THURSDAY MORNING

Applications in Nanoscience
One-Dimensional Materials Sponsored by COLL, Cosponsored by POLY, INOR, and NANO

Geochemical Processes, Reactivity, and Applications of Manganese Oxides
Sponsored by GEOC, Cosponsored by ENVR and INOR

Nanotechnology and the Environment: Emphasis on Green Nanotechnology
Nanomaterials for Clean Energy Sponsored by I&EC, Cosponsored by INOR and NANO

THURSDAY AFTERNOON

Applications in Nanoscience
Novel Structures Sponsored by COLL, Cosponsored by POLY, INOR, and NANO

Geochemical Processes, Reactivity, and Applications of Manganese Oxides
Sponsored by GEOC, Cosponsored by ENVR and INOR

MEDI

Division of Medicinal Chemistry

J. R. McCarthy, *Program Chair*

SUNDAY MORNING

Section A

Salt Palace Convention Center
Ballroom H

Metabolic Syndrome

P. Matyus, *Organizer*

9:00 1. Targeting genomic (FXR) and nongenomic (TGR5) bile acids receptor pathways for metabolic disorders: Discovery, S.A.R. and molecular modeling of potent and selective bile acids derivatives. **R. Pellicciari**, A. Macchiarulo, A. Gioiello, E. Rosatelli, C. Thomas, J. Auwerx
9:35 2. DGAT-1 Inhibitors as novel therapeutics for dyslipidemia. **A. J. Souers**, A. J. King, S. Mittelstadt, G. Zhao, A. S. Judd, B. D. Dayton, J. A. Segreti, K. Larson, M. Voorback, R. M. Reilly, M. Brune, P. R. Kym, C. A. Collins, B. F. Cox
10:10 3. Piperazine sulfonamides as potent, selective, and orally bioavaliable 11-beta-HSD1 inhibitors for the treatment of Type II diabetes and obesity. **E. Chenail**, Z-K. Wan, H-Q. Li, M. Ipek, J. Xiang, T. S. Mansour, J. Bard, V. Suri, J. Goodman, S. Hahm, X. Li, J. Tobin, E. Saiah
10:45 4. Potent and orally bioavailable stearoyl-CoA desaturase (SCD) inhibitors for the potential treatment of obesity and diabetes. **D. Koltun**, E. Q. Parkhill, N. I. Vasilevich, A. I. Glushkov, T. M. Zilbershtein, A. V. Ivanov, N. A. Zautke, S. A. Brunn, N. Mollova, K. Leung, J. W. Chisholm, J. Zablocki
11:20 5. Semicarbazide-sensitive amine oxidase (SSAO): A potential target for the treatment of diabetes and its complications. **P. Matyus**, P. Dunkel, E. Toth-Sarudy, G. Turos, M. Pihlavisto, K. Magyar, Z. Soltesz, C. Carpene

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Section B

Salt Palace Convention Center
Combo Ballrooms C&E

General Oral Session

J. McCarthy, *Organizer*

9:00 6. Progress toward an α-hemolysin heptamerization inhibitor. **B. S. Barth**, J. A. Chmielewski, M. A. Lipton
9:20 7. Identification of nonsulfonylurea P2Y12 inhibitors as a follow-up series to PRT060128. **S. M. Bauer**, M. M. Mehrotra, M. Venkataraman, P. B. Conley, M. Jurek, A. Hutchaleelaha, C. Ye, S. Hollenbach, R. Scarborough, A. Pandey
9:40 8. Design, synthesis, and biological evaluation of nonpeptidic, cell-permeable bivalent Smac mimetics as potent inhibitors of XIAP. **Y. Peng**, H. Sun, J. Lu, Z. Nikolovska-Coleska, C-Y. Yang, Q. Cai, S. Qiu, S. Wang
10:00 9. Community-based small molecule collaborative drug discovery for neglected infectious diseases and cancer. **B. A. Bunin**, S. Ernst, M. Hohman, K. Gregory
10:20 10. Biomimetic simulation of reactions postulated to occur during inhibition of ribonucleotide reductases by 2'-azido-2'-deoxynucleotides. **T. P. Dang**, A. J. Sobczak, M. Rapp, A. M. Mebel, S. F. Wnuk
10:40 11. Aleglitazar, a potent and balanced dual PPAR alpha/gamma agonist for the treatment of type II diabetes and dyslipidemia. **P. Mohr**, A. Bénardeau, J. Benz, A. Binggeli, B. Bittner, M. P. Boehringer, A. Costanzo, U. M. Grether, H. Hilpert, G. Hirth, H. Isel, B. Kuhn, H. P. Maerki, M. Meyer, K. Püntener, S. Raab, F. Ricklin, A. Ruf, E. Sebokova, U. Sprecher, P. Verry, N. Wyttenbach
11:00 12. Design and optimization of renin inhibitors: Orally bioavailable alkyl amines. **C. M. Tice**, Z. Xu, J. Yuan, R. D. Simpson, S. T. Cacatian, P. T. Flaherty, W. Zhao, J. Guo, A. V. Ishchenko, S. B. Singh, Z. Wu, B. B. Scott, Y. Bukhtiyarov, J. Berbaum, J. Mason, R. Panemangalore, M. G. Cappiello, R. K. Harrison, G. McGeehan, L. W. Dillard, J. J. Baldwin, D. A. Claremon
11:20 13. Discovery and pharmacological evaluation of dual FMS/Kit inhibitors. **P. N. Ibrahim**, J. Zhang, M. Nespi, R. Bremer, B. Burton, B. Wong, B. Powell, D. R. Artis, K. Zhang, B. West, P. Lin, C. Zhang, G. Habets, G. Tesch, G. Bollag, P. Hirth
11:40 14. Discovery of NA808: A novel host targeting anti-HCV agent. **K-I. Kawasaki**, H. Fukuda, T. Hayase, S. Komiyama, F. Watanabe, K. Takano, A. Mizutani, T. Katoh, N. Kimura, M. Murakata, T. Makino, A. Ohta, M. Masubuchi, H. Katoh, M. Aoki, H. Sakamoto, K. Okamoto, A. Katsume, Y. Aoki, M. Sudoh, T. Tsukuda, N. Shimma
12:00 15. Phenol-pyrazole inhibitors of mutant B-raf. **I. McAlpine**

Section C

Salt Palace Convention Center
Ballroom A

Nano Meets Neuro: Novel Challenges for Nanoscience in Probing Brain Chemistry
Cosponsored by ANYL, BIOL, COLL, and NANO‡

A. M. Andrews, *Organizer*

9:00 16. Quantum dot technologies for elucidating brain chemical signaling. **T. Q. Vu**
9:30 17. Probing the distribution and behavior of individual serotonin receptors in primary hippocampal neurons using quantum dots. **K. M. Fichter**, M. C. Flajolet, P. Greengard, T. Q. Vu
9:50 18. Drug-conjugated nanocrystal labeling and single protein tracking of the serotonin transporter protein. **S. J. Rosenthal**
10:20 Intermission.
10:30 19. Strategies for optical voltage-sensing in neuronal networks. **J. L. Nadeau**, D. R. Cooper
11:00 20. A biomolecular photodiode for imaging of cell membrane potential. **D. R. Cooper**, J. L. Nadeau

SUNDAY AFTERNOON

Section A

Salt Palace Convention Center
Ballroom H

Nano Meets Neuro: Novel Challenges for Nanoscience in Probing Brain Chemistry
Cosponsored by ANYL, BIOL, COLL, and NANO‡

A. M. Andrews, *Organizer*

1:00 21. In search of brain nanobiosensors: Small-molecule recognition and biomolecule capture as critical first steps. **A. M. Andrews**, A. Vaish, M. J. Shuster, P. S. Weiss
1:30 22. Enabling direct electrochemical and biological studies in living cells with multifunctional nanoscale needle probes. **M-F. Yu**
2:00 23. Single-walled carbon nanotube multimodal optical biosensors for genotoxin detection and identification. **D. A. Heller**, H. Jin, J-H. Kim, M. S. Strano
2:20 Intermission.
2:30 24. Nanoscale strategies to improve the reliability of chronic neural recordings. **R. V. Bellamkonda**, G. C. McConnell
3:00 25. Brain tissue responses to implanted analytical devices: Microdialysis probes and voltammetric microelectrodes. A. C. Michael, **A. Jaquins-Gerstl**
3:20 26. Microchip analysis of neuronal secretions by immunoaffinity capillary electrophoresis. **H. Kalish**, T. M. Phillips

Section B

Salt Palace Convention Center
Combo Ballrooms C&E

First Time Disclosure of Clinical Candidates
Financially supported by Sanofi-Aventis

A. J. Robichaud, *Organizer*

1:30 27. Discovery of BMS-708163: A potent and selective gamma-secretase inhibitor which lowers CSF beta-amyloid in humans. **J. E. Macor**, C. F. Albright, J. E. Meredith, R. C. Zaczek, D. M. Barten, J. H. Toyn, R. Slemmon, K. Lentz, J-S. Wang, R. Denton, G. Pilcher, O. Wang, H. Gu, R. Dockens, R. Berman, G. Tong, J. J. Bronson, M. F. Parker, R. A. Mate, K. McElhone, J. E. Starrett Jr., K. W. Gillman, R. E. Olson
2:05 28. Discovery of a novel, orally bioavailable CGRP receptor antagonist for the treatment of migraine. **I. M. Bell**
2:40 29. Discovery of AMG 221: An 11β-HSD1 inhibitor in the clinic for type 2 diabetes. **C. Fotsch**, J. Adams, M. Bartberger, E. A. Bercot, L. Cai, V. M. Castro, M. Chen, R. Cupples, M. Emery, J. Fretland, A. Guram, S. Gustafsson, A. Hague, C. Hale, N. Han, M. Hayashi, M. Henriksson, D. Hickman, E. Homan, R. W. Hungate, L. Johansson, S. Jordan, C. Kaiser, R. Komorowski, A. Li, Q. Liu, G. Matsumoto, K. McRae, G. Moniz, G. Palm, D. Pyring, D. J. St. Jean Jr., Y. Sun, M. Sydow-Bäckman, L. Tedenborg, H. Tu, S. Ursa, M. Véniant, M. Williams, G. Xu, Q. Ye, C. Yuan, J. Zhang, X. Zhang, M. Wang
3:15 30. Discovery of PF-2413873: A nonsteroidal progesterone receptor antagonist for the treatment of endometriosis. **K. R. Gibson**, K. N. Dack, S. E. Skerratt, P. S. Johnson, P. A. Bradley, T. Underwood, P. Bungay, N. Pullen, A. de Giorgio-Miller, N. M. Mount, D. Howe, B. Wittke

‡ Cooperative Cosponsorship

3:50 31. Physicochemical properties approach to the identification of a histamine H3 receptor antagonist for the treatment of ADHD. **T. T. Wager**
4:25 32. The discovery and development of selective androgen receptor modulator MK-0773. **R. S. Meissner**, J. J. Perkins, G. D. Hartman, C. Bai, D. B. Kimmel, C-T. Leu, B. L. Pennypacker, T. Prueksaritanont, M. E. Duggan, M. A. Gentile, P. Nantermet, J. Ray, A. Schmidt

Genetically Designed Molecular Materials
Peptide Binding, Kinetics and Assembly
Sponsored by NANO, Cosponsored by BIOL and MEDI

SUNDAY EVENING

Section A

Salt Palace Convention Center
Hall 5

General Poster Session
Financially supported by Nature Reviews Drug Discovery and Nature Chemistry

J. McCarthy, *Organizer*

7:00–9:00
33. Advances in medium pressure liquid chromatography. **J. E. Silver**, N. Fowler, P. Bellinghausen, C. Scanlon
34. Si-containing hydroxyapatite coating on titanium for implant application. S. R. Kim, **Y. Kim**, W. T. Kwon, Y. J. Lee
35. Synthesis and biological evaluation of potential RXR selective agonists: Novel bexarotene analogs. **C. E. Wagner**, P. W. Jurutka, P. A. Marshall, M. E. Graeber, E. Matro, I. T. Tran, J. N. Tedeschi, R. O. Khamees, J. E. Kwon, S. Moosavi, J. K. Furmick, B. V. Miguel, D. K. Grupe, J. S. Philp, A. Danishyar, J. W. Hart
36. SiliaSep HP flash cartridges: High performance separation tools. **L. Tremblay**, O. Marion, F. Béland
37. Comparative methods for analysis of protein covalent modification by electrophilic quinoids formed from xenobiotics. **B. Yu**, Z. Qin, G. Wijewickrama, P. Edirisinghe, J. L. Bolton, G. R. J. Thatcher
38. Design and synthesis small molecule inhibitors of alpha-synuclein and amyloid-beta fiber formation. E. Y. Hayden, S-R. Yeh, D. L. Rousseau, M. Blaufox, **B. C. Das**
39. Salicylamides as positive allosteric modulators of nAChR-alpha7. **T. R. Elworthy**, D. J. Du Bois, J. L. Tracy, S. Sahdeo, H. Maag
40. Monocyclic β-lactams as neuroprotective agents. **L. A. Girard**, C. Richards, T. Herbert, M. Konaklieva
41. Synthesis of inhibitors of the N-acetyl-L-ornithine transcarbamylase in Stenotrophomonas maltophilia. **T. Beck**, H. Morizono, M. Konaklieva
42. Monocyclic β-lactams as anti-Moraxella agents. **K. Baugh**, W. Lustig, J. Fritz, S. Sheftel, B. Plotkin, M. Konaklieva
43. Use of nitric oxide to enhance the efficacy of silver sulfadiazine as an antibacterial agent. **S. M. Deupree**, C. B. Johnson, M. H. Schoenfisch
44. Rational design of novel bacterial enzyme inhibitors. **T. R. Holguin**, M. Pass, M. J. Gage, C. C. Browder
45. Antibiotic activity of *Echinacea* herb in cultures of *Escherichia coli* and *Staphylococcus aureus*. K. Irvine, **R. Isovitsch**, **D. Iimoto**
46. Development of a novel activity assay describing the structure-activity-relationship of tetrabutylammonium counter-anions as antimicrobial agents. **M. L. Ingalsbe**, M. E. McGahan, J. D. St. Denis, W. W. Steiner, R. Priefer
47. New classes of novel gram-positive specific antimicrobials: Inhibitors of *E. coli*, *S. aureus*, and surrogates of the causative agents of methicillin-resistant *S. aureus*, tuberculosis and anthrax. **M. S. Kabir**, S. Ara, R. L. Polanowski, K. Engelbrecht, S. M. Krueger, M. E. Stemper, M. A. Rott, W. R. Schwan, A. P. Monte, J. M. Cook

48. Compounds targeting Lipid A as antibacterial agents. I. E. Crandall, Y. C. W. Yau, V. Waters, **W. A. Szarek**

49. Synthesis and evaluation of inhibitors selective for mycobacterial vs. human proteasomes. **H. Tao**, J. Schneider, G. Lin, C. Nathan, J. D. Warren

50. Inhibition of Sortase A in *Staphylococcus aureus*: A novel antibacterial target. **S. E. Velu**, B. Chenna, J. King, A. Lucius

51. Nonconventional antibiotic strategies: Suppression of virulence via QseC antagonism. J. Falck, **B. Lu**, N. Williams, R. Taussig, D. Stewart, V. Sperandio

52. Improving the potency of novel membrane targeted antibiotics by solution phase combinatorial chemistry. **S. K. Vooturi**, S. M. Firestine

53. MIF is a novel target for drug discovery in autoimmune and inflammatory diseases. **Y. Al-Abed**, K. F. Cheng

54. Discovery of highly selective matrix metalloproteinase-13 inhibitors for the treatment of osteoarthritis. **J. A. Scholten**, P. M. O'Brian, J. Nahra, M. Morris, W. H. Roark, C. E. Hanau, P. G. Ruminski, T. R. Fletcher, B. C. Hamper, H. S. Shieh, B. Collins, J. McDonald, M. D. Rogers, J. N. Carroll, A. Johnson, G. E. Munie, C-F. Man, S. L. Settle, O. Nemirovskiy, L. Vickery, A. Agawal, T. Sunyer, M. E. Schnute

55. Protective anti-inflammatory drugs containing NSAID esters with alkyl-aryl carbonate linkers. **K. Fabio**, N. Heindel, P. Mohanta, S. Young, J. Lacey, C. Guillon, M-T. Huang, D. Heck, J. Laskin

56. Synthesis and study of anti-inflammatory D-series resolvins. N. A. Petasis, **J. Winkler**, E. S. Nagengast, J. Uddin, C. N. Serhan

57. Kv1.3 blockers for treatment of autoimmune diseases. **S. Tasler**, T. Dreker, J. Kraus, S. Hamm

58. Discovery and synthesis of selective androgen receptor modulator MK-0773. **J. J. Perkins**, C. Bai, M. J. Breslin, F. Chen, D. B. Kimmel, A. Schmidt, R. S. Meissner

59. Cartilage biopolymers: Self-assembly and load-bearing properties. **F. Horkay**, D. C. Lin, I. Horkayne-Szakaly, C. Silva, E. K. Dimitriadis, P. J. Basser

60. 2-Aminopyrimidine agonists of the Wnt beta-catenin cellular messaging system 1: Lead optimization studies toward the discovery of WAY-262611. **J. T. Lundquist IV**, A. M. Gilbert, J. C. Pelletier, N. Alon, F. J. Bex, B. Bhat, M. Bursavich, V. Coleburn, L. Felix, D. Hauze, H-S. Lam, S. Lockhead, R. L. Magolda, J. Matteo, J. F. Mehlmann, R. Murrills, J. Wrobel, P. V. N. Bodine

61. 2-Aminopyrimidine agonists of the Wnt beta-catenin cellular messaging system 2: Additional lead optimization and in vivo studies on WAY-262611. **J. C. Pelletier**, J. T. Lundquist IV, F. J. Bex, B. Bhat, V. Coleburn, L. Felix, D. Green, P. Green, D. B. Hauze, Y. Kharode, H-S. Lam, S. Lockhead, J. Matteo, C. Milligan, R. Murrills, R. L. Magolda, J. F. Mehlmann, J. Pirrello, S. Selim, M. Sharp, M. D. Vera, J. E. Wrobel, P. V. N. Bodine

62. Synthesis of potent and selective nonzinc binding matrix metalloproteinase-13 inhibitors. **J. N. Carroll**, T. R. Fletcher, B. C. Hamper, J. A. Scholten, C. E. Hanau, P. G. Ruminski, M. D. Rogers, M. L. Grapperhaus, M. A. Massa, M. A. Schmidt, H. S. Shieh, N. Caspers, J. McDonald, G. E. Munie, D. M. Messing, S. Portolan, T. Sunyer, M. E. Schnute

63. Synthesis and biological evaluation of 2,4-diamino-6-(arylaminomethyl)pyrido[2,3-*d*]pyrimidines as inhibitors of *Pneumocystis jirovecii* and *Toxoplasma gondii* dihydrofolate reductase. A. Gangjee, W. Li, **S. Raghavan**, S. F. Queener

64. Synthesis of classical 6-substituted pyrrolo[2,3-*d*]pyrimidines as GARFTase inhibitors with folate receptor (FR) specificity and antitumor activity. A. Gangjee, **L. Wang**, L. H. Matherly, Y. Deng, R. L. Kisliuk

65. The importance of the glutamate moiety for folate receptor targeting and GARFT ase inhibitory activity in classical pyrrolo[2,3-d]pyrimidine antifolates. A. Gangjee, **Y. Wang**, Y. Deng, C. Cherian, Z. Hou, L. H. Matherly

66. Design, synthesis, evaluation of orally active small-molecule Smac mimetics as new anticancer drugs. **Q. Cai**, H. Sun, Y. Peng, Z. Nikolovska-Coleska, S. Qiu, L. Bai, C-Y. Yang, S. Kang, D. Yang, S. Wang

67. Design and synthesis of potent, specific and orally active small-molecule inhibitors of the MDM2-p53 interaction. **S. Yu**, D. Qin, J. Chen, G. Wang, K. Ding, Z. Nikolovska-Coleska, S. Kumar, S. Qiu, D. Bernard, Y. Lu, S. Kang, D. Yang, S. Wang

68. Synthesis and evaluation of a novel, potent and selective, orally bioavailable melanocortin-4 receptor antagonist for the treatment of cancer cachexia. **M. Soeberdt**, U. Abel, R. Bolliger, H. Deppe, A. Feurer, M. Henneböhle, H. Herzner, B. Hoffmann-Enger, S. Kervennic, A. Le Gall, G. Metz, S. Nordhoff, I. Ott, C. Rummey, H. Siendt, M. Terinek, P. Weyermann, C. Anklin, B. Cardel, I. Courdier-Fruh, R. Dallmann, J. Dubach-Powell, M. Hufschmid, J. P. Magyar, G. Santos, F. Schärer, C. Mondadori

69. The design, synthesis and biological evaluation of conformationally constrained Hsp90 inhibitors. **A. Duerfeldt**, B. Blagg

70. Exploring binding of HDAC isoforms with inhibitors by photoaffinity probes. **H. Bai**, S. Velaparthi, G. Pieffet, C. Pennington, R. van Breemen, S. Blond, P. Petukhov

71. Efficient synthesis of cruentaren A and preparation of analogs for the investigation of structure-activity relationships. **G. E. L. Brandt**, B. Blagg

72. Mechanistic studies on interaction of NiCR and NiCR-2H with DNA. **P. Chitranshi**, C-N. Chen, J. S. Faridi, P. R. Jones, L. Xue

73. Targeting the TNF-alpha/TNFR interaction with small molecule mimetics. **J. M. Davis**, C. Pace, R. Meister, R. Perrucci, C. Steele, C. Erin

74. Synthesis and biological evaluation of novel estradiol-platinum(II) hybrid molecules designed for site-specific treatment of female cancers. **C. Descôteaux**, C. Van Themsche, V. Leblanc, S. Parent, R. Hanna, É. Asselin, G. Bérubé

75. Investigation of new neo-tanshinlactone analogs as potent and selective anti breast cancer clinical trials candidates. **Y. Dong**

76. Synthesis, tubulin polymerization assays and cytotoxicity of D-seco paclitaxel analogs. S-R. Wang, C-G. Yang, Y. Zhao, I. Barasoain, J. F. Díaz, **W-S. Fang**

77. Discovery of CYT997, a potent vascular disrupting agent and inhibitor of tubulin polymerization. **J. Feutrill**, P. Bukczynska, C. Burns, E. Fantino, M. Harte, I. Kruszelnicki, I. Phillips, S. Su, L. Tranberg, B. Wang, Y. Wang, A. Wilks

78. Green tea polyphenols block the anticancer effects of boronic acid-based proteasome inhibitors. N. A. Petasis, **K. J. Gaffney**, E. B. Golden, S. G. Louie, T. C. Chen, A. H. Schönthal

79. Discovery of 1-benzoyl-3-cyanopyrrolo[1,2-*a*]quinolines as a new series of apoptosis inducers using a cell- and caspased-based high-throughput screening assay: Structure-activity relationships of the 4-, 5-, 6-, 7-, and 8-positions. **W. Kemnitzer**, J. Kuemmerle, S. Jiang, H-Z. Zhang, N. Sirisoma, S. Kasibhatla, G. Claassen, C. Crogan-Grundy, B. Tseng, J. Drewe, S. X. Cai

80. Synthesis and evaluation of γ-lactam derived small molecules as anticancer agents. S. Tekkam, P. Scott, S. C. Jonnalagadda, **V. R. Mereddy**

The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram/.

81. Discovery of novel angiogenesis inhibitors using transgenic zebrafish as a high-throughput phenotypic screening model. **J. Min**, S. Kurtkaya, B. Sneed, Y. Du, E. M. Sandberg, T. C. Baranowski, A. Sun, J. P. Snyder, D. C. Liotta, R. Dingledine

82. Investigation of indoloazepine as an adjuvant drug for cancer through chemoprotection. **T. N. Nguyen**, S. O'Reilly, G. Jin, J. J. Tepe

83. Structure activity relationship of dual acting histone deacetylase-topoisomerase II inhibitors. **V. Patil**, W. R. Guerrant, J. C. Canzoneri, A. K. Oyelere

84. Synthesis and evaluation of ether-linked dimers of epipodophyllotoxin. N. K. Dunlap, **T. L. J. Salyard**

85. Design, synthesis, and biological evaluation of indole-derived mitotic spindle poisons based on colchicine. **M. Shrestha**, A. Fowler, C. A. Ogle

86. Discovery and optimization of a selective inhibitor of oncogenic B-Raf. **W. Spevak**, H. Cho, S. Shi, B. Lam, Y. Guan, B. Powell, S. Shi, C. Zhang, K. Zhang, J. Tsai, G. Bollag, P. Ibrahim

87. Targeted photodynamic therapy of cancer using novel photosensitizer derivatives based on pyropheophorbide-a (PPa). **I. Stamati**, D. Phillips, G. Yahioglu, M. P. Deonarain

88. Discovery of pf-4217903-a highly potent and exquisitely selective c-met inhibitor. **M. Tran-Dubé**, H. Shen, M. Nambu, M. Pairish, L. Jia, H. Cheng, J. Hoffman, P. Le, C. Johnson, R. Kania, M. McTigue, N. Grodsky, K. Ryan, M. Parker, S. Yamazaki, H. Zou, J. G. Christensen, J. J. Cui

89. Withdrawn.

90. Discovery and in vivo efficacy of a novel, selective, and orally bioavailable Melanocortin-4 receptor antagonist for the treatment of cancer cachexia. **P. Weyermann**, R. Bolliger, H. Deppe, M. Henneböhle, H. Herzner, S. Kervennic, A. LeGall, G. Metz, S. Nordhoff, C. Rummey, H. Siendt, M. Soeberdt, M. Terinek, C. Anklin, B. Cardel, I. Courdier-Fruh, R. Dallmann, J. Dubach-Powell, M. Hufschmid, J. P. Magyar, G. Santos, F. Schärer, A. Feurer, C. Mondadori

91. Enhancing the antitumor activity of antibody-maytansinoid conjugates with hydrophilic linkers. **S. Wilhelm**, R. Zhao, R. Singh, W. Widdison, L. Clancy, E. Maloney, B. Kellogg, C. Audette, Y. Kovtun, M. Mayo, R. V. J. Chari

92. Photodynamic therapy for prostate cancer. **L. Y. Wu**, T. Liu, J. Choi, C. Berkman

93. Synthesis of 2-methyl-4-oxo-benzo[4,5]thieno[2,3-*d*]pyrimidines as TS inhibitor. A. Gangjee, **X. Zhang**, X. Zhou, R. L. Kisliuk

94. Design, synthesis and biological evaluation of 2-desamino-4-alkyl-5-[(substituted phenyl) ethyl]-7-substituted pyrrolo[2,3-d]pyrimidines as antitumor antimitoic agents. A. Gangjee, **S. Zhao**

95. Classical and nonclassical 2-amino-4-oxo-5-arylthio-substituted-6-isopropyl thieno[2,3-*d*]pyrimidine antifolates as potent thymidylate synthase inhibitors. A. Gangjee, **X. Zhou**, W. Li, R. L. Kisliuk

96. The stereospecific interactions of 3-deoxy-PI derivatives with the PTEN phosphatase domain. **Q. Wang**, M. F. Roberts, G. Krilov

97. Synthesis and structure activity relationship of D-homo cyclopamine analogs: A-ring fused heterocyclic analogs. **M. J. Grogan**, A. Lescarbeau, M. R. Tremblay, G. Lin, M. Hagel, K. McGovern, A. C. Castro

98. Synthesis and structure activity relationship of D-homo cyclopamine Hedgehog antagonists: 7-Membered A-ring lactam analogs. **A. Lescarbeau**, M. J. Grogan, M. R. Tremblay, S. J. Nair, J. Conley, K. McGovern, A. C. Castro

99. Synthesis and structure activity relationship of D-homo cyclopamine analogs: 3-Substituted analogs. **M. R. Tremblay**, A. Lescarbeau, M. J. Grogan, E. Tan, K. White, K. McGovern, A. C. Castro

100. Discovery of piperidine-4-carboxamides as potent chemokine receptor CCR2b antagonists, Part II: Reduction of hERG ion channel affinity and CYP450 liability. **P. Mohanty**, S. Koerner, R. Melendez, J. Lin, D. Chen, M. Fichman, E. Ben-Zeev, D. McCauley, A. Kolodziej, C. Kitsos, V. Jacques, Q. Deng, B. Das, S. Shacham, S. Jones, S. Ghosh, S. Dewitt

101. Discovery of piperidine-4-carboxamides as potent chemokine receptor CCR2b antagonists, Part I: Structure-based design and structure-activity relationship studies. **J. Lin**, R. Melendez, P. Mohanty, S. Koerner, M. Fichman, E. Ben-Zeev, D. McCauley, A. Kolodziej, C. Kitsos, V. Jacques, Q. Deng, D. Chen, B. Das, S. Shacham, S. Jones, Y. Marantz

102. Efficient syntheses of 8-substituted xanthine adenosine receptor antagonists. D. Ma, G. B. Jones, **A. E. Kallmerten**

103. Discovery of Lu AA21004: A novel compound for the treatment of mood disorders. **B. Bang-Andersen**, T. Ruhland, G. Smith, M. Jørgensen, B. Bjørnholm, K. Andersen, E. K. Moltzen, A. Mørk, L. T. Brennum, K. G. Jensen, T. B. Stensbøl, S. Hogg

104. Conformationally restricted tryptamine sulfonamides as novel and selective 5-HT6 receptor antagonists. **J. Konda**, R. S. Kambhampati, P. Kothmirkar, T. R. Bandyala, S. N. K. Yarra, S. Arepalli, M. A. Rasheed, A. K. Shinde, R. Nirogi

105. Identification of a potent, noncovalent series of fatty acid amide hydrolase (FAAH) inhibitors. **Z. Ma**, D. J. Gustin, Y. Li, C. Hedberg, X. Min, C. Guimaraes, Z. Wang, M. Lindstrom, A. Porter, D. Lester-Zeiner, F. Kayser

106. Design, synthesis and evaluation of heterocyclic peptide ketoamides as calpain inhibitors. **A. Ovat**, Z. Z. Li, J. C. Powers

107. Novel aryl sulfonamides: A new chemical class of selective 5-HT6 receptor antagonists. **A. K. Shinde**, A. V. Daulatabad, P. Gudla, V. Reballi, N. Rambabu, R. Badange, R. S. Kambhampati, R. Nirogi

108. Development of $GABA_A$ subtype selective agents for the treatment of alcohol abuse. **M. L. Van Linn**, W. Yin, D. Platt, E. M. Weerts, H. L. June, J. M. Cook

109. Lipoamino acid structure-anticonvulsant activity relationships of the systemically-active galanin analogs. **L. Zhang**, H. S. White, G. Bulaj

110. Synthesis of potential negative modulators of the dopamine D_2 receptor based on Pro-Leu-Gly-NH_2. **S. Bhagwanth**, R. L. Johnson

111. Exploration of the complex hydrogen-bonding network in the D1 dopamine receptor: Synthesis and evaluation of bicyclic catechol-containing dopamine analogs. **L. A. Bonner**, B. R. Chemel, U. Laban, J. I. Juncosa, V. J. Watts, D. E. Nichols

112. Antiviral drug design using computational chemistry. **H. A. Clifton**, J. W. Ribblett

113. Predicting UDP-glucuronosyltransferase of new structures. **K. Enslein**, R. Fraczkiewicz

114. Molecular docking and 3-D-QSAR studies of ranitidine analogs as acetylcholinesterase inhibitors in the treatment of Alzheimer's disease. **J. Gao**, J. M. Chapman Jr., C. McInnes

115. QSAR models of 5-HT2B receptor ligands and their application to predicting compounds that could cause valvulopathy. **R. Hajjo**, C. Grulke, A. Golbraikh, B. R. Roth, A. Tropsha

116. File enhancement: "Bench to Bedside" with "Iterative Efficiency". **C. Hulme**, G. M. Maggiora, N. Meurice, J. Petit

117. Molecular structure, inhibition, and docking studies of a family of polyaromatic hydrocarbons. **C. L. Klein Stevens**, N. Zhu, P. Jin, J. Liu, M. Foroozesh

118. Theoretical study of HIV-1 integrase inhibitors' tautomerism and their chelating complexes with two magnesium ions. **C. Liao**, M. C. Nicklaus

119. Identification of ligand features essential for TACE inhibitors by pharmacophore modeling. **P. R. Murumkar**, S. Das Gupta, R. Giridhar, M. R. Yadav

120. Computational correlation studies toward inactivation of O6-alkylguanine-DNA alkyltransferase by O6-benzylguanine analogs. A. E. Pegg, W. C. Guida, **S. L. Vankayala**, G. T. Pauly, N. Loktionova, Q. Fang

121. Ligand-based molecular modeling study on DNA G-quadruplex mediated telomerase inhibitors: 3-D-QSAR CoMFA/CoMSIA approach. **V. P. Zambre**, P. R. Murumkar, R. Giridhar, M. R. Yadav
122. Discovering potent molecules with human embryonic stem cells to treat heart disease. **C. B. Gilley**, M. Lanier, K. Okolotowicz, T. Wu, J. Ding, P. Bushway, J. Teixeira, E. Willems, M. Tsuda, A. Colas, Z. Xia, M. Mercola, M. Dawson, J. Cashman
123. Antioxidant activities of some potential drugs used in hypertension. **A. D. Oxton**, T. Brown, J. Rolfs, A. Pezeshk, D. Dalhouse
124. 17,18-Epoxyeicosatetraenoic acid, a potent antiarrhythmic EPA metabolite: SAR and stable analogs. J. Falck, **N. Puli**, G. Wallukat, C. Schmidt, R. Fischer, W-H. Schunck
125. Beneficial role of inducible nitric oxide synthase in thrombosis. **R. K. Upmacis**, H. Shen, L. E. S. Benguigui, D. P. Hajjar, K. A. Hajjar
126. Effects of flax oil on membrane fluidity and blood pressure of hypertensive and normotensive rats. **T. N. Brown**, J. Rolfs, A. D. Oxton, D. Dalhouse, A. Pezeshk
127. Novel inhibitors of Nav1.5 late current. **B. Jiang**, M. M. Abelman, C. Smith-Maxwell, K. Chan, M. Yang, H. Zou, J. Salcedo, L. Wu, C. Li, J. Hao, H-L. Sun, N. Chu, M. McGregor, J. Shryock, K. Leung, J. Zablocki
128. Inhibition models for cytochrome P450 1A2, 2C9, 2D6, and 3A4. **D. Zhuang**, J. Zhang, R. Fraczkiewicz, M. B. Bolger, M. Waldman, W. S. Woltosz, K. Enslein
129. Sansalvamide A binds to HSP90 and disrupts IP6K2 binding. **R. C. Vasko**, R. A. Rodriguez, C-M. Pan, S. R. McAlpine

MONDAY MORNING

Section A

Salt Palace Convention Center
Combo Ballrooms C&E

Smissman Award Symposium

D. J. Abraham, *Organizer*

9:00 130. New therapies for treating cancer and inflammation. **D. C. Liotta**
9:45 131. Design and synthesis of thrombin receptor antagonists. **W. J. Greenlee**, S. Chackalamannil, Y. Wang, Y. Xia, M. Clasby, K. Eagen, H. Tsai, X. Gao, G. Boykow, M. Chintala
10:30 132. Design, synthesis, and evaluation of fatty acid amide hydrolase inhibitors. **D. L. Boger**
11:15 Introductory Remarks.
11:20 133. Adventures in drug discovery: Enzyme inhibitors, receptor antagonists . . . and more. **B. E. Maryanoff**

Genetically Designed Molecular Materials Peptide-Based Molecular Erectors for Functional Systems Sponsored by NANO, Cosponsored by BIOL and MEDI

MONDAY AFTERNOON

Section A

Salt Palace Convention Center
Combo Ballrooms C&E

Latest Developments in Glutamate Receptors

J. M. Schkeryantz, *Organizer*

1:30 Introductory Remarks.
1:35 134. 20 Years of metabotropic glutamate receptor drug development.: An historical perspective on the discovery of the compounds which have been critical to our understanding of the physio-pathological involvement of these receptors. **V. Mutel**
2:15 135. Group II metabotropic glutamate receptors (mGluRs): Design and synthesis of small molecule modulators. **N. D. P. Cosford**
2:55 136. A novel series of group III metabotropic glutamate receptor (mGluR) agonists. **F. C. Acher**, C. Selvam, N. Triballeau, N. Ouaslati, I. Lemasson, C. Beurrier, S. Lopez, C. Goudet, P. Guibellini, M. Amalric, H.-O.Bertrand, J-P. Pin
3:35 137. Allosteric mGluR5 antagonists: From discovery to clinical development. F. Gasparini, **G. Bilbe**
4:15 138. The discovery and function of sweet taste enhancers. **M. Zoller**
4:55 139. Discovery, SAR and antiparkinsonian effect of novel positive allosteric modulators (PAMs) and ago-potentiators of metabotropic glutamate receptor subtype 4 (mGluR4). **C. W. Lindsley**

Section B

Salt Palace Convention Center
Ballrooms H&J

Recent Developments in Metalloprotease Inhibitors

F. Wu, Y. Xu, and J. O. Liu, *Organizers*

1:30 140. Metzincin clan of metalloproteinases as therapeutic targets. **Q-X. A. Sang**
2:05 141. Aggrecanase inhibitors. **K. E. Georgiadis**, J. Xiang, M. Ipek, Y. Hu, D. W. Hopper, M. D. Vera, D. How, J. Sabatini, P-E. Sum, E. L. Reifenberg, E. Feyfant, L. Mosyak, J. Skotnicki, M. G. Bursavich, S. Lombardi, A. M. Gilbert, S. Tam, E. A. Morris, T. S. Mansour
2:40 142. Methionine aminopeptidases as drug targets. **J. O. Liu**
3:15 143. Screening for exosite-targeting inhibitors of the anthrax lethal factor metalloproteinase. **B. E. Turk**
3:50 144. Bicyclic heterocycles as orally active and specific matrix metalloproteinase-13 inhibitors for the treatment of osteoarthritis. **J. J. Li**
4:20 145. Design of highly selective matrix metalloproteinase-13 inhibitors for the treatment of osteoarthritis. **M. E. Schnute**, P. G. Ruminski, M. A. Massa, J. W. Strohbach, C. E. Hanau, M. A. Schmidt, H. S. Shieh, N. Caspers, B. Collins, J. N. Carroll, T. R. Fletcher, B. C. Hamper, J. A. Scholten, M. D. Rogers, M. L. Grapperhaus, J. Hitchcock, J. Collins, J. McDonald, P. O'Brien, G. E. Munie, D. M. Messing, S. Portolan, S. L. Settle, O. Nemirovskiy, L. Vickery, T. Sunyer

Undergraduate Research Poster Session: Medicinal Chemistry Sponsored by CHED, Cosponsored by MEDI and SOCED

TUESDAY MORNING

Section A

Salt Palace Convention Center
Combo Ballrooms C&E

Novel Targets for the Treatment of Alzheimer's Disease
Financially supported by Bentham Science Publishers

A. Rivkin and I. Hills, *Organizers*

9:00 146. Novel targets for the treatment of Alzheimer's disease. **J. Buccafusco**
9:40 147. Metabolism of amyloid beta peptide and pathogenesis of Alzheimer's disease. **T. C. Saido**
10:20 148. Development of Hsp90 inhibitors as novel therapeutics for AD. **G. Chiosis**, W. Sun, W. Luo, A. Bretteville, K. Duff, P. Greengard
11:00 149. NADPH oxidase as a therapeutic target in Alzheimer's disease. **M. L. Block**
11:40 150. Alzheimer's disease drug discovery targeted to the nonamyloidogenic path of APP mRNA translation linked to Alpha-secretase (ADAM-17) expression. **J. T. Rogers**, C. M. Cahill, H. H. Cho, J. A. Moncaster, L. E. Goldstein, R. Moir, Z. Xie, X. Huang

Section B

Salt Palace Convention Center
Ballrooms H&J

Small Molecule Strategies for Inhibiting Human Viral Infections

M. Paige, *Organizer*

9:00 151. Inhibiting human papillomavirus infections. **R. Schlegel**
9:40 152. Discovery and development of nitazoxanide, a novel drug for the therapy of hepatitis B and hepatitis C virus infections. **B. E. Korba**
10:20 153. Small molecule strategies for inhibiting human viral infections. **K. H. Lee**
11:00 154. SAR studies on a series of inhibitors of human cytomegalovirus. **T. D. Cushing**
11:40 155. Discovery of GS-9131, an oral prodrug of a novel nucleoside phosphonate HIV reverse transcriptase (RT) inhibitor. **R. Mackman**, A. Ray, C. Boojamra, L. Zhang, H. Hui, J. Chen, J. Douglas, Y. Gao, D. Grant, G. Laflamme, K-Y. Lin, O. Petrakovsky, V. Prasad, J. Perry, A. Roy, J. Vela, M. Desai, C. Kim, T. Cihlar

Applications of Crystal Structure Information in Pharmaceutical Materials Development: Honoring Frank Allen Crystal Form Analysis, Experiment and Prediction Sponsored by CINF, Cosponsored by COMP, CHAL, and MEDI

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TUESDAY AFTERNOON

Section A

Salt Palace Convention Center
Combo Ballrooms C&E

Novel Antibiotics: Strategies for Discovery of Novel Antibacterial Targets and Inhibitors

M. R. Dobler and J. Leeds, *Organizers*

2:00 156. New drugs for bad bugs: Strategies for addressing the challenges of antibacterial drug discovery. **K. L. Widdowson**, S. F. Rittenhouse, D. J. Payne
2:45 157. Molecular machines that assemble biological membranes. **D. E. Kahne**
3:30 158. Novel DNA gyrase inhibitors: Fragment-based NMR screening to antibacterial agents. **B. A. Sherer**
4:15 159. Structural, mechanistic and inhibitory analysis of the transpeptidation/glycosyltransfer steps of peptidoglycan synthesis in MRSA. **N. C. J. Strynadka**, A. Lovering
5:00 160. The discovery of potent and selective inhibitors of undecaprenyl pyrophosphate synthase. **B. Hurley**

Section B

Salt Palace Convention Center
Ballrooms H&J

General Oral Session

J. R. McCarthy, *Organizer*

2:00 Introductory Remarks.
2:05 161. Award Address (E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances, sponsored by Schering-Plough Research Institute). Rational drug design of antiviral agents against influenza, HCV and HIV virus. **C. U. Kim**
2:35 162. Discovery of an allosteric activator of glucokinase. **R. F. Kester**, R. Sarabu, W. L. Corbett, N-E. Haynes, F. T. Bizzarro, K. R. Guertin, D. W. Hilliard, P. E. Mahaney, L. Qi, J. Tengi, G. W. Holland, A. Focella, J. F. Grippo, J. Grimsby, J. W. Coffey, L. Marcus, C. L. Spence, M. T. Dvorozniak
2:55 163. Discovery of BMS-754807, a small molecule inhibitor of IGF-1R in clinical development. **M. D. Wittman**, J. Carboni, Z. Yang, F. Y. Lee, G. Cantor, M. Antman, R. Attar, P. Balimane, C. Chen, S. Cheng, L. Discenza, C. Fairchild, F. G. Finckenstein, D. Frennesson, M. Gottardis, A. Greer, X. Gu, W. Hurlburt, A. Li, J. Li, P. Liu, W. Johnson, D. Langley, H. Mastalerz, A. Mathur, K. Menard, K. Patel, J. Sack, X. Sang, M. Saulnier, K. Stefanski, S. Traeger, G. Trainor, U. Velaparthi, S. Yeola, G. Zhang, K. Zimmermann, D. Vyas
3:15 164. EP-3 Receptor antagonists for Prostaglandin E-2 are novel potent antiplatelet agents that do not prolong bleeding. **A. Kiselyov**
3:35 165. Development of a CNS multiparameter optimization design tool increasing the probability of a compound survival by aligning metabolism, permeability, and safety properties in one molecule. **P. R. Verhoest**, X. Hou, A. Villalobos, T. Wager
3:55 166. Nonpeptide orally bioavailable glucagon receptor antagonists. **J. T. Kodra**, A. S. Jørgensen, B. Andersen, C. Behrens, C. L. Brand, I. T. Christensen, M. Guldbrandt, C. B. Jeppesen, L. B. Knudsen, P. Madsen, E. Nishimura, C. K. Sams, U. G. Sidelmann, J. Lau
4:15 167. Identification of potent, orally bioavailable nonnucleoside HCV RNA polymerase inhibitors. **P. S. Dragovich**, J. Brooks, D. M. Bartkowski, J. K. Blazel, K. Dao, D. A. Ellis, A. Gobbi, R. Kamran, S. H. Kim, L. A. LeBrun, L-S. Li, D. E. Murphy, T. G. Nolan, D. A. Norris, R. Patel, F. Ruebsam, M. V. Sergeeva, A. M. Shah, R. E. Showalter, N. Stankovic, Z. Sun, C. V. Tran, M. T. Tran, M. Tsan, S. E. Webber, A. X. Xiang, J. Zhao, L. Kirkovsky, Y. Zhou
4:35 168. 6, 9-Disubstituted purines as potent dual Src/Abl tyrosine kinase inhibitors targeting the "inactive" conformation. **W-S. Huang**, X. Zhu, Y. Wang, M. Azam, D. Wen, R. Sundaramoorthi, R. M. Thomas, S. Liu, G. Banda, S. Lentini, S. Das, Q. Xu, J. Keats, F. Wang, S. Wardwell, Y. Ning, J. T. Snodgrass, M. I. Broudy, K. Russian, J. Iuliucci, D. C. Dalgarno, T. P. Clackson, G. Q. Daley, T. K. Sawyer, W. C. Shakespeare
4:55 169. Discovery of 3-carboxamide isoxazoles as TRPV1 antagonists for the treatment of pain. **R. Palin**

Applications of Crystal Structure Information in Pharmaceutical Materials Development: Honoring Frank Allen Scientific and Regulatory Issues of Crystal Forms Sponsored by CINF, Cosponsored by COMP, CHAL, and MEDI

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WEDNESDAY MORNING

Section A

Salt Palace Convention Center
Combo Ballrooms C&E

From Poor to Rich: Optimization of Oral Bioavailability from Nonbioavailable Leads
Financially supported by Advanced Chemistry Development

J. F. Kadow and K-S. Yeung, *Organizers*

9:00 Introductory Remarks.
9:05 170. Discovery of orally active Bace-1 inhibitors for the treatment of Alzheimer's disease. **E. Demont**
9:40 171. If it's not one thing, it's another: Improving the Phase 1 and Phase 2 metabolic stability of a series of pyrazole-containing gamma-secretase inhibitors. **A. W. Garofalo**
10:15 172. Discovery of orally available aldosterone synthase (CYP11B2) inhibitors. **J. P. N. Papillon**, C. M. Adams, Q-Y. Hu, G. M. Ksander, J. Carvalho, C. Lou, A. K. Singh, C. Zhang, E. Gangl, W. M. Maniara, A. Amaral, M. Logman, S. Smith, A. Y. Jeng, D. F. Rigel, M. E. Beil, F. Fu, C-W. Hu, D. LaSala, S. Rajan
10:50 Intermission.
11:00 173. Optimization of oral pharmacokinetics in the discovery of clinical candidates for the treatment of sexual dysfunction. **D. Hepworth**, A. Cook, J. Blagg, C. Allerton, D. Miller, A. Baxter
11:35 174. Challenges in the development of orally bioavailable antagonists of the calcitonin gene-related peptide receptor, a family B GPCR: Discovery of telcagepant (MK-0974) for the treatment of migraine. **C. Burgey**
12:10 Concluding Remarks.

Section B

Salt Palace Convention Center
Ballrooms H&J

Targeting the Hedgehog Signaling Pathway for Therapeutic Opportunities in Cancer and Dermatology

S. Peukert and J. Kelleher, *Organizers*

9:00 Introductory Remarks.
9:05 175. Hedgehog pathway antagonists: New mechanisms and targets. **J. K. Chen**, J. M. Hyman, A. J. Firestone, C. A. Ocasio, V. M. Heine, Y. Zhao, K. Han, M. Sun, P. G. Rack, S. Sinha, J. W. Wu, D. E. Solow-Cordero, J. Jiang, D. H. Rowitch
9:45 176. GLI transcription factors as pharmacological targets. **R. Toftgård**, M. Lauth
10:25 177. Discovery of the Hedgehog antagonist GDC-0449 for the treatment of solid tumors. **D. P. Sutherlin**
11:05 Intermission.
11:15 178. Discovery of IPI-926, a semisynthetic clinical candidate that targets the Hedgehog pathway. **M. R. Tremblay**, A. Lescarbeau, M. J. Grogan, E. Tan, G. Lin, M. L. Benhke, B. C. Austad, L-C. Yu, M. Trudeau, L. Grenier, P. C-K. Lo, S. J. Nair, M. Hagel, K. White, J. Manna, T. Alvarez-Diez, J. Hoyt, J. R. Sydor, M. Pink, J. MacDougall, M. J. Campbell, K. McGovern, M. A. Read, V. J. Palombella, J. Adams, A. C. Castro
11:55 179. Inhibiting smoothened from inside: Rationally designed nanomolar inhibitors of the Hedgehog pathway. J. Remsberg, H. Lou, S. G. Tarasov, K. M. Adams, J. J. Barchi Jr., K. Gustafson, M. Dean, **N. I. Tarasova**

The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram/.

Symposium in Honor of Morris Robins
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WEDNESDAY AFTERNOON

Section A

Salt Palace Convention Center
Combo Ballrooms C&E

Importance and Utility of Screening Collections

D. G. Brown, *Organizer*

1:30 180. Evolution and utility of a corporate screening collection against CNS targets. **D. G. Brown**, T. A. Brugel, T. Hoerter, S. Wesolowski
2:10 181. Evolution of Eli Lilly screening collection. **R. J. Loncharich**
2:50 182. Approaches to front loading: Optimizing success with synthesis. **C. Hulme**
3:30 183. Building the NIH MLSMR screening collection for discovery of biological probes. **T. G. Lease**
4:10 184. Construction of a fragment-based screening collection. **C. W. Murray**

Section B

Salt Palace Convention Center
Ballrooms H&J

Optimizing the Stability of Clinical Candidates During Drug Discovery

E. Kerns and L. Di, *Organizers*

1:30 185. Metabolic stability challenges in drug discovery. **L. Di**
2:10 186. Inhibitors of respiratory syncytial virus fusion: Optimization from screening leads to potent, orally active compounds. **N. A. Meanwell**
2:50 187. PK/PD optimization of dihydropyridine allosteric FSH-receptor agonists. **C. Timmers**
3:30 188. Minimizing metabolic activation at the lead optimization stage: Challenges and solutions. **J-F. Lévesque**
4:10 189. The more we know the harder it seems: Past, present and future in metabolism optimization in drug discovery. **D. A. Smith**
4:50 Panel Discussion.

Symposium in Honor of Morris Robins
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WEDNESDAY EVENING

Section A

Salt Palace Convention Center
Hall 1

General Poster Session
Financially supported by American Chemical Society Book Division

J. R. McCarthy, *Organizer*

7:00–9:00
190. An artificial neural network model for prediction of logD. **M. Waldman**, R. Fraczkiewicz, W. S. Woltosz
191. Derivatives of fluoroquinolones: Synthesis and biological evaluation as potential antitumor agents. J. Azéma, B. Guidetti, J. Dewelle, B. Le Calve, T. Mijatovic, J. Vaysse, A. Korolyov, M. Malet-Martino, **V. Gilard**, R. Martino, R. Kiss
192. Genetic and biochemical analysis of MTA/SAH nucleosidase as a target for antibiotic development. **K. Cornell**, J. Jones, M. Wolter, M. Martinez, T. Martinez, N. Parveen
193. Discovery and structure-activity relationship investigations of 4-arylethynyldihydrocinnamic acid agonists of the antidiabetic target free fatty acid receptor 1. **E. Christiansen**, C. Urban, N. Merten, K. Liebscher, K. K. Karlsen, A. Hamacher, A. Spinrath, C. Drewke, S. Ullrich, M. U. Kassack, E. Kostenis, T. Ulven
194. Design and synthesis of azabicyclo octane derivatives as dipeptidyl peptidase IV inhibitors. T. Peng Cho, **Y. Fang Long**, L. Zhi Gang, L. He Jun, Z. Lei, Z. Fu Qiang, F. Jian Hong, W. Lin, S. Guang Yuan, G. Dong Liang, L. Xin
195. Design and synthesis of pyrrolidine amino amides as dipeptidyl peptidase IV inhibitors. T. Peng Cho, **Y. Fang Long**, Z. Lei, S. Guang Yuan, L. Jing Jing, L. Xin
196. Discovery of DNP-60502, a novel, potent AMPK activator for the treatment of metabolic syndrome. **K. Okano**, M. Hashimoto, T. Kodama, M. Iwata, C. Kohayakawa, D. Tanaka, A. Yano, J-I. Tsuji, F. Sato
197. Discovery of (4,4-difluoro-1,2,3,4-tetrahydro-5*H*-1-benzazepin-5-ylidene)acetamide derivatives as novel arginine vasopressin V_2 receptor agonists. **I. Tsukamoto**, H. Koshio, T. Kuramochi, S. Akamatsu, C. Saitoh, T. Yatsu, H. Yanai-Inamura, C. Kitada-Nozawa, E. Yamamoto, S. Sakamoto, S-I. Tsukamoto
198. Pharmacological characterization of AX-9657, a potent and selective neutrophil elastase inhibitor with good lung distribution. **J. Ishiyama**, K. Araki, M. Miura, Y. Kitamura, S. Izawa, E. S. Okerberg, E. C. K. Lin, K. R. Shreder, K. Murakami
199. Synthesis and optimization of 2-pyridin-3-yl-benzo[d][1,3]oxazin-4-one based inhibitors of human neutrophil elastase. **K. R. Shreder**, J. Cajica, L. Du, A. S. Fraser, Y. Hu, Y. Kohno, E. C. K. Lin, S. Liu, E. S. Okerberg, L. M. Pham, J. Wu, J. W. Kozarich
200. Vitamin D receptor antagonists from agonists: An unexpected discovery. **J. L. Gleason**, J. H. White, M. Lamblin, T-T. Wang, R. Spingarn, M. Burger
201. Aromatic analogs of geranyl- and digeranylbisphosphonate. **R. J. Barney**, A. J. Wiemer, R. J. Hohl, D. F. Wiemer
202. Design and synthesis of new inhibitors for protein Farnesyltransferase and Geranylgeranyltransferase type-I. **Y. Qiao**, J. Gao, D. Li
203. C2 N-Linked heterocyclic derivatives of the dihydroxypyrimidione-4-carboxamide HIV integrase inhibitor template. **M. A. Walker**, J. Banville, R. Remillard, S. Plamondon, G. Bouthillier, A. Martel, Y. Ueda, T. Connolly, J. Matiskella, B. Gulgeze, A. Torri, M. Casperson, S. Bollini, B. Terry, Z. Lin, H. Samanta, I. Dicker, M. Krystal, N. A. Meanwell
204. Optimization of compound efficiency in the context of discovering an amide keto-acid based HIV-integrase inhibitor with oral antiviral activity. **M. A. Walker**, J. Banville, T. Johnson, Z. Ma, R. Remillard, S. Plamondon, G. Bouthillier, A. Martel, A. F. Torri, M. Casperson, S. Bollini, B. J. Terry, Z. Lin, H. Samanta, M. Krystal, M. Zheng, N. A. Meanwell
205. Design, synthesis and HIV-1 integrase inhibitory activity of N-benzyl-4-hydroxy-5-oxo-2,5-dihydro-1H-pyrrole-3-carboxamides. **B. N. Naidu**, J. Banville, S. Bollini, G. Bouthillier, H. B. Gulgeze, T. Johnson, M. Krystal, Z. Lin, A. Martel, N. A. Meanwell, D. D. Parker, S. Plamondon, R. Remillard, H. Samanta, M. E. Sorenson, B. J. Terry, A. F. Torri, M. A. Walker, M. Zheng, M. Zupping
206. Binding to FKBP partitions a bifunctional HIV-1 protease inhibitor into blood cells and prolongs its lifetime in vivo. **P. S. Marinec**, J. E. Gestwicki
207. Solid phase synthesis of novel pyrrolidinedione analogs as potent HIV integrase inhibitors. **A. Pendri**, T. L. Troyer, S. W. Gerritz, M. J. Sofia, M. A. Walker, B. N. Naidu, J. Banville, N. A. Meanwell, Z. Lin, M. R. Krystal
208. C7-Heteroaryl-indoles as potent and orally bioavailable inhibitors of HIV attachment. **K-S. Yeung**, Z. Qiu, H. Fang, Z. Yin, M. E. Farkas, A. Trehan, B. Pearce, J. J. K. Wright, K. Ricarrdi, T. P. Spicer, P-Y. Shi, Y-F. Gong, R. J. Colonno, Z. Yang, L. Zadjura, C. J. D'Arienzo, M. R. Browning, S. Hansel, K. Santone, J. Barker, M. Taylor, R. Coxhead, R. Thomas, T. Coulter, P-F. Lin, N. A. Meanwell, J. F. Kadow
209. The development of a PSMA targeted imaging agent for prostate cancer. **J. Byers**, C. Berkman, P. Benny, T. Porter
210. Synthesis of a Gd(III)DOTA-lysine dendron specific contrast agent for cell receptor imaging by MR. **L. M. De Leon-Rodriguez**, A. J. M. Lubag, G. D. Udugamasooriya, T. Kodadek, A. D. Sherry
211. Synthesis and evaluation of methoxy-substituted deschloromazindols as potential PET radioligands for imaging the norepinephrine transporter. **K-S. Lin**, G-F. Huang, C. A. Mathis
212. Expeditious synthesis of labeled contrast agents for multimode cns imaging. **J. O'Neil**, G. Jones, C. C. Ferris
213. Synthesis of new carbon-11 labeled celecoxib derivatives as PET radioligands to image inflammation. **M. Gao**, M. Wang, G. D. Hutchins, Q-H. Zheng
214. Synthesis of [^{11}C]PBR28 as a PET radioligand for peripheral benzodiazepine receptors. **M. Wang**, M. Gao, B. E. Glick-Wilson, B. H. Mock, G. D. Hutchins, Q-H. Zheng
215. Synthesis of new carbon-11 labeled dual aromatase-steroid sulfatase inhibitors for PET imaging of aromatase and sulfatase in breast cancer. **M. Wang**, M. Gao, G. D. Hutchins, Q-H. Zheng
216. Structural activity relationship of imidazoline-based scaffolds as small molecules inhibitors of proinflammatory transcription factor NF-κB. **D. K. Kahlon**, T. A. Lansdell, J. S. Fisk, J. J. Tepe
217. Discovery of selective inhibitors of mutant b-raf. **J. G. Deal**, C. L. Palmer, W. H. Romines, J. Y. Park, L. C. Guo, L. Zehnder, T. J. Marrone, M. McTigue, D. DeLisle, J. Solowiej, X-H. Yu, S. Bagrodia
218. Small molecule inhibitors of Janus kinases. **J. Feutrill**, L. Andrau, D. G. Bourke, X. Bu, P. Bukczynska, C. Burns, N. Court, A. Donohue, E. Fantino, M. Farrugia, M. Joffe, M. Kling, M. Kurek, T. Nero, T. Nguyen, J. T. Palmer, H. Sikanyika, H. Treutlein, S. S. Wan, A. Wilks, J. Zeng
219. Novel N4-phenyl substituted tricyclic indeno[1, 2-d]pyrimidines as tyrosine kinase inhibitors and antiangiogenic agents. **A. Gangjee**, **Y. Zhao**, M. A. Ihnat
220. Evolution of a series of potent and efficacious PI3 kinase inhibitors. **T. P. Heffron**, M. Berry, G. Castanedo, C. Chang, I. Chuckowree, J. Dotson, A. Folkes, J. Gunzner, J. Lesnick, C. Lewis, K. Malesky, S. Mathieu, J. Nonomiya, A. Olivero, J. Pang, D. Peterson, L. Salphati, D. Sampath, D. P. Sutherlin, V. Tsui, M. Ultsch, N. C. Wan, S. Wang, C. Wiesmann, S. Wong, B-Y. Zhu
221. Discovery and development of novel furano-pyrimidine analogs as Aurora kinase inhibitors. **H-P. Hsieh**, M. S. Coumar, C-W. Lin, G. R. Reddy, M-T. Tsai, W-H. Lin, T-A. Hsu, S-Y. Wu
222. Synthesis and biological evaluation of potential EGFR Tyrosine kinase inhibitors: Aryl, benzyl and styryl coumarins. **V. R. Pallela**, S. C. Cosenza, M. R. M. Mallireddigari, E. P. Reddy, M. V. R. Reddy
223. 5-Bicyclic heteroaryl-3-pyridinecarbonitriles as PKC-theta inhibitors. **A. S. Prashad**, D. Wang, J. Chen, B. Wu, D. H. Boschelli, J. Lee, X. Yang, A. Brennan, D. Chaudhary
224. Hit to lead campaign of a series of cyclobutenediones as MAPKAP kinase 2 inhibitors for the treatment of inflammatory diseases. **J. E. Sabalski**, A. L. Banker, L. O. Resnick, J. A. Butera, R. Czerwinski, S. J. Kirincich, F. E. Lovering, I. J. McFadyen, L-L. Lin, J. Liu, K. Parris, K. Svenson, J-B. Telliez, W. Wang
225. New fluorescence-based binding assay for identification and characterization of kinase inhibitors. **U. Singh**, C. Lebakken, S. Riddle, W. J. Frazee, H. C. Eliason, J. K. Wolken, Y. Gao, L. Reichling, B. D. Marks, K. W. Vogel
226. Design, synthesis and evaluation of 5-chloro-N4-substituted phenyl-9H-pyrimido[4,5-b]indole-2,4-diamines as potential inhibitors of multiple receptor tyrosine kinases. A. Gangjee, **N. Zaware**, M. A. Ihnat
227. C-5 Substituted phenyl and monocyclic heteroaryl 3-pyridinecarbonitriles as PKC-theta inhibitors. **J. Chen**, D. Wang, B. Wu, C. Niu, D. H. Boschelli, J. Lee, X. Yang, A. Brennan, D. Chaudhary
228. Leishmanial choline kinase as a new therapeutic target. S. A. Pulido, J. A. Friesen, S. M. Robledo, D. L. Cedeño, **M. A. Jones**

229. Reversed chloroquines: Molecules that overcome malaria's resistance to chloroquine. **D. H. Peyton**, S. Burgess, C. Hodson, B. Gunasaru, K. Liebman, W. Morrill, S. Shomloo, J. X. Kelly
230. Development of novel chemotypes for negative allosteric modulation of mGluR5. **A. S. Felts**, C. W. Lindsley
231. Hit-to-lead optimization of 3,5-disubstituted-oxadiazoles as novel noncompetitive mGlu5 receptor antagonists. **G. M. Keserû**, K. Nógrádi, O. Nyéki, G. Wágner, C. Wéber, G. Domány, I. Greiner, A. Horváth, B. Kiss, A. Bielik, L. Molnár, K. Gál, Z. Szombathelyi
232. 5-Hydroxytryptophan-functionalized self-assembled monolayers capture native membrane-associated serotonin receptors. **A. Vaish**, P. S. Weiss, A. M. Andrews, M. J. Shuster
233. Measuring serotonin transporter function in rhesus peripheral blood lymphocytes using boron-doped diamond electrodes. **Y. S. Singh**, B. S. Beikmann, L. E. Sawarynski, B. A. Patel, A. M. Andrews
234. Improved resolution of closely related organic compounds with Reveleris™ flash cartridges. **R. Gaita**, S. Anderson, K. Lawrence
235. Novel dual detection flash instrument improves sample purity and productivity. **R. Gaita**, S. Anderson, K. Lawrence
236. Sulfonamides and sulfones as secondary pharmacophores in soluble epoxide hydrolase inhibitors. A. S. Kumar, B. R. Aavula, Z. N. Do, **R. D. Gless**
237. Discovery of a novel, potent and highly selective {beta}$_3$-adrenergic receptor agonist, SM-350300, for the treatment of overactive bladder syndrome. **M. Hashizume**, K. Hirota, T. Umezome, N. Sawada, Y. Ueno
238. Discovery of α-arylamino hydroxamic acids as novel anthrax lethal factor inhibitors. **G-S. Jiao**, L. Cregar-Hernandez, M. Moayeri, L. McKasson, S. Z. Millis, S. H. Leppla, A. T. Johnson
239. Design, synthesis, biophysical and biological studies of fluorescent Hoechst-polyamide hybrid molecules. R. Davis, A. Sielaff, J. Ruprich, L. Westrate, C. Tronrud, A. Ferguson, T. Brown, H. Mackay, J. Kluza, Y. Liu, D. Wilson, J. A. Hartley, **M. Lee**
240. New polymeric sorbents for postsynthesis reaction cleanup. **B. P. Murphy**, M. S. Young, D. Brousmiche, P. Iraneta, X. Zhang
241. Laser induced autofluorescence and anti-Stokes fluorescence spectroscopy in breast, colon and lung human biopsies. **M. Navas-Moreno**, Z. V. Vardeny
242. Characterization of novel inhibitors of the enzyme N5-CAIR synthetase. **H. Paritala**, S. M. Firestine, J. B. Thoden, H. M. Holden, J. M. Donnell
243. Design, synthesis and structural activity relationship of 1,3,6-trisubstituted-4-oxo-1,4,-dihydroquinoline-2-carboxylic acid as selective ET-A antagonists for prevention of preterm labor. H. J. Patel, K. Haranahalli, N. Olgun, I. Lengyel, S. Reznik, **R. A. Stephani**
244. Improved oral absorption of salmon calcitonin with AT-1002 peptide. **A. P. Tamiz**, Z. S. Teksin, K-H. Song, A. Tripathi, N. D. Eddington
245. The structure activity relationship studies of 3-(biaryl)-8-oxabicyclo[3.2.1]octane-2-carboxylic acid methyl esters. **L. Torun**, P. Meltzer
246. Redox-active liposome delivery agents as "smart" drug excipients. **N. Hollabaugh**, M. F. Mendoza, J. C. Forsythe, R. L. McCarley
247. Investigation of protein resistance on controlled triblock copolymers. **J-C. Yang**, **Q. Wang**, S. Z. D. Cheng, **J. Zheng**
248. Metabolic supplementing, sacrifice compensation and associated energy cooperation: Science in Chinese herb medicine. **Y. Zhang**, E. Wumanjiang
249. Acylcholine derivatives based on enantioenriched aminocyclanols. **R. W. Fitch**, R. R. Chase
250. The discovery of indeglitazar through scaffold based drug discover approach. **J. J. Lin**, U. Mehra, W. Wang, P. Bir Kohli, H. I. Krupka, C. Zhang, H. Nguyen, J. Cantwell, C. Settachatgull, D. Fong, A. Oh, S. Shi, B. Powell, G. Habets, B. West, K. Zhang, M. V. Milburn, P. Hirth, K. Nolop, G. Bollag, D. R. Artis, P. Ibrahim
251. Discovery of pyrrolopyridazines as novel DGAT1 inhibitors. **B. M. Fox**, K. Iio, K. Li, T. Inaba, S. Jackson, R. Choi, S. Sagawa, B. Shan, M. Tanaka, A. Yoshida, F. Kayser
252. Discovery of S-2367: A potent and selective NPY Y5 antagonist for the treatment of obesity. **T. Okuno**, H. Takenaka, Y. Aoyama, Y. Kanda, Y. Yoshida, T. Okada, H. Hashizume, M. Sakagami, T. Nakatani, K. Hattori, T. Ichihashi, T. Yoshikawa, H. Yukioka, K. Hanasaki, Y. Kawanishi
253. Discovery of novel diarylpyrazolyl thiadiazoles as cannabinoid CB1 receptor antagonists. **H. J. Seo**, S. H. Lee, S-H. Lee, M. E. Jung, K. Ahn, J. Kim, J. Lee
254. Novel adamantyl cannabinoids. **G. A. Thakur**, S. Bajaj, C. Paronis, Y. Peng, A. Makriyannis
255. Novel CB2 selective cannabinoids. **G. A. Thakur**, V. Shukla, A. Makriyannis
256. Discovery and optimization of oxazole based diacylglycerol acyltransferase 1 inhibitors for the treatment of obesity. **W. Yun**, D. R. Bolin, S. Li, M. Ahmad, S. J. Wertheimer, K. Conde-Knape, Y. Chen, S. Kazmer
257. Reduction of hERG inhibitory activity in the N-[piperidin-4-yl]urea series of H3 antagonists. **M. Berlin**, Y. J. Lee, C. Boyce, Y. Wang, K. McCormick, R. Aslanian, S. Sorota
258. Indole amines as novel, potent, and selective antagonists of the human histamine type 3 receptor. **W. R. Solvibile**, J-I. Kim, A. Adedoyin, S. Aschmies, J. Brennan, T. Comery, M. Day, L. Di, J. Golembieski, S. Grauer, J. Heinrich, W. D. Hirst, C. Kelley, K. Kubek, K. Marquis, R. Navarra, X. Ning, M. Pausch, G. J. Tawa, S. Rosenzweig-Lipson, M. J. Williams, G. Zhang, J. Gross, N. Brandon, A. J. Robichaud
259. Azacyclamine derivatives as Histamine-3 (H3) receptor antagonists. **M. J. Williams**, J. L. Gross, A. Adedoyin, S. Aschmies, J. Brennan, M. Day, L. Di, J. Golembieski, S. Grauer, W. D. Hirst, C. Kelley, J-I. Kim, K. Kubek, K. Marquis, R. Navarra, M. Pausch, W. R. Solvibile, G. M. Zhang, N. Brandon, T. Comery, A. J. Robichaud
260. Developing novel morphinanoids with dual actions at opioid receptors. F. Li, X. Xie, **A. Zhang**
261. Probes for narcotic receptor mediated phenomena: Binding studies on racemic cis benzofuro[2,3-c]pyridin-8-ols. **M. R. Iyer**, C. M. Dersch, R. B. Rothman, J. R. Deschamps, A. E. Jacobson, K. C. Rice
262. Identification and structure-activity relationship of an allosteric inhibitor of the dual specificity phosphatase Dusp6. **V. N. Korotchenko**, W. Dai, K. T. Debiec, K. A. Greene, G. Molina, A. Bakan, I. Bahar, M. Tsang, B. W. Day
263. Gold(I)-based inhibitors of protein tyrosine phosphatases. **D. Krishnamurthy**, M. R. Karver, N. Bottini, A. M. Barrios
264. Identifying protein tyrosine phosphatase inhibitors using a novel comparative screening approach. **R. A. Kulkarni**, A. M. Barrios
265. Selective PTP inhibitors with therapeutic potential. **R. A. Mathews**, A. M. Barrios
266. Development of a cellular assay for evaluating the permeability of novel neutrophil elastase inhibitors. **E. C. Lin**, L. Du, E. S. Okerberg, Y. Hu, A. S. Fraser, L. M. Pham, J. Cajica, C. M. Amantea, H. E. Brown, J. Kozarich, K. R. Shreder

Please refrain from using cellular telephones and cameras during technical sessions.

267. Assembly of a metal-binding fragment library to identify new chelators for inhibitors targeting metalloenzymes. **J. A. Jacobsen**, M. T. Miller, S. M. Cohen
268. Novel method for screening EGFR inhibitors using enzyme fragment complementation. **P. Angrish**, T. Naqvi, K. R. Olson
269. Endophytic analysis of tropical plants yields a platform for drug discovery. **B. Benham-Pyle**, S. A. Strobel
270. A new collaborative web-based database architecture for community-based pharmaceutical research. **S. Ekins**, B. A. Bunin, S. Ernst, M. Hohman
271. Multicomponent reactions for the generation of biologically active small molecules. **C. G. Evans**, J. E. Gestwicki
272. The pharmacodynamic screening of novel vinflunine derivatives. T. Peng Cho, **Y. Fang Long**, L. Xin Sheng, L. Xin, L. Yue, S. Yi, L. Li Guang
273. Pro-apoptotic screening of novel aza triterpenoids through structure-activity relationship investigation. **A. Koohang**, A. A. Mar, E. L. Szotek, D. A. Eiznhamer, Z-Q. Xu, M. T. Flavin
274. A high throughput screening FRET assay for identification of novel anthrax toxin lethal factor inhibitors. E. A. Amin, D. Hook, **S. Patil**, M. A. Walters, R. Francis, T-L. Chiu, J. Solberg, J. Nguyen
275. Design and synthesis of thallium-sensitive fluorescent probes for FLIPR assay of potassium channels. **G. G. Yi**, L. Leal, Z. Wang, G. Leung, S. Bhattacharyya
276. Design, synthesis, biochemical and biological evaluations of novel and potent small-molecule inhibitors of STAT3. **J. Chen**, L. Bai, N-C. Zaneta, J. Zhang, C. Gomez, Y. Han, K. Krzysztof, J. Sheng, P. Roller, S. Wang
277. Synthesis of dihydroquinoline derivatives as novel STAT3 inhibitors. **K. Park**, D. C. Cole, R. Ayyad, M. Asselin, S. A. Jelinsky, W. Hao, C-P. B. Chang, J. Xu
278. Two synthetic approaches to 6'-deaminocarbocyclic sinefungin. **Q. Chen**, W. Ye, S. W. Schneller
279. Synthesis of open-chain epothilones. **S. Fedorka**, N. Maurer, B. Baars, H. Haymour, R. Hudson, L. M. V. Tillekeratne
280. A practical synthesis of 6'-fluoroaristeromycins. **C. Liu**, S. W. Schneller
281. Design and synthesis of 3-deazaaristeromycin derivatives. **C. Chen**, S. W. Schneller
282. Synthesis of resveratrol using palladium catalyzed bond formation. **M. J. Panigot**, J. D. Green, C. Mathis, S. Hargrave
283. Hexachloroethane: A highly efficient reagent for the synthesis of chlorosilane from hydrosilane. **V. Pongkittiphan**
284. Nucleophilic selectivity in reactions of 3-chloromethylisoxazole-4,5-dicarboxylate. **G. J. Yu**, M. J. Kurth, B. A. Lorsbach
285. Fragment based drug design toward novel metalloprotein inhibitors. **A. Agrawal**, S. L. Johnson, M. Pellecchia, S. M. Cohen
286. Synthesis and in vitro biological evaluation of ring B abeosterols as novel inhibitors of Mycobacterium tuberculosis. **K. Nieves-Merced**, X. Wei, A. D. Rodriguez, Y. Wang, S. G. Franzblau
287. Synthesis and antitubercular activity of 4,6-diamino-1,3,5-triazine derivatives. **C-S. Yun**, Y-H. Choi, S-H. Lee, I-Y. Lee, P. Kim, T-H. Park, T. Oh, S-N. Cho, L. R. Camacho, D. Beer, V. Patel
288. Photodynamic inactivation with Mycobacterium smegmatis. **E. Feese**, R. A. Ghiladi
289. Novel pyridopyrimidine derivatives as inhibitors of STa induced cGMP synthesis. **E. A. Tanifum**, A. Y. Kots, F. Murad, S. R. Gilbertson
290. Design, synthesis and diversification on cyclohexen-1,4-dione libraries. **E. A. Tanifum**, A. M. Nyong, S. R. Gilbertson

THURSDAY MORNING

Section A

Salt Palace Convention Center
Ballroom C

Ion Channel Inhibitors for Pain and Atrial Fibrillation

J. Zablocki, *Organizer*

9:00 291. Novel 2-aminoalkylethers for the treatment of atrial fibrillation: Discovery of vernakalant. **G. N. Beatch**
9:40 292. Evaluation of potent and selective T-Type calcium channel antagonists in models of pain and insomnia. **T. S. Reger**, Z-Q. Yang, K-A. S. Schlegel, Y. Shu, R. V. Cube, C. Mattern, K. E. Rittle, P. L. Ngo, W. D. Shipe, V. Yang, C. Lindsley, J. Barrow, P. Coleman, G. D. Hartman, C. Tang, J. Ballard, Y. Kuo, T. Prueksaritanont, S. A. Kane, M. O. Urban, A. Liang, N. M. Sain, V. N. Uebele, C. E. Nuss, S. M. Doran, S. L. Garson, S. V. Fox, R. L. Kraus, J. J. Renger
10:20 293. Discovery and pharmacological evaluation of potent, selective blockers of the $Na_v1.8$ sodium channel with efficacy in models of neuropathic pain. **M. E. Kort**
11:00 294. Discovery, SAR and pharmacology of sodium channel Nav1.8 selective quinazolines. **A. Termin**
11:40 295. Novel dihydropyridines as inhibitors of Nav1.5 late current. **J. Zablocki**, M. Abelman, B. Jiang, C. Smith-Maxwell, K. Chan, M. Yang, H. Zou, J. Salcedo, L. Wu, C. Li, J. Hao, H-L. Sun, N. Chu, M. McGregor, J. Shryock, K. Leung

Section B

Salt Palace Convention Center
Ballroom H

General Oral Session

J. R. McCarthy, *Organizer*

9:00 296. Self-assembled quadruplex-DNA ligand. **M. García-Arriaga**, G. Hobley, J. M. Rivera
9:20 297. DNA-encoded libraries: A new resource for innovative hit identification. **T. L. Graybill**, B. W. King, D. T. Fosbenner, P. M. Keller, B. Morgan, M. A. Clark, J. Cuozzo
9:40 298. Prostate-specific membrane antigen-targeted imaging, diagnosis, and therapy of prostate cancer. **S. A. Kularatne**, P. S. Low
10:00 299. Retinoids, a new strategy for proteasome inhibition. M. Schmidt, Y. Leo, **B. C. Das**
10:20 300. Identification of a novel retinamide derivative that regulates cardiovascular development, using forward chemical genetic screen in zebrafish embryos. **T. Evans**, **B. C. Das**
10:40 301. Design, synthesis and evaluation of bivalent conformationally constrained Smac mimetics as inhibitors of IAP family proteins. **H. Sun**, J. Lu, L. Bai, N. C. Zaneta, C-Y. Yang, S. Qiu, H. Yi, D. McEachern, S. Wang
11:00 302. Predicting kinetic parameters for substrates of human cytochrome P450. **J. Zhang**, R. Fraczkiewicz, M. B. Bolger, M. Waldman, W. S. Woltosz, K. Enslein
11:20 303. Probing the mechanism of pseudopterosins. **W. Zhong**, C. Moya, R. S. Jacobs, R. D. Little
11:40 304. Synthesis of bis(difluoromethylene)triphosphonic acid and nonhydrolyzable nucleotide analogs. **M. Zibinsky**, R. Ismail, G. K. S. Prakash, T. G. Upton, B. A. Kashemirov, C. E. McKenna
12:00 305. Investigation of early steps in the pradimicin A biosynthetic pathway. **J. Zhan**, Y. Tang

‡ Cooperative Cosponsorship

THURSDAY AFTERNOON

Section A

Salt Palace Convention Center
Ballroom C

General Oral Session

J. R. McCarthy, *Organizer*

1:30 306. Design of hybrids with vitamin D receptor agonism and histone deacetylase inhibition as anticancer agents. **J. L. Gleason**, J. H. White, L. E. Tavera-Mendoza, T. D. Quach, B. Dabbas, J. Hudon, M. Lamblin, X. Liao, R. Spingarn, A. Palijan
1:50 307. Synthesis and biological evaluation of novel vitamin D3 derivatives. **W. Li**, M. A. Zmijewski, J. Chen, Z. Janjetovic, J. K. Zjawiony, T. Sweatman, D. D. Miller, A. T. Slominski
2:10 308. Synthesis, antibacterial activity, and new applications of aminoglycosides. **C. W. T. Chang**
2:30 309. Inhibition of aquaporin-4 by estrogen receptor modulators. **V. J. Huber**, M. Tsujita, T. Nakada
2:50 310. Addressing metabolism and toxicity in early drug discovery with rapid estimates of quantum mechanical descriptors. **R. Fraczkiewicz**, M. Waldman, J. C. Crison, W. S. Woltosz
3:10 311. The multistrategy for design of dopamine D1 and serotonin 5-HT1A receptor ligands. J. Zhang, X. Chen, X. Zhen, **A. Zhang**
3:30 312. Crystal structure of the naturally occurring Baeyer-Villiger monooxygenase MtmOIV. **M. Beam**, N. Noinaj, J. Rohr
3:50 313. Structural and thermodynamic characterization and comparison of RNA single mismatches. **A. R. Davis**, B. M. Znosko
4:10 314. Folate and antifolate synergism with nucleoside analogs. **A. R. Vortherms**, R. P. Doyle
4:30 315. Optimization of anthranilimide based glycogen phosphorylase inhibitors. **S. M. Sparks**, P. Banker, S. Thomson, A. Peat, F. X. Tavares, D. D. Sternbach, D. Garrido, K. Dwornik, J. Cooper, S. Dickerson, J. Weiel, D. M. Bickett, J. Boucheron, T. Wang, D. Clancy, R. T. Nolte, L. Wang, P. Golden, R. Graham

NUCL

Division of Nuclear Chemistry & Technology

M. A. Stoyer, *Program Chair*

SOCIAL EVENT:
Social Hour, 7-8pm: Mon

BUSINESS MEETINGS:
Business Meeting, 6-7pm: Mon
Executive Committee Meeting, 6:30-8:30pm: Sun

SUNDAY MORNING

Section A

Salt Palace Convention Center
251 D

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Kenton J. Moody

D. A. Shaughnessy and K. Czerwinski, *Organizers*

8:00 Introductory Remarks.
8:10 1. Award Address (Glenn T. Seaborg Award for Nuclear Chemistry, sponsored by ACS Division of Nuclear Chemistry and Technology). Some nuclear spectroscopy results. **K. J. Moody**
9:10 2. Heavy element production by the FLNR–LLNL collaboration. **Y. Oganessian**
9:40 3. Study of superheavy elements at the GSI SHIP. **S. Hofmann**
10:10 Intermission.
10:30 4. Heavy element production. **K. E. Gregorich**
11:00 5. Transfer and fusion aspects of the synthesis of heavy and superheavy nuclides. **M. Schädel**
11:30 6. From new actinide target technology to heavy element chemistry. **H. Nitsche**
12:00 7. Survival probabilities in hot fusion reactions. **W. Loveland**

SUNDAY AFTERNOON

Section A

Salt Palace Convention Center
251 D

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Kenton J. Moody

D. A. Shaughnessy and K. Czerwinski, *Organizers*

1:45 8. Chemical characterization of the heaviest elements at JAEA. **Y. Nagame**
2:15 9. Novel actinide separations and heavy element synthesis. **S. L. Nelson**
2:45 10. Study of absorption characteristics of Cm and Am to various Eichrom resins in several matrices. **N. Gharibyan**, A. Crable, S. Happel, R. Sudowe
3:15 11. Heavy element production and recovery at the Oak Ridge National Laboratory. **C. W. Alexander**, E. D. Collins, D. E. Benker
3:45 Intermission.
4:00 12. New developments in technetium-99 chemistry. **A. Sattelberger**
4:30 13. Developing the surrogate ratio methods with help from Ken Moody. **L. A. Bernstein**
5:00 14. Benchmarking (alpha, alpha' f) surrogate ratio in uranium. **S. Lesher**

MONDAY MORNING

Section A

Salt Palace Convention Center
251 D

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Kenton J. Moody

D. A. Shaughnessy and K. Czerwinski, *Organizers*

8:00 15. Stockpile stewardship challenges for radiochemistry. **Y. M. X. M. Dardenne**, J. M. Kenneally
8:30 16. University-national laboratory interactions for radiochemistry education. **K. R. Czerwinski**
9:00 17. An early investigation in contemporary nuclear forensic analysis at Livermore. **P. M. Grant**
9:30 18. Understanding the past, present and future – a tale of a hot particle: Part one. **R. C. Gostic**, J. M. Gostic, K. Czerwinski
10:00 Intermission.
10:15 19. Understanding the past, present and future – a tale of a hot particle: Part two. **J. M. Gostic**, R. C. Gostic, K. Czerwinski
10:45 20. Nuclear forensics: An emerging and still imperfect science. **I. D. Hutcheon**

The official technical program for the 237th National Meeting is available online at oasys2.confex.com/acs/237nm/techprogram/.

11:15 21. Development of radiochemistry experiments at the National Ignition Facility. **M. A. Stoyer**
11:45 22. Collection of solid debris for the National Ignition Facility. **D. A. Shaughnessy**

MONDAY AFTERNOON

Section A

Salt Palace Convention Center
251 D

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Kenton J. Moody

D. A. Shaughnessy and K. Czerwinski, *Organizers*

1:30 23. Highlights of spontaneous fission gamma spectroscopy. **J. O. Rasmussen**, Y-X. Luo
2:00 24. Nuclear isomers: Facts and fiction. **R. S. Rundberg**
2:30 25. Energy splitting of the ground-state doublet in the nucleus 229Th. **J. A. Becker**, B. R. Beck, P. Beiersdorfer, G. V. Brown, K. J. Moody, J. B. Wilhelmy, F. S. Porter, C. A. Kilbourne, R. L. Kelley
3:00 26. A new nuclear reaction for the production of 240Am. **P. A. Ellison**, L. Stavsetra, Z. Dvorakova, K. E. Gregorich, H. Nitsche
3:30 Intermission.
3:45 27. Separation methods for the isolation of Am-240 from proton-irradiated Pu-242 targets. **Z. Dvorakova**, P. A. Ellison, L. Stavsetra, H. Nitsche
4:15 28. Neutron capture and neutron-induced fission measurements on 241,242m,243Am at DANCE. **D. J. Vieira**, M. Jandel, T. A. Bredeweg, E. M. Bond, K. J. Moody, M. A. Stoyer, P. A. Wilk, C. Y. Wu
4:45 29. Nuclear structure of 242Am and (n,gamma) reaction on 242mAm. **C-Y. Wu**

TUESDAY MORNING

Section A

Salt Palace Convention Center
251 D

Nuclear Structure Using Rare Reactions

I-Y. Lee and M. A. Stoyer, *Organizers*

9:00 30. High-*K* isomers in deep-inelastic reactions. **G. D. Dracoulis**
9:30 31. Direct measurements of the goodness of the K quantum number in axially-deformed nuclei. **D. Cline**, A. B. Hayes
10:00 32. Shape, symmetry and structure in heavy nuclei. **P. Chowdhury**
10:30 Intermission.
10:45 33. Populating the 240U nucleus using the(18O,16O) reaction. **J. T. Burke**
11:15 34. Isomer spectroscopy of the heaviest nuclei. **R. M. Clark**
11:45 35. Octupole collectivity near N=126. **D. G. Sarantites**

Section B

Salt Palace Convention Center
251 E

Atom-at-a-Time Chemistry Cosponsored by NANO

R. A. Henderson, *Organizer*

8:00 Introductory Remarks.
8:05 36. Atom-at-a-time chemistry first used in discovery in 1955 of a new transuranium element 101. **D. C. Hoffman**
8:35 37. Atom-at-a-time chemistry. **A. Tuerler**
9:05 38. Chemical investigation of element 114. **R. Eichler**
9:35 39. Rapid chemical separation apparatus for atom-at-a-time chemistry of the heaviest elements. **Y. Nagame**, M. Asai, Y. Kasamatsu, T. K. Sato, A. Toyoshima, K. Tsukuda
10:05 Intermission.
10:35 40. The potential application of a diglycolamide-based resin for heavy element chemical separations. **J. M. Gostic**, K. Czerwinski, R. A. Henderson, D. A. Shaughnessy, K. J. Moody
11:05 41. Extraction chromatographic studies of Rf and Db homologs. **M. E. Bennett**, R. A. Henderson, D. A. Shaughnessy, R. Sudowe
11:35 42. Investigating the hydrolysis of uranium hexafluoride with DFT. **J. M. Becnel**, S. L. Garrison
12:05 Concluding Remarks.

TUESDAY AFTERNOON

Section A

Salt Palace Convention Center
251 D

Nuclear Structure Using Rare Reactions

I-Y. Lee and M. A. Stoyer, *Organizers*

1:30 43. Neutron-proton pairing and direct reactions. **A. O. Macchiavelli**
2:00 44. Beta-decay studies of N=Z nuclides at NSCL. **F. Montes**
2:30 45. Precision measurements of electromagnetic matrix elements in 10Be as a test of ab initio calculations. **C. J. Lister**, E. McCutchan, M. P. Carpenter, R. V. F. Janssens, T. L. Khoo, T. Lauritsen, E. F. Moore, D. Seweryniak, I. Stefanescu, S. Zhu
3:00 Intermission.
3:15 46. Voyage to the "Island of Inversion". **S. L. Tabor**
3:45 47. Nuclear halo and skin: A new era in nuclear physics. **R. Kanungo**
4:15 48. First experiments with the HELIOS spectrometer. **B. B. Back**

WEDNESDAY MORNING

Section A

Salt Palace Convention Center
251 D

Nuclear Structure Using Rare Reactions

I-Y. Lee and M. A. Stoyer, *Organizers*

9:00 49. In-beam gamma-ray spectroscopy at RI Beam Factory. **N. Aoi**
9:30 50. Measurements with rare isotope beams for nuclear astrophysics. **D. W. Bardayan**
10:00 51. Neutron spectroscopic factors of 34Ar and 46Ar from transfer reactions. **M. B. Tsang**, J. Lee, W. Lynch
10:30 Intermission.
10:45 52. Penning trap mass measurements of thermalized projectile fragments. **G. Bollen**
11:15 53. Studies of neutron-rich mass-80 nuclei with radioactive ion beams. **A. Galindo-Uribarri**, E. Padilla-Rodal
11:45 54. Approaching ^{78}Ni along the N=50 line using deep inelastic reactions. **M. P. Carpenter**, R. V. F. Janssens, S. Zhu, B. Fornal, R. Broda, A. Galindo-Uribarri, N. Hoteling, T. L. Khoo, F. G. Kondev, T. Lauritsen, C. J. Lister, E. Padilla-Rodal, D. Seweryniak, J. P. Ureggo-Blanco, W. B. Walters, I. Wang

WEDNESDAY AFTERNOON

Section A

Salt Palace Convention Center
251 D

Nuclear Structure Using Rare Reactions

I-Y. Lee and M. A. Stoyer, *Organizers*

1:30 55. Nonsystematic alpha decay and the structure of 101Sn and its neighbors. **R. K. Grzywacz**
2:00 56. Cd-128: A large problem or a small problem. **W. B. Walters**