

- 8:55 NUCL 52.** Exploring redox coordination chemistry in transuranic elements with various crown ethers and cryptands through lanthanides. **F.D. White, M.L. Marsh, D.E. Hobart, T.E. Albrecht-Schmitt**
- 9:20 NUCL 53.** Electrochemical studies to stabilize divalent californium. **M.L. Marsh, F.D. White, D.E. Hobart, T.E. Albrecht-Schmitt**
- 9:45 Intermission.**
- 10:10 NUCL 54.** Chelation past curium: Exploring trends in f-orbital bonding. **R.J. Aberget, G. Deblonde, J. Rees, C. Booth, W. Dejong, R. Strong**
- 10:35 NUCL 55.** Redox studies of the heaviest actinides. **Y. Nagame, A. Toyoshima**
- 11:00 Intermission.**
- 11:25 NUCL 56.** Heavy element chemistry research at Texas A&M University. **C.M. Folden**
- 11:50 NUCL 57.** Studying the fundamental chemistry toward the end of the periodic table: The Heavy Element Chemistry program. **P. Wilk**

### WEDNESDAY AFTERNOON

#### Section A

Grand Hyatt Washington  
Constitution D

#### Chemistry Past Curium

*Cosponsored by INOR*

T. E. Albrecht-Schmitt, D. E. Hobart, I. R. Triay, *Organizers*

- 2:30 NUCL 58.** Reactor production of actinide materials for super-heavy element research. **D.J. Dean, J. Roberto**
- 2:55 NUCL 59.** TODGA-based solvent extraction system: An alternative to CLEANEX for Cf production. **L.H. Delmau, C. Dryman**
- 3:20 NUCL 60.** Heavy actinide complexation thermodynamics: Chemical signatures arising from limited materials. **J. Braley, N. Bessen, M. Urban, P. Yang**
- 3:45 Intermission.**
- 4:10 NUCL 61.** Structural and thermodynamic considerations in the post-curium break. **T.E. Albrecht-Schmitt**
- 4:35 NUCL 62.** Single-ion manipulation in gas catchers and RF systems. **G. Savard**
- 5:00 NUCL 63.** Chemical studies of the transactinide elements. **A. Tuerler**

### WEDNESDAY EVENING

#### Section A

Grand Hyatt Washington  
Constitution C

Technical program information known at press time. The official technical program for the 254th ACS National Meeting is available at [www.acs.org/WDC2017](http://www.acs.org/WDC2017)

#### Nuclear Forensics

J. F. Corbey, K. L. Pellegrini, *Organizers*  
J. D. Auxier, *Organizer, Presiding*

- 5:30** Introductory Remarks.
- 5:35 NUCL 64.** High temperature uranium chemistry in condensing laser ablation plasmas. **D. Weisz, J.C. Crowhurst, H. Radousky, T. Rose, B. Koroglu, W. Siekhaus, J.M. Zaig, M. Azer, M. Finko, D. Curreli**
- 5:55 NUCL 65.** Preparation of surrogate post-detonation debris using a plasma torch. **P.A. Taylor**
- 6:15 NUCL 66.** High temperature aging study of UO<sub>2</sub> and U<sub>3</sub>O<sub>8</sub> for nuclear forensics. **A.M. Olsen, L.W. McDonald**
- 6:35 NUCL 67.** Quantitative morphological analysis of actinide materials. **K.L. Pellegrini, J.A. Soltis, E. Buck, L. Sweet, D.E. Meier**
- 6:55 Intermission.**
- 7:10 NUCL 68.** Dependence of UO<sub>2</sub> surface morphology on synthesis route. **E. Abbott, L.W. McDonald**
- 7:30 NUCL 69.** Three-dimensional morphological signatures for nuclear forensics. **B. Chung, D. Roberts, W. Talbot, D. Ashley, N. Teslich**
- 7:50 NUCL 70.** Impact of controlled storage conditions on the hydration and morphology of UO<sub>3</sub>. **I. Schwerdt, L.W. McDonald**
- 8:10 Intermission.**
- 8:25 NUCL 71.** Multi-variate statistical analysis enhancing preliminary morphological signature development strategies for nuclear forensic-related materials. **A.D. Lesiak**
- 8:45 NUCL 72.** NNSA Graduate Fellowship Program experience. **A. Gillens**

### THURSDAY MORNING

#### Section A

Grand Hyatt Washington  
Constitution D

#### Nuclear Forensics

J. D. Auxier, K. L. Pellegrini, *Organizers*  
J. F. Corbey, *Organizer, Presiding*

- 8:30** Introductory Remarks.
- 8:35 NUCL 73.** Detailed *in-situ* chemical characterization and Pb-Pb age dating of uraninite from North American deposits. **S. Lewis, L. Corcoran, A. Simonetti, P.C. Burns**
- 8:55 NUCL 74.** Atomistic insight into phase formation and alteration of uranium phases. **L.C. Shuller-Nickles**
- 9:15 NUCL 75.** Deposit type average rare earth element signatures for nuclear forensics. **T.L. Spano, A. Simonetti, G. Carpenter, D. Freet, E. Balboni, T. Wheeler, C. Dorais, P.C. Burns**
- 9:35 Intermission.**
- 9:55 NUCL 76.** Chemical characterization of altered and unaltered uraninites from various geological settings. **L. Corcoran, A. Simonetti, T.L. Spano, S. Lewis, P.C. Burns**
- 10:15 NUCL 77.** Novel dissolution chemistry for post detonation nuclear debris. **J.D. Brockman, N.T. Hubley, C. Mason, D. Wegge, J.D. Robertson**

- 10:35 NUCL 78.** Extraction of cesium ion with dibenzo-18-crown-6 from aqueous solutions using organic solvents. **R. Biswas, T. Banerjee, P. Ghosh, S. Ali**
- 10:55 Intermission.**
- 11:15 NUCL 79.** Withdrawn.
- 11:35 NUCL 80.** Phase-field modeling of the U,C-UC liquid-solid interface for the formation of UC microstructures. **D. Abrecht**
- 11:55 NUCL 81.** Chemist's stint with nuclear forensics at the State Department. **C.L. Cahill**

### THURSDAY AFTERNOON

#### Section A

Grand Hyatt Washington  
Constitution D

#### Nuclear Forensics

J. D. Auxier, J. F. Corbey, *Organizers*  
K. L. Pellegrini, *Organizer, Presiding*

- 12:30** Introductory Remarks.
- 12:35 NUCL 82.** Age dating of Sr-90 using DGA resin. **D. McLain**
- 12:55 NUCL 83.** Development of a Cs-Ba radiochronometry reference material for nuclear forensics. **K.B. Lavelle, K.P. Carney, J.T. Cessna, R.M. Essex, C.R. Hexel**
- 1:15 NUCL 84.** Gas chemical adsorption characterization of lanthanide chelates. **S. Stratz, H. Hall, J.D. Auxier**
- 1:35 Intermission.**
- 1:50 NUCL 85.** New K-edge densitometry calibration technique. **M.D. Yoho, D.T. Vo, D.R. Porterfield**
- 2:10 NUCL 86.** FBI nuclear forensics. **J. Blankenship**
- 2:30 Intermission.**
- 2:45 NUCL 87.** Nuclear Forensics International Technical Working Group collaborative materials exercises: Advancing the state and practice of nuclear forensic analysis since 1999. **J.M. Schwantes**
- 3:05 NUCL 88.** Software and analysis methods for the determination of americium in plutonium via alpha spectrometry. **M.D. Yoho, D.R. Porterfield, J. Rim**

## ORGN

### Division of Organic Chemistry

R. Broene and S. Silverman, *Program Chairs*

#### OTHER SYMPOSIA OF INTEREST:

**Insights on Medicinal Chemistry from Hardcore Practitioners** (see *MEDI*, Mon)

**Organometallic Chemistry** (see *INOR*, Sun, Tue, Wed, Thu)

**Synthesis & Chemistry of Agrochemicals** (see *AGRO*, Thu)

#### SOCIAL EVENTS:

**Social Hour**, 8:00 PM: Wed

#### BUSINESS MEETINGS:

**Business Meeting**, 1:00 PM: Sun

### SUNDAY MORNING

#### Section A

Walter E. Washington Convention Center  
Room 207A

#### Young Investigator Symposium

J. Aube, *Organizer, Presiding*

- 9:00 ORGN 1.** mPGES-1 inhibitors from start to clinic. **M. Schiffer**
- 9:20 ORGN 2.** Asymmetric hydrogen bonding catalysis for the synthesis of dihydroquinazoline-containing antiviral, letermovir. **Z. Liu**
- 9:40 ORGN 3.** Development of a robust process for venetoclax. **V.S. Chan**
- 10:00 ORGN 4.** Discovery, development and mechanistic study of catalytic transformations for the multi-kilogram scale synthesis of pharmaceutical intermediates. **E. Simmons**
- 10:20 ORGN 5.** New chemistries for antibody-drug conjugates. **T. Pillow**
- 10:40 ORGN 6.** Fueling the Alzheimer's BACE1 race with genetic insights and cyclopropyloxazine BACE1 inhibitors. **A.E. Minatti**
- 11:00 ORGN 7.** Synthesis of photo-reactive chemical probes through late-stage heterocyclic C-H functionalization of unmodified biologically active molecules. **K. Hesp**
- 11:20 ORGN 8.** New opportunities for synthetic chemistry to enable drug discovery: Discovery of [18F] MK-6240 a novel PET imaging agent for tau pathology. **A.M. Wajji**

#### Section B

Walter E. Washington Convention Center  
Room 202A

#### Flow Chemistry & Continuous Processes

R. D. Broene, *Organizer*  
Z. Li, *Presiding*

- 8:10 ORGN 9.** Continuous generation of anhydrous *tert*-butyl hydroperoxide and its application in flow oxidation. **Z. Li, S. Guinness, S.M. Hoagland, H.K. Kim, R.J. Maguire, J.C. McWilliams, J. Mustakis, J.W. Raggion, D. Campos, C. Voss, E. Sohodski, B. Feyock, H. Murnen, M. Gonzalez, M. Johnson, J. Lu**
- 8:30 ORGN 10.** Use of carbon monoxide gas in flow chemistry: Oxidative and reductive carbonylation chemistry. **C. Kappe**
- 8:50 ORGN 11.** Continuous flow synthesis of 1,4-benzoxazinones via a fully integrated nitration/hydrogenation/cyclization sequence. **D. Cantillo, B. Wolf, R. Goetz, C. Kappe**
- 9:10 ORGN 12.** Development of efficient and scalable amidation processes in flow: An inverse disconnection strategy. **J.D. Williams, S. Leach, W.J. Kerr**
- 9:30 ORGN 13.** High-throughput synthesis: A platform for rapid reaction development. **D. Battersby, R. Grainger, M. Gaunt**
- 9:50 ORGN 14.** On-demand electrochemical generation of oxidants and their applications in organic synthesis. **B.J. Deadman, S. Gian, X. Jin, L. Adrio, J. Zhu, K. Helligardt, M. Hii**

- 10:10 ORGN 15.** Shining new light on old reactions: A photocatalyst free, light enabled, Polonovski reaction for amide synthesis. M.P. Walsh, M. Baumann, M.O. Kitching, I.R. Bendanelle
- 10:30 ORGN 16.** Enabling organic synthesis with diazo acetonitrile: Technology and chemistry driven solutions. R.M. Koenigs
- 10:50 ORGN 17.** New synthetic route for the preparation of efavirenz. S. Chada
- 11:10 ORGN 18.** Scale up of continuous process in flow. G. Kai, X. Li

**Section C**

Walter E. Washington Convention Center Room 206

**Catalysis & Computation**

- R. Ruck, E. C. Sherer, *Organizers*  
D. Lehnher, *Presiding*
- 8:00** Introductory Remarks.
- 8:05 ORGN 19.** Insights into catalysis via gas phase methods. J. Lee
- 8:35 ORGN 20.** Computational insights into asymmetric organocatalysis. K.N. Houk
- 9:05 ORGN 21.** Understanding and design of organometallic reactivity with experimental and computational tools. F. Schoenebeck
- 9:35** Intermission.
- 9:50 ORGN 22.** Discovery and optimization of enantioselective catalysis through chemoinformatics. S.E. Denmark
- 10:20 ORGN 23.** Application of computational tools for process chemistry. E.C. Sherer
- 10:50 ORGN 24.** Computation of catalytic processes to guide reaction development including pathways involving dispersion or unpaired electrons. M. Kozlowski
- 11:20 ORGN 25.** Applying modern physical organic analysis tools to prediction in organic chemistry. M.S. Sigman

**Section D**

Walter E. Washington Convention Center Room 207B

**Biologically Related Molecules & Processes**

- R. D. Broene, *Organizer*  
M. A. Bertucci, *Presiding*
- 8:00 ORGN 26.** Isolation, functional evaluation, and total synthesis of Macrophilone A: A biologically active iminoquinone from the marine hydroid *Macrorrhynchia philippina*. W.M. Hewitt, K. Zlotkowski, P. Yan, H.R. Bokesch, M.L. Peach, M.C. Nicklaus, B.R. O'Keefe, J.B. McMahon, K.R. Gustafson, J. Schneekloth
- 8:20 ORGN 27.** Search for secondary structure: Synthesis and characterization of hydrophilic peptides. P.W. Peterson, J.G. Schmidt, R.D. Gilbertson, R.F. Williams, C.E. Strauss
- 8:40 ORGN 28.** New tools for the study of O-GlcNAc transferase in disease. S.E. Martin, Z.W. Tan, H. Itkonen, J. Janetzko, D.Y. Duveau, C.J. Thomas, P. Sliz, M.B. Lazarus, S. Walker
- 9:00 ORGN 29.** Discovery of new heterocycle ligands for a hepatitis C virus RNA switch. W. Frauman, T. Hermann

- 9:20 ORGN 30.** Self-immolative chemiluminescent polymers. S. Gnaim
- 9:40 ORGN 31.** Monitoring of protein interactions in frozen and freeze-dried solution states using small angle scattering techniques. V. Cristiglio, M. Castellanos, J.E. Curtis, I. Grillo, E. Shalav
- 10:00 ORGN 32.** Synthesis of phosphorodiamidate morpholino oligonucleotides and their chimeras using phosphoramidite chemistry. S. Paul, M.H. Caruthers
- 10:20 ORGN 33.** Thiophosphoramidate morpholino: A new class of antisense oligonucleotides. S. Paul, M.H. Caruthers
- 10:40 ORGN 34.** Strain-promoted double-click functionalised stapled peptides for inhibiting protein-protein interactions. K. Sharma, D.R. Spring
- 11:00 ORGN 35.** Harnessing intrinsic reactivity to understand covalent cancer metabolites. R. Kulkarni, T.T. Zengeya, D. Crooks, W. Linehan, J.L. Meier
- 11:20 ORGN 36.** X-Sept: Synthesis of indoxyl septanosides as chromogenic glycosidase substrates. A. Pote, Z. Cannone, A. Planas, M.W. Peczu
- 11:40 ORGN 37.** Experimental evidence of a stabilizing n $\rightarrow$  $\pi^*$  interaction in N-acyl homoserine lactone (AHL) hydrolysis. D. Schmucker, S.R. Dunbar, M.A. Bertucci

**Section E**

Walter E. Washington Convention Center Room 201

**Heterocycles & Aromatics**

- R. D. Broene, *Organizer*  
J. Xu, *Presiding*
- 8:00 ORGN 38.** Catalytic double carbon-boron bond formation for the synthesis of cyclic diarylborinic acids as versatile building blocks for  $\pi$ -extended heteroarenes. T. Igarashi, M. Tobisu, N. Chatani
- 8:20 ORGN 39.** Metal-free regioselective construction of indolin-3-ones via hypervalent iodine oxidation of N-substituted indoles. C. Jiang, C. Yang, G. Cheng, B. Huang, F. Xue
- 8:40 ORGN 40.** Improved synthesis of a nitrogen rich heterocyclic intermediate toward a RORC ligand. J. Xu, L. Sirois, R. Angelaud, D. Lao, F. Gosseil
- 9:00 ORGN 41.** BN heterocycles for molecular diversity. H.L. Van De Wouw, J. Lee, R.S. Klausen
- 9:20 ORGN 42.** Strained alkyne derived from 2,2'-dihydroxy-1,1'-biaryls: Synthesis and copper-free cycloaddition with azides. M. Wills, A. Del Grosso, L. Galanopoulos, C.K. Chiu, G. Clarkson, P.B. O'Connor
- 9:40 ORGN 43.** Biocatalysis meets organolithiums: Asymmetric synthesis of heterocyclic  $\alpha$ -tertiary amines. W. Zawodny, N. Turner, J. Clayden
- 10:00 ORGN 44.** Stereocontrolled synthesis of 2-substituted azetidines and spirocyclic 1,2-diazetidines. A. Pancholi, J. Geden, G. Clarkson, M. Shipman
- 10:20 ORGN 45.** Bisthiourea based efficient synthesis of iminothiazolidinone heterocycles. H. Rafique
- 10:40 ORGN 46.** Revisiting and extending the chemical and functional behavior of benzo[1,2-b:4,5-b']dithiophen-4-ol. A. Sotuyo, K.A. Abboud, I. Ghiviriga, R.K. Castellano

- 11:00 ORGN 47.** Building a library of 2-(hetero)arylchromanones via photoredox catalysis. J.K. Matsui, G.A. Molander
- 11:20 ORGN 48.** Microwave-assisted synthesis of imidazo[4,5-c]quino[lin-2-ones. X. Lu, H. Li, W. Huang

**Section F**

Walter E. Washington Convention Center Rooms 204A/B

**New Reactions & Methodology Alkynes & Rearrangements**

- R. D. Broene, *Organizer*  
Y. Xing, *Presiding*
- 8:20 ORGN 49.** Transition metal accelerated disrotatory 6 $\pi$ -electrocyclization reactions: Isolation of the first hexahapto metal complexes of acyclic conjugated trienes. J.M. O Connor, K.M. Veccharelli, S. Cope, K.K. Baldrige, C. Moore, A.L. Rheingold
- 8:40 ORGN 50.** Eneidyne cycloaromatization with incorporation of a halogen-atom from haloform and a hydrogen-atom from 1,4-cyclohexadiene. J.M. O Connor, D. Hitt, S. Cope, A.G. Raub, K.M. Veccharelli, C. Moore, A.L. Rheingold
- 9:00 ORGN 51.** Unlocking the elusive generation of carbyne equivalents with photoredox catalysis. Z. Wang, A.M. del Hoyo, A.G. Herraiz, M.G. Suero
- 9:20 ORGN 52.** Aryne-mediated metal-free Csp<sup>3</sup>-H bond activation. C. Majeste, F. Idris, G. Craven, C.R. Jones
- 9:40 ORGN 53.** *In situ* generation of iminoketenes from ynamides: Application in cycloadditions. E. Romero, M. Benchekroun, C. Minard, S. Ventre, K. Cariou, R. Dodd
- 10:00 ORGN 54.** Exploration on di-functionalization of alkynes and alkenes. Y. Xing
- 10:20 ORGN 55.** Regioselective reactions of new aryne precursors induced via 1,3-silyl group migration. Y. Kwon, Y. Jeon, W. Kim
- 10:40 ORGN 56.** Transition-metal-free cyclic iminium induced one-pot double annulation cascade: Direct access to dihydroisoquinolinium (DHIQ) based privileged scaffolds. V. Babu, S. Arepally, S.S. Duddu
- 11:00 ORGN 57.** From amino acids to octahydroquinolines: A new, facile and efficient one-pot five-transformation cascade. S. Gallagher Duval, G. Belanger
- 11:20 ORGN 58.** C-H activation and functionalization by Pd(II)/LA catalysts in organic synthesis. G. Yin

**Merck Research Award Symposium**

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

**What do Synthetic Chemists Want from Their Reaction Systems?**

Sponsored by CINF, Cosponsored by COMP, INOR, NUCL and ORGN

**SUNDAY AFTERNOON**

**Section A**

Walter E. Washington Convention Center Room 207A

**Young Investigator Symposium**

J. Aube, *Organizer, Presiding*

- 1:10 ORGN 59.** Next generation RET kinase inhibitor: Improved physicochemical and PK properties enhance local GI tissue distribution. M.P. Demartino, J. Russell, H.S. Eidam, G. Huijping, P.D. Gorycki, D. Rieman, M. Cooper, R. Groseclose, S. Castellino, E. Mohammadi, B. Greenwood-Van Meerveld, A. Oliff, S. Kumar, M. Cheung
- 1:30 ORGN 60.** Discovery of 2-pyridinone aminals: A prodrug strategy to advance a second generation of HIV-1 integrase strand transfer inhibitors. I.T. Raheem
- 1:50 ORGN 61.** Synthesis of active pharmaceutical ingredients (APIs): Difficulties in the synthesis of the parts can be greater than that of the whole. S. Bader
- 2:10 ORGN 62.** Development of a practical synthesis of small molecule intermediate for THIOAB-antibiotic conjugates (TACs). X. Linghu
- 2:30 ORGN 63.** Design and synthesis of novel natural product-inspired eIF4A inhibitors. C. Niewski, G.K. Packard, T.D. Michels, A.X. Xiang, C. Tran, P.A. Sprengeler, J.T. Ernst, S.H. Reich, B. Eam, S. Fish, N.P. Young, J. Chen, P.A. Thompson, K.R. Webster, C.J. Wegerski, A. Nevarez, J. Clarine, S. Sperry
- 2:50 ORGN 64.** Discovery and early enablement of PF-06747775: A next generation irreversible inhibitor of mutant EGFR for the treatment of NSCLC. D. Behenna
- 3:10 ORGN 65.** Design of highly potent allosteric integrase inhibitors. E. Velthuisen
- 3:30 ORGN 66.** Aldehyde oxidase metabolism in drug discovery. A.C. Burns

**Section B**

Walter E. Washington Convention Center Room 202A

**JOC OL Lectureship**

- T. Hanna, *Organizer*  
S. J. Miller, A. B. Smith, *Organizers, Presiding*
- 1:15** Introductory Remarks.
- 1:20 ORGN 67.** Unusual tools for the design of selective cyclization reactions of alkynes. I. Alabugin
- 1:50 ORGN 68.** Functionalization of sp<sup>2</sup> and sp<sup>3</sup> C-H bonds via deprotonative zincation. Q. Wang
- 2:20 ORGN 69.** Iron(III)-catalyzed carbonyl-olefin metathesis. C. Schindler
- 2:50 ORGN 70.** Palladium in peptide/protein synthesis and modification. A. Brik
- 3:20** The Journal of Organic Chemistry Award Presentation.

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or to stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from ACS.

**3:25 ORGN 71.** Industrial and academic applications of high throughput experimentation in reaction optimization. **M. Christensen**

**4:10 ORGN 72.** Nickel-catalyzed alkene hydrosilylation. **I. Buslov, X. Hu**

**4:55** Organic Letters Award Presentation.

**Section C**

Walter E. Washington Convention Center Room 206

**Small Splash, Big Waves: Research at Primarily Undergraduate Institutions**

Financially supported by Shimadzu Corp., Norton Publishing

S. M. Biros, T. A. Davis, Organizers, Presiding

**1:10** Introductory Remarks.

**1:15 ORGN 73.** Synthesis of readily diversified cyclopropyl peptidomimetics as enzyme inhibitors. **N.K. Dunlap**

**1:40 ORGN 74.** Design, synthesis and characterization of starch-functionalized dibromomaleimide for peptide delivery. **J.G. Schellinger**

**2:05 ORGN 75.** Trimethylsilyl trifluoromethanesulfonate as both silylating agent and Lewis acid catalyst in organic reactions new and old. **C.W. Downey**

**2:30 ORGN 76.** Lesson learned about resonance effects and inductive effects: Application of a vinyllogue methodology toward fundamental organic systems. **J.M. Karty**

**2:55** Intermission.

**3:10 ORGN 77.** Microwave-assisted copper-catalyzed amidation of aryl chlorides via concurrent tandem catalysis. **B.P. Clairmont, S. Lin, A.H. Roy MacArthur**

**3:35 ORGN 78.** Effect of ligand and carboxylic acid structure on under air direct arylation reactions. **J.A. Fritz, J. McAfee, L. Armstrong**

**4:00 ORGN 79.** Employing homogeneous gold catalysis to synthesize complex molecular structures. **T.A. Knoerzer, M. Marchioreto, J.L. Mascareñas**

**4:25 ORGN 80.** Synthesis, structure, and properties of supramolecular porphyrin metallocubes. **J.D. Thoburn**

**Section D**

Walter E. Washington Convention Center Room 207B

**Biologically Related Molecules & Processes**

R. D. Broene, Organizer  
D. Bandyopadhyay, Presiding

**1:00 ORGN 81.** Small-molecule organic NIR-II fluorophores for *in vivo* tumor imaging and image-guided surgery. **X. Hong**

**Technical program information known at press time.**

The official technical program for the 254th ACS National Meeting is available at [www.acs.org/WDC2017](http://www.acs.org/WDC2017)

**1:20 ORGN 82.** Probing protein prenyltransferase specificity using metabolic labeling with isoprenoid analogs. **K.F. Suazo, C. Palsuledesai, P. Lange, A. Jeong, C.C. Hsu, C. Schaber, A. Odom John, W.A. Tao, V. Tarakanova, L. Li, M.D. Distefano**

**1:40 ORGN 83.** Probe-guided strategy for selective C-H functionalization and late-stage diversification of the natural product micheliolide via P450-mediated chemoenzymatic synthesis. **H. Alwaseem, S. Giovani, J. Ponder, C.T. Jordan, R. Fasan, M. Crotti**

**2:00 ORGN 84.** Bio-orthogonal metalloporphyrin catalyzed modification of lantibiotics. **R. Maaskant, G. Roelfes**

**2:20 ORGN 85.** Efficient one-pot synthesis of FRET probes for *in vivo* and *in vitro* detection of redox homeostasis in cell. **Y. Li, T. Wang**

**2:40 ORGN 86.** Synthesis of oligosaccharides via construction of non-glycosidic linkages. **S. Truong, D.R. Mootoo**

**3:00 ORGN 87.** Chemical tools for carbonyl sulfide (COS) and hydrogen sulfide (H<sub>2</sub>S) delivery. **M.D. Pluth**

**3:20 ORGN 88.** Structural tuning of cyanine fluorophores for mitochondria and lysosome targeting: Highly selective series of fluorescent probes. **C.S. Abeywickrama, H.J. Baumann, L. McDonald, D. Dahal, F. Gombedza, N. Alexander, C. Wesdemiotis, M. Konopka, L. Shriver, S.M. Paruchuri, Y. Pang**

**3:40 ORGN 89.** Synthesis of novel flavonoid based dyes and their potential applications in zebrafish and eukaryotic cell imaging. **L. McDonald, B. Liu, F. Gombedza, A. Taraboletti, Q. Liu, Y. Pang**

**4:00 ORGN 90.** First synthesis of quaternary,  $\alpha$ -(1'-fluoro)vinyl amino acids via formal fluorovinylolation of AA enolates: A new class of potential mechanism-based PLP enzyme inactivators. **C.D. McCune, M.L. Beio, J.M. Sturdivant, R. de la Salud-Bea, B.M. Darnell, D.B. Berkowitz**

**4:20 ORGN 91.** Fluorescent sensors for lipids. **T.E. Glass, C.W. Littlefield, C. Ren, M. Xu**

**Section E**

Walter E. Washington Convention Center Room 201

**Heterocycles & Aromatics**

R. D. Broene, Organizer  
R. J. Hinkle, Presiding

**1:10 ORGN 92.** Gram scale synthesis of a  $\beta$ -secretase 1 (BACE 1) inhibitor. **B.D. Allison**

**1:30 ORGN 93.** Synthesis of novel ligands for platinum drugs. **A. Fraeyman, W. Jones, C.S. Chow, K.J. Friedrich**

**1:50 ORGN 94.** Synthesis of electronically diverse pyridine-triazoles: Structure and catalytic activity of corresponding palladium(II) complexes in Suzuki-Miyaura coupling reactions. **Z.L. Palchak, M.D. Sterling, C.H. Larsen**

**2:10 ORGN 95.** BODIPY-bacteriochlorin energy transfer arrays with tunable absorption and near-infrared emission. **A. Meares, A. Satraitis, M. Ptaszek**

**2:30 ORGN 96.** Direct access to highly functionalized heterocycles through the condensation of cyclic imines and  $\alpha$ -oxoesters. **A.Q. Cusumano, J.G. Pierce**

**2:50 ORGN 97.** Synthetic strategy for rapid access to *bis*(phenalenyl)-based polycyclic aromatic hydrocarbons. **M.S. Chen, C.M. Wehrmann**

**3:10 ORGN 98.** Synthesis of heterocycles driven by auto-tandem catalysis with acid catalysts. **G. Yanlong**

**3:30 ORGN 99.** Asymmetric synthesis of homoallylic amines for construction of substituted piperidines. **M.G. Donahue**

**3:50 ORGN 100.** Efficient preparation of oxazoles from 6-amino-5,6-dihydro-1,10-phenanthroline-5-ol derivatives. **E. Schoffers, D.L. Sellers, L. Kohler**

**4:10 ORGN 101.** Double palladium-catalyzed reductive N-heterocyclization: Synthesis of pyrroloindoles. **N.H. Ansari, M. Cummings, C.A. Dacko, B. Soderberg**

**4:30 ORGN 102.** Electronic effects in domino reactions toward tricyclic 1,4-dihydro-2H-benzof[*f*]isochromenes: Concerted alkylnyl-Prins and Friedel-Crafts reactions. **R.J. Hinkle, Y. Chen, S. Lewis, C. Nofi**

**Section F**

Walter E. Washington Convention Center Rooms 204A/B

**New Reactions & Methodology**

**Main Group**

R. D. Broene, Organizer  
S. D. Townsend, Presiding

**1:20 ORGN 103.** Sequential diboration/allylation/cross-coupling: A powerful method for diastereoselective carbocycle synthesis. **J.D. Shields, M. Eno, W.K. Chang, J.P. Morken**

**1:40 ORGN 104.** Chemoselective oxidation of aryl organoboron systems enabled by boronic acid-selective phase transfer. **J. molloy, A.J. Watson**

**2:00 ORGN 105.** Substrate-assisted, transition metal-free diboration of alkynamides with an unsymmetrical diboron reagent. **F. Astha, R. Snead, Y. Dai, C. Slebodnick, Y. Yang, H. Yu, F. Yao, W. Santos**

**2:20 ORGN 106.** Boronic acid catalyzed direct and ambient Beckmann rearrangement of oximes. **X. Mo, T.D. Morgan, D.G. Hall**

**2:40 ORGN 107.** Synthesis of tri-substituted alkenyl boronic esters: A second-generation boryl-Heck reaction. **W.B. Reid, D.A. Watson**

**3:00 ORGN 108.** Frustrated Lewis pair hydrogenation of a,b-unsaturated carbonyl compounds. **I. Khan, L. Morrill**

**3:20 ORGN 109.** Uncatalyzed 1,2-carboration of seven-membered-ring trans-alkenes. **J.R. Sanzone, K.A. Woerpel**

**3:40 ORGN 110.** Metal-free synthesis of unsymmetrical aryl, di-aryl, and glycosyl organoselenides. **S.D. Townsend**

**4:00 ORGN 111.** Progress towards the development of novel hypervalent iodine reactions. **I.D. Hyatt**

**4:20 ORGN 112.** Decoupling the Arrhenius equation via mechanochemistry. **J.M. Andersen, J. Mack**

**4:40 ORGN 113.** Synthesis of diverse imidazolindiones through a unified approach. **F. Xu, S. Shuler, D.A. Watson**

**5:00 ORGN 114.** Fluorinated diazoalkanes and beyond. **R.M. Koenigs**

**Science Communications: The Art of Developing a Clear Message**

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**What do Synthetic Chemists Want from Their Reaction Systems?**

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**SUNDAY EVENING**

**Section A**

Walter E. Washington Convention Center Hall D

**Asymmetric Reactions & Syntheses**

S. M. Silverman, Organizer

**5:30 - 7:30**

**ORGN 115.** Carbometallation/oxidation of cyclopropenes: An oasis of diastereomerically and enantiomerically enriched cyclopropanols and aldehydes possessing quaternary carbon stereocenters. **M. Simaan, I. Marek**

**ORGN 116.** Asymmetric autoinduction in the copper/phosphine catalyzed alkylation of carbonyl compounds. **T. Pellegrini, A.J. Minnaard, S.R. Harutyunyan**

**ORGN 117.** Exploitation of antagonistic electronic densities for the stereoselective reduction of ketones bearing masked amino surrogates. **R. Chew, M. Willis**

**ORGN 118.** Enantioselective synthesis of fluoro-dihydroquinazolones and -benzooxazinones by fluorination-initiated asymmetric cyclization reactions. **K. Hiramatsu, T. Honjo, V. Rauniyar, D. Toste**

**ORGN 119.** Exploitation of enantiomerically pure  $\alpha$ -trifluoromethyl  $\alpha$ -amino acids and conformational studies of their L-leucine-based peptides. **A. Ueda, T. Kasae, M. Oba, M. Doi, M. Tanaka**

**ORGN 120.** Stereoselective O-H insertion of  $\alpha$ -benzyl diazoesters by carboxylic acids activated by chiral oxazaborolidinium ion. **K. Kang, S. Kim, D. Ryu**

**ORGN 121.** Improvement of organocatalytic Robinson annulation by acid additives. **R. Fallek, Y. Shiloni, M. Portnoy**

**ORGN 122.** One-pot synthesis of perylene tetracarboxylic diester monoanhydride with labile substituents. **X. Zhao, B. Wang, H. Zhang, S. Jin**

**ORGN 123.** Withdrawn.

**ORGN 124.** Asymmetric Michael addition reactions catalyzed by alpha, alpha-disubstituted alpha-amino acid-containing helical peptides. **T. Umeno, A. Ueda, M. Doi, M. Tanaka**

**ORGN 125.** Enantioselective organocatalytic addition of carbon and sulfur nucleophiles to trisubstituted nitroalkenes via enantioselective protonation. **J. Phelan**

**ORGN 126.** 1-Hydrosilatane: A chiral Lewis base activated reducing agent for the asymmetric reduction of prochiral ketones to alcohols. **S. Varjosaaari, V. Skrypai, T.M. Gilbert, M.J. Adler**

**ORGN 127.** Stereoselective Lewis-base catalyzed TMSCF<sub>3</sub> additions of 2-halogenated carbonyls. **T.A. Davis, S. Rouleau, K. Russell, N. Heth**

†Cooperative Cosponsorship

- ORGN **128.** Stereodiverse synthesis of chiral aryl fluoroalkyl sulfones, from a single chiral precursor. **W. Wei**, R.K. Khangarot, L. Stahl, P. Pradhan, C. Veresmortean, B. Zajc
- ORGN **129.** Ni(II)-diamine complexes catalyzed asymmetric sequential Michael reactions of vinylketoesters and nitroalkenes for the synthesis of multifunctionalized cyclohexene derivatives. **B. Ni**, S. Huang
- ORGN **130.** Green direct reductive aminations using 1-hydrosilatane. **V. Skrypai**, S. Varjosaari, T.M. Gilbert, M.J. Adler
- ORGN **131.** Mechanistic investigation of reactions of rhodium(II) azavinyl carbenes. **J. Li**, J. Celajce, V.V. Fokin

**Section B**

Walter E. Washington Convention Center Hall D

**CH Activation**

S. M. Silverman, *Organizer*

5:30 - 7:30

- ORGN **132.** Exploring biosynthetic P450s as biocatalysts for multi-functional C-H oxidation. **J.L. Stachowski**, M. Demars, D.H. Sherman, J. Montgomery
- ORGN **133.** Chelation-directed amidation of aryl ketones using a heterogeneous Pd(II)-catalyzed C-H activation method. **Y. Timsina**, M. Burkholder, F. Gupton, K.C. Ellis
- ORGN **134.** Bridging C-H activation: Mild and versatile cleavage of the 8-aminoquinoline directing group. **M. Berger**, R. Chauhan, C. Rodrigues, N. Maulide
- ORGN **135.** Design and syntheses of scaffold and pincer catalysts. **A.A. Oppong**, B.L. DeBoef
- ORGN **136.** Iodine-catalyzed oxidative cyclizations for the construction of thienocarbazole derivatives. **A. Kivrak**, H. Koca
- ORGN **137.** Chemistry in water: Radical reactions of ketones using Fenton's reagent. **J.L. Meyer**, A. Duell, K.M. Baker, K.B. Mapeis, R.P. Hotz, A.R. Pinhas
- ORGN **138.** Copper catalyzed functionalization of un-activated sp<sup>3</sup> C-H bonds via carbon-carbon bond formation. **O.E. Okoromoba**, T.H. Warren
- ORGN **139.** Intramolecular C-H functionalization for the synthesis of structurally unique triazole-fused vinyl sulfams. **A. Cassity**, J. Jun, N.M. Windmon, N. Asad, A. Diepenbrock, C.D. Clay, P.R. Hanson
- ORGN **140.** Amide-directed alkane C-H borylation reactions. **S.N. Hyland**, M. Tortosa, T.B. Clark

**Section C**

Walter E. Washington Convention Center Hall D

**Metal-Mediated Reactions & Syntheses**

S. M. Silverman, *Organizer*

5:30 - 7:30

- ORGN **141.** Asymmetric catalysis of ketone reduction using ruthenium and iron-based catalysts. **M. Willis**, T. Hall, A. Del Grosso, Z. Fang, R. Hodgkinson
- ORGN **142.** Efficient and selective palladium-catalyzed direct aerobic oxidation of alcohols to esters. **Y. Hu**, B. Li

- ORGN **143.** High-throughput transition metal-catalyzed chemistry workflows at Pfizer. **J. Magano**, S. Monfette, N. Thomson
- ORGN **144.** Studies towards the total synthesis of trocheliophorolide A: A unique effort toward a one-pot hydroboration cyclization protocol. **K. Houghtling**, D. Verrico, T.G. Goudreau Collison, H.M. Simpson
- ORGN **145.** Synthesis of gold clusters with PNNP ligands. **J. Yang**, A.M. Echavarren
- ORGN **146.** Towards novel perfluoroalkylation of arenes. **K. Suppan**
- ORGN **147.** Rhodium(I)-complexes catalyzed 1,4-conjugate addition of arylzinc chlorides to N-boc-4-pyrindone. **M. Jeffries**, B. Graves, S. Graham, F. Guo
- ORGN **148.** Michael-Michael ring closing reactions promoted by TpMo(NC)(DMAP)(η<sup>2</sup>-naphthalene). **J.T. Myers**, M. Sabat, W.H. Myers, W.D. Harman
- ORGN **149.** Developing a modular synthesis of Eumelanin oligomers. **A.H. Aebly**, J.M. Belitsky
- ORGN **150.** Synthesis of small functionalized molecules using copper-catalyzed atom transfer radical addition (ATRA) and [3+2] azide-alkyne cycloaddition (CuAAC). **S. Fischer**, M. Baldwin, T. Pintauer
- ORGN **151.** Aluminum (III)-catalyzed synthesis of symmetrical Schiff base for aluminum sensor. **L. McDonald**, J. Wang, Y. Pang
- ORGN **152.** Sequential tandem addition reactions to a tungsten-trifluorotoluene complex. **K.B. Wilson**, J.T. Myers, M. Sabat, W.D. Harman
- ORGN **153.** Titanium-proline derived system for the asymmetric synthesis of propargyl alcohols. **C. Sweet**, D. Moustafa, P. Kaur
- ORGN **154.** Toward (Z)-selective alkene isomerization catalysts and potential anti-cancer agents. **E. Delgado**, E.R. Paulson, D.B. Grotjahn
- ORGN **155.** Dirhodium-mediated transfer of carbamate-derived nitrenes for aziridination-ring opening: A study on optimization and substrate scope. **E.C. McLaughlin**, M. Lasky, C.P. Anyanwu

**Section D**

Walter E. Washington Convention Center Hall D

**Peptides, Proteins & Amino Acids**

S. M. Silverman, *Organizer*

5:30 - 7:30

- ORGN **156.** Synthesis and conformational analyses of stapled peptides derived from allyl-tethered carbocyclic α,α-disubstituted α-amino acids. **K. Hirayama**, A. Ueda, M. Doi, M. Tanaka
- ORGN **157.** Characterizing proteins using SAXS on a hybrid laboratory x-ray scattering instrument. **J.E. Quinn**, N. Dadivanyan, A. Schierbeek, J. Bolze
- ORGN **158.** Thioamides: Improved incorporation methods and effects on protein stability. **D. Szantai-Kis**, C.R. Walters, T. Barrett, E. Petersson
- ORGN **159.** Synthesis and conformational analyses of peptides having α,α-disubstituted α-amino acids with (-)-menthyl skeleton. **A. Ueda**, S. Matsumoto, M. Doi, M. Tanaka
- ORGN **160.** Withdrawn.

- ORGN **161.** Development of a peptide library based on naturally occurring proteins from North American opossum (*Didelphis virginiana*) as potential inhibitors of snake venom metalloproteinases. **R.M. Werner**, J.M. Wickens, D. Webber
- ORGN **162.** Chiroptical sensing of cysteine in complex mixtures. **F.Y. Thanzeel**, C. Wolf
- ORGN **163.** Role of disulfide linkages in the folding and activity of scyllatoxin-based BH3 domain mimetics. **D.M. Berugoda Arachchige**, M. Harris, Z. Coon, J. Carlsen, J.M. Holub
- ORGN **164.** Spiro-cyclopropane type α-helix/β-strand mimetics targeting protein-protein interactions. **T. Kuwahara**, A. Mizuno, H. Fukuda, M. Watanabe, S. Shuto
- ORGN **165.** Small antimicrobial agents based on acylated reduced amide scaffold. **P. Teng**, J. Cai
- ORGN **166.** Helical 1:1 α/sulfono-γ-AA heterogeneous peptides with antibacterial activity. **F. She**, A. Nimmagadda, P. Teng, M. Su, X. Zuo, J. Cai
- ORGN **167.** High-throughput cyclic γ-AAPeptides screening library against EPHA2. **Y. Shi**, J. Cai
- ORGN **168.** Solid-phase synthesis of various peptoid structures. **S. Kim**, J. Song, H. Lim, Y. Kwon
- ORGN **169.** Conformational ensemble calculations of proteolytically stable β-hairpins containing bulky α,β-dehydroamino acids. **D. Kastner**, A. Jalan, S.L. Castle
- ORGN **170.** Development of a biaryl oxidative coupling-based route to the anti-tumor natural products TMC-95. **S. Burgeson**, E. Martin, L. Sanchez
- ORGN **171.** Alternative strategies for purification of fully protected peptides using flash chromatography. **E. Denton**, J.R. Bickler

**Section E**

Walter E. Washington Convention Center Hall D

**Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species**

S. M. Silverman, *Organizer*

5:30 - 7:30

- ORGN **172.** High performance nitrogen dioxide sensor based on organic field-effect transistor utilizing ultrathin CuPc/PTCDI-C8 heterojunction. **H. Fan**, J. Yu
- ORGN **173.** Mechanism of hydrolysis reactions of 2,2-disubstituted silo- and germocanes, 1-substituted sila- and germatranes. **Y.A. Vereshchagina**, D. Chachkov, R. Khanafieva, E. Ishmaeva
- ORGN **174.** Neighboring group participation in disulfide oxidation. **K. Fukuta**, T. Yamamoto, Y. Esaka, B. Uno
- ORGN **175.** Computational study on the stereospecific cross-coupling reactions of anomeric stannanes for the synthesis of C-aryl glycosides. **I. Kevlishvili**, P. Liu, M.A. Walczak, F. Zhu, T. Yang
- ORGN **176.** NMR spectroscopic studies for the behaviors of carbonyl compounds in various solvents. **S. Niwayama**, Y. Hiraga, S. Chaki

- ORGN **177.** Rh-catalyzed intramolecular C-H insertion reactions: Important considerations for controlling side products. **S.R. Hare**, D. Tantillo
- ORGN **178.** Analyzing the binding relationship between curcuminoids and HSA by steady state fluorescence spectroscopy. **O. Michels**, G.J. Myres
- ORGN **179.** Photoinduced bacterial inactivation by azosulfones. **R. Viswanathan**, S. Zachariah, S. Protti, M. Fagnoni, **A. Greer**
- ORGN **180.** Effect of irradiance on singlet oxygen generation and photobleaching of photosensitizer molecules immobilized on silica surfaces. **G. Ghoshi**, Y. Liu, A. Lyons, **A. Greer**
- ORGN **181.** Evidence for peroxide intermediates in intralipid photooxidations from 31P and 1H NMR studies: Implications for lipid peroxidations, photodynamic therapy, and tissue-simulating phantoms. **P.P. Mohapatra**, C. Chiemezie, A. Kligman, M. Kim, T. Zhu, **A. Greer**
- ORGN **182.** Sensitized photooxidations of mono-, di-, and tri prenylated phloroglucinol derivatives. **P.P. Mohapatra**, **A. Greer**
- ORGN **183.** Computational analysis of substitution effects on oxyluciferin and its analogues. **V.B. Satalkar**, E. Benassi, **Y. Shao**
- ORGN **184.** Combination calculation with experiment: Nitration mechanism for the one pot synthesis of 1-methyl-3,4,5-trinitropropyrazole. **Y. Xu**, C. Shen, P. Wang, M. Lu
- ORGN **185.** Synthesis of borazines derived from 1,2-aminoalcohols. **M. De Jesus**, M. Ortiz-Marciales
- ORGN **186.** Docking studies on novel 1-benzazepine analogues as potential multi-target drugs for the treatment of Alzheimer's disease. **C. Garcia**, S. Espinosa-Diaz, S. Ortiz, M. Ortiz-Marciales
- ORGN **187.** Lysosomes targeting probes with large Stokes' shifts via cyanine coupling with excited state intramolecular proton transfer (ESIPT). **D. Dahal**, L. McDonald, Y. Pang
- ORGN **188.** Realizing Aza Paternò-Büchi reaction. **S.K. Kandappa**, E. Kumarasamy, R. Raghunathan, S. Jockusch, J. Sivaguru
- ORGN **189.** Photoene vs. [2+2] photocycloaddition: A case study involving maleimides and alkenes. **S. Ahuja**, J. Sivaguru
- ORGN **190.** Bis-acetyl carbazole: Photoremovable protecting group for sequential release of two different functional groups and its application for therapeutic release. **Y. Venkatesh**, N. Pradeep Singh

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**ORGN 191.** Decarboxylation rates determined by measurement of dissolved CO<sub>2</sub>. **A. Campanella, M.D. Mosher**

**ORGN 192.** Synergy between solvation and aromatic substituent effects in CH-aryl interactions. **B.U. Emenike, R. Spinelle, A. Rosario**

**ORGN 193.** Controlling intramolecular [2+2] photocycloaddition of enones by axial chirality. **A. Clay**

**MONDAY MORNING**

**Section A**

Walter E. Washington Convention Center Room 207A

**Robert Burns Woodward Centennial Symposium**

P. A. Jacobi, R. M. Williams, *Organizers*  
P. N. Confalone, *Organizer, Presiding*

**8:30 ORGN 194.** R. B. Woodward: A larger-than-life chemist. **J. Seeman**

**9:30 ORGN 195.** Building bridges: Strategies and tactics for the synthesis of polycyclic natural products. **S.E. Reisman**

**10:30 ORGN 196.** Robert Burns Woodward: Bridging art and science. **C. Woodward**

**Section B**

Walter E. Washington Convention Center Rooms 202A/B

**Organometallics Distinguished Author Award**

P. J. Chirik, *Organizer, Presiding*

**9:00** Introductory Remarks.

**9:05 ORGN 197.** Design and application of 3,4-diazaphospholane ligands for enantioselective hydroformylation. **C.R. Landis, J. Wildt, J. Eshon, A.C. Brezny**

**9:40 ORGN 198.** Ti-catalyzed nitrene transfer reactions. **I. Tonks**

**10:15** Intermission.

**10:30 ORGN 199.** Catalytic  $\alpha$ -C-H alkylation of secondary amines: No directing auxiliary? No problem. **L. Schafer**

**11:05 ORGN 200.** New developments in the organometallic chemistry of high valent nickel. **M.S. Sanford**

**Section C**

Walter E. Washington Convention Center Room 206

**Modern Chemistry of the Amide Bond**

J. Aube, *Organizer, Presiding*

**8:10** Introductory Remarks.

**8:20 ORGN 201.** Testing delocalization of the nitrogen lone pair in bridgehead bicyclic lactams. **A. Greenberg**

**Technical program information known at press time. The official technical program for the 254th ACS National Meeting is available at [www.acs.org/WDC2017](http://www.acs.org/WDC2017)**

**9:00 ORGN 202.** Twists and turns of lactam research. **B.M. Stoltz**

**9:40 ORGN 203.** Twisted-amide mechanism of Pin1. **F.A. Etkorn**

**10:20 ORGN 204.** Cross-coupling of amides by N-C activation. **M. Szostak**

**11:00 ORGN 205.** Breaking amides using nickel catalysis. **N.K. Garg**

**Section D**

Walter E. Washington Convention Center Room 207B

**Biologically Related Molecules & Processes**

R. D. Broene, *Organizer*

L. J. Perez, *Presiding*

**8:00 ORGN 206.** Synthesis of oligodeoxynucleotides containing electrophilic groups using 1, 3-dithiane-2-yl-methoxycarbonyl (Dmoc) protection. **B. Halami, X. Lin, J. Chen, S. Shahsavari, N. Green, D. Goel, S. Fang**

**8:20 ORGN 207.** Truncated analogs of actin-targeting natural products: Synthesis and *in vitro* activity. **R.L. Grange, J.S. Allingham, A.W. Craig, P. Evans, S. Nersesian, D. Trofimova, R. Williams, J. Zhou**

**8:40 ORGN 208.** Design, synthesis, and antiviral evaluation of aryl and biaryl  $\alpha$ -hydroxytropolones against herpes simplex virus -1 and -2. **A. Garimalla, L. Morrison, B. Patel, S. Hoyt, S. Datla, J. Tavis, R.P. Murelli**

**9:00 ORGN 209.** Optochemical control of protein dimerization in living cells. **C. Aonbangkhen, H. Zhang, M. Lampson, D.M. Chenoweth**

**9:20 ORGN 210.** Synthesis of dimeric lysosomal inhibitors and their evaluation as anticancer agents. **M. Nicastri, J.D. Winkler, R. Amaravadi, V. Rebecca**

**9:40 ORGN 211.** Protein engineering for combinatorial synthesis: Rational design of a biocatalyst to enable a novel preparation of blockbuster statin drugs. **K. Belecki**

**10:00 ORGN 212.** Vitamin B2 related molecules that activate T cells. **J.Y. Mak, W. Xu, R.C. Reid, A.J. Corbett, B.S. Meehan, H. Wang, Z. Chen, J. Rossjohn, J. McCluskey, L. Liu, D.P. Fairlie**

**10:20 ORGN 213.** Genetic code and putative messages. **J. DeMassa**

**10:40 ORGN 214.** Sulfurization agents as capping reagents for phosphorothioate oligonucleotide synthesis. **J. Yang**

**11:00 ORGN 215.** Chemical signaling in *Pseudomonas aeruginosa* and design of species-specific inhibitors of this bacteria. **L.J. Perez**

**Section E**

Walter E. Washington Convention Center Room 201

**Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species**

R. D. Broene, *Organizer*

G. O. Jones, *Presiding*

**8:10 ORGN 216.** Photooxidative crosslinking and photoaffinity labeling of proteins with naphthalene imides and diimides. **S. Sova, L. Kelly**

**8:30 ORGN 217.** Photophysical & photoacoustic properties of dimethyl-amino terminated curcuminoid dyes containing the phenyl, naphthyl and thienyl  $\pi$ -spacers. **R.E. Borg, J.J. Rochford**

**8:50 ORGN 218.** Photochemical expulsion of leaving groups from a naphthothio-phenene-2-carboxamide anilide linked to a chromophore by a flexible polymethylene chain. **L. Li, G. Ndzaidze, M.G. Steinmetz**

**9:10 ORGN 219.** Photoreactions with a twist: Employing restricted bond rotations for controlling excited state transformations. **J. Sivaguru**

**9:30 ORGN 220.** Wavelength dependent rate acceleration in hybrid "photoisomerization-Bronsted acid catalysis". **J. Hioe, P. Renzi, G. Ruth Maria**

**9:50 ORGN 221.** Photophysics of naphthalene dimers controlled by the sulfur bridge oxidation. **C. Climent, D. Casanova**

**10:10 ORGN 222.** Chemistry of fingerprint visualization: New insights in the initiating step of the ethyl-2-cyanoacrylate polymerization reaction. **S.C. van der Lubbe, R. de Jong, F. Loadsman-Wammes, C. Fonseca Guerra, F. Bickelhaupt, M.A. van Bochove**

**10:30 ORGN 223.** Substituent effect on stability for rubrene analogues. **J.T. Ly, S. Thomas, M. Yamashita, H. Yamada, J.E. Bredas, L. Zhang, A.L. Briseno**

**10:50 ORGN 224.** Tuning the photochemical and redox properties of ethyl-flavinium ion. **B.D. Etz, S. Vyas**

**11:10 ORGN 225.** Evaluating stereospecificity of metal free visible light mediated acyl-migration. **A. Clay**

**11:30 ORGN 226.** Toward the origin of small chemical shift differences in diastereotopic X-CH<sub>2</sub>D groups. **O. Ogba, S. Elliott, D. Kolin, L.J. Brown, S. Cevallos, S. Sawyer, M. Levitt, D.J. O'Leary**

**Section F**

Walter E. Washington Convention Center Rooms 204A/B

**New Reactions & Methodology**

**Metals**

R. D. Broene, *Organizer*

V. W. Shurtleff, *Presiding*

**8:00 ORGN 227.** Electrochemical methods for Ni-catalyzed sp<sup>2</sup>-sp<sup>3</sup> cross-couplings. **R.J. Perkins**

**8:20 ORGN 228.** Synthesis of selectively difluorinated carbocycles through a novel gold(I) catalyzed cyclisation. **A. McCarter, C. Jamieson, J. Percy, D. Hirst**

**8:40 ORGN 229.** Construction of 1-heteroaryl-3-azabicyclo[3.1.0]hexanes by sp<sup>2</sup>-sp<sup>2</sup> Suzuki-Miyaura and Chan-Evans-Lam coupling reactions of tertiary trifluoroborates. **M. Harris, Q. Li, Y. Lian, J. Xiao, A.T. Londregan**

**9:00 ORGN 230.** Applications of light-gated cobalt catalysis to a [2+2+2] cycloaddition polymerization. **B. Ravetz, K.E. Ruhl, T. Rovis**

**9:20 ORGN 231.** Cobalt-catalyzed asymmetric hydroboration of prochiral 1,3-dienes. **K. Duvvuri, K.R. Dewese, T. RajanBabu**

**9:40 ORGN 232.** Palladium catalyzed decarboxylation of polyenoic acids. **M.H. Alhunit, M. Garr, M.P. Croatt**

**10:00 ORGN 233.** SmCpR<sub>2</sub>-mediated coupling of allyl and propargyl ethers with ketesters and a one-pot approach to complex cycloheptanols. **M. Plesniak, X. Just-Baringo, F. Ortu, D. Mills, D. Procter**

**10:20 ORGN 234.** Ni-catalyzed oxidative decarboxylative arylation of unactivated C-H bonds with (hetero)aryl benzoates. **A.P. Honeycutt, J.M. Hoover**

**10:40 ORGN 235.** Rhodium-catalyzed [(3+2)+1] carbocyclization reactions of alkynylidene cyclopropanes with carbon monoxide: Construction of polysubstituted dienones. **A. Burnie, P. Evans**

**11:00 ORGN 236.** Development of practical methods for tantalum-catalyzed hydroaminoalkylation. **P.M. Edwards, L. Schafer**

**11:20 ORGN 237.** Mechanistic investigation of reactions of 1-iodoaryl alkynes with organic azides in the copper (I)-catalyzed cycloaddition reaction. **A. Nazarova, V.V. Fokin**

**11:40 ORGN 238.** Reductive conversion of acyclic esters to ethers using ReactIR. **J.A. Pigza**

**Building a Safety Culture across the Chemistry Enterprise**

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**MONDAY AFTERNOON**

**Section A**

Walter E. Washington Convention Center Room 207A

**Robert Burns Woodward Centennial Symposium**

P. N. Confalone, R. M. Williams, *Organizers*  
P. A. Jacobi, *Organizer, Presiding*

**1:00 ORGN 239.** R. B. Woodward's insights into theory and mechanism. **K.N. Houk**

**2:00 ORGN 240.** Development of organocatalytic and photoredox catalyzed reactions. **D.W. MacMillan**

**3:00 ORGN 241.** Withdrawn.

**4:00 ORGN 242.** Working with Woodward. **R. Hoffmann**

**Section B**

Walter E. Washington Convention Center Rooms 202A/B

**Tetrahedron Prize for Creativity in Organic Chemistry Symposium**

*Financially supported by Elsevier*

S. F. Martin, *Organizer*

J. L. Wood, *Presiding*

**1:10** Introductory Remarks.

**1:15 ORGN 243.** Rise and promise of the mechanical bond in chemistry and beyond. **C. Pezzato, M.T. Nguyen, C. Cheng, J.F. Stoddart**

**2:05 ORGN 244.** New stereoselective, catalytic fluorination reactions. **E.N. Jacobsen**

†Cooperative Cosponsorship

**2:55 ORGN 245.** Hydrogel-actuated integrated responsive systems (HAIRS): Moving towards adaptive, homeostatic materials. J. Aizenberg

**3:45** Introduction of Awardee.

**3:55 ORGN 246.** Designing dynamic molecular systems: From switches to motors. B. Feringa

**4:55** Concluding Remarks.

### Section C

Walter E. Washington Convention Center  
Room 206

#### Cross-Electrophile Coupling

Financially supported by Pfizer, Novartis, Boehringer-Ingelheim

E. R. Jarvo, *Organizer*

D. J. Weix, *Organizer, Presiding*

**1:20 ORGN 247.** Enantioselective Ni-catalyzed cross-electrophile coupling. S.E. Reisman

**2:00 ORGN 248.** Nickel-catalyzed stereospecific reductive cross-electrophile coupling reactions. E.R. Jarvo

**2:40 ORGN 249.** Controlling selectivity and reactivity in nickel-catalyzed cross electrophile couplings. E.C. Hansen

**3:20 ORGN 250.** Cross-electrophile coupling of tertiary alkyl halides with other electrophiles. H. Gong

**4:00 ORGN 251.** Cross-electrophile coupling of challenging substrates. D.J. Weix

**4:40 ORGN 252.** Cobalt: A versatile catalyst to promote reductive cross-coupling reactions. C. Gosmini

### Section D

Walter E. Washington Convention Center  
Room 207B

#### Asymmetric Reactions & Syntheses

##### Miscellaneous

R. D. Broene, *Organizer*

Y. Yang, *Presiding*

**1:20 ORGN 253.** Developing chemical tools for accessing indolizidine alkaloids from dendrobatid frogs: Synthetic versatility of  $\alpha$ -methyl 2, 3-dihydropyridinones in building polyfunctional piperidines. Y. Yang

**1:40 ORGN 254.** Studies directed towards the synthesis of a sparteine surrogate. T.F. Higgins, J.D. Winkler

**2:00 ORGN 255.** Enantioselective total synthesis of cycloclavine. S.R. McCabe, P. Wipf

**2:20 ORGN 256.** Asymmetric synthesis of a HCV nucleoside cyclic prodrug. Y. Zhong, E. Cleator, Z. Liu, J. Yin, W. Morris, M. Alam, B. Bishop, A. Dumas, J. Edwards, A. Goodyear, P. Mullens, M. Shevlin, Z. Song, D. Thairisvongs, H. Li, R. Cohen, J. Yin, L. Tan, N. Yasuda, J. Limanto, P. Bulger, A. Davies, K.R. Campos

**2:40 ORGN 257.** Development of new Lewis-acid catalyzed methods for organic synthesis. P.S. Riehl, C. Schindler

**3:00 ORGN 258.** Asymmetric catalytic reactions: Recent use of TOX and SaBOX ligands. Y. Tang

**3:20 ORGN 259.** High-throughput phase-transfer catalyst synthesis and evaluation coupled with QSAR modeling as enabling tools for efficient catalyst optimization. K.M. Belyk, K. Lexa, E.C. Sherer, R. Ruck

**3:40 ORGN 260.** Metal-free stereospecific isomerization of electron-deficient allylic alcohols and allylic ethers. S. Martinez Erro, A. Sanz-Marco, A. Bermejo Gómez, A. Vázquez-Romero, M.S. Ahlquist, B. Martín-Matute

**4:00 ORGN 261.** H<sub>2</sub>PO<sub>2</sub>-catalyzed intramolecular stereospecific nucleophilic substitution of the hydroxyl group in stereogenic alcohols. A. Bunrit, R.A. Watile, C. Dahlstrand, S. Olsson, P. Srita, G. Huang, S. Biswas, F. Hirao, J.S. Samec

### Section E

Walter E. Washington Convention Center  
Room 201

#### Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

R. D. Broene, *Organizer*

H. Banks, *Presiding*

**1:00 ORGN 262.** Chemistry at the edges of doped graphenes: A computational study. H. Banks

**1:20 ORGN 263.** Exploring energetics in dirhodium paddle-wheel complexes with  $\pi$ -donors of different topologies. J. Li, A.Y. Rogachev

**1:40 ORGN 264.** Solving the density functional conundrum: Elimination of systematic errors to derive highly accurate reaction enthalpies of complex organic reactions. A. Sengupta, K. Raghavachari

**2:00 ORGN 265.** Conformational preferences and anomeric effect in light of attractive Coulomb interactions. M.J. Schmittl, A. Rana

**2:20 ORGN 266.** Theoretical studies on ring-opening polymerizations by alkoxides and (thio)ureas. G.O. Jones, X. Zhang, B. Lin, J. Hedrick, R.M. Waymouth

**2:40 ORGN 267.** Computational studies on the Z- and E-selective molybdenum catalysts for olefin metathesis. X. Dong, K.N. Houk

**3:00 ORGN 268.** Reductive desulfurization of thionated naphthalene diimides: Isolation of a new naphthalene derivative depicting attractive photophysical and electrochemical properties. A.J. Aytou

**3:20 ORGN 269.** Excited state equilibria and geometrical effects during fluorescence quenching of sterically-graded pyrenes by tertiary aliphatic amines and N,N-dialkylanilines. M.J. Bertocchi, R.G. Weiss, J. Moorthy, X. Zhang, A. Bajpai

**3:40 ORGN 270.** Mechanistic studies of samarium diiodide (SmI<sub>2</sub>) - amine complexes. C. Bartulovich, S. Maity, R.A. Flowers

**4:00 ORGN 271.** Pharmaceutical process development: Kinetic investigations and modeling. A.L. Dunn

**4:20 ORGN 272.** Design of stable organic electrolytes for Li-O<sub>2</sub> batteries. S. Feng, L. Giordano, M. Chen, J.A. Johnson, Y. Shao-Horn

**4:40 ORGN 273.** Racemization of cyclopropyl fused dihydroisoxazoles. K. Quasdorf, M.D. Bartberger

### Section F

Walter E. Washington Convention Center  
Rooms 204A/B

#### New Reactions & Methodology

##### Organocatalysis & General

R. D. Broene, *Organizer*

A. R. Narayan, *Presiding*

**1:30 ORGN 274.** Discovery and optimization of a new formal thiocyanopalladation/carbocyclization transformation via enzymatic screening. R.A. Swyka, G. Malik, G.A. Applegate, X. Fei, D.B. Berkowitz

**1:50 ORGN 275.** Organocatalyzed synthesis of epoxides from alkenes utilizing amino acids. S. Russell, J.J. Kiddle

**2:10 ORGN 276.** Organocatalytic methods for site-selective aliphatic C-H bond hydroxylation. W. Shuler, S.L. Johnson, D. Wang, C. Pierce, M.K. Hillinski

**2:30 ORGN 277.** Stereoselective synthesis of  $\alpha$ -hydroxy phosphonates/ $\alpha$ -amino phosphonates using manganese-proline derived catalytic system. P. Kaur, H. Lim, V. Datilus, R. Teriak, P. Chohan

**2:50 ORGN 278.** Chemoselective direct transformation of common amides: The chemistry for medicinal chemistry and total synthesis of natural products. P. Huang

**3:10 ORGN 279.** Withdrawn.

**3:30 ORGN 280.** Cofactors as a source of inspiration for discovering new modes of catalytic activation. M.D. Cliff

**3:50 ORGN 281.** Transaminase triggered aza-Michael approach for the enantioselective synthesis of chiral alkaloids. J. Ryan, B. Maciá, E. O'Reilly, V. Caprio

**4:10 ORGN 282.** Directing electrophilic aromatic substitution reactions from above and underneath aromatic rings. S.T. Schneebeil

**4:30 ORGN 283.** Phosphorus and sulfur-yliide mediated C(sp<sup>3</sup>)-C(sp<sup>3</sup>)-coupling reactions. K.J. Hock, U.P. Tran, L. Mertens, C.P. Gordon, J. Ho, T.V. Nguyen, R.M. Koenigs

**4:50 ORGN 284.** How mass spectrometry enables automatization and late stage functionalization workflows. I. Zamora, T. Radchenko, E. Ortega, B. Serra, G. Plasencia Gallofré, L. Morettoni, F. Fontaine

**5:10 ORGN 285.** Development of methods utilizing biocatalysts from natural product pathways. A.R. Narayan

#### Building a Safety Culture across the Chemistry Enterprise

##### Grassroots Approaches to Developing a Safety Culture

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### MONDAY EVENING

#### Section A

Walter E. Washington Convention Center  
Halls D/E

##### Sci-Mix

S. M. Silverman, *Organizer*

8:00 - 10:00

**116, 125, 130, 133-134, 138, 140-141, 147, 174, 177, 182, 184, 192.**  
See previous listings.

**387, 389, 392, 394, 403-405, 411, 415, 418, 433, 437-438, 447, 451, 454-455, 460, 462, 570-571, 578, 581-582, 586-587, 592-593, 598, 601, 604, 611, 619, 622, 624, 636-638, 640-641, 643, 646-647, 653, 659.** See subsequent listings.

### TUESDAY MORNING

#### Section A

Walter E. Washington Convention Center  
Rooms 202A/B

##### Arthur C. Cope Award Symposium

M. K. Boyd, *Organizer*

K. L. Lee, *Organizer, Presiding*

**8:00 ORGN 286. Award Address** (Arthur C. Cope Early Career Scholars Award Sponsored by Arthur C. Cope Fund). C-C and C-H functionalization of ketones. G. Dong

**8:40 ORGN 287. Award Address** (Arthur C. Cope Late Career Scholars Award Sponsored by Arthur C. Cope Fund). Transition metal catalysis and chemistry of bioactive molecules. M. Sodeoka

**9:20 ORGN 288. Award Address** (Arthur C. Cope Mid Career Scholars Award Sponsored by the Arthur C. Cope Fund). New vistas in the asymmetric construction of C-C bonds: Total synthesis of complex bioactive agents. P. Evans

**10:00 ORGN 289. Award Address** (Arthur C. Cope Mid Career Scholars Award Sponsored by the Arthur C. Cope Fund). Stereoselective saturated heterocycle synthesis via copper-catalyzed alkene difunctionalizations involving polar/radical cascades. S.R. Chemler

**10:40 ORGN 290. Award Address** (Arthur C. Cope Early Career Scholars Award Sponsored by Arthur C. Cope Fund). Chemically stable polycyclic aromatic hydrocarbon semiconductors for organic electronic applications. A.L. Briseno

**11:20 ORGN 291. Award Address** (Arthur C. Cope Late Career Scholars Award Sponsored by Arthur C. Cope Fund). Click, carry, and release: Building and transporting molecular function. M. Finn

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**Section B**

Walter E. Washington Convention Center  
Room 207A

**Young Academic Investigator Symposium**

H. M. Davies, L. McElwee-White, *Organizers, Presiding*

8:10 Introductory Remarks.

8:15 ORGN 292. Synthetic nucleic acid topology and their biological applications. Y. Weizmann

8:40 ORGN 293. New fluorophore scaffolds for chemical biology. C.I. Stains

9:05 ORGN 294. New recipes for biocatalysis: Expanding the cytochrome P450 chemical landscape. E.M. Brustad

9:30 ORGN 295. Chemical methods for tailoring glycan interactions at the cell-matrix interface. K. Godula

9:55 Intermission.

10:05 ORGN 296. Mechanistically-defined methods for synthesis of neuroactive small molecules. T.R. Newhouse

10:30 ORGN 297. Synthesis of designer organic nanowires and nanoribbons. A.A. Gorodetsky

10:55 ORGN 298. Strategic nanomaterial synthesis. R.S. Klausen

11:20 ORGN 299. Can single-molecule spectroscopy be a tool for mechanistic organometallic chemistry? R.H. Goldsmith

**Section C**

Walter E. Washington Convention Center  
Room 206

**Process Chemistry: New Developments in Pharmaceutical Process Development (IV)**

J. A. Pesti, R. Vaidyanathan, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ORGN 300. Science and innovation in API process design and continuous improvement. S. Cui

8:50 ORGN 301. Commercial route development of an SMO inhibitor. N. Do

9:35 ORGN 302. Development of scalable and cost-effective API synthesis through chemical innovation. C.H. Senanayake

10:20 ORGN 303. Invention of catalytic asymmetric methods for the commercial manufacture of complex drug targets. K.R. Campos

11:05 ORGN 304. Taming down those nitrogens: Design and development of the commercial synthesis of a novel tyrosine kinase inhibitor. K. Chen

11:50 Concluding Remarks.

**Technical program information known at press time.**

The official technical program for the 254th ACS National Meeting is available at [www.acs.org/WDC2017](http://www.acs.org/WDC2017)

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**Section D**

Walter E. Washington Convention Center  
Room 207B

**Asymmetric Reactions & Syntheses Metals**

R. D. Broene, *Organizer*

A. R. Angeles, *Presiding*

8:00 ORGN 305. Symmetric disubstituted heteroaryl-olefins: A new challenge for the enantioselective addition of Grignard reagents to electrophiles. T. Pellegrini, R.P. Jumde, S.R. Harutyunyan

8:20 ORGN 306. Enantioconvergent cross-coupling of racemic secondary organozinc reagents. R. Oost, A. Preinfalk, A. Misale, N. Maulide

8:40 ORGN 307. Pd-catalyzed synthesis of highly functionalized piperidines. B. Allen, J.P. Harrity

9:00 ORGN 308. Enantio-, diastereo-, and regioselective Pd-catalyzed allylic alkylation of fluoroenolates: Access to enantioenriched 3-fluorooxindoles with vicinal and four contiguous chirality centers. B. Kaluvu, C. Wolf

9:20 ORGN 309. Enantioselective oxidative homocoupling reaction: Vanadium(V)-catalyzed synthesis of novel 1,1'-bicarbazole-2,2'-diols. V. Peddiahgari, H. Kang, Y. Eun Lee, K. Niederer, P. Sung, M. Kozlowski

9:40 ORGN 310. Copper(I)-catalyzed enantioselective alkynylation of oxocarbenium and iminium ions to set diaryl tetra-substituted stereocenters. S. Dasgupta, J. Liu, T.E. Rivas, C. Shoffler, M.P. Watson

10:00 ORGN 311. Catalytic asymmetric synthesis of alkylsilanes enabled by stereoconvergent nickel-catalyzed cross-coupling. G.M. Schwarzwald, G.C. Fu

10:20 ORGN 312. Pd-catalyzed enantioselective intermolecular hydroamination of dienes with aliphatic amines. S. Malcolmson, N. Adamson, E. Hull

10:40 ORGN 313. Enantioselective cascade reaction for synthesis of quinolinones via synergistic catalysis using Cu-pybox and chiral benzotamisole as catalysts. X. Wu, X. Lu, L. Ge, C. Cheng

11:00 ORGN 314. N-sulfinyl metallo-dienamines in the total synthesis of (-)-albicycline. R.B. Andrade, V.K. Chatare

11:20 ORGN 315. Asymmetric synthesis of an active pharmaceutical ingredient: Discovery and development of novel photoredox-minisci formylation and KRED reactions. A.R. Angeles

**Section E**

Walter E. Washington Convention Center  
Room 201

**Peptides, Proteins & Amino Acids**

R. D. Broene, *Organizer*

L. Witus, *Presiding*

8:20 ORGN 316. Selective covalent derivatization of hexahistidine tag of recombinant proteins. A. Melman, V. Kadambar

8:40 ORGN 317. Metal-assisted folding of prolinomycin allows facile design of functional peptides. W. Wang, A.S. Hosseini, J. Gao

9:00 ORGN 318. Development of a colorimetric competitive displacement assay for the evaluation of catalytic peptides. A. Gest, E. Aguiluz Ramirez, L. Witus

9:20 ORGN 319. Role of single disulfide linkages in the folding and activity of scyllatoxin-based BH3 domain mimetics. J.M. Holub, D.M. Berugoda Arachchige, M.M. Harris, Z. Coon, J. Carlsen

9:40 ORGN 320. Engineered luciferases as off-the-shelf reporters of pathogenic bacteria. Z. Reinert, J.A. Prescher

10:00 ORGN 321. Lasso peptide benenodan-1 is a thermally actuated [1]rotaxane switch. C. Zong, M. Wu, J. Qin, A. Link

10:20 ORGN 322. Novel <sup>19</sup>F-amino acids as labels to study peptides by <sup>19</sup>F NMR. P. Mykhailiuk

10:40 ORGN 323. c-Myc reversibly associates into dynamic aggregates. V.S. Dobrev, A.C. de Dios, S.J. Metallo

**Section F**

Walter E. Washington Convention Center  
Rooms 204A/B

**New Reactions & Methodology**

**General**

R. D. Broene, *Organizer*

C. Brindle, *Presiding*

8:00 ORGN 324. Stereoselective cyclization reactions: New approaches to indole alkaloids. L. Wang, J. Zhu, L. Feng, H. Ren, Y. Tang

8:20 ORGN 325. Advancements using alkylsilicates for C-C bond construction. C. Kelly, S.B. Lang, N.R. Patel, R.J. Wiles, K. Lin, A.P. Siegenfeld, G.A. Molander

8:40 ORGN 326. Hydrazine and diethylenetriamine mediated direct cleavage of unactivated amides, carbamates, and ureas. M. Noshita, Y. Shimizu, H. Morimoto, T. Ohshima

9:00 ORGN 327. Phosphine oxide-catalyzed amide synthesis. P.H. Toy

9:20 ORGN 328. Withdrawn.

9:40 ORGN 329. Electrochemical synthesis and characterization of dicationic ionic liquids as electrolytes for safer lithium ion batteries. R.N. Manchanayakage

10:00 ORGN 330. Simple workup procedure for the removal of aldehydes. C. Brindle

10:20 ORGN 331. Catalytic insertion of isatins and aldehydes into aryl dihalonitromethyl ketones. R. Ding, P.R. Bakhshi, C. Wolf

10:40 ORGN 332. Oxidative cyclization reactions and the importance of controlling the nature of reactive intermediates. R. Feng, R.J. Perkins, K.D. Moeller

11:00 ORGN 333. Use of branched and dendritic scaffolds for controlling selectivity in organocatalysis. M. Portnoy, N. Ashush, A. Fallek, R. Palakuri, J. Karabine-Kuks, M. Weiss-Shtofman

11:20 ORGN 334. Oxidative C(sp<sup>2</sup>)-H trifluoromethylation of enamides using TMSCF<sub>3</sub>. S.B. Munoz, V. Krishnamurti, G.S. Prakash

11:40 ORGN 335. Bench-validated retrosynthetic cheminformatics tool to simplify the synthesis of novel chemical compounds. S.L. Trice

**Understanding the Chemistry of Our Planet**

**Chemistry's Role in our Earth System**

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**TUESDAY AFTERNOON**

**Section A**

Walter E. Washington Convention Center  
Rooms 202A/B

**Arthur C. Cope Award Symposium**

K. L. Lee, *Organizer*

M. K. Boyd, *Organizer, Presiding*

1:00 ORGN 336. Award Address (Arthur C. Cope Late Career Scholars Award Sponsored by Arthur C. Cope Fund). Themes and schemes: Some small molecule syntheses. K.A. Parker

1:40 ORGN 337. Award Address (Arthur C. Cope Mid Career Scholars Award Sponsored by Arthur C. Cope Fund). Synthesis of complex and diverse compounds from natural products leads to discovery of a broad-spectrum antibiotic. P.J. Hergenrother

2:20 ORGN 338. Award Address (Arthur C. Cope Late Career Scholars Award Sponsored by Arthur C. Cope Fund). Three-component hexadehydro-Diels-Alder (HDDA) reactions. T.R. Hoye

3:00 ORGN 339. Award Address (Arthur C. Cope Mid Career Scholars Award Sponsored by Arthur C. Cope Fund). Efforts in natural product synthesis design. C.D. Vanderwal

3:40 ORGN 340. Award Address (Arthur C. Cope Award Sponsored by the Arthur C. Cope Fund). Wild world of bioorthogonal chemistry. C.R. Bertozzi

4:40 Concluding Remarks.

**Section B**

Walter E. Washington Convention Center  
Room 207A

**Young Academic Investigator Symposium**

H. M. Davies, L. McElwee-White, *Organizers, Presiding*

1:10 ORGN 341. Strategies and methods for the synthesis of topologically complex natural products. J.L. Stockhill

1:35 ORGN 342. Catalysis at metal-metal bonds. C. Uyeda

2:00 ORGN 343. Transition metal catalyzed amination and amidation reactions. K.L. Hull

2:25 ORGN 344. Catalytic carbon-olefin metathesis. C. Schindler

2:50 ORGN 345. Catalytic hydroacylation and carboacylation of olefins: A platform for synthesis of heterocyclic and carbocyclic ketones. L.M. Stanley

3:15 Concluding Remarks.

Section C

Walter E. Washington Convention Center  
Room 206

Using Organic Chemistry to Illuminate Biological Systems

M. J. Schnermann, *Organizer, Presiding*

- 1:15 ORGN 346. Photocatalytic induction of tetrazine ligation with near IR light. J. Fox
- 1:45 ORGN 347. TMP-Tag: A chemical surrogate to the fluorescent proteins for live cell imaging. V.W. Cornish
- 2:15 ORGN 348. Optical control of protein function through genetic code expansion. A. Deiters
- 2:45 Intermission.
- 3:00 ORGN 349. Designing brighter dyes for advanced imaging experiments. L.D. Davis
- 3:30 ORGN 350. Illuminating the path for drug delivery. D.S. Lawrence

Section D

Walter E. Washington Convention Center  
Room 207B

Asymmetric Reactions & Syntheses

R. D. Broene, *Organizer*

C. Allais, *Presiding*

- 1:15 ORGN 351. Kinetic resolution of chiral racemic secondary allylboronates and their application in the synthesis of homoallylic amines. L. Villar, N. Orlov, N. Kondratyev, J.L. Vicario, A.V. Malkov
- 1:35 ORGN 352. Conjunctive cross-coupling reaction of bis(alkenyl) borates to afford enantioenriched allylboron reagents. E. Edelstein, S. Namirembe, J.P. Morken
- 1:55 ORGN 353. Two are better than one: New processes involving 1,1-diboronic acids. P. Starkov
- 2:15 ORGN 354. Enantio- and diastereoselective synthesis of 1,5-syn-(Z)-aminoalcohols via imine double allylboration: Synthesis of trans-1,2,3,6-tetrahydropyridines and total synthesis of and-rachicine. C. Allais, W.R. Roush
- 2:35 ORGN 355. Synthesis of axially chiral heterobiphenyl alkenes via dynamic kinetic asymmetric alkylation. V. Hornillos, A. Ros, P. Ramirez-López, J. Iglesias-Sigüenza, R. Fernández, J.M. Lassaletta
- 2:55 ORGN 356. Merging photoisomerization and Brønsted acid catalysis: Insight into transition states. P. Renzi, J. Hioe, G. Ruth Maria
- 3:15 ORGN 357. Chiral Lewis acid catalyzed enantioselective synthesis of cyclopropane and its retro-Claisen rearrangement to 2,5-dihydrooxepine. S. Shim, D. Ryu
- 3:35 ORGN 358. Chirality transfer intramolecular [2+2] cycloadditions of electron deficient allenes and alkenes. Y. Xu, M.K. Brown
- 3:55 ORGN 359. First two-step asymmetric  $\alpha,\alpha$ -bis-functionalization of ynone via unprecedented *tert*-*ra*-substituted 1,2-dialkyl enamines. S. Peng, Z. Wang, Y. Huang

Section E

Walter E. Washington Convention Center  
Room 201

Metal-Mediated Reactions & Syntheses

R. D. Broene, *Organizer*

C. Meyet, *Presiding*

- 1:10 ORGN 360. Choose your own adventure: Three-component copper chemistry reveals exclusive routes to either allene or propargylamine. C. Meyet, H. Banovetz, T. Beckwith, S. Kiledal, Z. Nusbaum, J. Olberding, J. Parker, K. Royer, J. Russell, S. Saccoman, E. Shankin, K.B. Shillingstad, E. Steger, Y. Xia
- 1:30 ORGN 361. Mechanistic studies on the conversion of metallacyclobutenes to highly substituted cyclopentadienes. J.M. O Connor, P. Qin, R.L. Holland, K.K. Baldrige, A.L. Rheingold, C. Moore
- 1:50 ORGN 362. Iron mediated *N*-arylation reactions. G. Douglas, S. Raw, S. Marsden
- 2:10 ORGN 363. Nickel-catalyzed reductive cross-electrophile coupling reactions of alkyl fluorides for cyclopropane synthesis. E. Lucas, L. Erickson, E. Tollefson, E.R. Jarvo
- 2:30 ORGN 364. Palladium catalyzed cross-coupling of 3-methylthiophene-2-carbonyl chloride with aryl/het-aryl boronic acids: A convenient method for synthesis of thienyl ketones. K. Rizwan, I. Karakaya, M. Zubair, N. Rasool, Z. Nazli, G.A. Molander
- 2:50 ORGN 365. One-pot cascade Suzuki-Miyaura/Diels-Alder approach to steroidal cores enabled by nucleophile chemoselectivity. J. Molloy, A.J. Watson
- 3:10 ORGN 366. Photosensitized, energy transfer-mediated organometallic catalysis through electronically excited nickel(II). E. Welin, C. Le, D.M. Arias-Rotondo, J.K. McCusker, D.W. MacMillan
- 3:30 ORGN 367. Iron-mediated aziridination. M. Shehata, S. Ayer, J.L. Roizen
- 3:50 ORGN 368. Development of cheap, recyclable cellulose-bonded palladium catalyst for cross coupling reactions. Z. Lu, J. Jasinski, S. Handa, G.B. Hammond
- 4:10 ORGN 369. Palladium-catalyzed tandem C-H functionalization/cyclization strategy for the synthesis of 5 hydroxy-benzofuran derivatives. S. Ichake, C. Yao
- 4:30 ORGN 370. Application of cyclic metal carbyne complexes in classical organic reactions. H. Zhang

Section F

Walter E. Washington Convention Center  
Rooms 204A/B

New Reactions & Methodology

Photoinduced & General

R. D. Broene, *Organizer*

T. Wang, *Presiding*

- 1:00 ORGN 371. Radical conjugate addition of alkyl bromides to  $\alpha,\beta$ -unsaturated amides and esters by visible-light photoredox catalysis. A. El Marrouni, J. Balsells
- 1:20 ORGN 372. Withdrawn.
- 1:40 ORGN 373. Withdrawn.

- 2:00 ORGN 374. Visible light mediated construction of pyrroloindolines via an amidyl radical cyclization/intermolecular radical alkene addition cascade: Total synthesis of ( $\pm$ ) flustramide B. T. Wang
- 2:20 ORGN 375. Withdrawn.
- 2:40 ORGN 376. Withdrawn.
- 3:00 ORGN 377. Synthesis and photophysical properties of novel organometallic hydrophorphyrins. N. Esemoto, M. Ptaszek
- 3:20 ORGN 378. Withdrawn.
- 3:40 ORGN 379. Development of a new methodology for synthesis of 1,4-oxazepines. M. Zora, Y. Kelgokmen, Y. Cayan
- 4:00 ORGN 380. Toward the ideal manufacturing process of active pharmaceutical ingredients at Merck. S.M. Silverman
- 4:20 ORGN 381. Base dependent chemo-divergent cascade reaction of dihydroxyfumarate with aldehydes. G.W. Ward, S.A. France, C.L. Liotta, R. Krishnamurthy, N.V. Hud
- 4:40 ORGN 382. Tandem reactions for the direct, catalytic synthesis of alpha-tetrasubstituted amines. C.H. Larsen, Z.L. Palchak, K.G. Nelson, M.D. Sterling

Understanding the Chemistry of Our Planet

Human Impacts to our Planet

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TUESDAY EVENING

Section A

Walter E. Washington Convention Center  
Hall D

Biologically Related Molecules & Processes

S. M. Silverman, *Organizer*

5:30 - 7:30

- ORGN 383. High-throughput post-synthetic chemical modification of RNA. D. Zewge, D.M. Tellers, I.W. Davies
- ORGN 384. Dynamic detection and visualization of RNA methylation by photochemical organic transformations. D. Kong, R. Wang, L. Xie, L. Cheng
- ORGN 385. Derivatizing lanosterol with improved water solubility for catalyzed treatment. Y. Cheng, H. Hsu
- ORGN 386. Sesterterpenoids from the marine sponge *Phorbasp* sp. activate latent HIV-1 provirus expression. M. Wang, I. Tietjen, M. Chen, D.E. Williams, J. Daoust, M.A. Brockman, R.J. Andersen
- ORGN 387. Design and synthesis of C2-substituted 8-aza-7-deaza-2'-deoxyadenosines as environmentally sensitive fluorescent nucleosides. Y. Saito, M. Yanagi
- ORGN 388. Detection of organochlorine pesticides in contaminated biological systems via cyclodextrin-promoted fluorescence modulation. J. Lynch, M. Levine, D.J. DiScenza

- ORGN 389. Glass surface adhered probe plate assay for characterization of protein binding partners of small molecules. S.J. Ramos-Hunter, K. Brandvold, C. Whidbey, A.T. Wright
- ORGN 390. Chemical route optimization of VAcHT gamma-carboline compounds. D. Billen, D.M. Sobieray, V. Westrick, O. Goethe
- ORGN 391. Inspired from naturally occurring bicyclic iminosugars to develop new molecular scaffolds and libraries. W. Chen, C. Chen, H. Lee, W. Cheng
- ORGN 392. Synthesis of a fluorinated C-glycoside of the immunostimulatory glycolipid KR7000. K. Ali, A.S. Altiti, D.R. Mootoo
- ORGN 393. Development and optimization of Glaser-Hay bioconjugations. D. Young
- ORGN 394. Targeting regulatory non-coding RNAs with druglike small molecules. C.M. Connelly, R.E. Boer, M.H. Moon, R.S. Sinniah, P. Gareiss, J. Schneekloth
- ORGN 395. Activity-based protein profiling of bile acid metabolism and host signaling in the gut microbiome. K. Brandvold, C. Whidbey, A.T. Wright
- ORGN 396. Water green synthesis of antitubercular dicoumarols. D. Bandyopadhyay, V.M. Cano, I.M. Chapa, A. Velasco, M.L. Vigilar, O. Espino, G. Rivera
- ORGN 397. Chemical investigation of avocado (*Persea americana*) seed husk: A waste of waste. D. Bandyopadhyay, O. Castillo, D. Villacana, V.M. Cano, T. Eubanks
- ORGN 398. Medicinally privileged compounds from *Magnolia grandiflora* green seed cones. D. Bandyopadhyay, A. Echeverria, B. Garza, T. Eubanks
- ORGN 399. Chemical investigation of southern live oak (*Quercus virginiana*) galls. D. Bandyopadhyay, A. Rodriguez, J.A. Rodriguez, J. Garcia, T. Eubanks
- ORGN 400. Poecillarin A: A new tri-indole alkaloid from a deep water *Poecillastra* sp. H. Liu, G. Lauro, R. O'Connor, K. Lohith, G. Bifulco, C.A. Bewley
- ORGN 401. Scalable synthesis and spectroscopic analysis of mercaptobenzamide thioester (SAMT) HIV inhibitors. H. Nikolayevskiy, M.T. Scerba, D.H. Appella

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- ORGN **402.** Withdrawn.
- ORGN **403.** Design, synthesis and biological evaluation of fucose-truncated monosaccharide analogues of ipomoeassin F. M. Hirsch, G. Zong, C. Mondrik, Z. Hu, W. Shi
- ORGN **404.** Stereoselective synthesis of flavonoid analogues and evaluation of biological performance diversity. L.N. Aldrich, E.M. Gerlach, T.R. Helgren, M.A. Korkmaz, M. Oleksyuk, I. Pavlinov, L.L. Xu
- ORGN **405.** Synthesis of solvatochromic probes to label the mycobacterial cell wall and their use in studies of host-pathogen interactions. S. Keyser, A. Utz, M. Kamariza, C.R. Bertozzi
- ORGN **406.** Withdrawn.
- ORGN **407.** Synthesis of amide isosteres of schweinfurthin-based stilbenes. D.P. Stockdale, J.A. Beutler, D.F. Wiemer
- ORGN **408.** Near-infrared fluorescent probes for sensitive and selective detection of pH changes in live cells though visible and near-infrared channels. W. Mazi, M. Fang, R. Adhikari, N. Dorh, J. Bi, J. Wang, A. Tiwari, F. Luo, H. Liu
- ORGN **409.** Efficient acylation of DNA-conjugated carboxylic acids with amines in aqueous media. M. Chung, H. Huang
- ORGN **410.** Tetraethylene glycol succinate 7-dehydrocholesterol derivative as vitamin D3 precursor. I. Jeong, H. Ryu, S. Bang, B. Chung
- ORGN **411.** Towards site-selective transformations in complex mixtures: DNA-catalyst conjugates for targeted ester hydrolysis. M.L. Flanagan, Y. Yao, Y. Zhang, A. Arguello, D. Colman, S. Krejci, D.J. Gorin
- ORGN **412.** Substitution effect on the luminescence of terpyridine zinc complexes: A study via low temperature fluorescence spectroscopy. X. Bi, Y. Pang
- ORGN **413.** Pushing the limits of biocatalysis with DERA variants to access the chiral side chain required for statin activity. C.M. Amarasekara, L.M. Foreman, K. Belecki
- ORGN **414.** Synthesis of ebelen derivatives and evaluation against *Mycobacterium tuberculosis*. A.D. Landgraf, S. Thanna, S.J. Sucheck
- ORGN **415.** Development of peptide nucleic acids for the optimization of assay sensitivity for quantitative determination of HIV viral load. M. Gould, E.E. Rastede, D.H. Appella
- ORGN **416.** Fluorescent kinase inhibitors: Novel modality for HER2 status of breast cancer cells. H. Lee, W. Liu, A. Brown, R. Landgraf, J.N. Wilson
- ORGN **417.** Synthesis and characterization of novel carbohydrate based macrocycles. A. Chen, L. Samankumara, G. Wang

Technical program information known at press time. The official technical program for the 254th ACS National Meeting is available at [www.acs.org/WDC2017](http://www.acs.org/WDC2017)

†Cooperative Cosponsorship

- ORGN **418.** Antihypertensive coumarins from *Mammea americana*. R. Fayad, D. Amaker, K. Jackson, O.E. Christian
- ORGN **419.** Design, synthesis and study of N-acetyl D-glucosamine based triazole derivatives as organogelators. D. Wang, A. Chen, G. Wang
- ORGN **420.** Antihypertensive activity of 7-epiclusianone and other bicyclic nonanes from *Hypericum hypericoides*. E. Hicks, K. Jackson, O.E. Christian
- ORGN **421.** Use of small molecule probe substrates, active site mutagenesis and molecular modeling to gain mechanistic insight into the PLP-enzyme, human serine racemase. D.L. Graham, M.L. Beio, D.L. Nelson, G.A. Applegate, D.B. Berkowitz
- ORGN **422.** 15-oxo-Lipoxin A<sub>2</sub>: Synthesis and use as a probe of electrophilic signaling. S.R. Woodcock, B. Singh, S. Gelhaus Wendell, F. Schopfer, B.A. Freeman
- ORGN **423.** Use of <sup>19</sup>F NMR to monitor thiol reactions of sultams, sulfonamides, and known drugs. C.D. Clay, J. Jun, A. Cassidy, J.S. Jha, P.R. Hanson

Section B

Walter E. Washington Convention Center Hall D

Chemistry of Fullerenes, Carbon Nanotubes & Graphene

- S. M. Silverman, *Organizer*  
5:30 - 7:30
- ORGN **424.** Synthesis and characterization of a [9]cycloparaphenylene derivative bearing three indeno[2,1-a]fluorene-11,12-dione-2,9-diyl units. S. Li, M. Aljhdli, H. Thakellapalli, B. Farajidzaji, Y. Zhang, N. Akhmedov, C. Milsman, B.V. Popp, K.K. Wang
- ORGN **425.** Design of novel graphene stabilisers. A. Alwattar
- ORGN **426.** Five regioisomers of dimethyl dodecahedrane derivatives: A hybrid DFT B3LYP study. K.H. Lee, S. Lee, Y. Cho
- ORGN **427.** Eclipsed isomer of C<sub>20</sub> fullerene by the hybrid density functional B3LYP methods. K.H. Lee, Y. Cho
- ORGN **428.** Influence of perfluoroalkylated fullerene acceptors on morphology and photodegradation of organic photovoltaic active layers. C.P. Brook, B. Larson, V.N. V., P.C. Ramamurthy, G. Paul, O.V. Boltalina, S.H. Strauss, A.J. Pal, W.A. Braunecker

Section C

Walter E. Washington Convention Center Hall D

Flow Chemistry & Continuous Processes

- S. M. Silverman, *Organizer*  
5:30 - 7:30
- ORGN **429.** Withdrawn.
- ORGN **430.** Rapid total synthesis of ciprofloxacin hydrochloride in continuous flow. H. Lin

Section D

Walter E. Washington Convention Center Hall D

Materials, Devices & Switches

- S. M. Silverman, *Organizer*  
5:30 - 7:30
- ORGN **431.** Study of carrier adjusting layer on electroluminescent and ultraviolet detectable performances of organic optoelectronic integrated device. D. Zhou, J. Yu
- ORGN **432.** Synthesis of a new hole-transport material (HTM) of conjugated reduced graphene oxide-thiophene for application in perovskite solar cells. B.A. Bregadiolli, L.C. da Silva Filho
- ORGN **433.** Visible light driven molecular rotary motors. G.D. Roke, S.J. Wezenberg, B. Feringa
- ORGN **434.** Water-soluble conventional and upconversion near-infrared luminescent probes for sensitive detection of pH changes in living cells. M. Fang, S. Zhang, H. Liu
- ORGN **435.** Synthesis and luminescence of novel organic viologens for electro-optic applications. E.N. Patel, R.B. Arthur, A.D. Nicholas, M. Brichacek, H.H. Patterson
- ORGN **436.** Non-symmetric dithienylene-based carboxylic acid photoswitches: Synthesis and acid-base properties. A.D. Sponza Mata
- ORGN **437.** Synthesis of rotaxane-based probes for hyperpolarized xenon-129 MRI. P.I. Fernando, B.L. DeBoef
- ORGN **438.** Cationic core-functionalized pyromellitic diimides. A.J. Greenlee, D.D. Cao
- ORGN **439.** Responsive luminescent dimethylamino-substituted dibenzoylmethane materials. F. Wang, T. Butler, M. Sabat, C.L. Fraser
- ORGN **440.** Photophysical studies, electronic properties, and computational modeling of 6,6'-diarylsubstituted isoindigo compounds. T.H. El-Assaad, D. Patra, B. Wex, B.R. Kaafarani
- ORGN **441.** Pyromellitic diimides tethered together. M.M. Modan, L. Schaller, D.D. Cao
- ORGN **442.** Ratiometric near-infrared fluorescent probes for sensitive detection of pH in live cells. J. Wang, M. Fang, H. Liu
- ORGN **443.** Modular form of CB6 for HYPER\_CEST imaging. D. Robinson

Section E

Walter E. Washington Convention Center Hall D

Molecular Recognition & Self-Assembly

- S. M. Silverman, *Organizer*  
5:30 - 7:30
- ORGN **445.** Probing the implications of tightness on molecular knot. L. Zhang, J. Lemonnier, F. Zerbetto, D.A. Leigh
- ORGN **446.** Synthesis and photophysical properties of multicomponent self-assemblies. M. Saha, Z. Zhou, X. Yan, H. Sepehrpour, P.J. Stang

- ORGN **447.** Chirality sensing via reversible Schiff base formation with a stereodynamic UV/CD probe. Z. De Los Santos, R. Ding, C. Wolf
- ORGN **448.** Self-assembly of cucurbit[7]uril based triangular [4]molecular necklaces and their fluorescence properties. S.K. Samanta, K. Brady, L.D. Isaacs
- ORGN **449.** Biomimetic comprehensive chirality sensing with pyridoxal-5'-phosphate. S.L. Pilicer, P.R. Bakshi, K. Bentley, C. Wolf
- ORGN **450.** Chemosensors for rapid detection of fluoride ion in water. S. Bae, N. Kim, Y. Choi
- ORGN **451.** Nanoreactors of self-assembled benzophenone bis-urea macrocycles: Improving the selectivity of singlet oxygen induced photooxidations. N. Noll, B. DeHaven, L.S. Shimizu
- ORGN **452.** Synthesis of (3, 8) torus knot via coordination-driven self-assembly. D. Kim, N. Singh, K. Chi
- ORGN **453.** Molecular recognition of amino acid amides by acyclic cucurbiturils. S. Zebaze Ndendjo, L.D. Isaacs
- ORGN **454.** Development of organic porous materials for the photo-re-activity of small molecules. A. Sindt, M.D. Smith, L.S. Shimizu
- ORGN **455.** pH switched assembly of a self-complementary supramolecular motif in polar solvent. X. Duan, J.W. Canary
- ORGN **456.** Tetrameric pseudo-peptide receptors with allosteric properties and [2]-catenanes with a responsive noncovalent network mimicking long-range responses in proteins. M. Chung, P.S. White, S.J. Lee, M.L. Waters, M.R. Gagne
- ORGN **457.** Stepwise self-assembly of giant metallo-supramolecules with multiple types of metal ions based on terpyridine ligand. L. Wang, X. Li
- ORGN **458.** Organoboron conjugated macrocycles. N. Baser-Kirazli, F. Jaekle
- ORGN **459.** Hydrated anions binding within the water-soluble hosts. W. Yao, M.R. Sullivan, P. Sokkalingam, B.C. Gibb
- ORGN **460.** Supramolecular catalyst for halogenation reaction. X. Cai, B.C. Gibb
- ORGN **461.** Withdrawn.

Section F

Walter E. Washington Convention Center Hall D

Nanomaterials

- S. M. Silverman, *Organizer*  
5:30 - 7:30
- ORGN **462.** Structure directing agents for organic polyhedral nanoparticles. D.K. Jones, N. Gavvalapalli
- ORGN **463.** Electronic and computational characterization of donor-acceptor nanostructures. N.N. Baughman, C. Huang, B. Farajidzaji, H. Thakellapalli, S. Li, K.K. Wang, B.V. Popp
- ORGN **464.** Phosphonic acid derivatives of DOTAZA for immobilization on nanoparticles. M. Holzapfel, W. Maison

WEDNESDAY MORNING

Section A

Walter E. Washington Convention Center  
Rooms 202A/B

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Kim D. Janda

R. D. Broene, *Organizer*  
R. M. Williams, *Presiding*

8:20 ORGN 465. Enantiomeric natural products: Synthesis, biogenesis and evolutionary origins. R.M. Williams

9:05 ORGN 466. Antibiotic adjuvants based upon nitrogen dense marine alkaloids. C. Melander

9:50 ORGN 467. Structure and mechanism of a nicotinic degrading enzyme, NicA2: Toward design of tools and therapeutics. K.N. Allen

10:35 Introduction of Awardee.

10:40 ORGN 468. Award Address (Alfred Bader Award in Bioinorganic or Bioorganic Chemistry Sponsored by the Alfred R. Bader Fund). Merging of chemistry and biology: In search of molecules with translational function. K.D. Janda

Section B

Walter E. Washington Convention Center  
Room 207A

Technical Achievements in Organic Chemistry

T. D. White, *Organizer, Presiding*  
8:20 Introductory Remarks.

8:25 ORGN 469. Synthetic modifications on amidine fused-ring scaffolds in a series of BACE inhibitors. J.C. Murray, J. Dutra, K. Ogilvie, P.J. Mikoichik, L. Buzon, L.A. Martinez-Alsina, E.A. LaChapelle, B.T. Oneill

8:55 ORGN 470. Complex organic synthesis in drug discovery: Examples from Lilly's BACE inhibitor program. L.L. Winneroski

9:25 ORGN 471. Control of a key hydrogenolysis-derived desfluoro impurity in the synthesis of LY2886721. R.J. Linder, M.M. Hansen, N. Zaborenko, M.D. Johnson, B. Campbell, T. Braden

9:55 Intermission.

10:10 ORGN 472. Investigations into the SAR of Isoclast™. A. Buysse, B.M. Nugent, M.R. Loso, R. Rogers, Y. Zhu, J.M. Babcock, N. Breaux, T. Johnson, T. Martin, M.P. Oliver, M. Ober, T.C. Sparks, N. Wang, G. Watson

10:40 ORGN 473. Opportunity, chirality, and mentors: A retrospective across therapeutic areas. J.G. Varne

11:10 ORGN 474. Synthetic efforts towards enablement of spliceostatin and calicheamicin natural products for antibody drug conjugate development. K.J. DiRico

Section C

Walter E. Washington Convention Center  
Room 206

From Bioinspired to Biocompatible Material Design for Organic Electronics

R. K. Castellano, J. D. Tovar, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ORGN 475. Structural and sequential factors affecting charge transport in self-assembled peptide fibrils. N. Ashkenasy

8:35 ORGN 476. Protein-inspired self-assembly of perylene diimide nanofibers. J. Hodgkiss

9:05 ORGN 477. Self-assembly of co-axial nanotube-polymer hybrids. J.R. Parquette, M. Ji

9:35 ORGN 478. Peptide-conjugated block copolymers and sequence controlled peptide-graphite composites: Conductive peptide hybrid materials with electronic activity. S.A. Sydlík, B. Holt, A. Arnold, Z. Wright

10:05 Intermission.

10:25 ORGN 479. Self-sorted peptide-based gels for organic electronics. D. Adams, E. Draper, E. Cross, R. Saberi Moghaddam

10:55 ORGN 480. Design rules for optimizing emergent optoelectronic properties in donor-acceptor films. A.B. Braunschweig, A. Levine

11:25 ORGN 481. Long-lived charge carriers in one-dimensional organic semiconductor nanostructures. H. Frauenrath

Section D

Walter E. Washington Convention Center  
Room 207B

Asymmetric Reactions & Syntheses

Organocatalysis

R. D. Broene, *Organizer*  
R. Foster, *Presiding*

8:20 ORGN 482. Organocatalytic stereoconvergent synthesis of  $\alpha$ -CF<sub>3</sub> amides: Triketopiperazines and their heterocyclic metamorphosis. R. Foster, E. Lenz, N. Simpkins, D. Stead

8:40 ORGN 483. Design of experiments (DoE): A rational approach towards non-covalent asymmetric organocatalysis. P. Renzi

9:00 ORGN 484. Enantioselective copper-catalyzed arylation-driven semi-pinacol rearrangement of allylic alcohols with diaryliodonium salts. D. Lukamto, M. Gaunt

9:20 ORGN 485. Asymmetric synthesis of multi-quaternary centre containing cyclopentanoids via the Nazarov reaction. R. Volpe, B.L. Flynn

9:40 ORGN 486. Fe(OTf)<sub>3</sub>-catalyzed intramolecular stereospecific substitution of stereogenic alcohols. R.A. Watlie, A. Bunrit, E. Lagerspets, T. Repo, J.S. Samec

10:00 ORGN 487. Oligourea foldamer-based asymmetric catalysis. D. Bécart, V. Diemer, G. Guichard, C.N. Palomo

10:20 ORGN 488. Two steps, (4+1) cycloaddition and kinetic resolution by Michael Henry-cascade reactions, leading to highly functionalized enantiomerically enriched spiro[4.5]decanes and spirooxindole polycycles. M. Sohail, J. Huang, F. Tanaka

10:40 ORGN 489. Application of chiral N,N'-dioxide-metal complex catalysts in asymmetric rearrangement reactions. X. Feng

Section E

Walter E. Washington Convention Center  
Room 201

Metal-Mediated Reactions & Syntheses

R. D. Broene, *Organizer*  
R. Lundgren, *Presiding*

8:10 ORGN 490. Withdrawn.

8:30 ORGN 491. Synthesis of substituted or  $\pi$ -extended triphenylenes via multiple C-H activations. S. Hong

8:50 ORGN 492. Cross-coupling of  $\alpha$ -hydroxy alkyltrifluoroborate with aryl electrophiles under photoredox/Ni dual catalysis. R. Alam, G.A. Molander

9:10 ORGN 493. Recoverable ruthenium-based olefin metathesis catalysts via host-guest complexation. H. Chung, B. Ondrusek, C. Kim

9:30 ORGN 494. Chan-Evans-Lam amination and etherification directly from organoboronate esters. T.B. Clark, K.A. McGarry, J. Marcum, V. Pérez, C.J. Ferber

9:50 ORGN 495. Pd-catalyzed Suzuki coupling reactions of aryl chlorides containing basic nitrogen centers with arylboronic acids in water in the absence of added base. Z. Li, C. Gelbaum, Z. Campbell, P. Gould, J. Fisk, B. Holden, A. Jaganathan, G. Whiteker, P. Pollet, C.L. Liotta

10:10 ORGN 496. Synthesis and evaluation of dithiolate-modified ruthenium olefin metathesis catalysts. T.P. Montgomery, R.H. Grubbs

10:30 ORGN 497. Chemo- and stereoselective rhodium-catalyzed ene-cycloisomerization of thioether-substituted alkenylidene cyclopropanes: Metal-mediated  $\beta$ -sulfide migration. Y. Su, P. Evans

10:50 ORGN 498. Palladium-catalyzed alkene difunctionalization reactions of heteroaromatic nucleophiles. J.K. Kirsch, J.P. Wolfe

11:10 ORGN 499. Binaphthyl-based scaffold for a chiral dirhodium(II) bis-carboxylate ligand with  $\alpha$ -quaternary carbon centers. K. Setthakarn, P. Chen, J. May

11:30 ORGN 500. Ambient decarboxylative cross-coupling reactions enabled by oxidative copper catalysis. R. Lundgren

Section F

Walter E. Washington Convention Center  
Rooms 204A/B

Molecular Recognition & Self-Assembly

R. D. Broene, *Organizer*  
N. J. Van Zee, *Presiding*

8:00 ORGN 501. Synthesis of biscalex[4] arene derivatives and their applications in molecular sensing and organogel materials. W. Chung

8:20 ORGN 502. G-quadruplex-templated oligomerization of a pore-forming peptide. L. Cozzoli, L. Gjonaj, G. Maglia, B. Poolman, G. Roelfes

8:40 ORGN 503. Stimuli-responsive multi-block molecules. T. Muraoka

9:00 ORGN 504. Chiral triarylamine-based supramolecular polymers: From pathway complexity to functional materials. B. Adelizzi, A. Palmans, E.W. Meijer

9:20 ORGN 505. Tailoring guanosine hydrogels for various applications. T.N. Plank, J. Davis

9:40 ORGN 506. Supramolecular orientational memory: A new route to complex supramolecular architectures. M. Peterca, D. Sahoo, B.E. Partridge, M.R. Imam, E. Aqad, P.A. Heiney, R. Graf, H.W. Spiess, X. Zeng, V. Percec

10:00 ORGN 507. 5' Modified guanosine-based hydrogel: Properties and environmental applications. S. Xiao, J. Davis

10:20 ORGN 508. Acyclic cucurbit[n]uril molecular containers with triptycene walls. X. Lu, S.K. Samanta, P.Y. Zavalij, L.D. Isaacs

10:40 ORGN 509. Synthesis and application of higher order cyclodextrin architectures for improved sensing and identification of medium-sized environmental toxicants. S. Chaudhuri, M. Levine

11:00 ORGN 510. Molecular containers bind drugs of abuse *in vitro* and reverse the hyperlocomotive effect of methamphetamine in rats. S. Ganapati, S.D. Grabitz, S.L. Murkli, F. Scheffebichler, P.Y. Zavalij, M. Eikermann, L.D. Isaacs

11:20 ORGN 511. Consequences of water content on the formation of chiral hydrogen-bonded aggregates. N.J. Van Zee, A. Palmans, E.W. Meijer

WEDNESDAY AFTERNOON

Section A

Walter E. Washington Convention Center  
Room 202A

CH Activation

R. D. Broene, *Organizer*  
D. Kalyani, *Presiding*

1:20 ORGN 512. Thiourea-catalyzed cross-dehydrogenative coupling of sp<sup>3</sup> C-H with nucleophiles: Mechanism and scope. Z. Zhang, K. Gu, Z. Bao, H. Xing, Q. Yang, Q. Ren

1:40 ORGN 513. Design and synthesis of novel thieno-dibenzothiophene derivatives. A. Kivrak, M. Aligso

2:00 ORGN 514. Direct C-H arylation of simple arenes: Ligand effect and mechanism. S. Hong

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- 2:20 ORGN 515.** Computational study of Ni-catalyzed C–H functionalization: Factors that control the competition of oxidative addition and radical pathways. H.B. Omer, K.M. Brummond, P. Liu
- 2:40 ORGN 516.** Electrochemical approach towards palladium-catalyzed C–H oxidation. A. Shrestha, M.S. Sanford
- 3:00 ORGN 517.** Copper-catalyzed intramolecular C–H amination for the synthesis of quinazolinone derivatives and rutaecarpine via ring-opening cyclization (ROC) strategy. S. Malipatel
- 3:20 ORGN 518.** Exploration of advance synthetic processes for generating heterocyclic scaffolds: Synthetic scope and mechanistic insight. S. Sharma, D.M. Sawant, R. Pardasani
- 3:40 ORGN 519.** Nickel catalyzed direct arylations of azoles using phenolic electrophiles and aromatic nitriles. D. Kalyani

**Section B**

Walter E. Washington Convention Center Room 207A

**Technical Achievements in Organic Chemistry**

T. D. White, *Organizer*

T. Braden, *Presiding*

**1:05** Introductory Remarks.

**1:10 ORGN 520.** Process development of GS-5734: An antiviral nucleotide analog for the treatment of Ebola. S. Neville

**1:40 ORGN 521.** Development of a commercial viable, highly regioselective copper catalyzed *N*-arylation of 3-methyl-1,2,4-triazole. J. Fan, W.P. Gallagher, M.C. Soumeillant, V. Iyer, J. Zhu, G. Beutner, A. Glace, A. Freitag, B. Cohen, K. Chen, M.D. Eastgate, D.A. Conlon

**2:10 ORGN 522.** Discovery of reversible LSD1 inhibitors. T. Kanouni

**2:40 ORGN 523.** Preparation of Rinskor™ active standards to support registration studies. P. Johnson, G. Whiteker, N. Giampietro, J.M. Renga, R. Ross, B. Canturk, C.V. Galliford, B. Peterson

**3:10** Intermission.

**3:25 ORGN 524.** Leveraging analytical technologies to impact medicinal chemistry projects. W.P. Farrell

**3:55 ORGN 525.** Reflections on the discovery of HCV polymerase, HCV NSSA, and bromodomain and extra-terminal domain (BET) inhibitors. J.K. Pratt

**4:25 ORGN 526.** Vignettes from my career in medicinal chemistry. C. Wang

**4:55** Concluding Remarks.

**Technical program information known at press time.**

The official technical program for the 254th ACS National Meeting is available at [www.acs.org/WDC2017](http://www.acs.org/WDC2017)

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**Section C**

Walter E. Washington Convention Center Room 206

**From Bioinspired to Biocompatible Material Design for Organic Electronics**

R. K. Castellano, J. D. Tovar, *Organizers, Presiding*

**1:15 ORGN 527.** Bio-integrated electronics: Interfacing semiconducting polymers with biology. E. Egap

**1:45 ORGN 528.** Bioinspired design of synthetic polymer-based Ca<sup>2+</sup> sensor for the realization of extracellular Ca<sup>2+</sup> imaging. F. Ishiwari, T. Fukushima

**2:15 ORGN 529.** Redefining melanin starting with Eumelanin-inspired materials. T.L. Nelson

**2:45 ORGN 530.** Functional conducting polymers: The molecules, the nano, the smart. H. Yu

**3:15** Intermission.

**3:35 ORGN 531.** Multicomponent macrocyclic assemblies from a DNA base toolkit. D. Gonzalez-Rodriguez

**4:05 ORGN 532.** Harnessing biologically relevant stimuli to control the structure and dynamics of hierarchical supramolecules. J.M. Rivera-Ortiz

**4:35 ORGN 533.** DNA architectures: DNA-based assembly of chromophores. H. Wagenknecht

**5:05** Concluding Remarks.

**Section D**

Walter E. Washington Convention Center Room 207B

**Materials, Devices & Switches**

R. D. Broene, *Organizer*

M. Kertesz, *Presiding*

**1:10 ORGN 534.** Carbon-carbon bond formation by a small molecule artificial molecular machine. C.T. McTernan, G. De Bo, D.A. Leigh

**1:30 ORGN 535.** Gated photochromism in a molecular motor - dithienylethene hybrid. G.D. Roke, C. Stuckhardt, W. Danowski, S.J. Wezenberg, B. Feringa

**1:50 ORGN 536.** Pancake bonded molecules as redox mechanical switches. M. Kertesz

**2:10 ORGN 537.** Sequence-specific beta-*homo* peptide synthesis by an artificial small-molecule machine. G. De Bo, M.A. Gall, M. Kitching, S. Kuschel, D.A. Leigh, D.J. Tetlow, J.W. Ward

**2:30 ORGN 538.** Rotary and linear molecular motors driven by pulses of a chemical fuel. U. Karaca, S. Erbas-Cakmak, S. Fielden, D.A. Leigh, C.T. McTernan, D.J. Tetlow, M. Wilson

**2:50 ORGN 539.** Artificial molecular machines that assemble oligomeric asymmetric catalysts. G. De Bo, M.A. Gall, S. Kuschel, J. De Winter, P. Gerbaux, D.A. Leigh

**3:10 ORGN 540.** Frame suspended into four Cucurbituril wheels: Meet the Ohio Bobcat Nanowagon. M. Ræsi, K. Kotturi, K. Perumal, R. Rabbani, S. Hla, E. Masson

**3:30 ORGN 541.** Efficient synthesis of *N*-heteroacenes, 1D graphene analogues, for organic electronics. R.C. Garcia, W. Zhang, C.B. Gorman

**3:50 ORGN 542.** Molecular electronic devices from selectively fluorinated self-assembled monolayers with controllable surface dipoles. R.C. Bruce, L. You, S. Pookpanratana, O. Pomeroy, C.A. Hacker

**4:10 ORGN 543.** Photoinduced electron transfer in conjugated oligomers. A.L. Jones, K.S. Schanze

**4:30 ORGN 544.** Development of high potential catholyte and low potential anolyte materials and their application in organic, non-aqueous redox flow batteries. K.H. Hendriks, C. Sevov, M. Cook, M.S. Sanford

**Section E**

Walter E. Washington Convention Center Room 201

**Total Synthesis of Complex Molecules**

R. D. Broene, *Organizer*

M. G. Donahue, *Presiding*

**1:15 ORGN 545.** Enantioselective total synthesis of the alkaloid (-)-haliclonin A. P. Huang

**1:35 ORGN 546.** Total synthesis of (+)-7-deoxypancratistatin from benzene. L.W. Hernandez, J. Pospech, U. Klöckner, D. Sarlah

**1:55 ORGN 547.** Synthetic studies toward dilemmaones A-C. K.E. Lambson, C.A. Dacko, J.M. McNeill, B. Soderberg

**2:15 ORGN 548.** Total synthesis and route optimization of Mcl-1 antagonist clinical candidate drug AZD5991. Q. Ye, A. Hird, J.W. Johannes, B. Peng, X. Zheng, Y. Wu, H. Wang, S. Mlynski, D. Perkins, C.A. Roberts, S. Stokes, D. Robbins, H. Huynh, M. Rego, M. Lindhagen, S. Karlsson, L. Thunberg, S. Swallow, C. Stewart, S. Li, C. Wu, Z. Liu, X. Zhao, X. Liu, H. Shen

**2:35 ORGN 549.** Selective, safe, scalable synthesis of a CC-90003, a covalent trifluoromethyl pyrimidine ERK 1&2 kinase inhibitor. J.F. Traverse, J. Han, N. Zou, R.M. Heid, A. Ferretti, K. Yong

**2:55 ORGN 550.** Chemical synthesis and absolute stereochemical determination of a ladderane phospholipid. C. Cohen, N.Z. Burns

**3:15 ORGN 551.** Enantioselective total synthesis of cannogenol and cannogenol-3-O-alpha-L-rhamnoside. B.T. Bhattacharai, P. Nagorny

**3:35 ORGN 552.** Spiro[4.5]cyclohexadienones as a platform for the synthesis of alkaloids and terpenes. M.G. Donahue

**Section F**

Walter E. Washington Convention Center Rooms 204A/B

**Molecular Recognition & Self-Assembly**

R. D. Broene, *Organizer*

M. Levine, *Presiding*

**1:20 ORGN 553.** Withdrawn.

**1:40 ORGN 554.** Intrahost interactions enhanced cation binding and π-π interactions in competitive solvents. X. Xing, Y. Zhao

**2:00 ORGN 555.** Water-soluble molecularly imprinted nanoparticles (MINPs) as turn-on fluorescence sensors. X. Xing, Y. Zhao

**2:20 ORGN 556.** Multistimuli-responsive release of dye/drug from cucurbit[7]uril functionalized MOP-based theranostic nanoparticle. S.K. Samanta, L.D. Isaacs

**2:40 ORGN 557.** Utilizing the G-quadruplex as a scaffold for [2+2] photocycloadditions of cinnamate esters. K. Sutyak, J. Davis

**3:00 ORGN 558.** Chiral self-recognition and supramolecular polymerization of [2.2]paracyclophane. D.E. Fagnani, M.J. Meese, K.A. Abboud, R.K. Castellano

**3:20 ORGN 559.** Molecularly imprinted cross-linked nanoparticles as artificial enzymes for biometric hydrolysis of activated esters. L. Hu, Y. Zhao

**3:40 ORGN 560.** Step-wise self-assembly and dynamic exchange of super snowflake shaped metallo-supramolecules. H. Wang, Z. Zhang, X. Li

**4:00 ORGN 561.** Metal ions fluorometric sensor based on [5]helicene derivatives. T. Sooksimuang, N. Wanichacheva, A. Petdum, N. Kaewnok, S. Jarutikorn, W. Klinpetch, W. Panchan, K. Kwanplod

**4:20 ORGN 562.** Self-assembly of oriented 2D porous organic cage crystals. S. Jiang, Q. Song, T. Hasell, A.I. Cooper

**4:40 ORGN 563.** Functionalized organic macrocycles for tunable anion and PAH detection. M. Levine, I. Tamgho

**WEDNESDAY EVENING**

**Section A**

Walter E. Washington Convention Center Hall E

**New Reactions & Methodology**

S. M. Silverman, *Organizer*

**7:00 - 9:00**

**ORGN 564.** Highly regioselective hydrochlorination of alkynes with a novel chlorinating reagent. S. Liang

**ORGN 565.** Efficient metal-free synthesis of perfluoroalkylated fluorenes. Z. Sun, Y. Wu, D. He, J. Chen, J. Han, H. Zhang, W. Cao

**ORGN 566.** Efficient synthesis of trifluoromethylated 5*H*-spiro[furan-2,3'-indolin]-2'-ones. L. Tao, J. Han, Z. Fan, J. Chen, H. Zhang, W. Cao

**ORGN 567.** Rh-catalyzed transannulation of 1,2,3-thiadiazoles with nitriles for the synthesis of isothiazoles. B. Seo, P.H. Lee

**ORGN 568.** Catalyst-dependent selectivity in sulfonium ylide cycloisomerisation reactions with pi-acid catalysts. R. Oost, J.D. Neuhaus, A. Oppedisano, N. Maulide

**ORGN 569.** Regiospecific synthesis of [2*H*]-indazoles from *N*-methoxyanthranilamides. E.J. Salaski, J. Esguerra, J. Etersque, M. Orlando, T. Puleo

**ORGN 570.** Development of enantioselective conjugative cross-coupling reactions. E. Edelstein, L. Zhang, G. Lovinger, A. Szymaniak, M. Chierchia, S. Namirembe, J.P. Morken

**ORGN 571.** Efficient copper-catalyzed amination from aryl chlorides to primary arylamines. J. Song, T. Yun, H. Jeon

ORGN **572**. NBS oxidation: The formation of esters. **J.D. Fair**, V. Bouch, M. Luderer, V. Causer

ORGN **573**. Design and synthesis of highly branched organocatalysts for site-selective acylation. **N. Ashush**, R. Palakuri, M. Portnoy

ORGN **574**. Brønsted base mediated regio- and stereoselective silaboration of alkynamides. **R. Fritzsche**, W. Santos

ORGN **575**. PhI-catalyzed  $\alpha$ -tosyloxylation of cyclopropyl methyl ketone. **W. Ma**, R.S. Ma, D.Z. Fang

ORGN **576**. Metal-free catalytic esterification of aldehydes with a variety of alcohols in the presence of poly(3,4-dimethyl-5-vinylthiazolium) iodide/DBU. **S. Chun**, Y.K. Chung

ORGN **577**. N-allylation by palladium-catalyzed cross-coupling of potassium allylBF<sub>3</sub>K and amines. **M. Al-Masum**, S. Alyahya, K. Liu

ORGN **578**. Diastereoselective intermolecular synthesis of medium sized cyclic ethers via prins-type cyclization. **A.J. Tomaine**, A.K. Ghosh

ORGN **579**. Chemoselective Baylis-Hillman reaction catalysis by Lewis base – metal bifunctional system. **A. Fallek**, M. Portnoy

ORGN **580**. One-pot concurrent synthesis of thiazolidinones and benzothiazepinones: A greener route. **D. Bandyopadhyay**, J. Strong

ORGN **581**. Stereochemical aspects of T3P amidations. **R.D. Barrows**, Z. Wang, T. Emge, S.A. Knapp

ORGN **582**. Reactivity of phenol in sulfur(VI) fluoride exchange chemistry. **J. Gurjar**, V.V. Fokin

ORGN **583**. Nucleophilic (radio)fluoro-click reaction enabled by of hydrogen bonding clusters. **X. Zeng**, B. Xu, G.B. Hammond

ORGN **584**. Development of iminium salt catalyzed nitrogen transfer reactions. **L.A. Combee**, B. Raya, D. Wang, M.K. Hillinski

ORGN **585**. Syntheses and electrochemical oxidation of disulfide compounds juxtaposing carbonyl groups. **T. Yamamoto**, K. Fukuta, Y. Esaka, B. Uno

ORGN **586**. Accessing highly substituted and functionalized beta-hydroxyboronate esters via dimerization and homologation of aldehydes. **T. Thane**, M.A. Nistler, C.J. Ferber, A.A. Ogtong, T.B. Clark

ORGN **587**. Synthesis of  $\alpha, \alpha, \alpha$ -dibromoketone catalyzed by 2-ast organosilane from alkynes. **J. Domena**, C. Chong, Y. Xing, B. Chauhan

ORGN **588**. Cobalt-catalyzed aerobic oxidative cyclization of 2-aminophenols with isocyanides. **J. Liu**, J. Hoover

ORGN **589**. Palladium catalyzed mono- $\gamma$ -arylation of 4-methylcoumarin. **M. Sexton**, J.R. Schmink

ORGN **590**. New method to synthesize thienopyridinone and thienodiazepinone derivatives. **N. Korkmaz Cokol**, M. Balci

ORGN **591**. Mn ter-pyridine complex catalyzed synthesis of imines through acceptorless dehydrogenation reaction of alcohol with amine. **H. Lim**, P. Chohan, P. Kaur

ORGN **592**. Transforming  $\alpha$ -amino acids to  $\alpha$ -aryl acids via nickel-catalyzed C–N bond activation. **K. Baker**, C. Basch, C. Shoffler, M. Hoerner, M.P. Watson

ORGN **593**. C–H trifluoromethylation of enamides: An oxidative approach. **V. Krishnamurti**, S.B. Munoz, G.S. Prakash

ORGN **594**. Shapiro elimination/epoxidation-based strategy for the synthesis of cage molecule building blocks. **L. Richert**, L. Sanchez

ORGN **595**. Development of metal-free bifunctionalization reaction of olefins leading to higher functionalized lactones. **S. Maejima**, A. Itoh, E. Yamaguchi

ORGN **596**. Investigating the reactivity of HCl/DMPU and HBr/DMPU reagents with unsaturated systems. **R. Ebulue**

ORGN **597**. Novel synthesis of phenanthridinones via oxidative C–H amidation using iodobenzene (PhI)-catalysis. **N.K. Nguyen**, D. Liang, W. Yu, J. Deschamps, G. Imler, Y. Li, A. MacKerell, C. Jiang, F. Xue

ORGN **598**. Methyl transfer from methylboronic acid or dimethyl carbonate for O–H and C–H alkylation. **M. Bartlett**, B. Habteselassie, Y. Zhu, N. Martinez-Munoz, C. Jacobson, S. Abreu, D.J. Gorin

ORGN **599**. Synthesis of 2-acylbenzo[b]thiophenes via Cu-catalyzed  $\alpha$ -C–H functionalization of 2-haloalcohols using xanthate. **S. Subramani**, S. Govindasamy

ORGN **600**. Progress towards the cross-coupling of sp<sup>3</sup> carbons using hypervalent iodine. **C. Mowdawalla**, F. Ahmed, L. Dave, G. Kim, I.D. Hyatt

ORGN **601**. Accessing fused ring systems through trimethylene-methane intermediates by initiation with hypervalent iodonium alkynyl triflates. **T. Li**, K. Pham, I.D. Hyatt

ORGN **602**. Novel synthesis of asymmetrical substituted diazidindinones from simple isocyanates. **R.M. Dare**, N. Cinti, L. Gerstein, G. Moura-Letts

ORGN **603**. Diastereoselective synthesis of complex heterocycles from the intramolecular cycloaddition of substituted alkenyldiaziridines. **A. Paneque**, A. Zinsky, G. Haun, G. Moura-Letts

ORGN **604**. Studies towards the stereoselective haloamination of alkenes. **L. Mir**, N. Chang, B. Selover, G. Moura-Letts

ORGN **605**. Multicomponent reactions for the direct stereoselective synthesis of complex vinyl-isooxazolidines. **D. Quinn**, L. Tumbelty, E. Moscarello, A. Paneque, A. Zinsky, M. Russ, G.J. Haun, G. Moura-Letts

ORGN **606**. Applying process intensification principles to the synthesis of the anti-retroviral drug lamivudine. **S.A. James**, F. Gupton, K. Belecki

ORGN **607**. Withdrawn.

ORGN **608**. Synthesis of cyclic ethers via oxidative rearrangement with (poly)cationic hypervalent iodine reagents. **J.C. Walters**, A.F. Tierno, S. Wengryniuk

ORGN **609**. Withdrawn.

ORGN **610**. Novel synthesis of fused-cyclic ethers via cycloaddition reactions of aldehydes and substituted cyclopropanes. **N.T. Bonney**, J.D. Horgan, G. Moura-Letts

ORGN **611**. Recyclable synthesis of  $\alpha, \alpha, \alpha$ -dibromoketones catalyzed by organosilanes from alkynes. **C. Chong**, J. Domena, Y. Xing, B. Chauhan

ORGN **612**. Electrophilic activation and domino reaction of arylated propargylic alcohols toward naphthyl(aryl)iodonium salts. **R.J. Hinkle**, S.E. Bredenkamp, S.J. Cheon

Section B

Walter E. Washington Convention Center Hall E

Heterocycles & Aromatics

S. M. Silverman, Organizer

7:00 - 9:00

ORGN **613**. Photophysical investigations of the solvent effect on the properties of thienophene-quinoline derivatives. **G.C. Santos**, L.C. da Silva Filho

ORGN **614**. Synthetic studies towards the indole alkaloids kottamides **A-E**. **R. White**, B. Copp, D. Barker

ORGN **616**. Withdrawn.

ORGN **617**. Synthesis of squaraine and croconine dyes for potential use in OPV solar cells. **J.A. Cody**, C.J. Collison, C. Zheng, A. Snyder, A. Murphy Shaw

ORGN **618**. Synthesis of pyrazole-fused 7-membered lactones via regioselective Claisen rearrangement and hydroesterification. **H. Ichikawa**, H. Takashima

ORGN **619**. Synthesis of bicyclic pyridines by iron mediated intramolecular radical cyclization. **J. Starr**, S. Bordi

ORGN **620**. Regiospecific *p*-brominations and *p*-iodinations: Perturbing secondary electronic effects. **S. Gumus**, J.R. Thomas, D.W. Slocum

ORGN **621**. Sustainable catalytic C–C bond formation with fluoroenolates. **M. Moskowitz**, C. Wolf

ORGN **622**. Regioselective alkylation of 5-alkyl-pyrazole-3-carboxylic esters: Application in the efficient synthesis of potent tankyrase inhibitors. **D. Dorsch**, D. Radtke, H. Buchstaller

ORGN **623**. Synthesis and cytotoxicity of functionalized heterocycles via multicomponent coupling reactions. **P. Suman**, A. Patel, D.C. Morgan, A.J. Vendola, R.M. Rutkoski, P.M. Mastoridis, S.C. Jonnalagadda

ORGN **624**. Green chemistry reaction of 1,4-naphthoquinone with anilines through an EDA complex. **E. Leyva**, A. Cárdenas-Chaparro, S. Loredó-Carrillo, M. Méndez-Sánchez, A. Martínez-Richa

ORGN **625**. Development and utilization of Mitsunobu glycosylation conditions to install pyrrolopyrimidine nucleobases onto a ribose core. **F. Wang**, D. Bernhardson, D. Richter, R. Patman, R. Maguire, I.J. McAlpine

ORGN **626**. Transition-metal-catalyzed one-pot synthesis of indole-fused polyaromatic heterocycles. **P. Sang**, J. Cai

ORGN **627**. Synthesis and chiral resolution of *N*-substituted 8-hydroxyphenylmorphans: Potential ligands for the Mu and delta opioid receptors. **T. Irvin**, Y. Peng, A.E. Jacobson, K.C. Rice

ORGN **628**. Synthesis of heterocyclic indolizines and its antibacterial activity study. **M. Zhang**, Y. Xing, K. Martin

ORGN **629**. Conformational changes in polyaromatic substituted 5,15-calic[4]pyrins upon anion binding. **S. Arora**, S. Chauhan

ORGN **630**. Synthesis of 2-(iodomethylene)-2,3-dihydro-1,4-oxazepines. **M. Zora**, E. Dikmen, Y. Kelgokmen

ORGN **631**. Strategies for the synthesis of Romeo and Juliet blue. **B. Dawson**, M.J. Samide, G.D. Smith, A.M. Wilson

ORGN **632**. Cyclization of  $\alpha, \beta$ -unsaturated oximes. **N.A. Burr**, M.D. Mosher

ORGN **633**. 2-(Pyrrole-2-yl)vinyl-substituted BODIPY as near-IR fluorophore. **S. Ansteatt**, M. Ptaszek

ORGN **634**. Synthesis of 2-substituted  $\alpha$ -carbonyl via synergistic methods. **F.G. Nguete Meke**, S. Wrenn, B. Cho, B.L. DeBoef, S.P. Mulcahy

ORGN **635**. Three-component cyclization of disubstituted pyrrol-2-ones: Synthesis and biological evaluation of the 5-hydroxyindole natural product, violacein. **A. Oppong-Holmes**, Z.E. Oppong-Holmes, J. Kaplitt, M.W. Norman, M. Hwee, E.C. McLaughlin

Section C

Walter E. Washington Convention Center Hall E

Photoredox Chemistry

S. M. Silverman, Organizer

7:00 - 9:00

ORGN **636**. Photoredox multicatalysis: Novel methods for the construction of C–C and C–heteroatom bonds. **V.W. Shurtliff**, J.A. Terrett, M. Shaw, J. Cuthbertson, D.W. MacMillan

ORGN **637**. Synthesis of aliphatic ketones via N–C bond cleavage of imides under photoredox/Ni dual catalysis. **R. Alam**, J. Amani, S. Badir, G.A. Molander

ORGN **638**. Direct diazomethylation of aromatic C–H bonds via photoredox catalysis. **Z. Wang**, A.M. del Hoyo, A.G. Herrera, M.G. Suero

ORGN **639**. Visible-light induced redox-neutral multicomponent radical reaction of  $\beta$ -functionalized  $\delta$ -diketones. **F. Pettersson**, G. Bergonzini

ORGN **640**. Photoredox catalyzed CH alkylation of heteroarenes: A mild approach for late stage functionalization. **J.K. Matsui**, G.A. Molander

ORGN **641**. Accessing *gem*-difluoroalkenes via photoredox catalysis. **R. Wiles**, S.B. Lang, C. Kelly, G.A. Molander

ORGN **642**. Withdrawn.

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ORGN **643.** Accessing uncharted chemical space via photoredox catalysis. C. Kelly, S.B. Lang, R. Wiles, K. Lin, G.H. Davies, C. Remeur, N. Patel, G.A. Molander

ORGN **644.** Enantioselective  $\alpha$ -alkylation of ketones by synergistic Lewis acid - photoredox catalysis: Formation of  $\beta$ -cyano ketones via a chiral iridium complex. J. Zbieg, A. Cholewczynski, L. Smith

**Section D**

Walter E. Washington Convention Center Hall E

**Total Synthesis of Complex Molecules**

S. M. Silverman, *Organizer*

7:00 - 9:00

ORGN **645.** Total synthesis, analysis and theoretical studies towards the characterisation of bioactive grape and wine metabolites. S. Tan, D. Barker, B. Fedrizzi

ORGN **646.** Ligand synthesis for aqueous metal detection. M.W. Fultz, M. Bright, J.P. Rickett

ORGN **647.** Asymmetric total synthesis of (+)-psiguadial B. M. Kinebuchi, R. Uematsu, K. Tanino

ORGN **648.** Total synthesis of four tricyclic azepinoindole alkaloids: Aurantioclavine, clavicipitic acid and hyrtioreticulon C and D. G. Ghimire, B. Soderberg

ORGN **649.** Synthesis and biological evaluation of 5,7-dihydroxyflavanone derivatives as potential antimicrobial agents. X. Zhang, O. Khalidi, S. Kim, R. Wang, V. Schultz, B. Cress, R.A. Gross, M. Koffas, R.J. Linhardt

ORGN **650.** Total synthesis of bioactive diterpene, parvifloron F. Y. Saito, M. Goto, K. Goto

ORGN **651.** Total synthesis of dictyodendrins by the gold-catalyzed intermolecular cascade cyclization of conjugated diynes with pyrroles. J. Matsuoka, Y. Matsuda, Y. Kawada, S. Oishi, H. Ohno

ORGN **652.** Withdrawn.

ORGN **653.** Synthesis of novel N6-substituted S-adenosyl-L-methionine analogues. N. Bremner-Hay, L. Comstock

ORGN **654.** Studies toward the synthesis of *ent*-artemisin: A potential anti-malarial compound. E. Steiner, M. Hejna, L. Sanchez

ORGN **655.** Synthetic studies towards the total synthesis of opaliferin. G. Opiyo, D.P. Furkert, M. Brimble

ORGN **656.** Progress toward the synthesis of the diospongin and related natural products. J. More, J. Deegan, M. Kirpas, D. Napack

ORGN **657.** Synthesis of ipomoeassin F analogs with a tail modified aglycone. A. May, G. Zong, E. Barber, W. Shi

ORGN **658.** Synthetic pathway to a modulator of mGluR5. W. Arce, B. Curtis, A. Cox, M. Flores, S. Sapati, E. Jurado Bustamante, K.J. Friedrich

ORGN **659.** Efforts towards the total synthesis of sanctolide A and the C2-epimer of sanctolide A. C.N. Ndi, J.L. Markley, G.C. Dissanayake, P.R. Hanson

ORGN **660.** Synthesis of complex small molecules with various biological activities: Total synthesis and structure design. R. Rafferty

**THURSDAY MORNING**

**Section B**

Walter E. Washington Convention Center Room 207A

**CH Activation**

R. D. Broene, *Organizer*

D. Powers, *Presiding*

8:10 ORGN **661.** Catalytic reductive ortho-C-H silylation of phenols with traceless, versatile acetal directing groups. P. Asgari, Y. Hua, T. Avullala, J. Jeon

8:30 ORGN **662.** Constructing new chemical bonds via transition metal catalyzed C-H activation and functionalization. L. Wang

8:50 ORGN **663.** Pseudohalide assisted aerobic oxidation of alcohols and alkanes in presence of visible-light. S. Shah, N.P. Singh

9:10 ORGN **664.** Palladium mediated C-H tritiation. A. Hoover, H. Yang, D. Hesk, N. Rivera

9:30 ORGN **665.** C-H fluorination mediated by a non-heme manganese complex. X. Chen, J.T. Groves

9:50 ORGN **666.** Pd(II) catalyzed allylic C-H oxidative amidation: Sustainable approach for functionalization of N-heterocycles. S. Vemula, D. Kumar, G.R. Cook

10:10 ORGN **667.** Cu catalyzed sp<sup>3</sup> C-H amidation: Catalyst controlled site selectivity. T.H. Warren, A. Bakhoda

10:30 ORGN **668.** New redox mediators for aerobic C-H oxidation chemistry. D. Powers, A. Maity, S. Hyun

**Section C**

Walter E. Washington Convention Center Room 206

**Chemistry of Fullerenes, Carbon Nanotubes, Nanomaterials & Graphene**

R. D. Broene, *Organizer*

K. E. Whitener, *Presiding*

8:20 ORGN **669.** Ultra-high thermal effusivity materials for resonant, ambient thermal energy harvesting. A. Cottrill, A.T. Liu, Y. Kunai, M. Strano

8:40 ORGN **670.** Synthesis and characterization of cucurbit[7]uril-based conjugated polyrotaxanes and further enhancement of their fluorescent quantum yields by embedding them into crystalline matrices. D. Tuncel

9:00 ORGN **671.** Development of prodrug approaches for long-acting nanoformulations of emtricitabine-based regimens. A. Al-Khouja, J.J. Hobson, D. Meyers, P. Curley, J.M. Siliciano, R.F. Siliciano, M. Siccardi, A. Owen, C. Flexner, S. Rannard, C.L. Meyers

9:20 ORGN **672.** Rational design of covalent organic cages via alkyne metathesis. T.P. Moneyppenny, J.S. Moore

9:40 ORGN **673.** Preserving chemically modified graphene from thermal and chemical loss of functionality. K.E. Whitener, W. Lee, R. Stine, J.T. Robinson, D.A. Kidwell, C. Tamanaha, P.E. Sheehan

10:00 ORGN **674.** Molecular dyads and triads based on phenothiazine, Ru(II) bisterpyridine complexes and fullerene. A. Winter, K. Barthelmes, Y. Luo, J. Kübel, M. Wächter, B. Dietzek, U.S. Schubert

10:20 ORGN **675.** Boranephosphonate DNA mediated metallization of single walled carbon nanotubes. S. Ganguly, S. Paul, O. Yehezkeili, J. Cha, M.H. Caruthers

10:40 ORGN **676.** Impact of graphitic nitrogen on bowl-shaped  $\pi$ -conjugated molecules: Supramolecular chemistry and reactivity. S. Hiroto, H. Yokoi, M. Takeda, H. Shinokubo

**Section D**

Walter E. Washington Convention Center Room 207B

**Materials, Devices & Switches**

R. D. Broene, *Organizer*

H. Liu, *Presiding*

8:10 ORGN **677.** Influences of out-of-plane lattice alignment on the OFET performance of TIPS-PEN crystal arrays. K. Wu, C. Wang

8:30 ORGN **678.** Organic optical material for broadband sensor protection. J. Shi, R. O'Donnell, W. Shensky, M. Ferry, T. Enslay

8:50 ORGN **679.** Novel oligo and polyacenes towards intramolecular singlet fission devices. A. Pun, L. Campos

9:10 ORGN **680.** Withdrawn.

9:30 ORGN **681.** Self-organizing derivatives of benzo[e][1,2,4]triazinyl and their magnetic behavior. P. Kaszynski, M. Jasinski, S. Kapuscinski, J. Szczytko, D. Pocięcha, A.C. Friedl

9:50 ORGN **682.** Are guanidinium organodisulfonates formally microporous? I. Brekalo, D. Deliz, K.T. Holman

10:10 ORGN **683.** Expanding the role of PDI in small molecule non-fullerene acceptors. J.A. Schneider, Y. Zheng, H. Wang, H. Nakayama, F. Wudl

10:30 ORGN **684.** Near-infrared fluorescent probes for selective and sensitive detection of lysosomal pH in live cells. H. Liu, H. Lee, A. Tiwari

10:50 ORGN **685.** New types of container molecules that can transport MCl<sub>2</sub> fragments. S. Kharel, J.A. Gladysz, J. Blumel

11:10 ORGN **686.** Boron dipyrrolylmethene (DIPYR) dyes: Shedding new light on pyridine-based chromophores. J.H. Golden, D.S. M. R., M.E. Thompson

11:30 ORGN **687.** Tuning of charge carriers using electron deficient thiophenes. J. Low, B. Capozzi, J. Cui, S. Wei, L. Venkataraman, L.M. Campos

**Section E**

Walter E. Washington Convention Center Rooms 204A/B

**Total Synthesis of Complex Molecules**

R. D. Broene, *Organizer*

R. Rafferty, *Presiding*

8:30 ORGN **688.** One-pot sequential strategies for the synthesis of natural products and their analogues. C.N. Ndi, P.R. Hanson

8:50 ORGN **689.** Synthesis and antibacterial screening of ( $\pm$ )-6,8-dihydroxy-3-undecyl-3,4-dihydroisochromen-1-one: A structural analog of metabolites from *Ononis natrix*. H. Rafique

9:10 ORGN **690.** Withdrawn.

9:30 ORGN **691.** Phosphate tether-mediated approach for the efficient syntheses of 13-desmethyl-lyngboullouside and simplified analogs. A. Ganguly, S. Javed, G.C. Dissanayake, D. Vithanage, P.R. Hanson

9:50 ORGN **692.** Total synthesis and SAR studies of the melokhanine family of natural products. P. Williams, J.G. Pierce

10:10 ORGN **693.** Lagunamide C: The quest for structural confirmation via total synthesis and biological evaluation. C. Weese, A. Fatino, L. Lawlor, Y. Zhang, R. Rafferty

10:30 ORGN **694.** Brocazine F&G: Total synthesis efforts and small molecule construction for investigations into molecular transport about complex barriers. W. Hulangamuwa, P. Desman, A.I. Lansakara, R. Rafferty

10:50 ORGN **695.** Synthesis of a regiomeric-7N-methyl-aspidostomide D, through epoxide opening strategy with Lewis acid. M.H. Althaf Hussain, F.A. Khan

**Section F**

Walter E. Washington Convention Center Room 201

**Molecular Recognition & Self-Assembly**

R. D. Broene, *Organizer*

M. D. Pluth, *Presiding*

8:00 ORGN **696.** Hierarchical assembly of a low energy gap p-conjugated oligomer via synergetic halogen and hydrogen bonding. A. Weldeab, S.T. Nyguen, D.J. Starkenburg, K.A. Abboud, J. Xue, R.K. Castellano, D.L. Watkins

8:20 ORGN **697.** Host-guest systems derived from deconstructed Hamilton receptors. M.D. Pluth

8:40 ORGN **698.** Foldamer-mediated structural rearrangement in A $\beta$  and vice-versa: A possible strategy for Alzheimer's therapeutics. S. Kumar, A. Hamilton

9:00 ORGN **699.** Design and self-assembly of different generation of metallomacrocycles from triphenylamine motif. L. Wang, X. Li

9:20 ORGN **700.** Reversed Hofmeister effects in synthetic hosts. J.H. Jordan, C.L. Gibb, A. Wishard, B.C. Gibb

9:40 ORGN **701.** Dual-stimuli induced shape transition of programmable DNA block copolymers. C. Kim, S. Park

**Technical program information known at press time.**

The official technical program for the 254th ACS National Meeting is available at [www.acs.org/WDC2017](http://www.acs.org/WDC2017)

†Cooperative Cosponsorship

**10:00 ORGN 702.** Artificial zinc enzymes based on molecularly imprinted cross-linked micelles for selective hydrolysis. M. Arifuzzaman, Y. Zhao

**10:20 ORGN 703.** Probing interactions between hydrocarbons and auxiliary guests inside cucurbit[8]uril. R. Rabbani, E. Masson

**10:40 ORGN 704.** Sequence control in dynamic metallo-supramolecular oligomers assembled with cucurbit[8]uril. K. Kotturi

**Synthesis & Chemistry of Agrochemicals**

Sponsored by AGRO, Cosponsored by ORGN

**THURSDAY AFTERNOON**

**Synthesis & Chemistry of Agrochemicals**

Sponsored by AGRO, Cosponsored by ORGN

**PHYS**

**Division of Physical Chemistry**

J. Shea, Program Chair

**OTHER SYMPOSIA OF INTEREST:**

**Advanced Electrocatalysis for Energy Conversion & Storage** (see CATL, Sun, Mon)

**Simulations of Polymeric Materials: Molecular- to Macroscale** (see POLY, Sun, Mon)

**Advances in Computational Catalysis** (see CATL, Mon, Tue, Wed)

**Photoresponsive Nanoparticles: From Fundamentals of Excitation to Applications Systems** (see ENVR, Mon, Tue, Wed, Thu)

**New Directions in Conformational Sampling Methods** (see COMP, Tue)

**SOCIAL EVENTS:**

JPC-PHYS Reception, 5:00 PM: Tue

**SUNDAY MORNING**

**Section A**

Walter E. Washington Convention Center Room 156

**Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets**

**PAHs & the Organic Inventory of the Gas Phase: Observations, Theory & Experiments**

P. Bera, X. Tielens, Organizers

J. Bouwman, Presiding

**8:00 PHYS 1.** Some key questions involving PAHs and astrochemistry. L.J. Allamandola

**8:35 PHYS 2.** Polycyclic aromatic hydrocarbons and related forms of interstellar carbon. G. Sloan

**9:05 PHYS 3.** Astronomical modelling of interstellar PAHs. O. Berné

9:35 Intermission.

**10:05 PHYS 4.** High-resolution IR spectroscopy of the isolated aromatic universe: Bad vibrations at work. W.J. Buma, E. Maltseva, A. Petrignani, J. Oomens, C. Mackie, A. Candian, X. Tielens, T.J. Lee, X. Huang

**10:35 PHYS 5.** Computation of the infrared spectra of polycyclic aromatic hydrocarbons. C.W. Bauschlicher

**11:05 PHYS 6.** Signatures and evolution of astronomical aromatic molecules. S.D. Wiersma, A. Candian, W. Roeterdink, J. Bakker, J. Oomens, W.J. Buma, A. Petrignani

**Section B**

Walter E. Washington Convention Center Room 152B

**Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann**

**Electronic Structure & Reactivity of Organic and Organometallic Compounds**

W. Grochala, E. Zurek, Organizers

O. G. Eisenstein, Presiding

8:00 Introductory Remarks.

**8:20 PHYS 7.** Structural chemistry, fuzzy logic and the law. J. Bernstein

**8:50 PHYS 8.** Rational design of Fe-based catalysts for Fischer-Tropsch synthesis from theoretical prediction to experimental confirmation. X. Wen, Y. Yang, Y. Li

**9:20 PHYS 9.** Ligand noninnocence in metallocorroles: Insights from optical and X-ray absorption spectroscopies. A. Ghosh

**9:40 PHYS 10.**  $\pi$ -stacking pancake bonding. M. Kertesz

10:00 Intermission.

**10:20 PHYS 11.** Planar hypercoordinate carbon atoms. G. Merino

**10:50 PHYS 12.** Roald Hoffmann's role in the development of the Woodward-Hoffmann Rules. J. Seeman

**11:20 PHYS 13.** Orbital control of single molecule conductivities and electrical switching properties of organometallic complexes. H. Berke, F. Lissel, F. Schwarz, G. Kastlunger, E. Lörtscher, R. Stadler, K. Venkatesan, H. Riel

**11:40 PHYS 14.** Organic chemistry at Stony Brook: Learning the basics with a glimpse at the complex yet to come. J.W. Lauher

**Section C**

Walter E. Washington Convention Center Room 152A

**Liquid Theory: Symposium in honor of Ben Widom**

K. Koga, R. F. Loring, Organizers

D. Ben-Amotz, Organizer, Presiding

8:00 Introductory Remarks.

**8:05 PHYS 15.** RNA branching, and the size of long RNA molecules. W.M. Gelbart, S. Singaram, A. Ben-Shaul

**8:35 PHYS 16.** From complex fluids and interfaces to very complex fluids and even more complex interfaces. K.A. Dawson

**9:05 PHYS 17.** Topology in biology. J. Yeomans

9:35 PHYS 18. Withdrawn.

10:05 Intermission.

**10:20 PHYS 19.** Van der Waals disappointed: First experimental tests of mean-field theory. J. Levelt Sengers

**10:40 PHYS 20.** Finding simplicity in complexity: Lessons I have learned from Ben Widom. M.A. Anisimov

**11:00 PHYS 21.** Integral equation theory of coarse-graining. M. Guenza

**11:20 PHYS 22.** Are there two forms of liquid water? Can the Widom Line settle the dispute? H.E. Stanley

**Section D**

Walter E. Washington Convention Center Room 151A

**Electronic Structure Methods for Complex Chemical Systems**

**Many-body Perturbation Theory, Random Phase Approximation & Beyond**

Cosponsored by COMP

F. U. Furche, S. Sharifzadeh, J. J. Shepherd, Organizers

A. Grüneis, Presiding

8:00 Introductory Remarks.

**8:05 PHYS 23.** Excited-state phenomena in condensed matter: GW, GW-BSE, and beyond. S.G. Louie

**8:30 PHYS 24.** Electronic excitations at solid-liquid interfaces. J. Lischner

**8:55 PHYS 25.** Real-space representation of electron-hole interaction kernel in excitonic systems. A. Chakraborty

9:10 Intermission.

**9:20 PHYS 26.** Effect of crystal packing on the electronic properties of molecular crystals. N. Marom

**9:45 PHYS 601.** Effect of crystal packing on the excitonic properties of rubrene polymorphs. X. Wang, T. Garcia, S. Monaco, B. Schatschneider, N. Marom

**10:00 PHYS 27.** The optical properties of stilbene from first-principles. K. Lewis, C.B. Rinderspacher, S. Sharifzadeh, J. Andzelm

**10:15 PHYS 28.** Beyond RPA: Kernels and renormalization. A. Ruzsinszky

**10:40 PHYS 29.** Convergence behavior of RPA renormalized many-body perturbation theory and applications to periodic systems. J.E. Bates, N. Sengupta, J. Sensenig, A. Ruzsinszky

10:55 Intermission.

**11:05 PHYS 30.** Self-consistent temperature dependent Green's function methods applied to solids and molecules. D. Zgid, A. Rusakov, S. Isakov

**11:30 PHYS 31.** Combining density functional theory and Green's function theory: Range-separated, non-local, dynamic hybrid functional. A. Kananenka, D. Zgid

**11:45 PHYS 32.** Towards rigorous *ab initio* quantum embedding for realistic systems in the framework of Green's function theory. L. Tran, A. Kananenka, D. Zgid

**Section E**

Walter E. Washington Convention Center Rooms 159A/B

**Spectroscopic & Computational Insights into Solid/Liquid Interfaces for Energy Conversion**

**First Principles Modeling of Liquid/Solid Interfaces**

K. L. Jungjohann, J. A. Keith, Organizers

A. Heyden, Presiding

**8:00 PHYS 33.** Modelling metal electrolyte interfaces from density functional theory based molecular dynamics. J. Le, M. Iannuzzi, A. Cuesta, J. Cheng

**8:20 PHYS 34.** Quantum/continuum simulations of solid/liquid interfaces under applied voltage. I. Dabo

**8:55 PHYS 35.** Integrating first principles theory and experimental characterization at the solid/liquid interface. K. Letchworth-Weaver

**9:30 PHYS 36.** Catalysis at the solid-liquid interface: Tools and challenges. A. Heyden, M.S. Saleheen

10:05 Intermission.

**10:20 PHYS 37.** Cation effects on Pt electrode surface chemistry – insights from DFT. M.J. Janik, I.T. McCrum

**10:55 PHYS 38.** Modeling solid-liquid interfaces in batteries: Degradation/acid-base reactions, electric double layers, and challenges. K. Leung

**11:30 PHYS 39.** *Ab initio* studies of ultrathin ionic liquid films on Au (111) surface. M. Liu, Q. Wu

**Section F**

Walter E. Washington Convention Center Rooms 158A/B

**Experimental & Computational Advances in Understanding Enzyme Specificity & Promiscuity**

**Catalytic Promiscuity & the Emergence of New Proteins**

Cosponsored by BIOL and COMP

Financially supported by Gaussian, Elsevier, Pfizer, DSM, SCM: Software for Chemistry and Materials, PCCP: Physical Chemistry Chemical Physics, F1000: Faculty of 1000

Q. Cui, G. J. Poelarends, N. Tokuriki, Organizers

S. C. Kamerlin, Organizer, Presiding

8:00 Introductory Remarks.

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