

# ORGN

## Division of Organic Chemistry

S. Silverman and E. McLaughlin, *Program Chairs*

### SUNDAY MORNING

Section A

San Diego Convention Center  
Room 7B

#### New Reactions & Methodology

S. M. Silverman, *Organizer*  
G. Alachouzos, *Presiding*

**8:00 ORGN 1.** Cyclization strategies for the synthesis of complex halocyclopentenes.  
**G. Alachouzos**, A.J. Frontier

**8:20 ORGN 2.** Chemoselective reductive N-alkylation of amines with carboxylic acids under hydrosilylation conditions and direct functionalization. **P. Trillo**, H. Adolfsson

**8:40 ORGN 3.** Turning waste into value: New trifluoromethylation reactions with fluoroform-derived  $\text{CuCF}_3$ . **G. Tsui**

**9:00 ORGN 4.** Application of bond cleavage reactions for removal of directing groups. **H. XIN**, T. Deguchi, W. Akkad, H. Morimoto, T. Ohshima

**9:20 ORGN 5.** Diastereoselective iridium catalyzed amination of biosourced isohexides through borrowing hydrogen methodology. M. Jacolot, S. Moebs, **F. Popowycz**

**9:40 ORGN 6.** Development of catalytic aza-Nazarov cyclization reactions. **Y.E. Turkmen**

**10:00 ORGN 7.** Iterative Csp<sup>3</sup> bond formation: Second-generation automated synthesizer. S. Chitti, D. Kostyra, S.G. Ballmer, R. Hansen, **D.J. Blair**, M.D. Burke

**10:20 ORGN 8.** Halogen bond organocatalysis. **P.H. Toy**

**10:40 ORGN 9.** Domino stereoselective synthesis of  $\beta,\gamma$ -unsaturated ketones from alkenylboronic acids and tosylhydrazone-tethered nitriles. **L. Florentino**, C. Valdés

**11:00 ORGN 10.** Olefin-accelerated C-N cross-coupling in the solid-state. **K. Kubota**, T. Seo, K. Koide, Y. Hasegawa, H. Ito

**11:20 ORGN 11.** Catalytic aerobic oxidations of alcohols and aldehydes. **S. Ma**

**11:40 ORGN 12.** <sup>18</sup>F-deoxyfluorination of phenols via Ru  $\pi$ -complexes for the synthesis of positron emission tomography (PET) tracers. **M. Beyzavi**, D. Mandal, M. Strebl, C. N. Neuman, E. D'AMATO, J. Chen, J. M. Hooker, T. Ritter

Section B

San Diego Convention Center  
Room 10

### **Asymmetric Reactions & Syntheses**

S. M. Silverman, *Organizer*  
T. Benkovics, *Presiding*

**8:00 ORGN 13.** Asymmetric nucleophilic fluorination under hydrogen bonding phase-transfer catalysis. **G. Pupo**, F. Ibba, D. Ascough, A. Vicini, J.M. Brown, R.S. Paton, V. Gouverneur

**8:20 ORGN 14.** Stereospecific nickel-catalyzed cross-coupling and cross-electrophile couplings of sulfonamides. **K.A. Hewitt**, E. Lucas, E.R. Jarvo

**8:40 ORGN 15.** Chiral derivatization of sulfinamides for <sup>1</sup>H NMR enantiomeric excess determination and chiral resolution. **R. Groleau**, T.D. James, S.D. Bull

**9:00 ORGN 16.** Accelerated asymmetric reaction screening and sensing of chiral compounds using small molecular probes. **F.Y. Thanzeel**, C. Wolf

**9:20 ORGN 17.** Iridium-catalyzed asymmetric allylic fluoroalkylation reactions.  
**T.W. Butcher**, J.L. Yang, J.F. Hartwig

**9:40 ORGN 18.** Stereodivergent synthesis of  $\beta$ -amino alkylboronic acids by diastereocontrolled mono-protodeboronation of *gem*-diboryl precursors. X. Li, **D.G. Hall**

**10:00 ORGN 19.** Catalytic asymmetric [3+2] annulation with allenylsilanes for the synthesis of spirocyclopentene oxindoles with vinylsilane functionality. **A. Cobos**, A.K. Franz

**10:20 ORGN 20.** Enantioselective carbene insertion into silanes: Access to chiral benzhydryl silanes. **J. Jagannathan**, A.K. Franz

**10:40 ORGN 21.** Catalytic asymmetric heteroatom Diels–Alder reactions catalyzed by VANOL-derived chiral borate catalysts. **L. Zheng**, X. Yin, W.D. Wulff

**11:00 ORGN 22.** Computer-assisted design of asymmetric copper-catalyzed borylation of terminal aliphatic alkenes. H. Iwamoto, T. Imamoto, **H. Ito**

**11:20 ORGN 23.** Iterative synthesis of Csp<sup>3</sup> rich small molecules by using bifunctional carbenoid-boronate building blocks. **S. Chitti**, D. Kostyra, D. Blair, M.D. Burke

**11:40 ORGN 24.** Ketoreductase enabled synthetic strategy to chiral bicyclic piperidine building blocks. **T. Benkovics**, J. McIntosh, A.J. Neel, D. Lehnerr, C.E. Suh

Section C

San Diego Convention Center  
Room 9

### **CH Activation**

S. M. Silverman, *Organizer*  
G. Hughes, *Presiding*

**8:00 ORGN 25.** Using two diarylacetylenes as an implicit benzofulvene for benzofulvenation of *o*-arylanilines through palladium-catalyzed C–H bond activation.  
**S. Chuang**

**8:20 ORGN 26.** Regio- and stereoselective palladium-catalyzed C(sp<sup>3</sup>)-H arylation of pyrrolidines and piperidines with C(3) directing groups. **D. Antermite**, J.A. Bull

**8:40 ORGN 27.** Weakly coordinating, ketone-directed cobalt(III)-catalyzed C-H allylation, alkenylation, and vinylation: Easy access to the simple and useful structural motifs. **M. Sk**, M. Maji

**9:00 ORGN 28.**  $\alpha$ -C-H activation of oxygen-containing heterocycles using organolithium reagents. **K. Kasten**, N. Seling, A. Kwong, M. Atobe, P. O'Brien

**9:20 ORGN 29.** Designing of templates to reach the distal C-H bond. **D. Maiti**

**9:40 ORGN 30.** Explaining the regioselectivity of rhodium(II)-catalyzed C-H functionalization of strained bicyclo[1.1.1]pentanes. **J.N. Sanders**, Z.J. Garlets, H.M. Davies, K.N. Houk

**10:00 ORGN 31.** Iridium-catalysed hydrogen isotope exchange of amino acid and peptide molecules. **A. Queen**, W.J. Kerr, D. Hesk, D.M. Lindsay, H. Yang

**10:20 ORGN 32.** Directed C-H activation using cobalt or iridium: Applications in medicinal chemistry. **M.J. Johansson**, L. Ackermann, B. Martin-Matute, S.D. Friis, E. Weis

**10:40 ORGN 33.** Iridium-catalyzed monoselective C-H iodination of benzoic acids: Development and mechanistic investigation. **E. Weis**, M.J. Johansson, B. Martin-Matute

**11:00 ORGN 34.** Heterocycle synthesis via C-H functionalization. **M. Shea**, D. Nagib, A. Prusnowski

**11:20 ORGN 35.** Site-selective C-H functionalization via palladium/norbornene catalysis. **J. Wang**, G. Dong

**11:40 ORGN 36.** Mechanistic insights and method development of selective photochemical fluorination of polycyclic terpenoid derivatives. **F. Ghorbani**, S.A. Harry, T. Lectka

Section D

San Diego Convention Center  
Room 8

## **Copper-Catalyzed C-Element Bond Cross-Coupling with Arylboronic Acids: Twentieth Anniversary of Chan-Lam Reaction Discovery**

Y. Du, A. J. Watson, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:35 ORGN 37.** Twentieth anniversary of Chan–Lam reaction. **P.Y. Lam**

**8:55 ORGN 38.** Copper-catalyzed *N*-arylation: From method development to discovery chemistry. **P. Das**

**9:25 ORGN 39.** Ionising cross-coupling inspired by the Chan-Lam mechanism. **A.J. Watson**

**9:55 ORGN 40.** Oxidative carbon-carbon bond forming processes inspired by the Chan-Lam reaction. **R. Lundgren**

**10:25 ORGN 41.** Chan–Lam couplings with tridentate sulfonate ligands: Small steps toward more general catalysts. V. Hardouin Duparc, **F. Schaper**

**10:55 ORGN 42.** Deaminative cross-couplings via C–N bond activation. **M.P. Watson**

**11:25 ORGN 43.** Drug discovery in academia: Success stories. **M.E. Jung**

Section E

San Diego Convention Center  
Room 7A

### **Young Investigator Symposium**

J. Aube, *Organizer, Presiding*

**8:00 ORGN 44.** Designing for bias: Computational methods to drive rational design of G-protein biased agonists. **R. Torella**

**8:30 ORGN 45.** Asymmetric atropisinduction. **C.A. Lewis**

**9:00 ORGN 46.** Rationally designed, conformationally constrained inverse agonists of ROR $\gamma$ t: Identification of a potent, selective series with biologic-like *in vivo* efficacy. **D. Marcoux**, J. Duan, Q. Shi, R.J. Cherney, A. Srivastava, L. Cornelius, D.G. Batt, Q. Liu, M. Beaudoin-Bertrand, C. Weigelt, P. Khandelwal, S. Vishwakrishnan, S. Kumaravel, A. Karmakar, A.K. Gupta, M. Basha, S. Ramlingam, N. Kulahalli, S. Vanteru, S. Karmakar, N. Rao, M. Vetrichelvan, A. Gupta, R. Rampulla, A. Mathur, H. Yip, P. Li, D. Wu, M. Ruzanov, J. Sack, J. Wang, M. Yarde, M. Cvijic, S. Li, D. Shuster, V. Borowski, J. Xie, K. McIntyre, M. Obermeier, A. Fura, K. Stefanski, G. Cornelius, J. Hynes, J.A. Tino, J.E. Macor, L. Salter-Cid, R. Denton, Q. Zhao, P.H. Carter, M. Dhar

**9:30 ORGN 47.** High-throughput experimentation in flow: From screening to compound production. **J.W. Tucker**

**10:00 ORGN 48.** High-throughput reaction screening enabled by small scale solid dispensing. **A.W. Dombrowski**

**10:30 ORGN 49.** Investigation of small molecule inhibitors of PLD for the treatment of ALS. **T. May-Dracka**

**11:00 ORGN 50.** Robust catalytic transformations: Value of mechanistic studies in process chemistry. **S.R. Wisniewski**

Section F

San Diego Convention Center  
Ballroom 20A

### **Organometallics Distinguished Author Award**

P. J. Chirik, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 ORGN 51.** Co-catalyzed hydroacylation. **V.M. Dong**

**9:05 ORGN 52.** Transition-metal-catalyzed asymmetric direct transformations of aromatic compounds. **S. You**

**9:35** Intermission.

**9:45 ORGN 53.** Development of Ni-catalyzed enantioselective reductive cross-coupling reactions. **S.E. Reisman**

**10:15 ORGN 54.** Ti-catalyzed nitrene transfer reactions: Harnessing the Ti<sup>II</sup>/Ti<sup>IV</sup> redox couple for new transformations. **I. Tonks**

## SUNDAY AFTERNOON

Section A

San Diego Convention Center  
Room 7B

### Metal-Mediated Reactions & Syntheses

S. M. Silverman, *Organizer*  
H. C. Johnson, *Presiding*

**1:00 ORGN 55.** Potential safety hazards associated with the Pd-catalyzed cross-coupling reactions. **Q. Yang**, N. Babij, S. Good

**1:20 ORGN 56.** Mesoporous nanoparticle supported nickel boron composite for the catalytic reduction of nitroarenes. **G. Amberchan**, J.L. Hauser, R. Manley, M. Tso, K. Bustillo, J. Cooper, J.H. Golden, B. Singaram, S. Oliver

**1:40 ORGN 57.** Efficient synthesis of chiral drugs facilitated by ligand design. **W. Tang**

**2:00 ORGN 58.** Computationally study of ligand effects using ligand substrate interaction model: Design of ligands that significantly improve the efficiency of CuH-catalyzed hydroamination reactions. A.A. Thomas, K. Speck, **I. Kevlishvili**, Z. Lu, P. Liu, S.L. Buchwald

**2:20 ORGN 59.** Nickel-catalyzed cross-electrophile coupling reactions of sulfonamides for diastereoselective cyclopropane synthesis. **E. Lucas**, K.A. Hewitt, E.R. Jarvo

**2:40 ORGN 60.** Efficient synthesis of 3-benzoyl benzo[*b*]thiophenes and raloxifene via mercury(II)-catalyzed cyclization of 2-alkylphenyl alkyl sulfoxides. **M. Wu**, S. Wen, C. Lin, C. Chen

**3:00 ORGN 61.** Palladium-catalyzed transfer hydrogenation of alkenes using tetrahydroxydiborane as the H atom donor. **M. Yaghoubi**, J. Ochoa, W. Spaller, H. Do, I. Gonzalez, B.J. Stokes

**3:20 ORGN 62.** Enantioselective synthesis of MK-8591 from benzalacetone via asymmetric ketone alkynylation and ozonolysis. **H.C. Johnson**, N. Patel, A.M. Whittaker

**3:40 ORGN 63.** Bifunctional palladium complexes bearing masked protic NHC ligands as highly active catalysts for sustainable cross-coupling reactions. **V. Lindsay**, J. Zhu

**4:00 ORGN 64.** Chromium-triggered cyclization and selective hydrogenation of conjugated dienes. **H. Steger**, J.M. O'Connor

**4:20 ORGN 65.** Chemo- and regioselective ruthenium-catalyzed cycloaromatization of conjugated dienes. **P. Qin**, J.M. O'Connor, D.M. Hitt, H. Steger, K.K. Baldrige

**4:40 ORGN 66.** Transition metal-catalyzed cycloaromatization of conjugated trienes. **P. Qin**, J.M. O'Connor, L. Wang, Y. Li, K.M. Veccharelli, K.K. Baldrige, J. Chen, B. Tufekci

Section B

San Diego Convention Center  
Room 10

## Chemistry & Water

S. M. Silverman, *Organizer*  
A. M. Hyde, *Presiding*

**1:00 ORGN 67.** Role of chalcogenide containing fluorescence in the analysis of reactive oxygen species (ROS) as neurodegenerative disease factor. **Y. Tesla**, D.G. Churchill

**1:20 ORGN 68.** First catalytic asymmetric total synthesis of the 6a-hydroxypterocarpan glyceollin I. **P. Ciesielski**, P. Metz

**1:40 ORGN 69.** Micellar gold catalysis: Three-component spirocyclization in bulk water. **N. Krause**



**2:00 ORGN 70.** Synthesis, characterization and evaluation of novel heterocyclic thiosemicarbazones against MRSA. **A. Delpe Acharige**, A.M. Almeida, S.H. Bossmann

**2:20 ORGN 71.** Towards the enantioselective synthesis of the sesquiterpenoid dehydrocostus lactone. **S. Nowotni**, P. Metz

**2:40 ORGN 72.** Enantioselective approach to (–)-dehydrocostus lactone by a domino ring-closing-metathesis strategy. **F. Kaden**, P. Metz

**3:00 ORGN 73.** Withdrawn.

**3:20 ORGN 74.** Estimation of polyamide interfacial polymerization reactivity ratios via solution-phase model studies. **M.J. Jansma**, T.M. Bechtel, S. Rosenberg, J.D. Wilbur

**3:40 ORGN 75.** Rhodamine–Hoechst positional isomers for highly efficient staining of heterochromatin. **J. Bucevičius**, J. Keller-Findeisen, T. Gilat, S.W. Hell, G. Lukinavicius

**4:00 ORGN 76.** Reductive etherification. **L. Whitaker**, K. Wheelhouse, W.J. Kerr, M. Reid

**4:20 ORGN 77.** Specific ion effects in organic chemistry: Improve your liquid-liquid extractions and reactions in water. **A.M. Hyde**

Section C

San Diego Convention Center  
Room 9

### **Total Synthesis of Complex Molecules**

S. M. Silverman, *Organizer*  
T. Davis, *Presiding*

**1:00 ORGN 78.** Towards the total synthesis of agariblazeispirol C. **R. Chung**, W.J. Kerr, T.A. Clohessy

**1:20 ORGN 79.** Synthesis of melokhanine E. **A. Cholewczynski**, P. Williams, J.G. Pierce

**1:40 ORGN 80.** Generation of dithianyl and dioxolanyl radicals exploiting photoredox catalysis: Application in the total synthesis of spiroketal natural products. **Y. Deng**, A.B. Smith

**2:00 ORGN 81.** Asymmetric synthesis of esketamine. **C. Chen**

**2:20 ORGN 82.** Total synthesis of alvaradoins E and F, uveoside, and 10-epi-uveoside. **K. Ng**, T.G. Minehan

**2:40 ORGN 83.** Total syntheses of sarpagine alkaloids and non-natural derivatives. **H. Rebmann**, T. Gaich

**3:00 ORGN 84.** Synthesis of polycyclic guanidinium alkaloids. **Y. Lin**, A. Ribaucourt, Y. Moazami, J.G. Pierce

**3:20 ORGN 85.** Enantioselective total synthesis of (+)-dihydro- $\beta$ -erythroidine. **S. Clementson**, M. Jessing, J. Langaard Kristensen, P. Vital

**3:40 ORGN 86.** Total synthesis of axially-chiral cannabinoids. **A.J. Grenning**

**4:00 ORGN 87.** Stereocontrolled and practical synthesis of conserved arylomycin macrocyclic core. **N. Wong**, X. Linghu, I. Young, F. Gosselin

**4:20 ORGN 88.** Uprifosbuvir: Innovating on the critical path. **P. Maligres**

**4:40 ORGN 89.** Commercial route development toward merck HCV NS5b inhibitor MK-3682. **T. Davis**

Section D

San Diego Convention Center  
Room 8

### **First-Generation Academic Faculty: Research Talks & Panel Discussion**

S. Zultanski, *Organizer, Presiding*

**1:15** Introductory Remarks.

**1:20 ORGN 90.** Reactive vapor deposition of conjugated polymers for textile electronics. **T.L. Andrew**

**2:00 ORGN 91.** Catalyst-controlled selectivity in iridium-catalyzed alkyl ether cleavage. **N.D. Schley**

**2:40 ORGN 92.** Synthesis of microbial fake IDs. **S.D. Townsend**

**3:20 ORGN 93.** Harnessing negative photochromic materials for synthesis of smart materials. **J. Read De Alaniz**

**4:00** Panel Discussion.

Section E

San Diego Convention Center  
Room 7A

### **Young Investigator Symposium**

J. Aube, S. M. Silverman, *Organizers*  
A. J. Grenning, *Presiding*

**1:00 ORGN 94.** New insights into acetylation & oncometabolism from chemoproteomics. **J.L. Meier**

**1:30 ORGN 95.** Process development in the pharmaceutical industry. **B. Sherry**

**2:00 ORGN 96.** Synthesis of bioactive flavagline analogues as inhibitors of cap-dependent translation: Discovery of eFT226. **T. Michels**

**2:30 ORGN 97.** Application of under-utilized transformations to the synthesis of pharmaceutically relevant molecules. **I. Young**

**3:00 ORGN 98.** Want to improve your (bio)performance? Take a closer look at the physical properties. **J.L. Terebetski**

**3:30 ORGN 99.** Polyolefin catalysts for the production of ethylene-based fluids. **B. Bailey**

**4:00 ORGN 100.** Impacting the pipeline through discovery synthesis groups: Cystic fibrosis, HCV, and immunology. **S.N. Greszler**

**4:30 ORGN 101.** Universal chromatographic methods and fit for purpose workflows in the research and development of new pharmaceuticals. **E. Regalado**, I. Haidar Ahmad, R.\. Bennett, V. D'Atri, A.A. Makarov, G.R. Humphrey, I.K. Mangion, D. Guillarme

Section F

San Diego Convention Center  
Ballroom 20A

### **JOC/OL Lectureship**

E. M. Carreira, S. J. Miller, *Presiding*

**1:00 ORGN 102.** Enantioselective and remote C–H activation reactions. **J. Yu**

**1:30 ORGN 103.** Bioorthogonal cyclopropenones for targeting and activating cellular proteins. **J.A. Prescher**

**2:00 ORGN 104.** Building bridges: Strategies for the synthesis of polycyclic natural products. **S.E. Reisman**

**2:30 ORGN 105.** Chemoenzymatic synthesis of sialidase inhibitors. **X. Chen**

**3:00** Introduction of Awardee.

**3:05 ORGN 106.** TCFH-NMI: Direct access to n-acyl imidazoliums for challenging amide bond formations. **G. Beutner**, I. Young, M.L. Davies, M.R. Hickey, H. Park, J.M. Stevens, Q. Ye

**3:45 ORGN 107.** Nature's medicine chest: Opportunities for synthesis and drug discovery. **M. Brimble**

**4:15** Introduction of Awardee.

**4:20 ORGN 108.** Recent advances in the preparative and mechanistic aspects of synthetic methods. **S.E. Denmark**

### **SUNDAY EVENING**

Section A

San Diego Convention Center  
TBD

## **Biologically-Related Molecules & Processes**

E. C. McLaughlin, *Organizer*

**5:30 - 7:30**

**ORGN 109.** Human vault nanoparticle targeted delivery of antiretroviral drugs to inhibit human immunodeficiency virus type 1 infection. **K. Tamshen**, A. Wollenberg, J. Fulcher, V. Kickhoefer, J. Mrazek, J. Elliot, F. Ibarando, P. Anton, L.H. Rome, H.D. Maynard, T.J. Deming, O. Yang

**ORGN 110.** Withdrawn.

**ORGN 111.** Design and synthesis of novel androstenedione-acridinium esters (AO-AEs) and their application in the ADVIA Centaur® androstenedione assay. Z. Zhao, P. Donovan, L. Parker, J. Driscoll, C. Higgins, M. Stranz, K. Garvey, J. Lyons, **Y. Zheng**

**ORGN 112.** Development of small molecules for the selective inhibition of the polysaccharide metabolism in human gut microbes. **K.C. Rees**, A.D. Santilli, K.J. Whitehead, D.C. Whitehead

**ORGN 113.** Efficient, microwave-assisted synthesis of N'-aryl/(alkyl)-substituted N-(4-hydroxy-6-phenylpyrimidin-2-yl)guanidines: Scope and limitations. **J. Singleton**, P. Machicao, R.K. Christensen, N.B. Lohner, M.A. Peterson

**ORGN 114.** Microwave-assisted synthesis of 3,6-disubstituted pyrazolo[1,5-a]-pyrimidines and progress toward discovery of anticancer activities. J. Singleton, **R. Dass**, M.A. Peterson

**ORGN 115.** Total synthesis and evaluating bioactivity of violaceoids A, B and their analogs. **T. Murata**, T. Kuboki, R. Ishikawa, T. Saitoh, S. Taguchi, K. Takeuchi, M. Shimonaka, I. Shiina

**ORGN 116.** Efficient syntheses of phenolic oxabicyclo[3.3.1]non-7-ene scaffolds for optimization of selectivity towards estrogen receptor targets. **T.A. Saxon**, R. Chinnasamy, J.B. Arterburn

**ORGN 117.** Trash-to-treasure transformation: Industrially and medicinally privileged compounds from Spanish moss, a neglected botanical. **D. Bandyopadhyay**, Z. Castillo, D. Gonzalez

**ORGN 118.** Highly efficient transition metal-free green synthesis of 4-aryl-2,4-dihydropyranopyrazoles. **D. Bandyopadhyay**, J. Escamilla, S. Wadekar, O. Castillo

**ORGN 119.** Withdrawn.

**ORGN 120.** DNA-compatible nitro reduction and multistep synthesis of benzimidazoles and oxadiazoles. **H. Du**, N. Simmons, M. Bangs, J. Faver, Z. Yu, M. Palaniappan, K. Riehle, M.M. Matzuk

**ORGN 121.** Optimization of guanidinylation of amines for the synthesis of protease-focused DNA-encoded chemical library. **S. Dawadi**, N. Simmons, M.M. Matzuk

**ORGN 122.** Withdrawn.

**ORGN 123.** Synthesis of novel rearranged stemodane diterpenoids and their biotransformation by *Exophiala jeanselmei* var. *lecanii-corni*. **R.K. Pryce**, P.B. Reese

**ORGN 124.** Adaption of ring-closing olefin metathesis and palladium-catalyzed hydroxycarbonylation reactions to a DNA-encoded chemical library platform. **N. Simmons**, J. Li, O. Monty, M.M. Matzuk

**ORGN 125.** Development of an efficient route to beta-lactamase inhibitor relebactam (MK-7655). **J.Y. Chung**, D. Meng, F. Xu, M. Shevlin, Q. Chen, A. Dumas, J.P. Scott

**ORGN 126.** Discovery of a novel, boron-containing macrolide as a mosquito-specific toxin for insecticide development. **J.M. Macho**, P. Fu, K. Vian, A. Khadilkar, J. Abrams, J. MacMillan

**ORGN 127.** Withdrawn.

**ORGN 128.** Broadening the activity of ribocil-C through application of the eNTRY rules. **S. Motika**

**ORGN 129.** Pd-catalyzed C–N cross coupling between on-DNA aromatic halides and amines. **Y. Chen**, N. Simmons, M.M. Matzuk

**ORGN 130.** Catalytic promiscuity vs. stereochemical fidelity: Toward an enzymatic dynamic reductive kinetic resolution (DYRKR) entry into valuable chiral synthons

and a model for the structural basis for enantio- and facial selectivity. **G.P. Kudalkar**, V.K. Tiwari, P. Madzelan, M.A. Wilson, D.B. Berkowitz

**ORGN 131.** Total synthesis of DHA-derived epoxides and their tissue regenerative sulfido-conjugates. **T.F. Lam**, R. Nshimiyimana, N.A. Petasis

**ORGN 132.** Bioluminescence and triplet excited states. N. DeHowitt, Z. Han, **R. Stanton**, N. Villasenor, M.C. Pirrung

**ORGN 133.** Synthesis and studies of porphyrin based bifunctional theranostic agents for magnetic resonance imaging and photodynamic therapy. **S. Singh**, A. Aggarwal, C.M. Drain

**ORGN 134.** Targeting BACE1 selectivity by spiro-1,3-oxazines and 1,4-oxazines . **C. Hsiao**, A. Peschiulli, F. Rombouts, H. Gijzen

**ORGN 135.** Antibacterial activity of multiflora Jamaican propolis. **S.B. Simpson**, A. Nawaz, D. Williams, O.E. Christian

**ORGN 136.** Synthesis of isotopically labeled guanosine diphosphate- $\alpha$ -D-[UL]- $^{13}\text{C}_6$ -mannopyranose. **A. Das**, J.P. Malerich

**ORGN 137.** Hydrolysis of salicylaldehyde imines by arylboronic acid catalysts. **C.C. Clement**, S. Zakia, M. Philipp

Section A

San Diego Convention Center  
TBD

## **Chemistry & Water**

E. C. McLaughlin, *Organizer*

**5:30 - 7:30**

**ORGN 138.** Exploration of *cis*-diamine-based conformationally locked chiral ligands in asymmetric synthesis. **C. van Beek**, V.V. Samoshin

**ORGN 139.** Mechanistic insights on the on-water Diels–Alder and Claisen rearrangement reactions. **M. Ibrahim**, T. Nizami, W. Cole, R.J. Saykally, H. Mishra

**ORGN 140.** Novel nanoprecipitation-based formulation technology to enhance catalytic activity of known catalysts in aqueous media. **D. Budai**, T. Bihari, F. Somodi, F. Darvas

**ORGN 141.** Sustainable drug discovery and development: SUDDEN Project. S. Karlsson, S. Kauppi, R. Kärkkäinen, M. Lundström, J. Martikainen, M. Miettinen, M. Mänttari, T. Sikanen, M. Sokero, H. Xhaard, **J.T. Yli-Kauhaluoma**

**ORGN 142.** Polymer fibers from reversibly cross-linked polysaccharide networks in water. **C. Chu**, A. Joseph, R. Langer, D.G. Anderson

**ORGN 143.** From detection to complexation: Detecting and removing aluminum from aqueous solutions. J.P. Rickett, **M.W. Fultz**

Section A

San Diego Convention Center  
TBD

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

E. C. McLaughlin, *Organizer*

**5:30 - 7:30**

**ORGN 144.** Fjord-edge nitrogen doped graphene nanoribbons. **Y.L. Li**, V. Basile, M. Flores, C. Zee, M. Muni, J.B. Lin, K.N. Houk, R.B. Kaner, S.H. Tolbert, Y.F. Rubin

**ORGN 145.** Synthesis and characterization of a red to near-IR absorbing donor-acceptor styrl-BODIPY conjugates. **A.D. Benitz**, F. D'Souza, M. Thomas

Section A

San Diego Convention Center  
TBD

### **Flow Chemistry & Continuous Processes**

E. C. McLaughlin, *Organizer*



**5:30 - 7:30**

**ORGN 146.** Multistep continuous flow synthesis of imatinib. **J. Szeto**, K. Rucker, D. Stout, J. Lim, s. mallya, J.D. White, J.P. Malerich, N. Collins

**ORGN 147.** Continuous flow *N*-Boc deprotection of amines using solid acid catalysts. **J. Wu**, C. Zeng, B. Li, J. Hawkins, S.L. Scott

**ORGN 148.** Improving multiphase catalytic microreactor productivity using a tube-in-tube membrane contactor. **M. Burkholder**, S. Gilliland, A. Luxon, C. Tang, F. Gupton

Section A

San Diego Convention Center  
TBD

### **Materials, Devices & Switches**

E. C. McLaughlin, *Organizer*

**5:30 - 7:30**

**ORGN 149.** Organic thin film transistor characteristics by using biosynthesized biosemiconductor named as *melanindigo*. **Y. Kim**, H. Park, P. Lee, K. Woo, K. Choi, H. Lee

**ORGN 150.** Thienopyrroledione-based photosensitizers as strong photoinduced oxidants: Oxidation of  $\text{Fe}(\text{bpy})_3^{2+}$  in a >1.3 V dye-sensitized solar cell. **R.R. Rodrigues**, A. Peddapuram, J.H. Delcamp

**ORGN 151.** Unique degradable guanidine derivatives and their polymers. **T. An**, Y. Lee

**ORGN 152.** Building a cocrystal via supramolecular synthons for pressure-accelerated heteromolecular azide-alkyne cycloaddition. **Y. Ma**

**ORGN 153.** Universal engineering of small organic dyes into fluorescent crystals by hierarchical assembly. C. Benson, L. Kacenauskaite, **K. VanDenburgh**, W. Zhao, B. Qiao, T. Sadhukhan, M. Pink, J. Chen, S. Borgi, C. Chen, K. Raghavachari, B. Laursen, A.H. Flood

**ORGN 154.** Thermosolient amphidynamic crystals: Effects of a phase transition on the motion at the molecular and macroscopic scales. **M.J. Jellen**, A. Colin-Molina, D. Karothu, R. Toscano, M.A. Garcia-Garibay, P. Naumov, B.V. Rodriguez-Molina

**ORGN 155.** Fabrication of black electrochromic device using a small molecule electroactive dye. **M. Baczkowski**, M. Li, O. Yassin, G. Sotzing

**ORGN 156.** Aziridine-based photochromic monomers for conductive polymers. **C. Udamulle Gedara**, M.C. Stefan, M.C. Biewer

**ORGN 157.** Development of highly soluble cyclopropenium salts leading to highly concentrated non-aqueous flow battery. **Y. Yan**, S.G. Robinson, K. Hendriks, M.S. Sigman, M.S. Sanford

Section A

San Diego Convention Center  
TBD

### **Molecular Recognition & Self-Assembly**

E. C. McLaughlin, *Organizer*

**5:30 - 7:30**

**ORGN 158.** Insights into supramolecular organization of cellulose nanocrystals in chiral nematic films. **O.V. Kulikov**, N. Wojtania, B.M. Novak

**ORGN 159.** Counter ion effect on the high-affinity binding of pyrophosphate by resorcinarene tetra-salt receptors. **J. Feder**, K. Twum, N. Schileru, M. Taimoory, S. Taimoory, J.F. Trant, N.K. Beyeh

**ORGN 160.** Allosteric control of photofoldamers for selecting between anion regulation and double-to-single helix switching. **F.C. Parks**, Y. Liu, S. Debnath, S. Stutsman, K. Raghavachari, A.H. Flood

**ORGN 161.** Free amino acid recognition: Bisbinaphthyl-based fluorescent probe with high enantioselectivity. **X. Wu**, Y. Zhu, S. Gu, L. Pu

**ORGN 162.** Using electron-transfer-induced proton transfer to control binding strength in a H-bond dimer. **H. Choi**, D.K. Smith

**ORGN 163.** Electrochemically controlled dimerization in ferrocene ureidopyrimidone derivatives: Effect of ferrocene position. **V. Mikhaylova, S. Murillo,** D.K. Smith

**ORGN 164.** Comparison of redox dependent H-bonding in simple electroactive ureas containing either ferrocene or phenylenediamine redox couples: Similar results with different mechanisms. D.K. Smith, **K. Logan, A. Elashmawy**

**ORGN 165.** Perturbation of ureidopyrimidinone polymerization via electrochemical oxidation of a ferrocene-substituted ureidopyrimidone. **M.R. Cedano,** K. Vuong, D.K. Smith

**ORGN 166.** Use of a redox-responsive 4 H-bond ureidopyrimidone (UPy) array to control polymerization in a UPy-Based supramolecular polymer. **K. Vuong, M.R. Cedano,** D.K. Smith

**ORGN 167.** Electrostatic control of macrocyclization reactions in water-soluble supramolecular capsules. **X. Cai,** B.C. Gibb

Section A

San Diego Convention Center  
TBD

### **Peptides, Proteins & Amino Acids**

E. C. McLaughlin, *Organizer*

**5:30 - 7:30**

**ORGN 168.** Silylated tag assisted peptide synthesis (STag-PS): Greener and continuous peptide synthesis for the congested amino acids. **H. Kubota,** S. Yano, T. Mori

**ORGN 169.** C18AQ flash column and its application in the purification of strong polar peptides. **B. Xu,** W. Qiu, A. Couture

**ORGN 170.** Fully automated optimized synthesis of linaclotide using orthogonally protected cysteine residues and on-resin oxidation chemistry. **E. Denton,** J.R. Bickler

**ORGN 171.** Contribution of bulky-  $\alpha$ ,  $\beta$ -dehydroamino acids to the proteolytic stability of 310-helices. **G. Damstedt,** M. Lee, J. Singh, S.L. Castle

**ORGN 172.** Responses of fluorescent probes to amyloid-beta peptides. **C. Chen**, S. Benavides, S. Mattei, J. Debrow, A. Hughes, O. Mantussova, S. Sahloul

**ORGN 173.** Synthesis and structural determination of chiral asymmetric ureas as  $\alpha,\beta$ -dipeptide derivatives. **S. García**, R. Guzmán-Mejía, J.A. Aviña-Verduzco

**ORGN 174.** Determining the susceptibility of various  $\alpha,\beta$ -dehydroamino acids to conjugate additions. **M. Lee**, J. Singh, G. Damstedt, S.L. Castle

**ORGN 175.** Design and synthesis of a peptide-aldoxorubicin conjugate to target triple negative breast cancer. **A. Saghaidehkordi**

**ORGN 176.** Peptide-doxorubicin conjugate for specific uptake by triple negative breast cancer cells. **e. ziaei**

**ORGN 177.** Challenges in the synthesis of peptidic macrocyclic biaryl ethers. **M.G. Gotz**, R. Dorn

**ORGN 178.** Peptide stapling by Lewis base-Brønsted acid catalyzed sulfenylation of tryptophan. **Z. Brown**, M.A. Saputra, H. Henriksen, I.W. Bell, J.J. Provost, J.L. Gustafson

**ORGN 179.** Structural studies of charged heptapeptides with point mutations using solution state two-dimensional NMR spectroscopy. **T. Bentley**, A. Xiong, C. Robinson, I. Fuson, K.V. Krishnan, K. Maitra

Section A

San Diego Convention Center  
TBD

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

E. C. McLaughlin, *Organizer*

**5:30 - 7:30**

**ORGN 180.** pH and temperature effects on process-scale degradation of clavulanic acid. **J.B. Washington**, M. Reid, S. Baillie

**ORGN 181.** Theoretical conformational studies of symmetric diesters including solvent effects. **S. Niwayama**, K. Osada, M. Yoshida, S. Matsushima

**ORGN 182.** Photooxidation of *o*-alkynylaryl oximes: Intramolecular cyclization reaction. **V.M. Espinoza Castro**, A. Council, E. Armenta, M. Ko, W.S. Kim, A.M. Abiad, A.S. Petit, P. De Lijser

**ORGN 183.** Mechanism of cinchona-alkaloid catalyzed asymmetric chloro-functionalization of alkenes. **A. Sarkar**, T. Kakeshpour, D. Steigerwald, S. Bedford, B. Soltanzadeh, R. Yousefi, B. Borhan, J.E. Jackson

**ORGN 184.** Withdrawn.

**ORGN 185.** Unusual KIE for ring-opening of short-lived intermediate formed by PCET reaction. **S. Alvi**, D.A. Singleton, H. Kurouchi

**ORGN 186.** Computational investigations of polymeric NHCs as catalysts for benzoin condensation. **K. Melancon**, T. Cundari

## MONDAY MORNING

Section A

San Diego Convention Center  
Room 7B

### New Reactions & Methodology

S. M. Silverman, *Organizer*  
A. Sanford, *Presiding*

**8:00 ORGN 187.** Palladium-catalyzed oxidative homocoupling of pyrazole boronic esters to access bipyrazoles for metal-organic frameworks. **M.K. Taylor**, M. Juhl, D. Hwang, G. Hadaf, E. Velasquez, J. Oktawiec, J.B. Lefton, T. Runcevski, J.R. Long, J. Lee

**8:20 ORGN 188.** Quaternary carbon synthesis by acid-catalyzed intermolecular hydroarylation of electron-deficient  $\alpha$ -methylstyrenes. **J. Alvarenga**, A. Keshavarz, B.J. Stokes

**8:40 ORGN 189.** Synthesis of novel renewable monomers from abundant monoterpenes. **S. Smith**, R. Stockman, S.M. Howdle

**9:00 ORGN 190.** Diisobutylaluminum borohydride (snelling salt): A versatile and efficient reducing agent. **G. Amberchan**, B. Singaram, E. Moya, M. Landi, K. Lutz

**9:20 ORGN 191.** Inquest for better selectivity and activity: Nucleophilic organocatalysts based on branched/dendritic design. **M. Portnoy**, N. Ashush, R. Fallek, A. Fallek, M. Weiss-Shtofman

**9:40 ORGN 192.** Nickel-catalyzed arylation of aldehydes to form secondary alcohols. **K.J. Garcia**, M.M. Gilbert, D.J. Weix

**10:00 ORGN 193.** I(I)/I(III) catalyzed *vicinal* dichlorination of alkenes. **J.C. Sarie**, J. Neufeld, C.G. Daniliuc, R. Gilmour

**10:20 ORGN 194.** Synthesis of pyrrolidines from sulfinamide azomethine ylide precursors. **D. O'Connor**, R.A. Stockman

**10:40 ORGN 195.** Single-electron reduction of iminium ions via ion pair charge-transfer. **K. Kohara**, M. Gaunt

**11:00 ORGN 196.** Nickel-catalyzed cross-electrophile coupling reactions of diol derivatives. **A. Sanford**, T.A. Thane, E.R. Jarvo

**11:20 ORGN 197.** Synthesis of sulfoximines and sulfonimidamides by highly chemoselective NH and O transfer. **J.A. Bull**, R. Luisi

**11:40 ORGN 198.** Copper-mediated stereospecific intramolecular deoxyfluorination using  $\text{CuF}_2$ . **D.E. Sood**, D.M. Dawson, Y.G. Andreev, S. Chabbra, B.E. Bode, A.J. Watson

Section B

San Diego Convention Center  
Room 10

**Peptides, Proteins & Amino Acids**

S. M. Silverman, *Organizer*  
S. Tower, *Presiding*

**8:00 ORGN 199.** Synthesis of (*R*)- $\alpha$ -methylselenocysteine and its application as a glutathione peroxidase mimic. **R.J. Wehrle**, E. Ste.Marie, R.J. Hondal, D.S. Masterson

**8:20 ORGN 200.** Bioorthogonal modification of dehydroalanine residues in RiPPS via Diels-Alder cycloadditions. **R. de Vries**, R. Oudshoorn, G. Roelfes

**8:40 ORGN 201.** Antimicrobial stapled peptide-drug conjugates. **J. Gaynard**, J. Parker, M. Welch, D.R. Spring

**9:00 ORGN 202.** Progress towards the total synthesis of yaku'amide A and analogues. **D. Joaquin**, C. Lo, D. Moya, A. Ramos, S. White, S.L. Castle

**9:20 ORGN 203.** Conformational analysis of lantibiotic peptides. **R. Dickman**, E.R. Danelius, M. Erdélyi, A.B. Tabor

**9:40 ORGN 204.** Developing a novel chemical approach for arginine modification. **M. Xu**

**10:00 ORGN 205.** Sulfatase-cleavable linkers for antibody-drug conjugates (ADCs). **J. Bargh**, S. Walsh, A. Isidro-Llobet, D.R. Spring

**10:20 ORGN 206.** Selective modification of proteins with fluoroalkyl radical precursors. **M. Imiolek**, B.G. Davis

**10:40 ORGN 207.** Chemical biology approaches to understanding the structure and function of Protoxin-II. **S. McCarthy**, J. Robinson, F. Reyes, S. Sanchez-Martinez, T. Gonen, M. Topf, K. Thalassinou, A.B. Tabor

**11:00 ORGN 208.** Preventing Huntington's disease using protein-like polymers. **W. Choi**, Y. Shang, X. Qi, N.C. Gianneschi

**11:20 ORGN 209.** Electron transfer reagents for selective photo-bioconjugation of proteins. **M. Taylor**

**11:40 ORGN 210.** Site-selective modification of tryptophan residues in peptides and proteins using redox active pyridinium salts and light. **S. Tower**, W. Hetcher, T. Myers, M. Taylor

San Diego Convention Center  
Room 9

**Materials, Devices & Switches**

S. M. Silverman, *Organizer*  
R. L. Greenaway, *Presiding*

**8:00 ORGN 211.** Observation of conformational transition of perfluorophenyl substituted benzanilide derivative. **R. Yamasaki**, M. Harada, R. Nagata, A. Ito, K. Fukuda, I. Okamoto

**8:20 ORGN 212.** Discotic liquid crystals: From quinoxalinophenanthrophenazine to isoindigo discotics. **B.R. Kaafarani**, S.H. Eichhorn

**8:40 ORGN 213.** High-voltage molecular engineered organic sensitizer-iron redox shuttle pair: 1.4 V DSC and 3.3 V SSM-DSC devices. **R.R. Rodrigues**, H. Cheema, J.H. Delcamp

**9:00 ORGN 214.** Understanding the diverse solution reactivity of N-DMBI-H with organic semiconductor molecules. **S. Jhulki**, H. Un, C. Risko, J. Pei, S. Barlow, S.R. Marder

**9:20 ORGN 215.** Hybrid discovery workflow for organic materials and supramolecular self-assemblies. **R.L. Greenaway**, V. Santolini, E. Berardo, M. Bennison, B. Alston, M. Little, R. Kearsey, M. Miklitz, K. Jelfs, A.I. Cooper

**9:40 ORGN 216.** Effect of thiol substitution on the thiol-ene polymerization: Kinetics and mechanical properties. **K. Long**, M. Olin, A. Ortega, S. Huang, C. Bowman

**10:00 ORGN 217.** Photoswitch generation using mechanical force. **X. Hu**, M.E. McFadden, R. Barber, M.J. Robb

**10:20 ORGN 218.** Photoinduced electron transfer in meso donor carrying bis styryl BODIPY bound to fullerene using “two point” self assembly strategy. **S. Shao**, H.B. Gobeze, P.A. Karr, F. D'Souza

**10:40 ORGN 219.** Enhanced purification of carbon nanomaterials. **V. Gangoli**, B. Brinson, A.R. Barron



**11:00 ORGN 220.** Synthesis of nanographenes via alkyne benzannulation reactions.  
**P. S**

**11:20 ORGN 221.** Atomically precise graphene nanoribbons: Bottom-up synthesis, characterization, and applications. **A. Sinitskii**

Section D

San Diego Convention Center  
Room 8

### **Organic Chemistry at Self-Assembling & Biological Interfaces**

S. M. Silverman, *Organizer*  
D. Bong, *Organizer, Presiding*

**8:00 ORGN 222.** Targeting structurally and functionally diverse nucleic acids with druglike small molecules. **J. Schneekloth**

**8:30 ORGN 223.** Isomorphous and isofunctional fluorescent nucleosides. **Y. Tor**

**9:00 ORGN 224.** Single chain polymeric nanoparticles containing transition metals as artificial metalloenzymes. **S.C. Zimmerman**, J. Chen, T. Xiong, E.S. Gracia Ramirez, Y. Xu

**9:30 ORGN 225.** Applications of a synthetic base-triple motif in nucleic acid structure-function, diagnostics, and delivery. **D. Bong**

**10:00 ORGN 226.** PNA-based sensors for disease-relevant miRNAs. **A.J. Kennan**, M. Schenkel, C. Henry

**10:30 ORGN 227.** Modulating noncovalent interactions at cellular interfaces. **K. Kumar**

**11:00 ORGN 228.** Exploring the human smORFeome. **A. Saghatelian**

**11:30 ORGN 229.** Toward novel therapeutics via directed remodeling of the gut microbiome. P. Chen, A. Black, P. Mukherjee, Y. Zhao, A.L. Sobel, B. Molparia, G.R. Aleman Muench, J. Wu, W. Chen, A. F. M. Pinto, B.E. Maryanoff, A. Saghatelian, P. Soroosh, A. Torkamani, L.J. Leman, **M.R. Ghadiri**

San Diego Convention Center  
Room 7A

### Young Investigator Symposium

J. Aube, *Organizer*  
H. Xu, *Presiding*

**8:00 ORGN 230.** Shifting the oxidation pathways of polyethylene to provide carbonaceous species in high yield. **B.E. Barton**

**8:30 ORGN 231.** Discovery and evolution of potent and selective heme-displacing IDO1 inhibitors. **M. McGowan**

**9:00 ORGN 232.** Design and development of catalytic processes for the synthesis of antiviral agents EFdA (MK-8591) and vaniprevir (MK-7009). **J. Kong**

**9:30 ORGN 233.** Convergent synthesis of the NS5B inhibitor GSK8175 enabled by transition metal catalysis. **I.I. Strambeanu**

**10:00 ORGN 234.** Organic molecules as forensic fuel markers. **R. Wright**

**10:30 ORGN 235.** Rational design of organic materials for advanced microlithography. **J.A. Kaitz**

**11:00 ORGN 236.** Development of PMC friendly approaches to the construction of synthetically challenging cyclopropane motifs. **M. Harris**

**11:30 ORGN 237.** Discovery of MK-8153: ROMK inhibitor as new mechanism diuretic for hypertension and heart failure. **S. Dong**

San Diego Convention Center  
Ballroom 20A

### Tetrahedron Prize

Financially supported by Elsevier  
S. M. Silverman, *Organizer*  
S. F. Martin, *Organizer, Presiding*

**8:00** Introductory Remarks.

**8:05 ORGN 238.** Control of polymer chain growth with external stimuli. **B.P. Fors**

**8:55 ORGN 239.** Using synthetic chemical tools to understand how toxic chemicals and drugs interfere with DNA replication and transcription. **S.J. Sturla**

**9:45 ORGN 240.** Synthesis and applications of complex natural products. **T.J. Maimone**

**10:35** Introduction of Awardee.

**10:45 ORGN 241.** Palladium-induced carbon-heteroatom bond-forming reactions for the functionalization of molecules big and small. **S.L. Buchwald**

**11:45** Concluding Remarks.

### **Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment**

Sponsored by BIOL, Cosponsored by COMP, ORGN and PHYS

### **Identification & Design of Catalytic Sites in Electrochemical Reactions**

Sponsored by ANYL, Cosponsored by ORGN

**MONDAY AFTERNOON**

Section A

San Diego Convention Center  
Room 7B

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

S. M. Silverman, *Organizer*  
C. J. Hall, *Presiding*

**1:00 ORGN 242.** Mechanism, selectivity, and orbital symmetry of CF<sub>3</sub>-Py ligand couplings at pentacoordinate phosphorous. **J. Alegre Requena**, R.S. Paton

**1:25 ORGN 249.** Withdrawn.

**1:50 ORGN 243.** Computational investigation of the thermal stability and temperature-dependent electronic properties of highly energetic material TKX-50. **J. Scher**, A. Chakraborty

**2:15 ORGN 244.** Contra thermodynamic, photocatalytic *E* to *Z* isomerization of alkenyl organoborons: Vectors to facilitate exploration of two dimensional chemical space. **J. Molloy**, J. Metternich, A.J. Watson, R. Gilmour

**2:40 ORGN 245.** Mechanistic analysis of trimethylanilinium salts: Implications for methylation and cross-coupling chemistry. **J.B. Washington**, M. Reid, S. Baillie

**3:05 ORGN 246.** Unique photochemistry of new strongly alkaline heterocyclic amine-based donor- $\pi$ -acceptor photoacids. **R. Bhide**, E. Schwartz, D. Fishman, S. Ardo

**3:30 ORGN 247.** Solvent-assisted, visible light RAFT polymerization. **M.D. Thum**, D. Falvey

**3:55 ORGN 248.** Investigation of the photochemistry of chlorinated flavins and flavinium cations. **B. Etz**, J. DuClos, J. Bingham, S. Vyas

**4:20 ORGN 250.** Investigation of the photochemistry and reactivity of diazidobenzene. **J.T. Bingham**, B. Etz, S. Vyas

Section B

San Diego Convention Center  
Room 10

## Heterocycles & Aromatics

S. M. Silverman, *Organizer*  
S. P. Mulcahy, *Presiding*

**1:00 ORGN 251.** Synthesis and functionalization of [b]-fused pyridine compounds. **F. Popowycz**, H. Lavrard

**1:20 ORGN 252.** Fascinating dynamic behavior of rare diazacyclobutenes. **C.J. Narangoda**, A. Kitaygorodskiy, C.D. McMillen, J.E. Jackson, D.C. Whitehead

**1:40 ORGN 253.** Trapping of *N*-acyliminium ions with enamides: Approach to medium-sized diaza-heterocycles. **L. Andna**, L. Miesch

**2:00 ORGN 254.** Parallel synthesis of benzimidazoles via oxidative cyclization. **D. Schmitt**, E. Arnold, P.K. Mondal

**2:20 ORGN 255.** Brønsted acid catalyzed one-pot benzannulation of 2-alkenylindoles under aerial oxidation: Route to carbazoles and indolo[2,3-*a*]carbazole-alkaloids. **S. SAHA**, M. Maji

**2:40 ORGN 256.** From late-stage oxidation to heterocyclic synthesis: New methodology for drug discovery. **E.P. Talbot**

**3:00 ORGN 257.** Synthesis and applications of the MR1 ligand precursor 5-amino-6-D-ribitylaminoouracil (5-A-RU). **J. Aube**

**3:20 ORGN 258.** Tandem transition metal catalysis in the synthesis of carboline heterocycles. **S.P. Mulcahy**

**3:40 ORGN 259.** Use of microwaves for synthesis of propargylic ethers as precursors of 1,2,3-triazoles in click reactions. L.C. García Sanchez, M.A. García Eleno, E. Cuevas Yañez, **A.F. Becerra Buitrago**, J.A. García Ortiz

**4:00 ORGN 260.** Readily accessible sp<sup>3</sup>-rich cyclic hydrazine frameworks exploiting nitrogen fluxionality. **C.L. Dean**, R. Sundaram, G.J. Clarkson, M. Jones, M. Wills, M. Shipman

**4:20 ORGN 261.** Tetrazole and oxadiazole heterocycles via multi-component reaction schemes. **M. Konstantinidou**, S. Kurhade, F. Sutanto, K. Kurpiewska, J. Kalinowska, A. Doemling

**4:40 ORGN 262.** Practical synthesis of 1-bromocodeine derivatives and the first synthesis of bismorphine A. **S. Mansouri**, A. Ali, J. Desaulniers, Y. Bolshan

Section C

San Diego Convention Center  
Room 9

### **Materials, Devices & Switches**

S. M. Silverman, *Organizer*  
D. Tilly, *Presiding*

**1:00 ORGN 263.** Stimuli responsive discotic semiconductors: From materials to devices. **B. Gomez-Lor**, A. Benito, M. Echeverri

**1:20 ORGN 264.** Donor-acceptor molecular switches as novel mechano-responsive chromophores. **Y. Liu**, A. Halmes, Q. Wu, J.S. Moore

**1:40 ORGN 265.** Macroscopic photon-powered actuators based on organized photomechanical nanocrystals. **F. Tong**, X. Dong, C.J. Bardeen

**2:00 ORGN 266.** Ligand induced polarity switch of dynamic ethylene-bridged non classical oligoureas. **D. Tilly**, D.T. Morris, J. Clayden

**2:20 ORGN 267.** Extending the bay-area: Synthesis, characterization, and application (OLED, OFET) of novel azaborinine-substituted coronene diimides. **J. Hoffmann**, M. Hissler, A. Staubitz

**2:40 ORGN 268.** Self-assembled azobenzene functionalized molecules for all-optical control of integrated photonics. **J. He**, A. Kovach, A.M. Armani

**3:00 ORGN 269.** Design and synthesis of electroactive chromophore for achieving black in electrochromic devices. **O. Yassin**, M. Baczowski, G. Sotzing

**3:20 ORGN 270.** Tuning properties of a hydroquinone chromophore. **H. Arslan**

**3:40 ORGN 271.** Synthesis and characterization of dicyanomethyl aryl radicals. **R. Zhang**

**4:00 ORGN 272.** Tale of redox-active organic radical polypeptides as electrode materials: From full organic batteries to electron-transfer kinetics. **T. Nguyen, A. Easley, N. Kang, C.H. Komatsu, C. Yu, J. Fan, R.A. Letteri, X. He, L. Su, J.L. Lutkenhaus, K.L. Wooley**

Section D

San Diego Convention Center  
Room 8

### **Artificial Intelligence in Organic Synthesis**

A. A. Shah, V. W. Shurtleff, *Organizers, Presiding*

**1:00** Introductory Remarks.

**1:05 ORGN 273.** (Un)supervised learning for the screening and classification of homogeneous catalysts. **C. Corminboeuf, B. Meyer, B. Sawatlon, M.D. Wodrich**

**1:50 ORGN 274.** Machine learning for organic chemistry reaction prediction and retrosynthesis. C.W. Coley, T.J. Struble, H. Gao, X. Wang, W. Lin, R. Barzilay, T. Jaakkola, W.H. Green, **K.F. Jensen**

**2:35** Intermission.

**2:40 ORGN 275.** Towards AI-based synthesis at scale. **M. Waller**

**3:25 ORGN 276.** Synthia™ (Chematica) retrosynthetic software for practicing chemists: Novel and efficient *in silico* pathway design validated at the bench. **S. Trice**

**4:10 ORGN 277.** Chemical reaction data reuse: Preparing ELN data for analytics and prediction. **S. Harrison**

**4:55** Concluding Remarks.

Section E

San Diego Convention Center  
Room 7A

## **Organic Chemistry for Next-Generation Therapeutics**

R. M. Franzini, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 ORGN 278.** Click and release: Unique approach to prodrugs of gasotransmitters.  
**B. Wang**

**1:35 ORGN 279.** Bioconjugation via zwitterionic boron-nitrogen heterocycles. T. Chio, H. Gu, K. Mukherjee, L. Tumey, **S.L. Bane**

**2:05 ORGN 280.** Click-cleavable antibody-drug conjugates (ADCs). **R. Rossin**

**2:35** Intermission.

**2:45 ORGN 281.** Controlled activation of RNA-based therapeutics. **M. Royzen**, M.V. Yigit

**3:15 ORGN 282.** SQ3370: Enhancing safety and efficacy of systemic cytotoxic prodrugs using bioorthogonal chemistry-driven local drug activation. S. Srinivasan, N.A. Yee, M. Royzen, **J. Mejia Oneto**

**3:45 ORGN 283.** Bioorthogonal reactions between isonitriles and tetrazines. **J. Tu**, R.M. Franzini

**4:15 ORGN 284.** Nucleophile-triggered cleavable linkage chemistry: Fundamentals and applications. **M. Finn**, S. Tekkam, L. DePascalis, C. Higginson, M. Yau

**4:45** Concluding Remarks.

Section F

San Diego Convention Center  
Ballroom 20A

**Tetrahedron Prize**



Financially supported by Elsevier  
S. M. Silverman, *Organizer*  
S. F. Martin, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 ORGN 285.** Break-it-to-make-it strategies for complex molecule synthesis. **R. Sarpong**

**1:55 ORGN 286.** Rh-catalyzed hydroacylation. **V.M. Dong**

**2:45 ORGN 287.** Multimetallic catalysis with palladium and nickel. **D.J. Weix**

**3:35** Introduction of Awardee.

**3:45 ORGN 288.** Catalytic substitution and C-H bond functionalization reactions.  
**J.F. Hartwig**

**4:45** Concluding Remarks.

### **Frontiers in Interdisciplinary Research: New Paradigms for Integration of Theory & Experiment**

Sponsored by BIOL, Cosponsored by COMP, ORGN and PHYS

### **Identification & Design of Catalytic Sites in Electrochemical Reactions**

Sponsored by ANYL, Cosponsored by ENFL and ORGN

### **MONDAY EVENING**

Section A

San Diego Convention Center  
TBD

## Sci-Mix

E. C. McLaughlin, *Organizer*

### 8:00 - 10:00

116, 119, 124-125, 132, 135, 139-142, 145-146, 150, 153, 157-158, 161, 166, 170-171, 177, 185-186. See Previous Listings.

389-390, 397-398, 400, 407, 409, 414, 428, 444, 448-449, 451-452, 458-460-461, 464, 467, 471, 476, 478, 481, 484, 597, 600, 607, 611-612, 616-617, 620, 622, 624, 633, 635-636, 641, 645, 648, 655-656, 669, 673, 675-676. See Subsequent Listings.

## TUESDAY MORNING

Section A

San Diego Convention Center  
Room 7B

### New Reactions & Methodology

S. M. Silverman, *Organizer*  
E. Corcoran, *Presiding*

**8:00 ORGN 289.** Dealkylative *N*-arylation of sulfonamides. **M. West**, B.J. Thomson, A.J. Watson

**8:20 ORGN 290.** Advancing the original cope rearrangement: Fundamental studies and applications in complex molecule synthesis. **A.J. Grenning**

**8:40 ORGN 291.** Decarboxylative amination of redox-active esters using diazirines. **P. Chandrachud**

**9:00 ORGN 292.** Diboron-mediated semireduction of terminal allenes. **A. Gates,** W.L. Santos

**9:20 ORGN 293.** Pd-Cu mediated decarboxylative *ortho*-halogenation of aryl carboxylic acids. **H. Cai,** Z. Fu, Y. Jiang, **G. Mei,** S. Wang

**9:40 ORGN 294.** Optimized semi-industrial electrochemical preparation of cyclic encarbamates and its application for the MedChem relevant building blocks synthesis. O.D. Tereshchenko, I.V. Knysh, M.Y. Perebiynis, O.V. Vasylets, A.A. Sorochenko, A. Borisov, S. Ryabukhin, **D.M. Volochnyuk**

**10:00 ORGN 295.** Scalable synthesis of MedChem relevant (Is)oxazole based building blocks. B.A. Chalyk, E.Y. Slobodyanyuk, O. Grygorenko, S. Ryabukhin, **D.M. Volochnyuk**

**10:20 ORGN 296.** Fascinating adventures in development of a drug from conception to commercialization: Personal perspective. **M. Chorghade**

**10:40 ORGN 297.** Visible-light-induced nickel-catalysed cross-coupling with alkylzirconocenes from unactivated alkenes. **C. Jiang,** X. Qi, Y. Gao, C. Yang

**11:00 ORGN 298.** New frontiers in Castagnoli–Cushman reaction. **S. Ryabukhin,** M. Adamovsky, O. Grygorenko, D.M. Volochnyuk

**11:20 ORGN 299.** Stimuli responsive additives: Transforming the future. **C. Roy,** C. Hayes, D. Saccomando, W. Barton

**11:40 ORGN 300.** Straightforward synthesis of all isomeric cyclo- and fluoro-alkylpiperidines. **S. Ryabukhin,** A. Subota, A. Lutsenko, O. Grygorenko, D.M. Volochnyuk

Section B

San Diego Convention Center  
Room 10

### **Biologically-Related Molecules & Processes**

S. M. Silverman, *Organizer*  
Y. L. Zhong, *Presiding*

**8:00 ORGN 301.** Shape-selective recognition of the major groove of DNA: Synthesis and DNA binding profile of monomeric, dimeric, and trimeric derivatives of crystal violet. **T.G. Minehan**, O. Nunez, R. Shaktah, B. Chavez

**8:20 ORGN 302.** Optical control of lipid metabolism and signaling. **J. Morstein**, A. Novak, D. Trauner

**8:40 ORGN 303.** Silicon polymethine fluorophores for the near-infrared and shortwave infrared. **M. Pengshung**, E.M. Sletten

**9:00 ORGN 304.** X-ray crystallographic investigations and molecular dynamics simulation studies with phospholipase A2 of some Leonard linker pyrazolo[3,4-d]pyrimidine compounds. **U. Yadava**

**9:20 ORGN 305.** From free radical chemistry to novel classes of bioactive molecules. Y. Guindon, M. Nemer, **M. Prévost**, S. Dostie, P. Mochirian, W. Maharsy, G. Kanaan

**9:40 ORGN 306.** Safe and high yielding synthesis of diazeniumdiolates and the application for synthesis of MK-8150. **Y. Zhong**, M.D. Weisel, G.R. Humphrey, D.J. Muzzio, L. Zhang, M.A. Huffman, W. Zhong, K.M. Maloney, K.R. Campos

**10:00 ORGN 307.** Design and stereospecific synthesis of atypical C1, C5, and C6-substituted carbapenem antibiotics. **M. Alqurafi**, T.Q. Nguyen, N.M. Al-Kharji, W. Chai, N. Nformi, M. Pan, J. Kim, A. He, S. Solanki, B. Meshram, C. Varner, K. Wong Wirth, S. Salinas Garcia, L. Newman, Y. Samadzada, J.D. Buynak

**10:20 ORGN 308.** Convergent synthesis of PI3K inhibitor GDC-0908 featuring palladium-catalyzed direct C-H arylation toward dihydrobenzothienooxepines. **H. Zhang**

**10:40 ORGN 309.** Near-infrared chemiluminescence probes for detection and imaging. **O. Green**, D. Shabat

**11:00 ORGN 310.** Flavylium polymethine fluorophores for multiplexed *in vivo* imaging with shortwave infrared light. **E.D. Cosco**, A.L. Spearman, S. Ramakrishnan, J.G. Lingg, M. Pengshung, M. Saccomano, S. Glasl, M. Warmer, R.R. McLaughlin, O.T. Bruns, E.M. Sletten

**11:20 ORGN 311.** Withdrawn.

**11:40 ORGN 312.** Synthesis of small molecule inhibitors to study fatty acid recycling. **K. Jaremko**, M. Currie, J. Beld

San Diego Convention Center  
Room 9

**Molecular Recognition & Self-Assembly**

S. M. Silverman, *Organizer, Presiding*

**8:00 ORGN 313.** Controlling chloride affinity swings of photofoldamers with arylazopyrazoles. **F.C. Parks**, S. Stutsman, Y. Liu, S. Debnath, K. VanDenburgh, X. Gao, K. Raghavachari, A.H. Flood

**8:20 ORGN 314.** Orthogonal metal templation strategy for the synthesis of unimolecular linear oligocatenanes. **N.D. Colley**, M. Nosiglia, C. Chang, L. Li, F. Solangi, J.C. Barnes

**8:40 ORGN 315.** Novel multicomponent fluorescent sensors for detection of glycolipids. **M. Xu**, T.E. Glass

**9:00 ORGN 316.** Small structural variations have large effects on the assembly properties and spin-state of room-temperature, high-spin Fe(II) iminopyridine cages. **T. Miller**, L.R. Holloway, R.J. Hooley

**9:20 ORGN 317.** Squaraine lasso peptides: New family of self-threaded fluorescent molecular probes. **C. Zhai**, C. Schreiber, S. Padilla, B.D. Smith

**9:40 ORGN 318.** Advances in porous liquids formed using porous organic cages. **R.L. Greenaway**, R. Kearsley, B. Egleston, M. Brand, A. Kai, A.I. Cooper

**10:00 ORGN 319.** Self-assembly of biohybrid materials with macrocyclic receptors. **N.K. Beyeh**

**10:20 ORGN 320.** Systematic construction of ternary assemblies through weak interactions. R. Puttreddy, M.D. Pour, M. Taimoory, **K. Twum**, F. Pan, K.T. Rissanen, J.F. Trant, N.K. Beyeh

San Diego Convention Center  
Room 8

## Remarkable Women in Organic Chemistry

Cosponsored by WCC

N. C. Goodwin, R. Ruck, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:10 ORGN 321.** Navigating the chemical space of amide activation to drug discovery. **E. Baker-Tripp**

**8:30 ORGN 322.** Innovative strategies toward complex molecule synthesis: Development of a fully biocatalytic manufacturing route for MK-8591. **N. Patel**

**9:00 ORGN 323.** Anion-catalyzed silicon Lewis acid activation of carbonyls. **M. Tekle-Smith**, K.S. Williamson, I. Hughes, J.L. Leighton

**9:20 ORGN 324.** Leaving their mark: From precision electrophile signaling to covalent ligand evolution. **Y. Aye**

**9:55** Intermission.

**10:05 ORGN 325.** Quest for enantioselective hydroamination reactions: Silver, gold, and serendipity. **A.G. Wenzel**

**10:35 ORGN 326.** Make it or break it with metal-hydrides. **V.M. Dong**

**11:10 ORGN 327.** Academic drug discovery: Playing to the strengths to address challenging targets and unmet medical needs in cancer and acute kidney injury. **D.M. Huryn**

Section E

San Diego Convention Center  
Room 7A

## Young Academic Investigator Symposium

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

**8:20** Introductory Remarks.

**8:25 ORGN 328.** Development of novel chemical tools for accessing unexplored chemical spaces. **M. Ngai**

**8:50 ORGN 329.** C–H and C–O functionalization via radical chaperones. **D. Nagib**

**9:15 ORGN 330.** Alcohol and amine derivatives guide position-selective C–H functionalization reactions. **J.L. Roizen**

**9:40 ORGN 331.** Catalytic strategies to selectively manipulate aryl radicals and strong C–F bonds. **N. Jui**

**10:05** Intermission.

**10:15 ORGN 332.** Enantioselective chemical synthesis methods via cooperative catalysis. **T.N. Snaddon**

**10:40 ORGN 333.** Development of high-valent aerobic oxidation catalysis. **D.C. Powers**

**11:05 ORGN 334.** Selective functionalization of pyridines, diazines, and pharmaceuticals via heterocyclic phosphonium salts. **A. McNally**

**11:30 ORGN 335.** Semiconducting polymer blends: Bringing the best of both worlds for organic electronics. **J. Mei**

Section F

San Diego Convention Center  
Ballroom 20A

### **Cope Award Symposium**

J. Aube, L. A. Marcaurelle, *Organizers*  
L. Marcaurelle, *Presiding*

**8:00** Introductory Remarks.

**8:10 ORGN 336. Award Address** (Arthur C. Cope Late Career Scholars Award sponsored by the Arthur C. Cope Fund). Organic chemistry in harsh reaction environments. **R.J. McMahan**

**8:45 ORGN 337. Award Address** (Arthur C. Cope Mid-Career Scholars Award sponsored by the Arthur C. Cope Fund). Organic & organometallic catalysts and Lewis pairs for polymer synthesis and biorefining. **E.Y. Chen**

**9:20 ORGN 338. Award Address** (Arthur C. Cope Late Career Scholars Award sponsored by the Arthur C. Cope Fund). Synthetic reactions driven by energy of photons. **M. Murakami**

**9:55** Intermission.

**10:10 ORGN 339. Award Address** (Arthur C. Cope Early Career Scholars Award sponsored by the Arthur C. Cope Fund). Design and synthesis of topologically controlled polymer networks. **J.A. Johnson**

**10:45 ORGN 340. Award Address** (Arthur C. Cope Late Career Scholars Award sponsored by the Arthur C. Cope Fund). Elements of marine bioorganic chemistry: From vanadium to iron. **A. Butler**

**11:20 ORGN 341. Award Address** (Arthur C. Cope Late Career Scholars Award sponsored by the Arthur C. Cope Fund). Assembly line synthesis. **V.K. Aggarwal**

## **Identification & Design of Catalytic Sites in Electrochemical Reactions**

Sponsored by ANYL, Cosponsored by ENFL and ORGN

## **TUESDAY AFTERNOON**

Section A

San Diego Convention Center  
Room 7B

## **Flow Chemistry & Continuous Processes**

S. M. Silverman, *Organizer*  
V. Vu, *Presiding*



**1:15 ORGN 342.** Scale-up of a continuous extraction process for driving an equilibrium-limited reaction to completion. **M.T. Tudesco**, E.G. Moschetta, E.A. Voight

**1:40 ORGN 343.** Centre for rapid online analysis of reactions (ROAR): Flow chemistry facility for the Dial-a-Molecule community. **B. Deadman**, P. Ferrini, M. Hii

**2:05 ORGN 344.** Development of a safe and high-throughput continuous manufacturing approach to N-(2-hydroxyethyl)thiomorpholine dioxide. **Y. Tan**, N. Strotman, M.C. Soumeillant, S.W. Leung, K. Powers

**2:30 ORGN 345.** Data-driven exploration of the catalytic reductive amination reaction. **P. Ferrini**, B. Deadman, M. Hii

**2:55 ORGN 346.** Diversity oriented synthesis of highly substituted heteroarenes using photochemistry and flow technology. **G. Sipos**, G. Ignacz, B. Fodi, T. Noel

**3:20 ORGN 347.** Tunable chiroptical induction and photolysis in flow. **A.C. Evans**

**3:45 ORGN 348.** Studies toward a general strategy for scaling photochemical reactions in flow. **E. Corcoran**, F. Levesque, J. McMullen, J.R. Naber

**4:10 ORGN 349.** Continuous synthesis of three nucleoside antivirals in one day on an automated flow chemistry system. **V. Vu**, J. Szeto, K. Rucker, D. Stout, J. Lim, J.P. Malerich, J.D. White, N. Collins

Section B

San Diego Convention Center  
Room 10

### **Biologically-Related Molecules & Processes**

S. M. Silverman, *Organizer*  
D. Bandyopadhyay, *Presiding*

**1:00 ORGN 350.** Functionalized nitrodibenzofuran-based protecting groups for biological applications. M. Hammers, F. Xu, S. Fang, A. Fenton, M. Hodny, A.T. Healy, D.A. Blank, **M.D. Distefano**

**1:20 ORGN 351.** Development of a reversible and repeatable thiol-ene reaction for controlled presentation of signaling proteins in hydrogels. **J.C. Grim**, B.A. Aguado, T. Brown, K.S. Anseth

**1:40 ORGN 352.** Synthesis of selective JAK3 inhibitor PF-06651600: Discovery to early clinical supplies. **J.I. Trujillo**, Y. Tao, N. Sach, S. Liang, K.E. Wigglesworth, T.M. Makowski, B. Samas, K. Girard, J.G. Mustakis, P.R. Rose, J.C. McWilliams, R. Mehta, A. Casimiro-Garcia, A. Thorarensen, J. Telliez, M.F. Brown, A.M. Gilbert, M.M. Hayward, J. Langille, J.I. Montgomery, R. Unwalla, F.F. Vajdos

**2:00 ORGN 353.** Turning PET on and off to sense amines with BODIPY fluorescence. **K. VanDenburgh**, A.H. Flood

**2:20 ORGN 354.** Synthesis and evaluation of 4-oxazolidinones as *Staphylococcus aureus* biofilm modulating agents. **B. Frohock**, J.G. Pierce

**2:40 ORGN 355.** Optimizing tetrazine amino acid size and reactivity for efficient protein labeling. **S. jana**

**3:00 ORGN 356.** Spontaneously blinking dyes and their utility in super-resolution microscopy. **F.M. Jradi**, T. Vu, T.A. Brown, J. Aaron, C. Galbraith, E. Jorgensen, L.D. Lavis

**3:20 ORGN 357.** Synthesis and mechanistic investigation of phospholipid-mimicking small molecules as synthetic modulators for liver receptor homologue-1. **A.R. Flynn**, N. Jui

**3:40 ORGN 358.** Imidazotetrazines for the treatment of glioblastoma and as synthetic diazoalkane precursors. **R. Svec**, P.J. Hergenrother

**4:00 ORGN 359.** Synthesis of an ideal selective estrogen receptor modulator. **R. LaLonde**

**4:20 ORGN 360.** Total synthesis of protectin and resolvin epoxide precursors and their tissue regenerative sulfidoconjugates. **R. Nshimiyimana**, T.F. Lam, N.A. Petasis

**4:40 ORGN 361.** Late-stage tailoring of natural product-like macrocycles: Structure and properties of functionalized [13]-macrolactones. **C. Chen**

San Diego Convention Center  
Room 9

## **Molecular Recognition & Self-Assembly**

S. M. Silverman, *Organizer*  
J. Meisel, *Presiding*

**1:00 ORGN 362.** Facile synthesis of a diverse library of mono-3-substituted  $\beta$ -cyclodextrin analogues and their applications. **K. Kellett**, M.K. Gilson

**1:20 ORGN 363.** Near-infrared rotaxane probes for fluorescence imaging and photothermal heating. **H.H. McGarraugh**, W. Liu, C. Schreiber, B.P. Matthews, B.D. Smith

**1:40 ORGN 364.** Micelle-encapsulated fluorescent probe: Chemoselective and enantioselective recognition of lysine in aqueous solution. **G. Du**

**2:00 ORGN 365.** Complexation thermodynamics between cyclodextrins and fatty acids. **X. Yao**, M. Bonizzoni, L. Kong

**2:20 ORGN 366.** Conversion of a weak DAD-ADA H-bond dimer to a much stronger DDD-AAA dimer via proton-coupled electron transfer. **D.K. Smith**, H. Choi

**2:40 ORGN 367.** Interaction of diazaperylenium guest with cucurbit[n]uril host. **A. Thangavel**, M. Macias, S. Tsumaki

**3:00 ORGN 368.** Rational control of geometry in pentacene macrocycles. **H.M. Bergman**, G.R. Kiel, R. Witzke, Y. Liu, T. Tilley

**3:20 ORGN 369.** Calix[5]arene-derived self-folding cavitand receptor for polycyclic aromatic hydrocarbons. **A. Lledo Ponsati**, D. Lozano, R. Álvarez-Yebra, R. López-Coll

**3:40 ORGN 370.** Heterofunctionalized proteomimetic foldamer libraries for biomolecular recognition. **J. Meisel**, A. Hamilton

Section D

San Diego Convention Center  
Room 8

## Remarkable Women in Organic Chemistry

Cosponsored by WCC

N. C. Goodwin, R. Ruck, *Organizers, Presiding*

**1:30** Introductory Remarks.

**1:35 ORGN 371.** Selective carbohydrate functionalization reactions. **A.E. Wendlandt**

**2:05 ORGN 372.** Design and synthesis of organic electronic materials. **M. Jeffries-El**, A.A. Burney-Allen, R. Chavez, D.L. Wheeler

**2:40 ORGN 373.** Owing your career: Personal reflections on creating a rewarding and successful career in industry. **E. Guidry**

**3:10** Intermission.

**3:20 ORGN 374.** Necessity is the mother of invention: Natural products and the chemistry they inspire. **S.E. Reisman**

**3:55 ORGN 375.** Career in medicinal chemistry: Transforming challenges into opportunities. **K.B. Goodman**

**4:25 ORGN 376.** Remarkable women in organic chemistry. **M. Faul**

Section E

San Diego Convention Center  
Room 7A

## Young Academic Investigator Symposium

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

**1:30 ORGN 377.** Stereoselective carbene annulations for assembling molecular complexity. **I. Sharma**

**1:55 ORGN 378.** Harnessing the indole heterocycle to rapidly access complex and diverse compounds from indole alkaloids. **R. Huigens**

**2:20 ORGN 379.** New methods and strategies in the synthesis of natural products. **S. Pronin**

**2:45 ORGN 380.** Biocatalysis and complex molecule synthesis. **A.R. Narayan**

**3:10 ORGN 381.** Flavylium polymethine fluorophores for imaging in the shortwave infrared region. **E.M. Sletten**

**3:35 ORGN 382.** Chemical tools that IMPACT lipid signaling. **J.M. Baskin**

**4:00** Concluding Remarks.

Section F

San Diego Convention Center  
Ballroom 20A

### **Cope Award Symposium**

L. A. Marcaurelle, *Organizer*  
J. Aube, *Organizer, Presiding*

**1:35 ORGN 383. Award Address** (Arthur C. Cope Early Career Scholars Award sponsored by the Arthur C. Cope Fund). Synthesis of complex terpenes from simple precursors. **T.J. Maimone**

**2:10 ORGN 384. Award Address** (Arthur C. Cope Mid-Career Scholars Award sponsored by the Arthur C. Cope Fund). Metal catalysts, clusters, and surfaces: Catalytic preparation of chiral bio-molecules and carbon-based self assembled monolayers. **C.M. Crudden**

**2:45** Intermission.

**2:55 ORGN 385. Award Address** (Arthur C. Cope Mid-Career Scholars Award sponsored by the Arthur C. Cope Fund). Versatile oxidative coupling reactions for site-selective protein modification. **M.B. Francis**

**3:30 ORGN 386. Award Address** (Arthur C. Cope Mid-Career Scholars Award sponsored by the Arthur C. Cope Fund). Stereocontrol in photochemical synthesis. **T.P. Yoon**

**4:05** Introduction of Awardee.

**4:15 ORGN 387. Award Address** (Arthur C. Cope Award sponsored by the Arthur C. Cope Fund). Research: A magical mystery tour. **D. Seebach**

## **Identification & Design of Catalytic Sites in Electrochemical Reactions**

Sponsored by ANYL, Cosponsored by ENFL and ORGN

## **TUESDAY EVENING**

Section A

San Diego Convention Center  
TBD

## **Heterocycles & Aromatics**

E. C. McLaughlin, *Organizer*

**5:30 - 7:30**

**ORGN 388.** First total synthesis of natural pyridocoumarins, goniotaline A and B. J. Jung, T. Lee, Y. Seo, **Y. Han**

**ORGN 389.** BODIPYs in the blue: New molecular design. **Z. Wu**, H. Fujita, N. Magdaong, J. Diers, D. Hood, S. Allu, D.M. Niedwiedzki, C.R. Kirmaier, D.F. Bocian, D. Holten, J.S. Lindsey

**ORGN 390.** Fluorocyclization of *N*-propargyl carboxamides by iodine(III) catalysts bearing coordinating substituents. **A. Saito**, S. Takahashi, Y. Umakoshi, A. Yoshimura, V.V. Zhdankin

**ORGN 391.** Withdrawn.

**ORGN 392.** Gold redox catalysis for cyclization/arylation of allylic oximes: Synthesis of isoxazoline derivatives. **A.A. Jimoh**, X. Shi

**ORGN 393.** Synthesis of 5-aromatic substituted tetrazoles: Modified catalytic approach. **S.C. Sarngadharan**, M. Malone, J. Faris, P. Pollet, C.L. Liotta

**ORGN 394.** Methodology to furnish imidazo[1,2,a]pyrimidines via the annulation of  $\beta$ -alkoxy acrylamides and activated aminoimidazoles. **K. Clagg**, N. White, L. Sirois, H. Zhang, F. Gosselin

**ORGN 395.** Vitamin catalysis: Photocatalytic synthesis of benzocoumarins via (–)-riboflavin-mediated electron transfer. **T. Morack**, J. Metternich, R. Gilmour

**ORGN 396.** Exploring the synthesis of oxazoles starting from amino acids treated with oxalyl chloride. **V.O. Cesare**, F. Guo, M. Fitzsimmons, D. Werner

**ORGN 397.** Synthesis of novel triazine-based aromatic boronic acids with potential for both antibacterial and flame-retardant applications. **B. Cromwell**, M. Levine

**ORGN 398.** Acid-mediated ring expansion of 2,2-disubstituted azetidine carbamates to 6,6-disubstituted 1,3-oxazinan-2-ones. **A.J. Boddy**, C. Cordier, K. Goldberg, A. Madin, A.C. Spivey, J.A. Bull

**ORGN 399.** 3,3-Diaryloxetanes: New opportunities for drug discovery. **M. Dubois**, J.J. Mousseau, C. Choi, J.A. Bull

**ORGN 400.** C(sp<sup>3</sup>)–H functionalization of saturated heterocycles at unactivated positions: Exploring 3D vectors for fragment growth. **D. Antermite**, D. Affron, O.A. Davis, J.A. Bull

**ORGN 401.** Copper-mediated cyclization of 1,2-dibromohomoallylic alcohols to versatile 3-bromodihydrofurans. **J. An**, J. Intano, M. Rhinehart, A.R. Howell

**ORGN 402.** Novel domino N<sub>2</sub>-extrusion/cyclization approaches for the synthesis of indoloquinolines and carbocycle-fused quinolines. **B. Akkachairin**, J. Tummatorn, N. Khamsuwan, C. Thongsornkleeb, S. Ruchirawat

**ORGN 403.** Synthesis and characterization of squaraine-containing macrocycles. **J. Pantano**, M. Levine

**ORGN 404.** Short strategy for the diastereoselective synthesis of 2,3-diaryl- $\gamma$ -butyrolactones: Total synthesis of cinnassin A<sub>1</sub>. **A.Y. Nuriye**, C. Craescu

**ORGN 405.** Practical preparation of a 1,3,5-trisubstituted pyridazin-4(1*H*)-one using selective C<sub>1</sub> unit insertion and cyclization. **A. Suzuki**, N. Fukuda, T. Kajiwara, T. Ikemoto

**ORGN 406.** Combinatorial synthesis of imidazo[2,1-*b*]thiazole acyl derivatives. **A.S. Bunev**

**ORGN 407.** 5-Cyano-2,4-diaminopyrimidine derivatives: Approaches to preparative synthesis. **A.S. Bunev**

**ORGN 408.** Synthesis of *bis*(thiazol-2-yl)amines. **A.S. Bunev**

**ORGN 409.** Sequential anionic intramolecular cyclization of bis-alkynylarene amides toward polycyclic isoindolo-isoquinolines and -benzazepines: Regioselectivity study. **G. Infante**

**ORGN 410.** Chemical explorations of the manzamenones from the tropical marine sponge, *Plakortis* sp. **H. Lee**, Y. Lee, J. Lee, J. Lee

**ORGN 411.** Pentacene-fused porphyrin dimer exhibiting high stability and solubility. **Y. Hu**, H. Wang

**ORGN 412.** Phenoxazine polymers for biosensor applications. **M.N. Almtiri**, C. Scott

**ORGN 413.** Suzuki catalyzed one-step access to photoluminescent D-A type diarylmalesimides. **J. Price**, E. Albright, B. Balonova, B. Blight, S. Eisler

**ORGN 414.** Synthesis of fluorinated 1,5-3*H*-benzodiazepines from substituted *o*-phenylenediamines and 2-fluoroalk-3-yn-1-ones. **T.L. Olson**, A. Kaspi-Kaneti, A. Walsh, R. Dembinski

**ORGN 415.** Design and synthesis of evodiamine and rutaecarpine analogues for biological evaluation. Y. Huang, **V. Sammeta**, R. Alshehry, S. Rasapalli

**ORGN 416.** Facile access to C-ring aromatic substituted luotoninins and vasicinones for Topo I inhibition via intramolecular aza-Michael reactions (IMAMRs) of quinazolinonyl chalcones. **V. Sammeta**, Z. Murphy, J. Golen, S. Rasapalli

**ORGN 417.** Design and synthesis of 4(3*H*)-quinazolinonyl chalcones and their derivatives for antibacterial and antibiofilm activity. Z. Murphy, **V. Sammeta**, S. Rasapalli



**ORGN 418.** Design and synthesis of 2-pyrazolyl quinazolinones as celecoxib analogs. G. vicente, V. Sammeta, Z. Murphy, **S. Rasapalli**

**ORGN 419.** Efficient approach to pyrroloquinazolinone alkaloids: Vasicinone and luotonin A. **V. Sammeta**, Y. Huang, S. Rasapalli

**ORGN 420.** Transition metal catalyzed synthesis of unsymmetrically substituted triazolium salts. **S. Hutchinson**

**ORGN 421.** Synthesis of C7-substituted-phenyl-[13]-macrodilactones, principal component analysis (PCA), and antiproliferation assays. **C. Chen**, M.W. Peczuh

**ORGN 422.** Quantification of hydrogen bond accepting ability of medicinally relevant N-heterocycles and alkaloid compounds using  $^{31}\text{P}$  NMR spectroscopy. **M. Milic**, K. Targos, J. Jennings, A.K. Franz

**ORGN 423.** Efficient routes to oxazolines through activation of aromatic amides. **H. Thompson**, M. Musa, S. Alhashim, **A. Dubrovskiy**

Section A

San Diego Convention Center  
TBD

## **New Reactions & Methodology**

E. C. McLaughlin, *Organizer*

**5:30 - 7:30**

**ORGN 424.** Fluorosulfonic anhydride: Another powerful reagent for the sulfur(VI) fluoride exchange (SuFEx) chemistry. **G. Li**

**ORGN 425.** Catalytic application of Eu(II)/Eu(III) redox cycles and photoluminescence tracking. S. Kim, **M. Kim**

**ORGN 426.** Facile synthesis of flavanones *via* Pd(II)-catalyzed  $\beta$ -arylation of chromanones with arylboronic acids. **H. Yoo**, N. Kim

**ORGN 427.** New strategies towards fine chemicals from HMF and GMF. W. Fan, C. Verrier, L. Wang, E. Dokmak, m. Ahmar, S. Moebs, **F. Popowycz**, Y. Queneau

**ORGN 428.** Mechanochemical iridium-catalyzed C-H borylation. **Y. Pang**, T. Ishiyama, K. Kubota, H. Ito

**ORGN 429.** Olefin-accelerated C–C cross-coupling reaction in solid-state. **T. Seo**, T. Ishiyama, K. Kubota, H. Ito

**ORGN 430.** Catalytic cascade dehydrogenative cross-coupling: One-pot process to break two B-H, one C-H, one X-H and construct new B-C and B-X (X = O, N) bonds. **Y. Au**, Y. Quan, Z. Xie

**ORGN 431.** Concise synthesis of potassium acyltrifluoroborates from aldehydes by borylation and oxidation. **T. Takeuchi**, J. Taguchi, R. Takahashi, F. Masero, H. Ito

**ORGN 432.** Formation of aryl(1-cyano-4-(dialkylamino)butadienyl)ketones from pyridines. **H. Gim**, M.E. Jung

**ORGN 433.** New polyallylsilane-based carbon-carbon bond forming reactions. **E.D. Tan**, **L.K. Baker**, G.W. O'Neil

**ORGN 434.** Reactivity enhancement in branched catalysts for phosphorylation reactions: Electronic and steric effects. **A. Fallek**, M. Portnoy

**ORGN 435.** Influence of bases and catalysts on substrate-selectivity in a model acylation reaction. **R. Fallek**, M. Portnoy

**ORGN 436.** Preparation, structure, and reactivity of phenolic arylodonium salts. **A. Yoshimura**, G. Rohde, V.V. Zhdankin, M. Yusubov, A. Saito

**ORGN 437.** *Ips*o-nitration of arylsilanes. **F. Fu**, S.B. Munoz, T. Mathew, S.G. Prakash

**ORGN 438.** Preparation of fluorinated selenium- and sulfur-containing compounds via reactions of selenols, diselenides, and disulfides with *in situ*-generated difluorocarbene and their potential uses for chalcogeno-fluorofunctionalization. **C. Barrett**, V. Krishnamurti, S.G. Prakash

**ORGN 439.** Synthesis of novel substituted dihydropyridines with potential pharmaceutical activity. **A.K. Ahmed**, **U. Siddika**, M. Shkooor

**ORGN 440.** Siladifluoromethylation and deoxo-trifluoromethylation of P<sup>V</sup>–H compounds with TMSCF<sub>3</sub>: Route to P<sup>V</sup>–CF<sub>2</sub><sup>–</sup> transfer reagents and P–CF<sub>3</sub> compounds. **V. Krishnamurti**, C. Barrett, S.G. Prakash

**ORGN 441.** Direct access to acyl fluorides and perfluoroalkyl carbonyl compounds from carboxylic acids using a phosphine-based deoxygenative reagent system. **X. Ispizua**, H. Dang, S.B. Munoz, T. Mathew, S.G. Prakash

**ORGN 442.** Withdrawn.

**ORGN 443.** Vinyl cations as cyclopentenone precursors via C–H insertion and alkene addition reactions. **M. Hensinger**, S. Cleary, M. Brewer

**ORGN 444.** Transition metal free selective  $N^2$ -arylation of 1,2,3-triazoles. **S. Roshandel**, M.J. Lunn, S.C. Suri, S.G. Prakash

**ORGN 445.** Tuning of regioselectivity by steric hindrance in Suzuki–Miyaura cross coupling reactions. **Y. Kwon**, W. Kim

**ORGN 446.** Cu(I)-catalyzed pentafluoroethylation of aryl iodides in the presence of tetrafluoroethylene and CsF. **N. Ishida**, K. Ando, Y. Hashimoto, A. Shigaki, K. Kikushima, M. Ohashi, S. Ogoshi

**ORGN 447.** Phosphorylation of carbon-oxygen bond mediated by *N*-phosphine oxide-substituted imidazolylidenes. **T. Asada**, Y. Hoshimoto, S. Ogoshi

**ORGN 448.** Exploring the reactivity of sulfur(VI) via sulfonimidate intermediates. **O. Goodrich**, R.A. Stockman

**ORGN 449.** 3-Aryloxetane-3-carboxylic acids: Two step process towards novel versatile building blocks for drug discovery programs. **M. Dubois**, J.J. Mousseau, C. Choi, J.A. Bull

**ORGN 450.** Diastereoselective nucleophilic substitution reactions of acyclic acetals. **A. Ramdular**, K.A. Woerpel

**ORGN 451.** Formation of strained rings through a nickel-catalyzed cross-electrophile coupling. **T. McGinnis**, A. Sanford, T.A. Thane, E.R. Jarvo

**ORGN 452.** Metal-free cyclopropanation of electrophilic olefins. **G.M. Batista**, P.P. Castro, A.G. Carpaneze, B. Horta, G.W. Amarante

**ORGN 453.** 4,5,6,7-Tetrahydropyrazolo[1,5-*a*]pyrazine: Lead-oriented scaffold with three diversity points. V.I. Bozhanov, O.V. Zarembo, A. Borisov, S. Ryabukhin, **D.M. Volochnyuk**

**ORGN 454.** Isoxazole and 1,2,4-oxadiazole-derived phosphonates via [3+2] cycloaddition. B.A. Chalyk, O. Grygorenko, S. Ryabukhin, **D.M. Volochnyuk**

**ORGN 455.** Synthesis of gem-difluorocycloheptanes building blocks. K.P. Melnykov, S. Ryabukhin, **D.M. Volochnyuk**

**ORGN 456.** Cu-catalyzed amination of (hetero)arylamines to disubstituted olefins. **S. Park**

**ORGN 457.** Synthesis of  $\beta$ -amino sulfones through copper-catalyzed hydroamination of allylic sulfones. **K. Kim, S. Park**

**ORGN 458.** Ni-catalyzed oxidative esterification of allylic  $sp^3$ -carbon followed by *in situ* reduction. **D. Moustafa, C. Sweet, P. Kaur**

**ORGN 459.**  $^{18}F$  deoxyfluorination of phenols via Ru  $\pi$  complexes. **D. Mandal, M. Beyzavi, M. G. Strebl, C. N. Neuman, J. Chen, J. M. Hooker, T. Ritter**

**ORGN 460.** Copper catalyzed  $S_N2'$  functionalization of fluoroalkylated alkenes. **J.L. Yang, T.W. Butcher, J.F. Hartwig**

**ORGN 461.** Alkyl-extended pinacol rearrangement. **N. Dao, J. Sader, J. Wulff**

**ORGN 462.** Synthesis of allylic amines through Cu-catalyzed aza-Michael addition of heterocycles to dienes. **H. Lee, S. Park**

**ORGN 463.** Studies directed toward the total synthesis of saxitoxin: Addition of 1,3-dihydro-2H-imidazol-2-one to aldehydes. **J. Lee, M. Ryu, H. Lee, Y. Lee, J. Lee**

**ORGN 464.** Efficient synthesis of L-ribonolactol derivative and their L-nucleoside analogs from D-ribose. **J. Cho, Y. Nam, S. Choi, J. Kim, D. Jung, J. Song, J. Park**

**ORGN 465.** Synthesis of homoallylic alcohols through addition of allylic aluminum reagents to carbonyls via Cu-catalyzed hydride addition to allenes. **S. Lee, S. Lee**

**ORGN 466.** Stereocontrolled multicomponent synthesis of amino acids and peptidomimetics in water. **K.M. Kossick, N.A. Petasis**

**ORGN 467.** Ion pair reactions in the high speed ball mill. **L.N. Trankina, J. Crain, C. Williams III, J. Mack**

**ORGN 468.** NMR quantification of halogen-bonding ability to evaluate catalyst activity. **Y. Chang, T. Tang, J. Jagannathan, N. Hirbawi, S. Sun, A.K. Franz**

- ORGN 469.** H<sub>2</sub>-mediated C-C bond formation via ruthenium-ketenimate intermediates. **M.M. Sikes**, L.V. Hale, N.K. Szymczak
- ORGN 470.** Hydroboration of carbodiimides using a carbodiphosphorane catalyst. **D. Chang**, A.L. Liberman-Martin
- ORGN 471.** One-step synthesis of sulfonamides from tosylhydrazones. A. Tsai, J.M. Curto, A. Dechert Schmitt, **G. Ingle**, V. Mascitti
- ORGN 472.** Survey and mechanism of the reductive cleavage of lignin-relevant aryl ethers by small molecule thiols. **G.E. Klinger**, J.E. Jackson, E.L. Hegg
- ORGN 473.** New  $\alpha$ -thioalkyl phosphonium salts as Wittig substrates for vinyl sulfide synthesis. **S. Dharavath**, J. Deobald, J. Magolan
- ORGN 474.** Process development of (S)-2-methylproline synthesis via microreactor. **M. Yu**, D. Zhang, I. Yu, **B. Zhang**
- ORGN 475.** Investigation of the 1,3-diaza-Claisen rearrangements in ring expansion of vinyl *N*-heterocycles. **T. Watanabe**
- ORGN 476.** Development of new difluormethylation reactions. **C. Brigham**, C. Malapit, M. Sanford
- ORGN 477.** Improved synthesis of *p*-SCN-Bn-HOPO for <sup>89</sup>Zr chelation. **N. Bhupathiraju**, A. Younus, J. Ali, M. Cao, S. Ponnala, H. Cicek, L.C. Francesconi, J. Lewis, J. Babich, C.M. Drain
- ORGN 478.** *In situ* enzymatic screening (ISES) approach to catalyst screening: Toward a new entry into halovinyl amino acids. **S.M. Ramos De Dios**, R.A. Dhokale, D.L. Graham, D.B. Berkowitz
- ORGN 479.** Stereoretentive Suzuki–Miyaura reaction enabling the synthesis of 1,3-disubstituted-cyclobutane. **T. Piou**
- ORGN 480.** Catalytic oxidative reactions of arylalkenes by *tert*-Butyl hydroperoxide: Mechanistic assessment. **L. De Angelis**, Y. Su, M.P. Doyle
- ORGN 481.** Biomimetic synthesis of kallosin. **V. Gharat**, P. Scesa, L. West
- ORGN 482.** Tailoring chemoenzymatic oxidation via *in situ* peracids. **R. Re**, J. Proessdorf, J.J. La Clair, M. Subileau, M.D. Burkart

**ORGN 483.** C–H functionalization of alcohols via radical-polar crossover. **R.K. Twumasi**, A. Prusinowski, E. Wappes

**ORGN 484.** Transition-metal catalyzed alkyne coupling reactions. **S. Acharya**, P. Zhao

**ORGN 485.** Hybrid synthetic-computational study of versatile approach to curcuminoids. **A. Guerrero**, J. Christensen, J. Cook, K. Wolmutt, V.A. Stepanova

**ORGN 486.** SuFEx click chemistry enabled late-stage drug functionalization. **Z. Liu**, J. Li, S. Li, G. Li, K.B. Sharpless, P. Wu

**ORGN 487.** Selective methylation of  $\alpha$ -methylene ketones. **S. Ryabukhin**, A. Frolov, E. Ostapchuk, D.M. Volochnyuk

**ORGN 488.** Synthesis and reactivity of N-difluorocyclopropyl-substituted pyrazoles. **S. Ryabukhin**, P. Nosik, M. Pashko, A. Poturai, K.P. Melnykov, O. Grygorenko, D.M. Volochnyuk

**ORGN 489.** Synthesis and properties of monoalkylsubstituted difluorocyclopropenes. **S. Ryabukhin**, P. Nosik, M. Pashko, D.M. Volochnyuk

**ORGN 490.** Expanding of the scope of Castagnoli–Cushman reaction: Anhydrides of cyclic 1,2-dicarboxylic acids. **S. Ryabukhin**, M. Adamovskyi, O. Smyrnov, D.M. Volochnyuk

**ORGN 491.** Expanding of the scope of Castagnoli–Cushman reaction: Trifluoroacetaldehyde monohydrate. **S. Ryabukhin**, M. Adamovskyi, D.M. Volochnyuk

## **WEDNESDAY MORNING**

Section A

San Diego Convention Center  
Room 7B

**New Reactions & Methodology**

S. M. Silverman, *Organizer*  
M. Jouffroy, *Presiding*

**8:00 ORGN 492.** Quaternary centers via dual-catalytic alkene hydroarylation. **S.A. Green**, R.A. Shenvi

**8:20 ORGN 493.** Condensation-driven assembly of bis(heteroaryl) motifs using a linchpin reagent. **C. Apte**, D. Diaz, A.K. Yudin

**8:40 ORGN 494.** Exploiting enzymes from (hyper)thermophiles for *in situ* enzymatic screening (ISES) at elevated temperature: Toward a catalytic, asymmetric entry into quaternary,  $\alpha$ -vinyl amino acids. **V.K. Tiwari**, G. Malik, J.A. Friest, R.A. Swyka, D.B. Berkowitz

**9:00 ORGN 495.** Distal control of aryne capture regioselectivity by an *in situ* formed boronate. **M. Hribersek**, C. Sollert, M. Ahlquist, L.T. Pilarski

**9:20 ORGN 496.** Calcium-catalyzed formal [5+2] cycloaddition of alkylidene  $\beta$ -ketoesters with substituted olefins: Chemodivergent synthesis of highly functionalized cyclohepta[b]indoles. **A.N. Parker**, M.C. Martin, R. Shenje, S.A. France

**9:40 ORGN 497.** Development of an electrocatalytic ruthenium-catalyzed C–H hydroxylation of amine derivatives. **S.G. Robinson**, J. Mack, J. Du Bois, M.S. Sigman

**10:00 ORGN 498.** Radical mediated S-atom transfer enabled strategies for chemical synthesis. **J. Lopp**

**10:20 ORGN 499.** Organocatalytic Mukaiyama Mannich reactions of 2,5-bis(trimethylsilyloxy)furan. **S.Y. Howard**, S.W. Laws, R. Mato, J.T. Shaw

**10:40 ORGN 500.** Selective hydrodefluorination and defluoroalkylation of a diverse range of trifluoromethyl arenes. **D. Vogt**, H. Wang, N. Jui

**11:00 ORGN 501.** Chemoselective nickel-catalyzed hydrogenation: Synthesis of highly substituted aromatic amines. **M. Tom**, P. Miller, R.L. Grange, D. Esau, G. Jerkiewicz, P. Evans

**11:20 ORGN 502.** Vinyl sulfides: New preparations and reactions. **J. Magolan**

**11:40 ORGN 503.** Direct C–H carbamoylation of nitrogen containing heterocycles.  
**M. Jouffroy**

Section B

San Diego Convention Center  
Room 10

## Heterocycles & Aromatics

S. M. Silverman, *Organizer*  
S. Malhotra, *Presiding*

**8:00 ORGN 504.** Synthesis of pyrene-pyrazole pharmacophores via copper-catalyzed *C-N* dehydrogenative cross-coupling and structure-activity studies for tubulin polymerization. **D. Sar**, I. Srivastava, D. Pan

**8:20 ORGN 505.** Selective intermolecular couplings of aryl radical species with olefins. **A.J. Boyington**, N. Jui

**8:40 ORGN 506.** Synthesis of 5-fluorocytosine from acyclic precursors: Improving global access to emtricitibine. **B. Derstine**, E. Crawford, J. Dietz, P. Moore, C. Peck, A.J. Arduengo, T. Opatz, T. McQuade, F. Gupton

**9:00 ORGN 507.** Carboxyboronate: An unusual C1 building block. **A.E. Holownia**, C. Tien, D. Diaz, R. Larson, A. Yudin

**9:20 ORGN 508.** Selectivity in the synthesis of 1-substituted and 1,8-disubstituted fluorenones by directed metalation. **S. Cope**, J.K. Pagano, B. Scott, L.A. Silks, J.L. Kiplinger

**9:40 ORGN 509.** Linking cyclopenta-fused polycyclic aromatic hydrocarbons via five-to-five connections. **K.N. Plunkett**

**10:00 ORGN 510.** Magnesium-catalyzed regioselective alkylation of 3-substituted pyrazoles. **D. Xu**

**10:20 ORGN 511.** Development of two simple building blocks for the biocatalytic synthesis of MK-8591. **C.M. Hong**



**10:40 ORGN 512.** Enabling the manufacturing process development of GPR40 MK-8666 through the highly efficient synthesis of the 6-5-3 fused heterocyclic ring system. **Z. Liu**, A.M. Hyde, A. Klapars, G.X. Zhou, J.Y. Chung, N. Yasuda, J. Limanto, K.R. Campos

**11:00 ORGN 513.** Withdrawn.

**11:20 ORGN 514.** Highly chemoselective functionalization of dihaloaromatics. **S. Malhotra**

Section C

San Diego Convention Center  
Room 9

### **Photoredox Chemistry**

S. M. Silverman, *Organizer*

C. Plummer, *Presiding*

**8:20 ORGN 515.** Difunctionalization of *N*-alkyl cyclobutyl and cyclopropyl amines via photoredox catalysis. **Q. Wang**, N. Zheng

**8:40 ORGN 516.** Mechanism and optimization of redox-mediated Ni-catalyzed cross coupling. **R. Sun**, Y. Qin, S. Ruccolo, C. Schnedermann, C. Costentin, D.G. Nocera

**9:00 ORGN 517.** Benzylic functionalization via visible-light induced photoredox catalysis. **Y. Xing**

**9:20 ORGN 518.** Computational characterization of photocatalytic processes with DFT-based methods. **F. Maseras**

**9:40 ORGN 519.** Arene cyanation via cation radical accelerated nucleophilic aromatic substitution. **N. Holmberg-Douglas**, D.A. Nicewicz

**10:00 ORGN 520.** Radical Stetter reaction enabled by merger of ion-pair photocatalysis with radical umpolung. **T. Morack**, C. Mück-Lichtenfeld, R. Gilmour

**10:20 ORGN 521.** Photocatalytic birch-like arylation via C–F functionalization. **J.D. Weaver**

**10:40 ORGN 522.** Contra-thermodynamic photocatalysis; Progress towards the synthesis of a hexaprismane. **J.D. Weaver**

**11:00 ORGN 523.** Stereoselective glycosides via copper-catalyzed cross couplings of anomeric sp<sup>3</sup> carbons with alkyl alcohols induced by visible light. **H.M. Nguyen, F. Yu, R. Schaugard, H.B. Schlegel**

Section D

San Diego Convention Center  
Room 8

### **Sustainable Catalysis: Discovery through Application**

S. M. Silverman, *Organizer*  
D. K. Leahy, *Organizer, Presiding*

**8:00 ORGN 524.** Development of regioselective hydro- and oxidative amination reactions. **K.L. Hull**

**8:45 ORGN 525.** Radical biocatalysis: Using light to reveal new enzyme functions. **T. Hyster**

**9:30 ORGN 526.** Development of reductive aminases: Useful tool for efficient chiral amine synthesis. **G. Hughes**

**10:00 ORGN 527.** Synthesis of enantiomerically enriched diaryl alkanes through a stereoconvergent Suzuki-Miyaura cross coupling reaction catalyzed by iron-based complexes. **J.A. Byers, C.R. Tyrol, N. Yone**

**10:45 ORGN 528.** Identifying novel ligand scaffolds for Cu-catalyzed C–O and C–N cross-coupling through library screening. **E. Swift**

**11:15 ORGN 529.** Developing practical catalysis for C–H activation reactions. **J. Yu**

Section E

San Diego Convention Center  
Room 7A

## **From Lab to Commercial Scale: The Challenges to Scaling Up Flow Chemistry in the Pharmaceutical Industry**

K. M. Maloney, *Organizer*

J. R. Naber, *Presiding*

**8:00** Introductory Remarks.

**8:05 ORGN 530.** Continuous manufacturing innovation journey: Lessons from Lilly. **S. O'Keeffe**

**8:45 ORGN 531.** Formylation with ethyl formate in flow: Reduction of process mass intensity (PMI) and CO generated. **D.A. Otte**

**9:25 ORGN 532.** Scaling photochemical reactions in flow using visible light. **E. Moschetta**

**10:05** Intermission.

**10:15 ORGN 533.** From R&D to commercialization: Successful integration of flow chemistry into manufacturing of API's and intermediates. **M.A. Gonzalez**

**10:55 ORGN 534.** Flowing away from batch: Continuous processing for metalation reactions. **S. Opalka**

Section F

San Diego Convention Center  
Ballroom 20A

### **Technical Achievements in Organic Chemistry**

T. Braden, J. Calvin, *Organizers, Presiding*

**8:40** Introductory Remarks.

**8:45 ORGN 535.** Process chemistry impacts at the interface of discovery and development. **A. Nolting**

**9:15 ORGN 536.** Novel technology platform developments to accelerate drug discovery. **N. Tu**

**9:45 ORGN 537.** Case studies in the use of machine learning models applied to small molecule therapeutic targets. **I. Aliagas**

**10:15** Intermission.

**10:30 ORGN 538.** Evolution of long and short acting pan-AMPK activators as exercise mimetics. **J. Apgar**, R. Wilkening, J. Hicks, D. Feng, L. Wei, K.J. Leavitt, J. Dropinski, L. Chu, X. Qian, A. Kekec, A. Kassick, A. Kim, H. Lu, G. Dong, H. Guan, K. Lu, X. Yang, J. Gorski, G. Eiermann, A. Gollapudi, M. Kurtz, M. Trujillo, R. Myers, D. Kemp, M. Hu, S. Xu, I.K. Sebhat

**11:00 ORGN 539.** Brief history of... a few good molecules. **J. Magano**

**11:30 ORGN 540.** Discovery of ambiphilic reagents for the synthesis of chiral pyrrolidines. **Q. Shi**, N.S. Greenwood, M.C. meehan, J. Coombs, W.P. Gallagher, C.A. Guerrero, J. Hynes, M. Dhar, F. Gonzalez Bobes, D. Marcoux

## **Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets**

Sponsored by ANYL, Cosponsored by COMP, ORGN and PHYS

### **WEDNESDAY AFTERNOON**

Section A

San Diego Convention Center  
Room 7B

### **New Reactions & Methodology**

S. M. Silverman, *Organizer*  
Z. Liu, *Presiding*

**1:00 ORGN 541.** Synthesis inspires design: Importance of synthetic innovations in drug discovery and development. **T. Lyons**

**1:20 ORGN 542.** Extraction reaction mechanism determination of powder river basin (PRB) coal in the supercritical CO<sub>2</sub>-ethanol system by <sup>1</sup>H, <sup>2</sup>H and <sup>13</sup>C nuclear magnetic resonance (NMR) spectroscopy. **X. He**, T. Wang, W. Lu, K. Sun, M. Fan

**1:40 ORGN 543.** SciFinder<sup>n</sup> in the age of computer-aided synthesis design. **O.Y. Ravitz**, J.W. Taylor

**2:00 ORGN 544.** New strategies for catalytic fluorination methods. **C. Brigham**, C. Malapit, M. Sanford

**2:20 ORGN 545.** BPh<sub>3</sub> catalyzed [2+3] cycloaddition of Ph<sub>3</sub>P=C=C=O with nitrones to 4-triphenylphosphoranylidene-5-isoxazolidinones. **A. Brar**, D. Unruh, C. Krempner

**2:40 ORGN 546.** Radical mediated hydroamination using N-hydroxyphthalimide. **S. Lardy**, V.A. Schmidt

**3:00 ORGN 547.** Copper mediated photochemical cycloadditions for the synthesis of small heterocycles. **D. Flores**, V.A. Schmidt

**3:20 ORGN 548.** Ligand-controlled chemodivergent Suzuki cross coupling using palladium-N-heterocyclic carbene catalysts. **E. Reeves**, S. Neufeldt

**3:40 ORGN 549.** Radical-chaperone mediated β,γ-difunctionalization of alcohols. **R.K. Twumasi**, A. Prusinowski, E. Wappes

**4:00 ORGN 550.** Systematic chemical diversity: Synthesis of fused Csp<sup>2</sup>-Csp<sup>3</sup> hybrid pyrano/furano pyridines for fragment based lead discovery. **S. Chamakuri**

**4:20 ORGN 551.** Synthesis of Cannabigerol derivatives via direct *ortho*-allylation of phenols. **N. Jentsch**, X. Zhang, J. Magolan

**4:40 ORGN 552.** Ligand-free rhodium-catalyzed regio- and diastereoselective allylic benzylation using unstabilized nucleophiles. **D. Pal**, T.B. Wright, P. Evans

Section B

San Diego Convention Center  
Room 10

## Asymmetric Reactions & Syntheses

S. M. Silverman, *Organizer*

C. M. Hong, *Presiding*

**1:00 ORGN 553.** Asymmetric synthesis of *P*-stereogenic compounds via thulium (III)-catalyzed desymmetrization of dialkynylphosphine oxides. **Y. Zhang**, X. Liu, X. Feng

**1:20 ORGN 554.** Nickel(II)-catalyzed asymmetric propargyl [2,3]-Wittig rearrangement of oxindole derivatives: Chiral amplification effect. **X. Xu**, X. Feng

**1:40 ORGN 555.** Asymmetric synthesis of 3-aminodihydrocoumarins via the chiral guanidine catalyzed cascade reaction of azlactones. **S. Ruan**, X. Liu, X. Feng

**2:00 ORGN 556.** Asymmetric synthesis of  $\alpha,\beta$ -epoxy- $\gamma$ -lactams by enantioselective Darzens/ring-closure reaction. **b. shen**, X. Liu, X. Feng

**2:20 ORGN 557.** Energy decomposition analyses reveal the origins of catalyst and nucleophile effects on regioselectivity in nucleopalladation of alkenes. **X. Qi**, P. Liu

**2:40 ORGN 558.** *De novo* synthetic study towards 11-deoxyandomycins. **J. Lee**, Y. Rhee

**3:00 ORGN 559.** Development of an asymmetric synthesis of ergoline derivatives. **R. Cannon**, P.J. Guiry

**3:20 ORGN 560.** Development of a metal-catalysed asymmetric carboxylation. **B. Roche**, P.J. Guiry

**3:40 ORGN 561.** Enantioselective synthesis of tricyclic steroidal analogs. **D. Townsend**, A.A. Cobb

**4:00 ORGN 562.** Improved generations of catalysts for asymmetric synthesis and stereoselective reactions. **M. Diéguez**, P. Norrby, F. Maseras, M.A. Pericas, O. Pamies

**4:20 ORGN 563.** Chemosynthetic livers: Predict, prepare and prove the structure, activity and toxicity of drug metabolites. **M. Chorghade**

**4:40 ORGN 564.** Synthesis and application of a novel family of modular ferrocenyl catalysts for asymmetric organocatalysis. **L. Cunningham**, C. Nottingham, P. Guiry

Section C

San Diego Convention Center  
Room 9

### **Photoredox Chemistry**

S. M. Silverman, *Organizer*  
J. D. Weaver, *Presiding*

**1:20 ORGN 565.** Synthesis and photochemical behavior of photoconversion-resistant triarylmethane fluorophores. **A.N. Butkevich**, M.L. Bossi, G. Lukinavicius, S.W. Hell

**1:40 ORGN 566.** Decarboxylative photoredox/nickel-catalyzed conversion of aryl halides to aryl aminooxetanes. **J.A. Terrett**, K. Kolahdouzan, R. Khalaf, J.M. Grandner, Y. Chen, M.P. Huestis

**2:00 ORGN 567.** Electron-catalyzed Diels-Alder reactions by TiO<sub>2</sub> photocatalysis. **Y. Okada**, K. Nakayama, N. Maeta, G. Horiguchi, H. Kamiya

**2:20 ORGN 568.** Radical conjugate addition of N-heterocycles and tertiary amines. **A. Aycock**, **H. Wang**, C.J. Pratt, D.B. Vogt, N.T. Jui

**2:40 ORGN 569.** Radical anions as reactive intermediates for the synthesis of complex molecules. **C. Seath**, N. Jui

**3:00 ORGN 570.** Facile preparation of spirolactones by an alkoxy carbonyl radical 5-*exo* cyclization cross-coupling cascade. **N.A. Weires**, Y. Slutskyy, L.E. Overman

**3:20 ORGN 571.** Visible light mediated alkene aminoarylation with benzenesulfonyl acetamides. **A.R. Allen**, R. McAtee, C. Stephenson

**3:40 ORGN 572.** Amine and heterocycle synthesis enabled by photoredox catalysis. **A.F. Garrido-Castro**, M. Maestro, J. Alemán

Section D

San Diego Convention Center  
Room 8

**Development of New Strategies for the Synthesis & Functionalization of Strained Rings for Applications as Bioisosteres in Biologically Active Compounds**

S. M. Silverman, *Organizer*  
J. Mousseau, *Organizer, Presiding*  
J. J. Mousseau, *Presiding*

**1:00** Introductory Remarks.

**1:05 ORGN 573.** Conformationally-restricted motifs as bioisosteres for aromatics: Playground for new methods development. **T. Fessard**

**1:35 ORGN 574.** Cubanes in medicinal chemistry. **M. Kassiou**

**2:20 ORGN 575.** Synthesis of new chemical motifs for drug discovery: 4-Membered heterocycles as fragments and bioisosteres. **J.A. Bull**

**3:05** Intermission.

**3:20 ORGN 576.** Use of aliphatic bioisosteres in medicinal chemistry. **A. Stepan**

**3:50 ORGN 577.** Strained rings in nature, medicines, and energetics. **P.S. Baran**

**4:50** Concluding Remarks.

Section E

San Diego Convention Center  
Room 7A

**From Lab to Commercial Scale: The Challenges to Scaling Up Flow Chemistry in the Pharmaceutical Industry**

J. R. Naber, *Organizer*  
K. M. Maloney, *Presiding*



**1:00 ORGN 578.** Enabling photochemistry: Moving from lab to pilot scale. **F. Lévesque**

**1:40 ORGN 579.** Drug substances continuous process development: From the bench to demonstration pilot. **M. Etienne**

**2:20 ORGN 580.** Development of continuous API manufacturing technologies at Pfizer. **A. Dion**

**3:00 ORGN 581.** Development of a continuous flow process from lab to production at Vertex Pharmaceuticals. **B. Lewandowski**

**3:40 ORGN 582.** Safe scale-up of an exothermic grignard reaction based on thermal hazard understanding and engineering control. **A. Allian**

**4:20 ORGN 583.** Enabling commercial continuous manufacturing through robust control strategies. **A. O'Brien**

Section F

San Diego Convention Center  
Ballroom 20A

### **Technical Achievements in Organic Chemistry**

T. Braden, J. Calvin, *Organizers, Presiding*

**1:40** Introductory Remarks.

**1:45 ORGN 584.** Discovery of potent small molecule inhibitors of the PICK1 PDZ-domain that modulate amyloid beta-mediated synaptic dysfunction. **E.Y. Lin**, L.F. Silvian, D. Marcotte, C.C. Banos, F. Jow, T.R. Chan, R.M. Arduini, F. Qian, D.P. Baker, C. Bergeron, C.A. Hession, R.L. Haganir, C.F. Borenstein, I. Enyedy, J. Zou, E. Rohde, M. Wittmann, G. Kumaravel, K.J. Rhodes, R.H. Scannevin, A.W. Dunah, K.M. Guckian

**2:15 ORGN 585.** Discovery of tetflupyrolimet: New mode-of-action herbicide that interferes with *de novo* pyrimidine biosynthesis. **K.A. Hughes**, T.P. Selby, A.D. Satterfield, A. Puri, D.A. Travis, M.J. Campbell, A.E. Taggi

**2:45 ORGN 586.** Discovery of pyrrolidine sulfonamides as TRPV4 antagonists. **E. Brnardic**

**3:15** Intermission.

**3:30 ORGN 587.** Use of structure-based design in the discovery of the BCL-2 selective inhibitor Venclexta® and the bromodomain and extra-terminal domain (BET) inhibitors mivebresib and ABBV-744. **L.A. Hasvold**

**4:00 ORGN 588.** Synthetic chemistry enabling hit-to-lead progression of T-type Ca<sup>2+</sup> channel antagonists and ASC-1 inhibitors. **K. Schlegel**

**4:30 ORGN 589.** Identification of a novel ASGPr ligand and application to receptor mediated delivery and cell-type specific gene editing with CRISPR-Cas9 ribonucleoproteins. **B. Thuma**

### **Covalent & Non-Covalent Dimers as Therapeutic Agents in Drug Discovery**

Sponsored by BIOL, Cosponsored by MEDI and ORGN

### **Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets**

Sponsored by ANYL, Cosponsored by COMP, ORGN and PHYS

## **WEDNESDAY EVENING**

Section A

San Diego Convention Center  
TBD

### **Asymmetric Reactions & Syntheses**

Cosponsored by MEDI‡  
E. C. McLaughlin, *Organizer*

**7:00 - 9:00**

**ORGN 590.** Multikilogram-scale synthesis of esomeprazole using enantioselective iron catalysis. **S. Nishiguchi**, T. Izumi, T. Kouno, J. Sukegawa, L. Ilies, E. Nakamura

**ORGN 591.** Design of helical peptide foldamers for asymmetric reactions. **T. Umeno**, A. Ueda, T. Kato, M. Doi, M. Tanaka

**ORGN 592.** Helical peptide-catalyzed asymmetric Michael addition reactions of malonates to  $\alpha,\beta$ -unsaturated ketones and their synthetic applications. **A. Ueda**, M. Higuchi, T. Umeno, A. Sugiyama, M. Tanaka

**ORGN 593.** New practical method for direct asymmetric reductive amination of *p*-trifluoromethoxy acetophenone. **M. Yamada**, K. Murai, M. Yamano

**ORGN 594.** Mechanism and stereoiduction of catalytic asymmetric propargylboration of hydrazonoesters. **S. Jonker**, C. Diner, G. Schulz, H. Iwamoto, L. Eriksson, K.J. Szabo

**ORGN 595.** Organocatalyzed three-component reaction of  $\gamma$ -arylenals and nitroalkenes. D. Majee, S. Jakkampudi, H.D. Arman, **C.C. Zhao**

**ORGN 596.** Asymmetric carbon atom synthesis by samarium (II)-water allylic benzoate reductions. **M.A. Leitch**, **D.R. Turner**, G.W. O'Neil

**ORGN 597.** Change the enantioselectivity of enzymes: Rational structural-modification of functional proteins catalyzing Diels-Alder reactions with the reversed enantioselectivity. **Y. Zou**, K.N. Houk

**ORGN 598.** Organoboron bifunctional catalysis of asymmetric nitro-Michael addition. **Y. Du**

**ORGN 599.** Gold catalyzed asymmetric intramolecular [4+3] cycloadditions. **R. Ma**

**ORGN 600.** Stimuli-responsive asymmetric catalysis. **S. Spring**, C.G. Frost

**ORGN 601.** Enantioselective formation of  $\gamma$ -lactams with multiple chiral carbon centers by Ni(0)-catalyzed asymmetric carbonylative cycloaddition. **K. Ashida**, Y. Hoshimoto, S. Ogoshi

**ORGN 602.** Synthesis and characterization of ethylenediamine-cored optoelectronic starburst materials. **T. Lee**, Y. Kim, K. Park

**ORGN 603.** Ir catalyzed asymmetric tandem reaction of meso-diols. **T. Suzuki**

**ORGN 604.** Atroposelective nucleophilic aromatic substitution of fluorinated pyrrolopyrimidines. **M.A. Saputra**, A. Weng, J.L. Gustafson

**ORGN 605.** Circularly polarized luminescence from chiral molecules based on planar chiral [2.2] paracyclophane. **Y. Morisaki**

**ORGN 606.** Diastereodivergent and enantioselective synthesis of  $\alpha$ -fluoro- $\beta$ -aminonitriles via copper(I) catalyzed asymmetric Mannich reaction. **R. Ding**, Z. De los Santos, C. Wolf

**ORGN 607.** Accessing pharmaceutically relevant 3-arylated *N*-heterocycles via atroposelective synthetic methodologies. **M.M. Cardenas**, M.A. Saputra, A.N. Sanchez, E. Valle, J.L. Gustafson

**ORGN 608.** Catalytic enantioselective synthesis of  $\alpha$ -allylic alcohol- $\alpha$ -aryl oxindoles. **E. Judge**, P. Guiry

**ORGN 609.** Atroposelective halogenation of biaryl anilines. **S.D. Vaidya**, S. Toenjes, J.L. Gustafson

**ORGN 610.** Asymmetric ring-opening of donor–acceptor cyclopropanes with primary arylamines catalyzed by a chiral heterobimetallic catalyst. **W. Luo**, H. Wang

**ORGN 611.** Development of late-stage functionalization of chiral bisphosphorylimides. **A. Smolin**, O. Apolinar, R.G. Iafe

**ORGN 612.** Enantioselective, copper-catalyzed alkynylation of cyclic iminium ions lacking stabilizing groups. **W. Guan**, J. Liao, M.P. Watson

**ORGN 613.** Enaminone, metal Lewis acid catalyzed inverse electron demand Aza–Diels Alder reaction to synthesize dihydropyridine derivatives. **H.N. Fernando**

Section A

San Diego Convention Center  
TBD

**CH Activation**

Cosponsored by MEDI  
E. C. McLaughlin, *Organizer*

**7:00 - 9:00**

**ORGN 614.** Mono- and bis-norbornene annulated biaryl amines through pseudo-Catellani intermediates by Pd-catalyzed C-H activation. **S. Chuang**

**ORGN 615.** Enantioselective  $\alpha$ -amino C-H functionalization by cooperative actions of B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> and chiral Mg-PyBOX complex. **J. Chan**, M. Wasa

**ORGN 616.** Pd-catalyzed C(4)-H functionalization of pyrrolidines and piperidines with C(3)-directing groups: Mechanistic insight into regio- and stereoselectivity. **D. Antermite**, J.A. Bull

**ORGN 617.** Unified approach to C-H amination via imidate radicals. **M. Shea**, D. Nagib, A. Prusinowski

**ORGN 618.** Mechanistic insights and kinetic studies of Lewis base chlorination of arenes and heterocycles. **A.N. Dinh**, L. Janke, S.M. Maddox, J. Gustafson

**ORGN 619.** Catalytic dimerization of terminal alkynes to *gem*-enynes using a binuclear Lewis acid-base complex. **A. Brar**, S. Mummadi, D. Unruh, C. Krempner

**ORGN 620.** Synthesis of  $\alpha$ -Keto esters using platinum-catalyzed C-H acylation reaction with ethyl chlorooxoacetate. **S. Huo**, E. Javed, J.D. Guthrie, G. Chirayath

**ORGN 621.** Chelation-assisted decarboxylative amidation. **K. Das**, P. Kilaru, P. Zhao

Section A

San Diego Convention Center  
TBD

### **Metal-Mediated Reactions & Syntheses**

Cosponsored by MEDI<sup>‡</sup>  
E. C. McLaughlin, *Organizer*

**7:00 - 9:00**

**ORGN 622.** Solid-state aldol reaction of lithium enolate of pinacolone. **H. Pang**, P.G. Williard

**ORGN 623.** Copper-catalyzed photoinduced radical domino cyclization of ynamides and cyanamides: Unified entry to rosettacin, luotonin A and deoxyvasicinone. **H. Baguia**, C. Deldaele, E. Romero, B. Michelet, G. Evano

**ORGN 624.** Stereoselective synthesis of mono and fused, carbo- and heterocyclic compounds via cobalt-assisted radical cyclizations. **N. Babayans**, E. Artashyan, S. Guarina, G.G. Melikyan

**ORGN 625.** Rhodium-catalyzed oxy-trifluoromethylthiolation of diazocarbonyl substrates. **M. Lübcke**, W. Yuan, K.J. Szabo

**ORGN 626.** Quaternary carbons via palladium-catalyzed aryl prenylation. **J. Leister**, M. Mendoza, K. Billingsley

**ORGN 627.** Intramolecular C–N bond formation: Reactivity and selectivity of hypervalent iodine oxidants in the generation of carbamate-derived nitrenes. **A. Bunnell**, M. Lasky, B. Lee, E.C. McLaughlin

**ORGN 628.** Copper-catalyzed hydro-oxycarboxylation of terminal alkynes. **Q. Tan**, S. Seo, M.C. Willis

**ORGN 629.** Tungsten dearomatization of electron deficient arenes: Synthesis of functionalized cyclohexenes via tandem additions. **S. Simpson**, W.D. Harman

**ORGN 630.** Regio- and enantioselective CuH-catalyzed ketone allylation with terminal allenes. **E. Tsai**, R.Y. Liu, Y. Yang, S.L. Buchwald

**ORGN 631.** Intermolecular Heck coupling with hindered alkenes directed by potassium carboxylates. **T.R. Huffman**, Y. Wu, A. Emmerich, R.A. Shenvi

**ORGN 632.** Exploring sulfonamide substrates for cyclopropane formation by cross-electrophile coupling. **A. Izad**, E. Lucas, K.A. Hewitt, E.R. Jarvo

**ORGN 633.** Synthesis of cyclopentenones via Ni-catalyzed formal [3+2] cycloaddition of cyclopropanones and internal alkynes. **Y. Jang**, V. Lindsay

**ORGN 634.** Expansion of scope for nickel-catalyzed cross-electrophile couplings of sulfonamides for cyclopropane synthesis. **Y. Tiemsanjai**, A. Castro, E. Lucas, K.A. Hewitt, E.R. Jarvo

**ORGN 635.** Non-precious metal catalyzed direct synthesis of Guerbet alcohol. **E. Sehovic**, P. Kaur

**ORGN 636.** Green preparation of Au(I) complexes via mechanochemistry. **F. Ingner**

**ORGN 637.** Stereocontrolled synthesis of (*E*)-stilbene derivatives by palladium-catalyzed Suzuki-Miyaura cross-coupling reaction. H.H. Rau, **N.S. Werner**

**ORGN 638.** Nickel-catalyzed Kumada cross-coupling reactions of sulfonamides. **A.C. Matus**, K.A. Hewitt, E.R. Jarvo

**ORGN 639.** Nickel catalyzed synthesis of alkynylphosphonates. **P. Kaur**

**ORGN 640.** Synthesis of fluorescent compounds to detect ethylene gas. **S. Rezgui**, S. Toussaint, B.W. Michel

**ORGN 641.** Selective deuteration of a broad variety of halogenated compounds using Pd/C-Al-D<sub>2</sub>O system as the deuterium source and reaction medium. **N. Zorigt**, **C. Schaefer**, **B. Torok**

**ORGN 642.** Mechanism of a chromium-salen catalyzed oxidative cross-coupling of phenols. **T. Paniak**, M. Kozlowski

**ORGN 643.** Mechanistic origins of site-selectivity in Pd-NHC-catalyzed cross-couplings. **E. Reeves**, S. Neufeldt

**ORGN 644.** Studies directed toward the development of transition metal-halloysite nanocomposite materials for organic transformations. **J. Hamdi**, B. Diehl, A. Blanco, J.B. Wiley, M. Trudell\*

Section A

San Diego Convention Center  
TBD

### **Photoredox Chemistry**

Cosponsored by MEDI<sup>‡</sup>  
E. C. McLaughlin, *Organizer*

**7:00 - 9:00**

**ORGN 645.** Enablement of  $C(sp^3)-C(sp^3)$  coupling for DNA encoded library synthesis: Decarboxylative alkylation of  $\alpha$  amino acids via mild, aqueous photoredox catalysis. D.K. Kölmel, **R.P. Loach**, T. Knauber, M.E. Flanagan

**ORGN 646.** Visible light-mediated radical process for the synthesis of C-glycoamino acids. **P. Ji**, Y. Zhang, Y. Wei, H. Huang, W. Hu, W. Wang

**ORGN 647.** Synthesis of chemical libraries and building blocks for drug discovery using photoredox catalysis. **K. Tai**, Y. Mori, C. Kikuchi, M. Kurimura, K. Kondo

**ORGN 648.** Organocatalytic thioesterification of aldehydes with visible light. **Y. Zhang**, P. Ji, W. Hu, Y. Wei, H. Huang, W. Wang

**ORGN 649.** Lead halide perovskites for photocatalytic organic synthesis. **X. Zhu**, Y. Lin, Y. Sun, D. Zhu, Y. Yan

**ORGN 650.** Withdrawn.

**ORGN 651.** Silicon for pharmaceutical molecule synthesis: Alkenyl-passivated Si quantum dots for C-H activation of tertiary amine. **Y. Sun**, J. San Martin, Y. Yan

**ORGN 652.** Radical cation vinylcyclopropane rearrangements by  $TiO_2$  photocatalysis. **N. Maeta**, H. Kamiya, Y. Okada

**ORGN 653.** Nitrene generation via visible-light photocatalysis: Aziridination from electrophilic amine sources. **V. Wu**, C.P. Anyanwu, W. Mohamed, E.C. McLaughlin

**ORGN 654.** Continuous flow photocatalytic Minisci reaction using *N*-(acetoxy)phthalimide esters. **G. Ignacz**, T. Noel, G. Sipos

**ORGN 655.** Silicon quantum dots for synthesis of pyrroles and pyrazoles. **J. San Martin**, Y. Sun, Y. Yan

**ORGN 656.** Carboamination strategy for sultam synthesis enabled by photoredox catalysis. R. McAtee, **E.A. Noten**, C. Stephenson

**ORGN 657.** Perovskite  $CsPbBr_3$  nanocrystal with a rich possibility of photocatalysis reactions. **D. Zhu**

**ORGN 658.** Chiral lead-halide perovskite as efficient photocatalysts for atroposelective pyrroles and indoles synthesis. **Y. Lin**, Y. Sun, C. Manabat, J. San Martin, D. Zhu, X. Zhu, Y. Yan



**ORGN 659.** Oxidative photo-catalyzed sulfenylation of substituted indoles and benzothiamides. A.N. Dinh, **A.D. Nguyen, E. Millan**, S. Albright, M.R. Cedano, D.K. Smith, J.L. Gustafson

Section A

San Diego Convention Center  
TBD

### **Total Synthesis of Complex Molecules**

Cosponsored by MEDI<sup>‡</sup>  
E. C. McLaughlin, *Organizer*

**7:00 - 9:00**

**ORGN 660.** Total synthesis and absolute configuration of simpotentin, a potentiator of amphotericin B activity. **M. Ohtawa**, R. Uchida, H. Tomoda, T. Nagamitsu

**ORGN 661.** Enantioselective total synthesis of (+)-ieodomycin B and its optical isomers: Synthesis and biological evaluation. D. Choi, J. Lee, Y. Lee, H. Lee, **J. Lee**

**ORGN 662.** Withdrawn.

**ORGN 663.** Asymmetric total syntheses of bridged indole alkaloids with medium sized ring via regioselective indolization. C. Cho, **J. Kim**, H. Kang

**ORGN 664.** Kinetically controlled Fischer indolization for the total syntheses of (+)-uleine, (-)-tubifolidine, (-)-tabersonine, and polyveoline. C. Cho, **D. Kim**, T. Jeon, Y. Kim, J. Lim

**ORGN 665.** Progress toward total synthesis of (-)-platensimycin and (-)-cyanthiwigin F by internal H-bonding mediated intramolecular Diels-Alder reaction. C. Cho, **H. Kim**, J. Lee, J. Oh

**ORGN 666.** Synthetic approach to ergotryptamine, norpsilocin, and aurantioclavine. **S. Rahman**

**ORGN 667.** Synthetic studies on strophasterols A-D. **S. Sato**, S. Kuwahara

**ORGN 668.** Synthesis of the N-Acyl amycolose moiety of amycolamicin and its methyl glycosides. **y. meguro**, S. Kuwahara

**ORGN 669.** Aleutianamine: Architecturally-complex pyrroloiminoquinone alkaloid with selective cytotoxicity toward pancreatic cancer cell lines. **Y. Zou**, X. Wang, J. Sims, B. Wang, P. Pandey, C. Welsh, R. Stone, M. Avery, R.J. Doerksen, D. Ferreira, C. Anklin, F.A. Valeriote, M. Kelly, M.T. Hamann

**ORGN 670.** Scalable and convenient syntheses of molecular baskets. **T.A. Neal, M. Gunther**, J. Badjic

**ORGN 671.** Total synthesis of unique monoterpene-polyketides, cryptolaevilactones, from *Cryptocarya laevigata*. **Y. Miura**, Y. Saito, K. Nakagawa-goto

**ORGN 672.** Structure-activity relationship study of antiproliferative abietane diterpenes: Syntheses of 4-*epi*-parviflorons and its derivatives. Y. Miyajima, **Y. Saito**, M. Takeya, M. Goto, K. Nakagawa-goto

**ORGN 673.** 11-step catalytic asymmetric synthesis of (–)-bilobalide. **M. Baker**, R. Demoret, M. Ohtawa, R.A. Shenvi

**ORGN 674.** Total synthesis of furanosteroids natural products: Viridin and nodulisporiviridin E. **Y. Ji**, S. Gao

**ORGN 675.** Studies towards the total synthesis of anguidine. **D. Zhao**, R. Manetsch

**ORGN 676.** Progress toward an enantioselective total synthesis of paecilomycine A. **J.M. Nguyen**, S.D. Townsend

**ORGN 677.** Synthesis and biological evaluation of illudalic acid derivatives: Inhibition of protein tyrosine phosphatase activity. **B.S. McCullough**, P. Batsomboon, G.B. Dudley, A.M. Barrios

## **THURSDAY MORNING**

Section A

San Diego Convention Center  
Room 7B

**New Reactions & Methodology**

S. M. Silverman, *Organizer*  
D. Weingarten, *Presiding*

**8:00 ORGN 678.** Aerobic C(sp<sup>2</sup>)-H hydroxylations of 2-aryloxazolines: Fast access to novel ESIPT-based luminophores. **D. Göbel**, B.J. Nachtsheim

**8:20 ORGN 679.** Synthesis of NIR dyes by C-H functionalization for applications in cellular imaging. **C. Rathnamalala**

**8:40 ORGN 680.** C-H activation: Viable route to materials. **C.N. Scott**, I. Rajapaksha, D. Feng, C. Rathnamalala

**9:00 ORGN 681.** Confirmation and quantification of fatty amides and nonamides in direct vegetable oil stripping. **O. Abel-Anyebe**, D. Keita, K.I. Ekpenyong, A. Sodipe, M. Yakubu

**9:20 ORGN 682.** Reverse pharmacology and systems approaches for chemical biology, drug discovery and development: Inspiration from the wisdom of mother nature. **M. Chorghade**

**9:40 ORGN 683.** Surveying iron-organic framework TAL-1 derived and related materials in ligandless heterogenous oxidative catalytic transformations. **K. Ping**, M. Alam, R. Bhadoria, P. Starkov

**10:00 ORGN 684.** Catalytic enantioselective C(sp<sup>2</sup>)-H and C(sp<sup>3</sup>)-H alkylation: From organocatalysis to transition metal catalysis. **S. Mukherjee**

**10:20 ORGN 685.** High throughput quantitative and qualitative analysis of high-density kinetic data leads to improved understanding of complex catalytic reactions. **A. Nazarova**, V.V. Fokin

**10:40 ORGN 686.** Cross-coupling of amides by N-C activation. **M. Szostak**

**11:00 ORGN 687.** Multicomponent reactions for the introduction of SCF<sub>3</sub> groups into diazocarbonyl compounds. **M. Lübcke**, W. Yuan, D. Bezhan, K.J. Szabo

**11:20 ORGN 688.** Chemoenzymatic approaches to the total synthesis of epoxyquinoid natural products. **J.A. Collins**, M.S. Duncan, W.B. Kline, Z.T. Clark

San Diego Convention Center  
Room 10

## Asymmetric Reactions & Syntheses

S. M. Silverman, *Organizer*  
A. Lo, *Presiding*

**8:00 ORGN 689.** Synthesis of axially chiral biaryl-carboxylic acids (BINA-Cox) and their evaluation as ligands in asymmetric titanium-catalyzed hydroalkoxylation. **S.L. Helmbrecht**, L. Hintermann

**8:20 ORGN 690.** Applications of boronic acids in asymmetric synthesis. **S. Jonker**, C. Diner, G. Schulz, H. Iwamoto, L. Eriksson, K.J. Szabo

**8:40 ORGN 691.** Diastereodivergent synthesis of tricyclic chromanone derivatives using modularly designed organocatalysts. **C.C. Zhao**, S. Jakkampudi, R. Parella, H.D. Arman

**9:00 ORGN 692.** Asymmetric synthesis of azepine-fused cyclobutanes via a gold(I)-catalyzed cyclopropanation/C-C cleavage/chirality-memorized Wagner-Meerwein rearrangement of yne-methylenecyclopropanes. **C. Li**, Z. Yu

**9:20 ORGN 693.** Asymmetric synthesis of fused bicyclic N,O- and O,O-acetals via cascade reaction by gold(I)/N,N'-dioxide-nickel(II) bimetallic relay catalysis. **B. Hu**, X. Feng

**9:40 ORGN 694.** Acyclic stereocontrol in the additions of nucleophilic alkenes to  $\alpha$ -chiral *N*-sulfonyl imines. **A. Lo**, L.C. Moore, J.T. Shaw, J.S. Fell

**10:00 ORGN 695.** Enantioselective [3 + 2] cycloaddition and rearrangement of thiazolium salts to synthesize thiazole and 1,4-thiazine derivatives. **X. Zhang**, X. Liu, X. Feng

**10:20 ORGN 696.** Bimetallic rhodium(II)/indium(III) relay catalysis for tandem insertion/asymmetric claisen rearrangement. **Y. Chen**, X. Liu, X. Feng

**10:40 ORGN 697.** Bimetallic catalytic asymmetric tandem reaction of  $\beta$ -alkynyl ketones to synthesize 6,6-spiroketal. **S. Ge**, X. Feng

**11:00 ORGN 698.** Enantioselective synthesis of 2,2,3-trisubstituted indolines via bimetallic relay catalysis of  $\alpha$ -diazoketones with enones. **J. Yang**, X. Liu, X. Feng

**11:20 ORGN 699.** Catalytic enantioselective ene-type reactions of vinylogous hydrazone: Construction of  $\alpha$ -methylene- $\gamma$ -butyrolactone derivatives. **H. Zhang**, X. Liu, X. Feng

Section C

San Diego Convention Center  
Room 9

### Heterocycles & Aromatics

S. M. Silverman, *Organizer*  
F. P. Lim, *Presiding*

**8:00 ORGN 700.** Magnesium ethoxide promoted conversion of nitriles to amidines and its application in 5,6-dihydro-imidazobenzoxazepine synthesis. **M.E. Dalziel**, J. Deichert, D. Carrera, D. Beaudry, C. Han, H. Zhang, R. Angelaud

**8:20 ORGN 701.** Withdrawn.

**8:40 ORGN 702.** Withdrawn.

**9:00 ORGN 703.** [4+2] Cycloaddition methodology for the synthesis of functionalised aromatic scaffolds. **B. Emery**, S.D. Bull

**9:20 ORGN 704.** Rapid assembly of saturated nitrogen heterocycles in one-pot for biological screening collections. **A.J. Boddy**, D. Affron, C. Cordier, E. Rivers, A.C. Spivey, J.A. Bull

**9:40 ORGN 705.** Synthesis of novel 3,3-disubstituted azetidines for medicinal chemistry: Divergent catalytic functionalization of 3-aryl-3-azetidins. **M. Dubois**, C. Denis, A. Lazaridou, V. Anne Sophie, R. Bureau, J.J. Mousseau, C. Choi, J.A. Bull

**10:00 ORGN 706.** Synthesis of small sensory models for develop as pH probes. **I. Rajapaksha**

**10:20 ORGN 707.** *In vivo* monitoring of carbonic anhydrases expression with fluorescence turn-on enrichment. **C. Chou**

**10:40 ORGN 708.** Synthesis of  $\beta$ -lactams via metal-catalyzed formal [3+1] cycloaddition of cyclopropanones. **C.M. Poteat**, Y. Jang, J.D. Johnson, V. Lindsay

**11:00 ORGN 709.** Regio- and stereoselective synthesis of isoindolinones through superbase-mediated iodoaminocyclization of 2-(1-Alkynyl)benzamides. **S. Mehta**, D. Brahmchari

**11:20 ORGN 710.** Unprecedented and efficient synthesis of DMDPP and its conversion to the arylalkenyl  $\pi$ -system through C-H transition-metal-free approach. **D. Feng**

**11:40 ORGN 711.** One-pot, multicomponent synthesis of azolo[1,3,5]triazines via selective 1,3,5-triazine ring annulation onto aminoazoles. **F.P. Lim**, A.V. Dolzhenko

Section D

San Diego Convention Center  
Room 8

### **Metal-Mediated Reactions & Syntheses**

S. M. Silverman, *Organizer*  
H. Shenouda, *Presiding*

**8:00 ORGN 712.** Nickel-catalyzed, ring-forming aromatic C-H alkylations with unactivated alkyl halides. **Q.D. Tercenio**, E.J. Alexanian

**8:20 ORGN 713.** Formation of new C-C bonds via H<sub>2</sub>-mediated coupling of ketenimines with carbonyl electrophiles. **M.M. Sikes**, L.V. Hale, N.K. Szymczak

**8:40 ORGN 714.** Transition metal-catalyzed highly regioselective azide-internal alkynes cycloaddition under mild conditions. **W. Song**

**9:00 ORGN 715.** Iron-catalyzed site-selective oxidation of phenols and anisoles. L. Göttemann, **M. Chojnacka**, A. Pan, K. Kou

**9:20 ORGN 716.** Synthesis of benzoxocine heliannuols via the intramolecular Nicholas reaction. **B. St Onge**, J.R. Green

**9:40 ORGN 717.** Stereospecific, manganese-catalyzed hydroxymethylation of unactivated alkyl tosylates. **H. Shenouda**, E.J. Alexanian

**10:00 ORGN 718.** Iridium catalyzed hydrogen-borrowing reactions of  $\beta$ -amino alcohols. **C.J. Hall**, W.R. Goundry, T.J. Donohoe

**10:20 ORGN 719.** Vinylation of benzylic amines via C-N bond functionalization of benzylic pyridinium salts. **W. Guan**, J. Liao, M.P. Watson

**10:40 ORGN 720.** Cyclic(alkyl)amino carbenes synthesis and applications. **R.F. Jazzar**, G. Bertrand

**11:00 ORGN 721.** Expansion of the Chan–Evans–Lam reaction with functionalized potassium vinyl trifluoroborates. **G.I. Elliott**, T.E. Cole

**11:20 ORGN 722.** Activation of trifluorotoluene towards hydroamination type reactions by a tungsten dearomatization agent. **K.B. Wilson**, H.S. Nedzbala, W.D. Harman

**11:40 ORGN 723.** Synthesis of long expanded helicenes via a diyne-selective [2+2+2] cycloaddition strategy. **G.R. Kiel**, T. Tilley

Section E

San Diego Convention Center  
Room 7A

### **Total Synthesis of Complex Molecules**

S. M. Silverman, *Organizer*  
R. Demoret, *Presiding*

**8:00 ORGN 724.** New strategies for the concise synthesis of complex terpenes. **P. Hu**

**8:20 ORGN 725.** Total synthesis of (-)- $\gamma$ -lycorane. **C.J. Hall**, I. Marriott, W.R. Goundry, T.J. Donohoe

**8:40 ORGN 726.** Biocatalytic C–H oxidation as an enabling tool for complex molecule total synthesis. **H. Renata**

**9:00 ORGN 727.** Biocatalyst-initiated *ortho*-quinone methide generation and diversification. **J. Perkins**, T. Doyon, E. Romero, S.A. Dockrey, K. Skinner, P.M. Zimmerman, A.R. Narayan

**9:20 ORGN 728.** Enantioselective syntheses of concave-substituted dioxabicyclo[3.3.0]octanone spongian diterpenoids. **T.K. Allred**, P. Zhao, G. Lackner, L.E. Overman

**9:40 ORGN 729.** Eleven-step synthesis of (–)-bilobalide. **R. Demoret**, M. Baker, M. Ohtawa, R.A. Shenvi

**10:00 ORGN 730.** Total synthesis of streptothricin F and streptolidine lactam. **M. Dowgiallo**, M. Kassu, J. Kirby, R. Manetsch

**10:20 ORGN 731.** Biocatalytic synthesis of anthelmintics using a cascade assembly approach. **S. Kelly**, A.E. Fraley, S. Newmister, Y. Ye, D.H. Sherman

**10:40 ORGN 732.** Stereodivergent, chemoenzymatic synthesis of azaphilones natural products. **J. Pyser**, S.A. Dockrey, L. Joyce, A. Rodriguez Benitez, R. Wiscons, A.R. Narayan

**11:00 ORGN 733.** Progress toward the synthesis of arimetamycin A. **E.D. Huseman**, S.D. Townsend

**11:20 ORGN 734.** Thioenamide synthesis inspired by peptide macrocycles. **J. Lutz**, C.M. Taylor

### **Interface between Experiments & Modeling in Unraveling the Physical & Chemical Properties of Charged Droplets**

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