Section G

Pennsylvania Convention Center
Hall D

Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals

N. S. Radu, *Organizer*

5:30 - 7:30

INOR **683.** Synthesis and investigation of macrocyclic Cr(III)-acetylide complexes: Emission properties and electron delocalization. **E. Judkins**, S.F. Tyler, T. Ren

INOR **684.** Synthesis and reactivity of molybdenum carbon dioxide complexes. **M. Graziani, L. Briggs, G.R. Lorzing, J.R. Vasta, M. Pogash, X. Duan, P.M. Graham**

Section H

Pennsylvania Convention Center
Hall D

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

5:30 - 7:30

INOR **685.** Synthesis, characterization, and photophysical properties of hybrid N-heterocyclic carbene complexes of copper. **L. Tahsini**, K. Moseni

INOR **686.** Synthesis and characterization of novel bis- and tris-cyclometalated iridium (III) complexes for potential use in OLED applications. **D.A. Laviska, R. Markese, A. Morris, F. Renner, T. Schreiber**

INOR **687.** Functionalized imidazole-based weakly coordinating anions paired with cationic transition metal catalysts. **D.I. Wozniak, A. Hicks, G. Dobereiner**

INOR **688.** Synthesis and reactivity of phosphine ligated palladium(II) (Ar)(CF_3) complexes. **D. Ferguson, J.R. Bour, M.S. Sanford**

INOR **689.** Accessibility and isolation of organometallic Ni^{IV} complexes using a diverse set of oxidants. **E.A. Meucci, N. Camasso, M.S. Sanford**

INOR **690.** Synthesis, characterization, and photophysical properties of platinum complexes containing benzothiophene-derived ligands. **C.M. Anderson, L.M. Duman, M.A. Weinstein, N. Oh, A. Hashmi, J. Tanski**

INOR **691.** Synthesis of high-valent nickel complexes supported by electron rich CCC pincer ligand platform. **C. Ocampo, G. Espinosa Martinez, A.R. Fout**

INOR **692.** Withdrawn.

INOR **693.** Exploring cooperative redox chemistry using iron dipyrrin pacman complexes. **E.J. Johnson, C. Kleinlein, T. Betley**

Technical program information known at press time. The official technical program for the 252nd ACS National Meeting is available at: www.acs.org/Philadelphia2016

‡ *Cooperative Cosponsorship*

MEDI

Division of Medicinal Chemistry

W. Young, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Merck Research Award Symposium (see *WCC*, Sun)

Effectively Harnessing the World's Literature to Inform Rational Compound Design (see *CINF*, Sun)

Chemistry For the People: Reflections from Perkin Medalists (see *CHED*, Mon)

SOCIAL EVENTS:

Hall of Fame Reception, 5:30 PM: Tue

BUSINESS MEETINGS:

MEDI Executive Meeting (Closed), 8:30 AM: Sun

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

SUNDAY MORNING

Section A

Pennsylvania Convention Center
Room 114

Renaissance of Estrogen Receptor-Based Therapy

S. Peukert, X. Wang, *Organizers*, *Presiding*

8:30 MEDI **1.** SERMs and SERDs as the cornerstone of endocrine therapy in ERα-positive breast cancer. **D. McDonnell**, K. Cocce, S. Wardell, J. Norris

9:10 MEDI **2.** Benzothiophene SERMs, SERDs, MERDs, SEMs, and ShERPAs in endocrine-independent ER+ breast cancer therapy. **G.R. Thatcher**, D.A. Tonetti, R. Xiong, H. Patel

9:45 MEDI **3.** GDC-0810: An orally bioavailable selective estrogen receptor degrader for breast cancer. **X. Wang**

10:20 MEDI **4.** Tetrahydroisoquinolines as selective estrogen receptor degraders with good oral bioavailability in preclinical species. **H. Burks**

10:50 MEDI **5.** Fifty shades of SERD: Designing and characterizing selective estrogen receptor degraders towards clinical candidates. **C. De Savi**, J.S. Scott, S.L. Degorce

Section B

Pennsylvania Convention Center
Room 113C

General Orals

W. B. Young, *Organizer*

J. B. Schwarz, *Presiding*

8:30 MEDI **6.** Structure-activity studies of IspD-targeting antimalarials related to MMV008138. Z. Yao, M. Ghavami, R. Elahi, M.E. Simpson, E.F. Merino, M.M. Totrov, M.B. Cassera, **P.R. Carlier**

8:50 MEDI **7.** Structure-activity relationship studies of the lipophilic tail region of indole derived sphingosine kinase 2 inhibitors. **M. Congdon**, Y. Kharel, K.R. Lynch, W. Santos

9:10 MEDI **8.** Discovery of the first subfamily-selective inhibitor of FTO for novel treatment of obesity and related metabolic syndrome. **E.C. Woon**, E. Tai, S. Toh, M. Liu, T. Song, M. Agrawal, W. Goh

9:30 MEDI **9.** Discovery of a novel binder of Lp-PLA_2 and subsequent optimization through rational target design. **J.E. Pero**, S. Aravapalli, V. Berdini, J. Coyle, P. Day, A. Dodson, P. Grondin, F. Holding, L. Lee, P. Li, E.S. Manas, J.P. Marino, A. Martin, B. McCleland, R. McMenamin, C. Murray, C. Neipp, L. Page, V. Patel, F. Potvain, S. Rich, R.A. Rivero, K. Smith, D. Somers, L. Trottet, R. Velagaleti, G. Williams, A. Woolford, R. Xie

9:50 MEDI **10.** Synthesis and biological characterization of a novel PTP4A3 inhibitor. **J.M. Salamoun**, K.E. McQueeney, E.R. Sharlow, J.S. Lazo, P. Wipf

10:10 MEDI **11.** Discovery of potent, selective, CNS-penetrant potentiators of glycine receptors. **E. DiMauro**

10:30 MEDI **12.** Isoform selective AMPK activators. **K.O. Cameron**

10:50 MEDI **13.** Discovery of the potent and selective pyridine M_1 PAM PF-06767832: Evaluation of efficacy and cholinergic side effects. **J.E. Davoren**

11:10 MEDI **14.** Discovery of a novel series of aminopyrazine-based A2a antagonists for the treatment of Parkinson's disease: Integration of an intramolecular H-bonding strategy in the design of brain-penetrant scaffold. **R. Kuang**, H. Wu, A. Ali, P.C. Ting, S.M. Levi, M.M. Lo, E. Metzger, T.J. Henderson, Y. Lim, Q. Deng, H. Wang, Y. Yu, R. Anand, K. Dykstra, T. Pereira, S.W. Krska, R. Hodgson, L. Hyde, E. Parker, D. Mullins, D.B. Prelusky, R.G. Aslanian, A.W. Stamford

11:30 MEDI **15.** Design and synthesis of a potent, reversible covalent, Oxaborininol inhibitor of Lp-PLA_2. **S. Hart**, V. Berdini, E.E. Boros, N. Curtis, P. Day, A. Daugan, N.E. Faucher, M. Fouchet, P. Grondin, I. Kaldor, W. Kerr, E.S. Manas, M. Mitchell, V. Patel, D. Somers, E. Talbot, M. Toczko, L. Trottet, G. White, A. Woolford

11:50 MEDI **16.** Discovery of 4-undecylpiperidine-2-carboxamides as selective positive allosteric modulators of the serotonin (5-HT) 5-HT_{2C} receptor. **E.A. Wold**, C. Wild, C. McAllister, C. Crawford, Y. Ding, N.C. Anastasio, R.G. Fox, S. Stutz, R.M. Hartley, H. Chen, M.A. White, K.A. Cunningham, J. Zhou

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WCC Merck Research Award Symposium

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SUNDAY AFTERNOON

Section A

Pennsylvania Convention Center
Room 114

General Orals

W. B. Young, *Organizer*, *Presiding*

1:30 MEDI **17.** Balancing selectivity and safety in a MAP4K4 kinase inhibitor: Advancing potent, selective, and orally bioavailable leads to preclinical toxicity. **S.K. Bhattacharya**, S.W. Bagley, L. Buckbinder, A.A. Carlo, C. Cortes, R.L. Dow, A.F. El-Kattan, G.B. Freeman, C.R. Guimaraes, A. Skoura

1:55 MEDI **18.** Discovery and structure-activity relationships of BMS-820132, a potent partial glucokinase activator. **Y. Shi**, Y. Wang, W. Meng, R. Brigance, D. Ryono, S. Bolton, H. Zhang, S. Chen, R.A. Smirk, S. Tao, J.A. Tino, K. Williams, R. Sulsky, B.A. Ellsworth, M. Wong, J. Sun, L. Leith, D.Z. Sun, D. Wu, A. Gupta, R. Rampulla, A. Mathur, B. Chen, A. Wang, H. Fuentes, L. Kunselman, M. Cap, J. Zalaznick, X. Ma, H. Liu, J. Taylor, R. Zebo, B. Jones, S. Kalinowski, J. Swartz, A. Staal, K. Omalley, L.M. Kopcho, J. Muckelbauer, C. Chang, S.R. Krystek, S. Spronk, J. Marcinkeviciene, G. Everlof, X. Chen, C. Xu, R. Langish, Y. Yang, Q. Wang, K. Behnia, A. Fura, E. Janovitz, N. Pannacciulli, S. Griffen, B. Zinker, J. Krupinski, M. Kirby, J. Whaley, R. Zahler, J.C. Barrish, J.A. Robl, P.T. Cheng

2:20 MEDI **19.** Discovery of ubrogepant (MK-1602): A potent, selective and orally bioavailable CGRP receptor antagonist for the acute treatment of migraine. **M.E. Fraley**

2:45 MEDI **20.** Discovery of AZN001: A broad-spectrum capsid-binding human rhinovirus inhibitor. **M.A. Cornebise**, J. Atherton, S. Bist, S. Butler, T.P. Grebe, M. Hentemann, J. Huang, K.D. Johnson, S.P. Kawatkar, C. McCrea, L. Martin, M. Mondal, M. Rooney, K. Thakur, C. Tiong-Yip, J. Wang, Q. Yu

3:10 MEDI **21.** Discovery of in vivo inhibitors of lactate dehydrogenase A (LDHA). **H.E. Purkey**

3:35 MEDI **22.** SAR evolution of C-17 amines triterpenoids leading to the discovery of the second generation HIV maturation inhibitor BMS-955176. **A. Regueiro-Ren**, Z. Liu, Y. Chen, N. Sin, S. Sit, J.J. Swidorski, J. Chen, B.L. Venables, Z. Juliang, B. Nowicka-Sans, T. Protack, Z. Lin, B. Terry, H. Samanta, S. Zhang, Z. Li, B.R. Beno, X. Huang, S. Rahematpura, D. Parker, R. Haskell, S. Jenkins, K. Santone, M. Cockett, M. Krystal, U. Hanumegowda, I.B. Dicker, N.A. Meanwell

4:00 MEDI **23.** Discovery of a first-in-class, potent, selective and orally bioavailable inhibitor of the p97 AAA ATPase (CB-5083). **H. Zhou**

4:25 MEDI **24.** Discovery of AZD2716: A novel, potent secreted phospholipase A2 (sPLA2) inhibitor for the treatment of coronary artery disease. **D. Pettersen**, F. Giordanetto, J. Sandmark, I. Starke, L. Larsson, E. Hurt-Camejo, P. Nordberg

4:50 MEDI **25.** Developing CDK8 inhibitors as tool compounds: A case study in lean decision making. **M. Koehler**, P. Bergeron, E.M. Blackwood, K. Bowman, K. Clark, J.R. Kiefer, M.L. McCleland, L. Salphati, S. Schmidt, J. Wu, M.H. Beresini, R. Firestein

Section B

Pennsylvania Convention Center
Room 113C

Role of Water in Ligand Design & Optimization

D. Shivakumar, A. Tebben, S. Wrobleski, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 MEDI **26.** Water, integral but often overlooked partner in protein-ligand binding. **G. Klebe**

2:20 MEDI **27.** Interacting with visible or not visible water molecules to gain potency and selectivity. **L. Schio**, H. Minoux, W. Sherman, D. Robinson

2:55 MEDI **28.** Water, water, everywhere, nor any space left to link? **P. Czodrowski**

3:30 MEDI **29.** Applying CSD- and PDB-derived binding hotspot analysis to water molecules to aid in ligand design. **C.J. Radoux**, P. Sanschagrin, E. Davis, W. Pitt

4:05 MEDI **30.** Water-centric methods in structure-based GPCR ligand design. **A. Bortolato**, J.S. Mason, F. Deflorian, B. Tehan, R. Smith, R. Cooke, A. Zhukov, F. Marshall

4:40 MEDI **31.** Navigating the ocean: Importance of understanding active site waters in drug discovery. **L. Frye**, R. Abel

5:15 Panel Discussion.

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Regional Small Chemical Businesses: Case Histories & Lessons Learned

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SUNDAY EVENING

Section A

Pennsylvania Convention Center
Hall G

General Posters

W. B. Young, *Organizer*

7:00 - 9:00

MEDI **32.** Transition of lipophilic imidazolium salts from *in vitro* to *in vivo* testing. **M. Southerland**, M. DeBord, N. Alexander, S.M. Paruchuri, L.P. Shriver, C. Wesdemiotis, C. Tessier, M. Panzner, W.J. Youngs

MEDI **33.** New bromodomain inhibitors with halogen bonding interactions. **A.S. Vincek**, E. Rusinova, J. Meslamani, A. Plotnikov, T. Zhou, M. Ohlmeyer, H. Long, K. Cheung, T. Shen, M. Zimmermann, F.M. Boeckler, M. Zhou

MEDI **34.** *N*-arylated 2-amino fused thiophene analogs as potential MEK5/ERK5 pathway inhibitors. **M. Gupta**, P.T. Flaherty, T. Wright, J. Cavanaugh

MEDI **35.** Utility of monomethyl auristatin (MMA) analogs as payloads for targeted therapies of cancer: Design and synthesis of MMAE and MMAF folate conjugates. **H.K. Santhapuram**, J.F. Vaughn, C.P. Leamon, I.R. Vlahov

MEDI **36.** Design and synthesis of *seco*-duocarmycin analogs as warheads in small molecule drug conjugates (SMDCs) for targeted cancer therapies. **G.L. Parham**, C.P. Leamon, I.R. Vlahov

MEDI **37.** Novel targets for small molecule drug conjugates: Design and synthesis of somatostatin analogs as targeting ligands and their conjugates with cytotoxic warheads. H.F. Klein, **F. You**, N. Zou, I.R. Vlahov

MEDI **38.** Design and synthesis of small molecule drug conjugates: Additional structural motifs. I.R. Vlahov, **N. Zou**, A. Felten, C.P. Leamon

MEDI **39.** Design, synthesis and early evaluation of hybrids of DNA minor groove binders and DNA-alkylating agents as warheads for small molecule drug conjugates (SMDCs) for targeted cancer therapies. I.R. Vlahov, **L. Qi**, S. Hahn, K.Y. Wang, H.K. Santhapuram, A. Felten, J.F. Vaughn, C.P. Leamon

MEDI **40.** Elucidating the binding mechanism of DAT inhibitors that result in abusable vs. non-abusable atypical DAT inhibitors. **B. Jean**, J.D. Madura, C.K. Surratt

MEDI **41.** Improved Grp94-selective inhibitors as therapies for glaucoma and metastasis. **V. Crowley**, B.S. Blagg

MEDI **42.** Discovery of anti-invasive tools and leads for the study and treatment of metastatic cancer: two case studies. **B.I. Roman**, S. Verhasselt, M.E. Bracke, C.V. Stevens

MEDI **43.** 3',4'-Dimethoxyflavonols: A new group of potential anti-prostate cancer agents. **X. Li**, G. Chen, X. Zhang, Q. Chen

MEDI **44.** Triazolopyrimidine derivatives as the first potent and selective inhibitors of the kinase GCN2. **D. Dorsch**, A. Wegener, G. Hölzemann, M. Busch, M. Calderini, O. Pöschke

MEDI **45.** Synthesis and development of new, potent ROCK inhibitors for the treatment of glaucoma. **J.M. Sturdivant**, S.M. Royalty, J.D. Yingling, C.L. Laethem, B. Sherman, G.R. Heintzelman, C.C. Kopczynski, M.A. deLong

MEDI **46.** Synthetic strategies for the generation of aliphatic and aromatic bis-imidazoles as carbonic anhydrase activators. **U.K. Mondal**, B. Draghici, J.P. Musco, M.A. Ilies

MEDI **47.** Synthesis and biological activity of triclosan based β-acetamido ketones. **A.B. Khade**, C.T. A, S.S. Kar, M. Tiwari, V. K.E., V.B. G, G.G. Shenoy

MEDI **48.** Discovery of BCL-3 inhibitor for the potential treatment of metastatic breast cancer. **C. Bordoni**, J. Soukupova, W. Yang, A.D. Westwell, R.W. Clarkson, A. Brancale

MEDI **49.** Aza-bodipy-steroid conjugates for fluorescence imaging. **S. Osati**, H. Ali, J.E. van Lier

MEDI **50.** Development of fused heterocyclic betulin conjugates as potential anti-cancer agents. S. Pathi, A. Patel, L. Solano, G. Jampana, T. Moosavi, **S.C. Jonnalagadda**

MEDI **51.** Synthesis of novel benzothiadiazole derivatives and their biological evaluation against the oncogenic SHP2 phosphatse. **W. Wang**

MEDI **52.** Design and synthesis of xanthone analogs based on α-mangostin analogs as new anti-cancer agents. **X. Fei**, S. Seo

MEDI **53.** Design, synthesis and evaluation of spiro[benzo[d][1,3] dioxine-2,1'-isobenzofuran] -3',4(1H)-dione derivatives as potential anticancer agents. **C. Yin**, Z. Chen, R. Stephani, V.L. Korlipara

MEDI **54.** Design and synthesis of 4-anilinoquinazoline-acylamino derivatives as VEGFR-2 inhibitors. **L. Sun**, H. Zhang, C. Zhang

MEDI **55.** Design of inhibitors for the human papillomavirus E6 protein. **D.P. Petrov**, V.J. Davisson, E. Androphy, A. Rietz

MEDI **56.** Synthesis and properties of curcumin conjugates as green cancer drug delivery system. **K. Punia**, C. Sun, S. Dolai, A. Mancuso, J.E. Fata, M. Castellanos, K.S. Raja

MEDI **57.** Breast cancer cell MDA viability of extracts from Taylor and Callahan counties of West-Central Texas plants: *Asclepias syriaca, Asclepias viridis, Solanum elaeagnifolium, Gaillardia pulchella,* and *Glandularia bipinnatifida*. **H. Shin**

MEDI **58.** Creating new from clinical agents: Discovery of combretastatin, a-4 inspired heterocycles as antitubulin anticancer agents. **N. Hura**, A. Shah, K. Guchhait

MEDI **59.** Synthesis and evaluation of benzamide and phenyl tetrazole derivatives with amide and urea linkers as BCRP inhibitors. **N. Gujarati**, L. Zeng, Z. Chen, V.L. Korlipara

MEDI **60.** Cytoxicity assay of *Combretum farinosum* extracts. **A.K. Addo-Mensah**, **E. Williams**

MEDI **61.** Computational studies of 2-phenyl indole inhibitors of p97 chaperone. **C. Lim**, J.C. Burnett, R. Gussio, D.M. Huryn, P. Wipf

MEDI **62.** Side chain optimizations of novel inhibitors of the AAA ATPase p97. **C. Alverez**, **M. Kovaliov**, M. Laporte, C. Lim, R. Colombo, Z. Yue, S. Bulfer, M. Arkin, D.M. Huryn, P. Wipf

MEDI **63.** Design and synthesis of heterocyclic inhibitors of the AAA ATPase p97. **M. LaPorte**, **M.J. Houghton**, R. Colombo, Z. Yue, C. Alverez, M. Kovaliov, C. Lim, L. Samankumura, Y. Yan, N. Green, W.J. Moore, B. Mroczkowski, S. Bulfer, J.R. Neitz, M. Arkin, D.M. Huryn, P. Wipf

MEDI **64.** Design and characterization of a mercaptophile library for screening cysteine-containing target. **C. Lim**, **T. Lewis**, **M. Liang**, A.J. Chatterley, Y. Tang, M. Arkin, D.M. Huryn, P. Wipf

MEDI **65.** 2-Phenyl indole piperazine inhibitors of AAA ATPase p97. **A.J. Chatterley**, E. Miller, C. Alverez, M. Kovaliov, C. Lim, R. Colombo, Z. Yue, M. LaPorte, L. Samankumura, S. Bulfer, M. Arkin, D.M. Huryn, P. Wipf

MEDI **66.** PEG-conjugated aromatic and heterocyclic sulfonamides as potent carbonic anhydrase inhibitors with anti-tumor activity. S. Akocak, **M.R. Alam**, A.M. Shabana, R.K. Sanku, H. Thompson, M.A. Ilies

MEDI **67.** Exploration of quinazoline derivates as MEK5 inhibitors. **P.T. Flaherty**, T. Wright, A. Motta, J. Cavanaugh

MEDI **68.** Prostate-specific membrane antigen targeted phosphoramidate-pronucleotides. **H. West**, S.C. Kumarapperuma, A. Hendricks, C.R. Wagner

MEDI **69.** Designing bispecific aptamers for increased stability in human serum. **G.E. Maio**, H. Zumrut, N. Van, S. Batool, P. Mallikaratchy

MEDI **70.** Structural requirements of histone deacetylase inhibitors: Suberoylanilide hydroxamic acid analogs modified at the C4 position display HDAC6 selectivity. **A.T. Negmeldin**, M.H. Pflum

MEDI **71.** Design, synthesis, and biological screening of novel CUCS-inspired estrone analogues towards treatment of hepatocellular carcinoma. **M. Mahnashi**, **S. Elgazwi**, **F.T. Halaweish**

MEDI **72.** Anti-tumor studies of N,N'-naphthylmethyl-2-alkyl and N,N'-quinolylmethyl-2-alkyl substituted imidazolium salts. **M. DeBord**, M. Southerland, A. Taraboletti, C. Tessier, S.M. Paruchuri, L.P. Shriver, M. Panzner, W.J. Youngs

MEDI **73.** Discovery of novel leucyl adenylate analogues as leucyl tRNA synthetase (LRS)-mediated mTORC1 inhibitors. **J. Lee**

MEDI **74.** Structure based design, synthesis, and study of potent and selective KDM5A/5B (JARID1A/1B) inhibitors. **Z. Nie**, L. Shi, C. Lai, S. O'Connell, J. Xu, R. Stansfield, J. Veal, J. Stafford

MEDI **75.** Regulation of neural stem cell proliferation and differentiation with molecules that stabilize nucleic acid secondary structure. **L. Fones**, **J. Cave**

MEDI **76.** Synthesis and biological evaluation of novel 6-substituted pyrrolo[2,3-*d*] pyrimidines with substituted nitrogen bridges as targeted antifolates. A. Gangjee, **L.K. Golani**, C.E. Dann, S. Deis, A. Wallace-Povirk, Z. Hou, L.H. Matherly

MEDI **77.** Inhibitors of the mitochondrial citrate transport protein for targeting lung cancer. **K. Kim**, S. Gadre, H. Fernandez, M. Girgis, A. Uren, M. Avantaggiati, M. Paige

MEDI **78.** Discovery and optimization of small molecule CSN5 inhibitors for the treatment of cancer. **E. Altmann**, B. Martoglio, M. Renatus, A. Schlierf, M. Schaefer, U. Hassiepen, K. Pfister, A.B. Jefferson, J. Quancard

MEDI **79.** Structure-activity and structure-toxicity relationships of 1,5-diarylpenta-1,4-dien-3-ones on prostate cell models. **M. Patanapongpibul**, X. Zhang, G. Ruiz, C. Chen, G. Chen, R. Wang, N. Subrahmanyam, J.Z. Keith, Q. Chen

MEDI **80.** Structure based design, synthesis and activity studies of small hybrid molecules as HDAC and G9a dual inhibitors. **M. Kondengaden**, L. Zang, P.G. Wang

MEDI **81.** *In silico* design and synthesis of novel thiourea and phenylsulfonyl-benzamide compounds as anti-prostate cancer agents. **M. Bassetto**, S. Ferla, A. Brancale, C. McGuigan

MEDI **82.** Exploiting biocatalysis for the production of novel cryptophycin anticancer agents. **J.J. Schmidt**, K.L. Bolduc, S.I. Brody, F.A. Valeriote, D.H. Sherman

MEDI **83.** Design, synthesis and evaluation antitumoral of quinazoline derivatives. **A.S. Matus-Meza**, M. Herrera-Martínez, P. Talamás-Rohana, F. Hernández-Luis

TECHNICAL PROGRAM

MEDI **84.** Discovery of indazole aldosterone synthase inhibitors as potential treatments for resistant hypertension. **S.B. Hoyt**, J.A. Taylor, C. London, A. Cooke, A. Ali, F. Ujjainwalla, J. Tata, M. Struthers, D. Cully, T. Wisniewski, N. Ren, C. Bopp, A. Sok, A. Verras, D.R. Mc Masters, Q. Chen, E. Tung, W. Tang, G. Salituro, J. Clemas, G. Zhou, R. Duffy, Y. Xiong

MEDI **85.** Discovery and structural development of novel natriuretic peptide receptor A (NPR-A) agonists. **T. Iwaki**, Y. Oyama, T. Tomoo, T. Tanaka, M. Sugiyama, A. Yamaki, M. Furuya

MEDI **86.** Design & synthesis of novel dihydropyrimidine derivatives as potential L- and T-type calcium channels blockers. **M.T. Ismail**, F. Zhang, O.H. Rizk, A.M. Farghaly, O.M. AboulWafa, G.W. Zamponi, H.T. Fahmy

MEDI **87.** ROCK kinase inhibitor prodrug to improve PK properties. **L. Wu**, Z. Chen, Y. Yao, X. Yang, D. Wu, Y. Li, R. Xu, J. Li, S. Chen

MEDI **88.** Reducing bleeding risks of anticoagulants through a novel partial inhibition approach. **D. Afosah**, S. Verespy, R.S. Boothello, R. Karuturi, U.R. Desai

MEDI **89.** Sulfonylated benzothiazole based inhibitors of endothelial lipase. **J. Johnson**, G. Tora, Z. Pi, M. Phillips, X. Yin, L. Abell, G. Locke, R. Yang, L. Zhao, A. Rose, K. Behnia, X. Chen, M. Galella, A. Chen, D. Taylor, H. Lu, M. Basso, C. Caporuscio, L. Adam, T. Kirchgessner, H. Finlay, R.R. Wexler

MEDI **90.** Discovery and optimization of novel chemotype $LpPLA_2$ inhibitors featuring a unique binding mode. **P. Li**, S. Aravapalli, A. Dodson, B. McCleland, E.S. Manas, J. Marino, C. Neipp, J.E. Pero, V. Patel, R.A. Rivero, C. Seath, D. Somers, R. Velagaleti, A. Woolford, R. Xie

MEDI **91.** Strategies toward structurally constrained diamide inhibitors of FXIa. **M.J. Orwat**, L. Smith, Y. Wang, S. Srivastava, W. Yang, K. Rossi, J. Luettgen, J. Bozarth, A. Wei, V. Ramamurthy, S. Sheriff, J. Myers, P. Morin, D. Seiffert, P.Y. Lam, R.R. Wexler, D. Pinto

MEDI **92.** Stat5 and chronic myeloid leukemia: Synthesis and biological evaluation of novel inhibitors. **L. Juen**, G. Prié, M. Viaud-Massuard, M. Brachet-Botineau, J. Bourgeais, F. Gouilleux

MEDI **93.** Monitoring the progression of structure-activity relationship information during lead optimization. **D. Dimova**, J. Bajorath

MEDI **94.** Design and synthesis of macrocyclic factor XIa inhibitor. **T. Fang**, J.R. Corte, H. Osuna, W. Yang, Y. Wang, Y.T. Jeon, K. Rossi, A. Rendina, J. Bozarth, S. Sheriff, J. Myers, T. Harper, Z. Lou, J. Zheng, J. Luettgen, D. Seiffert, P.Y. Lam, R.R. Wexler, M.L. Quan

Technical program information known at press time. The official technical program for the 252nd ACS National Meeting is available at: www.acs.org/Philadelphia2016

MEDI **95.** Structure-based design of novel RORgamma inverse agonists. **Y. Zheng**, **L. Jia**, J. Yuan, L.W. Dillard, L. Zhuang, K. Fan, C.M. Tice, C. Dong, A.P. Marcus, S.D. Lotesta, P. Noto, S. Meng, K. Lipinski, G. Kandpal, Y. Bukhtiyarov, Y. Zhao, D. Lala, J. Zhou, R. van Order, G. Chen, B.M. Mckeever, G. McGeehan, D.A. Claremon, S.B. Singh

MEDI **96.** Protease inhibitors from derivatives of tranexamic acid. **B.K. Bordoloi**, N. Sarma, R. Eisenberg

MEDI **97.** New small organic ligands for the natural cytotoxicity receptor NKp30. **P. Pinheiro**, J. Justino, M.M. Marques

MEDI **98.** Structural investigation of FISLE-412, a peptidomimetic compound derived from saquinavir that targets lupus autoantibodies. **M. He**, S. VanPatten, K. Cheng, S. Sun, A. Altiti, O. Bloom, B. Volpet, B. Diamond, Y. Alabed

MEDI **99.** Anti-DNA antibodies as a drug target in systemic lupus erythematosus. **S. Vanpatten**, A. Papatheodorou, V. Jeganat, J.M. Crawford, O. Bloom, B.T. Volpe, C. Grant, T. Coleman, B. Diamond, Y. Al-Abed

MEDI **100.** Discovery of potent and selective RORγt inverse agonists through scaffold hopping using CoreHop™. **Y. Fan**, Z. Liu, Y. Zheng, L. Jia, J. Yuan, L.W. Dillard, L. Zhuang, C.M. Tice, C. Dong, A.P. Marcus, S.D. Lotesta, P. Noto, S. Meng, K. Lipinski, G. Kandpal, Y. Bukhtiyarov, Y. Zhao, D. Lala, J. Zhou, R.V. Orden, G. Chen, B.M. Mckeever, G. McGeehan, D.A. Claremon, S.B. Singh

MEDI **101.** Discovery of novel $S1P_3$-sparing $S1P_1$ & $S1P_5$ receptor agonists for treatment of multiple sclerosis. **W. Son**, H. Kim, N. Cho, S. Seo, J. Park, K. Sim, J. Seong, S. Lim, K. Park, D. Baek, K. Jeong, A. Pae

MEDI **102.** Taurine prodrugs: a new class of amino acid anti-inflammatory drug devoid gastric toxicity. E.O. Vizioli, R.C. Chelucci, R. Chiqueto, P.L. Bosquesi, J.L. Santos, **C.M. Chin**

MEDI **103.** Structure-based design of 3-(4-aryl-1*H*-1,2,3-triazol-1-yl)-biphenyl derivatives as $P2Y_{14}$ receptor antagonists. A. Junker, R. Balasubramanian, A. Ciancetta, E. Uliasi, E. Kiselev, C. Martiriggiano, K. Trujillo, G. Mtchedlidze, **K.A. Jacobson**

MEDI **104.** Non selective PDE inhibitors as promising anti-inflammatory medicine. **L. Wu**, P. Zhang, L. Zhang, F. Gao, H. Jia, Z. Chen, R. Xu, J. Li, S. Chen, F. Geng, Y. Shen, B. Liu, X. Ma

MEDI **105.** Synthesis and development of novel compounds selectively targeting on sphingosine 1-phosphate receptor 1 (S1P1) for treatment of multiple sclerosis. **S. Yeon**, J. Park, T. Ha, J. Choi, B. Jang, S. Kim, Y. Lee, S. Shin, K. Park

MEDI **106.** 2,5-Isomers of triazole-pyrrolopyrimidine act as selective inhibitors of Janus kinase 2 (JAK2) compared to JAK1 and JAK3. **L. Sun-mi**, Y. Kim

MEDI **107.** Targeting pulmonary inflammation by pharmacological augmentation of leukotriene A_4 hydrolase with 4-methoxydiphenylmethane. **K. Lee**, S. Peyton, H. Lee, M. Burdick, E.M. Chung, S.M. Noble, Y.M. Shim, M. Paige

MEDI **108.** Design and characterization of peptide inhibitors of the interleukin-1β receptor signaling complex. **K. Lee**, A. Dailing, L. Liotta, A. Luchini, M. Paige

MEDI **109.** Design and synthesis of small molecule inhibitors of interleukin-1β for the treatment of osteoarthritis. **K. Kim**, A. Dailing, L. Liotta, A. Luchini, M. Paige

MEDI **110.** Discovery of a novel allosteric thyroid hormone binding site on macrophage migration inhibitory factor (MIF). **S. Sun**, Y. Al-Abed

MEDI **111.** Design and synthesis of 1,3,4-thiadiazoles as $S1P_1$ and $S1P_5$ selective agonists for the treatment of autoimmune diseases. **B. Enugurthi**, E. Martinborough, A.R. Yeager, L. Huang, J. Tamiya, M. Moorjani, M. Boehm, F. Scott, B. Clemons, J. Brooks, R. Powell, H. Dedman, H. Desale, G. Reinhart, G. Timony, R. Peach

MEDI **112.** Identification of novel arylpiperazinyl butyrolactones 5-HT_7 antagonists as potential inflammatory bowel disease (IBD) therapies. **K. Blattner**, **B.E. Blass**, D.J. Canney, R. Gao, J.C. Gordon, M. Abou-Gharbia, D.A. Pippin, H. Wang, W. Khan

MEDI **113.** Identification of Vps34 as a key-off target activity in the search for a suitable PI3Kδ oral inhibitor for the treatment of respiratory diseases and its potential impact on toxicity. **S. Bertrand**, A. Amour, N. Barton, K. Down, C. Edwards, P. Grandi, N. Hamblin, Z. Harrison

MEDI **114.** Asymmetric synthesis and preliminary biological evaluation of heteroaromatic lipoxin A_4 analogues. **A. Zanetti**, E. Butler, C. Loscher, P.J. Guiry

MEDI **115.** Asymmetric synthesis and biological evaluation of novel heteroaromatic lipoxin A4 analogues for biological evaluation. **K. Gahan**, E. Butler, M. de Gaetano, C. Godson, P.J. Guiry

MEDI **116.** Tryptamine derivatives, extracted from Syrian rue seeds, negatively affected *Leishmania tarentolae* in culture: A model study. **K. Eichenberg**, B. Dorsey, A. Broedlow, J. Wickline, M.A. Jones

MEDI **117.** Synthesis and biological evaluation of 5,7-dihydroxyflavanone derivatives as antimicrobial agent. **S.Y. Kim**, X. Zhang, O. Khalidi, R. Wang, S. Victor, B. Cress, R.A. Gross, M. Koffas, R.J. Linhardt

MEDI **118.** Inhibitors of LHR-1 as novel anti-parasitic drugs. **C.R. Johnson**, X. Yuan, I. Hamza, F. Xue

MEDI **119.** New vacuolar-ATPase inhibitors as antiviral therapies. **A. Lindstrom**, D.P. Petrov, R. Davey, D.J. LaCount, V.J. Davisson

MEDI **120.** Synthesis and biological evaluation of polyalthic acid derivatives for the treatment of neglected diseases. **C.S. Mizuno**, A.B. Souza, B.L. Tekwani, S.R. Ambrósio, R. Veneziani

MEDI **121.** Antibacterial activity of *Combretum farinosum* extracts. **I. Maldonado, A.K. Addo-Mensah**

MEDI **122.** Synthesis and biological evaluation of pyochelin analogs as potential antibacterial agents against pathogenic bacteria. **J. Kong**, S. Yoganathan

MEDI **123.** Multidisciplinary approach to design New Delhi metallo-β-lactamase-1 (NDM-1) inhibitors. **E.K. Kurbanov**, S. Cohen

MEDI **124.** Antimicrobial and exfoliative properties of silver(I) N-heterocyclic carbenes. **M. Stromyer**, M. DeBord, K.M. Tiemann, S.R. Crabtree, M.J. Panzner, C. Tessier, D.A. Hunstad, W.J. Youngs

MEDI **125.** Potent influenza endonuclease inhibitors developed from metal-binding pharmacophore library screen. **C.V. Credille**, S. Cohen

MEDI **126.** Synthesis and antimicrobial studies of hydrophilic pyrazole derivatives as potent antibacterial agents. M.A. Alam, **D. Allison**, **E. Delancey**, D. Jones, **A. Gottsponer**, D. Gilmore

MEDI **127.** Design, synthesis, and evaluation of a carbapenem antibiotic with improved activity against carbapenemase-producing *Klebsiella pneumoniae*. W. Chai, **M. Alqurafi**, T.Q. Nguyen, P. Nguyen, J. Kim, C. Edwards, B. Meshram, M. Lohry, M. Cox, D. Le, E. Kim, S. Casco, P. Oelschlaeger, S. Hartouni, J.W. Janc, J.D. Buynak

MEDI **128.** Development of azotochelin analogues as potential antibacterial leads. **N. Karadkhelkar**, S. Yoganathan

MEDI **129.** Synthesis of 2'-C-methyl pseudouridines for the inhibition of HCV RNA polymerase. **I. Sappy**

MEDI **130.** Boronic acid analogs of anti-HIV therapies: Synthesis and biological evaluation. **S. Burke**, J.W. Tomsho

MEDI **131.** Synthesis of solithromycin analogues with acyclic desosamine surrogates. **X. Jin**, R.B. Andrade

MEDI **132.** Structural characterization and inhibition of shikimate kinase from methicillin resistant *Staphylococcus aureus* through homology modeling and molecular docking simulations. A. Favela-Candia, R. Moreno-Silerio, E. Sierra-Campos, M.A. Valdez-Solana, J. Cisneros-Martínez, A. Téllez-Valencia, **C.I. Avitia-Domínguez**

MEDI **133.** Computer assisted drug design to find potential inhibitors of phosphoglycerate mutase 1 from *Plasmodium falciparum*. L. Ríos-Soto, M. Aguirre-Raudry, E. Sierra-Campos, M.A. Valdez-Solana, M. Gómez-Palacio, A. Téllez-Valencia, **C.I. Avitia-Domínguez**

MEDI **134.** Structure-based drug design (SBDD), synthesis and evaluation of peptides inhibitors of Y-49 β-lactamase from *Mycobacterium tuberculosis*. J. Gonzalez, **C.C. Clement**, M. Philipp

MEDI **135.** Development of inhibitors of the di-zinc metallo beta-lactamase NDM-1. **I.Y. Darwish**, M. Moore, C. Reidl, A. Stewart, P. Thomas, W. Fast, D.P. Becker

MEDI **136.** Design, synthesis, and evaluation of improved apramycin derivatives for the treatment of MDR infectious diseases. **A. Sonousi**, A. Vasella, E. Böttger, D. Crich

MEDI **137.** Withdrawn.

MEDI **138.** Fragment-based design, synthesis, and binding of non-peptide mimics of NS4A and their binding to HCV NS3/4A protease. **M.E. El-Araby**, A. Omar, M.T. Khayat, S. Soror, S. Arold, M. El-Faky, E. Elalem, F. Bamane, H. Asfour

MEDI **139.** Synthesis and development of the endophenazines as new antibacterial drugs. **M.M. Conda-Sheridan**, M.B. Samad, V.R. Udumula

MEDI **140.** Characterization of menoctone efficacy against *Plasmodium berghei*. **A. Shaikh**, I.D. Iyamu, L. Blake, S. Siegel, M. Johnson, D. Kyle, R. Manetsch

MEDI **141.** SAR study of novel anti-fungal agents targeting the synthesis of fungal sphingolipids. **K.H. Raghunandan**, K. Hu, C. Lazzarini, M. DelPoeta, I. Ojima

MEDI **142.** Estimated binding energies of molecules in the active site of HIV-1 integrase (1BIS.pdb): Results of drug-like and nondruglike molecules with consideration of mutations of1BIS. pdb using ICM-Pro (Molsoft L.L.C.). **J.B. Ealy**, H. Yazgi, N. Abouomar, J. Cogan

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MEDI **143.** Dipicolinic acid derivatives as inhibitors of New Delhi metallo-β-lactamase-1 (NDM-1). **Y. Chen**, C.R. Bethel, P. Thomas, R. Bonomo, W. Fast, S. Cohen

MEDI **144.** Towards enhanced treatment of tuberculosis: Discovery and development of indole-2-carboxamide scaffold. **J. Stec**, O.K. Onajole, S. Lun, H. Guo, B. Merenbloom, G. Vistoli, W.R. Bishai, A.P. Kozikowski

MEDI **145.** 8-Hydroxyquinoline as a scaffold for the development of New Delhi metallo-β-lactamase-1 Inhibitors. **R. Adamek**, C.V. Credille, W. Fast, S. Cohen

MEDI **146.** Withdrawn.

MEDI **147.** Synthesis of novel 2-methoxylated fatty acids as effective inhibitors of clinical isolates of methicillin-resistant *Staphylococcus aureus* (CLMRSA). **N.M. Carballeira**, N. Montano, D. Sanabria, Y. Rivera-Torres

MEDI **148.** Orally bioavailable antimalarial 4(1*H*)-quinolone prodrugs with single-dose cures. **F. Brockmeyer**, A. Monastyrskyi, A.N. LaCrue, T. Mutka, D. Kyle, R. Manetsch

MEDI **149.** Synthesis and kinetic characterization of mechanism-based inhibitors of tubercular BioA. **C. Eiden**, J.D. Lipscomb, C.C. Aldrich

MEDI **150.** Towards the synthesis of novel 1,3-azaborines as potential HIV-1 protease inhibitors. **K.M. Norris**, K. Sigurjonsson, M.D. Frank, L. Fabry-Asztalos

MEDI **151.** New bisabolenes isolated from *Calea urticifolia*. **V. Gogineni**, F. León, M. Núñez, S.J. Cutler

MEDI **152.** Inhibition of phosphoglycerate mutase from *Entamoeba histolytica* by benzimidazole derivatives. A. Luévano-De la Cruz, E. Sanabria-Chanaga, A. Hernandez Campos, L. Yépez-Mulia, M. Sarabia-Sánchez, C. Avitia-Domínguez, **A. Téllez-Valencia**

MEDI **153.** Design, synthesis, and biological evaluation of pyrrolo[2,3-*d*]pyrimidines as potent and selective dihydrofolate reductase inhibitors and potential anti-opportunistic agents. A. Gangjee, **K.S. Shah**, S.F. Queener, V. Cody, J. Pace

MEDI **154.** Synthesis and evaluation of boron-containing inhibitors of the non-mevalonate isoprenoid synthesis pathway. **J.M. Gamrat**, S.J. Burke, B.C. Figula, J.W. Tomsho

MEDI **155.** Hydroxymethylnitrofurazone (NFOH) in chronic Chagas disease animal model. C.B. Scarim, R.C. Consolin Chelucci, I. Martinez, E. Padilha, J.A. da Rosa, R.G. Peccinin, C.R. Andrade, J.L. Santos, **C.M. Chin**

MEDI **156.** Parmodulins: Biased ligands for protease-activated receptors (PARs). **C. Dockendorff**, D. Gandhi, R. Rosas, Jr., O. Aisiku, J. Dilks, R. Flaumenhaft

MEDI **157.** Three-ring scaffold with rich biological activity but no commercial availability. **A.S. Bayden**

MEDI **158.** Evaluation of brain migration and therapeutic effects of novel RXR partial agonist CBt-PMN on cognitive impairment in mice. **O. Shibahara**, M. Watanabe, S. Yamada, M. Akehi, T. Sasaki, T. Hanada, A. Akahoshi, H. Hirano, H. Kakuta

MEDI **159.** Syntheses of 3-aminopiperidinone amides as CGRP receptor antagonists. **C. Wang**, M.E. Fraley

MEDI **160.** Preparation and evaluation of a series of ^{18}F-enkephalin analogues: the first step in the design of potent and selective ^{18}F-labeled PET tracers for delta opioid receptor imaging. **A. Pirisedigh**, **Y. Dory**, **L. Gendron**, **B. Guerin**

MEDI **161.** Evaluation of 4-(2-fluoro-4-nitrophenoxy)-1-([^{11}C]methyl)-1,2,3,6-tetrahydropyridine as a MAO-A selective PET-MRI hybrid imaging probe. **L. Drake**

MEDI **162.** Pyrrolotriazines as potent inhibitors for a novel serine-threonine kinase for indication of neuropathic pain. **B. Dasgupta**, C.D. Dzierba, J.J. Bronson, R. Rajamani, J.E. Grace, J. Lippy, N. Surti, J.M. Brown, L. Hunihan, J. Allen, B. Hamman, K. Baker, K. Savelieva, B. Zambrowicz, C. Bourin, A. Easton, L. Bristow, D. Parker, J.K. Muckelbauer, J. Khan, D.M. Camac, C. Conway, W. Kostich, R. Westphal, J.E. Macor

MEDI **163.** Design and synthesis of new acetylcholine analogues acting as full agonists for the nicotinic acetylcholine receptor subtype α9α10. **E.G. Perez**, S. Tobias, D.J. Minter, J.C. Boffi, R. Reiff, E. Katz, C. Wedemeyer, A. Elgoyhen

MEDI **164.** Synthesis and evaluation of C10 and flexible analogues of (±)-stepholidine at dopamine D_3 and σ2 receptors. **S. Gadhiya**, W. Harding

MEDI **165.** Discovery of C6-truncated purine (N)-methanocarba nucleoside derivatives as selective A_3 adenosine receptor agonists. **D. Tosh**, A. Ciancetta, E.P. Warnick, R. O'Connor, Z. Chen, E. Gizewski, S. Crane, Z. Gao, J. Auchampach, D. Salvemini, K.A. Jacobson

MEDI **166.** Design, synthesis and in combo activity of selective σ-1 receptor ligands with robust antinociceptive effect. **G.J. Navarrete Vazquez**, B. Godínez-Chaparro, F.J. López-Muñoz, B. Wünsch, D. Schepmann, A. Austrich-Olivares, J. Espinosa-Juárez, L.A. Melo-Hernández, S. Hidalgo-Figueroa, . Torres-Gómez

MEDI **167.** 2,4-Dioxo-3-aza-bicyclo[3.1.0] hexane-6-carboxamide derivatives as atypical antipsychotics for the treatment of schizophrenia. **A. Mohammed**, A.K. Shinde, N. Bogaraju, K.R. Sastry, R. Subramanian, S. Edula, G. Bhyrapuneni, R. Nirogi

MEDI **168.** Design, synthesis and pharmacological characterization of novel amides as 5-HT_4 receptor agonist. **A.K. Shinde**, A. Mohammed, S. Saraf, V. Bhatta, K. Kandukuri, K.R. Sastry, R. Subramanian, V. Mekala, G. Bhyrapuneni, V. Benade, P. Jayarajan, R. Nirogi

MEDI **169.** Conjugated amides: Potent and selective histamine H_3 receptor ligands. R. Nirogi, **A.K. Shinde**, A. Mohammed, S. Saraf, K. Bojja, P. Achanta, K.R. Sastry, R. Subramanian, G. Bhyrapuneni, N. Muddana, P. Jayarajan

MEDI **170.** 1-Isopropyl-1H-pyrrolo[2,3-b] pyridine-6-carboxamide derivatives as 5-HT_4 receptor partial agonists. **A. Mohammed**, A.K. Shinde, S. Gagginapally, K.R. Sastry, R. Subramanian, V. Mekala, G. Bhyrapuneni, P. Jayarajan, R. Nirogi

MEDI **171.** Synthesis of [^{11}C] MK-1064 as a new PET radioligand for imaging of orexin-2 receptor. M. Gao, **M. Wang**, Q. Zheng

MEDI **172.** Tunable pH-sensitive linker for controlled release. **C. Choy**, C. Ley, J. Geruntho, B. Backer, A. Davis, C.E. Berkman

MEDI **173.** Technologies for assessing target engagement and their applications in drug discovery. **J. Xiao**, T. Engler, K.W. Furness, S.A. Haney, C.D. Jesudason, T.B. Durham, M.J. Blanco-Pillado

MEDI **174.** Long-term storage stability problems of screening libraries for drug discovery. **C. Laggner**, C. Johnson, Y. Shayo, C. Hendarto, C. Loomis

MEDI **175.** NCI small molecule screening libraries available to academic oncology HTS investigators. **R.N. Misra**, M. Eckert, C. Laggner

MEDI **176.** Methods for clean-up and enrichment of coporate screening collection. **M. Jorgenson**, M. Marigo, A.G. Sams, M. Langgard, L. David

MEDI **177.** Directed evolution of PET imaging agents by scanning unnatural protease resistance (SUPR) mRNA display. L. Kelderhouse, A.N. Hardy, F. Pisaneschi, Y. Peleg, B. Hu, A. Ornelas, P. Yang, S. Gammon, S. Howell, D. Piwnica-Worms, P. Wang, T. Takahashi, R.W. Roberts, S.V. Fiacco, **S.W. Millward**

MEDI **178.** [^{18}F]JNJ-3^{11}, a novel tau PET ligand. **F. Rombouts**, D. Moechars, J. Andres, G. Macdonald, V. Chupakhin, X. Langlois, G.M. Bormans, L. Declercq

MEDI **179.** Urea carboxylic acid derivatives as antischistosomal agents. **C. Wang**, J. Keiser, Y. Dong, J.L. Vennerstrom

MEDI **180.** Discovery and evaluation of the first small molecules targeting GOAT inhibition *in vivo*. **M.A. Martinez-Grau**, C. Dominguez, C.S. Galka, E.J. Hembre, N.A. Honigschmidt, C.D. Jesudason, S.J. Keding, C. Nevill, G. Ruano, A. Rubio, K.M. Ruley, D.L. Smith, R.A. Brier, M.M. He, Y. Chen, N.A. Reynolds, H. Yang

MEDI **181.** Withdrawn.

MEDI **182.** Design, synthesis, and applications of novel PUFA-taxoid probes for fluorescence imaging and ^{19}F NMR analysis. **S. Yan**

MEDI **183.** Studies of influence of plasma-activation of compounds on melanogenesis and tyrosinase activity. **F. Jabeen**, A. Ali, Z. Ashraf, E. Ha Choi, P. Attri

MEDI **184.** Crystallographic study of metalloenzyme inhibitors. **B. Dick**, S. Cohen

MEDI **185.** Chemoenzymatic synthesis and characterization of multifunctional fluoresceins for breast cancer diagnosis. **G. Shrikhande**, S. Sen, J.E. Puskas

MEDI **186.** Evaluation of silica stability in methanolic solvents. **J.R. Bickler**, E. Denton

MEDI **187.** Effective cannabinoid purification by flash chromatography. **J.R. Bickler**, E. Denton

MEDI **188.** Chemical make-up of plants used in herbal remedies and their applications. **B. Harvey**

MEDI **189.** Dirhodium catalyzed direct aryl amination. **M.P. Paudyal**, **A. Adebesin**, D. Ess, Z. Ma, L. Kurti, J.R. Falck

MEDI **190.** Synthesis of novel photoaffinity probes of antiangiogenic homoisoflavonoids. **W. Sun**, B. Lee, S. Seo, T. Corson

MEDI **191.** Peptide-based capsules for protein delivery. **Y. Li**, L. Lock, H. Cui

MEDI **192.** Synthesis of *cis-/trans-2*-tert-butoxycarbonylamino-cyclopropanecarboxylic acid. **G. Pan**, H. Jing, H. Li, M. Yang

MEDI **193.** Delivering phytochemical therapeutics through polymer nanofibers. **A. Mancuso**

Radiopharmaceutical Chemistry

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MONDAY MORNING

Section A

Pennsylvania Convention Center
Room 114

Small Change, Big Impact: Strategic Minor Structural Modifications in Drug Design

T. Tsukamoto, *Organizer*, *Presiding*

9:00 Introductory Remarks.

9:05 MEDI **194.** Strategic exploration of the magic methyl effect in drug design. **M.S. Egbertson**

9:40 MEDI **195.** Challenges and opportunities of implementing halogen bonds in molecular design. **F.M. Boeckler**

10:15 MEDI **196.** Some applications of fluorine in drug design. **N.A. Meanwell**

10:50 MEDI **197.** Improvement in aqueous solubility via small structural modifications. **M.A. Walker**

11:25 MEDI **198.** Strategies to reduce glucuronidation through structural modification. **S. Zimmermann**

Section B

Pennsylvania Convention Center
Room 113C

Small Molecule Approaches for the Treatment of Lupus

M. C. Bryan, *Organizer*, *Presiding*

J. B. Schwarz, *Presiding*

9:00 Introductory Remarks.

9:05 MEDI **199.** Testing new therapeutics in SLE: Unmet needs and strategies. **A. Davidson**

9:35 MEDI **200.** Translational studies evaluating Btk inhibition as a therapeutic strategy for the treatment of SLE. **A. Bender**, A. Pereira, K. Fu, E. Samy, Y. Wu, L.M. Liu-Bujalski, R. Caldwell, Y. Chen, H. Tian, F. Morandi, J. Head, M. Genest, S.L. Okitsu, D. Xu, P. Haselmayer, R. Grenningloh

10:05 MEDI **201.** Discovery of pyridine amide based inhibitors of interleukin receptor-associated kinase 4 (IRAK4) for the treatment of lupus. **J. Hynes**, S. Nair, W.J. Pitts, R. Bhide, R. Schmidt, S. Spergel, V. Ram Reddy Paidi, S. Ratna Kumar, R. Sistla, J.B. Santella, D. Gardner, H. Wu, J.V. Duncia, N. Murugesan, J. Tino, P.H. Carter, J. Carman, S. Dudhgaonkar, R. Srivastava, F. Deborah, C. Goldstine, S. Skala, X. Li, S. Maddi, A. Saxena, K. Palanisamy, A. Chimalakonda, S. Ruepp

10:35 MEDI **202.** Structure-based design of potent and selective inhibitors of NF-κB inducing kinase (NIK). **N. Blaquiere**, S.T. Staben, G. Castanedo

11:05 MEDI **203.** E6887: A novel and selective inhibitor of toll-like receptors 7 and 8. **L.D. Hawkins**

Section C

Pennsylvania Convention Center

Room 113B

Solute Carrier (SLC) Membrane Transporters as Emerging Drug Targets

M. P. Bourbeau, *Organizer*, *Presiding*

9:00 MEDI **204.** SLC transporters in drug response. **K. Giacomini**

9:30 MEDI **205.** Structure-based ligand discovery for nutrient transporters. **A. Schlessinger**

10:00 MEDI **206.** Discovery of a non-absorbable ASBT inhibitor clinical candidate for treatment of type 2 diabetes. **J.L. Collins**

10:30 MEDI **207.** Blocking lactic acid transport: A cancer metabolism-based strategy for finding new antitumor agents. **T.D. Bannister**, H. Wang, C. Wang, R.N. Nair, C. Yang, W.R. Roush, J.L. Cleveland

11:00 MEDI **208.** Development of selective uric acid reabsorption inhibitors (SURIs) for the treatment of gout. **J. Girardet**

11:30 MEDI **209.** Overview of the progression of Pfizer's SGLT2 inhibitor program from the discovery of ertugliflozin (PF-04971729) to successful POC. **V. Mascitti**

International Drug Discovery & Development Collaborations

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Shedding Light on the Dark Genome: Methods, Tools & Case Studies

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Mass Spectrometry for the Masses: Recent Developments in Mass Spectrometry Enabled Pharmaceutical Discovery, Development & Manufacturing

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Forced Degradations in the Pharmaceutical Industry

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MONDAY AFTERNOON

Section A

Pennsylvania Convention Center

Room 114

Medicinal Chemist's Toolbox: Scaffolds & Privileged Scaffolds in Drug Design

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

2:00 Introductory Remarks.

2:05 MEDI **210.** Computational analysis of molecular scaffolds. **J. Bajorath**

2:40 MEDI **211.** Spirocyclic scaffolds in drug discovery. **C.M. Tice**, Y. Zheng, S.B. Singh

3:15 MEDI **212.** Malaria as a proof of concept of how natural products have inspired the development of preclinical and clinical candidates with diverse mechanisms of action. **F. Calderon Romo**

3:50 MEDI **213.** Macrocyclic peptide scaffolds: Passive permeability and oral absorption beyond the rule of 5. **S. Lokey**

4:25 MEDI **214.** LipMetE assessment of bioisosteres in medicinal chemistry. **A.F. Stepan**

Section B

Pennsylvania Convention Center

Room 113C

Medicinal Chemistry of Chemical Biology

R. J. DeVita, *Organizer*, *Presiding*

2:00 MEDI **215.** Chemical probes for target validation. **M. Bunnage**

2:30 MEDI **216.** Selective modulation of p97-dependent protein homeostasis networks. **M. Arkin**

3:00 MEDI **217.** DrugTargetSeqR: An interdisciplinary approach to dissect the mechanisms of action of drugs and chemical probes. **T. Kapoor**

3:30 MEDI **218.** Sirtuin inhibitors as anticancer agents. **H. Lin**

4:00 MEDI **219.** Designed covalent inhibitors as chemical biology probes and drug development candidates. **T.D. Owens**

4:30 MEDI **220.** Chemical and proteome-wide reactivity profiling of covalent serine hydrolase inhibitor chemotypes. **M.J. Niphakis**

Section C

Pennsylvania Convention Center

Room 113B

Nucleic Acid Therapeutics

A. C. Bryant-Friedrich, *Organizer*

M. Manoharan, *Presiding*

2:00 Introductory Remarks.

2:10 MEDI **221.** Tuning the chemical properties of XNA nucleotides and oligomers for therapeutics and diagnostics. **J.M. Heemstra**, T. De Costa, Z. Chen, A. Rangel, K. Meek

2:45 MEDI **222.** RNAi therapeutics: From base pairs to bed side. **M. Manoharan**

3:20 MEDI **223.** Expanding the chemical diversity of therapeutic oligonucleotides for the treatment of neurodegenerative disorders. **A. Khvorova**

3:55 MEDI **224.** Development of nucleoside analogs as broadly active antiviral agents. **G. Painter**

4:30 MEDI **225.** Sequence-based design of small molecules targeting RNA. **M.D. Disney**, S. Velagapudi, S. Rzuczek

International Drug Discovery & Development Collaborations

Sponsored by SCHB, Cosponsored by MEDI, ORGN, POLY and PROF

Kavli Symposium on Chemical Neurotransmission: What Are We Thinking?

Sponsored by ANYL, Cosponsored by BIOL, BMGT, CHED, CINF, MEDI, PMSE and SCHB

Radiopharmaceutical Chemistry

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Tetrahedron Prize for Creativity in Organic Chemistry Symposium

Sponsored by ORGN, Cosponsored by BIOL, COMP and MEDI

Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

MONDAY EVENING

Section A

Pennsylvania Convention Center

Halls D/E

Sci-Mix

W. B. Young, *Organizer*

8:00 - 10:00

41, 44-45, 84, 94-95, 158. See previous listings.

273, 286-287, 345-347, 352, 354-355, 376, 387-388. See subsequent listings.

TUESDAY MORNING

Section A

Pennsylvania Convention Center

Room 114

Gut Reaction: Opportunities & Challenges of Gut-Specific Drug Targeting

B. P. Mc Kibben, D. Smith, *Organizers*, *Presiding*

8:30 MEDI **226.** Concepts in the design of intestinally targeted drugs. **K.J. Filipski**, M.V. Varma, A.F. El-Kattan, C.M. Ambler, R.B. Ruggeri, T.C. Goosen, K.O. Cameron

9:00 MEDI **227.** Discovery of TGR5 agonists with gut restricted action. **J.G. Lewis**, T. Chen, J.W. Jacobs, P. Finn, D. Rodriguez, J. Kohler, K. Kozuka, L. He, C. Carreras, S. Koo-McCoy, J. Tabora, J. Caldwell

9:30 MEDI **228.** Physical-property based design of gut-selective CCK1 receptor agonists. **K.O. Cameron**

10:00 MEDI **229.** Gut restricted oral peptides as therapeutics for inflammatory bowel disease. **L. Mattheakis**, X. Cheng, G. Zemede, L. Bai, V. Tran, H. Celino, B. Frederick, L. Zhao, M. Dogra, J. Tovera, S. Shah, N. Rao, G. Bourne, J. Zhang, J. McMahon, T. Annamalai, A. Bhandari, M. Smythe, D. Patel, D. Liu

10:30 MEDI **230.** Power of the gut microbiome. **G. Hecht**

11:15 MEDI **231.** Strategies to investigate the xenobiotic-metabolizing capabilities of the human gut microbiome. **E. Bess**, J. Bisanz, P. Spanogiannopoulos, P. Turnbaugh

11:45 Discussion.

Section B

Pennsylvania Convention Center

Room 113C

Emerging Isosteric Replacement Methods: A Fundamental Strategy in Drug Design

T. Fessard, *Organizer*, *Presiding*

8:30 Introductory Remarks.

8:35 MEDI **232.** Applications of bioisosteres in drug design. **N.A. Meanwell**

9:00 MEDI **233.** New computational methods to support bioisosteric replacement and molecular library design. **N. Brown**

9:25 MEDI **234.** Novel building blocks for discovery chemistry: New vistas and opportunities with bioisosteres. **E.M. Carreira**

9:55 MEDI **235.** Strategies towards increasing the 3-dimensionality of the medicinal chemistry design space. **A.F. Stepan**

10:20 MEDI **236.** Cubane: A benzene isostere! **C.M. Williams**

10:45 MEDI **237.** Isosteric replacement by catalytic fluorination, fluoroalkylation, borylation, silylation, and amination. **J.F. Hartwig**

11:15 MEDI **238.** Late-stage functionalization of marketed drugs: Synthesis and use of tetrazolones as a carboxylic acid bioisostere. **M.A. Duncton**, R. Murray, G. Park, R. Singh

11:40 MEDI **239.** Development of synthetic methods for the construction of isosteres. **G.A. Molander**

12:10 Concluding Remarks.

Connectivity & the Global Reach of Chemistry: Honoring the Life & Scientific Contributions of Ernest L. Eliel

Sponsored by ORGN, Cosponsored by BMGT, CHED, CINF, HIST, INOR, MEDI, MPPG, PMSE and SCHB

Polymeric Materials as Imaging Agents & Theranostics

Drug Delivery

Sponsored by POLY, Cosponsored by FLUO, INOR, MEDI and NUCL

TUESDAY AFTERNOON

Section A

Pennsylvania Convention Center

Room 114

MEDI Award Symposium

W. B. Young, *Organizer*

T. D. Bannister, *Presiding*

2:00 MEDI **240.** Optimization of a benzoxazepinoindazole series for human African trypanosomiasis. **D. Klug**, R. Diaz-Gonzalez, C. Cordon-Obras, D. Rojas-Barros, M. Navarro, M.P. Pollastri

2:20 MEDI **241.** Synthetic lethal targeting: A new anticancer strategy. **K.E. Knewtson**, C. Perera, B.R. Peterson

2:40 MEDI **242.** Reactivity-based and genome-guided natural product discovery. **J. Tietz**, D. Mitchell

3:00 MEDI **243.** Discovery of an agouti-related protein (AGRP) octapeptide macrocycle derivative with equipotent antagonist pharmacology at the mouse melanocortin-4 receptor as AGRP(87-132). **M. Ericson**, A. Wilczynski, Z. Xiang, N. Sorensen, C. Haskell-Luevano

3:20 MEDI **244.** Small molecule induced degradation of bromodomains. **D. Buckley**

3:40 MEDI **245.** Drug design for addiction: Targeting the dopamine D_3 receptor. **A.H. Newman**

4:25 MEDI **246.** Novel immunomodulators that target toll-like receptors. **H.H. Yin**

‡ *Cooperative Cosponsorship*

Section B

Pennsylvania Convention Center

Room 113C

Modulation of the Ubiquitin-Proteasome Pathway

E. Altmann, V. Cee, J. D. Hansen, *Organizers*, *Presiding*

2:00 MEDI **247.** Targeting the regulatory enzymes in protein ubiquitination. **N. Zheng**

2:30 MEDI **248.** New paradigm in drug action: Differentiated gain of function amongst IMiD® analogues binding the E3 ubiquitin ligase, CRL4^{CRBN}. **J.D. Hansen**

3:00 MEDI **249.** Proteolysis targeting chimera (PROTACS): Recruiting proteins to the cellular quality control machinery. **C.M. Crews**

3:30 MEDI **250.** Structure based design of COP9 directed inhibitors. **M. Renatus**, E. Altmann, A. Schlierf, M. Jones, U. Hassiepen, R. Assenberg, M. Schaefer, J. Quancard, M. Kiffe, A. Weiss, W. Christian, R.C. Sedrani, J. Eder, B. Martoglio, K. Pfister, A. Jefferson

4:00 MEDI **251.** Discovery of TAK-243: An investigational, first-in-class inhibitor of the ubiquitin activating enzyme. **J. Ciavarri**

Needs & Directions for the Future of Toxicology in Pharmaceutical Development

Sponsored by TOXI, Cosponsored by MEDI

Polymeric Materials as Imaging Agents & Theranostics

Medical Imaging

Sponsored by POLY, Cosponsored by FLUO, INOR, MEDI and NUCL

WEDNESDAY MORNING

Section A

Pennsylvania Convention Center

Room 114

Epigenetics

W. B. Young, *Organizer*

J. E. Macor, *Presiding*

9:00 MEDI **252.** From a novel HTS hit to a series of potent, selective, orally bioavailable KDM5 inhibitors: A success story utilizing structure- and property-based design. **J. Liang**

9:25 MEDI **253.** Isoxazole-derived amino acids are bromodomain-binding acetyl-lysine mimics when incorporated in histone H4 peptides and histone H3. A.R. Sekirnik, D. Hewings, N.H. Theodoulou, L. Jursins, K. Lewendon, L. Jennings, T. Rooney, **S.J. Conway**

9:50 MEDI **254.** Fragment-based, structure-enabled discovery of novel pyridone and pyridazinone macrocycles as potent selective BET family bromodomain inhibitors. **L. Wang**, J. Pratt, G.S. Sheppard, S. Fidanze, D. Liu, L.A. Hasvold, R. Mantei, C. Park, A. Sarthy, L. Li, D.H. Albert, X. Lin, S. Warder, E. Faivre, M.H. Bui, X. Huang, D. Wilcox, R. Wang, T. Magoc, G. Rajaraman, A. Petros, S. Panchal, G. Fang, S.W. Elmore, S. Rosenberg, Y. Shen, K. McDaniel, W. Kati

10:15 MEDI **255.** Discovery of an *in vivo* probe for the bromodomain of CBP that is efficacious in a MOLM-16 AML xenograft model. **A. Romero**

10:40 MEDI **256.** Discovery and structure-based optimization of novel allosteric inhibitors targeting the epigenetic methyltransferase PRC2. **A. Lingel**, D. Bussiere, J. Cantwell, M.P. Dillon, Y. Huang, M. Lindvall, M. Sendzik, W. Shu, B.R. Taft

11:05 MEDI **257.** Discovery of first-in-class reversible dual inhibitor of DNA methyl transferases and histone methyl transferase (G9a) with *in vivo* activity in different cancer models. E. San Jose, X. Agirre, O. Rabal, A. Vilas-Zornoza, J. Sanchez-Arias, E. Miranda, A. Ugarte, R. Alvarez, S. Roa, B. Paiva, N. Casares, V. Segura, J. Martin-Subero, G. Castellano, M. Garcia Fernandez de Barrena, J. Rodriguez-Madoz, M. Garcia-Barchino, J. Lasarte, M. Avila, J. Martinez-Climent, F. Prosper, **J. Oyarzabal**

11:30 MEDI **258.** Dual screening using protein-observed fluorine NMR uncovers the first selective inhibitor for BPTF. **A.K. Urick**, L.M. Hawk, M. Cassel, N.K. Mishra, S.E. Kirberger, P. Ycas, C. Dos Santos, W.C. Pomerantz

Section B

Pennsylvania Convention Center

Room 113C

General Orals

W. B. Young, *Organizer*

R. J. DeVita, *Presiding*

8:30 MEDI **259.** Structure-based drug design of aminobenzisoxazoles as orally available factor IXa (FIXa) inhibitors. **I. Sakurada**

8:55 MEDI **260.** Discovery and optimization of the first sub-micromolar, cell permeable, small molecule inhibitors of poly(ADP ribose) glycohydrolase (PARG). **A. McGonagle**, B. Acton, J. Ahmet, P. Chapman, E. Fairweather, L. Griffiths, N. Hamilton, N. Hamilton, J. Hitchin, C. Hutton, D. James, C. Jones, S. Jones, A.M. Jordan, D. Mould, D. Ogilvie, K. Smith, A. Stowell, H. Small, J. Tucker, I. Waddell, B. Waszkowycz

9:20 MEDI **261.** Discovery of ozanimod (RPC1063): A $S1P_{1R}$ and $S1P_{5R}$ selective agonist for the treatment of autoimmune disease. **J. Tamiya**, E. Martinborough, A.R. Yeager, L. Huang, B. Enugurthi, M. Moorjani, M. Boehm, F. Scott, B. Clemons, J. Brooks, R. Powell, H. Dedman, H. Desale, G. Reinhart, G. Timony, R. Peach

9:45 MEDI **262.** Structure-based design of highly potent and selective small-molecule reversible factor D inhibitors blocking *in vivo* alternative complement pathway activation. **J.K. Maibaum**, K. Anderson, A. Vulpetti, E. Lorthiois, N. Ostermann, S. Liao, S. Randl, O. Rogel, E. Paul, B. Gerhartz, U.A. Argikar, I. Müller, U. Hommel, B. Kinzel, F. Kolb, S. Rüdisser, F. Cumin, R.C. Sedrani

10:10 MEDI **263.** Potent, gut-restricted inhibitors of divalent metal transporter 1 (DMT1): Preclinical efficacy against iron overload and safety evaluation. **S. Chowdhury**, A. Cutts, L. Ratkay, M. Eyers, C. Young, R. Namdari, J. Cadieux, N. Chahal, M.E. Grimwood, Z. Zhang, S. Lin, I. Tietjen, C. Xie, L. Robinette, L. Sojo, M. Waldbrook, M.D. Hayden, T.S. Mansour, S. Pimstone, Y. Goldberg, M.J. Webb, C. Cohen

10:35 MEDI **264.** Development of novel, selective and irreversible PI3Kδ inhibitors. **S.E. Dalton**, S.A. Campos, J.T. Bush, D.A. Thomas, M.A. Convery, J.A. Murphy

11:00 MEDI **265.** *C*-linked benzyl triazolopyridine inhibitors of myeloperoxidase. **S. Shaw**, B.P. Vokits, L. Abell, M. Basso, C.G. Clark, A. Dilger, F. Duclos, G. Fernando, S. Halpern, S. Jusuf, J. Khan, L.M. Kopcho, X. Liu, F. Lo, G. Locke, R. Narayanan, R.J. Peterson, P. Sleph, J. Smallheer, A. Viet, R.R. Wexler, N. Wurtz, L. Zhao, E.K. Kick

11:25 MEDI **266.** Systematic study of the glutathione (GSH) reactivity of *N*-arylacrylamides. **V. Cee**, L.P. Volak, Y. Chen, M.D. Bartberger, D.J. Kopecky, C. Tegley, T. Arvedson, J. McCarter, A.S. Tasker, C.H. Fotsch

11:50 MEDI **267.** Discovery of BMS-212 as a potent, liver-selective glucokinase activator clinical candidate. **W. Meng**, R. Brigance, H. Zhang, D.S. Yoon, Y. Wang, R.A. Smirk, L. Nielsen, Y. Shi, S.S. Chen, S. Wu, S. Tao, R. Sulsky, R. Zhao, B. Wang, J. Sun, M. Wong, A. Mathur, Y. Yang, J. Taylor, H. Fuentes, X. Ma, R. Ponticiello, R. Zebo, X. Chen, K. Omalley, L.M. Kopcho, S. Johnson, J. Muckelbauer, C. Chang, Q. Wang, K. Behnia, B. Zinker, A. Wang, E. Janovitz, M. Kirby, J. Whaley, J.C. Barrish, J.A. Robl, P.T. Cheng

WEDNESDAY AFTERNOON

Section A

Pennsylvania Convention Center

Room 114

First Time Disclosures

L. A. Thompson, *Organizer*, *Presiding*

1:30 MEDI **268.** Discovery of AG-120: A first-in-class inhibitor of IDH1 mutant enzymes for the treatment of cancers harboring IDH1 mutations. **J.V. Popovici-Muller**, R.M. Lemieux, J. Saunders, F.G. Salituro, K. Yen, K. Straley, E. Tobin, F. Wang, S. Gross, E. Artin, L. Dang, H. Yang, L. Utley, Y. Chen, A. Olaharski, L. Silverman, S. Agresta, M. Su, S.A. Biller

2:00 MEDI **269.** JNJ-54175446: A P2X7 receptor antagonist clinical candidate for major depressive disorders. **B.M. Savall**

2:30 MEDI **270.** SAGE-217: A next-generation neuroactive steroid $GABA_A$ receptor positive allosteric modulator for the potential treatment of seizure disorders. **A.J. Robichaud**

3:00 MEDI **271.** Inhibition of autoimmune pathways with dual inhibition of JAK1 and TYK2: Discovery of PF-06700841. **A. Fensome**, M. Banker, M.F. Brown, J. Clark, M. Dowty, I.V. Efremov, B.S. Gerstenberger, A. Gopasamy, M. Hayward, M. Hegen, B. Hollingshead, J. Jussif, J. Knafels, T. Lin, B. Pierce, E. Saiah, R. Sharma, P. Symanovicz, F. Vajdos, F. Vincent, Z. Wan, L. Xing, X. Yang, X. Yang, J. Trujillo, L. Zhang

3:30 MEDI **272.** Discovery of a pseudokinase domain ligand as an allosteric inhibitor of TYK2 for the treatment of autoimmune diseases. **D.S. Weinstein**, S. Wrobleski, R. Moslin, S. Lin, Y. Zhang, S. Spergel, M. Mertzman, J.S. Tokarski, H. Sun, M. Chiney, P. Elzinga, N. Aranibar, A. Chimalakonda, J. Strnad, A. Zupa-Fernandez, L. Cheng, K. Gillooly, K. Mcintyre, P.H. Carter, L. Lombardo, J.R. Burke, J.E. Macor

4:00 MEDI **273.** Discovery of NVP-HDM201: Identification of a next-generation Mdm2 inhibitor with superior characteristics. **P. Holzer**, P. Chène, S. Ferretti, P. Furet, T. Gabriel, B. Gruenenfelder, V. Guagnano, F. Hofmann, J. Kallen, R. Mah, K. Masuya, R. Ramos, S. Ruetz, C. Rynn, A. Schlapbach, T. Stachyra-Valat, S. Stutz, A. Vaupel, S. Jeay

4:30 MEDI **274.** Discovery of DRX-065: Characterizing the non-PPARγ, mitochondrial function modulation and anti-inflammatory activity of thiazolidinedione (TZD) enantiomers using deuterium. A.W. Czarnik, **S.H. Dewitt**, V. Jacques, L. Van der Ploeg

Section B

Pennsylvania Convention Center

Room 113C

General Orals

W. B. Young, *Organizer*

A. W. Stamford, *Presiding*

1:30 MEDI **275.** Distributed drug discovery (D3) in action: Finding inhibitors of *P. aeruginosa*. **W.L. Scott**, J.G. Samaritoni, G. Anderson, K.A. Marrs, S. Colglazier, J.R. Hitchens, S.D. Burris, M.S. Ware, M.J. O'Donnell

1:50 MEDI **276.** Discovery of potent HCV NS5A inhibitors with pan-genotype activity. **W. Yu**, L. Chen, M.P. Dwyer, K. Keertikar, S. Kim, B.J. Lavey, A.G. Nair, R. Rizvi, S.B. Rosenblum, O. Selyutin, B. Shankar, L. Tong, M.K. Wong, D. Yang, Q. Zeng, G. Zhou, B. Hu, B. Zhong, D. Wang, J. Hao, R. Liu, S. Agrawal, D. Carr, L. Rokosz, S. Curry, P. McMonagle, P. Ingravallo, F. Lahser, E. Asante-Appiah, A. Nomeir, C.A. Coburn, J.A. Kozlowski

2:10 MEDI **277.** Discovery of LY3073084, a novel non-peptide small molecule ghrelin-O-acyl transferase (GOAT) inhibitor. **E.J. Hembre**, R.A. Brier, Y. Chen, C. Dominguez, C.S. Galka, M.M. He, N.A. Honigschmidt, C.D. Jesudason, S.J. Keding, M.A. Martinez-Grau, C. Nevill, N.A. Reynolds, G. Ruano, A. Rubio, K.M. Ruley, D.L. Smith, H. Yang

2:30 MEDI **278.** Biotin carboxylase inhibitors with improved antibacterial activity against gram-negative pathogens. **T. Kane**, A. Serio, C. Haglund, D. Hildebrandt, G.A. McEnroe, H. Le, K. Wlasichuk, L. Andrews, M. Linsell, P. Dozzo, R. Cirz, T. Machajewski, D. Neau, N. Anzalone, S. Pakhomova, G.L. Waldrop, F. Cohen

2:50 MEDI **279.** Discovery of allosteric WNK inhibitors and in vivo proof-of-concept as anti-hypertensive agents. **K. Yamada**

3:10 MEDI **280.** Optimization of a heteroaryl sulfonamide series of potent, selective and efficacious Nav1.7 inhibitors. **M.M. Weiss**, A. Boezio, J. Butler, T.A. Dineen, R. Graceffa, C. Kreiman, T. Kornecook, D.S. La, I.E. Marx, B. Milgram, B. Sparling, B. Moyer

3:30 MEDI **281.** Natural product-based drug abuse therapies through the investigation of salvinorin A. **R.M. Saylor**, T.E. Prisinzano

3:50 MEDI **282.** Development of a new class of ALK2 inhibitor for the study of the most aggressive paediatric brain cancer, DIPG. **L. Hudson**, H. Woodward, S. Hoelder

4:10 MEDI **283.** Leukotriene A_4 hydrolase aminopeptidase activity as a new target for chronic obstructive pulmonary disease. **M. Paige**, K. Lee, S. Peyton, L. Li, S. Fitzpatrick, K. Kim, H. Lee, M. Burdick, S.M. Noble, Y.M. Shim

4:30 MEDI **284.** Discovery of a novel, selective and orally bioavailable allosteric PRC2 inhibitor with robust anti-cancer efficacy. **Y. Huang**, J. Zhang, Z. Yu, A. Lingel, Z. Gao, L. Wang, X. Fu, Y. Sun, Q. Zhang, X. Jiang, J. Zhang, M.D. Shultz, Y. Mi, C. O-Yang

4:50 MEDI **285.** Efficient discovery of lead molecules for hundreds of target proteins in parallel via DNA encoded chemical library: A platform for prioritizing therapeutic targets in a single experiment. **G. Evindar**

WEDNESDAY EVENING

Section A

Pennsylvania Convention Center
Hall E

General Posters

W. B. Young, *Organizer*

7:00 - 9:00

MEDI **286.** Design and optimization of novel tetracyclic pyrrolopyridone BET family inhibitors. **S. Fidanze**, R. Mantei, L.A. Hasvold, J. Pratt, G.S. Sheppard, L. Wang, D. Liu, C. Park, A. Sarthy, L. Li, D.H. Albert, X. Lin, E. Faivre, M.H. Bui, X. Huang, D. Wilcox, R. Wang, T. Magoc, G. Rajaraman, G. Fang, S. Rosenberg, Y. Shen, W. Kati, K. McDaniel

MEDI **287.** Potential of silibinin derivatives in prostate cancer managements. **B. Vue**, S. Zhang, X. Zhang, M. Huang, T. Lee, G. Chen, Q. Chen

MEDI **288.** Synthesis and SAR of sulfonyl azide-derived NDM-1 inhibitors. **C. Reidl**, M. Moore, I.Y. Darwish, A. Stewart, P. Thomas, W. Fast, D.P. Becker

MEDI **289.** Design and synthesis of small molecule Hsp70 inducers. **T.F. Ali**, N. Taira, R. Koga, Y. Okamoto, M. Otsuka, M. Fujita

MEDI **290.** Discovery of ABI-231 analogs as a new generation of tubulin inhibitors targeting the colchicine binding site. Q. Wang, K. Arnst, D.D. Miller, **W. Li**

MEDI **291.** Biologically active ferrocene based guanidines: Synthesis, antimicrobial, and anti-cancer potential. **A. Altaf**, **A. Badshah**, R. Gul

MEDI **292.** Cytotoxic triterpenoids substituted in the position 2. **L. Borkova**, J. Sarek, J. Rehulka, P. Dzubak, M. Hajduch, M. Urban

MEDI **293.** Host-guest formulations of novel isozyme-selective carbonic anhydrase inhibitors for colon cancer detection and treatment. **O. Ozen Karakus**, R.K. Sanku, U.K. Mondal, M.A. Ilies

MEDI **294.** Design, synthesis, and biological evaluation of novel PAMAM dendrimer-based tumor-targeted drug delivery systems. **L. Wei**, T. Wang, Y. Sun, Y. Zhang, S. Bahl, Y.G. Teng, I. Ojima

Technical program information known at press time. The official technical program for the 252nd ACS National Meeting is available at: www.acs.org/Philadelphia2016

MEDI **295.** Withdrawn.

MEDI **296.** Selective DDRs inhibitors as novel therapeutic agents for human cancers and pulmonary fibrosis. **K. Ding**

MEDI **297.** Preparation of fenbufen boronopinacol, *meta*- and *ortho*-[^{18}F]fluorofenbufen boronopinacol and [^{18}F]fluorocelecoxib for boron neutron capture therapy of cholangio carcinoma. C. Yeh, C. Chang, I. Chung, Y. Chen, T. Chen, Y. Huang, H. Wang, S. Tien, **C. Yu**, Y. Chou, C. Liu, I. Hsie

MEDI **298.** Synthesis and evaluation of drug-DNA conjugated gold nanoparticles activated by cancer cell specific mRNA. **N. Li**, N.P. Gossai, J. Naumann, P.M. Gordon, J.A. Piccirilli

MEDI **299.** Discovery of hepatoselective inhibitors of diacylglycerol acyltransferase 2 (DGAT2). **K. Futatsugi**, D.W. Kung, K. Huard, S.T. Orr, S. Cabral, D. Hepworth, S. Bader, M. Boehm, P.A. Carpino, T.V. Magee, M. Herr, S.Y. Lavergne, Q. Li, K. Ahn, R.W. Clark, D.M. Erion, K. Kou, B.A. Pabst, S.M. Perez, J. Purkal, C.C. Jorgensen, J.R. Gosset, A.S. Kalgutkar, T.C. Goosen, M. Niosi, J.C. Pettersen, B. Goodwin

MEDI **300.** Discovery of human NMUR2 selective hexapeptidic agonists. **K. Taketa**, K. Takayama, K. Mori, Y. Sohma, A. Taguchi, N. Minamino, M. Miyazato, K. Kangawa, Y. Hayashi

MEDI **301.** Synthetic chemistry core at Albert Einstein College of Medicine. Recent contributions to chemical biology and drug discovery. **L. Nordstroem**

MEDI **302.** Design, synthesis, and biological evaluation of novel tumor-targeted drug delivery systems for a third-generation taxoid, combretastatin and their combination. **Y. Zong**, I. Ojima

MEDI **303.** Molecular mimics of classic P-glycoprotein as dual cytotoxic/MDR auto-suppressors or in combination with Paclitaxel. **M.T. Khayat**, M.E. El-Araby, A.M. Omar, A.M. Al-Abd

MEDI **304.** Novel selective estrogen receptor downregulators developed using endocrine-independent breast cancer cells lines. **R. Xiong**, J. Zhao, L. Gutgesell, D.A. Tonetti, G.R. Thatcher

MEDI **305.** Design, synthesis and evaluation of WZ4002 analogues as EGFR inhibitors. **A. Romu**, Z. Bin, Z. Chen, V.L. Korlipara

MEDI **306.** Exploring EGFR kinase-ligand interactions for optimizing dual action inhibitors. **A. Deschenes**

MEDI **307.** Synthesis of substituted trifluoromethyl ketone targeted antifolates as potential purine synthesis inhibitors. A. Gangjee, **W. Xiang**, L.H. Matherly

MEDI **308.** In silico design and synthesis of novel estrone analogs utilizing click chemistry targeting colorectal cancer. **F.S. Alotaibi**, F.T. Halaweish

MEDI **309.** Novel 6-substituted pyrrolo[2,3-*d*]pyrimidine classical antifolates as selective folate receptor substrates and antitumor agents. A. Gangjee, **X. Li**, A. Wallace-Povirk, C. O'Connor, M. Wilson, Z. Hou, L.H. Matherly

MEDI **310.** Withdrawn.

MEDI **311.** Design and synthesis of antifolates as targeted antitumor agents: Exploring the benefits of fluorine substitution on the side chain (het)aryl ring for improved selectivity and potency. A. Gangjee, **M.P. Ravindra**, A. Wallace-Povirk, C. O'Connor, M. Wilson, Z. Hou, L.H. Matherly

MEDI **312.** Small molecule mimics of a conserved TWXE/DFL motif targeting G-alpha-i3. **M.J. Koyack**, R. Rajnarayanan

MEDI **313.** Development of functionalized aminobenzoboroxoles as anti-cancer agents. S. Pathi, L. Solano, B. Patel, A. Kasibotla, **J. Seay**, **S.C. Jonnalagadda**

MEDI **314.** Synthesis and biological evaluation of amorfrutin analogs: A unique class of natural product that modulates PPARγ activity. **S. Yoganathan**

MEDI **315.** Discovery of an inhibitor of the Rpn11 proteasome subunit. **C. Perez**, S. Cohen, R. Deshaies, J. Li, M.J. Rouffet

MEDI **316.** Chemical modification and structure activity relationship (SAR) of fellutamide B, a natural product with anticancer and anti-tuberculosis activity. **N. Acharekar**, L. Barasa, S. Yoganathan

MEDI **317.** Scaffold replacement & 3D ligand optimization applied to the discovery of tyrosine kinase inhibitors. R. Alvarez, **H. Shadnia**

MEDI **318.** Design, synthesis, and anti-proliferation activity of cucurbitacin-inspired estrone analogs targeting pancreatic cancer. **K. Asleud**

MEDI **319.** New cephalotaxane derivatives for TKI resistant CML. **L. Wu**, Y. Yao, Z. Chen, F. Gao, J. Sun, X. Yang, C. Zhang, J. Li, S. Chen, Z. Zhang

MEDI **320.** Compounds designed to elevate reactive oxygen species (ROS) and their antiproliferative implications. **R. Elhaggar**, T. Abdelghany, A.M. Omar, M.T. Khayat, M.E. El-Araby

MEDI **321.** Identification of the small molecule inhibitor for STAT3 pathway through chemical structure focused library screening. **B. Seo**, K. Kim, S. Lee, J. Ahn, J. Hur, Y. Suh

MEDI **322.** Synthesis and cytotoxic effects of novel glycosylated thiosemicarbazides and their analogs as anticancer agents. A. Czubatka-Bienkowska, J. Sarnik, A. Macieja, **Z.J. Witczak**, T. Poplawski

MEDI **323.** Synthesis, characterization, molecular modeling, and potential anticancer activities of novel 1,3,4-thiadiazole derivative. A. Czubatka-Bienkowska, A. Macieja, J. Sarnik, **Z.J. Witczak**, T. Poplawski

MEDI **324.** Bicycloheptylamines and cyclohexylamines as σ_2 receptor ligands: Potential use as anticancer agents. **M. Alamri**, Z. Ates-Alagoz, A. Adejare

MEDI **325.** Synthesis and characterization of some new emetine amide derivatives for studies in prostate and breast cancer cells. **N. Brandy**, O. Bakare

MEDI **326.** Encapsulation and delivery of trastuzumab into human breast cancer cells using cholestosomes. **J. Cubello**, J.F. McArthur, J. Schentag, J. Hughes, L. Mielnicki, M.P. McCourt

MEDI **327.** Discovery and optimization of triazole compounds as novel BCL6 inhibitors. **H. Cheng**, F. Xue

MEDI **328.** Synthesis and pharmacological evaluation of new compounds useful to treat sickle cell disease. **T. Ferreira de Melo**, K. Barbieri, R.C. Consolin Chelucci, C. Lanaro, C.M. Chin, J.L. Santos

MEDI **329.** Synthesis and biological activity of new hybrids phthalimide-furoxan derivatives useful to treat sickle cell disease symptoms. **R.C. Consolin Chelucci**, K.P. Barbieri, M.E. Pires, M.C. Polesi, P.L. Bosquesi, S. Marcondes, I.Z. Carlos, J.L. Santos, C.M. Chin

MEDI **330.** Nitric oxide donor controllable with yellowish green light. **H. Okuno**, N. Ieda, Y. Hotta, M. Kawaguchi, K. Kimura, H. Nakagawa

MEDI **331.** Novel adamantane derivatives efficiently inhibit cisplatin resistant ovarian cancer cell line growth. A. Czubatka-Bienkowska, J. Sarnik, A. Macieja, **Z.J. Witczak**, T. Poplawski

MEDI **332.** Discovery of dihydrobenzofuran substituted chromene analog as a potent anticancer agent for ovarian cancer. R. Patil, A. Kulshrestha, G.K. Katara, K. Beaman, **S. Patil**

MEDI **333.** Design and synthesis of a library of 8-quinolinethiol based Rpn11 inhibitors. **Y. Ma**, J. Li, C. Perez, R. Deshaies, S. Cohen

MEDI **334.** Design, synthesis, and biological evaluation of novel metabolically stable (+)-discodermolide analogues. **B. Guo**, N. Zhang, H.M. McDaid, S.B. Horwitz, A.B. Smith

MEDI **335.** Withdrawn.

MEDI **336.** Development of diketopiperazine-type antitumor agent plinabulin prodrug with an IgG binding peptide for generating a tumor selective non-covalent-type antibody-drug conjugate. K. Muguruma, F. Yakushiji, R. Kawamata, D. Akiyama, R. Arima, T. Shirasaka, A. Taguchi, K. Takayama, **Y. Hayashi**

MEDI **337.** Towards a universal Mu-agonist template for alignment modeling of opioid ligands. **Z. Wu**, V.J. Hruby

MEDI **338.** Designing of selective gamma-secretase inhibitory benzenesulfonamides through comparative *in vitro* and *in silico* analysis. N. Masand, S. Gupta, R. Khosa, **V. Patil**

MEDI **339.** Exploiting solvent effects in drug design and optimization. **A. Ajamian**

MEDI **340.** Computational approach for performing medicinal chemistry transformations within a 3D active site. **R. Alvarez**, J. Leonard

MEDI **341.** Property assessment of medium size molecules: Connecting drug-like properties from *in vitro* to *in vivo.* **M.J. Blanco-Pillado**, I. Gonzalez Valcarcel, P. Desai, J. Barrett, G. Sawada, T.N. Vetman

MEDI **342.** Problem-based learning in drug discovery with MOE. **A. Bonin**

MEDI **343.** What rings do medicinal chemists use, and why? **M.D. Mackey**, T. Cheeseright, R. Lawrence

MEDI **344.** Amide-to-ester substitutions modify the permeability and ADME properties of natural and synthetic cyclic peptides. **M. Naylor**, A. Ly, J. Schwochert, P. Desai, I. Gonzalez Valcarcel, J. Barrett, G. Sawada, M.J. Blanco-Pillado, S. Lokey

MEDI **345.** Structure-based drug design of macrocyclic factor XIa inhibitors. **J.R. Corte**, T. Fang, H. Osuna, D. Pinto, K. Rossi, A. Rendina, J. Bozarth, S. Sheriff, J. Myers, T. Harper, Z. Lou, J. Zheng, J. Luettgen, D. Seiffert, P.Y. Lam, R.R. Wexler, M.L. Quan

‡ *Cooperative Cosponsorship*

MEDI **346.** Optimization of BTK inhibitors to mitigate kinase selectivity, PK and off target shortcomings. **D. Guiadeen**, J. Liu, A. Krikorian, X. Gao, J. Wang, S.B. Boga, A. Alhassan, J. Xu, J. Kelly, R. Anand, Y. Yu, O. Selyutin, W. Yu, S. Liu, C. Yang, H. Wu, J. Cai, K.M. Maloney, V. Honak, Y. Gao, S. Tyagarajan, T. Fischmann, J. Presland, M. Mansueto, Z. Xu, E. Leccese, J. Zhang-Hoover, I. Knemeyer, N. Bays, P. Stivers, P. Brandish, A. Hicks, R. Kim, J.A. Kozlowski

MEDI **347.** Discovery of low clearance PI3Kd templates for the treatment of respiratory disease. **S. Peace**

MEDI **348.** Synthesis of heteroaromatic lipoxin analogues for treatment of chronic inflammation. **C. Tighe**, M. de Gaetano, C. Godson, P.J. Guiry

MEDI **349.** Discovery of novel and orally active quinolyl oxazole-based PDE4 inhibitors for the treatment of chronic obstructive pulmonary disease and asthma. **R. Kuang**, H. Shue, D. Blythin, P.C. Ting, N. Shih, L. Xiao, X. Chen, D. Gu, J. Schwerdt, J. Cao, H. Wu, D.B. Prelusky, S. Sorota, P. Wu, J. Zhang, X. Zhang, C. Celly, M. Billah, P. Wang

MEDI **350.** 7-Heteroarylmethoxy-triazolopyridines as potent inhibitors of myeloperoxidase. **M. Valente**, N. Wurtz, A. Viet, S. Shaw, D. Andrew, J. Khan, S. Jusuf, G. Fernando, X. Liu, G. Locke, L.M. Kopcho, L. Abell, J. Gao, A. Dongre, R.R. Wexler, F. Duclos, E.K. Kick

MEDI **351.** Stable lipoxin analogues for biological evaluation. **D. Moran**, M. de Gaetano, C. Godson, P.J. Guiry

MEDI **352.** Lipobactins: A new class of antibiotics against gram-positive bacteria. **H. Yang**, K.H. Chen, J.S. Nowick

MEDI **353.** Design, synthesis, antimicrobial evaluation and molecular modeling studies of 4-(5-(2-aminothiazol-4-yl)-1,4-dihydro-2,6-dimethyl-4-aromatic substituted pyridin-3-yl)thiazol-2-amine derivatives. **P. Tigulla**, S. Vankadari

MEDI **354.** Exploring structural importances on penetration of the first line tuberculosis prodrug: Pyrazinamide. B. Peters, D. Crick, **D.C. Crans**

MEDI **355.** Ribosome templated azide-alkyne cycloadditions: Synthesis of potent macrolide antibiotics screening by in situ click chemistry. **S. Daher**, **I.M. Glassford**, **C.N. Teijaro**, R.B. Andrade

MEDI **356.** Discovery of iguratimod as a selective, steroid-sparing MIF inhibitor via specificity-guided screening. **J. Bloom**, C. Metz, S. Nalawade, K. Cheng, M. He, B. Sherry, T. Forsthuber, Y. Al-Abed

MEDI **357.** Elaboration of indole frameworks in the development of allosteric HIV-1 integrase inhibitors. **J. Antwi**, P. Koneru, M. Kobe, M. Kvaratskhelia, J. Fuchs

MEDI **358.** Parallel inhibition of amino acid efflux and parasite growth of erythrocytic *Plasmodium falciparum* by mefloquine and open-ring analogs: Implication for the mechanism of antimalarial action. **M. Ghavami**, C.H. Dapper, K. Holzschneider, M. Klemba, P.R. Carlier

MEDI **359.** Luminescence assay for natural product inhibitors of the *Mycobacterium tuberculosis* proteasome. **A. Gunderwala**, J.R. Porter

MEDI **360.** Biosynthetic intermediates of amicetin produced by engineering mutants. **H.B. Zhang**, C. Zhang

MEDI **361.** Multicationic quaternary ammonium compounds (MultiQACs): Potent antimicrobial and antibiofilm agents arising from a variety of scaffolds. **K.P. Minbiole**

MEDI **362.** Zinc-mediated binding of a low-molecular-weight stabilizer of the host anti-viral factor APOBEC3G. **M.O. Radwan**, S. Sonoda, T. Ejima, A. Tanaka, R. Koga, Y. Okamoto, M. Fujita, M. Otsuka

MEDI **363.** Arylation of 2-bromo-5-chloro thiophenes with aryl boronic acids, their structural investigations (X-ray and DFT), and in vitro antibacterial and scavenging activities. **N. Rasool**

MEDI **364.** Synthesis of novel allosteric inhibitors of HIV-1 integrase that bind to the LEDGF/p75 site. **Y. Mansour**, P. Koneru, M. Kobe, A. Hoyte, M. Mohamed, M. Kvaratskhelia, J. Fuchs

MEDI **365.** Synthesis and biological studies of dihydropyrido pyrimidinones. **M.A. Alam**, H. Alkhattabi, Z. Alsharif, D. Jones

MEDI **366.** Design, synthesis, and evaluation of novel anti-DENV compounds. **G. Giancotti**, V. Anastasi, I.M. Trist, J. Bugert, A. Brancale

MEDI **367.** 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**, S. Gallagher, E. Allen, N. Herrmann, M. Hashemzadeh

MEDI **368.** Some selected metal complexes of proguanil-sulphadiazine mixed ligands: Synthesis, characterization, and antimicrobial studies. J.A. Obaleye, A.O. Rajee, **F.H. Babamale**

MEDI **369.** Synthesis of benzoxaborole-metronidazole based compounds for *Clostridium difficile.* **L. Solano**, **E. Lueth**, **Z. Gardner**, **T. Schumacher**, S.K. Jonnalagadda, S. Gurrapu, D. Imtiaz, C. Ronayne, G.L. Nelson, V. Mereddy, S.C. Jonnalagadda

MEDI **370.** Antiplasmodial and other compounds from an *Aniba sp.* **Y. Du**, A. Latif, Y. Dai, S. Dalal, M.B. Cassera, M. Goetz, D.G. Kingston

MEDI **371.** Overcoming PK limitations via prodrugs to advance a second generation of HIV-1 integrase strand transfer inhibitors. **T.J. Hartingh**, I.T. Raheem, A.M. Walji, J. Schreier, M.W. Embrey, T.G. Steele, J.S. Wai, P.J. Coleman, K. Moore, J. Sisko, V.L. Rada, D. Hazuda, J. Truchon, S. Clas, P. Abeywickrema, D.J. Klein, J.M. Sanders, M.D. Miller, J.A. Grobler, N.D. Pajkovic, M.J. Hafey, P. Rearden, A. Bennet, M. Xu, S. Patel, D.C. Dubost, D.A. Powell

MEDI **372.** Optimization of macrocyclic peptide triazole HIV-1 inactivators. **A. Ahmed**, R. Aneja, K. Acharya, S. Zhang, I. Chaiken

MEDI **373.** Design and synthesis of novel nucleotide analogues targeting HCV NS5B. **B. Alabdullah**, A.C. Bryant-Friedrich

MEDI **374.** Potent, selective and orally efficacious inhibitors of *Plasmodium falciparum* protein kinase G (*Pf*PKG). **D. Harding**, S. Osborne, K. Birchall, N. Bouloc, J. Large, A. Merritt, E. Smiljanic-Hurley, M. Wheldon, K. Ansell, C. Kettleborough, D. Whalley, P. Bowyer, L. Stewart, D. Baker

MEDI **375.** Trisubstituted thiazoles as potent and selective inhibitors of *Plasmodium falciparum* protein kinase G (*Pf*PKG). **D. Harding**, S. Osborne, K. Birchall, N. Bouloc, J. Large, A. Merritt, E. Smiljanic-Hurley, M. Wheldon, K. Ansell, C. Kettleborough, D. Whalley, P. Bowyer, L. Stewart, D. Baker

MEDI **376.** Structure-activity-relationship of alkyl and alcohol analogs of omarigliptin, long acting DPP-4 inhibitors. **D. Feng**

MEDI **377.** Reversible small molecule inhibitors of endothelial lipase (EL) which increase high density lipoprotein (HDL) concentration *in vivo*. **S. Kim**, L. Abell, L. Adam, K. Behnia, M. Basso, C. Caporuscio, A. Chen, J. Jiang, J. Johnson, E. Liu, J. Lloyd, H. Lu, M. Phillips, Z. Pi, A. Rose, D. Taylor, G. Tora, T. Wang, R.R. Wexler, R. Yang, X. Yin, L. Zhao, H. Finlay

MEDI **378.** Fluorination of JQ1 slows its metabolism. **S.L. Holmes**, J. Williams, C. Santini, F. Li, D. Young

MEDI **379.** Finding hits for designing new antidiabetic drugs. Inhibition of protein tyrosine phosphatase 1B. M. Sarabia-Sánchez, P.J. Trejo, A. Hernandez Campos, R. Castillo-Bocanegra, A. Luévano-De la Cruz, C. Avitia-Domínguez, **A. Téllez-Valencia**

MEDI **380.** Synthesis and SAR of triazole analogs as potent glucokinase activator. **H. Zhang**, W. Meng, R. Brigance, Y. Shi, Y. Wang, R.A. Smirk, L. Nielsen, D.S. Yoon, S. Chen, S. Wu, S. Tao, R. Sulsky, S. Spronk, Y. Li, Y. Yang, J. Taylor, H. Fuentes, X. Ma, R. Ponticiello, R. Zebo, X. Chen, K. Omalley, L.M. Kopcho, S. Johnson, J. Muckelbauer, C. Chang, Q. Wang, K. Behnia, B. Zinker, A. Wang, E. Janovitz, M. Kirby, J. Whaley, J.C. Barrish, J.A. Robl, P.T. Cheng

MEDI **381.** Optimization of sulfonamide based GPBAR1 (TGR5) agonists. **C. Huang**, D. Shi, S.G. Kultgen, J. Healy, Y. Li, A.G. Cole, S. Nawoschik, K. Tovar, B. Fanelli, X. Ma, C. Ebert-Gallo, M. Hayward, J. Nickels, P.D. Stein, M. Webb, B.F. McGuinness, J.R. Beasley

MEDI **382.** GPBAR1 (TGR5) agonists with low systemic exposure. **C. Huang**, E. Sieber-McMaster, X. Xu, S. Nawoschik, K. Tovar, B. Fanelli, X. Ma, C. Ebert-Gallo, M. Hayward, J. Nickels, P.D. Stein, M. Webb, B.F. McGuinness, J.R. Beasley

MEDI **383.** Design, synthesis, and evaluation of (2S, 4R)-ketoconazole sulfonamide analogs as potential treatments for metabolic syndrome. **B.E. Blass**, P. Iyer, M. Abou-Gharbia, W.E. Childers, J.C. Gordon, M. Ramanjulu, G.C. Morton, P. Arumugam, J. Boruwa, J.W. Ellingboe, S. Mitra, R. Nimmareddy, S. Paliwal, J. Rajasekhar, S. Shivakumar, P. Srivastava, R.S. Tangirala, K. Venkataramanaiah, M. Yanamandra

MEDI **384.** Discovery of 2-thio-5-thiomethyl substituted imidazoles as potent and orally efficacious TGR5 receptor agonists for rreatment of type 2 diabetes. **X. Zhang**, Z. Sui, J. Kauffman, F. Du, T. Kirchner, C. Hou, Y. Liang, D. Johnson, W.V. Murray, K. Demarest

MEDI **385.** Ghrelin *O*-acyl transferase (GOAT) inhibitors: Optimization of the 6-chloro-2-methyl-5-[2-(4-piperidyl) ethyl]pyrimidin-4-amine scaffold. **G. Ruano**, C.S. Galka, E.J. Hembre, N.A. Honigschmidt, M.A. Martinez-Grau, C. Nevill, A. Rubio, R.A. Brier, M.M. He, Y. Chen, N.A. Reynolds, H. Yang

MEDI **386.** Discovery of a novel series of *N*-phenylindoline-5-sulfonamide derivatives as potent, selective, and orally bioavailable acyl CoA: monoacylglycerol acyltransferase-2 inhibitors. **K. Sato**, H. Takahagi, T. Yoshikawa, O. Kubo, K. Hidaka, S. Morimoto, T. Takai, M. Kamaura, R. Adachi, T. Ishii, T. Maki, K. Take, T. Mochida, S. Takekawa, M. Nakakariya, N. Amano, T. Kitazaki, T. Maekawa

MEDI **387.** Design, synthesis, and mechanism of action determination of flupirtine derivatives with enhanced neuroprotective activity. N. Kinarivala, F. Saadeh, J. Makoukji, R. Boustany, **P.C. Trippier**

MEDI **388.** Discovery and quantitative pharmacology of novel azetidine-containing PDE10A inhibitors. **Q. Liu**, A.K. Amegadzie, J.J. Chen, N. Chen, M.J. Frohn, E.H. Hu, M.R. Kaller, V. Ma, T. Nguyen, A. Pickrell, W. Qian, S. Rumfelt, R.M. Rzasa, K. Andrews, S. Zhao, C. Davis, J. Able, J. Shi, G. Hill Della Puppa, M. Dovlatyan, H. Chen, S. Miller, J. Treanor, T. Kornecook, W. Zhong, J.R. Allen

MEDI **389.** Design, synthesis and pharmacological evaluation of benzamide derivatives of 1,3,4-thiadiazole as acetylcholinesterase inhibitors for cognitive dysfunction. **A. Kulshreshtha,** P. Piplani

MEDI **390.** GC-MS and GC-IRD studies on S cathinones: Bath salt-type aminoketone designer drugs related to MDPV. **Y. Abiedalla**, C.R. Clark, J. DeRuiter, K. Abdelhay

MEDI **391.** Syntheses and evaluations of arylbicycloalkylamines as NMDAR antagonists. **M.B. Dybek**, A. Adejare

MEDI **392.** Synthesis and optimization of truxillic acid-based fatty acid binding protein inhibitors as anti-nociceptive and anti-inflammatory drugs. **K. Hu**, S. Tong, M. Elmes, M. Kaczocha, R.C. Rizzo, D. Deutsch, I. Ojima

MEDI **393.** Synthesis & evaluation of a dopamine D3 receptor-selective positron emission tomography probe. **M.N. Stewart**, B. Hockley, P. Scott

MEDI **394.** Synthesis and biological evaluation of novel fluorinated tacrine hybrids against Alzheimer's disease. **C.D. Obi**, A. Sledge, C.O. Okoro

MEDI **395.** Quinazoline and quinoline derivatives as inhibitors of adaptor associated kinase 1. **R.A. Hartz**, V. Ahuja, C.D. Dzierba, B. Dasgupta, W. Kostich, S. Nara, A. Easton, C. Bourin, L. Bristow, J. Brown, L. Hunihan, M. Gulianello, R. Westphal, R. Rajamani, S. Kiefer, D. Camac, J. Muckelbauer, M. Pokross, V. CM, R. Manepalli, S.K. Sarvasiddhi, S. H, S. Kandula, V. Patankar, R. Brown, N. Surti, J. Lippy, R. Padmanabha, K. Esposito, B. Hamman, J. Allen, K. Baker, K. Savelieva, B. Zambrowicz, S. Pattipati, M. Dokania, S. Elavazhagan, K. Dandapani, J.J. Bronson, J.E. Macor

MEDI **396.** Synthesis & optimization of vinyl sulfone compounds as Nrf2 activator. **J. Choi**, J. Park, T. Ha, S. Yeon, B. Jang, S. Kim, Y. Lee, S. Shin, K. Park

MEDI **397.** Synthesis of imidazobenzodiazepine oxazole bioisosteres as potential alpha 2, 3 selective GABA(A) receptors agonists with improved antiepileptic and antinociceptive efficacy. **K. Methuku**, G. Li, M.M. Poe, J.M. Witkin, J.M. Schkeryantz, J.M. Cook

MEDI **398.** Syntheses and pharmacological characterizations of arylbicycloheptylamines as uncompetitive NMDAR antagonists. **N. Filemban**, T. Colestock, J. Wallach, A. Adejare

MEDI **399.** Targeting ion channels, transporters, and GPCRs with monoclonal antibodies. **J. Rucker**

MEDI **400.** Novel sigma-2 receptor modulators for the treatment of Alzheimer's disease. **B.E. Blass**, **K. Blattner**, D.J. Canney, R. Bhandare, J.C. Gordon, M. Abou-Gharbia

MEDI **401.** Synthesis and profiling of CNS prodrugs of 5-lipoxygenase (5-LO) inhibitors. **R. Fan**, J.C. Gordon, B.E. Blass, M. Abou-Gharbia, W.E. Childers

MEDI **402.** New synthetic approach to procyanidins. **I.M. Geraskin**, G.A. Kraus

MEDI **403.** Development of a multikilogram scale synthesis of *trans*-4-(5-bromo-2-chloro-pyrrolo[2,3-d] pyrimidin-7-yl)-cyclohexanol: A key intermediate for MER/FLT3 dual inhibitors. L. Rong, **J. Li**, H. Li, X. Wu, M. Yang

MEDI **404.** Synthesis of α-fluoro nitriles and derivatives. **L. Zhang**, G. Liu, X. Wu, M. Yang

MEDI **405.** Drug patent lifecycle management through follow-on patents, extending the term of patents and regulatory exclusivities. **D. Chandran**, J. Ravula, R. Nirogi

MEDI **406.** Microneedles for transdermal delivery of traditional Chinese medicine. **B. Zhong**, H.T. Poon, K. Yeung

MEDI **407.** Synthesis of hollow mesoporous silica nanoparticles and their application for delivery of multiple peptides for melanoma immunotherapy. **J. Tao**, J. Zhu, Z. Zhang, **L. Qianqian**, C. Yang

MEDI **408.** Synthesis of d-labeled and unlabeled ethyl succinic anhydrides and application to quantitative analysis of peptides by MALDI and ESI mass spectrometry. **S. Niwayama**, M. Zabet-Moghaddam, S. Kurono, A. Shaikh, P. Kattanguru

MEDI **409.** On the structure-activity relationship of cADPR and cADPR analogs: a high-field NMR study. **S.M. Graham**, J. Plavec, U. Javornik

MEDI **410.** Electrochemical halogenation: A new method to synthesize intermediates for tritium labeling. **Z. Tan**, Y. Liu, R.M. Helmy, N. Rivera, D. Hesk, J. Su

MEDI **411.** Synthesis of biotinylated triterpenes and their use in target identification. **M. Urban**, M. Soural, J. Hodon, V. Sidova, J. Sarek, L. Borkova, S. Gurska, P. Dzubak, M. Hajduch

MEDI **412.** From propafenone to fumitremorgin C: Probing inhibitor selectivity for P-gp/BCRP. **T. Schwarz**, F. Montanari, A. Cseke, K. Wlcek, E. Urban, G.F. Ecker

MEDI **413.** Novel architectures for multicationic quaternary ammonium compounds (multiQACs). **S. Al-Khalifa**, M. Jennings, W.M. Wuest, K.P. Minbiole

MEDI **414.** Tunable polymersomes: Towards enzyme delivery through the blood-brain barrier. **J. Kelly**, D.R. Martin, M.E. Byrne

MEDI **415.** γ-Radiation generates active chlorine species (ACS) in physiological solutions. A novel mechanism of radioprotection by ACS scavengers. **A.V. Popov**, O.P. Mishra, R.A. Pietrofesa, M. Christofidou-Solomidou

MEDI **416.** Large-scale synthesis and sre-clinical characterization of a cationic iodinated imaging contrast agent (CA4+) and its use for quantitative computed tomography of *ex vivo* human hip cartilage. R.C. Stewart, **A.N. Patwa**, J.D. Freedman, M.C. Wathier, B.D. Snyder, A. Guermazi, M.W. Grinstaff

MEDI **417.** 1,2,3-Triazole inhibitors of *Porphyromonas gingivalis* biofilm formation. **F.A. Luzzio**, P.C. Patil, D.R. Demuth, J. Tan

MEDI **418.** Shape-dependent relaxivity of nanoparticle-based MRI contrast agent. **Y. Shin**, K. Culver, M. Rotz, T.J. Meade, M. Hersam, T.W. Odom

MEDI **419.** Formulation of insulin for oral dosing. **J. Catalano**, J.F. McArthur, J. Hughes, J. Schentag, L. Mielnicki, M.P. McCourt

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NUCL

Division of Nuclear Chemistry and Technology

J. Terry, D. Hobart and A. Hixon, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Radiopharmaceutical Chemistry (see *FLUO*, Sun, Mon)

SOCIAL EVENTS:

Social Hour, 6:00 PM: Tue

BUSINESS MEETINGS:

Business Meeting, 5:00 PM: Tue

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

SUNDAY MORNING

Section A

Philadelphia Downtown Courtyard by Marriott Grand Ballroom Salon II

Nuclear Forensics

T. A. Bredeweg, A. V. Giminaro, *Organizers*

J. D. Auxier, *Organizer*, *Presiding*

8:00 Introductory Remarks.

8:05 NUCL **1.** Deciphering a nuclear threat -- Nuclear forensic advances and pressing needs. **H.L. Hall**, J. Auxier II, M. Cook, R. Gilbreath

9:00 Intermission.

9:15 NUCL **2.** Morphology and chemical speciation of nuclear materials for forensic science. **M.P. Wilkerson**

9:35 NUCL **3.** Preparation and characterization of glass analogs for post-detonation debris material. R. Carter, C. Dorais, J. Coble, **A.E. Hixon**

9:55 NUCL **4.** Evaluation of ammonium bifluoride dissolution of refractory minerals for nuclear forensic analysis. **N.T. Hubley**, J.D. Brockman, J.M. Guthrie, J.D. Robertson

10:15 NUCL **5.** Neutron imaging studies of *in situ* growth of neutron and gamma detector materials. **J.Z. Larese**, C. Crain, **N.A. Strange**

SUNDAY AFTERNOON

Section A

Philadelphia Downtown Courtyard by Marriott Grand Ballroom Salon II

Nuclear Forensics

T. A. Bredeweg, A. V. Giminaro, *Organizers*

J. D. Auxier, *Organizer*, *Presiding*

1:00 Introductory Remarks.

1:05 NUCL **6.** Trace element and isotopic signatures of uranium ore concentrates: Forensic applications. **T.L. Spano**, A. Simonetti, E. Balboni, C. Dorais, A.E. Hixon, P.C. Burns

1:25 NUCL **7.** Online trace-level quantification of uranium in environmental water. **C.E. Duval**, T.A. Devol, S.M. Husson

1:45 NUCL **8.** Chemical and isotopic characterization of North America uraninite samples: forensic applications. **E. Balboni**, N. Jones, T.L. Spano, C. Dorais, A. Simonetti, A.E. Hixon, P.C. Burns

2:05 Intermission.

2:25 NUCL **9.** Rapid uranium isotopic analysis using ultrafiltration and alpha spectroscopy. **C.E. Duval**, T.A. Devol, S.M. Husson

2:45 NUCL **10.** New natural uraninite reference material for nuclear forensic analysis. **C. Dorais**, T.L. Spano, E. Balboni, A. Simonetti, A.E. Hixon, P.C. Burns

3:05 NUCL **11.** Divalent cation incorporation into actinide oxides. **M.E. Hoover**, L.C. Shuller-Nickles

3:25 NUCL **12.** Morphological effects of variable calcination conditions for the thermal decomposition of uranyl peroxide. **I. Schwerdt**, L.W. McDonald

SUNDAY EVENING

Radiopharmaceutical Chemistry

Sponsored by FLUO, Cosponsored by INOR, MEDI, NUCL and POLY

MONDAY MORNING

Section A

Philadelphia Downtown Courtyard by Marriott Grand Ballroom Salon II

Nuclear Forensics

T. A. Bredeweg, A. V. Giminaro, *Organizers*

J. D. Auxier, *Organizer*, *Presiding*

8:00 Introductory Remarks.

8:05 NUCL **13.** Using Sr resin with mixed acid matrices. **D. McLain**, C. Liu, R. Sudowe

8:25 NUCL **14.** Improving rapid separations for nuclear forensics through computational techniques. **D.A. Penchoff**, C. Peterson, J.D. Auxier, H.L. Hall, A.K. Wilson

8:45 NUCL **15.** Development of a chemical system for rutherfordium using TEHA and TEHP. **J. Rolfes**

9:05 NUCL **16.** Rare earth element sorption to UO_2. **R. Carter**, J. Coble, A.E. Hixon

9:25 Intermission.

9:40 NUCL **17.** Modern measurements of uranium decay rates. **T. Parsons-Moss**, J. Wimpenny, S. Padgett, S. Faye, R. Williams, T. Wang, P. Renne, T. Harrison, B. Bandong, K. Moody, K. Knight

10:00 NUCL **18.** Determination of Am-241 in weapons grade plutonium for chronometry applications. **M.D. Yoho**, D.R. Porterfield, J.H. Rim, D.J. Klundt

10:20 NUCL **19.** Structural characterization of hydrolyzed of the uranium tetrafluoride solids. **M. DeVore**, M.S. Wellons

Radiopharmaceutical Chemistry

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MONDAY AFTERNOON

Section A

Philadelphia Downtown Courtyard by Marriott Grand Ballroom Salon II

Physicochemical Characterization of Actinides & Fission Products

J. H. Terry, D. Velazquez, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 NUCL **20.** Understanding the surface chemistry of PuO_2. **D.T. Olive**, C. Booth, A. Pugmire, M.P. Wilkerson, F.J. Freibert

1:50 NUCL **21.** Determining speciation of U and Pu in spent nuclear fuel via electrospray ionization mass spectrometry. **L.W. McDonald**, T. Vercouter, J.A. Campbell, S.B. Clark

2:20 NUCL **22.** Thorium incorporation in phosphates matrices: the case of the rhabdophane and xenotime. **M. Adel**, N. Clavier, C. Gausse, D. Qin, S. Szenknect, J. Lozano-Rodriguez, N. Dacheux

2:50 Intermission.

3:10 NUCL **23.** Correlation between surface morphology and crystallographic orientation in polycrystalline UO_2. **Y. Miao**, K. Mo, T. Yao, J. Lian, J. Fortner, L. Jamison, R. Xu, A.M. Yacout

3:55 NUCL **24.** Structure and spectra of uranyl fluoride hydrates. **A. Miskowiec**, M. Kirkegaard, L. Trowbridge, B. Anderson

4:25 NUCL **25.** Withdrawn.

Radiopharmaceutical Chemistry

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TUESDAY MORNING

Section A

Philadelphia Downtown Courtyard by Marriott Grand Ballroom Salon II

Physicochemical Characterization of Actinides & Fission Products

J. H. Terry, D. Velazquez, *Organizers*, *Presiding*

8:00 NUCL **26.** Characterization of irradiated metallic fuels using synchrotron radiation and electron microscopy. **M. Okuniewski**, A. Aitkaliyeva, J. Harp, K.E. Wright, B.D. Miller, R. Seibert, D. Velazquez, J.H. Terry, H. Sharma, P. Kenesei, J.S. Park, J. Hunter, R. Pokharel, F. Zhang, V. Ganapathy, P. Cassutt, B. Hamilton, J. Almer

‡ *Cooperative Cosponsorship*