11:30 INOR **1005.** Strong magnetic coupling in dinuclear transition metal complexes bridged by redox-active ligands. **I. Jeon**, D. Harris

11:50 INOR **1006.** Magnetic and spectroscopic properties of linear two-coordinate transition metal complexes. **C. Lin**, G.J. Long, P.P. Power

Section I

Colorado Convention Center
Room 205

Inorganic Catalysts

S. A. Koch, *Organizer*
T. J. Hubin, *Presiding*

8:30 INOR **1007.** Structure-function relationships for electrocatalytic water oxidation by molecular $[Mn_{12}O_{12}]$ clusters. **Y. Yan**, D.A. Ruddy

8:50 INOR **1008.** Functional ordered mesoporous metal carbides. **M. Xu**, M.R. Nimlos, B.G. Trewyn, R.M. Richards

9:10 INOR **1009.** Withdrawn.

9:30 INOR **1010.** Single-crystal to single-crystal structural and chemical transformation of a Fe-based mononuclear electrocatalyst for hydrogen production. **X. Wang**, T. Liu, M. Bullock

9:50 Intermission.

10:00 INOR **1011.** Two 4-step mechanisms for nanoparticle nucleation, growth, bimolecular agglomeration, and then autocatalytic agglomeration or secondary autocatalytic growth. **P. Kent**, R.G. Finke

10:20 INOR **1012.** Progress in developing an aerobic hydrocarbon oxidation catalyst. **C.C. Scarborough**, G.J. Karahalis, C.T. Buru, A. Thangavel

10:40 INOR **1013.** Measurement of aqueous hydricities of transition-metal hydrogen evolution catalysts. **C. Tsay**, B. Livesay, J. Yang

11:00 INOR **1014.** Activation of CO_2 utilizing Lewis acid/base cooperativity from a NiFe bimetallic Robson-type complex. **S. Poteet**, J. Yang

11:20 INOR **1015.** Synthesis, structural studies, and oxidation catalysis of the late first row transition metal complexes of a 2-pyridylmethyl pendant armed ethylene cross-bridged cyclam. **T.J. Hubin**, D.G. Jones, A.D. Shircliff, G. Yin, T.J. Prior

Section J

Colorado Convention Center
Room 402

Organometallic Chemistry

Synthesis and Characterization

N. S. Radu, *Organizer*
S. Fortier, V. M. Iluc, *Presiding*

8:30 INOR **1016.** Metal-ligand interactions: E-H activation and metal-element multiple bonding. **V.M. Iluc**

8:50 INOR **1017.** Synthesis, characterization, and coordination chemistry of a new guanidinate ligand class possessing ketimine backbones. **A. Maity**, S. Fortier, L. Griego, A.J. Metta-Magana

9:10 INOR **1018.** Identification and characterization of an η2 nitrogen-nitrogen complex between diazoalkanes and lithium dimethylcuprate. **J. Morse**, M.D. Murphy, S.H. Bertz, C. Ogle

9:30 INOR **1019.** $U(bipy)_4$: A mistaken case of U(0)? **S. Fortier**, J. Le Roy, K. Ghiassi, M.M. Olmstead, D. Villagran, M. Murugesu, A.J. Metta-Magana

9:50 INOR **1020.** Structural and chemical study of iron supported by "super bulky" guanidinates. **S. Fortier**, A. Maity, L. Griego, A.J. Metta-Magana

10:10 INOR **1021.** Mechanochemical vs. solution syntheses of group 15 bulky allyl metal complexes. **N.R. Rightmire**, D.L. Bruns, T.P. Hanusa

10:30 INOR **1022.** C–H bond activation by iridium (III) pincer dicarboxylate complexes. **A.M. Wright**, K.I. Goldberg

10:50 INOR **1023.** Synthesis, characterization, and reactivity study of a masked "Ti(II)" complex. **R. Aguilar**, S. Fortier, A. Metta-Magana

11:10 INOR **1024.** Size effect and odd-even alternation in the melting of single and stacked silver alkanethiolate layers: Experiment and phenomenological model. **Z. Ye**, L. de la Rama, L. Hu, M. Efremov, L. Allen

11:30 INOR **1025.** Molecular switches: Exploring the counter-ion problem. **J.A. Christie**, R. Forrest, S. Corcelli, N.A. Wasio, R. Quardokus, S.A. Kandel, Y. Lu, C.S. Lent, A.G. Oliver, K.W. Henderson

THURSDAY AFTERNOON

Section A

Colorado Convention Center
Room 105

Nanoscience

Semiconductors

Cosponsored by PRES

R. M. Richards, *Organizer*
N. R. Neale, M. Zamkov, *Presiding*

1:30 INOR **1026.** Progress towards complete photocatalytic water splitting utilizing hybrid nanoparticles. **A.D. LaCroix**, J. Macdonald

1:50 INOR **1027.** Phase dependent visible to near-infrared photoluminescence of $CuInS_2$ nanocrystals. **A. Leach**, J. Macdonald

2:10 INOR **1028.** Silicon monoxide: A convenient precursor for near infrared emitting silicon nanocrystals and switching-on quantum size effects. **W. Sun**, C. Qian, G.A. Ozin

2:30 INOR **1029.** Growth of $CuInS_2$ nanoplatelets by cation exchange and mechanism study. **L. Mu**, W.E. Buhro

2:50 Intermission.

3:00 INOR **1030.** Sub-diffraction imaging of exciton diffusion in semiconductor nanocrystal solids. **M. Zamkov**, N.N. Kholmicheva, P. Moroz

3:20 INOR **1031.** Surface passivation of group 14 nanocrystals. **N.R. Neale**

3:40 INOR **1032.** Cu_2ZnSnS_4/Cu_2Se core/shell nanocrystal thin films: Manipulation of charge carrier transport through surface modification. **L. Korala**, A.L. Prieto

Section B

Colorado Convention Center
Room 301

Lanthanide and Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
P. C. Burns, N. E. Travia, *Presiding*

1:30 INOR **1033.** Withdrawn.

1:50 INOR **1034.** Coordination chemistry of the rare-earths in a tripodal nitroxide ligand framework: New chemistry for magnet recycling. **J.A. Bogart**, C.A. Lippincott, P.J. Carroll, E.J. Schelter*

2:10 INOR **1035.** Interactions of uranium and plutonium with phosphonate-functionalized mesoporous silica. **E.C. Uribe**, J. Shusterman, A. Bruchet, H. Mason, H. Nitsche

2:30 INOR **1036.** Exploring the chemistry of the f-elements with nitrogen-rich ligands. **N.E. Travia**, K. Browne, J.L. Kiplinger, D.E. Morris, A. Mueller, A. Nelson, A.J. Parkison, B. Scott, B.C. Tappan, J. Veauthier

2:50 Intermission.

3:00 INOR **1037.** Synthesis, characterization, and reactivity of U^{2+} in the $\{[C_5H_3(SiMe_3)_2]_3U\}^{1-}$ anion. **C.J. Windorff**, J.W. Ziller, W.J. Evans

3:20 INOR **1038.** Examining covalency in uranium-ligand multiple bonds through synthesis, spectroscopy, and theory. **N.C. Tomson**, L. Spencer, R.L. Shook, E.R. Batista, J.M. Boncella

3:40 INOR **1039.** Mechanistic insights into the early stages of crystallization of REE-carbonate. **J. Rodriguez Blanco**, K. Dideriksen, D. Tobler, K. Sand, B. Vallina, L. Benning, S.S. Stipp

4:00 Intermission.

4:10 INOR **1040.** Increasing the reactivity of actinide coordination compounds: Imidazolin-2-iminato actinide complexe. **I. Karmel**, N. Fridman, T. Bannenberg, M. Tamm, M. Eisen

Section C

Colorado Convention Center
Room 302

Chemistry of Materials

Metal-Organic Frameworks

C. G. Lugmair, *Organizer*
J. Jiang, J. V. Lockard, *Presiding*

1:30 INOR **1041.** Metal-organic frameworks for natural gas storage. **J.A. Mason**, M.K. Taylor, M.R. Hudson, Z. Hulvey, A. Guagliardi, C.M. Brown, N. Masciocchi, J.R. Long

1:50 INOR **1042.** Ultrastable piezofluorochromic metal-organic frameworks. **Q. Zhang**, H. Zhou

2:10 INOR **1043.** In situ spectroscopy studies of CO_2 adsorption in a dually functionalized microporous metal-organic framework. Y. Chen, H. Wang, J. Li, **J.V. Lockard**

2:30 INOR **1044.** Highly stable meso porous MOFs. **D. Feng**, K. Wang, T. Liu, J. Park, H. Zhou

2:50 INOR **1045.** Mechanistic insights into the gelation of cyanide-bridged coordination polymers. **I.C. Fortmeyer**, P.A. Hoijemberg, Y. Yan, I. Pelczer, A.B. Bocarsly

3:10 INOR **1046.** Alternative UiO-66 synthesis for HCl-sensitive nanoparticle encapsulation. **K.S. Walton**, K. Tulig

3:30 INOR **1047.** Prussian red: A carbon monoxide fused cyano bridging mixed valence FeII/III coordination polymer with unprecedented packing pattern and anisotropic negative thermal expansion. W. Lo, O. Ishal, D. Sultan, **J. Jiang**

3:50 INOR **1048.** Photochromic metal–organic frameworks toward control of singlet oxygen generation. **J. Park**, D. Feng, S. Yuan, H. Zhou

4:10 INOR **1049.** Solvothermally grown porphyrin metal-organic framework (MOF) thin films: Post metalation and electrocatalysis. C. Kung, **T. Chang**, L. Chou, J.T. Hupp, O.K. Farha, K. Ho

4:30 INOR **1050.** Novel phosphine coordination materials based on *bis*(phosphine) and methyl triarylphosphonium groups for applications in gas storage, separations, and sensing. **N. Waggoner**, A. Bohnsack, L. Cinninger, T. Kornfuehrer, B.J. Holliday, S.M. Humphrey

4:50 INOR **1051.** Pressure-induced switching in functional molecular materials. **G.J. Halder**, K.W. Chapman, A.A. Yakovenko, P.J. Chupas, A.M. dos Santos

Section D

Colorado Convention Center
Room 303

Coordination Chemistry

Characterization and Applications

D. C. Crans, *Organizer, Presiding*
A. C. Bowman, *Presiding*

1:30 INOR **1052.** Proton-responsive pincers: Enabling bifunctional Lewis acidic/Bronsted basic late metal complexes. **B. Cook**, C. Chen, M. Pink, R.L. Lord, K.G. Caulton

1:50 INOR **1053.** Synthesis and photocatalytic properties of a boron-centered ionic metal organic framework. **X. Zhang**, X. Zhang, Y. Chen, J. Zhang

2:10 INOR **1054.** Mechanism for ligand exchange processes in metal organic frameworks. **J. Byers**, C. Tsung, J.V. Morabito, L. Chou, Z. Li, R. Kyada

2:30 INOR **1055.** Highly dynamic coordination chemistry and redox chemistry of aromatic polyphosphorus complexes. **M. Fleischmann**, M. Scheer

2:50 INOR **1056.** $[Ru(bpy)_3]^{2+}$ linked with methyl viologen and phenothiazine substituted aminoethylglycines. **B. Biber**, M. Williams

3:10 INOR **1057.** Utilizing TREN-based copper complexes to calculate activation rate constant values in ideal atom transfer radical addition (ATRA) reactions. **K.A. Bussey**, K.D. Oshin

MEDI

Division of Medicinal Chemistry

W. B. Young, *Program Chair*

SUNDAY MORNING

Section A

Colorado Convention Center
Mile High Blrm 2A/2B

Applications of Positron Emission Tomography in Drug Discovery

D. Donnelly, C. D. Jesudason, *Organizers, Presiding*

9:00 MEDI **1.** Synthesis of radiopharmaceuticals and applications in functional positron emission tomography (PET) imaging. **P.J. Scott**

9:30 MEDI **2.** 18F-T807: A PET imaging compound for detecting tau in alzheimer's and non-alzheimer's neurodegenerative diseases. **G. Attardo**, A.T. Hoye, H. Xiong, X. Li, C.L. Horchler, K. Fan, N. Lim, F. Gomez, Y. Lin, Q. Liang, K. Conway, H. Kolb, D. Skovronsky, M. Mintun

10:00 MEDI **3.** Development of PET radioligands for imaging brain mGlu1 receptors. **P.W. Victor**

10:30 MEDI **4.** Preclinical peripheral enzyme occupancy and PK/PD modelling: A retrospective analysis of sildenafil. **C.D. Jesudason**, V.N. Barth, T.E. Eessalu, E. Yuen

11:00 MEDI **5.** Design, synthesis, and development of fluorine-18 and carbon-11 labeled lysophosphatidic acid receptor 1 (LPA1) PET radioligands for lung receptor occupancy imaging. **D. Donnelly**, S. Bonacorsi, S. Du, A. Pena, J. kim, W. Hayes, N. Nabulsi, J. Gallezot, Y. Huang, R. Carson

11:30 MEDI **6.** ImmunoPET imaging in the development of therapeutic antibodies. **J. Marik**

Section B

Colorado Convention Center
Mile High Blrm 1A/1B

Targeting the Microbiome

S. M. Firestine, *Organizer, Presiding*

9:00 MEDI **7.** Gut reactions: Understanding and manipulating chemistry from the human microbiota. **E.P. Balskus**

9:35 MEDI **8.** Chemical library in food presents the natural ligands for the gastrointestinal microbiome. **M.L. Heiman**

10:10 MEDI **9.** Discovery of small molecule therapeutics based on microbiome-host interaction analysis in inflammatory bowel disease. **T.Z. DeSantis**

10:45 MEDI **10.** Incorporation of therapeutic bacteria into the gut microbiome for treatment of obesity. **S.S. Davies**

11:20 MEDI **11.** Pharmaceutical control of the microbiome. **M. Redinbo**

Section C

Colorado Convention Center
Mile High Blrm 2C

General Oral Session

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

8:30 MEDI **12.** γ-AApeptides as a new class of peptidomimetics. **H. Wu**, Y. Niu, J. Cai

8:50 MEDI **13.** Improved inhibitors of inducible nitric oxide synthase (iNOS) through fragment assisted lead generation and optimization. **F. Edfeldt**

‡ *Cooperative Cosponsorship*

9:10 MEDI **14.** SAR enablement of multifunctional BACE templates: Thioamidines. **B.T. O'Neill**, E. Beck, M.A. Brodney, M.W. Bundesmann, C. Butler, L. Buzon, L. Chenard, J. Davoren, J. Dutra, C.J. Helal, K.E. Henegar, J.M. Humphrey, E.A. LaChapelle, B. Li, R. Lira, L.A. Martinez-Alsina, J.C. Murray, K. Ogilvie, L. Price, T.P. Tran, S. Sakya, Y. Zhang, A. Yu

9:30 MEDI **15.** Development of novel NLRP3 inflammasome inhibitors and their potential application. **S. Zhang**, J. Chojnacki, C. Marchetti, S. Toldo, A. Abbate

9:50 MEDI **16.** Methionine aminopeptidases (MetAPs) as promising targets toward discovery of novel anti-infective agents. P. Wangtrakuldee, **C. Chen**, B. Staker, J.M. Wilk, J.R. Horn, T.J. Hagen

10:10 MEDI **17.** Development of pyridopyrimidine-based inhibitors of HIV-1 reverse transcriptase. **C. Lacbay**, J. Mancuso, Y. Lin, N. Bennett, M. Menni, M. Gotte, Y.S. Tsantrizos

10:30 MEDI **18.** Open source malaria: A new approach to drug discovery. **A.E. Williamson**, M.H. Todd, P. Willis, O. Consortium

10:50 MEDI **19.** Development of non-incorporating small molecule inhibitors of antibody fucosylation. **M.J. Frohn**, J.G. Allen, C.H. Fotsch, M. Mujacic, T. San Miguel, O.R. Thiel, J. McCarter, A.J. Pickrell, M. Lo, J.B. Jordan

11:10 MEDI **20.** Discovery and opioid receptor SAR of AT-076, the first small-molecule opioid pan antagonist with nanomolar affinity at mu, delta, kappa and nociceptin opioid receptors. **V.B. Journigan**, N.T. Zaveri, W.E. Polgar

11:30 MEDI **21.** Discovery of oral FSHR (follicle stimulating hormone receptor) allosteric modulators. **H.N. Yu**

11:50 MEDI **22.** Small molecule activators of Pro-apoptotic BAX for cancer therapy. **E. Gavathiotis**

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Sponsored by COMP, Cosponsored by MEDI

SUNDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Blrm 1A/1B

General Oral Session

W. B. Young, *Organizer, Presiding*

1:30 MEDI **23.** Discovery of TAK-063, a novel phosphodiesterase 10A (PDE10A) inhibitor. **M. Fushimi**, J. Kunitomo, M. Yoshikawa, A. Kawada, J.F. Quinn, H. Oki, H. Kokubo, M. Kondo, K. Nakashima, T. Taniguchi

1:55 MEDI **24.** Discovery of a novel and potent dual orexin 1/orexin 2 receptor antagonist, E2006, for the treatment of sleep disorders. **T. Terauchi**

2:20 MEDI **25.** Discovery of the clinical candidate BMS-816336, an adamantyl acetamide based 11β-hydroxysteroid dehydrogenase type-1 (11β-HSD1) inhibitor. **X. Ye**, S. Chen, S. Wu, D.S. Yoon, H. Wang, Z. Hong, S.P. Oconnor, J. Li, J. Li, S. Walker, L.J. Kennedy, A. Apedo, A. Nayeem, S. Sheriff, P. Morin, D. Camac, T. Harrity, R. Zebo, J. Taylor, N. Morgan, R. Ponticiello, R. Golla, R. Seethala, M. Wang, T. Harper, B. Sleczka, B. He, M. Kirby, J. DiMarco, R. Scaringe, R.L. Hanson, Z. Guo, J. Li, J. Sun, M.K. Wong, B. Chen, L. Haque, D.K. Leahy, C. Chan, Y. Li, T. Zvyaga, L. Hansen, C. Patel, D.A. Gordon, J.A. Robl

2:45 MEDI **26.** Discovery, optimization, and human microdosing study of a novel series of H3 antagonists. **M. Chytil**, S. Engel, K. Fang, K. Spear

3:10 MEDI **27.** Cholesteryl ester transfer protein inhibitor BMS-795311. **J.X. Qiao**, T.C. Wang, A. Chen, D.S. Taylor, R.Z. Yang, P.G. Sleph, J.P. Li, D. Li, M. Chang, X. Chen, C. Xu, J. Li, D. Smith, D. Wu, L. Leith, L.S. Harikrishnan, M. Kamau, R. Rampulla, M.M. Miller, D. Bilder, R. Lawrence, M.A. Poss, P. Levesque, C.S. Huang, L.P. Adam, R.R. Wexler, H.J. Finlay, M.S. Salvati

3:35 MEDI **28.** Discovery of potent and kinase-selective p21-activated kinase 1 (PAK1) inhibitors. **J. Rudolph**, I. Aliagas, E. Blackwood, T. O'Brien, J. Crawford, J. Drobnick, L. Gazzard, C. Heise, W. Lee, L. Murray, C. Ndubaku, W. Wang, X. Zhao, K.P. Hoeflich

4:00 MEDI **29.** Liver targeted HIF-PHD inhibitors for the treatment of anemia. **C. Sinz**, Y. Chen, V.J. Colandrea, Q. Dang, B. DuBois, P. Liu, P.T. Meinke, R. Liu, J. Tan, F. Ujjainwalla, L. Wang, J.J. Hale, J. Cai, D. Stickens, B. Bishwokarma, M. Zielstorff, D. Zaller, C. Chiu, M. Cheng, C. Alpert, J. Metzger, L. Yang, S. Vincent, K. Bleasby, M. Hafey, R. Houle

4:25 MEDI **30.** Discovery of BMS-852927, a potent LXR partial agonist possessing LXRbeta functional selectivity. **E.K. Kick**, B. Busch, R. Martin, Y. Xie, M. Nanao, T. Stout, A. Plonowski, I. Schulman, G. Yan, W. Stevens, M. Nyman, L. Nguyen, R. Narayanan, K. Behnia, G. Cantor, J. Lupisella, P. Sleph, D. Grimm, J. Ostrowski, T. Kirchgessner, R.R. Wexler, R. Mohan

4:50 MEDI **31.** Building ERK inhibitors. Mitigaing their clearance. **J.T. Bagdanoff**, D. Poon, W. Han, S. Zhu, R. Jain, M. Lindvall

Section B

Colorado Convention Center
Mile High Blrm 2A/2B

Biased Agonism: An Emerging Paradigm in GPCR Drug Discovery

J. Herr, Z. Rankovic, *Organizers, Presiding*

1:30 MEDI **32.** Harnessing ligand-directed signaling to improve pain therapeutics. **L.M. Bohn**, C.L. Schmid, K. Lovell, N.C. Ross, T.D. Bannister

2:10 MEDI **33.** Engineering enhanced, receptor-specific, and signaling-biased arrestins. **V. Gurevich**

2:50 MEDI **34.** Discovery of TRV130, a G protein biased agonist of the μ-opioid receptor, for the treatment of acute severe pain. **A.L. Crombie**, X. Chen, P.M. Pitis, G. Liu, C. Yuan, D. Gotchev, D.S. Yamashita, J.D. Violin

3:30 MEDI **35.** Discovery of functionally selective ligands of fopamine D_2receptors. K. Butler, J. McCorvy, X. Chen, M. Caron, W. Wetsel, B.L. Roth, **J. Jin**

4:00 MEDI **36.** Novel GPR40 agonists for the treatment of type-2 diabetes: The effect of b-arrestin signaling. **C. Hamdouchi**

4:30 MEDI **37.** Biased signaling with allosteric modulators of GPCRs. **C.W. Lindsley**

5:00 Concluding Remarks.

Section C

Colorado Convention Center
Mile High Blrm 2C

Young Investigator in Medicinal Chemistry

Cosponsored by YCC

T. E. Prisinzano, *Organizer, Presiding*

2:00 MEDI **38.** First structural disclosure, discovery, preclinical characterization, and FTIH pharmacokinetics for GSK2878175, a second generation boron-based inhibitor of the HCV RNA-dependent RNA polymerase. **J. Shotwell**

2:30 MEDI **39.** Hedgehog pathway modulators as therapeutic agents. **M.K. Hadden**

3:00 MEDI **40.** Discovery of halogenated phenazine and halogenated quinoline small molecules with antibacterial and antibiofilm activities against *staphylococcal* biofilms. **R. Huigens**

3:30 MEDI **41.** Novel small molecule immunomodulators that target toll-like receptors. **H.H. Yin**

4:00 MEDI **42.** Discovery and adverse safety findings of two new mGluR5 NAM chemotypes. **A.F. Stepan**

4:30 MEDI **43.** Efficient small molecule inhibitors of the HDM2-p53 protein-protein interaction. **M.R. Machacek**

Drug Discovery

Structural Informatics & Target Based: Structure-Based

Sponsored by COMP, Cosponsored by MEDI

SUNDAY EVENING

Section A

Colorado Convention Center
Hall C

General Poster Session

W. B. Young, *Organizer*

7:00 - 9:00

MEDI **44.** Design, synthesis, and biological evaluation of novel tubulysin analogs as payloads for antibody-drug conjugates for the targeted treatment of cancer. Y. Huang, H. Xie, J. Jia, H. Guo, S. Gai, X. Li, L. Qu, X. Zuo, X. Zhou, S. Sun, Q. Yang, W. Li, C. Lin, H. Ye, **R.Y. Zhao**

MEDI **45.** Withdrawn.

MEDI **46.** New flash purification capabilities decrease run times up to 67%. **J.R. Bickler**

MEDI **47.** New high-performance C18 flash cartridge significantly improves resolution and fraction purity. **J.R. Bickler**

MEDI **48.** Rapid cleanup of peptides with mass-directed flash chromatography and spherical C18 silica. **W.J. Hartsock**, **J.R. Bickler**, V. Vandell, F.A. Kero

MEDI **49.** Purification of peptides by flash chromatography. J.E. Silver, R. Lewis

MEDI **50.** Design, synthesis, and biological evaluation of *Rickettsia prowazekii* methionine aminopeptidase (MetAP) Inhibitors. **T.R. Helgren**, C. Chen, P. Wangtrakuldee, C. Long, M. Hathuc, R. Small, B. Curran, J.R. Horn, T.J. Hagen

MEDI **51.** Mutual solubilities of the antibiotic/β-lactamase inhibitor drug combinations vancomycin, piperacillin, and tazobactam in aqueous solution. **H.S. Gray**, **H.N. Gray**, S.C. Butler, R.N. Mason

MEDI **52.** Molecular mechanism and ligand design of a PLP/GABA-dependent bacterial transcription regulator GabR. **E. Cybulla**, R. Wu, C. Reidl, D. Gawron, D.P. Becker, D. Liu

MEDI **53.** Synthesis, conformational analysis, and pharmacokinetics of fluorinated antituberucular nucleosides. **S. Dawadi**, K. Viswanathan, H. Boshoff, C.E. Barry, C.C. Aldrich

MEDI **54.** Protein structure-based virtual screening led to identification of novel natural product-derived hits as cannabinoid receptor 1 modulators. **P. Pandey**, K.K. Roy, R.J. Doerksen

MEDI **55.** Building on the success of the first generation of N-alkylthiol beta-lactams yields a multimodal, multiaction prodrug therapy for MRSA. **J.L. Borja**

MEDI **56.** Investigating the conformational states and ligand binding of voltage gated sodium channels by multiple spectroscopic techniques. **M. Colledge**, B. Wallace

MEDI **57.** Incorporation of triazoles as disulfide mimics in chimeric AGRP-melanocortin peptide template. **S.R. Tala**, A. Singh, C. Haskell-Luevano

MEDI **58.** Drug discovery and large-scale synthesis for 7-azaindoline derivatives as potent, orally available, selective M1 and M4 muscarinic acetylcholine receptors agonists. **Y. Uruno**, Y. Inoue, Y. Konishi, A. Suwa, K. Takai, K. Hashimoto, H. Matsuda, T. Nakako, M. Sakai, G. Hashimoto, T. Enomoto, A. Kitamura, Y. Uematsu, A. Kiyoshi, T. Sumiyoshi

MEDI **59.** Design, synthesis, and structure-activity relationships of flupirtine derivatives for the treatment of neuronal ceroid lipofuscinosis. **N. Kinarivala**, J. Makoukji, F. Saadeh, R. Boustany, P.C. Trippier

MEDI **60.** Exploiting the Sigma-2 receptor as a therapeutic target for cancer and various CNS diseases. **J. Chan**, J. Sahn, S.F. Martin, L. Scott, J. Pierce-Shimomura

MEDI **61.** Optimization of synthetically novel agonists of the putative cannabinoid receptor, GPR55, using an activated state model. **M.A. Lingerfelt**, L. Alfakhori, D.P. Hurst, P. Zhao, M.P. Croatt, M.E. Abood, P.H. Reggio

MEDI **62.** Rational fesign of fual-site scetylcholinesterase inhibitors: Multifunctional lead for Alzheimer's disease therapy. W. Yang, S. Yang, G. Yang

MEDI **63.** Discovery of novel, potent γ-secretase inhibitors. Z. Zhao

MEDI **64.** Novel amyloid binding compounds: A search for PET imaging probes for neurofibrillary tangles. B. Hurtle, L. Cai, B. Qu, V.W. Pike

MEDI **65.** Crystallographic evaluation of chelidamic acid congeners. **A.L. Green**, K.M. Lincoln, R.E. Saunders, K.N. Green

MEDI **66.** Rational design and bioevaluation for novel acetylcholinesterase inhibitors for treating Alzheimer's disease. **Q. Sun**, G. Yang, . Yang

MEDI **67.** Structural insights into the mechanism of activation of the human cannabinoid type 2 (CB_2) receptor: Molecular dynamics study of an agonist-bound state. **K.K. Roy**, P. Pandey, R.J. Doerksen

MEDI **68.** Discovery, SAR, and biological evaluation of a novel series of piperazine-based inhibitors of glycine transporter-1 (GlyT-1). **C.L. Cioffi**, S. Liu, M.A. Wolf, P.R. Guzzo, K. Sadalapure, V. Parthasarathy, J. Maeng, E. Carulli, D.T. Loong, X. Fang, P. Gupta, S. Panduga, K.N. Kalesh, L. Matta, S. Choo, R.N. Buckle, R. Davis, S.A. Sakwa, M. Hu, D.H. Dethe, B.J. Sargent, N.A. Moore, M.M. Luche, Y.L. Khmelnitsky, J. Ismail, H. Decornez, D.B. Kitchen, P.L. Love, M.A. Watson, J. Adolphson, G. Padilla, K. Waikins, S. Tom, A. Ngo, M. Chung, M. Bai, N. Johal, S. Swaminathan, A.J. Mhyre

MEDI **69.** Arylguanidine NAMs for α7 nAChRs: Where do they bind and why? **O.I. Alwassil**, S. Khatri, M.K. Schulte, M. Dukat

MEDI **70.** Structure activity relationship of tetrahydroisoquinoline *N*-methyl-D-aspartate receptor positive allosteric modulators can be modified to target GluN2B-containing receptors. **K.L. Strong**, D.S. Menaldino, K.K. Ogden, S.F. Traynelis, D.C. Liotta

MEDI **71.** CPM: A potential moiety to reduce opioid dependence. **Z. Wu**, V.J. Hruby

MEDI **72.** Curcumin/melatonin hybrids as neuroprotective agents for Alzheimer's disease. **J. Saathoff**, K. Liu, J. Chojnacki, S. Zhang

MEDI **73.** Application of machine learning and regression techniques in developing novel homologous recombination inhibitors. **J. Zhu**

MEDI **74.** Simple and integrated approach to compound progress and work-request tracking. **J.W. Sager**, T.E. Mansley, P. Mounteney, C.P. Snyder

MEDI **75.** In silico modeling workflows in support of exploratory computational toxicology. **M.R. Goldsmith**, D. Chang, A. Deschenes, C. Williams, A. Ajamian

MEDI **76.** Importance of visualization in lead discovery: Supporting the medicinal chemist in designing compounds more efficiently. **C. Detering**

MEDI **77.** Chemoinformatics analysis of natural products databases: Toward the identification of tubulin polymerization inhibitors. **R. Aguayo-Ortiz**, R. Castillo-Bocanegra, A.M. Hernandez Campos, J.L. Medina-Franco

MEDI **78.** Discovery and synthesis of triphenylethanamine derivatives as highly potent cholesteryl ester transfer protein Inhibitors. **T. Wang**, J.X. Qiao, A. Chen, D.S. Taylor, R.Z. Yang, P.G. Sleph, J.P. Li, D. Li, M. Chang, X. Chen, C. Xu, J. Li, P. Levesque, C.S. Huang, L.P. Adam, M.S. Salvati, H.J. Finlay, R.R. Wexler

MEDI **79.** Identification of a novel class of covalent modifiers of hemoglobin as potential antisickling agents. **A.M. Omar**, M.A. Mahran, M. Ghatge, N. Chowdhury, F.H. Bamane, M.E. El-Araby, O. Abdulmalik, M. Safo

TECHNICAL PROGRAM

MEDI **80.** Process of blood coagulation investigated through the interactions of aspirin with bovine red blood cell lipid extract membrane monolayers. **K.A. Miller**, A. Sostarecz

MEDI **81.** Novel coumarin based monocarboxylate transport 1 & 4 inhibitors as anticancer agents. L. Solano, C. Ronayne, G.L. Nelson, S. Gurrapu, S.K. Jonnalagadda, V. Mereddy

MEDI **82.** Potent dual monocarboxylate transporter 1 & 4 inhibitors for triple negative breast cancer treatment. **L. Solano**, **G.L. Nelson**, **C. Ronayne**, V. Mereddy, S.K. Jonnalagadda, S. Gurrapu

MEDI **83.** Development of collagen films coated with synthetic photoreactive peptides that support cardiovascular repair and regeneration. **J. Malcor**, D. Bax, D. Bihan, S. Hamaia, R. Farndale

MEDI **84.** Withdrawn.

MEDI **85.** Total synthesis of clavatadine A analogs to produce a viable reversible inhibitor for factor XIa. **C.E. Malmberg**, S. Chamberland

MEDI **86.** Discovery of novel, potent, and highly selective factor xIa inhibitors from HTS hit with X-ray crystallography-based rational design. T. Nishiyama, T. Kondo, K. Hisaichi, K. Ochi, A. Kinoshita, R. Miwa, **A. Imagawa**, S. Flanagan, C.J. Yarnold, S. Courtney, M. Gohda, K. Suzuki, T. Ono, S. Koyama, T. Hagio, M. Sakai, H. Habashita, K. Kawabata

MEDI **87.** Structure-based design, synthesis, and evaluation of novel peptide inhibitors of thrombin-induced activation of platelets aggregation. **C.C. Clement**, J. Gonzalez, A. Babinska, M. Philipp

MEDI **88.** Picomolar K_D ligands can be obtained by increasing the binding rate instead of decreasing the dissociation rate: Surprising structure-kinetic relationship among very similar thrombin inhibitors. **M.T. Khayat**, A.S. Murkin, M.M. Murphy, T.e. Ryan, B. Sathyamoorthy

MEDI **89.** Synthesis of resorufin derivatives as inhibitor indicators of cytochrome P450 enzymes. **L. Lovings**, J. Liu, M. Foroozesh

MEDI **90.** Radical-induced oxidation of tobacco-specific nitrosamines under physiological conditions. B.R. Daws, **S.P. Mezyk**, J.J. Kiddle

MEDI **91.** Pyrano- and furanochromones as specific inhibitors of human cytochrome P450 1A2. **J. Liu**, P. Pham, L. Lovings, N. Goyal, M. Foroozesh

MEDI **92.** Investigation of regulation of cytochrome P450 2J2 in adult human primary cardiomyoctyes. **R. Rowlands**, E. Evangelista, B. Raccor, R. Totah

MEDI **93.** Metabolic stability assessment of tumor-targeted drug delivery systems with fluorine-labeled taxoid probes by 19F NMR. **B. Lichtenthal**, J.D. Seitz, J.G. Vineberg, L. Wei, C. Lin, J. Kahn, I. Ojima

MEDI **94.** Drug release by remotely controlled magnetic anisotropy. **M. Shin**, B. Kang, S. Han, E. Jang, J. Suh, Y. Huh, S. Haam

MEDI **95.** Modular platform for the synthesis of a targeting and pH-responsive lipopeptide ligand in nanovectors. **M. Salinas**, G.R. Negrete

MEDI **96.** Fibrosis toolbox: Small molecules to investigate fibrosis pathways and mechanisms. **R. Hatley**

MEDI **97.** Novel Nrf2 activators from microbial transformation products suppress oxidant stress-induced cellular damage in ARPE-19 cells. **Y. Nakagami**, K. Masuda, E. Hatano, T. Inoue, S. Komoriya

MEDI **98.** Discovery of potent and selective S1P2 antagonists. **K. Kusumi**, A. Naganawa, H. Kurata, K. Shinozaki

MEDI **99.** Monster Mas agonist: Revealing the beauty in the beast. **J. Redmond**, S. Peace, G. Inglis, G. Vitulli, J. Barrett

MEDI **100.** Quatenary-ammonium salt derivatives as bifunctional muscarinic antagonist and beta2 agonist (MABA) for the treatment of COPD and asthma. **J. Igarashi**, E. Mitsuyama, T. Ida, H. Sugiyama, K. Segawa, J. Nomura

MEDI **101.** Novel strategy for the treatment of asthma by targeting $GABA_A$ receptors in the lung. **R. Jahan**, M.R. Stephen, G. Gallos, C.W. Emala, J.M. Cook

MEDI **102.** Design and synthesis of anti-inflammatory steroids with improved therapeutic index: Discovery of an inhaled dissociated steroid (selective glucocorticoid receptor modulator). **P.J. Biju**

MEDI **103.** Achieving desired levels of selectivity for a series of "acyclic-based" JAK inhibitors. **J. Kempson**, S.H. Spergel, S. Wrobleski, J. Das, L.M. Doweyko, J. Guo, J. Hynes, J. Duan, B. Jiang, Z. Lu, R.V. Moquin, S. Lin, H. Wu, B.V. Yang, S.M. Stachura, J.S. Tokarski, A. Gupta, J.C. Barrish, P.H. Carter, G.L. Schieven, W.J. Pitts

MEDI **104.** Determinants of activity at human toll-like receptors 7 and 8: Quantitative structure-activity relationship (QSAR) of diverse heterocyclic scaffolds. **E. Yoo**, D.B. Salunke, D. Sil, X. Guo, A.C. Salyer, A.R. Hermanson, M. Kumar, S.S. Malladi, R. Balakrishnan, W.H. Thompson, H. Tanji, U. Ohto, T. Shimizu, S.A. David

MEDI **105.** Enhancement of potency of the TLR7 ligand by conjugation to polysaccharide. **H. Shinchi**, T. Hayashi, M. Chan, A. Ahmadiiveli, S. Zhang, B. Crain, Y. Suda, H.B. Cottam, D. Carson

MEDI **106.** Design and synthesis of a dual-targeting liposomal spherical nucleic acid. **J. Ferrer**, N. Chernyak, J. Wertheim, C.A. Mirkin

MEDI **107.** Human toll-like receptor 8-selective agonistic activities in 1-alkyl-1*H*-benzimidazol-2-amines. **M. Beesu**, S.S. Malladi, L.M. Fox, C.D. Jones, A. Dixit, S.A. David

MEDI **108.** Design, synthesis, and testing of macrocyclic β-strand as protease inhibitors. **A.D. Pehere**, M. Pietsch, N.M. Paul, D.F. Callen, M. Gütschow, A.D. Abell

MEDI **109.** Single cell imaging and analysis for macrophage uptake of nanoparticles using fluorescent organosilica nanoparticles. **M. Nakano**, M. Nakamura, K. Hayashi, T. Kanadani, K. Miyamoto

MEDI **110.** Mitochondria targeted cardiolipin based high density lipoprotein mimicking nanoparticles for atherosclerosis. **R. Wen**, S. Dhar

MEDI **111.** Investigation on cellular uptake of functionalized gold nanoparticles and their biological effects. N. Ma, **C. Ma**, X. Mou, N. He

MEDI **112.** Molecular beacon-functionalized gold nanoparticle as miRNA detecting probe for cellular classification in gastric cancer. **K. Jisun**

MEDI **113.** Wire-framed gold nanoparticles for a multistep photothermic driven drug release system. **T. Lee**, D. Bang, J. Suh, Y. Huh, S. Haam

MEDI **114.** Virus-mimicking antimicrobial polymer brushes: The nanostructure and activity. **Y. Jiang**, W. Zheng, H. Liang

MEDI **115.** Targeting mitochondrial genome by cisplatin prodrug and its nanoparticle formulation to overcome chemoresistance. **R. Pathak**, S. Marrache, S. Dhar

MEDI **116.** Syntheses, characterization, and biomedical applications of novel organosilica nanoparticles. **M. Nakamura**

MEDI **117.** Activatable two-component photosentisizer: selective targeting and killing of cancer cells. **J. He**, Y. Wang, M.P. Bruchez

MEDI **118.** Withdrawn.

MEDI **119.** Silybin derivatives as antiprostate cancer agents: Synthesis and antiproliferative activity. **B. Vue**, S. Zhang, X. Zhang, K. Parisis, Q. Chen

MEDI **120.** Fluorescein hydrzones as novel nonintercalative topoisomerase catalytic inhibitors with low DNA toxicity. **A.M. Rahman**, S. Park, Y. Kwon, A.A. Kadi

MEDI **121.** Design and synthesis of a novel tri-branched asymmetric bowtie PAMAM dendrimer-based drug conjugate as a cancer theranostic agent. **L. Wei**, T. Wang, Y.G. Teng, I. Ojima

MEDI **122.** Synthesis and antitumor activity of *N,N'*-bisnaphthylated imidazole salts with lipophilic or hydrophilic substituents on the imidazole and benzimidazole rings. **K.L. Shelton**, P.O. Wagers, M.R. Southerland, M.A. DeBord, M.J. Panzner, N.K. Robishaw, C.A. Tessier, W.J. Youngs

MEDI **123.** Disrupting reactive oxygen species mediated pathways in human cancer models with ferrocenylated *N*-heterocyclic carbenes. **J.F. Arambula**, K. Arumugam, D.J. Magda, C. Bielawski, J.L. Sessler

MEDI **124.** Targeting the hypoxia-adenosinergic pathway via $A_{2A}R$ antagonists; Toward cancer immunotherapeutics. **G. Yuan**, S. Hatfield, M. Sitkovsky, M.J. Ondrechen, G. Jones

MEDI **125.** Triterpenoid derivatives and their biological activities. **M. Urban**, J. Sarek, M. Hajduch, J. Rehulka, P. Dzubak, L. Borkova

MEDI **126.** Development of a novel class of hydroxylated 2, 4-diphenyl indenopyridines as a selective non-intercalative topoisomerase IIα catalytic inhibitor. **T.M. Kadayat**, T. Thapa Magar, G. Bist, A. Shrestha, Y. Kwon, E. Lee

MEDI **127.** Preliminary structure-activity relationship studies of a fungal metabolite ophiobolin A – promising antiglioblastoma agent. **R. Dasari**, V. Mathieu, R. Kiss, A. Evidente, A.V. Kornienko

MEDI **128.** Identification of the first selective small molecule GRPR (BB2) antagonists. **N.D. Harriott**, S.B. Ravula, G. Beaton, N.J. Ashweek, J.P. Williams, S.R. Hoare, J. Fan

MEDI **129.** Withdrawn.

MEDI **130.** Bishomoisoprenoid triazoles as inhibitors of geranylgeranyl diphosphate synthase. **V.S. Wills**, J.I. Metzger, C. Allen, S.A. Holstein, D.F. Wiemer

MEDI **131.** Synthesis and structure-activity studies of drugs that affect a cancer causing mechanism and reduce cell growth. **A. Jelowicki**, K.E. Tan, E.H. Li, C. Wen, C.M. Ott, N.V. Patel, P. De Lijser, C.A. Martindale

MEDI **132.** Click chemistry approach to diversification of novel base-modified thymidine analogs that exhibit anticancer activity. **P.R. Wolfkiel**, K.M. Borland, E.J. Merino, M.C. Tranter, V.A. Litosh

MEDI **133.** Two-faced, biphenyl-based synthetic α-helix mimetics are effective inhibitors of the Mcl-1 oncoprotein. **M. Lanning**, P. Wilder, S. Fletcher

MEDI **135.** Structure-based design of functionalized salicylates as potent Mcl-1 inhibitors. **L. Chen**, J. Chauhan, J.L. Yap, P.T. Wilder, S. Fletcher

MEDI **136.** Design and synthesis of coumerin-aminoethylphenol hybrids as potential epigenetic modulators. **M. Branscum**, **T. Rowe**, J. Brider, M.A. Alam

MEDI **137.** Design and chemoproteomic functional characterization of a chemical probe targeted to bromodomains of BET family proteins. **B.A. Lefker**, K.F. Geoghegan, S.W. Wright, D.C. Limburg, J. Shin, C.M. Williams, P. Sahasrabudhe, P. Bonin, S. Ramsey

MEDI **138.** Identification and characterization of cellular histone deacetylase active site alterations Induced by deacetylase complex components. **T. Hanigan**, I. Kastrati, J. Frasor, P.A. Petukhov

MEDI **139.** Comparison of local and tropical plants used as herbal remedies and their chemical make-up. **M.D. Mann**

MEDI **140.** Transformations of allicin from garlic: The discovery of allylselenoalkylsulfonylpyridazines and Its antitumor activity. **M. Park**, **C. Kim**, **D. Shin**, M. **Choi**

MEDI **141.** Docking studies to develop GLI-associated oncogene inhibitors from natural products. **Y. Rifai**

MEDI **142.** Discovery of novel hit molecules for Sphingosine kinase -1 inhibitory activity by structure based virtual screening. C. Selvam, **B.C. Jordan**, S. Doshi

MEDI **143.** Novel method for targeting sphingosine kinase 2: Design, synthesis, and evaluation of bisubstrate inhibitors. **T.K. Dawson**, R. Dyer, Y. Kharel, K. Lynch, T.L. Macdonald

MEDI **144.** Serotonin-linked NSAIDs as inhibitors of FAAH, TRPV1, and COX 2. **T.M. Rose**, C.A. Reilly, C.E. Deering-Rice, C. Brewster, C. Brewster

MEDI **145.** Discovery of second generation P2X3 receptor antagonists for the treatment of chronic pain. **A. Ginnetti**, D. Paone, S. Stauffer, C. Potteiger, A. Shaw, J.Z. Deng, D.N. Nguyen, C. Segerdell, C.S. Burgey, S. Graham, J. Anquandah, A. Calamari, G. Cheng, S. Cook, S. Kane, M. Leitl, A. Liang, E. Moore, J. Panigel, C. Salvatore, M. Urban, J. Wang, K. Fillgrove, C. Tang

MEDI **146.** Design, synthesis, and in vitro evaluation of novel inhibitors of fatty acid amide hydrolase (FAAH). **S. Cramer**, J. Johnson, A. El-Alfy, J. Stec

MEDI **147.** Targeted far-red light activatable prodrugs: folate receptor-targeting, optical imaging, and a combination of photodynamic therapy and site-specific chemotherapy. G.N. Nkepang, **M. Bio**, P. Rajaputra, S.G. Awuah, Y. You

MEDI **148.** Synthesis of tripartite prodrugs via N → C amidative-installation of the Katzenellenbogen-spacer: Application of the *traceless* Staudinger ligation. **T. Kirby**, B.L. Barthel, T.H. Koch

MEDI **149.** Exploring CatSper channel openers and binding site interactions: Discovery of steroidal channel blockers. **E. Carlson**, J. Hawkinson, G.I. Georg

MEDI **150.** Enzyme sensitive conjugates as a macromolecular delivery platform for siRNA. **J.C. Carlson**, J. Benson, A. Sokoloff, D. Rozema, A.V. Blokhin

MEDI **151.** Development of a catalytic Mitsunobu reaction. **J.A. Buonomo**, C.C. Aldrich

MEDI **152.** Flow hydrogenation: A tool for creating 3D shaped molecules from flat precursors. **L. Kocsis**, S. Fekete, J. Gerencsér, G. Makara, F. Darvas

MEDI **153.** Discovery of potent α_{1L}-adrenoceptor agonists: Design and synthesis of bicyclic derivatives. **S. Suzuki**

MEDI **154.** Density functional calculations of the structural, thermodynamic, and spectroscopic properties of tautomers of avigan. F.L. Nesbitt

MEDI **155.** Novel 3-nitrotriazole-based amides and carbinols as bifunctional anti-chagasic agents. **M.V. Papadopoulou-Rosenzweig**, W.D. Bloomer, G.I. Lepesheva, H.S. Rosenzweig, M. Kaiser, E. Chatelain, J. Ioset

MEDI **156.** Syntheses and binding studies of novel benzimidazole compounds targeting the hepatitis C virus internal ribosome entry site. **A. Kanner**, A. Cholewczynski, D. Schmit, U. Milewicz, R. Wolkowicz, M.A. Boerneke, T. Hermann, M.B. Bergdahl

MEDI **157.** Discovery of MK-8325: A silyl proline containing HCV NS5A inhibitor with pan-genotype activity. **A.G. Nair**, Q. Zeng, S.B. Rosenblum, O. Selyutin, Y. Jiang, D. Yang, K. Keertikar, G. Zhou, M.P. Dwyer, S. Kim, S. Bandarpalle, W. Yu, L. Tong, R. Mazzola, J.P. Caldwell, H. Tang, R. Liu, E. Asante-Appiah, S. Agrawal, E. Xia, S. Curry, P. Ingravallo, J.A. Kozlowski

MEDI **158.** Discovery of silyl proline containing HCV NS5A inhibitors: SAR development. **J.A. Kozlowski**, N. Anilkumar, O. Selyutin, S.B. Rosenblum, Y. Jiang, D. Yang, K. Keertikar, G. Zhou, M.P. Dwyer, S. Kim, B. Shankar, W. Yu, L. Tong, R. Mazzola, J.P. Caldwell, H. Tang, S. Agrawal, E. Asante-Appiah, S. Curry, P. McMonagle, S. Black, A. Nomeir

MEDI **159.** Design and synthesis of dual-tropic HIV entry inhibitors that utilize a homologous CCR5/ CXCR4 binding site. **S. Gupta**, A.R. Prosser, B.D. Cox, L.J. Wilson, D. Liotta

‡ *Cooperative Cosponsorship*

MEDI **160.** Synthesis and biological evaluation of substituted pyrimidines. **B.S. Clark**, J. Kudrysch, S.Q. Smith, V.E. Zottig

MEDI **161.** Star-branched polymers with antioxidant activities. **U.G. Huynh**, C.Y. Lee, A. Sharma

MONDAY MORNING

Section A

Colorado Convention Center
Mile High Blrm 2A/2B

Innate Potential: Advances in Non-Biologic Modulation of Innate Immune Targets

A. J. Dyckman, J. Hynes, D. S. Weinstein, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 MEDI **162.** Structure-based design of small molecule modulators of TLR8. **S.A. David**

9:45 MEDI **163.** Development of novel IRAK4 inhibitors for the treatment of inflammation related disorders. **W.M. Seganish**, W.T. McElroy, S. Brumfield, G. Li, D. Tulshian, J. Tata, R. Herr, B.J. Lavey

10:15 MEDI **164.** Identification of highly potent and mono-selective RIP1 kinase inhibitors for the treatment of TNF-dependent diseases. **P.A. Harris**

10:45 MEDI **165.** Designing RIP2 kinase inhibitors for innate immunity-driven Indications. **L. Casillas**

11:15 MEDI **166.** Identification of selective TYK2 inhibitors and their role in IL12- and IL23-pathway signaling. **S. Magnuson**, J. Liang, V. Tsui, Y. Lai, B. Zhang, K. Williams, C. MacLeod, Y. Wenqian, S. Sohn, J. DeVoss, I. Peng, J. Lesch, M. Balazs, A. Van Abbema, K. Barrett, P. Bir Kohli, W. Blair, C. Chang, A. Johnson, L. Berezhkovskiy, J. Driscoll, P. Fan, A.N. Sambrone, P. Chiang, C. Eigenbrot, S. Shia, M. Ultsch, N. Ghilardi, L. Wu

11:45 MEDI **167.** Oligonucleotide inhibitors of endosomal toll-like receptors: Novel approach to treatment of autoimmune diseases. **S. Agrawal**

Section B

Colorado Convention Center
Mile High Blrm 1A/1B

Recent Advances in Targeting the Nav1.7 Sodium Channels

M. Chu-Moyer, *Organizer*
E. H. Harrington, *Organizer, Presiding*

9:00 MEDI **168.** Recent advances in therapeutic targeting of NaV channels. **D.C. Pryde**, B. Marron, N. Swain, C.W. West

9:30 MEDI **169.** Imaging pain generators in vivo using radiolabeled sodium channel toxin derivatives. **D. Behera**, A. Hoehne, W.H. Parsons, B. Shen, D.C. Yeomans, S. Biswal, F.T. Chin, J. Du Bois

10:00 MEDI **170.** Potent and selective Nav1.7 inhibitory peptides from tarantula venom. **K. Biswas**, J.K. Murray, B. Wu, J. Long, K. Sham, A. Zou, D. Liu, J.A. Ligutti, L. Poppe, J.B. Jordan, K.L. Andrews, S. McDonough, L.P. Miranda, B.D. Moyer

10:30 MEDI **171.** Identification of GNE-131: A potent and selective hNa$_v$1.7 inhibitor for the treatment of pain. **B.S. Safina**, G. Bankar, P. Bichler, C. Chabot, E. Chang, J. Chang, C. Chen, S. Chowdhury, C.J. Cohen, S. Decker, C.M. Dehnhardt, T. Focken, M.E. Grimwood, D. Hackos, I. Hemeon, K. Khakh, C. Koth, R. Kwan, S. Lin, K. Nelkenbrecher, D.F. Ortwine, J. Pang, J. Payandeh, L. Robinette, T. Sheng, S. Sun, M. Waldbrook, A. White, M. Wilson, C. Xie, C. Young, A. Zenova, Y. Zhang, D. Sutherlin

11:00 MEDI **172.** Design of subtype selective Na$_v$1.7 inhibitors for the treatment of pain. **N. Swain**

11:30 MEDI **173.** Development of oral Na$_v$1.7 inhibitors with excellent selectivity over Na$_v$1.5 for the treatment of pain. **M. Layton**, A.J. Roecker, J.E. Pero, M.S. Egbertson, B. Gomez, K. Jones, Z. Zhao, S. Wolkenberg, J. Mulhearn, M.J. Kelly, M.A. Rossi, H.D. Fiji, L. Zhao, P.J. De Leon, D. Li, K. Gilbert, A.K. Houghton, R. Kraus, B. Klein, M. Clements, C. Daley, J. Wang, T. Finger, J. Majercak, V. Santarelli, I. Gregan, M. Cato, T. Filzen, A. Jovanovska, Y. Wang, D. Wang, X. Peng, X. Wang

Section C

Colorado Convention Center
Mile High Blrm 2C

Approaches to Targeting RNA with Small Molecules

N. A. Meanwell, R. E. Olson, *Organizers, Presiding*

8:30 MEDI **174.** Rational design of small molecules to target the DNA/RNA of trinucleotide repeat (TNR) diseases. **S.C. Zimmerman**, L. Nguyen, L. Luu, J.Lee

9:05 MEDI **175.** New chemical and analytical tools for understanding RNA recognition. **B.L. Miller**

9:40 MEDI **176.** Identification of biologically active, RNA-binding small molecules using small molecule microarrays. **J. Schneekloth**

10:15 MEDI **177.** High-throughput platform assay technology for the discovery of pre-microRNA-selective small molecule probes. **A.L. Garner**

10:50 MEDI **178.** Giving SMN2 a push in the right direction: The discovery of small molecule splicing modulators. **M.G. Woll**, H. Qi, A. Turpoff, N. Zhang, X. Zhang, G. Chen, N.A. Naryshkin, A. Dakka, J. Narasimhan, V. Gabbeta, M. Weetall, X. Zhao, N. Risher, J. Sheedy, G.M. Karp

11:25 MEDI **179.** Progress on the development of rational methods to target RNA with small molecules. **M.D. Disney**

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

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Drug Discovery

Structural Informatics & Target Based: Structure-Based

Sponsored by COMP, Cosponsored by MEDI

MONDAY AFTERNOON

Section A

Colorado Convention Center
Mile High Blrm 1A/1B

New Models for Drug Discovery: Public, Private, and Non-Profit

J. Crawford, A. A. Estrada, B. Shotwell, *Organizers, Presiding*

2:00 MEDI **180.** Investigation of highly optimized LRRK2 kinase inhibitors in preclinical safety studies via a Michael J. Fox Foundation–Genentech collaboration. **A.A. Estrada**

2:30 MEDI **181.** New collaborative ways of discovering and developing anti-malarial therapies. **P. Willis**

3:00 MEDI **182.** ENABLE(ing) drug discovery: A public private partnership addressing antimicrobial resistance in serious gram negative infections. **A.T. Price**

3:30 MEDI **183.** Development of antiviral agents to treat poliovirus infections. **M. McKinlay**

4:00 MEDI **184.** Foundation-directed therapeutic development: Pfizer collaboration on PDE inhibitors. **C. Dominguez**

4:30 MEDI **185.** First small molecule clinical candidate discovered in Africa. **K. Chibale**

Section B

Colorado Convention Center
Mile High Blrm 2A/2B

Modulators of the Nuclear Receptor RORc

B. P. Fauber, S. J. Taylor, *Organizers, Presiding*

2:00 MEDI **186.** Development of RORalpha/beta/gamma subtype selective ligands. **T.P. Burris**

2:25 MEDI **187.** Small molecule inhibitors of RORgamma t: Their development to study the function of inflammatory immune cells. **J. Huh**

2:50 MEDI **188.** Structural basis for the inverse agonism of novel RORγt Inhibitors. **X. Li**

3:15 MEDI **189.** Optimization of quinoline tertiary alcohols as modulators of RORgt. **K. Leonard**, A. Fourie, X. Xue, M.J. Urbanski, H. Venkatesan, K. Barbay, D.A. Kummer, R. Nishimura, R.L. Wolin, K.D. Kreutter, C.R. Woods, V.M. Tanis, A. Wang, W. Jones, K. McClure, S.D. Goldberg, E. Fennema, C. Martin, J. Pierce, G. Bacani, J. Spurlino, C. Schalk-Hihi, C. Milligan, P. Wilkinson, T. Cao, M.C. Abad, R. Luna, K. Herman, A. De Leon, E. Nulton, M. Nelen, J. Yu, M.D. Cummings, B. Scott, K. Sepassi, S. Nguyen, M. Sablad, N. Rozenkrants, Y. Zhang, T. Rao, A. Ndifor, S. Branum, J. Spink, C.A. Teleha, D. Pippel, R. Russell, T. Schlueter, J.P. Edwards

3:40 MEDI **190.** Dealing with a highly lipophilic binding pocket: design and development of novel RORg inverse agonists with the consideration of ligand polarity and conformational diversity. **J. Chao**

4:05 MEDI **191.** Reversed sulfonamide series of selective RORc inverse agonists. **M.B. van Niel**, B.P. Fauber, M. Cartwright, S. Gaines, J.C. Killen, O. René, S.I. Ward, G.d. Boenig, Y. Deng, C. Eidenschenk, C. Everett, E. Gancia, A. Ganguli, A. Gobbi, J. Hawkins, A.R. Johnson, J.R. Kiefer, H. La, P. Lockey, M. Norman, W. Ouyang, A. Qin, N. Wakes, B. Waszkowycz, H. Wong

4:30 MEDI **192.** Discovery of novel RORγ antagonists. **M. Shiozaki**

Section C

Colorado Convention Center
Mile High Blrm 2C

Symposium in Honor of Richard Gibbs

B. Blagg, T. E. Prisinzano, *Organizers, Presiding*

2:00 MEDI **193.** Targeting indenoisoquinoline topoisomerase I inhibitors to cancer cells. D.E. Beck, T. Nguyen, W. Lv, P.N. Reddy, M. Abdelmalak, K. Agama, C. Marchand, Y. Pommier, J. Roy, A. Kanduluru, C. Venkatesh, P. Low, **M. Cushman**

2:35 MEDI **194.** Inhibition of geranylgeranyl diphosphate synthase by isoprenoid bisphosphonates. **D.F. Wiemer**

3:10 MEDI **195.** Small molecule epigenetic modulators for the treatment of cardiovascular disorders. C.J. Kutz, S.L. Holshouser, **P.M. Woster**

3:45 MEDI **196.** Protein prenylation: From enzymology to biotechnology and therapeutic application. **M.D. Distefano**, Y. Wang, C.C. Palsuledesai, J.K. Dozier

4:20 MEDI **197.** Biosynthesis of squalene: A new pathway in bacteria. J. Pan, **C.D. Poulter**

Medicinal & Aromatic Crops: Production, Phytochemistry, & Utilization

Sponsored by AGFD, Cosponsored by AGRO and MEDI

Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

Drug Discovery

ADME & Informatics

Sponsored by COMP, Cosponsored by CINF and MEDI

MONDAY EVENING

Section A

Colorado Convention Center
Halls C/D

Sci-Mix

W. B. Young, *Organizer*

8:00 - 10:00
44, 53, 56, 68, 70, 78, 84, 96, 99, 128, 137.
See previous listings.
278, 286, 294, 298, 323, 331, 333, 338, 343.
See subsequent listings.

TUESDAY MORNING

Section A

Colorado Convention Center
Mile High Blrm 2A/2B

E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances: Symposium in Honor of Ruth R. Wexler

Cosponsored by WCC

W. B. Young, *Organizer*
J. E. Macor, *Presiding*

9:00 MEDI **198.** Lessons learned in the practice of medicinal chemistry. **P.S. Anderson**

9:35 MEDI **199.** In search of small molecule modulators for the treatment of autoimmune and inflammatory diseases. **J.C. Barrish**

10:10 MEDI **200.** Thrombin receptor antagonists for the prevention of arterial thrombosis: Discovery of vorapaxar (zontivityTM). **W.J. Greenlee**

10:45 MEDI **201.** Structure-based design of serine protease inhibitors: The quest for safer and efficacious anticoagulants. **M.L. Quan**

11:20 MEDI **202. Award Address** (E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances sponsored by Merck Research Laboratories). Adventures in cardiovascular drug discovery: New frontiers and lessons learned. **R.R. Wexler**

Section B

Colorado Convention Center
Mile High Blrm 1A/1B

Observations from Recent Drug Launches: The Rules of Today May Not Apply Tomorrow

J. B. Schwarz, *Organizer, Presiding*

9:00 MEDI **203.** Discovery of macitentan: Can we apply rules of yesterday tomorrow? **M.H. Bolli**

9:30 MEDI **204.** Discovery and development of covalent BTK inhibitors. **W. Chen**

10:00 MEDI **205.** Chiral, nonracemic hemi-aminals to the rescue: The discovery of the HIV-1 integrase inhibitors dolutegravir and cabotegravir. **B.A. Johns**

10:30 Intermission.

10:45 MEDI **206.** Discovery of thalidomide and amino substituted analogs as anticancer agents. **R. DAmato**

11:15 MEDI **207.** Ponatinib, a pan-Bcr-Abl kinase inhibitor approved for leukemia treatment, potently inhibits the T315I mutant and overcomes mutation-based resistance. **W. Huang**

11:45 MEDI **208.** Pirfenidone and optimized pirfenidone analogs for antifibrotic indications. J.Y. Ramphal, L. Pan, C. Schaefer, S.D. Seiwert, B.O. Buckman, **J.B. Schwarz**

Section C

Colorado Convention Center
Mile High Blrm 2C

Why You Should Have Paid Attention in P-Chem: Thermodynamics in Drug Discovery

A. J. Peat, B. Shotwell, *Organizers, Presiding*

9:00 MEDI **209.** Thermodynamic-based approach to the inhibition of HIV-1 cell infection. **E. Freire**

9:30 MEDI **210.** Thermodynamics guided lead discovery and optimization. **G.M. Keseru**

10:00 MEDI **211.** Ligand-protein binding thermodynamics from fragments to drugs. **G. Ferenczy**

10:30 Intermission.

10:45 MEDI **212.** Exploring applications and origins of binding kinetics in structure-based drug discovery. **D. Meinhold**

11:15 MEDI **213.** Accelerating drug discovery: the role of free energy calculations. **R. Abel**, R. Friesner, R. Farid, T. Lin, L. Frye, J. Knight, G. Krilov, L. Wang

11:45 MEDI **214.** Lipophilic efficiency as a tool for identifying and optimizing enthalpic interactions. **M.D. Shultz**

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

Phenolic & Polyphenolic Chemistry in Food Processing

Reactions/Properties

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

Drug Discovery

Methodology

Sponsored by COMP, Cosponsored by CINF and MEDI

TUESDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Blrm 1A/1B

Smissman Award: Symposium in Honor of Dennis Liotta

W. B. Young, *Organizer*

J. E. Macor, *Presiding*

2:00 MEDI **215.** Nucleoside analogs: Synthesis and medicinal chemistry. **Y. Guindon**, M. Prévost, S. Dostie, P. Mochirian, G. Tambutet

2:45 MEDI **216.** Therapeutic opportunities of chemical targeting of mitochondria. **P. Wipf**

3:30 MEDI **217.** Targeting protein-protein interactions for new cancer therapeutics. **S. Wang**

4:15 MEDI **218.** Discovery of novel therapeutics for treating various types of viral diseases, cancers, and inflammatory disorders. **D. Liotta**

Section B

Colorado Convention Center

Mile High Blrm 2A/2B

The Role of Rings in Drug Design

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

2:00 MEDI **219.** Rings in drugs. **R. Taylor**

2:35 MEDI **220.** Small, medium, and large ring systems: Observations and examples of their roles in molecular recognition and drug design. **D.L. Cheney**

3:10 MEDI **221.** Development of novel transition metal-catalyzed approaches toward heterocycles. **V. Gevorgyan**

3:45 MEDI **222.** Rings in (candidate) drugs: Case stories. **J. Boström**

4:20 MEDI **223.** Sulfur-containing heterocycles in drug design. **M.D. Bartberger**

GSSPC: Designed by Nature, Developed by Science: Interdisciplinary Perspectives on Biocatalysis

Sponsored by CHED, Cosponsored by ANYL, BIOL, CATL, ENVR, I&EC, MEDI, ORGN and PRES

Phenolic & Polyphenolic Chemistry in Food Processing

Sources

Sponsored by AGFD, Cosponsored by AGRO, BIOT, COMP and MEDI

Drug Discovery

Methodology

Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY MORNING

Section A

Colorado Convention Center

Mile High Blrm 2A/2B

General Oral Session

W. B. Young, *Organizer*

J. Rudolph, *Presiding*

8:30 MEDI **224.** Discovery and synthesis of first-generation single-drug "cocktails" to combat HIV. **A.R. Prosser**, B.D. Cox, S. Gupta, L.J. Wilson, D.C. Liotta

8:55 MEDI **225.** B-DNA structure-based removal of genotoxicity from a series of inhibitors of the IκB-kinase IKK2. **L. Borjesson**, **I. Shamovsky**, M. Andersson, T. Brimert, C. Ekström, A.K. Ray, P. Zlatoidsky, P. Åberg

9:20 MEDI **226.** Selective inhibition of group-II p-21-activated kinases (PAKs). **S.T. Staben**, J. Feng, W. Wang

9:45 MEDI **227.** Discovery of novel indole derived mineralocorticoid receptor antagonists. **A.K. Ogawa**

10:10 MEDI **228.** Discovery of phosphonic acid containing LpxC inhibitors as broad spectrum antibacterial agents. **Q. Dang**, P. McNicholas, D. Olsen, P.T. Meinke

10:35 MEDI **229.** Discovery of novel anti-chagas agents targeting *T. cruzi* CYP51. **J. Choi**, D. Vieira, C. Claudia, J. Siqueira-Neto, D. Kellar, J. Gut, J. Johnston, M. Cameron, J. McKerrow, L. Podust, W.R. Roush

11:00 MEDI **230.** Potent and selective pyridone BTK inhibitors with activity against mutant forms of BTK. **J. Crawford**

11:25 MEDI **231.** Understanding our love affair with *para*-chlorophenyl: Scientific rationale or unsubstantiated bias? **D.G. Brown**, M. Gagnon, J. Boström

11:50 MEDI **232.** Learning from experience: 15 years of protein-fragment X-ray crystal structures and the consequences for fragment library design. **D. Norton**

Section B

Colorado Convention Center

Mile High Blrm 1A/1B

Advances in the Treatment of Fibrotic Diseases

P. Devasthale, *Organizer*

W. B. Young, *Presiding*

8:30 MEDI **233.** Organ and tissue fibrosis: Principles and prospects for therapy. **S. Friedman**

9:00 MEDI **234.** Therapeutic targeting of Nox4 leads to reversal of age-associated persistent fibrosis. **L. Hecker,** N. Logsdon, L.H. Hurley, V. Thannickal, J. Garcia

9:30 MEDI **235.** Development of a small molecule inhibitor of integrin αvβ1. **W.F. Degrado**

10:00 MEDI **236.** Development of novel sGC activators that protect against the progression of diabetic nephropathy in ZSF-1 rats. **C.R. Sarko**, J. Brenneman, T. Bosanac, C. Boustany, H. Chen, H. Clifford, R. Fryer, J. Ginn, P.C. Harrison, J.I. Levin, K. Lincoln, H. Qian, S. Pullen, G. Reinhart, J. Richman, H. Wang, D. Wong, K. Gueneva-Boucheva

10:30 MEDI **237.** Galectin-3 antagonists with therapeutic implications in fibrosis. **U.J. Nilsson**, H. Leffler, H. Schambye, A. Mackinnon, T. Sethi

11:00 MEDI **238.** Needs and challenges in anti-fibrosis drug discovery: Experience from JNK inhibitors. **Y. Satoh**

11:30 Discussion.

Section C

Colorado Convention Center

Mile High Blrm 2C

Small Molecule Approaches to Autism Spectrum Disorder Therapy

K. A. Emmitte, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 MEDI **239.** Harnessing rodent models to develop new therapeutic targets in autism spectrum disorder. **J. Veenstra-VanderWeele**

9:40 MEDI **240.** Therapeutic strategies for restoring excitatory/inhibitory balance in Rett syndrome: Focus on BDNF/TrkB signaling. **D. Katz**

10:15 MEDI **241.** Utility of NMDA antagonists for the treatment of Rett syndrome. **R.J. Mather**

10:50 MEDI **242.** Development of a highly selective and CNS penetrant $mGlu_5$ NAM: An in vivo tool for further elucidating the role of group II mGlus in psychiatric disorders. J.L. Engers, L.C. Konkol, A.L. Rodriguez, R.D. Morrison, F.W. Byers, A.D. Thompson Gray, J.S. Daniels, C.M. Niswender, C.K. Jones, P.J. Conn, C.W. Lindsley, **K.A. Emmitte**

11:25 MEDI **243.** Approaches toward the identification of rodent models of autism spectrum disorder suitable for use in lead optimization efforts. **C.K. Jones**

Drug Discovery

Ligand-Based

Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY AFTERNOON

Section A

Colorado Convention Center

Mile High Blrm 1A/1B

First Time Disclosures

L. A. Thompson, *Organizer, Presiding*

1:30 MEDI **244.** Discovery of JNJ-42847922, a selective orexin-2 antagonist for the treatment of insomnia disorder. **M.A. Letavic**, P. Bonaventure, K.S. Ly, Z. Aguilar, L. Aluisio, N.I. Carruthers, S. Chaplan, C. Dugovic, R. Halter, T. Koudriakova, B. Lord, T.W. Lovenberg, M. Kramer, K.L. Morton, A. Ndifor, M. Rizzolio, C. Shah, J. Shelton, J. Shoblock, S. Sutton

2:05 MEDI **245.** Discovery and optimization of the human histamine H4 antagonist Toreforant (JNJ38518168) for the treatment of inflammatory diseases. **J.D. Venable**, D.E. Kindrachuk, D.J. Buzard, P.J. Dunford, L. Karlsson, R.L. Thurmond, J.P. Edwards

2:40 MEDI **246.** Discovery of MK-8931: A BACE inhibitor in Phase 3 clinical development for Alzheimer's disease. **J.N. Cumming**, J.D. Scott, S.W. Li, M. Cartwright, X. Chen, K. Cox, M. Forman, E.J. Gilbert, R. Hodgson, L. Hyde, Y. Jin, I. Kazakevich, R. Kuvelkar, X. Liang, H. Mei, J. Misiaszek, P. Orth, J. Stone, C. Strickland, J.H. Voigt, H. Wang, B. Werner, J. Wong, E.M. Parker, W.J. Greenlee, M.E. Kennedy, A.W. Stamford

3:15 MEDI **247.** Discovery of GSK2881078A: A selective androgen receptor modulator (SARM) for the treatment of muscle wasting disorders. **P. Turnbull**, R. Cadilla, Y. Shen, C. Poole, E. Stewart, R. Gampe, R. Clark, B.R. Henke, A. Russell

3:50 MEDI **248.** Discovery of a next generation irreversible inhibitor targeting the resistance mutation T790M and activating mutations in NSCLC with a broad selectivity margin over EGFR wild type. **S. Planken**, B.W. Murray, J. Lafontaine, S. Weinrich, M. Hemkens, J.C. Kath, S.K. Nair, T.O. Johnson, H. Cheng, S.C. Sutton, M. Zientek, M. Yin, J. Solowiej, A. Nagata, K. Gajiwala

4:25 MEDI **249.** Discovery and early development of vibegron (MK-4618): A potent and selective β_3-AR agonist for the treatment of overactive bladder. **S. Edmondson**, C. Zhu, N.F. Kar, R. Berger, S.D. Goble, B. Harper, G. Morriello, C. Moyes, L. Wang, P.N. Brown, K.H. Dingley, J. DiSalvo, A. Fitzmaurice, T. Frenkl, S.A. Green, A.L. Hurley, N. Jochnowitz, S. Khalilieh, R.R. Miller, H. Nagabukuro, J.D. Ormes, B. Sacre-Salem, G.M. Salituro, D. Stickens, A.A. Kulick, A.T. Sanfiz, A. Stevenson, K. Villa, L.A. Wickham, B.A. Zamlynny, M. Struthers, A.E. Weber

Section B

Colorado Convention Center

Mile High Blrm 2A/2B

MEDI Award Symposium

W. B. Young, *Organizer*

J. E. Macor, *Presiding*

2:00 MEDI **250.** Phenylalkylaminome: Scaffolding for drugs of abuse, with a focus on synthetic cathinones. **R.A. Glennon**

2:45 MEDI **251. Award Address** (George and Christine Sosnovsky Award for Cancer Research sponsored by the George and Christine Sosnovsky Endowment Fund). Design and development of ligand-targeted therapies and imaging agents for multiple human diseases. **P.S. Low**, C.P. Leamon, J. Reddy, I.R. Vlahov

3:30 MEDI **252. Award Address** (George and Christine Sosnovsky Award for Cancer Research sponsored by the George and Christine Sosnovsky Endowment Fund). Personalized medicine using targeted small molecule drug conjugates and companion imaging agents for cancer therapy. **C.P. Leamon**

4:15 MEDI **253. Award Address** (Earle B. Barnes Award for Leadership in Chemical Research Management sponsored by the Dow Chemical Co. Foundation). Getting the chemistry right: Catalyzing translational innovation at NIH. **C.P. Austin**

Section C

Colorado Convention Center

Mile High Blrm 2C

General Oral Session

W. B. Young, *Organizer*

J. J. Bronson, *Presiding*

1:30 MEDI **254.** Design, synthesis, and biological evaluation of manassantin analogues for HIF-1α inhibition. **D. Kwon**, K. Park, D. Weitzel, S. Lee, T. Stephenson, C. Lee, J. Chi, R. Mook, M. Dewhirst, Y. Lee, J. Hong

1:50 MEDI **255.** First discovery of a single digit nanomolar small molecule protein-protein interaction blocker. L.K. Petersen, F. Sloek, P. Blakskjaer, L. Larsen, J. Holmkvist, A.B. Christensen, J. Rasmussen-Dietvorst, T. Hansen, **N. Hansen**

2:10 MEDI **256.** Discovery of the mGlu5 receptor NAM HTL14242 by fragment based drug discovery. M. Congreve, S.J. Aves, K.A. Bennett, J.A. Christopher, A.S. Doré, J.C. Patel, B. Tehan, F.H. Marshall

2:30 MEDI **257.** Small molecules targeting XBP-1s expression in CLL. **J.R. Del Valle**, S. Ranatunga, C. Kang, C. Hu

2:50 MEDI **258.** Stabilized cyclopropane analogs of the spliceosome Inhibitor FD-895. **M.D. Burkart**

3:10 MEDI **259.** Investigating aromaticity effects In the tail region of sphingosine kinase 2 selective guanidine-based inhibitors. **M.D. Congdon**, Y. Kharel, K. Lynch, W. Santos

‡ *Cooperative Cosponsorship*

3:30 MEDI **260.** Repurposing aspartic protease inhibitors as novel antimalarial agents. **M.J. Meyers**

3:50 MEDI **261.** Chemical optimization of novel inhibitor classes selectively targeting PI4KIIIbeta: A host lipid kinase crucial for enterovirus replication. **A. Leivers**, A. Maynard, A.J. Peat, E. Nartey, J. Shotwell, J. Botyanszki, J. Gobel, J. Catalano, J.F. Miller, J. Seal, L. Want, L. Shewchuk-Chapman, P.Y. Chong, P. Xiong, S. Dickerson, S. You, V.W. Tai

4:10 MEDI **262.** Variation in ADC linker composition generated from aldehyde-tagged antibodies impacts both efficacy and PK. **A.W. Garofalo**

4:30 MEDI **263.** HIV microbicide development using a combination of QSAR and structure-based approaches. **L. Guasch**, A.V. Zakharoz, M.C. Nicklaus

4:50 MEDI **264.** Dihydroquinazolines: A novel class of hOCT3 inhibitors. **M. Dukat**, X. Pan, M. Argade, K.A. Iyer, P.D. Mosier, D. Sweet

Drug Discovery

Ligand-Based

Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY EVENING

Section A

Colorado Convention Center

Four Seasons Ballroom

General Poster Session

W. B. Young, *Organizer*

7:00 - 9:00

MEDI **134.** Amphipathic α-helix mimetics based on a 1,4-disubstituted 2,3,4,5-tetrahydro-1*H*-benzo[e][1,4]diazepine: Inhibition of the Mcl-1 oncoprotein. **L. Chen**, K. Jeong, S. Fletcher

MEDI **265.** Physical compatibility of co-solubilized vancomycin, piperacillin, and tazobactam in aqueous solution. **R.N. Mason**, S.C. Butler, H.N. Gray, H.S. Gray

MEDI **266.** Development and validation of RP-HPLC method for simultaneous determination of guaifenesin impurities in multidrug combinations. **R. Grigoryan**

MEDI **267.** Carbon monoxide releasing property of amine carboxyboranes. **N.N. Dingra**

MEDI **268.** Use of Fc receptor affinity separation resin to obtain high potency glycoforms (nonfucocylsated) of antiviral immunoglobulin. **A. Boesch**, G. Bolton

MEDI **269.** Structure-activity relationships of prazole fragment inhibitors of *T. vaginalis* uridine nucleoside ribohydrolase using NMR-based activity and binding assays. **T.A. Shea**, M.A. VanAlstine-Parris, B.J. Stockman

MEDI **270.** Aminomethyl spectinomycins as novel therapeutics for drug resistant respiratory tract and sexually transmitted bacterial infections. **S.L. Waidyarachchi**, D.F. Bruhn, J. Liu, D.B. Madhura, D. Shcherbakov, Z. Zheng, Y. Abdelrahman, A. Singh, C. Rathi, R. Belland, B. Meibohm, J. Rosch, E. Böttger, R.E. Lee

MEDI **271.** Targeting *Mycobacterium tuberculosis* biotin protein ligase (MtBPL): Synthesis and evaluation of nucleoside-based bisubstrate adenylation inhibitors. **M.R. Bockman**, A. Kalinda, D. Tiwari, T. De la Mora, B. Finzel, D. Schnappinger, C.C. Aldrich

MEDI **272.** Hybridization of metronidazole with natural product tetramic acids improves its antidifficile efficacy. **P.T. Cherian**, X. Wu, R.E. Lee, J. Hurdle

MEDI **273.** Lipidated cyclice gamma-AA peptides display both antimicrobial and anti-inflammatory activities. **Y. Li**, C. Smith, H. Wu, S. Padhee, H.H. Yin, J. Cai

MEDI **274.** Design and biological evaluation of novel Cdc42 inhibitors. **B.J. Aguilar**, **B. Hinckley**, S. Huo, Y. Chen, Q. Lu

MEDI **275.** Development of $\alpha_4\beta_3\gamma_2$-subtype selective ligands for $GABA_A$ receptors. **R.S. Verma**, C. Witzigmann, J.M. Cook

MEDI **276.** Quantitative structure-activity relationship (QSAR) investigations of abuse-related neurochemical and behavioral effects of para-substituted methcathinone derivatives. **F. Sakloth**, R. Kolanos, M. Barnier, P.D. Mosier, J. Partilla, M.H. Baumann, R.A. Glennon

MEDI **277.** Structure-activity studies on the α-modified analogs of the abused substance methylenedioxypyrovalerone (MDPV) as reuptake inhibitors at the dopamine transporter (DAT). **F. Sakloth**, R. Kolanos, A.D. Jain, J. Partilla, M.H. Baumann, R.A. Glennon

MEDI **278.** Synthesis, SAR, and progress toward orally available, brain penetrant P2X7R antagonists for the treatment of neuroinflammatory disorders. **C. Chrovian**

MEDI **279.** Structure-activity relationships of iminoheterocyclic BACE1 inhibitors: Discovery of MK-8931 for the treatment of Alzheimer's disease. **J.D. Scott**, S.W. Li, X. Chen, K. Cox, J. Cumming, M. Forman, E.J. Gilbert, W.J. Greenlee, R. Hodgson, C. Huang, L. Hyde, Y. Jin, U. Iserloh, I. Kazakevich, R. Kuvelkar, G. Li, X. Liang, J. Misiaszek, P. Orth, E.M. Parker, C. Strickland, J.H. Voigt, H. Wang, B. Werner, J. Wong, M.E. Kennedy, A.W. Stamford

MEDI **280.** Robust and efficient amination route toward the development of N-substituted piperazines as serotonergic ligands for autism spectrum disorder. **J. Dhuguru**, S.W. Goldstein, A. Khalil, O.M. Ghoneim

MEDI **281.** Computational approach for performing medchem transformations within a 3D active site. **M.R. Goldsmith**

MEDI **282.** Applying extended Huckel theory to pharmacophore modeling. **A. Deschenes**

MEDI **283.** Exploring the role of solvation in drug design and optimization. **M.L. Drummond**, J. Truchon, C. Williams, P. Labute

MEDI **284.** Performance of structure based and ligand based virtual screening methods for ten selected anticancer targets. **C. Selvam**, T. Ramasamy

MEDI **285.** Scaffold hopping: Balancing novelty, accessibility, and physicochemical properties. **T. Cheeseright**, S. Tomásio, P. Tosco, M. Mackey

MEDI **286.** Discovery of KSI-6666, a novel S1P1 antagonist for the treatment of autoimmune disease. **Y. Ohsawa**, **H. Inoue**, T. Suzuki, Y. Maruyama, K. Ohno, N. Arisaka, S. Muto, Y. Okuhara, M. Hayashi, A. Yamamoto, K. Kaidoh, H. Mukaiyama, M. Hiratochi

MEDI **287.** Discovery of a new indole-based group IVA cytosolic phospholipase A_2 inhibitor as a promising drug candidate for treatment of respiratory diseases. **T. Tomoo**, T. Nakatsuka, T. Katayama, Y. Hayashi, Y. Fujieda, M. Terakawa, K. Nagahira

MEDI **288.** Controlled-release mechanism for sulfur mustard anti-inflammatory drugs based on polyamine platform. C.J. Lacey, J. Saxena, **C.D. Guillon**, G.M. Composto, L.B. Joseph, D.E. Heck, J.D. Laskin, N.D. Heindel

MEDI **289.** Synthesis and anti-inflammatory activity of three nitro chalcones. **A. Gómez** Rivera, C.E. Lobato Garcia, H. Aguilar Mariscal, N. Romero Ceronio

MEDI **290.** Microwave assisted synthesis, pharmacological activities, and molecular docking studies of Ethyl 2-substituted-4-(2-thienyl) thiazole-5-acetates. **M. Attimarad**, M.A. Khedr, B.E. AlDubaib

MEDI **291.** Toward a bioisosteric alkahest: Targeting the human dehydroorotate dehydrogenase (hDHODH) by a scaffold hopping bioisosteric approach using hydroxylated pentaatomic heterocycles. **M.L. Lolli**, A.C. Pippione, S. Sainas, S. Mensa, M. Giorgis, M. Piccinini, E. Lupino, S. Al-Kadaraghi, D. Boschi

MEDI **292.** Discovery of thienopyrimidinones as a new series of potent phosphodiesterase 7 inhibitors. **Y. Endo**, K. Kawai, T. Asano, S. Amano, K. Sawada, K. Ogura, N. Ueo, N. Takahashi, Y. Sonoda, M. Nagai, N. Kamei

MEDI **293.** Development of fluorescent affinity probes for the $P2Y_{14}$G protein-coupled receptor. **E. Kiselev**, M. Barrett, E. Hammes, V. Katritch, R. Balasubramanian, A. Yin, S. Paoletta, C. Weitzer, Q. Zhao, R. Stevens, T. Harden, K. Jacobson

MEDI **294.** Design, evolution, and in vivo profile of a novel series of GPBAR 1 agonists for the treatment of diabetes and metabolic syndrome. **R. Kurukulasuriya**, S.K. Shah, J. Dellureficio, S. Fung, L. Guo, J. Szewczyk, M. Trujillo, R.P. Nargund, W.K. Hagmann, A. Pocai, R.J. Devita

MEDI **295.** Withdrawn.

MEDI **296.** Benzothiazolyl substituted iminothiazolidinones and benzamido-oxothiazolidines as potent and partly selective aldose reductase inhibitors. **J. Iqbal**

MEDI **297.** Design and bioevaluation of novel human 4-hydroxyphenylpyruvate dioxygenase inhibitors. **H. Lin**, G. Yang, W. Yang

MEDI **298.** Targeting integrin $\alpha_v\beta_3$ receptors with multivalent RGD peptidomimetics. **J.L. Teh**, R.N. Hanson, S. Sridhar

MEDI **299.** Design, synthesis, topoisomerase I and II inhibitory activity, cytotoxicity, and structure-activity relationship study of novel 2-phenyl-4-aryl indenopyridines. **G. Bist**, T.M. Kadayat, T. Thapa Magar, A. Shrestha, Y. Kwon, E. Lee

MEDI **300.** Importance of side chain orientation on large macrocycles: Structure activity relationship of sanguinamide B analogs on colon cancer HCT-116 cells. **A. Pietkiewicz**, H. Wahyudi, J. McConnell, S. McAlpine

MEDI **301.** Synthesis, characterization, and in vitro anticancer activity of quinolylmethyl- and napthylmethyl-substituted imidazolium salts. **P.O. Wagers**, M. DeBord, M.J. Panzner, C. Tessier, W.J. Youngs

MEDI **302.** Development of novel casein kinase 1 nhibitors. **R.L. Schroeder**, N.A. Pham, P. Tram, T. Stone, K. Nguyen, J. Geathers, D.Q. Nguyen, E. Skripnikova, M.R. Bratton, J. Sridhar

MEDI **303.** Synthesis and biological evaluation of novel naphthoquinones as HER2 inhibitors for the treatment of trastuzumab resistant breast cancer. **R.L. Schroeder**, M.E. Sfondouris, M.R. Bratton, N.A. Pham, P. Tram, T. Stone, K. Nguyen, J. Geathers, D.Q. Nguyen, C.L. Stevens, F.E. Jones, J. Sridhar

MEDI **304.** Anthracenyl isoxazole amides (AIMs) stabilize quadruplex DNA structures in telomeric and c-MYC promotor sequences. **S. Stump**, M.J. Weaver, N.S. Duncan, A.K. Kearns, N.R. Natale, H.D. Beall

MEDI **305.** Design, synthesis, and biological screening of novel estrone analogs toward treatment of hepatocellular carcinoma. **M. Mahnashi**

MEDI **306.** Synthesis, structure-activity relationship (SAR) study, and mode of action study of cationic triazole analogs of 1,4-naphthoquinone: A new class of highly potent anticancer agent. **J.P. Shrestha**, C.T. Chang

MEDI **307.** ZMPSTE24 protease inhibitors as senescence agonists for cancer chemotherapy. **D. Xanthopoulos**, A. Matralis, H. de Vries, G. Huot, G. Ferbeyre, Y.S. Tsantrizos

MEDI **308.** Thio-sugars can sensitize human cervixadenocarcinoma (Hela) cancer cells to Bleomycin and ROS generator. J. Sarnik, A. Czubatka, T. Poplawski, **Z.J. Witczak**

MEDI **309.** Low glucose level enhances the cytotoxicity of CARB-pharmacophore to cancer cells. A. Czubatka, J. Sarnik, T. Poplawski, Z.J. Witczak

MEDI **310.** N,N'-bisquinolylmethyl-2-alkyl and N-quinolylmethyl-N'-naphthylmethyl-2-alkyl substituted imidazolium salts as potential therapeutics for the treatment of lung cancer: Synthesis, characterization, and in vitro anticancer activity. **M. DeBord**, P.O. Wagers, M.J. Panzner, C. Tessier, W.J. Youngs

MEDI **311.** 2,4-Diaryl-indenopyridine derivatives: Design, synthesis, topoisomerase I and II inhibition, cytotoxicity, and structure-activity relationship study. **T. Thapa Magar**, T.M. Kadayat, G. Bist, A. Shrestha, Y. Kwon, E. Lee

MEDI **312.** Mechanistic studies of imidazolium salts as antitumor agents. **M.R. Southerland**, P.O. Wagers, M. DeBord, K.L. Shelton, L. Shriver, S.M. Paruchuri, C. Tessier, M.J. Panzner, W.J. Youngs

MEDI **313.** Design, synthesis, and in vitro anticancer activities the 7-chloro-6-fluoro-N-subsituted-2-phenylquinoline-4-carboxamide derivatives. **A.P. Patel**, H.G. Bhatt

MEDI **314.** Synthesis of pyrazole derivatives as potential cytotoxic agents. **T. Rowe**, **J. Brider**, M. Branscum, M.A. Alam

MEDI **315.** Synthesis of curcumin mimics with substituted triazolyl groups and their sensitization effect of TRAIL against brain cancer cells. **S. Lee**, S. Oh, D. Kwon, Y. Park, W. Shin

MEDI **316.** 10-oxy-anthracenyl isoxazole amides (AIMs) as potential G-quadruplex stabilizing antitumor agents. **N.S. Duncan**, N.R. Natale, H.D. Beall

MEDI **317.** Ferrocenyl derivatives as promising scaffolds for anticancer and antileishmanial agents. **S. Zaib**, J. Iqbal, M. Hassan, F. Macaev, A.K. Powell

MEDI **318.** Improved efficacy for a novel class of G-quadruplex binding anti-tumor agents. **M.J. Weaver**, N.R. Natale

MEDI **319.** Design, synthesis, and antineoplastic evaluation of isoform selective inhibitors of AKR1C3. **K. Verma**, T. Zhang, T.M. Penning, P.C. Trippier

MEDI **320.** Discovery and development of a series of irreversible EGFR_T790M 7H-pyrrolo[2,3-d]pyrimidine inhibitors with high selectivity over EGFR wild type. **S. Planken**, S.K. Nair, J.C. Kath, J. Lafontaine, S. Weinrich, H.K. Cheng, S.C. Sutton, T.O. Johnson, M. Zientek, A. Nagata, K. Gajiwala, J. Solowiej, B.W. Murray, M. Yin, M. Hemkens

MEDI **321.** Synthesis of PF-06459988; a next generation irreversible EGFR_T790M inhibitor for resistant non-small cell lung cancer. **K.T. Tran**, D.C. Behenna, S. Cho-Schultz, S. Kephart, J. Matthews, S.K. Nair, M.A. Ornelas, S.T. Orr, M.A. Pairish, P. Richardson, D.T. Richter, N. Sach, H. Shen, S.C. Sutton, R. Zhou

MEDI **322.** Synthesis of warhead containing scaffolds on irreversible 7H-pyrrolo[2,3-d] pyrimidine EGFR T790M inhibitors. **J.J. Matthews**, S.E. Kephart, R. Zhou, M.A. Pairish, D. Behenna, S. Cho-Schultz, S.K. Nair, M.A. Ornelas, S.T. Orr, D.T. Richter, H. Shen, S.C. Sutton, K.T. Tran

MEDI **323.** Exploring EGFR kinase-ligand interactions for optimizing dual action inhibitors. C. Williams, A. Ajamian, **P. Kamya**, B. Jean-Claude, Z. Rachid

MEDI **324.** Fully automated radiosynthesis of [11C]AZD8931 as a new PET agent for imaging of EGFR, HER2 and HER3 signaling. **M. Wang**, M. Gao, Q. Zheng

MEDI **325.** Synthesis of carbon-11-labeled aminoalkylindole derivatives as new candidate CBR radioligands for PET imaging of alcohol abuse. M. Gao, A. Gao, **M. Wang**, Q. Zheng

MEDI **326.** Development of isoform selective compounds for Grp94 inhibition. **S. Mishra**

MEDI **327.** Targeting Hsp90: Development of C-terminal inhibitors. **M. Anyika**

MEDI **328.** Deuterated dabrafenib (BRAF kinase inhibitor): Metabolism and pharmacokinetics. **J.M. Ralph**, L.E. Richards-Peterson, T. Wilde, D. Bershas, E.A. Minthorn, A. Kaura, M. Bleam, S. Laquerre, M. Arnone, C. Manning, J.L. Adams

MEDI **329.** Combination therapy with epothilone and aurora kinase inhibitors induces a novel form of cell death. **L. Woods**, R.E. Taylor, K.T. Vaughan

MEDI **330.** Identification of 2-(4-benzamidophenyl)-7-phenyl-5H-benzo[c] pyrimido[4,5-e]azepines as potent aurora kinase inhibitors. **R.E. Gershman**, S.G. Stroud, D.A. Janowick, T.B. Sells, M. Rezaei, C.F. Claiborne, S.J. Critchley

MEDI **331.** Rational design of ALK2 small molecule inhibitors for treatment of fibrodysplasia ossificans progressiva (FOP). **Y.L. Luo**, A. Alsamarah

MEDI **332.** Discovery and SAR exploration of a novel series 8-oxo-8,9-dihydro-7H-purine-6-carboxamides as mTOR kinase inhibitors. **P. Papa**

MEDI **333.** Discovery of substituted morpholinothiophene and morpholinothiazole carboxylic acids as selective inhibitors of PI3Kb kinase. **Z. Shi**, D. Cardin, J. Chouitar, J. Ecsedy, K. Galvin, R. Griffin, P. Hales, M. Hirose, T. Hu, N. Natasha Iartchouk, D.A. Janowick, Y. Kawakita, M. Rezaei, T. Sells, M. Smith, S. Stroud, L. Takaoka, S. Vyskocil, D. Deborah Wysong, T. Xu, W. Zhang

MEDI **334.** Inhibition of the inositol phosphatase SHIP utilizing quinoline-based small molecules. C.M. Russo, A.A. Adhikari, D.R. Wallach, R. Brooks, F. Sandra, A.N. Balch, W.G. Kerr, **J.D. Chisholm**

MEDI **335.** Disruption of STAT3 phosphorylation by novel pyrimidino-thiazinones, PI3K-α and δ inhibitors. **B. Akula**, D. Subbaiah, M.R. Mallireddigari, S. Cosenza, V. Bharathi, V. Pallela, G. Panda, . Reddy, M. Reddy

MEDI **336.** Structure based design, synthesis, and anticancer evaluation of human neutrophil elastase inhibitors. Q. Sun, Y. Li, J. Li, W. Yang, **G. Yang**

MEDI **337.** Synthesis and biological evaluation of potential isoform-selective benzimidazole-4-carboxamide inhibitors of poly(ADP-ribose)polymerases. **J. Pickles**, C. Cano, B. Golding, S. Harnor, S. Jackson, H. Newell, J. Travers, R. Griffin

MEDI **338.** Novel strategies for improving the pharmacological properties of platinum-acridine anticancer agents. **S. Ding**, A. Pickard, G. Kucera, U. Bierbach

MEDI **339.** Labeling of TSPO PET radioligands by [18F]fluorination of diarylsulfoxide precursors. **F.G. Simeon**, E. Barresi, S. Lu, S. Taliani, F. Da Settimo, V.W. Pike

MEDI **340.** Red blood cell-mediated photodynamic therapy for improved cancer treatment. **W. Tang**, J. Xie, Z. Zhen

MEDI **341.** Molecular modeling studies of choline acetyltransferase inhibitors as potential PET probes. **R. Kumar**, T. Darreh-Shori

MEDI **342.** Target identification and mechanism elucidation of chalcones' cytotoxicity via photoaffinity probes. **B. Zhou**, X. Yu, C. Zhuang, P. Jiang, S.S. Wickramaratne, Y. Lin, J. Lü, C. Xing

MEDI **343.** Activity-based probe for acyl protein thioesterases. **Y. Chen**, M. Zompa, R. Bisiewicz, C.T. Seto

MEDI **344.** Design and application of lipid probes for proteomic characterization of protein binding partners. **S. Eni**, M. Best, S. Mattern-Schain, K. Tscherch

MEDI **345.** Design and synthesis of novel fluorinated amines. **P. Mykhailiuk**

MEDI **346.** Synthesis of conformationally restricted scaffolds by double-Mannich reaction of cyclic ketones. **P. Mykhailiuk**

MEDI **347.** Synthesis of novel unique pyrrolidines by [3+2]-cycloaddition of azomethine ylides with electron-deficient alkenes. **P. Mykhailiuk**

MEDI **348.** Affinity selection-mass spectrometry screening: Development and validation of a 384-well ultrafiltration format for drug discovery. **R.E. Williamson**, D. Terry, G. Roth

MEDI **349.** Plasma treatment of dentin surfaces for improving dental composite restoration bonding. X. Dong, M. Cheng, Y. Wang, H. Li, **Q. Yu**

MEDI **350.** Synthesis and evaluation of inhibitors of the salicylate synthase (Mbtl) involved in siderophore biosynthesis in *mycobacterium tuberculosis*. **F. Liu**, Z. Liu

MEDI **351.** Large scale storage stability analysis of molecules in the MLSMR. **C. Laggner**, Y. Shayo, C. Hendarto, C.R. Johnson, C.R. Loomis

MEDI **352.** Development of novel nitrogen based heterocyclic antibiotic advjuvants. **R.E. Furlani**, C. Melander

NUCL

Division of Nuclear Chemistry and Technology

J. C. Braley and D. E. Hobart, *Program Chairs*

SOCIAL EVENTS:

Social Hour, 6:30 PM: Mon

BUSINESS MEETINGS:

NUCL Executive Business Meeting, 5:30 PM: Sun

NUCL Business Meeting, 5:30 PM: Mon

SUNDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, *Organizers, Presiding*

8:30 NUCL **1.** Studies of the thermodynamics of actinide reactions: A tribute to Heino Nitsche. **K.L. Nash**

8:50 NUCL **2.** Treatment of contaminated water at Fukushima. D. Hobbs, R. Peterson, **K. Yamaguichi**, M. Yamamoto

9:20 NUCL **3.** Thermodynamics and predicting actinide behavior in repository science. **D.T. Reed**

9:40 NUCL **4.** Spatially resolved characterization techniques for next generation nuclear forensics signature development. J.M. Schwantes, **L. Sweet**, E. Buck, T.J. Johnson, D.D. Reilly, D. Abrecht, E. Mausolf

10:10 Intermission.

10:30 NUCL **5.** Investigation of silica-grafted CMPO-modified calix[4]arenes for radionuclide separations. **E.M. May**, Y. Wanglee, A. Solovyov, Y. Matvieiev, A.S. Katz, V. Kalchenko, H. Nitsche

10:50 NUCL **6.** Interactions of plutonium and ordered mesoporous materials. **T. Parsons-Moss**, D. Olive, S. Jones, J. Wang, D. Zhao, Z. Dai, M. Zavarin, A. Kersting, H. Nitsche

11:10 NUCL **7.** FIONA: A new mass analyzer for superheavy elements. **N. Esker**, J.M. Gates, G.K. Pang, K.E. Gregorich, H. Nitsche

11:30 NUCL **8.** Solid-phase extractants for sequestration and separation of actinides and lanthanides. **J. Shusterman**, A. Bruchet, H. Mason, E.C. Uribe, H. Nitsche

11:50 NUCL **9.** DTRA basic research for combating weapons of mass destruction. **S. Wilk**

Uranium in Seawater

Sorbents and Analysis

Sponsored by I&EC, Cosponsored by CEI, MPPG‡ and NUCL

SUNDAY AFTERNOON

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, *Organizers, Presiding*

1:20 NUCL **10.** Scientific contributions of Heino Nitsche to actinide and transactinide chemistry. **C. Düllmann**, R. Wilson

1:40 NUCL **11.** Heavy element studies at Berkeley. **K.E. Gregorich**

2:10 NUCL **12.** Impact of [Ca_2 UO_2 $(CO_3)_2$] aq.-complex formation on environmental behavior of uranium. **G. Bernhard**, G. Geipel, V. Brendler

2:40 NUCL **13.** Molecular scale investigations towards actinide retention at mineral surfaces. **H. Geckeis**

3:10 Intermission.

3:30 NUCL **14.** Applications of molten salts in nuclear technology. **T. Fanghänel**, O. Beneš, J. Glatz, R. Konings, R. Malmbeck, P. Souček

4:00 NUCL **15.** Advances in the production and chemistry of the heaviest elements. **A. Tuerler**

4:30 NUCL **16.** Laser-induced spectroscopy of actinides: From simple metal systems to species in living cells. **G.C. Geipel**

5:00 NUCL **17.** Toward A and Z identification of superheavy elements. **J.M. Gates**

5:30 NUCL **18.** Chronology of 239/240Pu and of 236U in the Miaergou glacier from eastern Tien Shan, China. **H.W. Gaeggeler**, S. Hou, C. Wang, M. Christl, S. Maxeiner, H. Synal, C. Vockenhuber

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Fission Product Studies

A. Klingensmith, R. S. Rundberg, *Organizers*

T. A. Bredeweg, *Organizer, Presiding*

1:00 NUCL **19.** Energy dependence of fission product yields from 235U, 238U and 239Pu for incident neutron energies between 0.5 and 14.8 MeV. **M. Gooden**, C. Arnold, T.A. Bredeweg, J. Wilhelmy, D. Vieira, A. Tonchev, M.A. Stoyer, W. Tornow

1:25 NUCL **20.** Measurement of fission product yields and nuclear reaction crossSections using mono-energetic neutrons from a dense plasma focus. **R.S. Rundberg**

1:50 NUCL **21.** Fission product chain yields from fission spectrum irradiations at NCERC. T.A. Bredeweg, **K.R. Jackman**, A.C. Olson, S.M. Bowen, A. Schake, S.A. Kozimor

2:15 NUCL **22.** SPIDER: New instrument for fission mass yield measurements. **K.C. Meierbachtol**, F. Tovesson, C. Arnold, T.A. Bredeweg, M. Devlin, M. Jandel, J. Lestone, R. Nelson, A. Sierk, D. Shields, M. White, A. Hecht, R. Blakeley

2:40 NUCL **23.** Relative fission product yield determination in varying neutron environments. **M. Koehl**, J. Braley

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Separations

T. A. Bredeweg, A. Klingensmith, *Organizers*

R. S. Rundberg, *Organizer, Presiding*

3:20 NUCL **24.** Synthesis of rapid separation targets by hydrothermal methods. **J.M. Dorhout**, K. Czerwinski

3:45 NUCL **25.** Thermochromatographic separations of volatile rare earth compounds for nuclear forensics analysis. **J.D. Auxier**, S.A. Stratz, D.E. Hanson, M.L. Marsh, A.V. Jones, H.L. Hall

4:10 NUCL **26.** Synthesis and characterization of Ln[fod]$_x$ and Ln[dpm]$_x$ compounds for the development of rapid gas-phase separation methods. **S.A. Stratz**, J.D. Auxier, M.L. Marsh, D. Hanson, A.V. Jones, H.L. Hall

4:35 NUCL **27.** Determination of decontamination factor for various radioisotopes during the PUREX process of irradiated DUO_2. **T.K. Bhardwaj**, P. Mendoza, R. Du, M. Bencomo, J. Allred, M. Swinney, C.M. Folden, S. Chirayath

5:00 NUCL **28.** Source facility determination based on PUREX process trace metal signatures. **A. Baldwin**, J.C. Braley

Uranium in Seawater

Sorbents and Analysis

Sponsored by I&EC, Cosponsored by CEI, MPPG‡ and NUCL

MONDAY MORNING

Section A

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom A

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Heino Nitsche

C. Duellman, T. Fanghänel, D. E. Hobart, A. Kersting, R. Wilson, *Organizers, Presiding*

8:10 NUCL **29.** Actinide sorption to aluminum (hydr)oxides: Influence of sorption site acidity. **T. Baumer**, P.E. Kay, A. Ko, A.E. Hixon

8:30 NUCL **30.** Pu transport mechanisms in the environment: Field evidence, conceptual models, and experimental data. **M. Zavarin**, J. Begg, C. Joseph, P. Zhao, A. Kersting

8:50 NUCL **31.** Separating uranyl nanoclusters using ultrafiltration membranes. **M. Sharifironizi**, C.R. Andrews, J.E. Syzmanowski, G.E. Sigmon, W.A. Phillip, P.C. Burns

9:10 NUCL **32.** Superheavy element discovery and chemistry program at LLNL. **D.A. Shaughnessy**, R. Henderson, K. Moody, N. Gharibyan, J. Despotopulos

9:30 Intermission.

9:50 NUCL **33.** Biotransformation of plutonium. **T. Ohnuki**, A.J. Francis

10:10 NUCL **34.** Plutonium hydrolysis and condensation. **L. Soderholm**, S. Skanthakumar

10:40 NUCL **35.** Role of multinucleon transfer reactions in making neutron-rich transactinide nuclei. **W. Loveland**, R. Yanez, S. Barrett

11:00 NUCL **36.** Relativistic quantum theory for chemical identification of the heaviest elements. **V. Pershina**

11:30 NUCL **37.** Heino Nitsche's contributions to the understanding of Pu reactions at mineral:water interfaces and their implications on present reactive transport modeling. **B.A. Powell**, D. Kaplan

Section B

Embassy Suites Denver–Downtown Convention Center

Crestone Ballroom B

Nuclear Forensics

Surrogates

T. A. Bredeweg, R. S. Rundberg, *Organizers*

A. Klingensmith, *Organizer, Presiding*

8:15 NUCL **38.** Mass transport in aerodynamic fallout glass from a near-surface nuclear explosion. **D. Weisz**, S.G. Prussin, K. Knight, B. Jacobsen, N.E. Marks, I.D. Hutcheon

8:40 NUCL **39.** Constraints on fallout melt glass formation from a near-surface nuclear test. **G.R. Eppich**, K.B. Knight, G. Spriggs, I.D. Hutcheon

9:05 NUCL **40.** Production of activation species for use with realistic surrogate debris materials. **B.B. Bandong**

‡ *Cooperative Cosponsorship*