**2:10** INOR **1561.** Long route from hexagonal-$AMn^{3+}O_3$ to $AMn^{2+}O_{2.5}$. **M. Olivier**, T. Pussacq, M. Huvé, F. Tessier, H. Kabbour

**2:30** INOR **1562.** Withdrawn.

**2:50** INOR **1563.** Thermolytic molecular precursor methods to germanium-doped single-sites on silica. **J.P. Dombrowski**, T.D. Tilley, A.T. Bell

**3:10** INOR **1564.** Beyond thioureas: Highly monodisperse CdS nanocrystal syntheses via thiocarbonates, thiocarbamates, and thioureas. **L. Hamachi**, I. Jen-La Plante, G. Cleveland, J.S. Owen

**3:30** INOR **1565.** Withdrawn.

**3:50** Intermission.

**4:05** INOR **1566.** Simple method to predict the electronic spin configuration of Fe(II) tris-diimine complexes. H. Phan, J. Hrudka, **M. Shatruk**

**4:25** INOR **1567.** Non-covalent interactions in superatomic crystals. **J.L. Shott**, M. Freeman, N. Saleh, D.S. Jones, C. Bejger

**4:45** INOR **1568.** Water confinement properties of a metal-organic nanotube. **M. Payne**, A.S. Jayasinghe, D. Unruh, T. Forbes

**5:05** INOR **1569.** Synthesis and characterization of magnesium oxychloride as a fire resistant construction material. **R.F. Gochez**, C.L. Kitchens

**5:25** INOR **1570.** Industrial outlook on the development of cost effective $SiO_2$ mesoporous cellular foams technology. **B.A. Kilos**, A.M. Kelly-Rowley, S. Matteucci, C.L. Tway, K. Mabe, H. Clements

**5:45** INOR **1571.** Centimeter-sized epitaxial h-BN as a flexible & transferrable template for heteroepitaxial growth of semiconductor thin films. **H. Oh**, K. Chung, J. Jo, Y. Tchoe, H. Yoon, H. Lee, S. Kim, M. Kim, B. Sohn, G. Yi

### Section L

Moscone Center
3003

#### Nanoscience

B. G. Trewyn, *Organizer*

E. Johlin, *Presiding*

**1:30** INOR **1572.** Monocrystalline nanopatterned films made by nanocube assembly and chemical welding. B. Sciacca, A. Berkhout, M. van Huis, B. Brenny, A. Polman, **E. Garnett**

**1:50** INOR **1573.** Graphene oxide membranes with strong stability in aqueous solutions and controllable lamellar spacing. **J. Hu**, Y. Xi, Z. Liu, R. Xie, X. Ju, W. Wang, L. Chu

**2:10** INOR **1574.** Photovoltage, effective bandgap and photochemical charge transfer in nanoscale transition metal (Cu, Fe, Mn, Ni) doped $SrTiO_3$ photocatalysts. **X. Ma**, F.E. Osterloh

**2:30** INOR **1575.** Semiconductor nanocrystals with compact fluorinated shells. **P. Xia**, M.L. Tang

**2:50** INOR **1576.** 3D Nanostructure imaging via multi-energy deconvolution SEM. **E. Johlin**, M. de Goede, B. Sciacca, F. Boughorbel, E. Garnett

**3:10** INOR **1577.** Opportunities and limitations for nanoscale photovoltaics to surpass the Shockley-Queisser limit. **S.A. Mann**, R. Grote, R.M. Osgood, A. Alu, E. Garnett

**3:30** Intermission.

**3:40** INOR **1578.** Metal halide perovskite nanowire arrays for photodetection with significantly improved stability. **Z. Fan**, L. Gu, M. Tavakoli, A. Waleed

**4:00** INOR **1579.** Exploring of the scope of polyarylboranes. **M.W. Lee**, T. Wang

**4:20** INOR **1580.** Efficiency of magnetic induction heating for single crystal iron oxide nanoparticles. R.R. Shah, T.P. Davis, A.L. Paulson, C.S. Brazel, **D.E. Nikles**

**4:40** INOR **1581.** Elucidation of synthesis and characterization of non-precious nanoscale mixed metal oxides for green chemistry catalysis. **A.M. York**, C.A. Cadigan, R.M. Richards

**5:00** INOR **1582.** Carrier selective contacts for nanowire solar cells. **S. Oener**, A. Cavalli, J. Haverkort, E. Bakkers, E. Garnett

**5:20** INOR **1583.** TERS: Nanoscale Raman characterization of 0-1-and 2D materials. **A. Krayev**, M. Chaigneau

# MEDI

## Division of Medicinal Chemistry

**A. Stamford**, *Program Chair*

**OTHER SYMPOSIA OF INTEREST:**

**ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin** (see *COMP*, Tue)

**ACS Chemical Biology Award Symposium** (see *BIOL*, Tue)

**Chemical Biology: Enabling Drug Discovery** (see *ORGN*, Wed)

**SOCIAL EVENTS:**

**Poster Sessions & Socials,** 7:00 PM: Sun, Wed

**BUSINESS MEETINGS:**

**Business Meeting (Open),** 5:30 PM: Sun

**Executive Committee Meeting (Closed),** 8:30 AM: Sun

**Long-Range Planning Committee Meeting (Closed),** 5:30 PM: Mon

## SUNDAY MORNING

### Section A

Moscone Center
3002/3004

#### Macrocycles & Cyclopeptides in Medicinal Chemistry

M. J. Blanco-Pillado, *Organizer*

M. Blanco, *Presiding*

**9:00** Introductory Remarks.

**9:05** MEDI **1.** Simple ADME rules for complex molecules and life beyond the rule of 5. **S. Lokey**

**9:40** MEDI **2.** Discovery of oral and BBB permeable eribulin analogs by taking advantage of its macrocyclic properties. **W. Zheng**

**10:15** MEDI **3.** Peptides as shuttles for drug delivery to the brain. **E. Giralt**

**10:50** MEDI **4.** Macrocyclic peptides as potential treatments for pain and drug abuse. **J.V. Aldrich**, S. Senadheera, T.F. Murray, J.P. McLaughlin

**11:25** MEDI **5.** Milla molecule inhibitors of IAP proteins. **Y. Zhang**

**12:00** Concluding Remarks.

### Section B

Moscone Center
3006/3008

#### General Orals

A. W. Stamford, *Organizer*

I. M. Bell, *Presiding*

**8:30** MEDI **6.** Development of a potent and selective bromodomain chemical probe. **M. Moustakim**, P. Brennan, D. Dixon

**8:50** MEDI **7.** Structure-based computer-aided IL-6/GP130 Protein-Protein Interaction (PPI) inhibitor design. **G. Shi**, L. Mao, V. Kumari, C. Li

**9:10** MEDI **8.** Disclosure of a development candidate to treat severe acute pancreatitis through a drug discovery partnership between GlaxoSmithKline and the University of Edinburgh. **J. Liddle**

**9:30** MEDI **9.** Expanding screening decks by innovative MCR scaffolds. **A. Doemling**, P. Patil, R. Madhavachary

**9:50** MEDI **10.** Metamorphosis of paroxetine into a highly potent and selective GRK2 inhibitor via structure-based drug design. **H. Waldschmidt**, K. Homan, O. Cruz - Rodriguez, M. Cato, R. Bouley, M. Wilson, A. Cannavo, J. Song, J. Cheung, P. Kirchhoff, W. Koch, J. Tesmer, S.D. Larsen

**10:10** MEDI **11.** Discovery of novel potent and selective agonists of the serotonin (5-HT) $5\text{-}HT_{2C}$ receptor as neurotherapeutics. **H. Mack**, G. Backfisch, G. Blaich, W.M. Braje, T. Erhard, A. Haupt, A. Kling, V. Lakics, J.J. Lynch, M. Mugnaini, F. Pohlki, A.L. Relo, K. Schaefer

**10:30** MEDI **12.** Assessment of MCHr1 target engagement in the brain using PET imaging. **A. Johansson**, M. Antonsson, A. Hogner, M. Fredenwall, M. Hayes, P. Johnstrom, M. Schou

**10:50** MEDI **13.** Redox-responsive hyaluronic acid-taxoid nanoconjugate for CD44-targeted cancer chemotherapy. **Y. Zhang**, I. Ojima

**11:10** MEDI **14.** Targeting ubiquitin pathway enzymes for cancer immunotherapy. **J. Wu**, H. Wang, S. Kumar, F. Wang, I. Sokirniy, C. Riling, M. Mattern, J. Weinstock

**11:30** MEDI **15.** Synthesis and biological profiling of 2-azabicyclo[2.1.1]hexane-based proline isosteres as antagonists of TRPA1 ion channel. **D. Shore**, M. Volgraf, B. Safina, V.A. Verma, E. Villemure, H. Chen, L. Wang, A.A. Estrada, J.P. Lyssikatos, A. Kolesnikov, S. Do, S. Shields

**11:50** MEDI **16.** Cyclophilin D inhibitors rational and fragment based design: From 7 mM to 7 nM potency. **C. Jorand-Lebrun**, X. Jian, T. Johnson, U. Graedler, D. Schwarz, B. Leuthner, A. Marx, D. Roche, M. Gilardone, H. Lemoine, S. Kulkarni, F. Bernard

#### LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

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

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

## SUNDAY AFTERNOON

### Section A

Moscone Center
3002/3004

#### General Orals

A. W. Stamford, *Organizer, Presiding*

**1:30** MEDI **17.** Discovery of AZD9977: A non-steroidal mineralocorticoid modulator for treatment of diabetic kidney disease. **K.L. Granberg**, Z. Yuan, B. Lindmark, K. Edman, K. Bamberg, A. Hogner, J. Kajanus, M. Malmgren, C. Löfberg, A. Nordqvist, J.Å. Lindberg, J. Brånalt, G. OMahony, M. Kossenjans, D. Liu, A. Aagaard, M. Billger, S. Bäckström, P. Cornwall, H. Ericsson, F. Erlandsson, E.L. Hansson, A. Hayen, M. Hermansson, I. Ivarsson, R. Jansson Löfmark, U. Johansson, U. Karlsson, X. Li, G. Nikitidis, P. Nordberg, A. Nordin, B. Polentarutti, N. Selmi, A. Turner, L. William-Olsson, C.E. Wingolf, J. Hartleib

**1:55** MEDI **18.** Discovery of BMS-962212 a highly potent, selective inhibitor of coagulation FXIa. **D. Pinto**, M.J. Orwat, L. Smith II, S. Shrivastava, M.L. Quan, P.Y. Lam, K. Rossi, A. Apedo, J. Bozarth, Y. Wu, J. Zheng, B. Xin, N. Toussaint, P. Stetsko, O. Gudmundsson, E. Crain, P. Wong, Z. Lou, T. Harper, S. Chacko, J. Myers, S. Sheriff, H. Zhang, X. Hou, A. Mathur, D. Seiffert, J. Luettgen, R.R. Wexler

**2:20** MEDI **19.** Development of new therapies for asthma based on compounds that specifically target $GABA_A$ receptors in the lung. **L. Arnold**, G.S. Forkuo, N.Y. Yuan, R. Kodali, O.B. Yu, N.M. Zahn, R. Jahan, G. Li, M.R. Stephen, M. Guthrie, A.N. Nieman, M.M. Poe, G.T. Yocum, C.W. Emala, D.C. Stafford, D.A. Steeber, J.M. Cook

**2:45** MEDI **20.** Discovery of AGN-241689: A potent, orally-acting CGRP receptor antagonist for migraine prophylaxis. **I.M. Bell**

**3:10** MEDI **21.** Discovery of BMS-986142: A reversible inhibitor of Bruton's Tyrosine Kinase (BTK) conformationally constrained by two locked atropisomers. **S.H. Watterson**, G.V. De Lucca, Q. Shi, C.M. Langevine, D.G. Batt, Q. Liu, M. Beaudoin Bertrand, H. Gong, J. Dai, H. Yip, P. Li, D.Z. Sun, D. Wu, C. Wang, Y. Zhang, S.C. Traeger, M.A. Pattoli, S. Skala, L. Cheng, M.T. Obermeier, R. Vickery, L.N. Discenza, C.J. D'Arienzo, Y. Zhang, E. Heimrich, K. Gillooly, T.L. Taylor, C. Pulicicchio, K. Mcintyre, M.A. Galella, A.J. Tebben, J.K. Muckelbauer, C. Chang, L. Salter-Cid, J.C. Barrish, P.H. Carter, A. Fura, J. Burke, J.A. Tino

**3:35** MEDI **22.** Hydrogen bond interaction geometries in protein-ligand complexes: From large-scale statistics to single cases. **E. Nittinger**, T. Inhester, G. Lange, R. Klein, M. Rarey

**4:00** MEDI **23.** Discovery of selective SETD8 inhibitors via structure-based approach. **A. Ma**, W. Yu, K. Butler, F. Li, W. Tempel, N. Babault, P. Fabio, J. Shao, J. Wang, M. Luo, M. Vedadi, P. Brown, C.H. Arrowsmith, J. Jin

**4:25** MEDI **24.** Discovery of a noncovalent, mutant-selective epidermal growth factor receptor inhibitor. **B.K. Chan**, E.J. Hanan, K. Bowman, M.C. Bryan, D. Burdick, E. Chan, Y. Chen, S. Clausen, T. Dela Vega, J. Dotson, C. Eigenbrot, R. Elliott, R. Heald, P. Jackson, J. Knight, H. La, M. Lainchbury, S. Malek, H.E. Purkey, G. Schaefer, S. Schmidt, E. Seward, S. Sideris, L. Shao, S. Wang, S. Yeap, I. Yen, C. Yu, T.P. Heffron

**4:50** MEDI **25.** Discovery of 4-(((2R,3R)-1,3-dihydroxybutan-2-yl)amino)-6-phenylpyrrolo[1,2-b]pyridazine-3-carboxamide (BMT-1438), a potent JAK1/3 inhibitor and the use of a phosphate prodrug in demonstrating efficacy in a rheumatoid arthritis model. **S.H. Spergel**, M. Mertzman, J. Kempson, J. Guo, S.M. Stachura, L. Haque, J. Lippy, R. Zhang, M.A. Galella, S. Pitt, G. Shen, A. Fura, K. Gillooly, K. Mcintyre, V. Tang, J.S. Tokarski, J. Sack, J. Khan, P.H. Carter, J.C. Barrish, S. Nadler, L. Salter-Cid, G.L. Schieven, S. Wrobleski, W.J. Pitts

### Section B

Moscone Center

3006/3008

### Medicinal Chemists' Toolbox: Factors Influencing Oral Bioavailability & Case Studies

N. A. Meanwell, P. M. Scola, K. Yeung, *Organizers*, *Presiding*

**2:00** Introductory Remarks.

**2:05** MEDI **26.** Drug absorption and disposition influencing oral bioavailability: An industrial perspective and literature review. **C. Huang**

**2:40** MEDI **27.** First-pass intestinal glucuronidation as a potential obstacle for oral absorption of small molecule drug candidates: When should we worry? **A.S. Kalgutkar**

**3:15** MEDI **28.** Role of drug metabolizing enzymes in oral bioavailability. **C. Khojasteh**

**3:50** MEDI **29.** Role of early solubility measurements in predicting bioavailability challenges and subsequent formulation strategies to enable compounds. **W.P. Wuelfing**

**4:25** MEDI **30.** Mesenteric lymph: A conduit to enhanced oral bioavailability and immune cell targeting. **C. Porter**

### Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

*Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF*

### LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

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

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

## SUNDAY EVENING

### Section A

Moscone Center

West Hall

### General Posters

A. W. Stamford, *Organizer*

**7:00 - 9:00**

MEDI **31.** Aminobenzimidazoles and structural isomers: Design, synthesis, pharmacological evaluation and computational studies of novel dual-acting butyrylcholinesterase inhibitors and *h*$CB_2$ receptor ligands for the treatment of Alzheimer's disease. **D. Dolles**, E. Sawatzky, J. Möller, M. Nabissi, A. Drakopoulos, A. Strasser, H. Wittmann, M. Lohse, M. Decker

MEDI **32.** Development of small molecules to modulate Apoe and Abca1/Ldlr levels for Alzheimer's therapy. **N. John**, I. Boginski, A. Voigt, R. Remotigue, J. Kim, J. Kim, S. Maitra

MEDI **33.** Design, synthesis and biological evaluation of 3-hydroxy-4H-pyranone derivatives as potent MTDLs for Alzheimer's disease. **R. Sheng**, J. Liu, L. Jiang, L. Tang

MEDI **34.** Acetyl cholinesterase inhibitory and toxicity profiles of tacrine-curcumin hybrids. **R. Alavala**, G. Tipparapu, **S. Boyapati**, U. Kulanthaivelu, R. Ajmeera, B. Mantriprgada

MEDI **35.** Design, synthesis, and in vitro evaluation of novel sigma-2 receptor modulators: An opportunity in Alzheimer's disease therapy. **K. Blattner**, D.J. Canney, R. Gao, R. Bhandare, J.C. Gordon, M. Abou-Gharbia, N.J. Izzo, N. Knezovich, C. Silky, K. Mozzoni, S. Catalano, G. Rishton, B.E. Blass

MEDI **36.** Discovery of multi-target-directed ligands for the treatment of Alzheimer's disease. **W. Huang**, Z. Shen, C. Li, Q. Li, X. Zhen, Z. Ma, M. Liang

MEDI **37.** Biased agonism at CB2 cannabinoid receptors: Implications for drug development. **R. Hutchison**, P. Prather

MEDI **38.** Synthesis and biological evaluation of dual-target peripheral $CB_1R$ antagonists. **M.R. Iyer**, R. Cinar, A.R. Katz, G. Kunos

MEDI **39.** Profiling signaling bias of synthetic cannabinoid New Psychoactive Substances (NPS) at the Cannabinoid Type 1 Receptor (CB1R). **S. Banister**, K.K. Kumar, B.K. Kobilka, S.V. Malhotra

MEDI **40.** Synthesis and SAR studies of somatostatin subtype-4 agonists for the treatment of Alzheimer's disease. **M. Minaeian**, A.M. Crider, I. Daryaei, M. Kontoyianni, W.M. Kolling, W.L. Neumann

MEDI **41.** Discovery of tetrahydroquinoline-containing CXCR4 antagonists with improved ADMET properties. **E.J. Miller**, E. Jecs, V. Truax, B. Katzman, K. Kuo, M.B. Kim, R.J. Wilson, H.H. Nguyen, Y.A. Tahirovic, M. Saindane, T. Wang, C. Sum, J. Chen, M.E. Cvijic, D.R. Shen, N. Burford, C. Chen, H. Zhang, A.J. Tebben, L.J. Wilson, G.M. Schroeder, D. Liotta

MEDI **42.** Synthesis of novel TIQ-15 analogs with improved drug properties. **E. Jecs**, E.J. Miller, R.J. Wilson, H.H. Nguyen, Y.A. Tahirovic, M.B. Kim, B.M. Katzman, V.T. Truax, K. Kuo, J. Chen, M. Cvijic, D.R. Shen, C. Chen, H. Zhang, A.J. Tebben, C. Sum, T. Wang, N. Burford, G.M. Schroeder, L.J. Wilson, D. Liotta

MEDI **43.** Synthesis and SAR of TIQ-15 based CXCR4 antagonists: Identification of tetrahydroquinoline replacements. **R.J. Wilson**, E.J. Miller, E. Jecs, V.T. Truax, L.J. Wilson, H.H. Nguyen, Y.A. Tahirovic, D. Liotta, G.M. Schroeder, T. Wang, H. Zhang, M. Kim

MEDI **44.** Synthesis of 2,4,6-trisubstituted pyridines using palladium-catalyzed cross-coupling reactions and in vitro anticancer evaluation. **A. Hernandez Campos**, P.J. Trejo, I. González, L. Yépez-Mulia, J. Pérez-Villanueva, M.A. Cerbón-Cervantes, R. Castillo-Bocanegra

MEDI **45.** First steps in hit-to-lead optimization towards AKT inhibition. **E.E. Sanabria-Chanaga**, R. Castillo-Bocanegra, A. Hernandez Campos

MEDI **46.** Design, synthesis and biological evaluation of quinazoline derivatives as cytotoxic molecules of breast cancer triple-negative. **A.S. Matus-Meza**, F. Hernández-Luis, M.A. Velasco-Velázquez

MEDI **47.** Targeting specific interactions to improve EGFR-ligand binding. C. Williams, A. Ajamian, N. Thorsteinson, **N. Li**, B. Jean-Claude

MEDI **48.** Molecular design and synthesis of inhibitors of EGFR kinase: New quinazoline derivatives. A.S. Bunev, E.V. Sukhonosova, **S. Sokov**

MEDI **49.** Derivatives of 5-(imidazo[2,1-*b*]thiazol-6-yl)-4-methylthiazol-2-amine new effective EGFR-kinase inhibitors. A.S. Bunev, E.V. Sukhonosova, **K. Talina**

MEDI **50.** Discovery of atropisomeric quinolinone sulfonamide (AM-0466), a potent and selective $Na_v1.7$ inhibitor with robust *in vivo* analgesic activity. **R. Graceffa**

MEDI **51.** Discovery of non-zwitterionic aryl sulfonamides as $Na_v1.7$ inhibitors with efficacy on preclinical behavioral and translational measures of pain. **Y. Wu**, J. Guernon, A. McClure, G. Luo, R. Rajamani, A. Ng, A. Easton, A. Newton, C. Bourin, D. Parker, K. Mosure, O. Barnaby, M. Soars, R.J. Knox, M. Matchett, R. Pieschl, J. Herrington, P. Chen, D. Sivarao, L.J. Bristow, N.A. Meanwell, J.J. Bronson, R.E. Olson, L.A. Thompson, C.D. Dzierba

MEDI **52.** Synthesis and structure-activity relationships of morpholine-based aryl sulfonamide $Na_v1.7$ inhibitors. **J.M. Guernon**, A. McClure, R. Rajamani, R.J. Knox, M. Matchett, R. Pieschl, J. Herrington, L.J. Bristow, N.A. Meanwell, R.E. Olson, L.A. Thompson, C.D. Dzierba, Y. Wu

MEDI **53.** Structure-based design of ATP citrate lyase inhibitors and their anticancer activities. F.E. Jernigan, S.K. Koerner, J. Hanai, V.P. Sukhatme, **L. Sun**

MEDI **54.** Withdrawn.

MEDI **55.** Bioassay protocols: Semantic annotation to enable informatics. **A. Clark**

MEDI **56.** Design, synthesis, and evaluation of a new privileged scaffold for use in drug discovery. **M.J. Stocks**, C. Schwehm, B. Kellam, A. Garces, N. Kindon, T. Bradshaw, J. Li, S.J. MacDonald, J. Rowedder

MEDI **57.** From chemical similarity to rational polypharmacology. **M.J. O'Meara**, X. Huang, B.L. Roth, B. Shoichet

MEDI **58.** Quantum chemistry calculation-aided optimization of novel microtubule-targeting agents binding to colchicine site. **C. Zheng**, J. Jiang, J. Liu, J. Zhu, Y. Zhou

MEDI **59.** Enhanced delivery of HIV integrase inhibitors with prodrugs designed for polymeric nanocarriers. **W.E. Afunugo**, M.E. Ebner, A.M. Bever, S. Cao, Y. Jiang, K.A. Woodrow, I.T. Suydam

MEDI **60.** Synthesis and biological evaluation of sulfonyl piperazine derivatives for LpxH inhibition. **M. Lee**, J. Zhao, J. Cho, D. Kwon, P. Zhou, J. Hong

MEDI **61.** Creating new from clinical agents: Discovery of Combretastatin A-4 inspired heterocycles as antitubulin anticancer agents. **N. Hura**, S.K. Guchhait

MEDI **62.** Matching medium characterization for microwave brain stroke imaging. T. Yilmaz, G.A. Eken, E. Yildirim, **M.H. Acar**, I. Akduman

MEDI **63.** Synthesis of functionalized benzofulvenes and their possible application towards thioredoxin reductase inhibition and cancer treatment. A. Glass, **K. Caspary**

MEDI **64.** Hologram QSAR and structure-based design of novel small-molecule inhibitors of choline acetyltransferase. **R. Kumar**, T. Darreh-Shori

MEDI **65.** Virtual hit-to-lead drug development program FRESH and success across carbonic anhydrase II and phosphatidylinositol 3-kinase α. **T. Kaiser**, Q. Shi, Z. Dentmon, P. Burger, J. Snyder, D. Liotta

MEDI **66.** Dopamine transporter ligands with short and long residence time. **S. Kukk**, J. Jarv

MEDI **67.** Structure function studies of silent agonists of the alpha 7 nicotinic acetylcholine receptor. **M. Quadri**, C. Stokes, R. Papke, C. Sanon, N. Horenstein

MEDI **68.** Dual soluble Epoxide Hydrolase (sEH) and Fatty Acid Amide Hydrolase (FAAH) inhibitors for treating. **S.D. Kodani**, K. Wagner, S. Hwang, K.S. Lee, C. Morisseau, B.D. Hammock

MEDI **69.** Low-cost high-impact route to kill MRSA with beta-lactam antibiotics. **C.V. Rice**, M. Foxley, M. Xiao, S. Wright, S. Strange

MEDI **70.** Clickable 4-*N*-alkanoyl and 4-*N*-alkylgemcitabine analogues with silicon-fluoride acceptors. **C. Gonzalez**, A. Sanchez, S.F. Wnuk

MEDI **71.** Novel 5-nitroimidazole and 5-nitrothiazole piperazine derivatives and their antiparasitic activity. **H.A. Saadeh**, M. Khasawneh, Y. Abou-Zeid, I. El-Haty, S. Nsangou, K. Goyal, R. Sehgal, A. Samadi

MEDI **72.** Matched molecular pair analysis and collaboration: Finding rules to the age-old problem. **A. Dossetter**, E.J. Griffen, A.G. Leach, S. Montague

MEDI **73.** Diketo acids and their hybrid bioisoster derivatives as bacterial biofilm and Methionine Aminopeptidase (MetAP) inhibitors. **A. Mohammad**, P. Hasan, V. Pillalamarry, M. Irfan, A. Perwez, B. Ahmad, U. Yadava, M. Rizvi, C. Daniliuc, R. Maguire, K. Kavanagh, A. Addlagatta

MEDI **74.** Studies aimed at the synthesis of Hsp90 inhibitors as antileishmaniasis agents. **L. Barbeto**, J. Leahy, D. Kyle

‡ *Cooperative Cosponsorship*

MEDI **75.** Synthesis and biological activity studies of C1-substituted carbapenem antibiotics. **T. Nguyen**, J. Kim, P. Nguyen, M. Cox, M. Bennett, B. Meshram, L. Phung, C. Watanabe, A. Shi, M. Alqurafi, J.D. Buynak

MEDI **76.** 2-Nitrobenzenesulfonyl fluoride is a novel small molecule pharmacophore for the development of new antibiotics. **B. Park**

MEDI **77.** Gold-phosphines and gold-phosphine-modified human serum albumin as potent inhibitors of T-cell proliferation. **T.C. Dean**, M. Yang, M. Liu, P.K. Langston, J. Lee, C.M. Furdui, J. Grayson, U. Bierbach

MEDI **78.** Insulin: Its structure, function, and interaction in model cell membranes. **K. Saulcy**, D.C. Crans, A. Sostarecz

MEDI **79.** Synthetic and mechanistic studies of cyclotriazadisulfonamide (CADA) down-modulators of human CD4. **T.W. Bell**

MEDI **80.** Facile synthesis of Benzalkonium Chloride (BAC)-derived mesoporous silica nanoparticles as antibacterial material. **H. Wang**, T.B. Shrestha, J. Covarrubias, A.P. Malalasekera, S.O. Wendel, J. Yu, P. Thapa, L. Chlebanowski, O. Covarrubias Zambrano, D.L. Troyer, S.H. Bossmann

MEDI **81.** Withdrawn.

MEDI **82.** Advanced carbapenem antibiotics: The synthesis and activity studies of C6 substituted carbapenems. **M. Alqurafi**, J. Kim, D. Le, M. Lohry, C. Watanabe, A. Shi, T. Nguyen, J.D. Buynak

MEDI **83.** Impact of pH on solubility, hydrolysis kinetics, and pharmacokinetics of tenofovir disoproxil fumarate delivered from intravaginal rings. **J.A. Moss**, M.M. Baum, M. Gunawardana, C.S. Miller, I. Butkyavichene, S. Calvez, F. Yang, K.L. Vincent, R.B. Pyles

MEDI **84.** Withdrawn.

MEDI **85.** Use of substrate analogues and Tetrahydroisoquinolines (THIQ) as potential inhibitors for *Mycobacterium tuberculosis* enzyme MshC and synthesis of mycothiol. **K. Patel**, A. Reddy Maddirala, P.R. Andreana

MEDI **86.** MRI probe loaded HDL mimicking nanoparticles for diagnosis and therapy of atherosclerosis. **B. Banik**, S. Dhar

MEDI **87.** Copper responsive gadolinium-based MRI contrast agents. **N.N. Paranewithana**, A.F. Martins, G. Meloni, S. Chirayil, P. Zhao, A. Sherry

MEDI **88.** Novel, real-time analysis of nanomaterial inhibition of *E. coli*. **P.A. Sermon**

MEDI **89.** Organizing 3D project data for structure-based drug design. H.J. Feldman, A. Ajamian, **E. Metwally**

MEDI **90.** Fast generation of novel leads using virtual screening and fast MCR chemistry. **A. Doemling**, C.J. Camacho

MEDI **91.** Tumor suppressor $P27^{Kip1}$ regulation by tissue transglutaminase and its potential application in cancer therapeutics. **L. Zhang**, R.J. Sheaff

MEDI **92.** Withdrawn.

MEDI **93.** Dual targeting of the cancer antioxidant network with redox active gold(I) N-heterocyclic carbene complexes. R. McCall, J. Kocerha, J.L. Sessler, V. Sittaramane, K. Arumugam, **J.F. Arambula**

MEDI **94.** Fluorescent chemosensing for chloride and nucleotides based on artificial receptors in water. **A. Dorazco Gonzalez**

MEDI **95.** D-peptides as inhibitors of Proteinase 3-membrane interactions. K. Maximova, T. Venken, N. Reuter, **J. Trylska**

MEDI **96.** Molecular investigation of cyclic β- and γ-peptoids. **R. Grams**, D. Marron, M. Kassu, J.S. Josan

MEDI **97.** Mapping of cell surface receptors using silver nanodiscs. **J.S. Josan**, M. Kassu, G. Liu, A. Khan, R. Grams

MEDI **98.** Late-stage functionalization of complex molecules. **R. Karimov**, A. Sharma, J.F. Hartwig

MEDI **99.** Synthesis of novel imidazobenzodiazepine oxazole bioisosteres as potential alpha 2, 3 subtype selective GABA(A) receptors agonists with excellent metabolic stability, pharmacokinetics, and anxiolytic efficacy. **G. Li**, K.R. Methuku, M.M. Poe, J.M. Witkin, J.M. Schkeryantz, M. Ernst, J.M. Cook

MEDI **100.** Study and isolation of chemical compounds of *Guaiacum sanctum* for cytotoxicity and antitumor activities. **A.A. Laureano**

MEDI **101.** Synthesis and evaluation of increased binding affinity analogues of fosmidomycin as inhibitors of the non-mevalonate isoprenoid biosynthesis pathway. **B.C. Figula**, J.W. Tomsho, J.M. Gamrat

MEDI **102.** Design and synthesis of alpha-helix mimetics for treatment of high-risk human papillomavirus infection. **S. Rendon**

MEDI **103.** Design of ER beta selective agonists for hippocampal memory enhancements. **K. Perera**, W. Donaldson, A. Schulitz, D. Sem, J. Kim, K. Frick

MEDI **104.** Rational design, synthesis, and *in vitro* evaluation of mPGES-1 inhibitors as next-generation of anti-inflammatory drugs. **K. Ding**, Z. Zhou, Y. Yuan, F. Zheng, C. Zhan

MEDI **105.** Delivery of flavonol-based photoCORMs to mitochondria. **T. Soboleva**, H. Esquer, S. Anderson, A. Benninghoff, L.M. Berreau

MEDI **106.** Exploring the mechanism of action of a newly-discovered therapeutic peptide for blinding retinal diseases by identifying its receptors. **D. Zhou**, Z. Shao, J.A. Kornfield

MEDI **107.** Design of new irreversible arginase inhibitors. **X. Guo**, C. Seto

MEDI **108.** Development of biodegradable microneedles using dexamethasone and Poly Lactic-co-Glycolic Acid (PLGA) for cochlear drug delivery. **C. Bravo**

MEDI **109.** Alpha-helix mimetics as potential drugs for Human Papillomavirus (HPV). **V. Do**

MEDI **110.** Discovery of a novel irreversible and potent FLT3 inhibitor FF-10101 under clinical investigation. **M. Takasaki**, A. Hirai, D. Terada, M. Okubo, T. Tsujino, K. Sato, S. Tanabe, S. Inuki, S. Mizumoto, N. Fujikawa, D. Hirano, T. Yamaura

MEDI **111.** Discovery of CCT251236 from an HSF1 phenotypic screen: A pirin ligand with efficacy in an ovarian adenocarcinoma model. **E. Pasqua**, M. Cheeseman, N.E. Chessum, C. Rye, M.J. Tucker, B. Wilding, L.E. Evans, S. Lepri, M. Richards, S.Y. Sharp, S. Ali, M. Rowlands, L. O'Fee, A. Miah, A. Hayes, A.T. Henley, M. Powers, R. Te Poele, E. De Billy, L. Pellegrino, F. Raynaud, R. Burke, R.L. van Montfort, S.A. Eccles, P. Workman, K. Jones

MEDI **112.** Bruton's Tyrosine Kinase (BTK) program: Quick systematic SAR development utilizing parallel synthesis. Y. Yu, R. Anand, D. Sha, H.A. Vaccaro, M. Maletic, R. Mazzola, Z. Shi, M. Alhassan, S.B. Boga, J.L. Duffy, **X. Gao**, D. Guiadeen, J. Kelly, A. Krikorian, J. Liu, K. Maloney, O. Selytin, J. Wang, J. Xu, W. Yu, M. Altman, B.M. Andresen, Y. Liu, M. Martinez, T. Siu, S. Liu, C. Yang, H. Wu, J. Cai, Y. Gao, T. Fischmann, J. Presland, M. Mansueto, Z. Xu, E. Leccese, J. Zhang-Hoover, I. Knemeyer, C. Garlisi, N. Bays, P. Stivers, P. Brandish, A. Hicks, R. Kim, J.A. Kozlowski

MEDI **113.** Withdrawn.

MEDI **114.** Leucine's role of dry powder inhaler performance of salbutamol sulphate containing spray dried mannitol. **C. Molina**

MEDI **115.** Effects of varying $H_2S$ concentrations on sulfhemoglobin complex formation. **N.E. Crespo Rosado**

MEDI **116.** Discovery of novel inhibitors of NF-kB Inducing Kinase (NIK) from an FBDD approach. **L. Kwok**

MEDI **117.** Utilizing the message-address concept to develop selective mu opioid receptor antagonists as potential treatment of opioid addiction. **S. Obeng**, A. Jali, D. Stevens, W.L. Dewey, D.E. Selley, Y. Zhang

MEDI **118.** Structure-activity relationships of phosphatidylinositol-3-kinase δ inhibitors for the treatment of inflammatory respiratory diseases. **A. Garces**, C. Schwehm, M.J. Stocks, N. Kindon, S.J. MacDonald, J. Rowedder, T. Bradshaw

MEDI **119.** Analysis of the binding parameters of the reversible inhibitor Argyrin B at the active sites of the constitutive and immunoproteasomes. D. Allardyce, C. Bell, **E. Loizidou**

MEDI **120.** Flavonol-based CO-releasing molecules: Tunability and albumin binding properties. **M. Popova**, T. Soboleva, L.M. Berreau

MEDI **121.** Identification of ligand-efficient inhibitors of *Trichomonas vaginalis* adenosine/guanosine preferring nucleoside ribohydrolase using NMR-based fragment screening. **S.N. Muellers**, A.L. Benzie, D.G. Brown, S. Cowen, D.W. Parkin, B.J. Stockman

MEDI **122.** Design, synthesis and employment of Flupirtine-derivative chemical probes for neuroprotective target identification. **N. Kinarivala**, F. Saadeh, J. Makoukji, R. Boustany, P.C. Trippier

MEDI **123.** Development of imidazopyridines and anti-proliferative effect against castration resistant prostate cancer cells. **I. Wazeerud-Din**, A. Millena, S. Khan, J. Bu

MEDI **124.** Novel chemotype of histone demethylase family KDM4 inhibitors. **M. Siklos**, M. Korczynska, T.A. Bates, B. Shoichet, D.G. Fujimori

MEDI **125.** Progress towards a novel class of immune modulators: Covalent toll-like receptor-7 agonists. **A.C. Chon**, A. Esser-Kahn

MEDI **126.** Novel prodrugs of transition state inhibitors of norovirus 3CL protease. **A. Galasiti Kankanamalage**, Y. Kim, K. Alliston, A.D. Rathnayake, M. Butler, S. Cardinale, T.L. Bowlin, K. Chang, W. Groutas

MEDI **127.** Cyclopropylthiazines as potent BACE1 inhibitors for Alzheimer's disease: Challenging chemistry and *in-vivo* data of this new pre-clinical series. **A. Siegmund**, K. Kong, M. Frohn, N. Nishimura, A. Pickrell, M.D. Bartberger, D. Hickman, J.R. Allen, S. Wood, M.P. Bourbeau

MEDI **128.** Threading the needle: Exploiting a P1-P3 ether linkage in the development of novel BACE inhibitors. **S.P. Walsh**, A. Shahripour, E. Kim, W. Li, J.D. Scott, D. Rindgen, L. Hyde, P. Orth, H. Wang, M. Kennedy, J. Cumming

MEDI **129.** Novel ROS activated prodrugs as kinase inhibitors: A strategy to improve selectivity. **P.N. Gurjar**, S. Abdul Salam, E.J. Merino

MEDI **130.** Design and synthesis of selective HADC6 inhibitors as potential agents against glioblastoma. **S. Fung**, A.A. Sadani, K. Wu, J. Chern

MEDI **131.** Solid-state structure and absolute configuration of enantiomers of 3-ethyl-3-phenylpyrrolidin-2-one. **A.V. Krivoshein**, S.V. Lindeman, V.N. Khrustalev, T.V. Timofeeva

MEDI **132.** Chemical correction of cellular dysfunction caused by progranulin deficiency in frontotemporal dementia. **M. Telpoukhovskaia**, K. Liu, C. Ludwig, J. Etchegaray, F. Sayed, Y. Zhou, M.S. Bogyo, S. Ding, L. Gan

MEDI **133.** Discovery and structure-activity relationship of thienopyridine derivatives as bone anabolic agent. **T. Shinozuka**, K. Saito, A. Nakao, K. Shimada, S. Matsui, N. Daisuke, N. Yoko, N. Satoru

MEDI **134.** Molecular modeling studies for a series of benzimidazole derivatives as cruzain inhibitors with anti-*Trypanosoma cruzi* activity. I. Pauli, **L. Ferreira**, M.L. de Souza, R. Ferreira, M. Dessoy, B. Slafer, G. Oliva, L.C. Dias, A.D. Andricopulo

MEDI **135.** Improving new molecule design using electrostatics. **T. Cheeseright**, M.D. Mackey

MEDI **136.** Structure-kinetics relationships for LpxC inhibition. **B. Lichtenthal**, C. Gu, F. Daryaee, R. Basu, M. Babar, P.J. Tonge

MEDI **137.** Problem based learning with MOE. **A. Bonin**

MEDI **138.** Exploiting solvent effects in drug design and optimization. R. Alvarez, A. Ajamian, **C. Williams**

MEDI **139.** Synthesis of novel efflux pump inhibitors which target the AcrAB-TolC multidrug efflux system in *Escherichia coli*. **K.M. Haynes**, N. Abdali, j. Parks, J.L. Chaney, A.T. Green, D. Wolloscheck, J.K. Walker, N. Wood, V.V. Rybenkov, J.Y. Baudry, J. Smith, H.I. Zgurskaya

MEDI **140.** Design of mGlu2 negative allosteric modulators for the treatment of neuropsychiatric disorders. **S. Conde**

MEDI **141.** Phosphonamidate inactivators of *Mycobacterium tuberculosis* (*Mtb*) *BlaC*. **D.S. White**, C. Choy, C.E. Berkman

MEDI **142.** Development of covalent caspase-6 inhibitors derived from disulfide trapping (tethering). **K.S. Van Horn**, D. Wang, C. Bryant, D. Medina-Cleghorn, P. Jaishankar, P. Lee, M. Arkin, A.R. Renslo

MEDI **143.** What do recently approved oral drugs look like? A year-by-year analysis of FDA approved drugs in 2007-2016. **A. Ritzén**, L. David

MEDI **144.** μCyclic peptides containing tryptophan and arginine residues: Antibacterial activities and structure-activity relationship. **N. Riahifard**, T. Aldakhil, S. Nasser, F. Nunez, K. Zoghebi, S. Mozaffari, J. Yamaki, K. Parang, R.K. Tiwari

MEDI **145.** Synthesis and evaluation of antimicrobial activity of levofloxacin-[$R_4W_4$] and Q-levofloxacin-[$R_4W_4$] conjugates and comparison with the corresponding physical mixtures. **N. Riahifard**, K. Tavakoli, J. Yamaki, R.K. Tiwari, K. Parang

MEDI **146.** Anti-malarials targeting the heat shock 90 protein of *Plasmodium falciparum*. **N. Everson**, J. Bach, T. Sisley, M. Walls, S.C. Eagon

MEDI **147.** Synthesis of anti-malarial compounds targeting the ATP4 protein in *Plasmodium falciparum*. G. Koch, J. Tryhorn, K. Ahn, B. Belanger, K. Yniguez, **H. Lazaro**, A. Kashtanova, S.C. Eagon

MEDI **148.** Novel high-affinity dopamine D4 receptor-selective ligands. **C.A. Boateng**, T.M. Keck, B. Free, C. Wu, A. Bonifazi, A.H. Newman, D.R. Sibley

MEDI **149.** Optimized chemical tools to probe the function of thioredoxin-interacting protein as therapeutic target. **O. Mirguet**, S. Nicolas, M. Aumis, K. Daeron-Courté, F. Perron-Sierra, S. Guizzetti, C. Vinson, A. Caliez, C. Chesneau, B. Cremers, M. Sadlo, I. Wehrle, G. Zanirato, P. Delerive, C. Bernard

MEDI **150.** Structure activity relationship of novel piperazino-enaminones (JOAB series) as pro-inflammatory cytokines suppressants. A. Bill, D. Szollosi, J. Dhuguru, I. Edafiogho, **O.M. Ghoneim**

MEDI **151.** Phytochemical evaluation of antimicrobial properties of *Combretum igneiflorum* extracts. **I. Maldonado**, A.K. Addo-Mensah

MEDI **152.** Next generation small molecule inhibitors of 5'-Methylthioadenosinenucleosidase (MTN) as novel antimicrobial agents. J.H. Thurston, K. Cornell, **L. Wayment**

MEDI **153.** Synthesis and evaluation of choline-derived Deep Eutectic Solvents (DES) as biofilm eradicating antibiotics. **A.W. Jemas**, D. Jacobs

MEDI **154.** Structure Activity Relationship (SAR) studies of EP2 receptor antagonists. **T. Ganesh**, R. Dingledine

MEDI **155.** Identification of vacuolar ($H^+$)-ATPase modulators by virtual screening process. R. Patil, A. Kulshrestha, A. Tikoo, S. Fleetwood, G. Katara, W. Seibel, A. Gilman-Sachs, **S. Patil**, K. Beaman

MEDI **156.** Identification of a novel chemotype of ASK1 inhibitors for heart failure utilizing structure-based drug design. **A.L. Chambers**

MEDI **157.** Determination of partition and distribution coefficients using $^1$H NMR spectroscopy time domain Complete Reduction to Amplitude-Frequency Table (CRAFT) analysis. **D.P. Soulsby**, J. Chica

MEDI **158.** Synthesis, cytotoxic evaluation and docking studies of novel 9-anilinothiazolo[5,4-*b*]quinoline derivatives bearing polar groups at the anilino ring. **A. Lira-Rocha**, V. Tinajero-Delgado, **J. Solano-Becerra**

MEDI **159.** Identification of R419, an indirect AMPK activator. **S.J. Shaw**, D. Goff, D.C. Carroll, R. Singh, D. Sweeny, G. Park, D. Lau, Y. Jenkins, V. Markovtsov, T. Sun, Y. Li, A. Pan, Y. Hitoshi, K. Baltgalvis, H. Nguyen, T. Kinsella, D. Payan

MEDI **160.** Effects of propolis on cancer cell membranes and bacterial cell membranes studied with Langmuir monolayers. **B. Book**, A. Sostarecz

MEDI **161.** Langmuir monolayer investigation in to the antibacterial properties of essential oils. **A. Axup**, A. Sostarecz

MEDI **162.** Synthesis and antiproliferative activities of doxorubicin thiol conjugates and doxorubicin-S-S-cyclic peptide. **S. Darwish**, N. Sadeghiani, **R. Tiwari**, **K. Parang**

MEDI **163.** Radiosynthesis of $P2X_7$ receptor radioligands [$^{11}$C]GSK1482160 and [$^{11}$C] GSK1482160 isomer under different base conditions. **M. Gao**, M. Wang, Q. Zheng

MEDI **164.** Fully automated synthesis of [$^{11}$C]Me-GDC-0068 as a PET tracer for imaging of Akt in cancers. **M. Gao**, M. Wang, H. Shannon, B. Bailey, K. Pollok, H. Zarrinmayeh, Q. Zheng

MEDI **165.** Natural product-inspired agents and their anticancer activity against glioblastoma multiforme cells. **V. Kumar**, S. Banister, H. Hunter Kaufman, J. Vittimberga, S.A. Jacobo, S.S. Gambhir, S.V. Malhotra

MEDI **166.** CDD vault: A modern approach for drug research project team informatics. **W.W. Smith**, B.A. Bunin, K. Gregory

MEDI **167.** Novel tetrahydro isoquinoline derivatives as LXR modulators. **A. Chatterjee**, T.P. Burris, K. Griffett, S. Banerjee, Z. Doerer, A. Avdagic, T. Boehm, **J.K. Walker**

MEDI **168.** From photochemically responsive crystals to anticancer compounds: Discovery of novel anthracene analogs as antineoplastic agents. **I. Islam**, A. Nehdi, R.O. Al-Kaysi, A. Alaskar, M. Boudjelal

MEDI **169.** Design, synthesis, and biological properties of a fluorescent duocarmycin analog: HxTfA. K. Kiakos, P.C. Patil, S. Yanow, J.A. Hartley, **M. Lee**

MEDI **170.** Evaluated as potential hypocholesterolemic agent, the preparation and characterization of steroidal ∝,ß-unsaturated ketones. E.J. Parish, **D. Ren**, Y. Lo, G. Ren, **H. Honda**

MEDI **171.** Novel approaches to the chemical preparation and characterization of kinsenoside. **D. Ren**, Y. Lo, E.J. Parish, **H. Honda**

MEDI **172.** New compounds for the treatment of *Mycobacterium abscessus* infections. **K.D. Combrink**, F. Maurer, K. Elizondo, A. Ramirez-Ramos, S. Spring

MEDI **173.** Anticancer activity of *exo*-cyclic carbohydrate enones containing thiophene and pyrolle moieties. J. Sarnik, A. Czubatka-Bienkowska, A. Macieja, **Z.J. Witczak**, R. Bielski, T. Poplawski

MEDI **174.** Novel carbohydrate functionalized thiosemicarbazides evoked DNA damage in cancer cell lines. A. Czubatka-Bienkowska, J. Sarnik, **Z.J. Witczak**, T. Poplawski

MEDI **175.** Enhanced chemical diversity through library *in situ* pre-metabolism: Using biological chemistry for novel lead discovery. N.J. Ayon, **W.G. Gutheil**

MEDI **176.** Actinomycete antibiotic compounds from soil bacteria at an ancient Roman site. **A. Hoffman**

MEDI **177.** Inhibitors of the protein-protein interaction of Class IIa HDACs with MEF2 as potential anticancer agents. **C.M. DeAngelo**, K.J. Gaffney, M.A. Sainz, J.A. Jarusiewicz, N. Jayathilaka, L. Chen, S.G. Louie, N.A. Petasis

MEDI **178.** Development and screening of new cathepsin B and K inhibitors utilizing substituted thiosemicarbazones. **R. McConnell**, H. Sarepalla, P.G. Akula, B. Guda, D. Yermala, N. Kadasala, K. Sayyar, W. Godwin, L. Wen

MEDI **179.** Novel mPGES-1 inhibitors identified from structure-based virtual screening based on new acting mechanism. **S. Zhou**, Z. Zhou, Y. Yuan, C. Zhan

MEDI **180.** Nanomolar-potency aminophenyl-1,3,5-triazine CFTR chloride channel activators for pro-secretory therapy of dry eye diseases. **S. Lee**, P. Phuan, C. Felix, M.H. Levin, A. Verkman

MEDI **181.** Development of novel anti-biofilm compounds for the prevention and treatment of Candidiasis. **M. Valdez**

MEDI **182.** Anti-bacterial activity of isoxazole rifamycin derivatives against *Mycobacterium abscessus*. **A. Ramirez Ramos**, K.D. Combrink, F. Maurer, S. Schmidl, S. Spring, K.N. Elizondo

MEDI **183.** Identical HIV populations and levels of proviral expression in lymph nodes and PBMCs in individuals on antiretroviral therapy. **V. Musick**

MEDI **184.** Synthesis and evaluation of 1, 3, 5 (10) estratriene aminoalkyloxy,16-formyl derivatives of Estrone as potential anti-breast cancer agents. **C. Sullen**, J.S. Cooperwood

MEDI **185.** Modulation of Glioblastoma tumor area is time dependent on the application of G4-OH PAMAM dendrimer. **M. Jeakle**

MEDI **186.** Polymorphs and solvates of erlotinib and dasatinib. **T. Maddox**, R. Quinones

MEDI **187.** Computer-aided design of negative allosteric modulators of metabotropic glutamate receptor 5 (mGluR5):CoMFA studies on aryl ether derivatives. S. Chelliah, **B. Jordan**, R. Thilagavathi

MEDI **188.** Chemo-enzymatic approach towards the synthesis of vancomycin and its analogs. **S. Ozturk**

MEDI **189.** EGCG and Sylibins as treatment for inherited cardiomyopathies: Binding simulations to cardiac troponin. **J. Eiros Zamora**, G. Hoben, A. Sheehan, A. Messer, A. Chaudhry, D. Biedermann, V. Kren, S.B. Marston, I.R. Gould

MEDI **190.** Derivatives of L-tryptophanhydroxamic acid as potential inhibitors of *Burkholderia pseudomallei* IspF. **C. Muller**

MEDI **191.** Synthesis and evaluation for biological activity of cyclic guanidine containing natural product analogues. **V. Sammeta**, **S. Rasapalli**

MEDI **192.** Exploring the chemical biology of secondary metabolites: Scalable synthesis of majusculamide D. **E.J. Caro-Diaz**, W.H. Gerwick

MEDI **193.** Prostate cancer targeted nanoparticle cocktail for combination therapy. **U. Basu**

MEDI **194.** Direct thrombin inhibitors with a novel, reversible, covalent mechanism of action. M. Sivaraja, S. Sizikov, D. Williams, C. Xu, D. Clemens, S. Dash, K. Lin, M. Reddy, G. Neckermann, S. Yau, E. To, L. Igoudin, S. Chang, S. Keutzer, P. Zalicki, N. Sandoval, J. Zhang, T. Shiau, **K. Short**, M. Estiarte, A. Datta, D. Kita

MEDI **195.** Cheminformatics analysis of WNK-inhibitor interactions. **M.A. Kuenemann**, D. Fourches

MEDI **196.** Computational structural-based design and structure and activity study of fluorinated combretastatin analogues. **Y. Zong**

MEDI **197.** Benzoate derived pH sensitive phosphoramidate-based linkers for controlled release. **B. Backer**, A. Davis, C. Choy, C.E. Berkman

MEDI **198.** New vacuolar-ATPase inhibitors as antiviral therapies. **A. Lindstrom**, D.P. Petrov, D. LaCount, R. Davey, V.J. Davisson

MEDI **199.** Design and synthesis of curcumin analogues for cytotoxicity against head & neck cancer. **S. Chelliah**, B. Jordan, B. Kumar, R. Thilagavathi, P. Kumar

MEDI **200.** Withdrawn.

MEDI **201.** Interactions of isoniazid with model membranes. **A. Groninger**, B.J. Peters, J.B. Hough, F. Fontes, G. Cardiff, D.C. Crick, D.C. Crans

MEDI **202.** Synthesis and biological evaluation of novel casein kinase 1d inhibitors for treatment of Alzheimer's disease. **V. Jha**, C. Gettridge, R. Schroeder, M. Bratton, P. Tram, J. Sridhar

MEDI **203.** Exploring the interactions between the anti-tuberculosis agent, pyrazinamide/pyrazonoic acid, and lipid model membrane systems. **J.B. Hough**, A.S. Groninger, B.J. Peters, F. Fontes, D.C. Crick, D.C. Crans

MEDI **204.** Aza-peptide aldehydes and ketones: A new class of proteasome inhibitors. **T. Corrigan**, K. Kasper, R. McCauslin, R.J. Yoder, C.M. Hadad, Ö. Doğan Ekici

MEDI **205.** Synthesis of oligothiophene tris(2,2'-bipyridyl)-type ruthenium (II) conjugate as electrochemiluminescence-luminophore. **L. Lantz**, P. Nilsson

MEDI **206.** Molecular dynamic simulation and pharmacophore model of parasitic cysteine proteases. **D. Gomes Vital Fujii**, **G.M. Monteiro Ferreira**, **J. da Fonseca Rezende e Mello**, **G.H. Trossini**

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MEDI **207.** Comparison of the efficacy of ester substituents in their specificity and effectiveness for reducing cell growth in certain cancer cell lines. **R. Nguyen**, A. Jelowicki, M. Young, C. Bunye, K. Soriano, E. Guglielmo, E. Lavassani, A. Nguyen, N. Patel, P. De Lijser

MEDI **208.** Synthesis of KS15 derivatives as CRY-mediated circadian clock modulators. **Y. Choi**, Y. Son, S. Chung, G. Son, K. Kim, Y. Suh, J. Jung

MEDI **209.** Synthesis and evaluation of xanthurenic acid analogs for impeding transmission of *Plasmodium falciparum* from host to vector. **A. Kanwar**, J. Leahy, D. Kyle, T. Mcgaha

MEDI **210.** Withdrawn.

MEDI **211.** Magnetite nanoparticles effect on *Escherichia coli* growth. **M.A. Gratacos**, E. Acevedo

MEDI **212.** Withdrawn.

MEDI **213.** Developing dual colorimetric and fluorogenic probes for visualizing tyrosine phosphatase activity and high throughput screening. **S. Biswas**, B. S. McCullough, E. S. Ma, D. LaJoie, C. W. Russell, G. Brown, J. L. Round, K. S. Ullman, M. A. Mulvey, A.M. Barrios

MEDI **214.** Photoswitchable dualsteric M1 ligand. **L. Agnetta**, M. Kauk, M. Canizal, R. Messerer, U. Holzgrabe, C. Hoffmann, M. Decker

MEDI **215.** Synthesis of chemical probes for serine/threonine protein phosphatase 5C based on a natural product template. **M. Tuttle**, L. Yet, R. Honkanen, M. Swingle

MEDI **216.** Development and synthesis of β-lactam prodrugs for tuberculosis. **M. Cole**, J. Buonomo, C.C. Aldrich

MEDI **217.** Synthesis and biological evaluation of a novel series of GPER antagonists for the treatment of gallstone formation. **C. DeLeon**, C.K. Arnatt, D. Wang, M. Wilhelm, P. Sweeney

MEDI **218.** Design, synthesis and SAR study of truxillic acid-based fatty acid binding protein inhibitors as anti-nociceptive and anti-inflammatory drugs. **S. Yan**, K. Hu, S. Tong, M. Awwa, Q. Gan, M. Elmes, J. Sweeney, H. Hsu, M. Kaczocha, H. Li, R.C. Rizzo, D. Deutsch, I. Ojima

MEDI **219.** SB-T-1214 and biotin functionalized gold nanoparticles. **X. Wang**, I. Ojima

MEDI **220.** Discovery of a novel series of potent and selective Phosphatidylinositol-3-Kinase delta (PI3Kδ) inhibitors for the treatment of inflammatory and autoimmune diseases. **N. Aguilar**, J. Fernandez, B. Hernandez, M. Carrascal, P. Niño, A. Lopez, L. Vazquez, E. Lozoya, M. Maldonado

MEDI **221.** Development of cancer stem cell depleting ALDH1A selective inhibitors as potential therapeutics for ovarian cancer. **B. Huddle**, C. Buchman, K. Yang, M. Chtcherbinine, I. Chefetz-Menaker, C. Morgan, R. Buckanovich, T. Hurley, S. Larsen

MEDI **222.** Photoaffinity probes for protein N-terminal methyltransferases. **B. Mackie**, R. Huang

MEDI **223.** Novel selenorhodamine dyes as photosensitizers in varying applications. **J. Hill**, M.W. Kryman, G.A. Schamerhorn, M.R. Detty, Z.A. McIver

MEDI **224.** Design, synthesis and preclinical study of novel taxoid-based Small Molecule Drug Conjugates (SMDCs) using folate/Dimethyltetrahydrofolate (DMTHF) as tumor targeting module. **C. Wang**, Y. Wang, M. Tortorella, I. Ojima

MEDI **225.** Structure-based discovery of novel small molecule Wnt/β-catenin signaling inhibitors. **S. Guzman**, A. Nguyen, P. De Lijser, N. Patel

MEDI **226.** Identification and lead optimization of pyrazole carboxamides with antiviral activity. **K. Paulvannan**

MEDI **227.** Inhibition of arginase from *Leishmania mexicana* by benzimidazole derivatives. **I. Betancourt**, A. Chaidez-Avila, A.G. Vazquez-Raygoza, C.I. Avitia-Domínguez, A. Romo-Mancillas, A. Hernandez Campos, A. Téllez-Valencia

MEDI **228.** Design and development of a novel class of structurally-enhanced allosteric modulators of hemoglobin for sickle cell disease treatment. **P. Pagare**, O. Abdulmalik, M.K. Safo, Y. Zhang

MEDI **229.** Generation of novel leads for γ-secretase modulation. **M. Mandal**

MEDI **230.** Synthesis of benzimidazole derivatives for uridine nucleoside ribohydrolase targeting. **A.S. Leonardo**, M.A. Vanalstine-Parris

MEDI **231.** Synthesis and biological evaluation of the first triple inhibitors of human topoisomerase 1, tyrosyl-DNA phosphodiesterase 1 (Tdp1), and tyrosyl-DNA phosphodiesterase 2 (Tdp2). P. Wang, **M.S. Elsayed**, C. Plescia, E. Kiselev, C. Marchand, O. Zeleznik, K. Agama, Y. Pommier, M. Cushman

MEDI **232.** Transcarbamoylation of sulfonyl carbamates to generate new Angiotensin II Type 2 Receptor (AT2R) ligands. J. Wannberg, **R. Isaksson**, M. Hallberg, M. Larhed

MEDI **233.** Development of new novel therapeutics for refractive breast cancer. **K. Crosby**, **K. Johnson**

MEDI **234.** Design, synthesis and pharmacological evaluation of 1,3,6-trisubstituted-4-oxo-1,4-dihydroquinoline-2-carboxylic acid derivatives as selective $ET_A$ antagonists. **N.S. Khadtare**, R. Stephani, V.L. Korlipara

MEDI **235.** Withdrawn.

MEDI **236.** Structure-based design of small-molecular inhibitors targeting the Menin-MLL protein-protein interaction. **S. Xu**, T. Xu, K. Zheng, A. Aguilar, L. Huang, D. Bernard, D. McEachern, S. Przybranowski, J. Stuckey, S. Wang

MEDI **237.** Novel pirfenidone derivatives: Potent antifibrotic agents. **Z. Ma**, C. Yu, Q. Chen, W. Huang, Z. Wang, C. Zhang, Z. Shen

MEDI **238.** Synthesis and biological activity of novel TU-100 derivatives. **O.J. Alao**, R.J. Sheaff, J.C. Dicesare

MEDI **239.** New α-helix mimetics targeting the E6 protein in the human papillomavirus. **E. Armenta**, A. Orchard

MEDI **240.** Finding hits for designing new antidiabetic drugs. Inhibition of protein tyrosine phosphatase 1B. M.J. Sarabia-Sánchez, P.J. Trejo, E. Sierra, M. Valdez-Solana, A. Hernandez Campos, C.I. Avitia-Domínguez, **A. Téllez-Valencia**

MEDI **241.** Identification of small molecular activators on the unfolded protein response in leukemia cells. **N. Mahmoud**, D. Garshott, Y. Xi, A. Brownell, M. Callaghan, A. Fribley

MEDI **242.** Constrained peptides that inhibit HIV-1 fusion. **O. Bolarinwa**, J. Cai

MEDI **243.** Design and optimization of small molecule inhibitors blocking the menin-MLL interaction. **T. Xu**, S. Xu, K. Zheng, A. Aguilar, L. Huang, K. Chinnaswamy, D. Bernard, D. McEachern, S. Przybranowski, J. Stuckey, S. Wang

MEDI **244.** Discovery of LLM4 as potent and specific IL-6/gp130 protein-protein interaction inhibitor for potential cancer therapy. **L. Mao**, G. Shi, C. Li

MEDI **245.** ML418: The first selective, sub-micromolar pore blocker of $K_v$7.1 potassium channels. **H. Kurata**, D.R. Swale, S.V. Kharade, J. Sheehan, R. Raphemot, K.R. Voigtritter, E.E. Figueroa, J. Meiler, A.L. Blobaum, C.W. Lindsley, J.S. Denton, C.R. Hopkins

MEDI **246.** Effect of magnetite chitosan/alginate beads infused with the antibiotic oxytetracycline hydrochloride on *E. coli* growth rates. **R.M. Zamora**, A. Chardon, F. Alvarez, A. Zapata, V. Fernandez-Alos, F. Roman, O. Perales

MEDI **247.** Design and solid-phase synthesis of Muramyl dipeptide (MDP) surrogates as NOD2 signaling activating agents. **I. Kekessie**, T. Goncharov, J. Tom, D. Vucic, A. Song

MEDI **248.** Discovery of preclinical candidate SCH 900577: A prodrug of hydantoin based TACE inhibitor. **L. Tong**, S. Kim, L. Chen, A. Kosinski, B. Shankar, V. Girijavallabhan, D. Yang, W. Yu, G. Zhou, N. Shih, K. Rosner, D. Li, C. Dai, J. Popovici-Muller, L. Yang, A. Siddiqui, Z. Guo, P. Orth, S. Chen, M. Hu, D. Lundell, X. Niu, S. Umland, J.A. Kozlowski

MEDI **249.** Probing conformational preference: (S)- and (N)-methanocarba 7-deazaadenosine analogues as inhibitors of human adenosine kinase. **K.S. Toti**, D. Osborne, A. Ciancetta, D. Boison, K.A. Jacobson

MEDI **250.** Synthesis and NMDA receptor activity of various ketamine metabolites. **P.J. Morris**, P. Zanos, R. Moadell, C.A. Zarate, T. Gould, C.J. Thomas

MEDI **251.** Discovery of potent glucagon receptor antagonists for the treatment of type 2 diabetes. **G. Xu**, M.D. Gaul, F. Song, B. Zhao, Y. Liang, F. Du, K. Diloreto, N. Huebert, B.C. Shook, D. Rentzeperis, R. Santulli, A. Eckardt, C. Smith, K. Demarest

MEDI **252.** Synthesis and two- and three-dimensional *in vitro* studies of hyaluronic acid porphyrin conjugates. **N. Bhupathiraju**, C. Farley, N. Berisha, B. Begum, C.M. Drain

MEDI **253.** Preformulation analysis and stability of hydrophobic small molecular echinomycin for injection formulation. **J.H. Lee**, M. Tran, P. Yuan, G.K. Potti

MEDI **254.** Withdrawn.

MEDI **255.** Design, synthesis and biological evaluation of specific ARK5 inhibitor. **M. Reddy**, S. Athuluri-Divakar, B. Akula, M.R. Mallireddigari, S.C. Cosenza, V. Dandu, V. Bharathi, V. Pallela, P. Reddy

MEDI **256.** Discovery of novel class IIa-selective histone deacetylase inhibitors using an in silico virtual screening approach. **H. Tseng**, C. Liu, C. Chen, K. Hsu, W. Huang

MEDI **257.** Hybridization approach to selective RIPK2 inhibitors by targeting inactive kinase conformations. **C. Suebsuwong**, A. Degterev, G. Cuny

MEDI **258.** Design and synthesis of tricyclic and tetracyclic fused coumarin sulfonate derivatives, and their inhibitory effects on LPS-induced nitric oxide and $PGE_2$ productions in RAW 264.7 macrophages. **M.I. El-Gamal**, C. Oh, K. Lee, D. Baek

MEDI **259.** Novel benzamides as capsid assembly modulators for the hepatitis B virus. **N. Hwang**, M. Campagna, K. McGuire, S. Wu, J. Guo, Y. Du

MEDI **260.** Computational design, synthesis and characterization of novel mPGES-1 inhibitors. **Z. Zhou**, K. Ding, S. Zhou, Y. Yuan, F. Zheng, C. Zhan

MEDI **261.** Evaluation of 2-amino-pyrimidine derivatives as antimicrobial agents and IspF inhibitors. **S. Watkins**, D. Ghose, C.A. Muller, Z. Zhang, J.M. Blain, Z. Lazowski, S.T. McDonald, T. Riggins-Walker, J.R. Horn, R. Meganathan, H. Hofstetter, T.J. Hagen

MEDI **262.** Design and synthesis of 1-(2-(2,4-difluorophenyl)-2-hydroxy-3-(1H-1,2,4-triazol-1-yl)propyl)-2-(1-((methyl(3-(((methylcarbamoyl)oxy)methyl)pyridin-2-yl)carbamoyl)oxy)ethyl)-1H-1,2,4-triazol-2-ium. **L. Peyton**, M. Hashemzadeh, S. Gallagher

MEDI **263.** Fragment-based lead discovery of a novel Map4k4 inhibitor. **L. Wang**

MEDI **264.** SDAP substrate analog enantioselective synthesis and ninhydrin-based enzyme assay for the dapE-encoded bacterial enzyme diaminopimelate desuccinylase (DapE). **T. Heath**, M. Lutz, C. Reidl, B. Nocek, M. Ballicora, R.C. Holz, K. Olsen, D.P. Becker

MEDI **265.** Discovery of a new class of highly potent small-molecule degraders of BET bromodomain proteins. **F. Xu**, J. Hu, B. Zhou, Z. Chen, M. Lin, L. Bai, C.Y. Yang, D. McEachern, S. Przybranowski, E. Fernandez-Salas, B. Wen, D. Sun, S. Wang

MEDI **266.** Glyoxylate shunt as an antibacterial drug target. **S. Bartlett**, A. McVey, A. Crousilles, M. Welch, D.R. Spring

MEDI **267.** Synthesis of monomers with enzymes and chemical reagents for preparing polyester. **K. Kim**, C. Song, K. Jeong, C.S. Cheong

MEDI **268.** Exploit ionic liquids to significantly improve asymmetric reduction of 3,5-bis(trifluoromethyl) acetophenone catalyzed by *T. asperellum* ZJPH0810 cells. **J. Li**, W. Du

MEDI **269.** Microwave-promoted/assisted method for rapid prepararation of biaryl seven-membered lactones. **W. Du**

MEDI **270.** Potent but potentially non-cardiotoxic anthracycline anti-cancer analogs. **J.A. Holdaway**, A.L. Petty, P.L. Barnes, P. Moon, K. Cornell, D.L. Warner

MEDI **271.** Targeting the colchicine binding site in tubulin for cancer treatment: Structural optimization of ABI-231 leads to improved potency and microsomal stability. **Q. Wang**, K. Arnst, D.D. Miller, W. Li

MEDI **272.** Novel, highly selective direct thrombin inhibitors: *In vivo* studies demonstrate efficacy with lower bleeding risk. C. Xu, D. Clemens, S. Dash, K. Lin, M. Reddy, G. Neckermann, S. Yau, E. To, L. Igoudin, S. Chang, S. Keutzer, P. Zalicki, N. Sandoval, S. Sizikov, D. Williams, M. Sivaraja, J. Zhang, T. Shiau, K. Short, **M. Estiarte**, A. Datta, D. Kita

MEDI **273.** Synthesis of a known binder of the GRB2 SH2 domain from naphthaldehyde. **A. Bowlsby**, C. Arpin

MEDI **274.** Novel synthetic strategies to disarm the myeloid cell leukemia-1 oncoprotein. **S.J. Hughes**, B. Drennen, M.E. Lanning, S. Fletcher

MEDI **275.** Improving the *in vitro* and *in vivo* performance of a $^{177}$Lu-labeled phosphoramidate-based PSMA inhibitor with an albumin-binding motif. **C.J. Choy**, X. Ling, J.J. Geruntho, S. Beyers, J. Latoche, B. Langton-Webster, C.J. Anderson, C.E. Berkman

MEDI **276.** Synthesis and evaluation of phenyl tetrazole derivatives with amide or urea linkers as BCRP/ABCG2 inhibitors. **N. Gujarati**, L. Zeng, Z. Chen, V.L. Korlipara

MEDI **277.** Two-faced synthetic α-helix mimetics based on heterocyclic cores as dual BCL-2/MDM2 inhibitors. I.L. Conlon, **B. Drennen**, M.E. Lanning, L. Chen, S.J. Hughes, P.T. Wilder, S. Fletcher

MEDI **278.** Kröhnke pyridine synthesis permits facile access to novel Mcl-1 inhibitors. **I.L. Conlon**, D. Van Eker, J. Chauhan, P.T. Wilder, S. Fletcher

MEDI **279.** Dual stimuli-activatable oxidative stress amplifying hybrid anticancer drugs. **J. Noh**, D. Yoo, E. Jung, D. Lee, **J. Lee**

MEDI **280.** Covalent-docking based protocol for the rational design of covalent inhibitors. **X. Wan**

MEDI **281.** Study of the chemical composition, cytotoxic and antitumor activities of *Croton discolor*. **A.D. Ramos Vicente**

MEDI **282.** *Trypanosoma cruzi* sirtuin-2 construction by modeling threading and molecular dynamics. **G.M. Monteiro Ferreira**, G.H. Trossini, F.D. Emery, V.G. Maltarollo

MEDI **283.** DFGmodel: Modeling protein kinases in inactive conformations and its applications in drug discovery. **P. Ung**, A. Schlessinger

MEDI **284.** Virtual screening for potential inhibitors of neuraminidase for influenza treatment. **E.C. Gomez-Suarez**

MEDI **285.** Anthranilic acid derivatives as potential multi-target drugs for metabolic syndrome treatment. **A. Bravo**, H. González Álvarez, M. Loza-Mejía

MEDI **286.** Design and synthesis of N-substituted acridone derivatives as potential antibacterial and antiviral agents. **L.J. Jimenez Sanchez**, D. Juan-Guadarrama, M. Loza-Mejía

MEDI **287.** Developing a chimeric heterobivalent platform as a selective imaging probe for MMP-14. **M. Pun**, R. Rios, C.E. Berkman

MEDI **288.** Structural characterization, homology modelling and virtual screening studies in shikimate kinase from methicillin resistant *Staphylococcus aureus*. **A. Favela**, A. Téllez-Valencia, H. Nájera, J. Cisneros, M. Gómez-Palacio, A. Hernandez Campos, C.I. Avitia-Domínguez

MEDI **289.** Selective inactivation of triosephosphate isomerase from *Trypanosoma brucei*. **A.G. Vazquez-Raygoza**, I. Betancourt, R. Castillo-Bocanegra, C.I. Avitia-Domínguez, E. Sierra, M. Valdez-Solana, A. Téllez-Valencia

MEDI **290.** Design, synthesis, and biological evaluation of novel C3-sustituted β-carboline-based HDAC inhibitors with potent antitumor activities. **Y. Ling**, J. Feng, J. Miao, J. Guo, Y. Peng, Y. Zhang

MEDI **291.** Design and development of reversible inhibitors of lysine specific demethylase 1. **D.P. Mould**, A. McGonagle, M. Geitmann, U. Bremberg, A.M. Jordan, D. Ogilvie

MEDI **292.** Withdrawn.

MEDI **293.** Development of allosteric hydrazide-containing class I histone deacetylase inhibitors for use in acute myeloid leukemia. **J.J. McClure**, C. Zhang, E.B. Inks, Y.K. Peterson, J. Li, C. Chou

MEDI **294.** Withdrawn.

MEDI **295.** Translational feasibility of novel methionyl-tRNA synthetase inhibitors. **M. Bassiri**

MEDI **296.** Identification and development of small molecule inhibitors of the aggregation of amyloid β. **S. Collins**, F. Gielen, L. van Vliet, G. Kaminski, F. Hollfelder, D.R. Spring

MEDI **297.** Drug-target residence time affects *in vivo* drug efficacy through multiple pathways. **K.S. Lee**, J. Yang, K. Wagner, C.J. Ng, J. Niu, A. Dickson, B.D. Hammock

MEDI **298.** Cytotoxicity study of α-hydroxy-β-dicarbonyl bearing synthetic metabolites of poecilosclerid sponge. **S.V. Malhotra**, M.P. Doyle, P. Truong, D. Sharma, A. Nagalingam, W.C. Reinhold, J.R. Alleyn, Y. Yu

MEDI **299.** Second-generation fluorescent ligands for nicotinic acetylcholine receptors. **R.W. Fitch**

## MONDAY MORNING

### Section A

Moscone Center

3002/3004

**Actually it does Work: Success with Allosteric Kinase Ligands & Phosphatase Modulators**

L. Lombardo, D. S. Weinstein, *Organizers*

R. Moslin, J. B. Schwarz, *Organizers*, *Presiding*

**9:00** MEDI **300.** Discovery of ARQ 092: A potent, selective allosteric inhibitor of AKT1, 2, 3 and AKT1-E17K in clinical development for cancer and rare diseases. **J. Lapierre**, S. Eathiraj, Y. Yu, R.E. Savage, G. Abbadessa, B. Schwartz

**9:30** MEDI **301.** Allosteric inhibitors of Interleukin-2-inducible T cell kinase that selectively target its inactive conformation. **A.E. Aulabaugh**

**10:00** MEDI **302.** BCR-ABL allosteric inhibitors targeting the myristoyl pocket: Optimization and pharmacological evaluation of substituted N-(4-(trihalomethoxy)phenyl)nicotinamide derivatives towards ABL001. **J. Schoepfer**

**10:30** Intermission.

**10:40** MEDI **303.** Identifying allostery in signaling enzymes. **W. Peti**

**11:10** MEDI **304.** Selective inhibition of a phosphatase to treat neurodegenerative diseases. **A. Bertolotti**

**11:40** MEDI **305.** Allosteric inhibition of SHP2 phosphatase. J. Garcia Fortanet, C. Chen, Y. Chen, Z. Chen, Z. Deng, B. Firestone, P. Fekkes, M. Fodor, P. Fortin, C. Fridrich, D. Grunenfelder, S. Ho, Z. Kang, R. Karki, M. Kato, N. Keen, L. Labonte, J. Larrow, F. Lenoir, G. Liu, S. Liu, F. Lombardo, D. Majumdar, M. Meyer, M.G. Palermo, L. Perez, M. Pu, T. Ramsey, W. Sellers, M.D. Shultz, T. Stams, C. Towler, P. Wang, S. Williams, J. Zhang, **M.J. LaMarche**

### Section B

Moscone Center

3006/3008

**Residence Time: Not Just Affinity for Drug Design**

B. Blagg, *Organizer*

P. J. Tonge, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35** MEDI **306.** Drug-target residence time model: A 10-year retrospective. **R. Copeland**

**9:10** MEDI **307.** Protein dynamics and allostery in kinase activation. **N. Ahn**

**9:45** MEDI **308.** Drug target residence time in the early drug discovery phase: HSP90, a model to gain insight into the molecular mechanism of kinetics. **M. Frech**

**10:20** MEDI **309.** Determination of *in vivo* enzyme occupancy utilizing inhibitor dissociation kinetics. **M. Lai**, D. Murphy, Y. Ou, D. Euler, K. Wessner, S. Adamski, B. Luo, G. Wesolowski, R. Vogel, H. Glantschnig, L. Lubbers, S. Carroll

**10:55** MEDI **310.** Linking target engagement and *in vivo* drug activity: Insights into target vulnerability. **P.J. Tonge**, F. Daryaee, Z. Zhang, K. Gogarty, S.L. Fisher

**11:30** Concluding Remarks.

**Advances in High-Throughput Screening**

*Sponsored by CINF, Cosponsored by COMP and MEDI*

**Science for a Sustainable Energy Future**

**Energy Storage**

*Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF*

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

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

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

## MONDAY AFTERNOON

### Section A

Moscone Center

3002/3004

**Kinase Inhibitors for Immuno-Inflammatory Diseases**

J. Ramanjulu, *Organizer, Presiding*

L. Krim Gavrin, *Presiding*

**2:00** MEDI **311.** Discovery of GDC-0853: A potent & selective BTK inhibitor for the treatment of lupus & rheumatoid arthritis. **W.B. Young**

**2:30** MEDI **312.** Development of the selective, allosteric RIPK1 kinase inhibitors. M. Najjar, C. Suebsuwong, S. Ray, G. Cuny, **A. Degterev**

**3:00** MEDI **313.** Identification of a first-in-class RIP1 kinase inhibitor in phase 2a clinical trials for immuno-inflammatory diseases. **P.A. Harris**

**3:30** MEDI **314.** Targeting NF-kB pathways in toll-like receptor and antigen receptor signaling. **H. Wu**

**4:00** MEDI **315.** Approaches to TYK2 pseudokinase: A unique mode of allosteric kinase inhibition. **R. Moslin**, S. Wrobleski, Y. Zhang, S. Lin, D. Gardner, J.B. Santella, J.V. Duncia, C. Liu, J. Lin, S. Spergel, M. Mertzman, J.S. Tokarski, H. Sun, M. Chiney, P.A. Elzinga, N. Aranibar, A. Chimalakonda, J. Strnad, A. Zupa-Fernandez, L. Cheng, K. Gillooly, K. Mcintyre, P.H. Carter, L. Lombardo, J. Burke, J.E. Macor, D.S. Weinstein

**4:30** MEDI **316.** Design of JAK3 covalent inhibitors for the interrogation of JAK3 signaling in humans. **A. Casimiro-Garcia**, A. Thorarensen, J. Telliez, P. Balbo, M.E. Banker, M.F. Brown, Y. Che, J. Chrencik, J.W. Coe, R. Czerwinski, M.E. Dowty, A.M. Gilbert, M.M. Hayward, M. Hegen, B. Juba, J. Jussif, J. Langille, L. Leung, S. Liang, T. Lin, J.I. Montgomery, S. Soucy, J. Trujillo, R. Unwalla, F.F. Vajdos, F. Vincent, X. Yang

### Section B

Moscone Center

3006/3008

**Misfolded Proteins in Neurodegenerative Diseases**

A. M. Walji, *Organizer, Presiding*

**1:30** Introductory Remarks.

**1:35** MEDI **317.** Targeting intrinsically disordered proteins: Taming alpha-synuclein with small molecules. J. Tao, A. Berthet, D. Agard, **L. McConlogue**

**2:10** MEDI **318.** Current status of the development of PET radiotracers for imaging alpha synuclein aggregates in Lewy bodies and Lewy neurites. **R.H. Mach**

**2:45** MEDI **319.** HDAC6 inhibitors, autophagy, mitochondrial movement, and disease modification. **A.P. Kozikowski**

**3:20** Intermission.

**3:35** MEDI **320.** Imaging mutant huntingtin aggregates: Development of potential PET ligand. **C. Dominguez**

**4:10** MEDI **321.** Small molecule modulators of ER stress for the treatment of neurodegenerative diseases. **N.D. Cosford**, H. Zou, A. Limpert, J. Zou, A. Dembo, D. Grant, R. Ardecky, A. Pinkerton, G. Magnuson, M. Goldman, J. Rong, D. Sheffler, J. Reed

‡ *Cooperative Cosponsorship*

**4:45** MEDI **322.** Discovery of the P7C3 class of neuroprotective compounds. **J. Ready**

**5:20** Concluding Remarks.

**Science for a Sustainable Energy Future**

**Chemical & Biological Conversions Approaches to Energy Conversion**

*Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF*

**Advances in High-Throughput Screening**

*Sponsored by CINF, Cosponsored by COMP and MEDI*

**Eminent Scientist Lecture with Dr. Carolyn Bertozzi**

*Sponsored by SOCED, Cosponsored by MEDI*

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

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

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

**Undergraduate Research Posters**

**Medicinal Chemistry**

*Sponsored by CHED, Cosponsored by MEDI and SOCED*

## MONDAY EVENING

### Section A

Moscone Center

Hall D

**Sci-Mix**

A. W. Stamford, *Organizer*

**8:00 - 10:00**

**111-112, 117, 136, 148, 154, 177, 182, 216, 234, 242, 245, 258, 266, 277, 290.** See previous listings.

**452, 457, 462, 473.** See subsequent listings.

## TUESDAY MORNING

### Section A

Moscone Center

3002/3004

**MEDI Awards Symposium**

A. W. Stamford, *Organizer*

W. B. Young, *Presiding*

**9:00** MEDI **323.** Withdrawn.

**9:45** MEDI **324. Award Address** (E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances sponsored by Merck Research Laboratories). Present and future of antisense technology. **S. Crooke**

**10:30** MEDI **325. Award Address** (ACS Award for Creative Invention sponsored by ACS Corporation Associates). CPP-115: A novel GABA aminotransferase inactivator and potential new treatment for epilepsy, addiction, and hepatocellular carcinoma. **R.B. Silverman**

**11:15** MEDI **326.** Bristol-Myers Squibb Smissman award lecture: Receptor structures enable drug discovery. **K.A. Jacobson**

### Section B

Moscone Center

3006/3008

**Antibiotic Drug Discovery: The Next Frontier**

E. D. Brown, C. L. Freel Meyers, *Organizers*, *Presiding*

**8:30** MEDI **327.** Targeting bacterial bioenergetics and central metabolism: Challenges and opportunities. **K. Pethe**

**9:10** MEDI **328.** Targeting bacterial nutrient biosynthesis with natural products. **E.D. Brown**

**9:50** MEDI **329.** Antibacterial agents that target adenylating enzymes in *Mycobacterium tuberculosis*. **C.C. Aldrich**

**10:30** MEDI **330.** Targeting a branch point in bacterial metabolism through inhibition of DXP synthase. **C.L. Freel Meyers**

**11:10** MEDI **331.** Co-therapy strategy to enhance target vulnerability in *Mycobacterium tuberculosis*. **N.S. Sampson**

**11:50** MEDI **332.** Discovery of ETX2514, a novel, rationally designed inhibitor of class A, C and D β-lactamases, for the treatment of Gram-negative infections. **T.F. Durand-Reville**

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

*Sponsored by COMP, Cosponsored by BIOL, MEDI and WCC*

**Green Chemistry Adoption: Progressive Changes by Different Industry Sectors**

*Sponsored by ENVR, Cosponsored by CEI, MEDI, ORGN and SCHB‡*

## TUESDAY AFTERNOON

### Section A

Moscone Center

3002/3004

**Drug Discovery for ALS: Putting the Ice Bucket to Work**

L. Bruijn, G. M. Dubowchik, *Organizers*, *Presiding*

**2:00** MEDI **333.** Challenges and opportunities for drug discovery in ALS. **L.I. Bruijn**

**2:40** MEDI **334.** Identification and preclinical pharmacology of antisense oligonucleotides targeted to human SOD1 for the treatment of ALS. **E.E. Swayze**

**3:20** MEDI **335.** Design and study of small molecules targeting r(G4C2) repeats in ALS and FTD. **M.D. Disney**

**4:00** Intermission.

**4:15** MEDI **336.** Dual leucine zipper kinase inhibitors for the treatment of neurodegenerative diseases. **M. Siu**

**4:55** MEDI **337.** Development of small-molecule autophagy inducers that mitigate neurodegeneration in models of ALS and other disorders. **S. Finkbeiner**

### Section B

Moscone Center

3006/3008

**General Orals**

A. W. Stamford, *Organizer*

A. Ali, *Presiding*

**1:30** MEDI **338.** γ-Functionalized hydrocarbon stapled peptides for inhibiting mutant estrogen receptor/coactivator interaction. **T. Speltz**, C.G. Mayne, S. Fanning, E. Tajkhorshid, G. Greene, T.W. Moore

**1:55** MEDI **339.** Discovery of BMS-986104: Moving from direct-acting, full agonists to pro-drug, partial agonists in the identification of a differentiated S1P1 modulator with an improved safety profile. **A.J. Dyckman**, M. Dhar, D. Marcoux, H. Xiao, Z. Xiao, J.L. Gilmore, L. Li, A. Mathur, J. Xie, X. Yang, T.L. Taylor, R. Thomas, K. Mcintyre, L. Lehman-McKeeman, H. Shi, P. Levesque, P. Balimane, H. Sun, A.M. Marino, Z. Yang, D. Shen, M. Cvijic, B.M. Warrack, G. Cornelius, C.J. D'Arienzo, L. Salter-Cid, J.C. Barrish, P.H. Carter

**2:20** MEDI **340.** Phenotypic screening identifies a small molecule anti-secretagogue of PCSK9 that acts via a novel mechanism of action. D. Petersen, J. Hawkins, W. Ruangsiriluk, K. Stevens, B. Maguire, T.N. O'Connell, B.N. Rocke, M. Boehm, R.B. Ruggeri, T. Rolph, D. Hepworth, P. Loria, **P.A. Carpino**

**2:45** MEDI **341.** Discovery of chemical biology probes inhibiting activation of SGK3 kinase in cancer cells. **M. Lindvall**, G.A. Nishiguchi, C. Bellamacina, W. Shu, L. Tian, E.J. Martin, S. Ma, E. Fang, T. Zavorotinskaya, E. Park, D. Duhl, A.C. Rico, V. Tamez, L. Doyle, M. Doyle

**3:10** MEDI **342.** Unveiling the truth about PAK1 with medicinal chemistry. **J. Rudolph**, L.J. Murray, C.O. Ndubaku, T. O'Brien, E. Blackwood, W. Wang, I. Aliagas, L.J. Gazzard, J.J. Crawford, J. Drobnick, W. Lee, X. Zhao, D. Favor, P. Dong, H. Zhang, C.E. Heise, A. Oh, C. Ong, H. La, P. Chakravarty, C. Chan, D. Jakubiak, J. Epler, S. Ramaswamy, R. Vega, G. Cain, D. Diaz, Y. Zhong

**3:35** MEDI **343.** Discovery of the potent and selective, broad spectrum fungal CYP51 inhibitor VT-1598. **C.M. Yates**, E.P. Garvey, R.J. Schotzinger, S.R. Shaver, W.J. Hoekstra

**4:00** MEDI **344.** Discovery of the brain penetrant Phosphodiesterase 1 (PDE1) inhibitor Lu AF64386. **J. Kehler**, A.I. Parachikova, H. Lindgren, L.K. Rasmussen, M. Langgard, C.T. Christoffersen, C. Bundgaard, K. Juhl, L. Skibsbye, J. Agner, J. Nielsen

**4:25** MEDI **345.** Impact of P-gp susceptibility on brain penetration for a series of potent, selective, and orally bioavailable TrkA inhibitors. **M.E. Fraley**

**4:50** MEDI **346.** Discovery of ruzasvir (MK-8408), a 2nd generation HCV NS5A inhibitor. **W. Yu**, L. Tong, L. Chen, O. Selytin, M.P. Dwyer, A.G. Nair, R. Mazzola, J. Kim, D. Sha, J. Yin, R. Ruck, I.W. Davies, B. Hu, B. Zhong, J. Hao, T. Ji, S. Zan, R. Liu, S. Agrawal, E. Xia, S. Curry, P. Mcmonagle, K. Bystol, F. Lahser, D. Carr, L. Rokosz, P. Ingravallo, S. Chen, K. Feng, M. Cartwright, E. Asante-Appiah, J.A. Kozlowski

**Entrepreneurship in Biotechnology, Advanced Materials, Drug Discovery & Information Systems**

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## WEDNESDAY MORNING

### Section A

Moscone Center

Gateway Ballroom 103/104

**First Time Disclosures**

J. B. Schwarz, *Organizer, Presiding*

**8:00** MEDI **347.** Discovery of highly efficacious potentiators for the treatment of cystic fibrosis. **S. Van der Plas**, H. Kelgtermans, T. De Munck, S. Martina, L. Tomaskovic, T. Christophe, M. Jans, E. Van der Aar, M. Borgonovi, L. Nelles, M. Gees, P. Stouten, J. Van Der Schueren, O. Mammoliti, M. Andrews, K. Conrath

**8:30** MEDI **348.** Discovery of ABBV/GLPG-2222: A potent, efficacious CFTR corrector for the treatment of cystic fibrosis. **X. Wang**

**9:00** MEDI **349.** Discovery of clinical candidate BMS-986158, an oral BET inhibitor for the treatment of cancer. **A.V. Gavai**, D. Norris, G.V. De Lucca, D. Tortolani, D.P. O'Malley, Y. Zhao, C.A. Quesnelle, W. Han, P. Gill, W. Vaccaro, T. Huynh, V. Ahuja, D. Dodd, C. Mussari, L.S. Harikrishnan, M. Kamau, J.S. Tokarski, R. Rampulla, D. Wu, J. Li, H. Zhang, P. Li, D.Z. Sun, H. Yip, C. Wang, Y. Zhang, A. Mathur, H. Zhang, C. Huang, Z. Yang, A. Ranasinghe, C.J. D'Arienzo, C. Tye, C. Su, G. Everlof, L. Zhang, N. Raghavan, K. Menard, M. Wen, J.T. Hunt, M. Poss, G. Vite, R. Westhouse, F. Lee

**9:30** MEDI **350.** Discovery of a novel class of potent, selective, and orally bioavailable histone methyltransferase Enhancer of Zeste Homolog 2 (EZH2) inhibitors and the identification of development candidate PF-06821497. **P. Kung**, S. Bergqvist, P. Bingham, J.F. Braganza, A. Brooun, M.R. Collins, W. Diehl, Y. Deng, D. Dinh, C. Fan, V.R. Fantin, H.J. Gukasyan, W. Hu, B. Huang, R. Kania, W. Liu, S. Kephart, M. Kraus, C. Krivacic, R.A. Kumpf, G. Li, K. Maegley, I.J. McAlpine, L. Nguyen, S. Ninkovic, M.A. Ornelas, D. Richter, E. Rui, M. Ryskin, S.A. Scales, J. Spangler, A. Stewart, S.C. Sutton, J. Tatlock, C. Tsao, D. Verhelle, F. Wang, H. Wang, P. Wells, M. Wythes, S. Yamazaki, B. Yip, X. Yu, L. Zehnder, W. Zhang, P. Zhu, J. Zhu, R.A. Rollins, S. Sharma, M.P. Edwards

**10:00** MEDI **351.** Discovery and development of BLU-554: A potent, highly selective covalent inhibitor of Fibroblast Growth Factor Receptor 4 (FGFR4) in development for the targeted treatment of advanced Hepatocellular Carcinoma (HCC) patients with amplified and overexpressed FGF19. **C.V. Miduturu**, M. Hagel, M. Sheets, N. Rubin, W. Weng, N. Bifulco, L.V. Dipietro, J. Kim, N. Brooijmans, B.L. Hodous, N. Stransky, K. Hoeflich, V.J. Kadambi, N. Kohl, C. Lengauer, T. Guzi

**10:30** MEDI **352.** Discovery of PRN1371: A highly selective, irreversible inhibitor of FGFR1-4 in clinical development for the treatment of solid tumors. **K.A. Brameld**

**11:00** MEDI **353.** FGF401: A reversible-covalent inhibitor of FGFR4 for the treatment of hepatocellular carcinoma. **R.A. Fairhurst**, T. Knoepfel, P. Furet, N. Buschmann, C. Leblanc, R. Mah, M. Kiffe, D. Graus-Porta, A. Weiss, J. Kinyamu-Akunda, M. Wartmann, J. Trappe, T. Gabriel, F. Hofmann, W. Sellers

**11:30** MEDI **354.** Interdiction at a protein-protein interface: Structure-based design of the Mcl-1 inhibitor AMG 176. **S.P. Brown**

### Section B

Moscone Center
3006/3008

#### Targeting Epigenetic Writers & Erasers

J. Jin, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35** MEDI **355.** Probing the epigenome for therapeutic targets. **C.H. Arrowsmith**

**9:05** MEDI **356.** Tazemetostat, a first-in-class inhibitor of EZH2: From bench to bedside to bench. **R. Copeland**

**9:35** MEDI **357.** Sirtuin inhibitors as promising anticancer agents. **H. Lin**

**10:05** Intermission.

**10:20** MEDI **358.** Targeting histone lysine methylation regulatory pathways in cancer. **P. Trojer**

**10:50** MEDI **359.** Exploring novel models of interaction to inhibit protein methyltransferases. **M. Luo**

**11:20** MEDI **360.** Chemical probes targeting the protein arginine deiminases. **P.R. Thompson**

**11:50** Concluding Remarks.

## WEDNESDAY AFTERNOON

### Section A

Moscone Center
Gateway Ballroom 103/104

#### First Time Disclosures

J. B. Schwarz, *Organizer, Presiding*

**1:30** MEDI **361.** Discovery of clinical candidate PF-06648671: A potent, highly brain penetrant gamma secretase modulator for the treatment of Alzheimer's disease. **M. Pettersson**, C. am Ende, T.W. Butler, P.H. Dorff, I.V. Efremov, E. Evrard, S.A. Eisenbeis, C.J. Helal, M.E. Green, J.M. Humphrey, G.W. Kauffman, P.B. Mullins, C.J. O'Donnell, D.A. Rankic, A.F. Stepan, C.M. Stiff, N. Patel, C. Subramanyam, T.P. Tran, E.X. Yang, L. Xie, K.R. Bales, E. Hajos-Korcsok, B.A. Pettersen, L.R. Pustilnik, S.J. Steyn, K.M. Wood, R. Qiu, P.R. Verhoest

**2:00** MEDI **362.** Discovery of a small molecule αvβ6 inhibitor for idiopathic pulmonary fibrosis. **S.J. MacDonald**, J. Pritchard, N. Anderson

**2:30** MEDI **363.** Identification of AZD9567, an anti-inflammatory glucocorticoid receptor modulator with improved side effect profile. **L. Ripa**, M. Dearman, G. Edenro, K. Edman, R. Hendrickx, M. Lepistö, L. Öberg

**3:00** MEDI **364.** Discovery and early clinical profile of a non-catchol dopamine 1 receptor agonist. **D.L. Gray**, R. Kozak, S. Mente, J.E. Davoren, D. Nason, S. ONeil, I.V. Efremov, A. Harris, R. O'Connor, M. Salafia

**3:30** MEDI **365.** Discovery and development of BLU-285: A potent, highly selective inhibitor of KIT and PDGFRα activation loop mutants. **B.L. Hodous**, E. Evans, A. Gardino, A. Davis, J. Zhu, D.P. Wilson, K. Wilson, L.V. Dipietro, J. Kim, N. Brooijmans, V.J. Kadambi, A. Shutes, Y. Zhang, N. Kohl, C. Lengauer, T. Guzi

**4:00** MEDI **366.** NVP-LXS196, a novel PKC inhibitor for the treatment of uveal melanoma. **M. Visser**, J.P. Papillon, J. Fan, M. Luzzio, W. Michael, R. Wang, A. Zhang, C. Straub, S. Mathieu, M. Kato, M.G. Palermo, C. Chen, M.J. LaMarche, T.M. Ramsey, A. Vattay, R. Guo, V. Cooke, A. Bric, F. Chung, G. Liang, M. Romanowski, A. Wylie

**4:30** MEDI **367.** Discovery of selonsertib (GS-4997): A first in class, selective inhibitor of apoptosis signal-regulating kinase 1. **G.T. Notte**, B. Corkey, E. Lansdon, D. Breckenridge, O.L. Saunders, M. Graupe, B. Murray, C. Venkataramani, J. Guerrero, J. Farand, J.A. Zablocki, K. Babaoglu, J. Liles, G. Budas, S. Wise, K. Koch, L. Castonguay, M.C. Desai

**5:00** MEDI **368.** Discovery of a selective inhibitor of indoleamine-2,3-dioxygenase for use in the therapy of cancer. **A. Balog**

### Section B

Moscone Center
3006/3008

#### General Orals

A. W. Stamford, *Organizer*

J. Ramanjulu, *Presiding*

**1:30** MEDI **369.** Teaching old drugs new tricks: Reprogramming ethionamide's bioactivation to fight multidrug resistant *Mycobacterium tuberculosis*. **N. Willand**, M. Gitzinger, B. Deprez, A. Baulard

**1:50** MEDI **370.** Preclinical development and characterization of MYC inhibitors. **N. Jacob**, P. Miranda, P. Serrano Navarro, J. Hart, P.K. Vogt, K.D. Janda

**2:10** MEDI **371.** Discovery of PF-06748962: A potent and selective lactam-based EP3 antagonist. **K. Futatsugi**

**2:30** MEDI **372.** Novel pyrrolomycins as potent antibacterial agents against *ESKAPE* pathogens and biofilms. **R. Li**, Z. Yang, J. Ahn, Y. Liu, Y. Chhonker, D. Murry, H.A. Zhong, K. Bayles

**2:50** MEDI **373.** Development and application of an NMR-based activity and inhibition assay for mycobacterial isocitrate lyase. **R.P. Bhusal**, K. Patel, B. Kwai, G. Bashiri, J. Reynisson, J. Sperry, I.K. Leung

**3:10** MEDI **374.** LEGO®-inspired drug design: Discovery of novel fungal Plasma membrane $H^+$-ATPase (Pma1) inhibitors from small molecule libraries: An introduction of HFSA-SBS_DOS-RD strategy in drug discovery. **T. Tung**, T. Dao, M.B. Palmgren, A.T. Fuglsang, S.B. Christensen, **J. Nielsen**

**3:30** MEDI **375.** Reducing cycle time in medicinal chemistry drug discovery. **J.S. Wai**, T. Wang

**3:50** MEDI **376.** Enzymatic tandem carboxylation-amidation as a bioactivity-potentiating strategy in the production of natural and unnatural thiolactomycin antibiotics. **J. Li**, X. Tang, S. Mckinnie, T. Awakawa, B.S. Moore

**4:10** MEDI **377.** Structure-based design of highly potent small-molecule inhibitors of DCN1-UBC12 protein-protein interaction. **H. Zhou**, J. Lu, L. Liu, D. Bernard, J. Stuckey, Y. Sun, S. Wang

**4:30** MEDI **378.** CDK8 inhibitors with long residence time emerging from a retro-design approach: New opportunities for cancer treatment. J.C. Benningshof, B. Aerts, **G. Müller**, J. Veerman, E. Damen, M. Kubbutat, J. Ehlert, H. Holger, F. Totzke

**4:50** MEDI **379.** Structure-based design, synthesis, biological evaluation, and x-ray crystallographic analysis of novel, highly potent HIV-1 protease inhibitors to address multi-drug resistant HIV. A.K. Ghosh, **H.L. Osswald**, J. Agniswamy, Y. Wang, I. Weber, M. Amano, H. Mitsuya

## WEDNESDAY EVENING

### Section A

Moscone Center
West Hall

#### General Posters

A. W. Stamford, *Organizer*

**7:00 - 9:00**

MEDI **380.** Inhibition of Aβ-40 and Aβ-42 aggregation by piceatannol and cis-piceatannol. **J.M. Chapman**, M. Moss, Y. Wang

MEDI **381.** Photoelectrocatalytic inhibition of Alzheimer's β-amyloid aggregation in vitro by hole-derived radicals. **K. Kim**, B. Lee, Y. Chung, W. Choi

MEDI **382.** Synthesis of Yakuchinone-derived compounds that inhibit β-amyloid aggregation. **L. Chen**, C. Yen, H. Tseng, Y. Huang, Y. Lu, W. Hou, K. Hsu, I. Pan, K. Huang, W. Huang

MEDI **383.** Photoexcited ruthenium complex for highly sensitive inhibition of β-amyloidogenesis. **G. Son**, C. Park, B. Lee, Y. Chung

MEDI **384.** New hydroxyquinoline-based derivatives as potent modulators of amyloid-b aggregations. **M. Hu**

MEDI **385.** Potential multimechanistic therapeutic effects of dihydropyridine calcium channel blockers: Mechanistic study of effects on amyloid-beta aggregation associated with Alzheimer's disease. **J.M. Chapman**, M. Moss, J. Tseng

MEDI **386.** Withdrawn.

MEDI **387.** Development of MBRI-001, a deuterium-substituted plinabulin, as a potent anti-microtubule agent for anticancer. Z. Ding, H. Cheng, S. Wang, Y. Hou, J. Zhao, H. Guan, **W. Li**

MEDI **388.** β-Sheet propensity of competitive peptide inhibitor's residue is crucial in binding to proteases: PACE4 inhibitors as a case study. **V. Dianati**, A. Shamloo, A. Kwiatkowska, R. Desjardins, A. Soldera, R. Day, Y. Dory

MEDI **389.** Hepsin-targeted ligands for prostate cancer imaging and therapy. **Y. Byun**, S. Son, H. Kwon

MEDI **390.** X-ray crystallographic structures of teixobactin analogues. **H. Yang**, D.R. Du Bois, J.W. Ziller, J.S. Nowick

MEDI **391.** Withdrawn.

MEDI **392.** Long wavelength, orthogonal release of internalized anti-inflammatory compounds from cellular vehicles. **R.M. Hughes**, C. Marvin, Z. Rodgers, S. Ding, N. Oien, W.J. Smith, D.S. Lawrence

MEDI **393.** Amino acid and peptide conjugates are potential drug candidates. **S.S. Panda**

MEDI **394.** Withdrawn.

MEDI **395.** Directed immune responses via covalently linked TLR agonist combinations for a Q-fever vaccine. **T.J. Albin**, J. Tom, S. Manna, A. Gilkes, A. Jain, M. Supnet, H. Davies, A. Nalca, A. Burkhardt, P. Felgner, A.P. Esser-Kahn

MEDI **396.** Development of antidotes against nerve agent inhibited acetylcholinesterase – the transformation of an inhibitor into a reactivator. **C. Lindgren**, N. Forsgren, C. Akfur, L. Berg, D. Andersson, M. Hillgren, W. Qian, F. Worek, F. Ekström, A. Linusson

MEDI **397.** Generating site-specific antibody-drug conjugates with high drug to antibody ratios using a tandem Knoevenagel dondensation-Michael addition. **R. Kudirka**, R. Barfield, J. McFarland, P. Drake, A. Carlson, S. Banas, W. Zmolek, A. Garofalo, D. Rabuka

MEDI **398.** Synthesis of truncated tirandamycin A-D derivatives as new antihelminthic agents. **T. Jimenez**, M. Grotli, C. Wallentin

MEDI **399.** Beyond IC50 and simple PK models – considerations for discovery chemists. **R. Fraczkiewicz**, M.B. Bolger, W. Woltosz

MEDI **400.** Synthesis and evaluation of antitubercular agents 2-aminothiophenes and benzo-1,2-selenazol-3(2H)-ones targeting Pks13 and Ag85C respectively. **S. Thanna**, S.E. Knudson, C.M. Goins, F. Salem, S. Kapil, A. Grzegorzewicz, M. Jackson, D.R. Ronning, R.A. Slayden, S.J. Sucheck

‡ *Cooperative Cosponsorship*

MEDI **401.** Novel pyrimidine compounds as potent JAK inhibitors. **Y. Chen**, H. Li, R. Yen, T. Heckrodt, D. McMutrie, N. Lin, R. Singh, V. Taylor, M. Chan, E. Masuda, G. Park, D. Lau, D. Payan

MEDI **402.** Synthesis and evaluation polythiophene containing rhodamine dyes for biological and photochemical applications. **M.K. Linder**, J.N. Nasca, K.S. Gast, G. Sawada, D. Watson, M.R. Detty

MEDI **403.** Synthesis of β-configured clickable [$^{18}$F]FDGs as novel $^{18}$F-fluoroglycosylation tools for PET *in vivo* imaging. **M. Elgland**, P. Nordeman, T. Fyrner, P. Konradsson, G. Antoni, P. Nilsson

MEDI **404.** Small-molecule anti-virulence agents for the prevention of dental biofilms. **B. Nijampatnam**, H. Wu, S.E. Velu

MEDI **405.** Discovery of novel pyrrolomycins as potential anticancer agents. **Y. Liu**, T. McGuire, Z. Yang, D. Coulter, Y. Chhonker, D. Murry, J. Sharp, H.A. Zhong, **R. Li**

MEDI **406.** Design and synthesis of small molecule inhibitors bearing 1,2,3-triazole/sulfonate pharmacophore from natural precursors for the treatment of bacterial infections. **B. Aneja**, S. Alam, M. Azam, A. Perwez, R. Haque, M. Rizvi, R. Maguire, K. Kavanagh, U. Yadava, C. Daniliuc, A. Azam, A. Mohammad

MEDI **407.** New N-substituted indazole-5-carboxamides as subnanomolar, selective monoamine oxidase B and dually active MAO-A/B inhibitors with BBB and GI permeability. **M. Gastreich**, C. Detering, L. Antonov, S. Hristova, H. Stammler, N.T. Tzvetkov

MEDI **408.** Withdrawn.

MEDI **409.** Glycosylated porphyrins for use in PET and PDT: Synthesis and characterization. **K. Arja**, M. Elgland, P. Nilsson

MEDI **410.** Selective nicotinic acetylcholine receptor activities from the areca nut. **N. Horenstein**, C. Stokes, R. Papke

MEDI **411.** Withdrawn.

MEDI **412.** Differentiating antiproliferative and chemopreventive modes of activity for electron-deficient aryl isothiocyanates against human MCF-7 cells. **J.R. Mays**

MEDI **413.** Application of the boronic acid as an isostere of the phenolic hydroxyl group in optimization of Selective Estrogen Receptor Downregulators (SERDs). **J. Liu**, S. Zheng, S. Guo, Q. Zhong, M. Bratton, T.E. Wiese, G. Wang

MEDI **414.** Withdrawn.

MEDI **415.** Substituted acylsulfonamides as surrogates of a terminal carboxylic acid: More effective small-molecule blockade of the Mcl-1 oncoprotein. **M.E. Lanning**, S. Fletcher

MEDI **416.** Novel class of substituted phenoxyacetamide derivatives as serotonin reuptake inhibitors and serotonin autoreceptor antagonists for repetitive behavior modulation in autism spectrum disorder. V.M. Gancarczyk, J. Dhuguru, A. Khalil, **O.M. Ghoneim**

MEDI **417.** Polymersomes for targeting and eradicating intracellular parasites. **L. Rizzello**, J. Robertson, P. M. Elks, T. McHugh, S. A. Renshaw, G. Battaglia

MEDI **418.** Two-in-one approach to modulate repetitive behaviors in autism spectrum disorder: N-arylpieprazines as key motifs towards developing bi-functional serotonergic ligands. **O.M. Ghoneim**

MEDI **419.** Zinc(II)-dipicolylamine coordination complexes are strongly active against cutaneous leishmaniasis. **M. Betancourt**, D. Rice, P. Vacchina, B. Norris-Mullins, M.A. Morales, B.D. Smith

MEDI **420.** Peptide-based nanosponges. **S.H. Bossmann**, H. Wang, A.S. Yapa, S.O. Wendel, N. Kariyawasam, T.B. Shrestha, M. Pyle, P.E. Smith, D.L. Troyer

MEDI **421.** Heterocyclic mimetics of crinine alkaloids – Novel scaffolds against drug-resistant cancer cells. **L.V. Frolova**

MEDI **422.** Characterization of histone lysine methyltransferase and discovery of NSD2 inhibitors. **J. Kwiatkowski**, A. Hung, Y. Tan, N. Ahmad, G. Lin, A. Ngo, Y. Li, H. Ng, J. Wee, X. Koh-Stenta, P.Z. Kwek, E.H. Ong, J.K. Joy, A. Poulsen, C. Kang, J. Hill, T.H. Keller

MEDI **423.** Computational rationalisation of ligand specific T-cell activation by the lipid presenting proteins CD1b and CD1c: Different means to the same end? **C. Cave-Ayland**, A. Chancellor, I. Tews, S. Mansour, C. Skylaris, J.W. Essex

MEDI **424.** Pharmacophore construction of Cyclooxygenase-2 (COX-2) selective inhibitors based on QSAR models. R.A. Gomes, G.L. Luiz Genesi, V.G. Maltarollo, **G.H. Trossini**

MEDI **425.** Perturbing dissimilar biomolecular targets from natural product scaffolds and focused chemical decoration. **J. Nielsen**, **T. Tung**, T. Holm Jakobsen, T. Dao, A.T. Fuglsang, M. Givskov, S.B. Christensen

MEDI **426.** Design of novel GPCR family-targeted scaffolds: Synthetic and cheminformatic exploration of novel medicinal chemistry space. **J.C. Benningshof**, G. Müller, T. Berkenbosch, D. Stumpfe, J. Bajorath

MEDI **427.** Synthesis and biological evaluation of C24 20*S*(OH)D3 analogs as anti-inflammatory agents. **Z. Lin**, S. Marepally, E. Goh, C.Y. Cheng, A.E. Postlethwaite, Z. Janjetovic, T. Kim, A.J. Slominski, R.C. Tuckey, N. Rochel, D.D. Miller, W. Li

MEDI **428.** Multi-omic approach to unraveling the microbial ecology of *Euphorbia* plant latex. M. Gunawardana, E. Hyde, S. Rivera, S. Webster, A. Castonguay, M. Anderson, S. Lahmeyer, B. Dorsey, T. La Val, D. VanderVelde, P. Webster, R. Knight, **M.M. Baum**

MEDI **429.** Discovery of novel indolinone derivatives as potent MELK inhibitors. **R. Edupuganti**, J.M. Taliaferro, Q. Wang, X. Xie, E.J. Cho, V. Sharma, P. Ren, C. Bartholomeusz, E.V. Anslyn, K.N. Dalby

MEDI **430.** Sphingosine analogues as inhibitors of Sphingosine Kinase (SK1). A. Cardona, M. Escudero-Casao, M. Corro, J. Hernandez, Y. Diaz, I. Matheu, S. Garcia-Vallve, M. Mulero, G. Pujadas, **S. Castillon**

MEDI **431.** Biological screening of *Moringa oleifera* for cytotocixity and antitumor activities. **E.P. Rodriguez**, C.A. Ospina

MEDI **432.** Design of a nucleic acid aptamer to achieve localization of a ROS-activated anti-cancer agent. **K.G. Earnest**, E.J. Merino

MEDI **433.** Exploring the binding site of GPR119 receptor inverse agonists. **E. Kotsikorou**, **S. Kowalski**

MEDI **434.** Methicillin-resistant *Staphylococcus aureus* becomes vulnerable to β-lactam antibiotics when in combination with branched polyethylenimine. **M. Foxley**, M. Xiao, S. Wright, S. Strange, A. Lam, K. Grogan, C.V. Rice

MEDI **435.** Old and new privileged scaffolds for medicinal chemistry. **P. Schneider**, G. Schneider

MEDI **436.** Vienna LiverTox Workspace: Towards predicting liver toxicity. **F. Montanari**, E. Kotsampasakou, B. Knasmüller, M. Pinto, M. Grandits, L. Richter, G.F. Ecker

MEDI **437.** Pyrrole-based antitubulin agents at the colchicine site: SAR of C-5 analogues in explicitly solvated models. **A.J. Obaidullah**, C.C. Rohena, J.A. Sikorski, S. Mooberry, J.T. Gupton, G.E. Kellogg

MEDI **438.** Design, synthesis, and biological evaluation of small molecule Gi$\alpha$2-androgen inhibitors in prostate cancer therapy. **S. Tapadar**, S. Caggia, S. Khan, A.K. Oyelere

MEDI **439.** Synthesis of GRB2 SH2 domain inhibitors: Analogues of sclerotiorin. **J.J. Gladfelder**, C. Arpin

MEDI **440.** Phytoestrogens: New ligands targeting the estrogen receptor domains. **V.J. Thakor**, M. Noolvi

MEDI **441.** Structure-based design of macrocyclic tetrapeptides intended to modulate the opioid receptors. **M.J. Ferracane**, J.V. Aldrich

MEDI **442.** MOEsaic: Making SAR analysis easier through the use of matched molecular pairs and R-group profiling. **A. Ajamian**

MEDI **443.** In search of AKT inhibitors as anticancer agents, an in silico approach. **P.J. Trejo**, A. Hernandez Campos, A. Romo-Mancillas, J.L. Medina-Franco, R. Castillo-Bocanegra

MEDI **444.** Design, synthesis and biological evaluation of Liver X Receptor (LXR) ligands. **R. Komati**, K.M. Lamark, K.A. Payne, M. Ndukwe, D. Spadoni, J. Sridhar, K. Riley

MEDI **445.** Amido phthalimides as CDKs and VEGF inhibitors. **R. Komati**, V.C. Miles, M. Ismail, F. Joseph, H. McFerrin, J. Sridhar

MEDI **446.** Withdrawn.

MEDI **447.** Discovery of Lu AF64196 a highly ligand efficient, brain penetrant and selective PDE1 inhibitor. **L.K. Rasmussen**, M. Langgard, C.T. Christoffersen, J. Nielsen, C. Bundgaard, J. Kehler

MEDI **448.** Repurposing for G-protein couple receptors by structure-based discovery: Transformation of adenosine derivatives into $5HT_{2B}$/$5HT_{2C}$ serotonin receptor antagonists. **D. Tosh**, A. Ciancetta, E.P. Warnick, S. Crane, Z. Gao, K.A. Jacobson

MEDI **449.** Discovery of highly selective Itk inhibitors with *in vivo* IL-2 inhibition. **S. Takai**, H. Takeda, A. Watanabe, K. Tsuboi, R. Suzuki, A. Hiramatsu, Y. Iyoda, T. Inukai, A. Kinoshita, H. Kohno, B. Liu, R. Shetty, K. Moriarty, M. Kurono, S. Umemura, H. Egashira, J. Zou, Z. Konteatis, R. Omi, H. Namboodiri, W. Sawada, M. Murata, T. Koike, R. Komaki-Nishikawa, N. Yada, T. Yoshizawa, J. McCool, M. Bukhtiyarova, M. Kelly, J. Takeuchi

MEDI **450.** Decoupling proton motive force to overcome antibacterial resistance. **J. Buonomo**, C.C. Aldrich

MEDI **451.** Adverse drug reactions triggered by the common HLA-B*57:01 variant: Virtual screening of DrugBank. **G. Van Den Driessche**, D. Fourches

MEDI **452.** Optimization of 4(1*H*)-quinolone antimalarials for oral bioavailability and in vivo efficacy. **C. Lichorowic**, J.R. Maignan, R. Neelarapu, A. Monastyrski, J.V. Giarrusso, T. Mutka, L. Blake, D. Casandra, A. LaCrue, D. Kyle, R. Manetsch

MEDI **453.** Design of inhibitors for the human papillomavirus E6 protein. **D.P. Petrov**, V.J. Davisson, E. Androphy, A. Rietz

MEDI **454.** Scaffold replacement and 3D ligand optimization applied to the discovery of tyrosine kinase inhibitors. **A. Deschenes**

MEDI **455.** Discovery of the first low-molecular-weight *Mycobacterium tuberculosis* MabA (FabG1) inhibitors using a fragment-based approach. C. Pintiala, M. Moune, K. Bourbiaux, R. Frita, K. Djaout, C. Piveteau, B. Deprez, A. Baulard, N. Willand, **M. Flipo**

MEDI **456.** Structure-based, in molecular design and synthesis of inhibitors of protein kinase family of receptors of epidermal growth factor. **A.S. Bunev**, E.V. Sukhonosova, G. Lisnik, N. Yabbarov, G. Ostapenko

MEDI **457.** *In vivo* structure-efficacy studies of regioisomeric artemolane-like endoperoxides. **B.R. Blank**, J. Gut, P.J. Rosenthal, A.R. Renslo

MEDI **458.** Optimization of peptide substrates for conjugate modification of macromolecular mediated RNAi delivery. **J.C. Carlson**, J. Benson, A.V. Blokhin, D. Rozema, A. Sokoloff

MEDI **459.** Impact of activation of GPR68 by metal cations on high throughput screening. **C. Wang**, S. Lin, L.D. Fader, A. Granger

MEDI **460.** Synthesis of 1,2,4-substituted imidazoles for a fragment-based drug discovery library. **T. Lafferty**, J. Patrone

MEDI **461.** Identification and optimization of 5-aryl benzimidazolones as AMPA receptor negative modulators selective for TARP-γ8. **S. Ravula**, **M. Ameriks**, **B.M. Savall**, **J.M. Ziff**, **B.T. Shireman**, **M.J. Seierstad**, **N. Wu**, **B. Lord**, **M. Maher**, **N.I. Carruthers**, **T.W. Lovenberg**

MEDI **462.** Design and synthesis of L-neplanocin analogues as antiviral agents. **Q. Chen**, C. Liu, S. Schneller, **A. Davidson**, **M. Stout**

MEDI **463.** Targeted isolation and simplified structure elucidation of new analogues of dolastatin 10 from marine cyanobacteria using MS/MS molecular networking. **B. Naman**, J. Almaliti, L. Keller, A. Remmel, E. Glukhov, P.C. Dorrestein, W.H. Gerwick

MEDI **464.** MELK as a valid cancer therapeutic target? From virtual screening to highly selective in vivo tool compounds. **S. Mathieu**, B. Toure, J. Giraldes, T. Smith, E. Sprague, Y. Yang, Z. Chen, Y. Mishina, Y. Feng, Y. Yan-Neale, D. Chen, M. Meyer, C. Straub, D. Sage, K. Wright, X. Chen, S. Kim, E.J. Martin, K. Hurov

MEDI **465.** P(NIPAM) microgel embedding p(AAm) hydrogel interpenetrating polymer networks for controlled drug delivery vehicles. **N. Sahiner**, A. Yasar, F. Onder, M. Ay

MEDI **466.** Evaluation of antimicrobial properties of *Combretum laxum* extracts. **J.G. Escobar**, **I. Maldonado**, **A.K. Addo-Mensah**

MEDI **467.** Development of a new class of fluorophores and their applications as biological imaging agents and chemical sensors. **J.R. Zimmerman**

MEDI **468.** Inhibition of pilocarpine-induced fluid secretion by ethylatropine bromide. **T. Ganesh**, A. Rojas, A. Walker, R. Dingledine

MEDI **469.** Structure-Based Drug Design (SBDD) of allosteric inhibitors for HSC-70 using a combination of pharmacophore searching with ZINCPharmer and AutoDock Vina molecular docking. **C.C. Clement**, J. Gonzalez, M. Philipp

MEDI **470.** Bioguided fractionation and isolation of chemical constituents of the chloroform extract from the Puerto Rican plant *Simarouba tulae*. **C.A. Ospina**, P. Vivas, E. Hernandez

MEDI **471.** Synthesis of amino derivatives of dehydroleucodine and dehydroparishin-B as potential anti-proliferative against breast cancer and B16 melanoma cells. **A. Sanchez**, M. Veisaga, S.F. Wnuk, M. Barbieri, L.A. Lopez

MEDI **472.** Design and evaluation of cyclic peptides containing arginine, lysine and tryptophan residues as a cellular drug delivery system and establishing structure-activity relationship. S. Mozaffari, N. Sadeghiani, R. Tiwari, **K. Parang**

MEDI **473.** Design, synthesis and evaluation of potent inhibitors of PARP-14/ARTD8, a mono-ADP-ribosyltransferase. **M. Meyers**, **K. Upton**, A. Thorsell, H. Schuler, D. Ferraris



MEDI **474.** Design, synthesis, and evaluation of potent DNA-alkylating agents for use in Antibody-Drug Conjugates (ADCs). **K.E. Archer**, E.E. Reid, M. Shizuka, A. Wilhelm, N.C. Yoder, C. Bai, N. Fishkin, M. Bogalhas, P. Salomon, L. Harris, E.K. Maloney, O. Ab, R.V. Chari, M.L. Miller

MEDI **475.** Improved trifluoromethylation via organic electrochemistry. **J. Chen**, J. Starr

MEDI **476.** R996, an orally-bioavailable and selective activator of nuclear factor (erythroid-derived 2)-like 2 (Nrf2), is active in a Murine model of multiple sclerosis. **M.A. Duncton**, A. Owyang, F. San Pablo, A. Torneros, G. Park, D. Lau, E. Masuda, D. Payan, R. Singh

MEDI **477.** New small molecule inhibitors of Ghrelin O-acyltransferase. **J.D. Chisholm**, N.S. Mahajani, K.R. McGovern-Gooch, A. Garagozzo, A.J. Schramm, L.G. Hannah, M.A. Sieburg, J. Hougland

MEDI **478.** Fused imidazole derivatives as TGF-β inhibitors. **J. Yu**, I.S. Darwish, M. Gelman, R. Ding, A. Friera, G. Godinez, W. Lang, W. Li, K. McCaughey, J. McLaughlin, H. Nguyen, I. Smith, K. White, G. Yam, T. Kinsella, V. Taylor, S. Braselmann, C. Lamagna, E. Masuda, H. Ren, L. Chou, G. Park, R. Basile, B. Samant, D. Sweeny, M. Standlee, D. Lau, A. Torneros, F. San Pablo, G. Clemens, D. Payan, R. Singh

MEDI **479.** Fused pyrazole derivatives as TGF-β inhibitors. **I.S. Darwish**, J. Yu, M. Gelman, R. Ding, A. Friera, G. Godinez, W. Lang, W. Li, K. McCaughey, J. McLaughlin, H. Nguyen, I. Smith, K. White, G. Yam, T. Kinsella, V. Taylor, S. Braselmann, C. Lamagna, E. Masuda, H. Ren, L. Chou, G. Park, R. Basile, B. Samant, D. Sweeny, M. Standlee, D. Lau, A. Torneros, F. San Pablo, G. Clemens, D. Payan, R. Singh

MEDI **480.** Collaborative web-based architecture for fragment-based drug discovery data. **W.W. Smith**, B.A. Bunin

MEDI **481.** Planar aryl triazenes inhibit cytochrome P450 1A1 and 1B1 as a potential means to prevent cancer. **R. Nakamura**, **R. Moran**, **R.A. Isovitsch**, **D.S. Iimoto**

MEDI **482.** Discovery of BPR1K871 – a quinazoline based multi-kinase inhibitor for the treatment of AML and solid tumors: Rational design, synthesis, in vitro and in vivo evaluation. **H. Hsieh**, W. Wang, H. Shiao, Y. Ke, W. Lin, J. Hsu, C. Chen, T. Yeh

MEDI **483.** Novel approaches to the chemical synthesis of haloindoles for the development of ergot alkaloids compounds. **G. Ren**, E.J. Parish, D. Ren, Y. Lo, **H. Honda**

MEDI **484.** Novel approaches to the structure activity relationship study of citronellol type compounds useful as enzyme inhibitors. E.J. Parish, **L. Lv**, G. Ren, Y. Lo, **H. Honda**

MEDI **485.** Novel approaches to the synthetic study of lanost-8-en-3ß-ol-7,11-dione, an inhibitor of cholesterol biosynthesis. **G. Ren**, E.J. Parish, Y. Lo, **H. Honda**

MEDI **486.** Second generation inhibitors of *Porphyromonas gingivalis* biofilm formation. **F.A. Luzzio**, P.C. Patil, D.R. Demuth, J. Tan

MEDI **487.** Preparative method development from analytical columns. **J.E. Silver**, R.L. Lewis, F. Nancy, L.M. Esther

MEDI **488.** Synthesis of organic azides via flow chemistry. **J.E. Silver**, L.M. Esther, R.L. Lewis, F. Nancy

MEDI **489.** Development and screening of new cathepsin D inhibitors. **R. McConnell**, K. Malayala, K. Yarlagadda, K. Sayyar, C. Trana, W. Godwin, L. Wen

MEDI **490.** Greener reversed-phase flash chromatography using acetone instead of acetonitrile. **J.R. Bickler**

MEDI **491.** Acetonitrile as a replacement for methanol in normal-phase flash chromatography. **J.R. Bickler**

MEDI **492.** NCI/NExT discovery HTS resources: Oncology Interrogation Tools Library. **R.N. Misra**, M. Eckert, C.R. Johnson, C. Laggner

MEDI **493.** Synthesis and solubility determination of a highly water soluble phosphonooxymethyl prodrug. **R. Castillo-Bocanegra**, J. Victoria-Miguel, A. Hernandez Campos, H. Jung-Cook

MEDI **494.** Inhibition of *Candida albicans* biofilm formation with biaryl amides. **D.A. Hinojosa**

MEDI **495.** Center for innovative in drug discovery collaborative programs: Structure based drug design, synthesis and evaluation of new antischistosomal agents. **R. Tarpley**

MEDI **496.** Fragment based drug discovery of allosteric FAK inhibitors. **O. Cossio**, R. Campos-Olivas, C. Santiveri Martín-Varés

MEDI **497.** Discovery of novel small molecule inhibitors of oncoprotein EYA2 for breast and ovarian cancers. **B. Campos**, S.F. McHardy, A. Lopez, H. Wang, **D. Wilson**, **D. Wristers**, R. Li, Y. Bin, S. Smith, S. McCowen

MEDI **498.** Synthesis of N-functionalized chiral 3-hydroxyphenylpyrrolidines and their evaluation as selective $D_3$ receptor ligands. **A. Omran**, S. Eslamimehr, A.M. Crider, W.L. Neumann

MEDI **499.** Anti-cancer drug discovery efforts target two kinases on the non-canonical NF-κB pathway. **G. Chan**, O. Demir, G. Ghosh, R.E. Amaro

MEDI **500.** Novel mitochondrial complex I inhibitors for anti-cancer therapeutics. **J. Holmes**, K. Damera, J. Yancey, M. Zhu, N. Devi, S. Kaluz, E. Van Meir, B. Wang

MEDI **501.** Efforts to expand our antibiotic arsenal to eradicate persistent bacterial biofilms. **R. Huigens**

MEDI **502.** Design, synthesis, and biological evaluation of heteroaryl amine derivatives for anticancer activity. **M. Besan**, R. Srivastava, S. Srivastava

MEDI **503.** Luminescent Conjugated Oligothiophenes (LCOs) for detection and characterization of disease-associated protein aggregates and cells. **M. Bäck**

MEDI **504.** Drugging the undruggable with MCR scaffold manifold: The design and synthesis of covalent inhibitors and macrocycles. **T. Zarganes-Tzitzikas**, P. Patil, A. Doemling, K. Neochoritis

MEDI **505.** Synthesis of novel agents for the treatment of neurodegenerative diseases. **B.J. Eduful**, J. Leahy, D. Kang, M. Chin, A. Rashedi, O. Jallow

MEDI **506.** Withdrawn.

MEDI **507.** Artificial macrocycles by multicomponent reactions. **A. Doemling**

MEDI **508.** Cocrystal of 5-fluorouracil with nicotinamide to improve its biopharmaceutical attributes using crystal engineering approach. **M.K. Gautam**, R. Chadha

MEDI **509.** Solving challenging structural motifs in natural products using concerted DFT modeling and 2-D INADEQUATE NMR. J.R. Powell, **T.M. McCullough**, R. Iuliucci, J.K. Harper

# NUCL

## Division of Nuclear Chemistry and Technology

**A. Hixon**, *Program Chair*

**OTHER SYMPOSIA OF INTEREST:**

**Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution** (see *GEOC,* Wed)

**Frontiers in Heavy Element Electronic Structure** (see *INOR,* Wed)

**Hollyweird Chemistry** (see *CPRC,* Sun, Mon)

**I&EC Division Early Career Fellow Symposium: Honoring Dr. Leigh Martin** (see *I&EC,* Wed)

**Lanthanide & Actinide Chemistry** (see *INOR,* Sun, Tue, Wed, Thu)

**SOCIAL EVENTS:**

**Social Hour,** 6:00 PM: Tue

**BUSINESS MEETINGS:**

**Executive Committee Meeting (Closed),** 5:00 PM: Sun

**Business Meeting,** 5:00 PM: Tue

## SUNDAY MORNING

### Section A

Moscone Center

Esplanade Ballroom 301

### Nuclear Fission

R. S. Rundberg, *Organizer*

T. A. Bredeweg, *Organizer, Presiding*

**9:00** Introductory Remarks.

**9:05** NUCL **1.** Total kinetic energy release and fission product mass distributions in the fast neutron induced fission of $^{235}$U, $^{232}$Th, $^{239}$Pu and $^{233}$U. **W. Loveland**

**9:40** NUCL **2.** U-235 fission mass yield dependence on resonance and neutron energy. **R.S. Rundberg**, T.A. Bredeweg, M. Koehl, J. Braley

**10:15** NUCL **3.** Energy dependence of fission product yields for $^{235}$U, $^{238}$U, and $^{239}$Pu with monoenergetic neutrons between thermal and 14.8 MeV. **M. Gooden**, T.A. Bredeweg, M.M. Fowler, D.J. Vieira, J. Wilhelmy, A. Tonchev, M.A. Stoyer, M. Bhike, F. Krishichayan, W. Tornow

**10:50** Intermission.

**11:10** NUCL **4.** Theory of fission-fragment angular distributions. **W. Younes**

**11:45** NUCL **5.** Survival of excited nuclei produced in warm fusion reactions. **C.M. Folden**

‡ *Cooperative Cosponsorship*