chloride sensor. **K. VanDenburgh**, Y. Liu, B. Qiao, A.H. Flood
- . Highly selective small potassium transporter induces cancer cell death. **F. Shen**, D. Yang
- . Evaluating the effect of lipophilicity on antimicrobial potency, cytotoxicity, and combinatorial library design. **J.A. Turkett**, K. Bicker
- . Determinants of the pKa value of catalytic residue in de novo designed enzymes. K. Hiebler, C. Castaneda, **O. Makhlynets**
- . Allosteric control of histone demethylase KDM5A. **J.E. Longbotham**, C. Chio, M. Kelly, D.G. Fujimori
- . Pathological mutations in the prion protein modulate the metal driven cis interaction. **G.P. Roseman**
- . Electrophilic Reactive Carbonyl Species: Participation in the Nonenzymatic Covalent Protein Modification of Human Hemoglobin. **P. Ropski**, J. Pattan, B. Park, R.W. Holman, K. Rodnick

- . Towards a Mechanistic Understanding of Nonenzymatic Glycation of Human Hemoglobin: Diverse Effects of Inorganic Phosphate on the Initial Noncovalent Binding of Glucose. **A. Hendricks, C. Mottishaw**, J. Mitchell, P. Ropski, B. Smith, G. Titus, B. Park, M. Finkbeiner, R.W. Holman, K. Rodnick
- . Fine-tuning triazabutadiene stability for controlled aryl diazonium release. **L. Guzman**, J.C. Jewett
- . Self-Assembling nanoluciferase fragments as probes for alpha-synuclein solubility. **T. Truong**, C. Bilyeu, J. Zhao, T. Nelson, C.I. Stains
- . Effects of DNA bending on T=C CPD deamination. **K. Wang**, J.S. Taylor
- . Development of targeted stigmaterol-solid lipid nanoparticles by hyaluronic acid and transferrin for lung cancer therapy. **Z. Torres**, Y. Delgado, K. Griebenow
- . Use of infrared spectroscopy to study the structural changes of calreticulin upon the addition of ligand. **A. Farquharson**, C. Thomas, L. Maynard
- . Functional implications of iron-sulfur cluster MUTYH variants associated with colorectal cancer. **K. Bradshaw**
- . Cyclopropene neurotransmitters for biorthogonal imaging of neural circuits. **P. kumar**, S. Li, D. Shukhman, S.T. Laughlin
- . Effect of caffeine on lipophagy in mammalian skeletal muscle cells. **D.S. Enyart**, J. Stansell, J.V. Ruppel, S. Kinsey, B. Baumgarner
- . Use of CDNB assay to determine calreticulin domain responsible for autoacetylation. **C. Nnebe**, C. Thomas, L. Maynard
- . Design of biomimetic antimicrobial peptide-polymer conjugates as building blocks for reactive/responsive membranes: A water purification approach. **V. Ortiz Gomez**, V. Rodriguez, E. Nicolau
- . Effect of 4,4' DDT, 4,4' DDE, 4,4' DDD, and 2,4' DDD on dihydrotestosterone binding to and releasing from the androgen receptor. **T. Resto**, F. Dean, A. Chavez, V. Flores
- . Synthesis and evaluation of Nebraska red derivatives for protein labeling studies. **L. Lesiak**, X. Zhou, C.I. Stains
- . Tryptophan derivatives as novel fluorescent probes for studying protein conformational changes and DNA-protein interaction. **P. TALUKDER**, S. Chen, B. Roy, P. Yakovchuk, S. Hecht
- . Photo-uncaging of reactive species and fluorescence with visible light and NIR. **S. Dai**, D. Yang

- . Investigating the evolution of acyl carrier proteins' structure and function. **V.V. Courouble**, B. Kokona, R. Fairman, L.K. Charkoudian
- . Molecular dynamics simulations of metabolite fibrils. **P. Rehak**, L. Vukovic, P. Kral
- . Physiological and behavioral adaptations of *Vibrio cholerae* to fatty acids in a continuous culture (bioreactor) model. **R.A. Boeger**, A. Turgeson, D. Giles, B. Harris
- . Binding mechanism study of coomassie brilliant blue species and bovine serum albumin. **R.N. Ngo**, C. Wei, E.A. Fabry
- . Using comb-branched DNA to construct deoxyribozyme-based biosensors. **M.R. Polaske**, E. Teselle, D.A. Baum
- . Effects of heterocyclic diamidine antiparasitic agent binding to DNA on restriction enzyme kinetics. **T.M. Rodriguez**, S.A. Winkle
- . Developing FRET assays to study the binding and regulation of fibroblast growth factor to its receptor. **M. Mohale**
- . Mechanistic studies of StyA1 styrene monooxygenase from *Rhodococcus Opacus*. **J.L. Diaz**, G.T. Gassner, d. Tischler
- . Development of a fluorescence polarization assay for RhlI. **N.R. Rexrode**, J. Taffin, N. Lam, R. Nagarajan
- . Bioluminescence and photoluminescence properties of the earthworm *Eisenia lucens*. **P. Taborsky**, O. Pes
- . Toward Raman-based diagnostics for amatoxins: Synthetic, computational, and spectroscopic studies on analogs for the substituted tryptathionine sulfoxide core of amanitins, the peptide toxins of *Amanita phalloides*. **K. Yniguez**, T.G. Moreno, A. Ringer McDonald, S.C. Eagon, E. Jones
- . Hyper obesity suppression by the products of *Rhinacanthus nasutus*: A study in rats. **T. Kedam**
- . Energy depletion in vitro potentially caused immunosuppression: A multi-omics characterization of pathogenic threat in spaceflight. **N. Chakraborty**, A. Cheema, A. Gautam, S. Miller, A. Hoke, M. Jett, R. Hammamieh
- . Investigation of catalytic activity of stable  $\beta$ -keto-acyl-ACP substrate analogs in quorum sensing signal synthesis. **N. Lam**, D. Dudekula, I. Csik, N. Collingwood, E.C. Brown, R. Nagarajan
- . Structural analysis of tau peptide interactions with lipid membranes using Fourier transform infrared spectroscopy. **P. Engen**, L. Masterson

- . Growth based complementation assay in *E. coli* for inhibitor screening of S-adenosylmethionine synthetase. **G.G. Parungao**, R.M. Blumenthal, R.E. Viola
- . Effect of the antimicrobial peptide combi-2 on vesicles of membrane mimicking systems of normal and cancer cells. **B.M. Almarwani**, A. Sunda-Meya, N. Phambu
- . Quantification of the minimum numbers of TLR2 agonists necessary to elicit a detectable immune response. **W.J. Howitz**, B. Moser, A. Esser-Kahn
- . Development of a novel, neural-activity triggered split enzyme. **B. O'Neill**, S. Laughlin
- . Enzyme-enzyme proximity stimulates iNOS activity. **K.M. Fomchenko**, D.J. Hirsh
- . Investigating the conformational landscape in a signaling protein complex with optical tweezers. **J.P. England**
- . Reactivity of bovin serum albumin with ligands of cisplatin analogs. **N.C. Puckett**, K. Williams
- . Selective in vivo cell labeling mediated cancer targeting. H. Wang, **K. Cai**, R. Wang, J. Cheng
- . Isolation, Structural Elucidation and Biosynthetic Characterization of HIV-1 Nef Accessory Protein Inhibitors. **L. Gomez-Rodriguez**
- . *In vitro* biochemical studies of the midgut serine protease AaSPVII of the Zika vector *Aedes aegypti*. **J.T. Nguyen**, A. Rascon
- . From synthesis to pathology: Identifying glucosepane's role in diabetes and aging. **M. Streeter**
- . Elucidating the temporal dynamics of caspase activity within the mitochondrial pathway of apoptosis. **R.D. Reif**, S. Morris
- . Characterization of menaquinone-2. **E. Magallanes**, J.T. Koehn, B.J. Peters, C.N. Beuning, M. Zhu, D.C. Crick, D.C. Crans
- . Allosteric inhibition via two-step enzyme isomerization of human herpesvirus protease protein-protein interaction decreases viral infectivity of Kaposi's sarcoma-associated herpesvirus in mammalian cells. **T. Acker**, J. Gable, M. Bohn, P. Jaishankar, A.R. Renslo, C. Craik
- . Chemical imaging of neuron-astroglia interactions. **A. Preston**, J. Farr, S. Laughlin
- . Computational study of relative thermodynamic stability of mutant base pairs between keto, enol and deprotonated forms of guanine and thymine at DNA polymerase  $\lambda$  active site. **S.N. Maximoff**, J. Eloge, S. Kamerlin, J. Florian
- . Dipyrimidine sequence library for determining the sequence dependence of UV-induced *cyclobutane pyrimidine dimer* formation. **C. Lu**, J.S. Taylor

- . Direct observation of breathing dynamics at the mismatch induced DNA bubble by smFRET measurement. **T. Paul**, P. Mishra
- . DNA Editing in DNA/RNA hybrids by adenosine deaminases that act on RNA. **Y. Zheng**, C. Lorenzo, P.A. Beal
- . Probing RNA recognition by human ADAR2 using a high-throughput mutagenesis method. **Y. Wang**, P.A. Beal
- . Successful screening of aptamers for an early diagnosis of a periodontitis. **B. Lee**, J. Park, Y. Ko, M. Gu
- . Single-molecule FISH of specific mRNAs using click chemistry. **S.H. Rouhanifard**, A. Raj
- . Dynamics of the *E. coli* beta clamp and its influence on DNA loading. **B. Koleva**, J. Baez, J. Conway, A. Wu, P.J. Beuning
- . T4 DNA ligase-catalyzed polymerization of modified oligonucleotides: Discovery and application of a high-fidelity codon set to the evolution of modified aptamers. **Y. Lei**, D. Kong
- . Design and synthesis of thiol cleavable self-immolative linkers and their conjugation to proteins. **C.M. Sadlowski**, N. Murthy
- . Tools for controlled microdomain formation and protein localization in artificial phospholipid membranes. **A.K. Rudd**, N.K. Devaraj
- . Site-Specific nanocluster synthesis in biomolecular hosts. **S. Teymorian**, A. West, M. Griep
- . Fourier transform infra red spectroscopy based spectral biomarker identification: Applications in classifying lung cancer subtypes. **A. Sarkar**, A. Sadhu, S.B. Thakur
- . Understanding the structures and dynamics of type II carrier proteins using molecular dynamics simulations. **A. Patel**, M.D. Burkart, J. McCammon
- . ROS responsive self-cyclization for hydroxyl radical detoxification. **J. Liu**, S. Abdul Salam, H. Zhu, E.J. Merino
- . New design for twin reactive oxygen species activated anti-tumor agents. **H. Zhu**, S. Abdul Salam, J. Liu, E.J. Merino
- . Investigation of catalytic activity of stable  $\beta$ -keto-acyl-ACP substrate analogs in quorum sensing signal synthesis. **N. Lam**, D. Dudekula, I. Csik, N. Collingwood, E.C. Brown, R. Nagarajan
- . Examination of essential genes involved in the biosynthesis of key metabolite by *Chlamydia trachomatis*. **T. Nguyen**, D.G. McCafferty

. Versatile site-specific modification of native protein N termini using a panel of engineered peptide ligases. **A. Weeks**, J.A. Wells

## MONDAY MORNING

Section A

Venue  
Placeholder

### **Nucleic Acid Therapeutics: Mechanisms & Applications-Invited, Oral**

M. Manoharan, *Organizer*  
M. J. Damha, *Presiding*

**8:00** Introductory Remarks.

**8:10** . Design and assembly of artificial proteins using nucleic acid hybridization. **j. wengel**

**8:45** . This is your brain on antisense oligonucleotides: Distribution, activity and application to the treatment of severe neurodegenerative disease. **E.E. Swayze**

**9:20** . Applying the chemist's toolbox for studying nucleic acid structure and function. **M.J. Damha**, H. Abou Assi, D. O'Reilly, E. Malek-Adamian, M. Habibian, D. Vlaho, J. Bogojeski, S. Jana, S. Martinez-Montero, C. Gonzalez

**9:55** Intermission.

**10:10** . Advances in RNAi therapeutics: Chemistry, mechanism and applications. **M. Manoharan**

**10:45** . Structure-based insights into stability, activity and protein interactions of chemically modified oligonucleotides. **M. Egli**

Section B

Venue  
Placeholder

### **Early Career Investigators in Biological Chemistry-Oral**

L. Hedstrom, *Organizer*

**8:30** Introductory Remarks.

**8:35** . Mechanistic insights into protein amyloidogenesis. **D. Du**, H. Liu, E. Elbassal

**8:55** . Introduction of D-glutamate at a key site of A $\beta$ 42 stabilizes a soluble aggregation intermediate and enhances toxicity. **J.A. Raskatov**, C.J. Warner, S. Dutta, A. Foley

**9:15** . Human monomeric insulin derived from cone snail venoms. **D. Chou**

**9:35** . Chemically modified macrophages for cancer imaging and drug delivery. M. Mingroni, J.J. Elliott, J. Hardie, **M.E. Farkas**

**9:55** Intermission.

**10:05** . Development of peptide-based tools to study quorum sensing in streptococci. Y. Yang, B. Koirala, C.R. Bikash, N.R. Phillips, L.A. Sanchez, S.R. Hamry, **Y. Tal-Gan**

**10:25** . Chemical biology strategies illuminating how the proteostasis network modulates evolutionary excursions in sequence space by RNA viruses. **M. Shoulders**

**10:45** . Profiling endogenous protein phosphatase activity using direct activity probes. **C.I. Stains**

**11:05** . Pushing click chemistry to its limits: An in-vitro sample generation pipeline for high-throughput single-molecule FRET-based screening of proteins and ribosome-bound nascent chain libraries. **K.M. Hamadani**, P. Wu, J. Cate, S. Marqusee

## **LGBT Graduate & Postdoctoral Student Chemistry Research Symposium-Oral**

### **Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries**

Sponsored by PROF, Cosponsored by ANYL<sup>‡</sup>, BIOL<sup>‡</sup>, CHED, COLL, COMP, CWD, ENVR, INOR<sup>‡</sup>, MEDI, MPPG, ORGN, PHYS, PMSE<sup>‡</sup>, POLY, PRES<sup>‡</sup> and WCC

### **Cellulose Structure & Biosynthesis-Oral**

#### **Mechanism of Cellulose Synthesis**

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

**MONDAY AFTERNOON**

Venue  
Placeholder

**Nucleic Acid Therapeutics: Mechanisms & Applications-Invited, Oral**

M. Manoharan, *Organizer*  
M. Egli, *Presiding*

**1:00** Introductory Remarks.

**1:05** . New roles for G-quadruplexes in gene expression and infectious disease. **C.J. Burrows**,  
A. Fleming, Y. Ding

**1:40** . Advances in the chemistry of microRNA-based therapeutics. **C. Allerson**

**2:15** Intermission.

**2:30** . Potent delivery of LUNAR™ nanoparticles containing synthetic mRNA for therapeutic protein expression. **P. Chivukula**

**3:05** . Homologous DNA recombination *in vivo* with the delivery of Cas9 ribonucleoprotein and donor DNA complexed to gold nanoparticles. **K. Lee**, m. conboy, f. jiang, H. kim, m. dewitt, h. park, j. corn, J. Doudna, I. Conboy, N. Murthy

**Rising Star Award Symposium-Invited, Oral**

Sponsored by WCC, Cosponsored by BIOL

**LGBT Graduate & Postdoctoral Student Chemistry Research Symposium-Oral**

**Advances in Medicinal & Biological Chemistry: From Therapeutics to Education**

Sponsored by PROF, Cosponsored by ANYL<sup>‡</sup>, BIOL<sup>‡</sup>, CHED, CMA, COLL, COMP, CWD, ENVIR, INOR<sup>‡</sup>, MEDI, MPPG, ORGN, PHYS, PMSE<sup>‡</sup>, POLY, PRES<sup>‡</sup> and WCC

**ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer-Invited, Oral**



Sponsored by I&EC, Cosponsored by ANYL, BIOL, COLL, INOR, ORGN, PMSE and POLY

**Cellulose Structure & Biosynthesis-Oral**

**Cellulose Synthase Trafficking & Synthesis of plant (1->3),(1->4)-D-glucans**

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

**Undergraduate Research Posters: Biochemistry-Poster**

**Biochemistry**

Sponsored by CHED, Cosponsored by BIOL and SOCED

**MONDAY EVENING**

Section A

Venue  
Placeholder

**Sci-Mix**

L. Hedstrom, *Organizer*

**8:00 - 10:00**

**TUESDAY MORNING**

Section A

Venue  
Placeholder

**Metalloprotein-Initiated Signaling Transduction Response to Redox Stress-Invited, Oral**

Cosponsored by INOR  
A. Liu, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05** . Screening of small molecule inhibitors of human pirin. **H. Osada**

**8:40** . Enzymology of hydrogen sulfide signaling. **R. Banerjee**

**9:15** . Probing heme trafficking, signaling, and dynamics in health and disease. **A.R. Reddi**

**9:50** Intermission.

**10:00** . Enzyme mechanism-driven DNA-protein crosslinks during attempted DNA repair. **B. Demple**

**10:35** . Signal transduction mechanisms in heme-dependent gas-sensing transcription factors. **J.N. Burstyn, J.P. Hines, H. Bowman, M.R. Dent, D.J. Stevens**

**11:10** . How metal-dependent oxidation can redirect AAA+ proteases to new protein substrates. **B. Ah, B. Brown, S. Calmant, J. Kardon, T. Baker**

Section B

Venue

Placeholder

### **Chemical Epigenetics-Invited, Oral**

D. G. Fujimori, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35** . Advanced chemical genetics for epigenetics: Bump-and-hole and PROTACs. **A. Ciulli**

**9:05** . Regulation of catalysis and novel inhibitor chemotypes for histone demethylases. **D.G. Fujimori**

**9:35** . Discovery of A-395: A novel protein-protein interaction inhibitor of EED. **B. Pappano**

**10:05** Intermission.

**10:20** . Development of irreversible small molecule epigenetic modulators to block menin-MLL in cancer. **J.E. Grembecka, D. Borkin, S. Klossowski, H. Miao, K. Kempinska, J. Pollock, T. Purohit, B. Wen, D. Sun, T. Cierpicki**

**10:50** . On the mechanisms of generation, recognition, and erasure of DNA and histone modifications. **X. Cheng**

## **Cellulose Structure & Biosynthesis-Oral**

### **Biochemistry and Cellular Biology of Cellulose Biosynthesis**

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

### **ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin**

Sponsored by COMP, Cosponsored by BIOL, MEDI and WCC

### **Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges-Invited,Oral**

Sponsored by INOR, Cosponsored by BIOL

## **TUESDAY AFTERNOON**

Section A

Venue  
Placeholder

### **ACS Chemical Biology Award Symposium-Invited, Oral**

Cosponsored by WCC  
A. Weidmann, *Organizer*  
L. L. Kiessling, *Organizer, Presiding*

**2:00** Introductory Remarks.

**2:05** . Profiling acetyltransferases to understand cancer's metabolic cues. **J.L. Meier**

**2:35** . Privileged First-Responding redox sensors in isozyme-specific apoptosis regulation. **Y. Aye**

**3:05** . Chemical tools for probing bacterial peptidoglycan activation of the innate immune system. **C.L. Grimes**

**3:35** . Cross-reactive cysteine modifications. **B.R. Martin**

**4:05** Introduction of Awardee.

**4:10** . Activity-based proteomics – protein and ligand discovery on a global scale. **B.F. Cravatt**

**ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin**

Sponsored by COMP, Cosponsored by BIOL, MEDI and WCC

**Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges-Invited, Oral**

Sponsored by INOR, Cosponsored by BIOL

**TUESDAY EVENING**

Section A

Venue  
Placeholder

**Current Topics in Biochemistry-Poster**

L. Hedstrom, *Organizer*

**7:00 - 9:00**

. Label free proteomics profiling unveils downregulation of thrombin mediated signaling and aggregation of human platelets upon treatment with thrombin inhibitors. **C.C. Clement**, A. Babinska, J. Gonzalez

. Allosteric and catalytic of UDP-sugar pyrophosphorylases suggest a new approach to anti-parasitic treatments. J.T. Cramer, J.I. Führung, F.H. Routier, A. Lamerz, J. Schneider, P. Baruch, R. Gerardy-Schahn, **R. Fedorov**

. Development of novel substrate inhibitors of bacterial phospholipid biosynthesis as new antibacterial agents. **P. Saklani**, **J. Luo**, D.P. Brown

. Analysis of chemotypes in retail *Cannabis* strains. R.M. Hyslop, **C.E. Brown**, A. Schwabe, S. Desa, M. McGlaughlin

- . Novel application of TEC-disulfide replacement showcased in the synthesis of SFTI-1. **J. Barbaretta**, A.J. Wommack
- . Self-assembled synthetic ion channels. **D. Yang**
- . Discovering and manipulating miRNA biology utilizing click-chemistry. **D. Lorenz**, A. Garner
- . Synthesis & spectroscopic characterization of xenometabolite, biomarkers for the diagnosis of fatty acid  $\beta$ -oxidation disorder. **H.F. Sobhi**, S. Adams, M. Ekwuru, . Teasley
- . Study of aminoglycosides binding to mitochondrial rRNA. **L. Garmo**, P. Madubashitha, E. Jones, C.S. Chow
- . Bioorthogonal metal catalysed transformation of dehydroalanine in peptides and proteins. **A. de Bruijn**, G. Roelfes
- . *In vitro* anti-neoplastic activity of specific phytocannabinoids of *Cannabis sativa*. **R.M. Hyslop**, A. Saviola, S. Bydalek, C.E. Brown, S. Desa, M. Thomas, A. Magiotta, S. Mackessy, C. Hansen, M. Brown
- . Quantifying the relative amounts of PrP polymorphisms present in prions isolated from heterozygous prion-infected animals. **C.J. Silva**, M.L. Erickson-Beltran, C. Hui, J.J. Badiola, J.R. Requena, R. Bolea
- . Novel application of scaffold treatment procedure with minimum side effects by using an engineered biodegradable scaffold. Y. Lo, G. Ren, E.J. Parish, **H. Honda**
- . Novel approaches to the developmental relationship of retinol binding protein and clinical phenotype of coronary heart disease. L. Lv, E.J. Parish, **D. Ren, G. Ren, H. Honda**
- . Novel application of new methodology in the treatment of enzyme as a preparation method for biocompatible material. G. Ren, E.J. Parish, Y. Lo, **H. Honda**
- . *In vitro* activation of purified *Aedes aegypti* mosquito wild-type Early Trypsin (AaET) versus the inactive AaET mutant. **R.M. Lucero**, A. Rascon
- . Genetically modifying T-cells to target CD19 and CD22 antigens. **N.P. Joseph**
- . Importance of Ser26 in the Folate Half-Reaction of *E. coli* MTHFR. **R. Li**
- . Interfacial Interactions of Glycine and Short Glycine Peptides in Confined Spaces. **K. Doucette**, P. Chaiyasit, D.L. Calkins, K. Martinez, M.J. Fisher, D.C. Crans, A. Tongraar
- . Developing small molecule adjuvants from contact allergens. **S. Kim**, A. Esser-Kahn

- . Synthesis of 2-Arachidonoylglycerol: An endocannabinoid with potential as an anti-cancer drug. **S. Bydalek**, R.M. Hyslop
- . Purification and characterization of adenosine aminohydrolases from *Pisum Sativum*. **L. Thicklin**, P.C. Kline
- . Photoactivatable innate immune receptor for optogenetic inflammation. **B. Moser**, A. Esser-Kahn
- . Investigation of Cu(II) complexation with fourth microtubule-binding repeat of tau protein by ESI-MS, IMS-MS and NMR. **S. Ahmadi**, S. Zhu, R. Dutta Majumdar, R. Soong, D. Wilson, A. Simpson, H. Kraatz
- . Conformational sampling and non-dimer aggregates of HIV-1 protease containing darunavir promoted mutations. **L. Pham**, Z. Liu, L. Hu, X. Huang, A. Bhatt, K. Bentz, T. Tran, D. Savin, R. McKenna, G. Fanucci
- . Synthesis of fluorogenic phosphatidylcholine derivatives for kinetic studies of phospholipase A<sub>2</sub> enzymes. **L. Zelaya**, J. Hajdu, T.G. Minehan
- . Enhancing efficacy of protease drugs through site-directed mutagenesis. **A. Amorello**, A. Batt, T. Baird
- . Investigating a new paradigm in melanocortin signaling and energy balance. **V. Chen**
- . Affinity ligand purification for pyridine dinucleotide binding proteins. **D. Andy**, J. Slama, T. Walseth
- . Elucidating Met18 Functionality in Iron-Sulfur Cluster Biogenesis Pathway. **C. Lee**, A. Vo, J. Cosman, D. Perlstein
- . Engineering a Polymerase for Accurate Bypass of Damaged DNA Samples. **T. Coulther**, P.J. Beuning, M.J. Ondrechen
- . Topology study of one CpTat component, Hcf106, in resting and precursor binding state. **A.G. Habtemichael**, G. Thomas, C. Dabney-Smith
- . Single molecule imaging of protein activity in living cells. **N. Pinkin**, J. Smith, B. Liu, C.J. MacNevin, K.M. Hahn
- . Assessing the functionality of active site threonine substituted trypsin with disulfide residue serine variants. **J. Schuder**, B. Caswell, T. Baird
- . HPLC analysis of sulfation of dopamine derivatives by SULT1A3. **K. Reed**, J. Rogowiec, M.L. Cafiero, L.W. Peterson

- . Cloning of IME4 to establish a new model system to probe N6-methyladenosine modification of mRNA. **A. Barnaby**, C. Schoose, J. Dunkle
- . Gene expression in a synthetic tissue of artificial cells. **H. Niederholtmeyer**, N.K. Devaraj
- . Cobalticinium derivatives as mediators for bioelectrochemical catalysis with P450. **W. Bae**
- . Characterization of Sup35, Rnq1, and Ure2 Cotranslational Prion Aggregation in *Saccharomyces cerevisiae*. **B.T. Allwein**, D. Cameron
- . Construction of hydrophobic nanoparticles based surface plasmon resonance biosensor for lysozyme detection. **Y. Saylan**, F. Yilmaz, A. Derazshamshir, A. Denizli
- . Photoswitchable immunostimulants for optical control of TLR activity. **A. Love**, T.J. Albin, A.P. Esser-Kahn
- . Solid phase peptide cyclization and development of PRC2 Inhibitors. **G. Zhang**
- . Relationship between metal binding and protein stabilization of an ancestral  $\beta\gamma$ -crystallin from the *Ciona intestinalis* tunicate. **N. Kozlyuk**, S. Sengupta, J. Bierma, R.W. Martin
- . Using light and a photoactivated insulin depot to control insulin release and blood glucose in-vivo. **B.R. Sarode**, K. Kover, P.Y. Tong, C. Zhang, S.H. Friedman
- . *C9orf72* repeat expansion disrupts nucleocytoplasmic transport. **S. Bifulco**, K. Zhang
- . Development of highly specific carbohydrate-nucleic acid reagents for lectin recognition. **C. Gordon**, J. Niu, A. Pusuluri, A. Csordas, C.J. Hawker, H. Soh
- . Synthesis of solvatochromic probes to study the effect of host microenvironment on mycobacterial cell wall dynamics during infection. **S. Keyser**, A. Utz, C.R. Bertozzi
- . Cryptic antibiotic discovery in the filamentous cyanobacterium *Scytonema* sp. UTEX LB 1163. **M.L. Hillwig**
- . Chemo-enzymatic synthesis of an effective bifunctional NAADP analog for isolation and purification of the NAADP receptor. **P. Su**, T. Walseth, J. Slama
- . Ribonucleotide reductase enzyme a target for titanium complexes: A strategy to cure cancer. **K. Gaur**, S.C. Perez, E. Akam, E. Tomat, M. Saxena, R.K. Sharma, A.D. Tinoco
- . Inhibition of cancer cell viability and selective inhibition of lysyl oxidase with small-molecule Inhibitors. **K. Johnston**, K.M. Lopez
- . Plausible reaction mechanism of the deamination of histidine catalyzed by histidine-ammonia lyase. **S. Minkowicz**, Y. Sheng

- . Unraveling the role of ligands in the hydrogen evolution mechanism catalyzed by [NiFe] hydrogenases. **S. Qiu**, L.M. Azofra, D.R. MacFarlane, C. Sun
- . Highly responsive and selective fluorescent probes to image ATP in live cells. **Y. Fan**, H. Ai
- . Design of a two-step fluorogenic strategy for tyrosine specific labeling of proteins. **M. Shadmehr**, M. Stagg, J.C. Jewett
- . Development of a direct activity probe for a critical regulator of metastatic signaling. **T. Hamada**, J.R. Beck, G.R. Casey, M. Kelly, X. Zhou, C.I. Stains
- . Spatial and temporal control of lysine acetyl transferases (KATs): Ligand gated split KATs. **C.S. de Silva**
- . Determination of metal affinities of *Halobacterium salinarum* cysteinyl-tRNA synthetase. **L. Cobani**, J. Kuhlmeier, J. Rosentreter, C.M. Evilia
- . Irradiation-controlled disassembly of peptide hydrogels and dye release via photolabile Lys(Nvoc). **J. Pellegrino**, R.M. Abaskharon, F. Gai
- . DNA repair proteins XLF and XRCC4 interact with telomeric proteins TRF1 and RAP1. **P. Zaibaq**, **M. Guirette**, E. Castle, K. Vu, N. Fahmy, J. Jabbur, A. Ribes-Zamora
- . Evolved luciferases improve activity with pyridone luciferins. **B.S. Zhang**, K.A. Jones, D.C. McCutcheon, J.A. Prescher
- . Development of antifungal  $\alpha/\beta$ -peptides mimetics of the antimicrobial peptide Aurein 1.2. **M. Lee**, N. Raman, A. Rodriguez-Lopez, S.H. Gellman, D.M. Lynn, S. Palecek
- . Engineering Modular Polyketide Synthases for Generation “Drop In” Biofuels. **C.B. Bailey**, A. Zargar, R. Anayah, S. Curran, L. Katz, J.D. Keasling
- . Development of *Streptomyces* as heterologous hosts for the production of branched fatty acids for biofuels. **R. Krishna**, **J. Blake-Hedges**, R. Haushalter, J.D. Keasling
- . Synthesis and biochemical assessment of hydroxytyrosol. **I. Kady**, E. Onobun, S. Mumford
- . Proline-rich peptides inhibit polymerization of sickle cell hemoglobin. **B.B. Brennan**, L. Steenberge
- . Investigation of the effect of gold nanoparticles on the structure and catalytic function of *Escherichia coli* prolyl-tRNA synthetases. **S. Mitchell**, **O. Hurst**, A. Lato, J.A. Dahl, S. Hati
- . LGN protein purification for X-ray crystallography. A. Howard, A.H. Smith, R. Elnicki, J. Galardi, L.B. Cook, **B.M. Sreenilayam**



- . Measuring metabolite consumption by *Sinorhizobium meliloti* using  $^1\text{H}$  NMR spectroscopy and time domain complete reduction to amplitude frequency table (CRAFT). **D.P. Soulsby**, D.B. Wacks, N. Stubb
- . Development of a cannabinoid-based Cell-in-a Box® therapeutic system targeted toward malignant tumors. R.M. Hyslop, **C.E. Brown**, A. Magiotta, B. Morgan, M. Brown, T. Sherman, D. Petty, S. Desa, J. O'Neil, S. Flora, K. Kellogg, C. Hansen, S. Bydalek, T. Cale, C. Laster, J. Folsom, A. Hawkinson
- . Cartilage: Function and supramolecular structure. **F. Horkay**, E.K. Dimitriadis, I. Horkayne-Szakaly, P.J. Bassar
- . Novel porphyrin derivatives for photodynamic therapy. **T.E. Hayes**, T. White, M.E. Scarbrough, J.E. Bradshaw
- . Photosensitized oxidation of biotinylated dyes. **R.A. Haack**, Q. Ruan, K.M. Swift, S. Tetin
- . Purification of a putative tartrate-resistant acid phosphatase from *Penicillium spinulosum*. B.A. Schofield, J. Carsella, **S.J. Bonetti**
- . Evaluation of potential functions of two previously uncharacterized bacterial GNAT threonine N-acetyltransferases from *Clostridium difficile* and *Staphylococcus aureus*. J. Baumgartner, D. Tran, **M.L. Kuhn**
- . Discovery of endogenous and synthetic ligands for orphan nuclear receptor TLX. **A.C. Cao**, P. Kandel, M. Maletic-Savatic, D. Young
- . Synthesis, characterization and biological studies of cobalt(II) Schiff bases derived from *o*-vanillin with series of aromatic amines. **R.O. Shaibu**
- . Spectroscopic and computational studies on the comparative interaction of cationic single-chain and gemini surfactants with hen egg white lysozyme. **R. Patel**
- . Evaluating Fmoc-amino acids as butyrylcholinesterase inhibitors. **J.P. Schwans**, J. Ramirez, J. Gonzalez
- . Site-selective modification of native proteins and antibodies. **G. Bernardes**
- .  $\beta$ -2-Himachalen-6-ol: A novel anticancer sesquiterpene unique to the Lebanese wild carrot. **R.I. Taleb**, C. Daher, M. Mroueh, M. ElSibai
- . Reverse transport of 1-methyl-4-phenylpyridinium (MPP<sup>+</sup>) is mediated by extracellular calcium in dopaminergic MN9D cells. **V.Q. Le**, K. Wimalasena, S. Mapa
- . Glycoconjugated site-selective DNA-methylating agent targeting glucose transporters on glioma cells. M. Buchanan, N. Chase, N. Neill, M. White, C. Kelly, K. Mastro-Kishton, L.

Chauvigne-Hines, T. Goodwin, A. McIver, L.J. Bartolotti, A. Bourdelais, A. Frampton, **S. Varadarajan**

. Linker strategy for addressing unprecedented photochemistry in coumarin-caged Tamoxifen. P.T. Wong, E.W. Roberts, S. Tang, J. Mukherjee, J. Cannon, M.F. Krummel, **S. Choi**

. Disabling WTA to kill MRSA with beta-lactam antibiotics. **C.V. Rice**, M. Foxley, M. Xiao, S. Wright, S. Strange

. Cloning, expression and NMR spectroscopy of purified MerF transmembrane protein isolated from mercury resistant *Enterobacter* sp. AZ-15. **A. Amin**, S. Opella, Z. Latif

. Heteromultivalency in melanoma with GPCR ligands: Target validation and use of orthogonal chemistries towards a heterobivalent scaffold. **J.A. Rodriguez Corrales**, D.H. Clark, P. Kohnke, J.S. Josan

. Engineered luciferases as off-the-shelf reporters of pathogens. **Z. Reinert**, J.A. Prescher

. NitroTyrosine: Gain-of-function alterations to calcium signaling. **J. Porter**, R.A. Mehl

. Traversing the challenges of extended conjugation: Bacteriochlorins and aza-bodipys, a new era in photomedicine. **M. Cheng**, R.W. Boyle

. Bioelectrochemical detection of endocrine disrupting compounds. **A.L. Furst**, A. Hoepker, M.B. Francis

. Cytochrome c-induced permeabilization of cardiolipin-containing phospholipid membranes is induced through the selective interaction of cytochrome c with cardiolipin. **J.P. Kitt**, D.A. Bryce, S.D. Minter, J.M. Harris

. Correlation between melatonin and cortisol levels in hair and their validity as biomarkers. **A. Alarbi**, W. Potter

. Synthetic Foldamers as Inhibitors of A $\beta$  Self Assembly. **S. Kumar**, A. Hamilton

. Propargyl-linked antifolates potently inhibit US clinical *S. aureus* isolates with newly identified dfrG and dfrK resistance genes. **S.M. Reeve**, A.C. Anderson, D. Wright

. Development and application of novel small molecule calcium sensors for investigating neuronal activity. **A.A. Contractor**

. Engineering alternative radical rebound chemistry the  $\alpha$ KG oxygenase Factor Inhibiting Hypoxia Inducible Factor (FIH). **V.D. Chaplin**, M. Knapp

. Engineered cardiolipin nanoparticle for Barth syndrome. **R. Wen**, S. Dhar

- . Determination of calreticulin-ligand complex formation using fluorescence spectroscopy. **C. Thomas**
- . Isomerically pure tetramethylrhodamine voltage reporters. **P. Deal**, E. Miller
- . Design and application of new voltage sensitive dyes for *Ex vivo* brain imaging. **R. Kulkarni**, E. Miller
- . Narrowing down the minimal recognition motif for ligand sensing in the leucine-rich repeat domain of Nod2. **M.L. Lauro**, E. D'Ambrosio, B.J. Bahnson, C.L. Grimes
- . Investigating active site dynamics in a thermophilic enzyme through FTIR and 2DIR spectroscopy. **T.D. Hill**, H.H. Lepird, D.A. Price, S.D. Moran
- . Dynamics of thrombin generation and flux from clots during whole human blood flow over collagen/tissue factor surfaces. **S. Zhu**, Y. Lu, T. Sinno, S. Diamond
- . Internally quenched synthetic peptides for the study of yeast Ste24p proteolytic activity. **E.A. Krautkramer**, E. Hsu, C. Hrycyna, M.D. Distefano
- . Tissue-specific ascaroside production in the nematode *Caenorhabditis elegans*. **A.E. Akagi**, P. Sternberg, F. Schroeder
- . Stable-on-the-table enzymes: Interlocking of laccase in Whatman filter paper. **C. Riccardi**, C.V. Kumar, R. Kasi
- . Synthetic foldamers as inhibitors of A $\beta$  aggregation. **s. Kumar**, A. Hamilton
- . Characterization of cold adaptation in Antarctic toothfish eye lens proteins. **J. Bierma**
- . Host cell entry of Zika virus may be mediated by glycosaminoglycans. **S.Y. Kim**, J. Zhao, X. Liu, L. Lin, X. Zhang, F. Zhang, R.J. Linhardt
- none** . Fibrinogen  $\alpha$ C (233-425): A model protein for characterizing cross-linking by the transglutaminase factor XIII. **K. Mouapi**, J. Bell, K. Smith, R. Ariens, H. Philippou, M.C. Maurer
- . Copper containing sulphonamide analogs for biological targets. **M. Danish**, **A. Altaf**
- . Ionic Interactions of Collagen and Thermosetting Resin Composites. **A. Lorts**, A. Stewart, R. Quirino
- . Characterizing the atypical protein kinase 9 in *Plasmodium* . **A. Eubanks**, R. Raphemot, E. Derbyshire

. For Better or Worse: Site-Specific Protein Attachment. **K. Kean**, R. Bednar, W.J. Brown, J. Porter, P. Karplus, R.A. Mehl

**none** . Investigating the ability of small molecule gibberellins to inhibit the NF- $\kappa$ B pathway. **J. Annand**, A.R. Henderson, A.K. Mapp, A.N. Koehler, C. Schindler

. On the mechanism of slowing down cancer cell migration in the gold nanoparticles treatment. **Y. Wu**, M.R. Ali, M.A. El-Sayed

. Purification and kinetic assays of recombinant AaCHYMO from the *Aedes aegypti* female mosquito. **O.E. Burata**, A. Rascon

. Characterizing the genetic fitness landscape of virus-like particles. **E. Hartman**, C. Jakobson, D.T. Ercek, M.B. Francis

. Mechanistic studies in Flavin Dependent Thymidylate Synthase (FDTS). **k.u. karunaratne**, M. LeFebvre, J. Villalobos, A. Kohen

. Insight into the mechanism of a bifunctional diguanylate cyclase enzyme in *Agrobacterium vitis*: A catalytic loop 6, nitric oxide signaling and bacterial biofilm formation. **D. Williams**, N.M. Nesbitt, E.M. Boon

. Investigation of oligomeric assemblies within the claudin tight junction protein family: A combined computational and experimental approach. **D. Shastry**, F.J. Irudayanathan, S. Nangia, P. Karande

. Design, synthesis, and conformational analysis of proposed  $\beta$ -turn mimics from isoxazoline-cyclopentane aminols. **M. Memeo**, **M. Mella**, V. Montagna, P. Quadrelli

. Design and synthesis of lysine-56 targeting covalent inhibitors of HSP72. **J. Pettinger**, M. Cheeseman, Y. Le Bihan, M. Widya, R.L. van Montfort, K. Jones

. Exploiting the peptide-binding site to design inhibitors of the KDM4 subfamily. **J. Maw**, Y. Le Bihan, N. Mok, K. Boxall, A. Tumber, V. Bavetsias, J. Blagg

. Repurposing an aminomutase from *Taxus* plants: Enzymatic conversion of cinnamate epoxides into ring-opened, chiral phenylserines. **P.K. Shee**, N. Ratnayake, O. Goethe, E.E. Onyeozili, K.D. Walker

. Branched polyethylenimine disables teichoic acid function leading to altered morphologies of Gram-positive bacteria. **M. Foxley**, S. Wright, M. Xiao, S. Strange, C.V. Rice

. Protein power: Enzyme-hydrogels for efficient sugar-to-power conversion in a biofuel cell. **A. Ghimire**, A. Pattammattel, R. Kasi, C.V. Kumar

. Protein phosphor materials: A new generation of biodegradable, multi-functional, protein-based, hydrogels for white emission, sensing of small molecules, and detection of pH over a wide range (3-11). **K.R. Benson**, A. Ghimire, R. Kasi, C.V. Kumar

. Inhibition of fibrillar assemblies of l-phenylalanine by crown ethers: A potential approach toward phenylketonuria. **D. Banik**

. Assay interference and off-target liabilities of reported histone acetyltransferase inhibitors. **J.L. Dahlin**, K.M. Nelson, J.M. Strasser, D. Barsyte-Lovejoy, J.H. Shrimp, J.L. Meier, C.H. Arrowsmith, P. Brown, J.B. Baell, M.A. Walters

. Epigenetics and *O*-GlcNAc cycling: The relationship between dynamic *O*-linked glycosylation and transcriptional regulation. **K.R. Harwood**, J. Hanover

. Analysis of how trimethyllysine is recognized by epigenetic reader proteins. **J. Poater**, F. Bickelhaupt, J. Mecinovic

. Enzymatically self-assembled functional RNA nanostructures and their therapeutic applications. **H. Kim**, J. Lee

. Altered protein motions modified the chemical step in thymidylate synthase. **A.K. Ghosh**, T. Abeysinghe, A. Kohen

. Supramolecular assembly of artificial metalloenzymes: Influence of the second coordination sphere of the LmrR in catalysis. **L. VILLARINO PALMAZ**, S. Chordia, E. Reddem, G. Roelfes

## WEDNESDAY MORNING

Section A

Venue

Placeholder

### Self-Assembly of Small Molecules in the Cellular Milieu-Invited, Oral

B. Xu, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35** . Molecular prosthetics for missing ion transport proteins. **M.D. Burke**

**9:10** . Protein responsive supramolecular assembly for live cell imaging. **I. Hamachi**

**9:45** . Enzyme-instructed self-assembly in cellular milieu: Bioinspired targeting of cancer cells without drug resistance. H. Wang, Z. Feng, J. Zhou, X. Du, **B. Xu**

**10:20** Intermission.

**10:35** . Self-assembly of chemotherapeutic colloidal drug aggregates. **M.S. Shoichet**, A. Ganesh, C. McLaughlin, J. Logie, S.C. Owen, B. Shoichet

**11:10** . Mechanism of cell death induced by a small-molecule forming fibrils. **O. Julien**, J.A. Wells

Section B

Venue

Placeholder

### **Mid-Career Investigators in Biological Chemistry-Oral**

L. Hedstrom, *Organizer*

**8:30** Introductory Remarks.

**8:35** . Nanobody activation immunotherapeutics. **B. McNaughton**

**8:55** . Inhibitors of the coenzyme A biosynthetic enzyme phosphopantothencysteine synthetase: Design, mechanism and selectivity. R. Domingo, W.J. Moolman, K.J. Mostert, L. Barnard, **E. Strauss**

**9:15** . Highly selective and sensitive fluorescent probes for superoxide, peroxyxynitrite, hypochlorous acid, hydrogen peroxide and hydroxyl radical. J. Hu, N. Wong, T. Peng, X. Bai, M. Lu, S. Ye, **D. Yang**

**9:35** . Allosteric modulation of G protein coupled receptors: The P2Y<sub>1</sub> receptor as an example. **Z. Gao**, K.A. Jacobson

**9:55** Intermission.

**10:05** . Role of intrinsic dynamics on substrate binding and catalysis of *Escherichia coli* prolyl-tRNA synthetase. **S. Hati**

**10:25** . Chemical probes for the investigation of natural product assembly: Biosynthetic insights and novel opportunities. **M. Tosin**, C. Ho, I. Wilkening, E. Riva, J. Havemann

**10:45** . Targeting RNA with branched peptide boronic acids: unnatural amino acids, molecular recognition, and in vitro activity against HIV-1 RRE RNA. **W.L. Santos**, Y. Dai, J. Wynn, A. Peralta , D. Rekosh, M. Hammarskjold

**11:05** . Chemical biology tools to study protein-protein interactions of the fatty acid synthase – updates from the interface. **M.D. Burkart**

## **Chemical Biology: Enabling Drug Discovery**

Sponsored by ORGN, Cosponsored by BIOL

### **WEDNESDAY AFTERNOON**

Section A

Venue  
Placeholder

## **Chemical Probes for Bacterial Imaging-Invited, Oral**

E. E. Carlson, *Organizer, Presiding*

**2:00** Introductory Remarks.

**2:05** . Chemical technologies for illuminating *Mycobacterium tuberculosis*. **K.E. Beatty**

**2:50** . Probing the dynamics of peptidoglycan biosynthesis with fluorescent D-amino acids (FDAAs). **M. Van Nieuwenhze**

**3:35** Intermission.

**3:50** . Activity-Based probes for selective imaging of an essential PBP in *Streptococcus pneumoniae*. **E.E. Carlson**

**4:35** . Chemical insights into methicillin-resistant *Staphylococcus aureus*. **S. Walker**

**5:20** Concluding Remarks.

Section B

Venue  
Placeholder

## Graduate Student & Postdoctoral Fellow Symposium-Oral

L. Hedstrom, *Organizer*

**2:00** Introductory Remarks.

**2:05** . Utilizing selenocysteine for expressed protein ligation and bioconjugations. **J. Liu**, Q. Chen, S. Rozovsky

**2:20** . Genetic targeting of small molecule voltage indicators using SpyTag/SpyCatcher. **V. Grenier**, E. Miller

**2:35** . Translating unnatural amino acids with phenotypically-diverse computationally-engineered EF-Tu variants. **V. Cox**, E. Gaucher

**2:50** . Constructing de novo small molecules responses via signal-induced protein proximity in mammalian cells: Chemically engineer cell behaviors & signaling. **G. Zeng**, W. Xuan, H. Li, R. Zhang, Y. Wei, L. Breden, F. Liang, W. Wang

**3:05** . Direct proximity tagging of small molecule proteins targets. **Z.B. Hill**, S.B. Pollock, M. Zhuang, J.A. Wells

**3:20** Intermission.

**3:35** . Development of novel far-red to near-infrared fluorophores for chemical biology. **X. Zhou**, L. Leisak, R. Lai, J.R. Beck, J. Zhao, C. Elowsky, H. Li, C.I. Stains

**3:50** . Probing innate immunity with tunable synthetic glycopeptides. **M. Zhou**, C. Delaveris, J. Kramer, C.R. Bertozzi

**4:05** . Monitoring thioredoxin redox in live cells with a genetically encoded red fluorescent protein biosensor. **Y. Fan**, H. Ai, M. Makar

**4:20** . SAMDI Mass spectrometry assay for the high-throughput profiling of protein interaction domains with peptide ligands and its application to chromodomains. **P.T. O'Kane**, M. Mrksich

**4:35** . Engineered luciferase-luciferin pairs for highly sensitive bioluminescence *in vitro* and *in vivo*. **H. Yeh**

**4:50** . Generation of allosteric chaperones for Glucose-6-Phosphate Dehydrogenase (G6PD) deficiency. **S. Hwang**

**THURSDAY MORNING**



Venue  
Placeholder

**Graduate Student & Postdoctoral Fellow Symposium-Oral**

L. Hedstrom, *Organizer*

**8:30** Introductory Remarks.

**8:35** . Exploring vectorial chain translocation in assembly line polyketide synthases. **M. Ostrowski**, C. Khosla

**8:50** . What machinery controls the release of peptide mimetics from endosomes? A genome-wide analysis. **A. Steinauer**, J.R. LaRochelle, R.F. Wissner, A. Schepartz

**9:05** . Influenza Hemagglutinin Fusion Domain by Advanced NMR using Novel Orthogonal Refinement and BICS Curvature Measurements. **S.T. Smrt**, A. Draney, J. Lorieau

**9:20** . Discovery of a bacterial gene in the gut microbiome encoding metabolism of dietary lignans. **E. Bess**, J. Bisanz, P. Spanogiannopoulos, E. Waligurski, P. Turnbaugh

**9:35** . Targeting phospholipase A<sub>2</sub> to diminish inflammation by developing novel inhibitors. **V. Mouchlis**, **J. McCammon**, **E.A. Dennis**

**9:50** . Investigating the Regiospecificity of an Unusual Bacterial Acyl-CoA Dehydrogenase. **J. Blake-Hedges**, J. Pereira, J. Chen, P.D. Adams, J.D. Keasling

**10:05** Intermission.

**10:20** . Characterization of a drug-inactivating enzyme from a prominent human gut microbe. **N. Koppel**, J. Bisanz, P. Turnbaugh, E.P. Balskus

**10:35** . Investigating the molecular basis of algal-bacterial symbioses. **R. Wang**, M. Wilson, M. Seyedsayamdost

**10:50** . Engineering protein structure and small molecule transport of the bacterial microcompartment. **M. Slininger Lee**, C. Jakobson, D.T. Ercek

**11:05** . Structural insight from activity: Functional screening of the entire *Arabidopsis* GT1 family enables cheminformatic-bioinformatic predictions of glycosyltransferase reactions and protein features. **C. Fehl**, M. Yang, K.V. Lees, E. Lim, W. Offen, G.J. Davies, D. Bowles, S.J. Roberts, B.G. Davis

**11:20** . Enzymatic mechanisms for decorating phenazine antibiotics from *Lysobacter antibioticus*. **J. Jiang**, Y. Zhao, S. Wright, L. Du