5:00 INOR **934.** One-step synthesis of substituted 2-(2'-pyridyl)quinoline ligands and investigation of the solution and solid phase behavior of the corresponding gold(III) complexes. **M.D. Sterling**, L. Bishop, A.L. Rheingold, C.H. Larsen

5:20 INOR **935.** Synthesis, structure and bonding in metal complexes of P-stereogenic phosphiranes. **J.A. Muldoon**, M. Deegan, R.P. Hughes, D.S. Glueck, C. Moore, A.L. Rheingold

Section D

Renaissance Washington, DC Downtown
Congressional C

Bioinorganic Chemistry

Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

M. I. Galinato, M. D. Pluth, *Presiding*

1:30 INOR **936.** Selection of peptidic inhibitors against sortase A by using phage display library. **M. Koksal**, N. Ersoz, F. Dudak

1:50 INOR **937.** Quantitatively probing photosystem II with a rotating ring disk electrode assembly. **N. Kornienko**, R. van Grondelle, A. Rutherford, E. Reisner

2:10 INOR **938.** Fast hydrogen atom abstraction by a hydroxo iron(III) porphyrazine. **H. Gao**, J.T. Groves

2:30 INOR **939.** Investigating the bioinorganic chemistry of H_2S using small molecule model systems. **M.D. Pluth**

2:50 INOR **940.** OEC model complexes via application of a tunable carboxamide ligand scaffold. **N. McMillion**, J.S. Anderson

3:10 Intermission.

3:20 INOR **941.** Spectroscopic and electrocatalytic reduction studies of nitrite to NO by human serum albumin-heme. **M.I. Galinato**, E.M. Luteran, G.A. Fye, J.A. Bennett

3:40 INOR **942.** Functional role for the [4Fe4S] cluster in human DNA primase as a redox switch using DNA charge transport. **E. OBrien**, M. Holt, M.K. Thompson, L.E. Salay, A.C. Ehlinger, W.J. Chazin, J.K. Barton

4:00 INOR **943.** Revision of hydroxylamine oxidoreductase activities and bacterial ammonia oxidation pathways. **J.D. Caranto**, K.M. Lancaster

4:20 INOR **944.** Elucidating the reactivity of ferrous heme-P460 cofactors. **M. Smith**, K.M. Lancaster

4:40 INOR **945.** Metallodithiolenes revealed as unique chemical chameleons. **J.H. Enemark**, B.W. Stein, J. Yang, R. Mtei, N. Wiebelhaus, D. Kersi, D.L. Lichtenberger, M.L. Kirk

Section E

Renaissance Washington, DC Downtown
Grand Ballroom North

Organometallic Chemistry

Applications to Organic Transformations

N. S. Radu, *Organizer*

D. Lehnherr, A. N. Vedernikov, *Presiding*

1:30 INOR **946.** Redox activity of carbene ligands: Convergent and divergent radical-type pathways of metal-bound carbene radicals. **B. de Bruin**

1:50 INOR **947.** Cp*Ir(III)-catalyzed ortho halogenation of benzamides via C-H bond activation. **A.J. Guzman-Santiago**, E. Ison

2:10 INOR **948.** Mechanistic studies of a Re-catalyzed mono-alkylation of phenols. **D. Lehnherr**, M.D. Weisel, X. Wang, Y. Lam, H. Sheng, F. Peng, J.R. Naber, K.M. Maloney, I.W. Davies

2:30 INOR **949.** Bioinspired Mn(I) catalysts for CO_2 hydrogenation and transfer hydrogenation reactions. **A. Dubey**, J.R. Khusnutdinova

2:50 INOR **950.** Nonprecious metal catalysts for hydrogenation, hydrofunctionalization and dehydrogenative coupling reactions. **G. Zhang**

3:10 INOR **951.** Withdrawn.

3:30 INOR **952.** Large bite angle early transition metal biphenolate complexes as tunable catalysts for amine addition to alkenes. **J. Soltys**, A. Roller, K. Hultzsch

3:50 INOR **953.** Mechanistic studies of the Zn(II)/SiO2-catalyzed hydroamination of alkynes. **A.K. Cook-Sneathen**, C. Coperet

4:10 INOR **954.** Formation of carbazoles and indolines via oxidative intramolecular C-N coupling of amido aryl and amido alkyl Pd(II) complexes with H_2O_2 as oxidant: A mechanistic analysis. E. Abada, P.Y. Zavalij, **A.N. Vedernikov**

4:30 INOR **955.** Acceleration of Pd-catalyzed amide N-arylations using co-catalytic metal triflates: Substrate scope and mechanistic study. **J. Becica**, G. Dobereiner

4:50 INOR **956.** Expansion of boracarboxylated vinyl arenes: Exploring the synthetic elaboration of the carbon-boron bond through cross-coupling. **T. Perrone**, S. Knowlden, B.V. Popp

5:10 INOR **957.** Withdrawn.

Section F

Renaissance Washington, DC Downtown
Grand Ballroom Central

Bioinorganic Chemistry

DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

A. G. Tennyson, Y. Zheng, *Presiding*

1:30 INOR **958.** Synthesis, characterization, and biological activity of DNA mismatch-targeting rhodium complexes. **K. Boyle**, J.K. Barton

1:50 INOR **959.** Photoactivation of two fluorescent dyes via ruthenium(II) polypyridyl ligand exchange. **T.N. Rohrabaugh**, J.K. White, C. Turro

2:10 INOR **960.** Synthesis and characterization of dinuclear ruthenium complexes as mitochondrial calcium uptake inhibitors. **S.R. Nathan**, J. Urgiles, J. Woods, J. Wilson

2:30 INOR **961.** Withdrawn.

2:50 INOR **962.** Withdrawn.

3:10 Intermission.

3:20 INOR **963.** Rhodium-cyanine fluorescent probes for detection and signaling of mismatches in DNA. **A. Nano**, J.K. Barton

3:40 INOR **964.** Hydride donation by NAD^+ in biologically-relevant redox catalysis. **A.G. Tennyson**

4:00 INOR **965.** Nanoprecipitation of metallocages for platinum-based anticancer drug delivery. **Y. Zheng**, Z. Yue, H. Wang

4:20 INOR **966.** Withdrawn.

Nanoscale Sensing in Foods & Other Complex Media

Sponsored by AGFD, Cosponsored by ANYL, COLL, ENVR and INOR

MEDI

Division of Medicinal Chemistry

A. Stamford, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Chemical Biology of Infectious Disease (see *BIOL*, Wed)

Drug Discovery: Cheminformatic Approaches (see *CINF*, Wed)

Glycomimetics as Antibiotic-Sparing Therapeutics for Infectious Disease (see *CARB*, Sun)

Informatics & Chemical Biology: Identifying Targets & Biological Pathways (see *CINF*, Tue)

Toxicological Considerations in Antibody Drug Conjugate Design & Development (see *TOXI*, Tue)

What do Synthetic Chemists Want from Their Reaction Systems? (see *CINF*, Sun)

SOCIAL EVENTS:

MEDI Hall of Fame Reception (Open), 5:30 PM: Tue

Poster Session & Social Hour, 7:00 PM: Sun, Wed

BUSINESS MEETINGS:

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

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

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

SUNDAY MORNING

Section A

Walter E. Washington Convention Center
Room 146B

Treatment of Chronic Neuropathic Pain

K. A. Jacobson, D. Salvemini, *Organizers, Presiding*

8:30 MEDI **1.** Purine receptors as drug targets in pain. **K.A. Jacobson**, D.K. Tosh, A. Ciancetta, D. Salvemini

9:05 MEDI **2.** A_3 adenosine receptor subtype agonists as novel non-narcotic analgesics for neuropathic pain. **D. Salvemini**, K.A. Jacobson, D.K. Tosh, G. Bennett

9:40 MEDI **3.** Design of new antagonists of P2X and P2Y receptors. **C.E. Mueller**

10:15 MEDI **4.** Endocannabinoid system as a target for neuropathic pain treatment. **A. Makriyannis**

10:50 MEDI **5.** Benzo[c][2,7]naphthyridin-5(6*H*)-one and 5H-chromeno[3,4-*c*] pyridine as potent inhibitors of a novel serine/threonine kinase for the potential treatment of neuropathic pain. **C.D. Dzierba**

11:25 MEDI **6.** Biasing opioid receptor signaling away from opiate side effects. **L.M. Bohn**, T.D. Bannister

Section B

Walter E. Washington Convention Center
Room 146A

General Orals

A. W. Stamford, *Organizer*

J. R. Allen, *Presiding*

8:30 MEDI 7. 6-((2-Oxo-1-substituted-1,2-dihydropyridin-3-yl)amino)imidazo[1,2-b] pyridazine derivatives as potent, selective, and orally active Tyk2 JH2 inhibitors. **C. Liu**, J. Lin, R. Moslin, J.S. Tokarski, J. Muckelbauer, H. Park, P. Li, D. Wu, J. Strnad, A. Zupa-Fernandez, L. Cheng, C. Chaudhry, C. Huang, J. Chen, C. Chen, H. Sun, P. Elzinga, C. D'Arienzo, K. Gillooly, T.L. Taylor, K.W. McIntyre, L.M. Salter-Cid, L. Lombardo, P.H. Carter, N. Aranibar, J.R. Burke, D.S. Weinstein

8:50 MEDI **8.** Discovery of small molecule protease-activated receptor 2 (PAR2) antagonists and agonists using DNA-encoded library (DEL) screening technologies. **D.G. Brown**, A. Ferguson, H. Chen, L. Sundstrom, S. Geschwinder, A. Snijder, M. Saxin, J. Zhang, Y. Wu, H. Souter, D.M. Troast, C. Dumelin, G.A. Brown, R.K. Cheng, C. Fiez-Vandal, R. Cooke, R. Prihandoko, B. Tehan, G. Wiggin, A. Zhukov, M.S. Congreves, B. Teobald, O. Schlenker, Q. Liu, W. Yang, R. Chen, S. Johnstone, R. Burli, N. Dekker

9:10 MEDI **9.** Creating the ideal vaccine formulation: Attenuating inflammation while maintaining the adaptive response. **B. Moser**, R.C. Steinhardt, A.P. Esser-Kahn

9:30 MEDI **10.** High confidence protein-ligand complex modeling by NMR-guided docking enables early hit optimization. **A. Lingel**, D. Bussiere, A. Proudfoot

9:50 MEDI **11.** Identification of potent, selective, and cellularly-active KDM2B inhibitors by utilizing structure- and property-based design. **J. Liang**

10:10 MEDI **12.** Selectively targeting *MYC* expression with nucleic acid binding small molecules. **D. Calabrese**, E. Leon, S. Gaikwad, X. Chen, S. Alden, Z. Phyo, W. Hewitt, T. Hilimire, K. Walters, B. Mock, J. Schneekloth

10:30 MEDI **13.** Different modes of activation of the four regulatory pyruvate dehydrogenase kinases by the E2 and E3 binding protein components of the human pyruvate dehydrogenase complex. **E.L. Guevara**, L. Yang, N.S. Nemeria, J. Zhou, F. Jordan

10:50 MEDI **14.** Discovery of a selective androgen receptor degrader (SARD) for treatment of castration-resistant prostate cancer. Z. Yao, S.E. Wardell, I. Spasojevic, J.D. Norris, J.A. Katzenellenbogen, D.P. McDonnell, **J.S. Josan**

11:10 MEDI **15.** EGFR triple mutant: Recent set-backs and new hopes in fighting mutant non-small cell lung cancer. **S.A. Laufer**, M. Guenther, M. Juchum, E. Doering, M. Keul, J. Lategahn, H. Tumbrink, J. Engel, D. Rauh

11:30 MEDI **16.** Development and optimization of a selective MYST histone acetyltransferase inhibitor that induces cellular senescence. **D.J. Leaver**, B. Cleary, N. Nuyen, M. Chung, B.N. Sheikh, H. Falk, A.K. Voss, T. Thomas, J.B. Baell

11:50 MEDI **17.** Mnk1/2 and Abl inhibitions for the treatment of blast crisis chronic myelogenous leukemia. **K. Nacro**, J. Cherian, H. Yang, Y. Yeap, Z. Poh, L.R. Chennamaneni, S. Ang, E.S. Tan, A.J. Duraiswamy, A. Poulsen, J.K. Joy, B. Liu, E. Ong, M. Choon, P. Kwek, V. Pendharkar, V. Manoharan, V. Susmitha, C. Low, M. Lee, K. Sangthongpitag, S. Lim, C. Chua, S. Ong, J. Hill, T.H. Keller, A. Matter

Merck Research Award Symposium

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Glycomimetics as Antibiotic-Sparing Therapeutics for Infectious Disease

Targeting P. Aeruginosa Bacterial Lectins & Other Anti-Virulence Strategies

Sponsored by CARB, Cosponsored by MEDI

What do Synthetic Chemists Want from Their Reaction Systems?

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

SUNDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 146B

General Orals

A. W. Stamford, *Organizer, Presiding*

1:30 MEDI **18.** Integration of x-ray crystallography, computational modelling and NMR conformational analysis data in fragment-based drug design. **E. Tamanini**

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

1:55 MEDI **19.** NMR conformational signatures guide the design of macrocycle drug cell activity and permeability: AstraZeneca case studies. **A.Y. Balazs**, R. Carbajo, N. Davies, E. Chiarparin

2:20 MEDI **20.** Discovery of CC-671: A TTK/CLK2 inhibitor for the treatment of triple negative breast cancer. **J.R. Riggs**

2:45 MEDI **21.** Optimization of macrocyclic ring containing Mcl-1 inhibitors through SAR and rational design. **T. Kohn**

3:10 MEDI **22.** Discovery of GDC-0077: A highly selective inhibitor of PI3K-alpha that induces degradation of mutant-p110 alpha protein. **M. Braun**, C. Chan, S. Clausen, K. Edgar, C. Eigenbrot, R. Eliott, N. Endres, L. Friedman, K. Gerland, X. Gu, P. Hamilton, C. Han, E.J. Hanan, R. Hong, P. Jackson, S. Kelly, J. Knight, M. Lee, A. Lu, C. MacLeod, A. McKenzie, M. Nannini, R. Narukulla, A. Nguyen, J. Pang, H.E. Purkey, L. Salphati, D. Sampath, S. Schmidt, L. Schutt, R. Heald, K. Song, M. Ultsch, J. Xin, K. Yeap, A. Young, Z. Zhong, S.T. Staben

3:35 MEDI **23.** Discovery of the JAK1 selective kinase inhibitor AZD4205. **Q. Su**, J. Kettle, N. Grimster, M. Vasbinder, S. Kawatkar, S. Throner, R. Woessner, H. Chen, C. Chuaqui, G. Bebernitz, K. Bell, E. Anderson, L. Ruston, J. Winter-Holt, W. Yang, P. Lyne

4:00 MEDI **24.** Discovery of LY3200882: A highly specific and potent TGFβRI small molecule inhibitor. **S. Parthasarathy**

4:25 MEDI **25.** Discovery of BMS-135: An orally active imidazo[2,1-f][1,2,4]triazine pan-CK2 inhibitor for the treatment of cancer. **A.V. Purandare**, K. Zimmermann, W. Johnson, H. Wan, A.C. Hart, C.M. Tarby, L. He, B.E. Fink, A.V. Gavai, G. Vite, Y. Zhao, W. Vaccaro, T. Huynh, H. Mastalerz, J.A. Inghrim, J.S. Tokarski, X. Sang, B. Rupnow, C. Yu, J. Fargnoli, B. Henley, F. Lee, A. Fura, M. Oberneier, P.A. Elzinga, W. Foster, B. Sleczska, P. Arunachalam, A. Gupta, M. Vetrichelvan, N. Raghavan, Z. Yang, A. Mathur, R. Rampulla, D. Wu, P. Li, H. Klei, G. Everlof, S. Zhong, G. Locke, J.T. Hunt, J. Muckelbauer, W. Yong, T. Wong

4:50 MEDI **26.** Discovery of CC-90003: A covalent ERK1/2 inhibitor. **L. Qiao**

Section B

Walter E. Washington Convention Center
Room 146A

Biophysical Methods in Drug Discovery

M. J. Blanco, *Organizer*

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

2:00 Introductory Remarks.

2:05 MEDI **27.** Two photon fluorescence polarization microscopy for imaging and quantifying drug target binding *in vitro* and *in vivo*. **C. Vinegoni**, R. Weissleder

2:40 MEDI **28.** Cryo-EM applications from viruses to nanoparticles. **P.L. Stewart**

3:15 MEDI **29.** Discovering drug leads by practical NMR strategies. **S. Laplante**

3:50 MEDI **30.** Applications of SPR to drug discovery: Understanding LXRb agonist binding profile to two key serum proteins. **M.R. Witmer**, K. Behnia, S. Johngahr, Q. Wang, J. Smalley, D. Calambur, P. Marathe, D. Rodrigues, E.K. Kick

4:25 MEDI **31.** Not all sites are equal: Using biophysics to probe the biological relevance of fragment binding sites. **S. Saalau**

Glycomimetics as Antibiotic-Sparing Therapeutics for Infectious Disease

Targeting Uropathogenic *E. coli* Bacterial Adhesins & Other Anti-Virulence Strategies

Sponsored by CARB, Cosponsored by MEDI

What do Synthetic Chemists Want from Their Reaction Systems?

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

SUNDAY EVENING

Section A

Walter E. Washington Convention Center
Hall E

General Posters

A. W. Stamford, *Organizer*

7:00 - 9:00

MEDI **32.** New selective 5-HT_2B receptor antagonists for the treatment of fibrosis. **L. Pettersson**

MEDI **33.** Novel pirfenidone derivatives: Potent antifibrotic agents. **Z. Ma**, C. Yu, Q. Chen, W. Huang, Z. Wang, C. Zhang, Z. Shen

MEDI **34.** Discovery of novel benzo[*b*] thiophene tetrazoles as non-carboxylate GPR40 agonists. **M.R. Player**, H. Huang, M.P. Winters, S.K. Meegalla, S.P. Lee, T. Martin, J. Liu, M. Towers, F. Xu, H. Lim, J. Silva, M. Otieno, E. Arnoult, A. Pocai

MEDI **35.** GPR40 full agonists for the treatment of type 2 diabetes. **M.R. Player**, S.K. Meegalla, H. Huang, T. Martin, J. Xu, S. Zhao, J. Liu, M. Towers, J. Gunnet, Y. Wang, S.P. Lee, J. Silva, M. Otieno, E. Arnoult, A. Pocai

MEDI **36.** Discovery of clinical candidate MR1704: A novel isothiazole based GPR40 agonist for diabetes. **M. Okochi**

MEDI **37.** Discovery of a novel series of heterocycles as potent EP3 antagonists for the treatment of type 2 diabetes. **X. Zhang**, L. Guo, I. Bakaj, M. Rankin, G. Ho, K. Jack, S.P. Lee, L. Norquay, M.J. Macielag

MEDI **38.** Synthesis of 5-(3-(2-[18F] fluoroethoxy)phenyl)-1,3-dihydro-2*H*-benzofuro[3,2-e][1,4]diazepin-2-one as a new potential PET radioligand for P2X4 receptor. **M. Wang**, M. Gao, J. Meyer, J. Peters, H. Zarrinmayeh, P. Territo, G. Hutchins, Q. Zheng

MEDI **39.** Novel and widely-applicable method to uncover pharmacologically active metabolites using metabolic biotransformation, affinity selection-mass spectrometry, and 2D NMR technique. **X. Yang**, P. Dandliker, T. Zhang, E.C. Sherer, R.M. Helmy

MEDI **40.** Structural optimization of atropisomeric pyrrolopyrimidine RET kinase inhibitors. **S. Toenjes**

MEDI **41.** Molecular docking of potent MmpL3 inhibitors based on the indole-2-carboxamide scaffold. **J. Stec**, O. Onajole, S. Lun, H. Guo, B. Merenbloom, G. Vistoli, W. Bishai, A.P. Kozikowski

MEDI **42.** Longitudinal murine biodistribution and MRI study of a gavage-administered gadolinium pegylated metallofullerene nanoparticle. **Y. Kim**, T. Li, D. Smiley, A. Eltahir, D. Karolyi, S. LaConte, H.C. Dorn

MEDI **43.** Withdrawn.

MEDI **44.** Urea TrkA kinase inhibitors: How the hinge helped open the door to improved potency. **K. Jones**

MEDI **45.** Repurposing of a conformationally locked nucleoside scaffold: Enhanced activity at the dopamine and norepinephrine sodium symporters. **D. Tosh**, A. Janowsky, A. Eshleman, E. Warnick, Z. Gao, Z. Chen, E. Gizewski, J. Auchampach, D. Salvemini, K.A. Jacobson

MEDI **46.** Structure-based fragment growing and serendipity: First discovery of S1 benzylamine-derived potent and selective reversible inhibitors binding to an 'unlocked' conformation of the serine protease Complement Factor D. T. Yoon, A. Vulpetti, N. Ostermann, O. Rogel, A. Mac Sweeney, F. Cumin, S. Randl, E. Lorthiois, O. Simic, S. Rüdisser, P. Erbel, **J.K. Maibaum**

MEDI **47.** Organizing 3D project data for structure-based drug design. **E. Metwally**

MEDI **48.** Targeting specific interactions to improve EGFR-ligand binding. **N. Li**

MEDI **49.** MOEsaic: Application of matched molecular pairs to interactive SAR exploration. **A. Ajamian**

MEDI **50.** Exploiting solvent effects in drug design and optimization. **C. Williams**

MEDI **51.** Design, synthesis, and evaluation of potent and selective inhibitors of mono-(ADP-ribosyl)transferases, PARP10 and PARP14. **J. Holechek**, R. Lease, A. Thorsell, R. Grant, A. Keen, T. Karlberg, H. Schuler, D. Ferraris

MEDI **52.** Development of azole antifungal analogues to treat cancers dependent on Hedgehog signaling. **K.A. Teske**, J.R. Pace, A.M. DeBerardinis, M.K. Hadden

MEDI **53.** Development of novel NK3 receptor antagonists with reduced environmental impact. **K. Yamamoto**, H. Ohno, N. Fujii, S. Oishi

MEDI **54.** Synthesis of [11C]methyl 3-((2,2-difluoro-5*H*-[1,3]dioxolo[4',5':4,5] benzo[1,2-*d*]imidazol-6-yl)carbamoyl) benzoate as a new potential PET agent for imaging of casein kinase 1. M. Gao, **M. Wang**, Q. Zheng

MEDI **55.** Strategies for improving flash chromatography efficiency. **J.R. Bickler**, E. Denton

MEDI **56.** Mass-directed flash purification – a new tool for isolating natural products. **J.R. Bickler**, E. Denton

MEDI **57.** Synthesis and Structure–Activity Relationship (SAR) of tetra-substituted cyclohexyl diol inhibitors of pan-PIM kinases. **W. Han**

MEDI **58.** Morphing of antimicrobial peptides towards selective antibiotic agents. **A.T. Mueller**, J.A. Hiss, G. Schneider

MEDI **59.** Problem-based learning in drug discovery with MOE. **A. Bonin**

MEDI **60.** Identification and characterization of small molecule scaffolds as inhibitors of the translesion synthesis pathway. **Z. Ozen**, M.K. Hadden

MEDI **61.** Development of affinity probes for identification of the molecular target for a novel series of Rho/MRTF/SRF-mediated gene transcription inhibitors. **D. Kahl**, E. Mathes Lisabeth, S. Haynes, B. Martin, R. Neubig, S.D. Larsen

MEDI **62.** Asymmetric synthesis of novel antimalarial agents with fluorene core. J. Schneider, A. Dassonville-Klimpt, **J. Becker**, P. Sonnet

‡ *Cooperative Cosponsorship*

MEDI **63.** Small molecule and peptidic ligands as PCSK9-LDLR inhibitors. **S.K. Bhattacharya**, M. Ammirati, K.A. Borzilleri, O. Cheneval, B. Chrunyk, D. Craik, N. Daly, R. Dullea, M.C. Griffor, A.S. Kamlet, C. Limberakis, P. Sahasrabudhe, S. Liu, P.M. Loria, K.F. Mc Clure, E. Menhaji-Klotz, D. Petersen, D.W. Piotrowski, M. Popovska-Gorevski, D. Price, A. Reyes, R.B. Ruggeri, C. Schroeder, K. Song, J. Swedberg, I.A. Stock, M. Tu, J. Withka

MEDI **64.** Novel Wnt/β-catenin inhibitors for the treatment of colorectal cancer. **Y. Ai**, W. Yang, Y. Li, Y. Shu, F. Xue

MEDI **65.** Selective inhibition of Hedgehog (Hh) signaling by analogues of vitamin D3 and calcitriol. **C. Maschinot**, M.K. Hadden

MEDI **66.** Studies towards the identification of small molecule regulators of SWI/SNF chromatin remodeling. **A. Zaino**, M.K. Hadden

MEDI **67.** Imine-based dynamic combinatorial chemistry for discovery of multivalent RNA-binding ligands. **A. Umuhire-Juru**, A. Jan, A.E. Hargrove

MEDI **68.** Diversification of nitrogen containing fused heterocycles for selective recognition and binding to RNA. **N.N. Patwardhan**, B.S. Morgan, J. Forte, A.E. Hargrove

MEDI **69.** Targeting the EWS-FLI1 pre-mRNA in Ewing sarcoma through small molecule microarray screening. **R. Boer**, C. Neckles, D. Calabrese, G. Rangel-Rivera, S. Kim, N.J. Caplen, J. Schneekloth

MEDI **70.** Exploiting amino acid differences: Design, synthesis and biological evaluation of substituted pyrido[3,2-*d*]pyrimidines as potent and selective dihydrofolate reductase inhibitors for pneumocystis pneumonia infection. A. Gangjee, **K.S. Shah**, M.P. Ravindra, D.W. Seybert, M.T. Cushion

MEDI **71.** Chemistry of Canadian medical cannabis. **M.M. Lewis**, Y. Yang, E. Wasilewski, L.P. Kotra

MEDI **72.** Identification of a potent *in vivo* candidate inhibiting SHMT, an underexploited antimalarial target. **G. Schwertz**, M. Witschel, M. Rottmann, U. Leartsakulpanich, P. Chitnumsub, K. White, F.N. Diederich

MEDI **73.** Macrocyclic triazolopyridines as potent inhibitors of myeloperoxidase. **C.H. Hu**, J.M. Smallheer, M.N. Valente, O.S. Halpern, S.J. Jusuf, J. Khan, S.A. Shaw, B.P. Vokits, G.A. Locke, L.M. Abell, F.J. Duclos, R.R. Wexler, E.K. Kick

MEDI **74.** Design, synthesis, and anti-neoplastic evaluation of dimeric amino-naphthoquinones against acute myeloid leukemia (AML) cells. **P. Truong**, O. Kipe, V. Lam, B.A. Carter-Cooper, S. Dash, R.G. Lapidus, A. Emadi, D. Ferraris

MEDI **75.** Discovery and characterization of 1*H*-pyrazol-5-yl-2-phenylacetamides as novel, non-urea containing GIRK1/2 potassium channel activators. **S. Sharma**, J.M. Wieting, A.K. Vadukoot, K.K. Abney, T.M. Bridges, B. Vo, A. Andersone, K.D. Wickmane, C. Weaver, C.R. Hopkins

MEDI **76.** Design and development of new potent and selective inhibitors of NaV1.7. **P. Bergeron**, S. McKerrall, B. Safina, D.P. Sutherlin, D.F. Ortwine, T. Nguyen, C.M. Dehnhardt, S. Sun

MEDI **77.** Novel indole pharmacophore series of irreversible MPO inhibitors. **A. Patnaik**, L. Axford, N. Dales, L.G. Hamann, J. Marcinkeviciene, M. Marro, A.W. Patterson

MEDI **78.** Novel inhibitors of the NLRP3 inflammasome. **J. Fulp**, L. He, Y. Jiang, S. Zhang

MEDI **79.** Synthesis of novel tanshinones for probing the inflammatory response in zebrafish. **M.J. Foulkes**, S. Jones, S.A. Renshaw

MEDI **80.** Small molecule activators of the leukotriene A4 hydrolase enzyme for pulmonary inflammation. **K. Lee**, G. Petruncio, M. Burdick, S.M. Noble, Y.M. Shim, M. Paige

MEDI **81.** Synthesis, docking and biological evaluation of certain class of nonsteroidal anti-inflammatory drugs as fatty acid amide hydrolase inhibitors. **I.S. Saad**, F.A. Alasmary, M.E. EL-Araby

MEDI **82.** Anti-proliferative and anti-inflammatory estrogen receptor modulators. **K. Cagasova**, S. Rajalekshmi Devi, A. Arneson, N. Fox, S. Srinivasan, K. Carlson, T. Martin, J.A. Katzenellenbogen, K. Nettles, J.S. Josan

MEDI **83.** Synthesis of natural 1α,20S-dihydroxyvitamin D3 as a potent vitamin D receptor agonist and anti-inflammatory agent. **Z. Lin**, H. Chen, A. Belorusova, J. Bolinger, E. Tang, Z. Janjetovic, T. Kim, J. Wu, D.D. Miller, A. Slominski, A. Postlethwaite, R. Tuckey, N. Rochel, W. Li

MEDI **84.** Phospholipase A2: A pharmaceutical target to diminish inflammation. **V.D. Mouchlis**, J. McCammon, E.A. Dennis

MEDI **85.** Design and synthesis of curcumin conjugates as potential anti-inflammatory agents. **S.S. Panda**, A.S. Girgis, S.J. Thomas

MEDI **86.** Selective JAK1 inhibitors for treatment of inflammatory diseases: Design and synthesis. **M.D. Parikh**, R.P. Robinson

MEDI **87.** Design and synthesis of *N*-alkylated tubulysin analogs and their folate conjugates. I.R. Vlahov, **F. You**, K.Y. Wang, H.K. Santhapuram, H.F. Klein, M. Vetzel, J. Reddy, C.P. Leamon

MEDI **88.** Pro-Pyrrolobenzodiazepine (pro-PBD) bioconjugates, part 1: Design and synthesis of pro-PBD conjugates containing a cleavable disulfide linker. I.R. Vlahov, **L. Qi**, P.J. Kleindl, S.J. Hahn, K.Y. Wang, J.F. Vaughn, H.K. Santhapuram, M. Vetzel, M. Nelson, J. Reddy, C.P. Leamon

MEDI **89.** Targeted folate-aminopterin anti-inflammatory conjugates: Synthesis and activity of an enzymatically labile lysine-linked conjugate and its pegylated analogs. **P.J. Kleindl**, F. You, H.K. Santhapuram, H.F. Klein, S.J. Hahn, J. Lu, S. Rao, M. Pugh, V. Cross, C.P. Leamon, I.R. Vlahov

MEDI **90.** Targeted folate-aminopterin anti-inflammatory conjugates: Optimization of a reductively/enzymatically labile cysteine-derived linker system. **P.J. Kleindl**, F. You, H.K. Santhapuram, J.F. Vaughn, H.F. Klein, J. Lu, S. Rao, M. Pugh, V. Cross, C.P. Leamon, I.R. Vlahov

MEDI **91.** Pro-Pyrrolobenzodiazepine (pro-PBD) bioconjugates, part 2: Design and synthesis of pro-PBD conjugates containing an enzyme-responsive linker. I.R. Vlahov, **N. Zou**, A. Felten, K.Y. Wang, S.J. Hahn, C.P. Leamon

MEDI **92.** Withdrawn.

MEDI **93.** Discovery of potent antiallodynic agents for neuropathic pain targeting P2X3 receptors. **Y. Jung**, Y. Kim, H. Lin, J. Cho, J. Park, S. Lee, J. Bae, K. Kang, Y. Kim, A. Pae, H. Ko, C. Park, M. Yoon, Y. Kim

MEDI **94.** Pyrrolo-triazine derivatives as atypical antipsychotics for the treatment of schizophrenia. **M. Rasheed**, A.K. Shinde, M. Dasoju, S. Gagginapally, V. Middekadi, R. Subramanian, G. Bhyrapuneni, P. Jayarajan, V. Nirogi

MEDI **95.** Preclinical characterization of indole carboxamide derivatives: Novel, potent and selective muscarinic M1 positive allosteric modulators. **A.K. Shinde**, M. Rasheed, R.K. Badange, V. Reballi, K. Bojja, S. Kommineni, S. Manchineela, V. Goyal, S. Pandey, V. Benade, P. Jayarajan, V. Nirogi

MEDI **96.** Towards the development of a peptide-PROTAC conjugate targeting a viral protein: Rational design and optimization of a stapled alpha-helical peptide that binds HPV16 E2 protein. **S.L. Richardson**, M.C. Hartman

MEDI **97.** Synthesis and biological evaluation of phosphoantigens for gamma-delta T cell stimulation. **M.M. Poe**, C. Hsiao, A.J. Wiemer

MEDI **98.** Synthesis and evaluation of vitamin D3-based probes for cellular target(s) verification. **J. Wen**, M.K. Hadden

MEDI **99.** Design and synthesis of siderophore-antibiotic conjugates. J. Jourdan, A. Dassonville-Klimpt, C. Mullié, **J. Becker**, P. Sonnet

MEDI **100.** Design and validation of a peptidomimetic ligand as a translesion synthesis inhibitor. **R. Dash**, M.K. Hadden

MEDI **101.** Strategies for the modulation of protease-activated receptors (PARs). **D. Gandhi**, M. Majeswski, R. Rosas, T.J. Foster, K. Kentala, A. Stephans, K. Kurtenbach, R. Engel, K. Lucknow, C. Dockendorff

MEDI **102.** Withdrawn.

MEDI **103.** Discovery of novel class of alpha selective PI3K inhibitors. **K. Garland**, E.J. Hanan, S.T. Staben, M. Braun, K. Edgar, N. Endres, L. Friedman, A. Nguyen, J. Pang, H.E. Purkey, L. Salphati, S. Schmidt, K. Song, M. Ultsch, A. Jaochico, C. Chan, C. Eigenbrot, C. MacLeod, P. Jackson, R. Narukulla, J. Knight, K. Yeap, K. Messick, N. Valle, R. Heald, M. Nannini, P. Hamilton, S. Clausen, A. Young, D. Sampath, R. Hong, M. Lee, T. Blench, R. Elliott, A. Lu, X. Gu, J. Xin

MEDI **104.** Discovery of pan-active and isoform selective inhibitors of class I phosphoinositide-3-kinases (PI3Ks) utilizing a DNA-encoded discovery platform. **C.D. Hupp**, D.I. Resnicow, D. Gikunju, M.A. Clark, Y. Zhang, A.D. Keefe, J.W. Cuozzo, E.A. Sigel, P.A. Centrella, M.A. Guie, S. Habeshian, K.M. Kennedy

MEDI **105.** Potent and selective PI3Kδ inhibitors: Structure-activity relationships of 8-alkoxy-2-(benzimidaz-ol-1-yl)-6-morpholinopurines. **J. Li**, B. Safina, Z.K. Sweeney, D.P. Sutherlin

MEDI **106.** Discovery of naldemedine (S-297995): A potent and orally available opioid receptor antagonist for treatment of opioid-induced adverse effects. **M. Inagaki**, M. Kume, Y. Tamura, S. Hara, Y. Goto, T. Hasegawa, N. Haga, K. Koike, H. Chiba, M. Imai, T. Nakamura, S. Mihara, S. Ohnishi, Y. Ishihara, T. Kanemasa, H. Kai

MEDI **107.** Synthesis and biological evaluation of matrix metalloproteinase 9 inhibitors for cancer therapeutics. **X. Ren**, V. Alford, Q. Gan, M. Awwa, I. Ojima

MEDI **108.** Addressing a large active site: Inhibition of trypanothione reductase with cyclohexylpyrrolidine-based ligands. **R.E. De Gasparo**, E. Persch, S. Bryson, M. Kaiser, E.F. Pai, R. Krauth-Siegel, F.N. Diederich

MEDI **109.** Stereoselective synthesis of rhodotorulic acid analogues with potential siderophore properties. T. Garnerin, A. Dassonville-Klimpt, **J. Becker**, P. Sonnet

MEDI **110.** Structure-based drug design of novel ASK1 inhibitors using an integrated lead optimization strategy. **T.S. Gibson**, B. Johnson, A. Fanjul, P. Halkowycz, D.R. Dougan, D.C. Cole, S. Swann

MEDI **111.** Lead identification of activators of the Nrf2 pathway via targeting repression of Bach1. **H. Nie**, A. Davis, J.F. Callahan, R. Carr, J.K. Kerns, A. Lakdawala-Shah, T. Li, B. McCleland, J. Kou, R. Osborn, W. Rumsey, Y. Sanchez, T. Sweitzer, L. Wolfe, J. Yonchuk, H. Yan

MEDI **112.** Novel thiophene analogs as potential MEK5/ERK5 inhibitor. **M. Gupta**, P.T. Flaherty, A. Bhatt, T. Wright, J. Cavanaugh

MEDI **113.** Design and synthesis of phenylthiourea emetine analogs for studies in prostate cancer. **N. Idris**, E.S. Akinboye, O. Bakare

MEDI **114.** Improving solubility, permeability and bioavailability of imatinib using crystal engineering approach with nicotinamide and glutamic acid. **M. Kumar Gautam**, M. Besan, R. Chadha

MEDI **115.** Identification of novel 5,6-dimethoxy indan-1-one derivative as potent antiviral agent. S.A. Patil, V. Patil, R. Patil, K. Beaman, **S. Patil**

MEDI **116.** Phosphatase-stable peptidomimetic ligands of the polo-like kinase 1 polo-box domain. **D. Hymel**, T.R. Burke

MEDI **117.** Exploration of intramolecular protein-protein interaction inhibitors of polo-like kinase 1. **K. Tsuji**, D. Hymel, T.R. Burke

MEDI **118.** Application of oxime-diversification to optimize ligand interactions within a cryptic pocket of the polo-like kinase 1 polo-box domain. **X. Zhao**, D. Hymel, T.R. Burke

MEDI **119.** Novel 5-substituted pyrrolo[2,3-*d*]pyrimidines with pyridine glutamate side chain as selective folate receptors and proton-coupled folate transporter substrates: Potential targeted chemotherapeutic agents. A. Gangjee, **A.B. Doshi**, L.H. Matherly, Z. Hou, A. Dekhne, C. O'Connor, A. Wallace-Povirk

MEDI **120.** Design of alkylarylsubstituted targeted thieno[2,3-*d*]pyrimidines as cancer chemotherapeutic agents with fluorine insertion on aryl the side chain. **N. Tong**, A. Gangjee, L.H. Matherly, Z. Hou, C.E. O'connor, A.W. Povirk, A.S. Dekhne

TECHNICAL PROGRAM

MEDI **121.** Optimizing the cystargolide scaffold for the selective treatment of cancer by proteasome inhibition. **L. Hallada**, D. Niroula, S. Ganegamage, M. Groll, C. Le Chapelain, S. Rogelj, R. Tello-Aburto

MEDI **122.** Coupled enzyme assay for screening of effector molecules of nicotinamide mononucleotide adenylyltransferase (NMNAT). **B.A. Haubrich**, C. Ramesha, D.C. Swinney

MEDI **123.** Identification and characterization of a new series of calcium/calmodulin-dependent protein kinase kinase-2 (CAMKK2) inhibitors. **Y. Liang**, R. Counago, M. Stashko, T. Willson, C. Zhang, W.J. Zuercher, D. Drewry

MEDI **124.** Palladacycle-facilitated ligand-free Suzuki coupling of hindered aryl bromides yields potent and selective COX-2 inhibitors. **M.S. Elsayed**, S. Chang, M. Cushman

MEDI **125.** Design, synthesis and evaluation of 8-(methylamino)-2-oxo-1,2-dihydroquinoline derivatives as novel DNA gyrase and topoisomerase IV inhibitors. **F. Ushiyama**, H. Amada, T. Yoshizumi, Y. Mihara, J. Yamagishi, A. Masuko, K. Fujita, M. Mima, H. Okumura, H. Sugiyama, N. Ohtake

MEDI **126.** Evaluation of a FLT3 inhibitor as an anti-leukemic agent for acute myeloid leukemia. **P. Jeong**, J. Lee, H. Lee, J. Baek, J. Choi, Y. Chin, Y. Choi, Y. Kim, S. Han

MEDI **127.** Incorporation of a biguanide scaffold enhances uptake by organic cation transporters (OCT) 1 and 2. **A. Coutinho**, O.N. Obianom, W. Yang, H. Yang, F. Xue, Y. Shu

MEDI **128.** P38 MAPK kinase inhibitor for steroid insensitive asthma. **L. Wu**, L. Zhang, L. Zhao, J. Sun, D. Yu, J. Wang, X. Li, S. Han, J. Li, S. Chen

MEDI **129.** Design, synthesis and biological evaluation of heteroaryl amine derivatives as potential anticancer agents. **M. Besan**, S. Shrivastava, R. Srivastava

MEDI **130.** Method for the analysis and quantification of 3-methylene furanone: A biomarker of oxidative damage to DNA. **H.T. Tchienga**, M. Bedi, A.C. Bryant-Friedrich

MEDI **131.** Discovery of (3S,4R)-1-(1-(2-chloro-6-cyclopropylbenzoyl)-4-fluoro-1H-indazol-3-yl)-3-hydroxypiperidine-4-carboxylic acid as potent and selective allosteric inhibitors of RORγt for the treatment of autoimmune diseases. **H. Zhang**, K.J. Barr, N.J. Anthony, C. Correll, H. Ferguson, G. Parthasarathy, J. Maclean, M. Richard, B. Trotter

MEDI **132.** Design, synthesis, and biological evaluation of flexible acyclic nucleoside analogues against human coronaviruses and filoviruses. **M. Yates**, A. Falat, K.L. Seley-Radtke

MEDI **133.** Dentification of novel inhibitors of glucose transporter 3 (GLUT3) through structure-based virtual screening. **S. Zhang**, C. Libby, C.E. Augelli-Szafran, A.B. Hjelmeland, W. Zhang

MEDI **134.** Withdrawn.

MEDI **135.** Glutathione as an herbal molecule with potential for zinc chelation therapy. **M. Russo**, A. Mousavi

MEDI **136.** Non-psychoactive cannabinoid CBD modulates the orphan receptor GPR3. **P. Morales Lázaro**, A. Laun, D. Hurst, Z. Song, P. Reggio

MEDI **137.** Reduced synthesis time of an acidic α-diimine ligand using flow chemistry. **J.E. Silver**, C. Reber, R. Sorgo, E. Bitz, R. Ivy, R. Lewis

MEDI **138.** Panamanian cyanobacterial metabolite with antitrypanosomal activity. **K. Ahmed**, C. Spadafora, K.J. Tidgewell

MEDI **139.** Investigating the impact of pore size and chain length when purifying peptides. **J.E. Silver**, C. Reber, R. Sorgo, E. Bitz, R. Ivy, R. Lewis

MEDI **140.** Optimal light conditions and nitrogen treatments for growth and for accumulation of phytochemical groups in *Calendula officinalis*. **P. Tuladhar**

MEDI **141.** Identification and optimization of 4-anilinoquinolines as selective inhibitors of cyclin G associated kinase. **C.R. Asquith**, T. Laitinen, J.M. Bennett, P.H. Godoi, G.J. Tizzard, J.M. Elkins, T. Willson, W.J. Zuercher

MEDI **142.** Targeted antitumor agents for the inhibition of one-carbon metabolism associated with purine biosynthesis: Altering sterics, electronics and conformation for tumor selectivity and potency. A. Gangjee, **M.P. Ravindra**, A. Wallace-Povirk, C. O'Connor, A. Dekhne, Z. Hou, L.H. Matherly

MEDI **143.** Discovery of N-substituted 2-phenylcyclopropylmethylamines as functionally selective serotonin 2C (5-HT2C) receptor agonists for potential use as antipsychotic medications. **G. Zhang**, J. Cheng, J.D. McCorvy, P.J. Lorello, B.J. Caldarone, B.L. Roth, A.P. Kozikowski

MEDI **144.** Design and synthesis of 1,4-benzodioxane-6-carboxylic acid derivatives for studies in prostate cancer drug development. **N. Idris**, O. Bakare

MEDI **145.** Development of thiol specific fluorogenic agents for cell surface thiol imaging in live cells. **Y. Alqahtani**, S. Wang, X. Guan

MEDI **146.** Efforts towards the development of new ERRg modulators via structure-based drug design. **C.S. Hampton**, K.M. Haynes, S. Banerjee, S. Sitaula, C. Billon, K. Griffett, J.C. Chrivia, T.P. Burris, J.K. Walker

MEDI **147.** Targeting inhibitor of apoptosis proteins: Identification of potent dimeric antagonists of IAPs. **H.L. Perez**, K.S. Kim, E.M. Stang, D.D. Wei, L. Zhang, G. Vite, J.T. Hunt, R.L. Talbott, J. Gan, R.M. Borzilleri

MEDI **148.** Optimization of quinazoline derivatives as selective MEK5 inhibitors. **S.B. Patel**, A.J. Motta, P.T. Flaherty, A. Bhatt, T. Wright, J. Cavanaugh

MEDI **149.** Potent and selective inhibitors of receptor-interacting protein kinase 1 that lack an aromatic back pocket group. **G. Hamilton**

MEDI **150.** Novel 6-substituted pyrrolo[2,3-*d*] pyrimidines with substituted nitrogen bridges and fluorinated benzoyl regioisomers as selective folate receptor substrates and antitumor agents. A. Gangjee, **X. Li**, A. Wallace-Povirk, C. O'Connor, A. Dekhne, Z. Hou, L.H. Matherly

MEDI **151.** Design, synthesis and *in combo* antidiabetic bioevaluation of multitarget phenylpropanoic acids. **G. Navarrete Vazquez**, B. Colin-Lozano, S. Estrada-Soto, J. Almanza-Pérez, X. Xie, U. Mura

MEDI **152.** Phytochemical approach for therapeutic efficacy enhancement of FeNP: As biomedicine. **A. Mubayi**, G. Watal

MEDI **153.** PTX-NPs encapsulated by metal-polyphenol: Synthesis and cytotoxicity. **M. Hung**, P. Li, W. Liu, Y. Yang

MEDI **154.** Synthesis of α,β-unsaturated phosphonate esters as DXR inhibitors. **K. Heidel**, R.C. Brothers, R. Edwards, A. Haymond, H.I. Boshoff, M.J. Meyers, S. Arnett, A. Rodriguez, A.R. Odom, C.S. Dowd

MEDI **155.** Synthesis of enantiopure 10-nornaltrexone as potential TLR-4 antagonist and opioid receptor ligand. **C.A. Herdman**, A.E. Jacobson, K.C. Rice

MEDI **156.** Targeted BET protein degradation for the treatment of acute myeloid leukemia (AML) and acute lymphoma leukemia (ALL). **J. Hu**, F. Xu, E. Fernandez-Salas, D. McEachern, S. Przybranowski, B. Wen, D. Sun, S. Wang

MEDI **157.** Design, synthesis and evaluation of potent DNA-alkylating agents for use in antibody-drug conjugates (ADCs). E.E. Reid, K.E. Archer, C. Bai, N.C. Yoder, D. Vitharana, L. Lanieri, M. Bogalhas, R. Wu, Q. Qu, E.K. Maloney, O. Ab, J.F. Ponte, R.V. Chari, **M.L. Miller**

MEDI **158.** Towards a structure-based pharmacophore for the transient potential melastatin 8 (TRPM8) ion channel: Ligand recognition at the menthol receptor. **V.B. Journigan**, C.E. Heffner

MEDI **159.** Development of bis{*N,N'*-rhodamine-7,7'-aminosulfonyl(benzo[c][1,2,5]oxadiazol-4-yl)}sulfane (BiROS) as a thiol specific fluorogenic agent for mitochondrial thiol imaging in live cells. **S. Wang**, H. Yin, Y. Li, X. Guan

MEDI **160.** Design, synthesis, and evaluation of glutathione-cholesterol sulfide and its derivatives as brain-targeting agents. **Y. Huang**, S. Wang, A. Najmi, X. Guan

MEDI **161.** Defining the pharmacokinetic and pharmacodynamic parameters of potent and selective heteroaryl sulfonamide NaV1.7 inhibitors with robust *in vivo* analgesic activity. **B. Milgram**

MEDI **162.** Novel isoprenoid triazole bisphosphonates as potential GGDPS inhibitors. **R.A. Mattheissen**, M.L. Varney, S.A. Holstein, D.F. Wiemer

MEDI **163.** Withdrawn.

MEDI **164.** Design and synthesis of bicyclic piperazine sulfonamides leading to highly potent HIV protease inhibitors. **C.J. Bungard**

MEDI **165.** Identification of potent 17β-hydroxysteroid dehydrogenase type 3 (17β-HSD3) inhibitors by systematic structural modifications of the lead compound RM-532-105. **F. Cortés-Benítez**, J. Roy, M. Perrault, R. Maltais, D. Poirier

MEDI **166.** Targeting cancer cell metabolism using sugar-based small molecules. **F. Ndombera**

MEDI **167.** Smart and targeted delivery of an anticancer active copper complex: *In vitro* and *in vivo* studies. A. Pramanik, K. Somasundaram, **A.G. Samuelson**

MEDI **168.** Ferrocene based Fe-Sn heterobimetallics: Synthesis and DNA binding potentials. **A. Altaf**, N. Khan, A. Badshah, B. Lal

MEDI **169.** Design and synthesis of novel pH-responsive multifunctional lipid-like carriers for siRNA delivery. **Z. Sun**, H. Jiang, J. Qin, D. Sun, Z. Lu

MEDI **170.** 3D imaging detection method of HER2: Application of conjugated affibody-quantum dots probes and ratiometric analysis. **P.I. Pérez Treviño**, H. Hernández de la Cerda, N. García, J. Altamirano

MEDI **171.** Improving solubility of thieno[2,3-*d*]pyrimidine based FLT3 inhibitor via structural modifications at the C_2 and C_6 position. **C. Oh**, H. Kim, G. Han

MEDI **172.** Dendrimer-based multifunctional conjugates of new-generation taxoids for tumor-targeted drug delivery. **Y. Sun**, L. Wei, I. Ojima

MEDI **173.** Synthesis of flexible, purine analogue inhibitors of NCp7. **T. Ku**, K.L. Seley-Radtke, Y. Arefeayne

MEDI **174.** Discovery of novel series of LasR quorum sensing inhibitors in *Pseudomonas aeruginosa*. P. Suman, L.J. Perez, **S.C. Jonnalagadda**

MEDI **175.** Cefiderocol (S-649266): A new siderophore cephalosporin exhibiting potent activities against *Pseudomonas aeruginosa* and other gram negative-pathogens including multi-drug resistant bacteria: Structure activity relationship. **T. Aoki**, H. Yoshizawa, K. Yamawaki, K. Yokoo, J. Sato, S. Hisakawa, Y. Hasegawa, H. Kusano, M. Sano, H. Sugimoto, Y. Nishitani, Y. Yamano, T. Sato, M. Tsuji, R. Nakamura, T. Nishikawa

MEDI **176.** Inhibiting effect of essential oils and methylglyoxal with carrier oils on the growth of *Pseudomonas aeruginosa*. **A. Patel**, J.P. Mack, A. Rojtman

MEDI **177.** Inhibition of the *Pseudomonas aeruginosa* heme oxygenase. **E. Robinson**, D. Liang, K. Hom, A. Wilks, F. Xue

MEDI **178.** Discovery of 1H-benzo[d] imidazol-2-yl-methyl-spiro [cyclopropane-1,3′-indolin]-2′-one derivatives as fusion inhibitors for treatment of respiratory syncytial virus infection. **H. He**

MEDI **179.** Molecular-based design, synthesis and docking studies of new benzimidazole derivatives as potential bacterial peptide deformylase inhibitors. **S.E. Kassab**

MEDI **180.** Discovery of small molecules that inhibit the LRS-RagD interaction and their potential use as anti-cancer drugs. **K. Jung**, C. Lee, G. Han

MEDI **181.** First insight into structure-activity relationships of selective Meprin β inhibitors. **D. Ramsbeck**, A. Hamann, D. Schlenzig, S. Schilling, M. Buchholz, H.U. Demuth

MEDI **182.** Evaluating p97 inhibitor analogues for potency against different p97-p97 cofactor complexes. **T. Chou**

MEDI **183.** Examining the activity of HIV protease inhibitors against human endogenous retrovirus-K: A potential treatment for amyotrophic lateral sclerosis. **R. Abrams**, R. Tyagi, W. Li, M. Bianchet, A. Nath

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

‡ *Cooperative Cosponsorship*

MEDI **184.** Evaluating fosmidomycin analogs as antimicrobial agents through 1-Deoxy-D-xylulose-5-phosphate reductoisomerase (Dxr) inhibition. **X. Wang**, R. Edwards, A. Haymond, R.C. Brothers, H.I. Boshoff, R.D. Couch, A.R. Odom, C.S. Dowd

MEDI **185.** Withdrawn.

MEDI **186.** N6-benzyladenosine derivatives inhibit replication of RNA viruses from *Flavivirus* and enterovirus geni. **A. Orlov**, M.S. Drenichev, V.E. Oslovsky, L.I. Kozlovskaya, G.G. Karganova, V.A. Palyulin, S.N. Mikhailov, D.I. Osolodkin

MEDI **187.** Pharmacolofical protection of mitochondrial function mitigates acute limb ischemia/reperfusion injury. **X. Yan**, S. Hou, L. Bi

MEDI **188.** Catch and release strategy to treat bacterial infections. **M. Royzen**, J.M. Mejia Oneto

MEDI **189.** Multi-target molecular profiling using MOE: A CYP450 isoform selectivity case study. **M.R. Goldsmith**, C. Williams, A. Ajamian, P. Labute

MEDI **190.** Phytoestrogens: New ligands targeting the estrogen receptor domains. **V. Thakor**, A. Shaikh, M. Noolvi

MEDI **191.** Structure-based drug design of new indole and benzpyrazole analogs with expected activity. **A. Shaikh**, V. Thakor

MEDI **192.** Rapid identification and optimization of a novel CGRP receptor antagonist chemotype. **B.M. Crowley**, C.M. Potteiger, D.N. Nguyen, J. Lim, C. Wang, H. Mitchell, K. Schirripa, M. McWherter, R. Gilfillan, M. Patel, K.L. Arrington, E.L. Moore, J.G. Bruno, A. Kemmerer, A. Soni, R.B. White, D. Cui, A. Danziger, S.T. Harrison, J.C. Culberson, H. Su, G. Parthasarathy, I.M. Bell, M.E. Fraley, S.D. Mosser, C. Fandozzi, C.A. Salvatore, C.S. Burgey

MEDI **193.** Discovery of (*E*)-(4-(3-methylbut-2-en-1-yl)-3-(3-phenylpropanamido) cinnamic acid as highly potent and selective inhibitor of AKR1C3 for the treatment of castration-resistant prostate cancer (CRPC) and acute myeloid leukemia (AML). **K. Verma**, T. Zang, T.M. Penning, P.C. Trippier

MEDI **194.** Synthesis of *β*-monoadducts using oligonucleotides. **W.G. Aguilar**, E. Champeil

MEDI **195.** Profiling CD8 T cells in tumor microenvironment using PEGylated single domain antibodies and immunoPET. **M. Rashidian**, M. Dougan, J. Ingram, A. Dongre, K. Whang, H. Ploegh

MEDI **196.** Synthesis of ^{11}C labeled RXR partial agonist CBt-PMN by [^{11}C] carbon dioxide fixation via organolithiation of trialkyltin precursor and PET imaging thereof. **O. Shibahara**, M. Watanabe, M. Akehi, T. Sasaki, T. Hanada, A. Akahoshi, H. Hirano, H. Kakuta

MEDI **197.** Predicting ADME and PK properties of antivirals for Ebola. **M.A. Lingerfelt**, K. Zorn, J.S. Freundlich, M. Anantpadma, G. Rao, R. Davey, P. Madrid, S. Ekins

MEDI **198.** Interdiction at a protein—protein interface: Structure-based design and optimization of spirocyclic Mcl-1 inhibitors. **K. Li**, S.P. Brown

MEDI **199.** Indole-TEMPO conjugates alleviate ischemia-reperfusion injury via attenuation of oxidative stress and preservation of mitochondrial function. **S. Hou**, X. Yan, L. Bi

MEDI **200.** Development of prolinol based derivatives targeting sphingosine kinase-1. **H. Li**, Y. Kharel, K. Lynch, W.L. Santos

MEDI **201.** Aryl ring modifications of sphingosine kinase 2 selective inhibitors. **C. Sibley**, Y. Kharel, K.R. Lynch, W. Santos

MEDI **202.** Investigation of the oprin protein from North American opossum (*Didelphis virginiana*) as a potential inhibitor of Western diamondback rattlesnake (*C. atrox*) venom metalloproteinases. **R.M. Werner**

MEDI **203.** Synthesis and cytotoxicity of Baylis-Hillman reaction derived betulinic acid analogs. P. Suman, A. Patel, L. Solano, A. Indukuri, S.K. Kommineni, **R.M. Rutkoski**, M. Collins, **S.C. Jonnalagadda**

MEDI **204.** Design of *α*-(benzoboroxolyl) and *α*-(benzoboroxolylmethyl) acrylamides as potential anti-cancer agents. P. Suman, M. Ur Rahman, M. Islam, P.M. Mastoridis, R. D'Souza, **S.C. Jonnalagadda**

MONDAY MORNING

Section A

Walter E. Washington Convention Center
Room 146B

Insights on Medicinal Chemistry from Hardcore Practitioners

J. Barrow, *Organizer, Presiding*

8:30 MEDI **205.** Roles of chemists and chemical technology in a changing drug discovery environment. **P.R. Bernstein**

9:05 MEDI **206.** Adventures in the discovery of excitatory amino acid antagonist therapeutics: The value of perseverance. **P.L. Ornstein**

9:40 MEDI **207.** Role of tacit knowledge in medicinal chemistry. **R.L. Dow**

10:15 MEDI **208.** Find out what you don't know: A recurring lesson from years of lead generation research. **M.R. Wiley**

10:50 MEDI **209.** Tales from the hood: Three vignettes focused on optimization of human dose. **H.B. Wood**

Section B

Walter E. Washington Convention Center
Room 146A

Addiction: The Unmet Medical Need of the 21st Century

J. V. Aldrich, *Organizer*

M. J. Blanco, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 MEDI **210.** Addictive diseases: Molecular neurobiology, behavior, human genetics, and treatments. **M. Kreek**

9:15 MEDI **211.** Discovery of selective orexin-1 receptor antagonists. **B.T. Shireman**, C. Preville, J.M. Ziff, C.A. Dvorak, H. Coate, C. Gelin, T. Lebold, P. Bonaventure, C. Dugovic, T. Koudriakova, B. Lord, D. Nepomuceno, J. Shelton, T. Lovenberg, N.I. Carruthers

9:50 Intermission.

10:05 MEDI **212.** Targeting the dopamine D3 receptor for treatment of opioid and cannabis use disorders. **A.H. Newman**

10:40 MEDI **213.** Substance use disorders: Vaccination as a therapeutic strategy. **K.D. Janda**

11:15 MEDI **214.** Development of M5 muscarinic acetylcholine receptor negative allosteric modulators for the treatment of opioid use disorder. **C.K. Jones**

11:50 Concluding Remarks.

Modeling & Measuring Protein-Ligand Kinetics & Residence Times

Sponsored by COMP, Cosponsored by MEDI and PHYS

MONDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 146B

Encoded Technologies for Lead Generation, Successes & Challenges

H. Deng, K. Leftheris, N. V. Prabhu, *Organizers*

J. Messer, *Organizer, Presiding*

K. Leftheris, *Presiding*

1:30 Introductory Remarks.

1:40 MEDI **215.** ALIS affinity selection in pharmaceutical discovery. **P. Dandliker**

2:10 MEDI **216.** Synthesis strategies to DNA-encoded small molecule libraries – of a chemoresistant sequence, and micellar nanoreactors. **A. Brunschweiger**, M. Klika Skopic, H. Salamon

2:40 MEDI **217.** DNA-encoded library technology (ELT): Challenges and advances in chemistry and library development. **Y. Ding**

3:10 Intermission.

3:25 MEDI **218.** *In vitro* selection assays: New approaches and applications. **C.J. Krusemark**, K.E. Denton, D. Kim, R. Jetson

3:55 MEDI **219.** Revolution will be compartmentalized: Technology for next-generation small molecule discovery. **B. Paegel**

4:25 MEDI **220.** Application of DNA-encoded technology to lead generation of challenging targets. **Y. Zhang**

Section B

Walter E. Washington Convention Center
Room 146A

Off Targets No More: CYP450 Enzymes as Drug Discovery Targets

S. B. Hoyt, *Organizer*

S. Hoyt, *Presiding*

1:30 MEDI **221.** Steroidogenic cytochrome P450 enzymes as drug targets. **R.W. Hartmann**, J. Emmerich, L. Yin, A. Ali, S. Hoyt, Q. Hu, C. van Koppen

2:20 MEDI **222.** LFF269: A cortisol-sparing CYP11B2 inhibitor that lowers aldosterone in human subjects. **J.P. Papillon**

3:00 MEDI **223.** Using fragment-based approaches to probe the Mycobacterium tuberculosis CYPome. **C. Abell**

3:40 MEDI **224.** CYP51 inhibitors for Chagas disease. **G. Lepesheva**

4:20 MEDI **225.** Discovery of selective CYP11B2 inhibitors as potential treatments for resistant hypertension. **S.B. Hoyt**, W. Petrilli, M.K. Park, J.A. Taylor, C. London, A. Cooke, J. Cai, E. Carswell, J. Robinson, J. Maclean, L. Brown, S. Belshaw, T. Clarkson, D.J. Bennett, K. Liu, G. Liang, F. Ujjainwalla, J. Tata, Q. Hu, L. Yin, C. van Koppen, R.W. Hartmann, B. Kulkarni, S.K. Samanta, R. Saxena, M. Struthers, D. Cully, T. Wisniewski, N. Ren, C. Bopp, A. Sok, T. Cai, S. Stribling, L. Pai, X. Ma , J. Metzger, A. Verras, D. McMasters, Q. Chen, E. Tung, W. Tang, G. Salituro, N. Buist, J. Clemas, G. Zhou, M. Rosenbach, Y. Xiong, A. Ali

Modeling & Measuring Protein-Ligand Kinetics & Residence Times

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Undergraduate Research Posters

Medicinal Chemistry

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MONDAY EVENING

Section A

Walter E. Washington Convention Center
Halls D/E

Sci-Mix

A. W. Stamford, *Organizer*

8:00 - 10:00

51, 56, 61, 66, 70, 74-75, 78-79, 97, 101, 112, 119-120, 122-123, 130, 142-143, 146, 177-178.
See previous listings.

286, 303, 305, 318-320, 323-324, 328, 331, 338, 341, 353, 364.
See subsequent listings.

TUESDAY MORNING

Section A

Walter E. Washington Convention Center
Room 146B

Award Symposium

A. W. Stamford, *Organizer*

W. B. Young, *Presiding*

8:30 MEDI **226.** Synthesis and evaluation of itraconazole analogues for the treatment of medulloblastoma. **J.R. Pace**, M.K. Hadden

8:55 MEDI **227.** Discovery of new quinazolinone antibiotics for the treatment of methicillin-resistant *Staphylococcus aureus*. **R. Bouley**, M. Suckow, J. Hermoso, M.F. Chang, S. Mobashery

9:20 MEDI **228.** Harnessing a catalytic lysine residue for the rapid, one-step preparation of homogeneous antibody-drug conjugates. **A.R. Nanna**, X. Li, E. Walseng, L. Pedzisa, R.S. Goydel, D. Hymel, T.R. Burke, W.R. Roush, C. Rader

9:45 MEDI **229.** Dual inhibition of the oncoproteins MCL-1 and BCL-2 by rationally designed polypharmacology. **B. Drennen**, S.J. Hughes, S. Fletcher

10:10 MEDI **230.** Novel HIV-1 protease inhibitors: Design, synthesis, and biological evaluation. **H.L. Osswald**

10:35 MEDI **231.** From endocrine regulation to bacterial quorum sensing (QS): Design and optimization of compounds for the treatment of endocrine disorders and infectious diseases. **R.W. Hartmann**, Q. Hu, C. van Koppen, S. Marchais-Oberwinkler, C. Maurer, M. Empting

11:20 MEDI **232.** Activity-based proteomics: Protein and ligand discovery on a global scale. **B.F. Cravatt**

Section B

Walter E. Washington Convention Center
Room 146A

Recent Advances in the Treatment of HIV-1 Infection & Approaches to a Cure

N. A. Meanwell, B. N. Naidu, S. Runyon, *Organizers, Presiding*

E. Velthuisen, *Presiding*

8:30 Introductory Remarks.

8:35 MEDI **233.** Curing HIV infection: Going beyond N = 1. **R.F. Siliciano**

9:10 MEDI **234.** Exploring epigenetic regulatory proteins and their inhibition for HIV latency disruption. **L.I. James**

9:45 MEDI **235.** Long acting HIV antiretroviral agents: Moving beyond one pill once a day. **B.A. Johns**, E. Velthuisen

10:20 MEDI **236.** Second generation HIV-1 maturation inhibitors: The discovery of BMS-955176. **A. Regueiro-Ren**

10:55 MEDI **237.** Phosphonamidate prodrugs GS-7340 (tenofovir alafenamide) and GS-9131 for the treatment of HIV. **R.L. Mackman**

11:30 MEDI **238.** Withdrawn.

Innovations in Healthcare in the Global Economy

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

Informatics & Chemical Biology: Identifying Targets & Biological Pathways

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Modeling & Measuring Protein-Ligand Kinetics & Residence Times

Sponsored by COMP, Cosponsored by MEDI and PHYS

TUESDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 146B

Recent Advancements & Therapeutic Opportunities in Muscarinic Receptors

M. P. Bourbeau, R. Mazzola, *Organizers, Presiding*

1:30 MEDI **239.** Mutant muscarinic receptors as novel chemogenetic tools to identify new therapeutic targets. **J. Wess**

2:00 MEDI **240.** Allosteric regulation and oligomerization of muscarinic cholinergic receptors. **R.V. Shivnaraine**

2:30 MEDI **241.** Convulsion and cholinergic toxicity of subtype selective M1 positive allosteric modulators (PAMs). **J.E. Davoren**

3:00 MEDI **242.** Targeting positive allosteric modulators of the M1 muscarinic receptor: Identification of MK-7622. **D.C. Beshore**

3:30 MEDI **243.** Discovery, development, mechanisitic insights and therapeutic potential of M_4 PAMs. **C.W. Lindsley**

4:00 MEDI **244.** Discovery and clinical progression of highly selective M_1 agonists utilizing structure-based drug design. **G.A. Brown**

Section B

Walter E. Washington Convention Center
Room 146A

General Orals

A. W. Stamford, *Organizer*

J. Ramanjulu, *Presiding*

1:30 MEDI **245.** Design of liver-targeting, glucose-responsive insulin. **D.A. Pissarnitski**, S. Lin, L. Yan, Z. Zhao, A. Kekec, Y. Zhu, D.N. Hunter, P. Huo, D. Feng, C. Moyes, B. Pipik, J.L. Duffy, E. Guidry, J. Mu, M. Van Heek, P. Zafian, T. Kelly, E. Carballo-Jane, R.P. Nargund

1:55 MEDI **246.** Identification of potent and selective covalent monoacylglycerol lipase (MAGL) inhibitors for treatment of neuroinflammation. **L.A. McAllister**, E.M. Beck, M.A. Brodney, C. Butler, A.M. Gilbert, A.R. Harris, C.J. Helal, D.S. Johnson, S. Mente, J.I. Montgomery, S.V. O'Neil, J.R. Piro, B.N. Rogers, T. Samad, D. Webb

2:20 MEDI **247.** Discovery of molidustat (BAY 85-3934): A small-molecule oral HIF-prolyl hydroxylase (HIF-PH) inhibitor for the treatment of renal anemia. **H. Beck**

2:45 MEDI **248.** Discovery of potent and orally bioavailable macrocyclic FXIa inhibitors. **W. Yang**

3:10 MEDI **249.** Cleavable photoprobes enable binding site identification of a gamma secretase inhibitor. **C. am Ende**, N. Gertsik, K.F. Geoghegan, C. Nguyen, P. Mukherjee, S. Mente, U.I. Seneviratne, D.S. Johnson, Y. Li

3:35 MEDI **250.** Identification of LYS228: A Novel monobactam with activity against extended spectrum β-lactamase expressing and carbapenem-resistant enterobacteriaceae. **A. Casarez**, A. Bermingham, J. Blais, V. Capka, R. Colvin, C. Dean, A. Fekete, W. Gong, E. Growcott, H. Guo, X. Lin, M. Lindvall, S. Lopez, D. McKenney, H. Moser, D. Rasper, V. Sethuraman, X. Shen, R. Simmons, D. Tang, M. Tjandra, N. Turner, T. Uehara, C. Vitt, S. Whitebread, A. Yifru, X. Zang, Q. Zhu, F. Reck

4:00 MEDI **251.** Chemoinformatic-driven design and synthesis of an RNA-targeted small molecule library. **B. Morgan**, J. Forte, B. Sanaba, Y. Zhang, D. Karloff, D. Bertan, A.E. Hargrove

4:25 MEDI **252.** Discovery and optimization of a novel class of selective NaV1.7 antagonists. **C.M. Dehnhardt**, **S. Chowdhury, S. Sun**, M.S. Wilson, A. Hasan, I. Hemeon, M.E. Grimwood, W. Gong, J. Andrez, T. Focken, P. Bergeron, S. Lin, Q. Jia, P. Bichler, G. Bankar, E. Chan, **K. Khakh**, D. Hackos, S. McKerrall, **D.F. Ortwine, A. Zenova, S. Decker, J. Johnson**, J. Chang, B.D. Sellers, **C. Cohen, B. Safina, D. Sutherlin**

4:50 MEDI **253.** Discovery of clinical candidate GDC-0276: A selective NaV1.7 inhibitor for the treatment of pain. **D.P. Sutherlin**, S. Sun, S. Chowdhury, Q. Jia, A. Zenova, M.S. Wilson, T. Focken, J. Li, P. Bichler, S. Decker, M.E. Grimwood, I. Hemeon, T. Sheng, J. Andrez, D. Hackos, G. Bankar, K. Khakh, E. Chang, R. Kwan, S. Lin, K. Nelkenbrecher, D.F. Ortwine, J. Chang, J. Pang, L. Sojo, P. Chiang, A.N. Sambrone, M. Tagen, A. White, C. Chen, J. Chen, J. Lovelidge, X. Ding, R. Takahashi, M. Waldbrook, Z. Xie, C. Young, L. Robinette, C. Cohen, R. Oballa, C.M. Dehnhardt, B. Safina

Innovations in Healthcare in the Global Economy

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Toxicological Considerations in Antibody Drug Conjugate Design & Development

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WEDNESDAY MORNING

Section A

Walter E. Washington Convention Center
Rooms 146B/C

First Time Disclosure of Clinical Candidates

J. B. Schwarz, *Organizer, Presiding*

9:00 MEDI **254.** Discovery and initial clinical evaluation of trigriluzole: A tripeptide prodrug of riluzole for the treatment of glutamate-associated disorders such as ataxia. **J.C. Pelletier**, J. Wrobel, H. Bian, G.R. Smith, S. Chen, R.M. Berman, V. Coric, A.B. Reitz

9:35 MEDI **255.** Allosteric antagonists of sigma-2/PGRMC1 complex: Brain penetrant orally active amyloid oligomer-displacing agents for the treatment and prevention of mild cognitive impairment and Alzheimer's disease. **G.M. Rishton**, G.C. Look, Z. Ni, J. Zhang, Y. Huang, X. Wu, N. Izzo, K. Mozzoni, C. Silky, C. Rehak, R. Yurko, S.M. Catalano

10:10 MEDI **256.** Discovery of RG7314: A vasopressin 1a receptor antagonist for the treatment of social communication deficits in autism spectrum disorders. **P.D. Schnider**, B. Biemans, C. Bissantz, C. Dolente, E. Goetschi, R. Jakob-Roetne, W. Muster, N. Parrott, E. Pinard, H. Ratni, C. Risterucci, M. Rogers-Evans, M. Schmitt, C. Grundschober

10:45 MEDI **257.** Discovery of TAK-041: Potent and selective GPR139 agonist for treatment of negative symptoms associated with schizophrenia. **H. Reichard**, H. Monenschein

11:20 MEDI **258.** Discovery of a ketohexokinase inhibitor for the treatment of NAFLD/NASH: Fragment-to-candidate via structure-based drug design and parallel chemistry. **B. Raymer**, T.V. Magee, K. Futatsugi, A.C. Smith, K. Huard, M. Tu, G.J. Tesz, J. Gutierrez, J. Withka, K. Parris, J. Pandit, Y. Weng, G. Xing, S. Perez, A. Tsai, D. Fernando, M.S. Dowling, B. Thuma, A. Shavnya, H. Wisniewska, S.B. Coffey, K.A. Borzilleri, J.D. Knafels, K. Ahn, J. Zhou, D.A. Tess, S. Gut Ruggeri, V. Somayaji, A. Bergman, G.E. Sonnenberg, J.A. Pfefferkorn, D. Price, S. Liras

Section B

Walter E. Washington Convention Center
Room 146A

Unusual Protein-Ligand Interactions in the Design of Novel Pharmaceuticals

D. F. Ortwine, *Organizer*

H. E. Purkey, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 MEDI **259.** 40 Years of structure-based design: What have we learned? **F.N. Diederich**

9:20 MEDI **260.** Binding pockets make the difference: Morphing banal water–ligand interactions into determining ones. **S.G. Krimmer**, J. Cramer, M. Betz, V. Fridh, R. Karlsson, A. Heine, G. Klebe

9:50 MEDI **261.** Tales from the trenches: Case histories of exploiting surprising interactions in drug discovery. **N. Nevins**

10:20 MEDI **262.** Quantum mechanical approaches to structurally informed design. **A. Heifetz**

10:50 MEDI **263.** Noncovalent sulfur interactions in drug design: Conformational control and intermolecular association. **M.D. Bartberger**

11:20 MEDI **264.** How significant are unusual intermolecular interactions? **B. Kuhn**, O. Korb

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WEDNESDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Rooms 146B/C

First Time Disclosure of Clinical Candidates

J. B. Schwarz, *Organizer, Presiding*

2:00 MEDI **265.** S-033188: A novel, first-in-class, orally bioavailable inhibitor of influenza virus cap-dependent endonuclease. **M. Kawai**, M. Miyagawa, T. Akiyama, Y. Taoda, K. Takaya, T. Shishido, R. Yoshida

2:35 MEDI **266.** First time disclosure of BAY 1128688: A novel AKR1C3 inhibitor for the treatment of endometriosis. **U. Bothe**, M. Busemann, A. Steinmeyer, P. Droescher, O. Fischer, M. Peters, T. Zollner, F. Sohler, A. Rotgeri, K. Denner, N. Barak, M. Hillmann, P. Savy, N. Ray

3:10 MEDI **267.** Discovery and evaluation of clinical candidate IDH305: A brain penetrant mutant IDH1 inhibitor. **Y. Cho**, J.R. Levell, G. Liu, T.R. Caferro, C.M. Shafer, A. Costales, J.R. Manning, Q. Zhao, M. Sendzik, M.D. Shultz, J. Dooley, G. Chenail, A. Farsidjani, J. Chen, R. Kulathila, X. Xie, S. Dodd, T. Gould, G. Liang, T. Heimbach, K. Slocum, M. Pu, R. Pagliarini, J.D. Growney

3:10 MEDI **268.** Discovery of M2951: A selective, covalent inhibitor of BTK for the treatment of autoimmune diseases. **A. Goutopoulos**

3:45 MEDI **269.** Discovery of a macrocyclic peptide inhibitor of programmed death-ligand 1 (PD-L1). **P.M. Scola**, E.P. Gillis, K.M. Boy, D. Langley, D. Donnelly, M. Miller, L. Lombardo, M. Poss, C. Mapelli, K. Gillman, K. Yeung, L. Sun, K. Grant-Young, M.P. Allen, M. Poirier, M.S. Bowsher, J. Zhu, L. Li, V. Lafont, N. Sanghvi, C. Yan, J.A. Easter, V. Lee, Y. Zhang, J. Goodrich, S. Bonacorsi, E. Cole, E. Mull, A. Mathur, J. Kempson, D. Wu, Q. Zhao, M. Wichroski, S. Campellone, M. Loubeau, M. Cockett, M. Gao, A. Korman, M. Selby, Y. Wang, V. Chauhan, P.C. Reid, J. Nishikawa, H. Goto, R. Logan, J. Cutrone, R. Denton, R. Haskell, K. Johnson, Y. Benitex, K. Robbins, D. Critton, M. Donoso, D. Drexler, X. Huang, H. Park, S. Du, J. Kim, A. Pena, W. Hayes, P. Chow, R.A. Smith, J. Newitt, M. Soars, D. Tenney, N.A. Meanwell, P.H. Carter

Section B

Walter E. Washington Convention Center
Room 146A

General Orals

A. W. Stamford, *Organizer*

A. Ali, *Presiding*

1:30 MEDI **270.** Bayesian models for Chagas disease. **K.M. Zorn**, M.A. Lingerfelt, J.L. Siqueira-Neto, A. Clark, S. Ekins

1:50 MEDI **271.** Identification of novel small molecule inhibitors against NS2B/NS3 serine protease from Zika virus. **H. Lee**, J. Ren, S. Nocadello, I. Ojeda, S. Light, G. Minasov, D. Nagarathnam, W.F. Anderson, M. Johnson

2:10 MEDI **272.** Bacterial natural products as a renewed source of novel antibiotics: Isolation, characterization, and evaluation of antibacterial agents produced by soil bacteria. **A.L. Wolfe**

2:30 MEDI **273.** Targeting the influenza RNA-dependent RNA polymerase. **D. Beylkin**, G. Kumar, W. Zhou, J. Park, T. Jeevan, C. Lagisetti, R. Harfoot, R. Webby, S.W. White, T. Webb

2:50 MEDI **274.** Inhibitors of the DNA repair enzyme AAG as leads for potential new chemoprotectives and stroke treatments. **D. Whelligan**, B. Al Yahyaei, E. Mas, S. Chu, R. Elliott, B. Howlin, L. Meira

3:10 MEDI **275.** Exploration of A, C, and D-ring SAR of the IspD-targeting antimalarial agent MMV008138. **M. Ghavami**, Z. Yao, L. Liu, E. Merino, J. Butler, M. Casasanta, D. Slade, M. Totrov, M. Cassera, P.R. Carlier

3:30 MEDI **276.** Synthesis of ADMDP-typed iminosugars to develop pharmacological chaperones for the treatment of Fabry disease and potential enhancers to increase enzyme replacement therapy efficiency. **W. Cheng**

3:50 MEDI **277.** Dipeptidyl boronates as ClpP1P2 inhibitors: A novel approach to anti tuberculosis therapy. **A. Poulsen**, P. Gopal, S. Santhanakrishnan, K. Jihao, C. Huang, B. Chia, Y. Qiu, U. Lakshmanan, M. Li, J. Sarathy, W. Moreira, C. Low, M. Gengenbacher, K. Sangthongpitag, T.H. Keller, B.W. Dymock, T. Dick

4:10 MEDI **278.** Discovery and synthesis of 4-phenylpiperidine-2-carboxamides as selective 5-HT2C receptor positive allosteric modulators. **E.A. Wold**, C. Wild, N.C. Anastasio, R.G. Fox, S. Stutz, H. Chen, J.A. Allen, K.A. Cunningham, J. Zhou

4:30 MEDI **279.** Selective small molecule Nociceptin (NOP) agonist for the treatment of anxiety related disorders. **T.M. Ross**, G. Bignan, P.J. Connolly, J. Moyer

4:50 MEDI **280.** Modular total synthesis approach towards salvinorin A inspired designer opioids. **A.M. Sherwood**, S. Williamson, R.M. Saylor, T.E. Prisinzano

WEDNESDAY EVENING

Section A

Walter E. Washington Convention Center
Hall E

General Posters

A. W. Stamford, *Organizer*

7:00 - 9:00

MEDI **281.** Essential oil content of the seeds of wonderful kola, African walnut and guinea plum and their potentials on hyperlipidemic male Wistar rats. **E.O. Nwaichi**, J.O. Osuoha, M.O. Monanu

MEDI **282.** Promising antibacterial sesterterpenes: Cybastacine A and B from blue-algae cyanobacteria *Nostoc sp*. **V. Tena Pérez**, A. Hernández Cabanillas, D. Rosero Valencia, S. Maderuelo Corral, M. Ortega Doménech, Á. Rumbero Sánchez

MEDI **283.** Organometallic iridium compounds: Cytotoxic potential against p53wt and p53-/- human colon cancer HCT116. **R.M. Lord**, I. Henderson, P. McGowan

MEDI **284.** Novel ensemble approach to providing small molecule support for validation of cellular targets confirms that glycolysis is a viable antiproliferative strategy in leukemic cells. **A. Zweifach**

MEDI **285.** Generation of natural products-based screening libraries for drug discovery. **F.A. Egbewande**, M.J. Coster, R.A. Davies

MEDI **286.** Stabilization of quadruplex DNAs by tetraurea macrocycles: Synthesis, DNA binding and beyond. **C. Detchou**, B. Gong

MEDI **287.** Production of the antidote of cyanide poison (sodium and hydrogen cyanide) known as soda-sulphanecobalamin. **S.N. Olatunji**

MEDI **288.** Design and structural modification of adamantane analogs for their anti-cancer activity. **V. Thakor**, A. Shaikh

MEDI **289.** Design, synthesis and biological evaluation of new quinazolinone derivatives as potent antimicrobial agents. **S. Nanduri**, S. Gatadi, M.V. Yeddanapudi, S. Chopra

MEDI **290.** Withdrawn.

MEDI **291.** Discovery of a novel dual functional compound (IADB) as chemo-sensitizing and cardio-protective agent. **L. Bi**

MEDI **292.** Design and synthesis of PC-PLC selective self quenching near-infrared fluorescing probes. **B.K. Liebov**, E.J. Delikatny, A.V. Popov

MEDI **293.** Andrographolide: A versatile natural product for the generation of structurally diverse bioactive diterpenes. **S. Nanduri**, S.S. Kandanur, N. Golakoti

MEDI **294.** Isoprenoid pathway as a valid target to control parasitic diseases. **J.B. Rodriguez**, S.H. Szajnman, M.N. Chao

MEDI **295.** Lead optimization and drug development of antiproliferative constituents from *Phyllanthus poilanei*. **A.C. Huntsman**, A. Young, J.L. Woodard, H. Chai, Y. Ren, M.A. Phelps, A.D. Kinghorn, J.E. Burdette, J. Fuchs

MEDI **296.** Sensing bacterial growth and measuring antibiotic susceptibility via laser diffraction. **N.K. Kotoulas**, M. Goh

MEDI **297.** Binding at the telomeric G-quadruplex-duplex interface: A computational study. C. Radicella, T. Fasano, V. Persad, **C. Wu**

MEDI **298.** Triggering a peptidomimetic's oxidative activity to reduce survival of intracellular pathogens. **A.M. Angeles Boza**, M. Libardo

MEDI **299.** Addressing antibiotic-resistance targeting ketolide drugs by developing novel analogs generated via click & *in situ* click chemistry. **S. Daher**

MEDI **300.** Synthesis, design and computational studies of anti-cancer agents. **M. Kuanar**

MEDI **301.** New motif for targeting isoprenoid biosynthetic pathway enzymes. **N.H. Bhuiyan**, M.L. Varney, S.A. Holstein, D.F. Wiemer

MEDI **302.** Design, synthesis, and biological evaluation of small molecule drug conjugates targeting carbonic anhydrase IX positive cancers. **I. Marks**

MEDI **303.** Design, synthesis, and evaluation of derivatives of glutathione linked to cholesterol via a link for brain-targeting drug delivery. **A. Najmi**, S. Wang, Y. Huang, X. Guan

MEDI **304.** Synthesis and evaluation of 1, 3, 5 (10) estratriene aminoalkyloxy,16-formyl derivatives of estrone as potential anti-breast cancer agents. **C. Sullen**

MEDI **305.** Novel computer-assisted drug design (CADD) AKT pathway inhibitors. **N. Uko**, J. Shim, O.F. Guner, J.P. Bowen, D. Matesic

MEDI **306.** Discovery of selective low molecular weight VAV1 guanine nucleotide exchange factor inhibitors. **M. Gerspacher**, P. Skaanderup, V.M. Stucke, E. Vangrevelinghe, M. Knapp, M. Klumpp, A. Lingel, P. Chene, D. Erdmann, M. Duckely, L. Leder, G. Pardee, J. Narberes, T. Tsang, P. Imbach-Weese, F. Sirockin, W.R. Sellers, F. Hofmann

MEDI **307.** Synthesis and preliminary biological evaluation of [11C]methyl (2-amino-5-(benzylthio)thiazolo[4,5-*d*] pyrimidin-7-yl)-*D*-leucinate as a new potential PET radioligand for the fractalkine receptor (CX3CR1). **M. Gao**, M. Wang, J. Meyer, J. Peters, H. Zarrinmayeh, P. Territo, G. Hutchins, Q. Zheng

MEDI **308.** Macrocyclic factor XIa inhibitors containing phenyl azole carboxamide P1 groups. **J.R. Corte**, D. Pinto, T. Fang, H. Osuna, W. Yang, Y. Wang, A. Lai, Y.T. Jeon, I. Delucca, P. Gilligan, K.B. Pabbisetty, L.M. Smith, M.J. Orwat, C.G. Clark, N.D. Yadav, K.A. Rossi, J.E. Myers, S. Sheriff, Z. Lou, J.J. Zheng, T.W. Harper, C. Huang, J.M. Bozarth, Y. Wu, P. Wong, C. Watson, E. Crain, J.M. Luettgen, D.A. Seiffert, P.Y. Lam, R.R. Wexler, W.R. Ewing

MEDI **309.** Design of HIV co-receptor derived peptides that inhibit viral entry at submicromolar concentrations. **S. Mandadapu**, K. Bobyk, K. Lohith, C.A. Bewley

MEDI **310.** Study co-aggregations of nucleic acid nanostructures with tetracycline molecules and their potential applications in smart drug delivery. **N. Alzahrani**, J. Fu, D. Yang, Z. Wang

MEDI **311.** Investigation of a new DMC-DNA monoadduct. **O. Zacarias**, E. Champeil

MEDI **312.** Re-engineering the natural product, emetine, towards achieving a therapeutically useful drug. **O. Bakare**, E.S. Akinboye, N. Idris, N.Z. Brandy, M. Lewis, C.C. Mouamba, L. Abdulrahman

MEDI **313.** Novel selective dopamine D3 receptor modulators for the treatment of cocaine addiction. **P. Chen**, B.E. Blass, J.C. Gordon, R. Luedtke, M. Taylor, K. Korzekwa, M. Ye

MEDI **314.** Structure based discovery of host-targeted antiviral (HTA) small molecules: Ribosomal protein RACK1 as a potential broad antiviral target. **S. Dakshanamurthy**, I. Malli, H. Ullah

MEDI **315.** Withdrawn.

MEDI **316.** Formulating a toothpaste that intraorally delivers vitamin D using penetration enhancers. **N. Kim**, J. Lee

MEDI **317.** Synthesis and biological evaluation of novel thiophene, pyrrole and aromatic *exo*-cyclic carbohydrate enone derivatives. Part II. A. Macieja, J. Sarnik, A. Czubatka-Bienkowska, **Z.J. Witczak**, T. Poplawski

MEDI **318.** Novel cell directed glutaminase inhibitors as chemotherapeutic agents for hematological malignancies. **S. Zimmermann**, A. Gadiano, J. Alt, L. Tenora, G. Furtmueller, C. Garrett, P. Majer, R. Rais, B. Slusher

MEDI **319.** Structure-activity relationships for rigid amphipathic fusion inhibitors suppressing tick-borne encephalitis virus reproduction. **A. Orlov**, A.A. Chistov, G.V. Proskurin, N.M. Ivanov, V.A. Palyulin, L.I. Kozlovskaya, G.G. Karganova, D.I. Osolodkin, V.A. Korshun

MEDI **320.** Design and synthesis of selective histone deacetylase 6 inhibitors based on nexturastat A and evidence of efficacy in melanoma xenograft models. **S. Shen**, M.T. Tavares, M. Hadley, Z. Kutil, C. Barinka, A. Villagra, A.P. Kozikowski

MEDI **321.** Design, synthesis, and biological evaluation of novel histone deacetylase inhibitors as anti-cancer agents. **A. Al-Hamashi**, L. Tillekeratne, S. Dlamini

MEDI **322.** Surfing the kinetic and thermodynamic map in a hit to lead process. **S. Panchal**, R. Edalji, Y. Wang, H. Zhu, C. Jakob, S. Djuric, A. Vasudevan, C. Sun

MEDI **323.** PROTAC design of Mdm2 degraders: A novel efficient approach for cancer therapy. **Y. Li**, J. Yang, A. Aguilar, J. Lu, D. McEachern, D. Bernard, S. Wang

MEDI **324.** Synthesis of FR900098 analogs as inhibitors of *Plasmodium Falciparum* and *Mycobacterium tuberculosis* 1-deoxy-D-Xylulose-5-Phosphate Reductoisomerase (Dxr). **R. Wang**, R. Edwards, A. Haymond, H.I. Boshoff, A.R. Odom, R.D. Couch, C.S. Dowd

MEDI **325.** Revitalizing an old molecule: Investigating acidomycin as an inhibitor of *Mycobacterium tuberculosis* biotin synthase. **M. Bockman**, C. Engelhart, D. Schnappinger, C.C. Aldrich

MEDI **326.** Withdrawn.

MEDI **327.** Synthesis and microbiological evaluation of 2-amino-4,5,6,7-tetrahydrothieno[2,3-c]pyridines against sensitive and drug resistant *Mycobacterium tuberculosis*. **F. Salem**, S.J. Sucheck, S. Thanna

MEDI **328.** New carbapenem antibiotics with activity against *Mycobacterium tuberculosis* and *Mycobacterium abscessus*. T. Nguyen, **M.A. Alqurafi**, W. Chai, M. Netherton, R. Gupta, P. Nguyen, M. Cox, B. Meshram, J. Kim, C. Jacobson, O. Marx, S. Smriti, M. Bennett, C. Watanabe, A. Shi, L. Phung, D. Le, K. Rohde, J.D. Buynak

MEDI **329.** Imparting intrinsic flourescence as an approach towards rapid inhibitor screening and mechanistic evaluation of tuberculosis shikimate kinase. **R. Fuanta**, J. Simithy, T. Childers, A. Calderon, D.C. Goodwin

MEDI **330.** Novel pyrimidine antituberculars discovered through machine-learning Bayesian method. **D. Inoyama**, S.D. Paget, R. Russo, P. Kumar, E. Singleton, M. Tuckman, M.D. Zimmerman, H. Ho, A.L. Perryman, V. Dartois, N. Connell, J.S. Freundlich

MEDI **331.** Discovery of 2-aminobenzimidazoles that sensitize *M. smegmatis* and *M. tuberculosis* to β-lactam antibiotics in a pattern distinct from β-lactamase inhibitors. **V. Nguyen**, C. Melander

MEDI **332.** Rational design, synthesis and preliminary biological evaluation of novel C8-linked pyrrolobenzodiazepine-5′-*O*-[*N*-(salicyl)sulfamoyl] adenosine conjugates (PBD-Sal-AMS) as anti-tubercular probes with dual mode of action. **L. Ferguson**, S. Bhakta, F. Brucoli

MEDI **333.** Synthesis, optimization, and biological evaluation of novel analogs of DG85 as antitubercular agents. **R. Gallardo-Macias**

MEDI **334.** Evaluation of 5-substituted 1,10-phenanthroline and nickel complexes as G4 ligands and telomerase inhibitors. **S. Wang**, W. Liu, I.A. Dotsenko, V.V. Samoshin, L. Xue

MEDI **335.** Discovery of potent BET inhibitors as potential treatments for cancer: Optimization of pharmacokinetic and pharmaceutics properties. **M.D. Hill**, H. Fang, D. Norris, W.D. Schmitz, C. Huang, R. Westhouse, M. Kramer, J. Morrison, C. Tye, E. Shields, H. Zhang, M. Sinz, J. Simmermacher-Mayer, F. Lee, A.V. Gavai, A.P. Degnan

MEDI **336.** Discovery of highly potent BET protein degraders based on novel inhibitors inducing complete and durable tumor regression in human acute leukemia xenografts. **C. Qin**, S. Wang

MEDI **337.** N7-substituted pyrrolo[3,2-*d*] pyrimidine analogues - new small molecule anticancer agents. **B. Cawrse**

MEDI **338.** Late-stage modification of tigloyl moiety to ipomoeassin F to enable SAR studies of the natural product. **L. Whisenhunt**, G. Zong, Z. Hu, W. Shi

MEDI **339.** Highly-active influenza endonuclease inhibitors developed from a designer metal-binding pharmacophore library screen. **C.V. Credille**, S. Cohen

MEDI **340.** Cholestosome™ mediated delivery of nucleic acids into MCF7 cells. **A. Kovacs**, M. Irving, J. McArthur, J. Hughes, J. Schentag, L. Mielnicki, M. McCourt

MEDI **341.** Thiohydroxypyridinones as a scaffold for the development of potent New Delhi metallo-ß-lactamase-1 inhibitors. **R. Adamek**, C.V. Credille, P. Thomas, W. Fast, S. Cohen

MEDI **342.** Therapeutic effects of novel benzylguanidine derivative on neuroblastoma tumor cells. **O. Ozen Karakus**, M. Rajabi, M. Yalcin, D.J. Bharali, S. Mousa

MEDI **343.** Discovery of potent and selective Axl/Mer dual inhibitors. **T. Inukai**, K. Tsuboi, A. Hiramatsu, Y. Nomura, A. Yoshida, H. Kohno, K. Otsuki, M. Kurono, T. Fujimoto, S. Umemura, H. Egashira, R. Omi, T. Yasuhiro, R. Fujikawa, K. Tanaka, T. Yoshizawa, M.A. Wolf, V.D. Pawar, S.K. Chittimalla, C. Bandi, A. Chakrabarti, J. Takeuchi

MEDI **344.** Design, synthesis and biological evaluation of 6-aminopenicillanic acid and 7-aminocephalosporanic acid derivatives of emetine. **C.C. Mouamba**, L. Abdulrahman, N. Idris, O. Bakare

MEDI **345.** Synthesis of azotochelin analogues as antibiotic leads. **N. Karadkhelkar**

MEDI **346.** Design, synthesis and *in vitro* antiproliferative evaluation of quinazoline 2,4,6-triamine and 6-aminoquinazoline-4-(3*H*)-one derivatives in ovarian cancer skov-3 cell line. **A. Matus-Meza**, F. Hernández-Luis, M. Velasco-Velazquez

MEDI **347.** Withdrawn.

MEDI **348.** Closing the loop between synthesis and design: Balancing optimisation of potency with selectivity. P. Hunt, **T. Mansley**, E. Champness, N. Foster, M. Segall

MEDI **349.** Structure-based drug design (SBDD) and SAR of tetrapeptides competitive inhibitors of Y-49 β-lactamase. **C.C. Clement**, J. Gonzalez, M. Philipp

MEDI **350.** Design and synthesis of novel uridine analogue with possible anti-HCV activity. **B. Alabdullah**, A.C. Bryant-Friedrich

MEDI **351.** Synthesis of 2'-C-methyl pseudouridines for the inhibition of HCV RNA-polymerase. **I. Sappy**, A.C. Bryant-Friedrich

MEDI **352.** Discovery of multi-target-directed ligands for the treatment of Alzheimer's disease. **W. Huang**, Z. Shen, C. Li, Q. Li, X. Zhen, Z. Ma, M. Liang

MEDI **353.** Design and development of pramipexole-donepezil hybrids as potential therapeutics for Alzheimer's disease. **M.A. Barmade**, M. Shidore, S. Rajyaguru, J. Machhi, P.R. Murumkar, M. Yadav

MEDI **354.** SUVN-502, A novel, potent and pure 5-HT6 receptor antagonist - proof-of-concept study design in moderate Alzheimer's disease patients. **V. Nirogi**, K.R. Sastry, A.K. Shinde, M. Rasheed, R.K. Badange, T. Bandyala, V. Bhatta, v. reballi, P. Achanta, K. kandukuri, K. Bojja, S. Saraf, K. Mudigonda, P. Jayarajan, G. Bhyrapuneni, V. Goyal, V. Jasti

MEDI **355.** Pyrimidine carboxamide derivatives as muscarinic acetylcholine subtype 1 positive allosteric modulators (M1 PAM) for the treatment of cognitive deficits in Alzheimer's disease. **V. Nirogi**, M. Rasheed, A.K. Shinde, P. Kalukuri, D. Kancharla, N. Bogaraju, R. Subramanian, N. Muddana

MEDI **356.** Design and synthesis of novel [F18]-labeled histone deacetylase inhibitors as potential molecular imaging agents for Alzheimer's disease. **L. Hsin**, Y. Chen

MEDI **357.** REAL fragment-like covalent modifiers: N-arylsulfamoylbenzenesulfonyl fluorides as potent protease inhibitors. **O. Gavrylenko**, A. Chupryna, O. Vasylchenko, M. Platonov, P. Borysko, Y. Moroz

MEDI **358.** Synthesis and SAR studies of positive allosteric modulators of mGluR2 for treatment of neurological and psychiatric diseases. **Z. Meng**, R.J. Mattson, M. Parker, L. Gurenon, A. Easton, W. Kostich, M. Seager, C. Bourin, L. Bristow, K. Johnson, R. Miller, J. Hogan, V. Whiterock, M. Gulianello, M. Ferrante, Y. Huang, A. Hendricson, A. Alt, J. Macor, J.J. Bronson

MEDI **359.** Design, synthesis and application of novel building blocks to Escape the Flatland. **P. Mykhailiuk**

MEDI **360.** [2+2]-photochemical synthesis and application of bicyclic amines: Advanced building blocks for MEDIcinal chemistry. **P. Mykhailiuk**

MEDI **361.** Synthesis and application of unnatural Proline analogues: Advanced building blocks for MEDIcinal chemistry. **P. Mykhailiuk**

MEDI **362.** Rapid access to novel multifunctional spirocyclic cores for drug discovery. **Y. Moroz**

MEDI **363.** Synthesis of triazole as GABA analogues. **L. Diaz**, M. Fernandez

MEDI **364.** Novel deuterated GABAAR-α6 subtype selective ligands with improved metabolic stability and enhanced bioavailability: Targeting trigeminal orofacial pain, neuropsychiatric disorders, & depression. **D.E. Knutson**, R.S. Verma, M.R. Stephen, R. Kodali, L. Arnold, M.M. Savic, M.D. Mihovilovic, M. Ernst, W. Sieghart, J.M. Cook

MEDI **365.** Second-generation inhibitors of the hepatitis C virus NS3/4A protease: Discovery of BMS-986144 with pan-genotypic antiviral activity. **L. Sun**, E. Mull, Q. Zhao, E.P. Gillis, M.S. Bowsher, S. D'Andrea, Z. Zheng, X.A. Wang, A. Mathur, R. Rampulla, S. Kandhasamy, N. Pulicharla, S. Vishwakrishnan, S. Reddy, R. Trivedi, S. Sinha, A. Rao, S. Desai, K. Ghosh, R. Rajamani, J. Friborg, S. Levine, C. Chen, P. Falk, Y. Wang, H. Fang, S. Jenkins, M. Kramer, R. Haskell, K. Johnson, J. Loy, P. Levesqu, J. Zhu, M. Cockett, N.A. Meanwell, F. McPhee, P.M. Scola

MEDI **366.** Toxicological evaluation of magnetic nanoparticles. H. Huang, V. James, P. Villarreal, S. Bashir, **J.L. Liu**

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

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SUNDAY MORNING

Section A

Grand Hyatt Washington
Constitution D

General Topics in Radiochemistry

L. H. Delmau, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 NUCL **1.** Chromatographic separation of medically-related radionuclides from proton-irradiated thorium targets. **T. Mastren**, V. Radchenko, J.W. Engle, A. Owens, R. Copping, M. Brugh, F.M. Nortier, E.R. Birnbaum, K.D. John, M.E. Fassbender

9:00 NUCL **2.** Building a reference database for thermodynamic sorption modelling. **F. Bok**, A. Richter, V. Brendler

9:25 NUCL **3.** Dabco/quinuclidine increases the radiofluorinations of 2-halopyridines. **L. Cai**, G.R. Naumiec, S. Lu, V.W. Pike

9:50 Intermission.

10:15 NUCL **4.** Accumulation of specific radioisotopes by fish in offshore Fukushima, Japan. H. Katsura

10:40 NUCL **5.** Cesium ion partitioning with ionophores in ionic liquid-water biphasic systems. R. Biswas, T. Banerjee, P. Ghosh, S. Ali