Division of Medicinal Chemistry

Abstracts-233rd ACS National Meeting
Chicago, IL
March 25-29, 2006
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Final Program, 233rd ACS National Meeting, Chicago, IL, March 25-29, 2007

D. P. Rotella, *Program Chair*

SOCIAL EVENT:
Social Hour: Sun

SUNDAY MORNING

Section A

Unknown Site -- Unknown Room

Fragment-Based Drug Discovery

Cosponsored with Teledyne Isco
J. S. Albert, *Organizer, Presiding*
9:00 —1. Fragment based drug design. **M. Shapiro**

9:40 —2. Fragment screening and its application to drug design: The discovery of low molecular weight, non-peptidic, nanomolar inhibitors of beta-secretase. **P. D. Edwards**

10:20 —3. Fragment to lead evolution using chemical microarray screening. **H -D. Junker**, T. Neumann, I. Ott, K. Burkert, O. Keil, K. Schmidt, R. Sekul

11:00 —4. Structure activity relationships by mass spectrometry: Discovery of novel MMP3 inhibitors. **D. A. Ockey**, T. R. Gadek

11:40 —5. Fragment-based drug discovery: From crystal to clinic. **S. Howard**

12:20 —6. Strategies and experiences in fragment-based drug discovery. **R. E. Hubbard**

Section B

Unknown Site -- Unknown Room

General Oral Session

D. P. Rotella, *Organizer*

9:00 —7. Easier and better exploitation of PhysChem properties in medicinal chemistry. **S. Bhal**, G. Pearl, K. Kassam

9:20 —8. Independent expression of two genes using modified ecdysone receptors and small molecule actuators of a single chemotype. **R. E. Hormann**, O. Chortyk, J. L. Friz, C. S. Thompson, P. Kumar, C. Tice, B. Vertin, R. Palli, M. Kumar, A. Meyer, T. Meteyer, H. Smith, D. E. Cress, B. Li

9:40 —9. Modeling subtype-selective agonists binding with a4b2 and a7 nicotinic acetylcholine receptors: Effects of local binding and long-range electrostatic interactions. X. Huang, F. Zheng, X. Chen, **C -G. Zhan**

10:00 —10. Computational and experimental studies of free and enzyme-bound N-alkyltacrine derivatives. P. R. Carlier, **L. D. Williams**

10:20 —11. Synthesis and structure-activity relationships of a series of sigma receptor ligands. **R. Nahas**, J. R. Lever, S. Z. Lever

10:40 —12. Peptide ligands of regulators of G-protein signaling 4 (RGS4) identified by screening of a focused one-bead, one-compound peptide library. **R. A. Roof**, D. L. Roman, A. J. Turbiak, R. Neubig, H. I. Mosberg

11:00 —13. Synthesis and biologic evaluation of radioiodinated 5-chloro-2-(6-iodo-4-oxo-3,4-dihydroquinazolin-2-yl)phenyl phosphate (125IQ2-P, 5-Cl) for enzyme-mediated insolubilization therapy. **K. Wang**, S. J. Adelstein, A. Wang

11:20 —14. Synthesis, biological evaluation and docking studies inside PPAR alpha of resveratrol analogs. **C. S. Mizuno**, A. Patny, M. A. Avery, W. H. Yokoyama, A. M. Rimando

Claude S. Hudson Award in Carbohydrate Chemistry: Symposium in Honor of Pierre Sinay

Sponsored by CARB, Cosponsored with HIST, MEDI, and ORGN

SUNDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

First Time Disclosure of Clinical Candidates

A. W. Stamford, *Organizer, Presiding*

1:30 —15. Identification of GSK625433: A novel clinical candidate for the treatment of hepatitis C. **D. Haigh**, E. M. Amphlett, G. S. Bravi, H. Bright, V. Chung, C. L. Chambers, A. G. Cheasty, M. A. Convery, M. R. Ellis, R. Fenwick, D. F. Gray, C. D. Hartley, P. D. Howes, R. L. Jarvest, K. J. Medhurst, A. Mehbob, D. Mesogiti, F. Mirzai, F. Nerozzi, N. R. Parry, N. Roughley, T. Skarzynski, M. J. Slater, S. A. Smith, R. Stocker, C. J. Theobald, P. J. Thomas, P. A. Thommes, J. H. Thorpe, C. S. Wilkinson, E. Williams

2:10 —16. Identification and development of inhibitors of PI3K and related protein kinases for cancer treatment. M. Maira, F. Stauffer, P. Furet, H -G. Capraro, P. Holzer, **C. Garcia-Echeverria**

2:50 —17. Preclinical antitumor activity of BMS-690514, a panHER/VEGFR2 kinase inhibitor. **A. V. Gavai**, P. Chen, D. Norris, B. E. Fink, H. Mastalerz, Y. Zhao, W -C. Han, G. Zhang, W. Johnson, E. Ruediger, P. Dextraze, J -P. Daris, S -H. Kim, K. Leavitt, K. Kim, S. Lu, P. Zheng, A. Mathur, D. Vyas, J. S. Tokarski, C. Yu, S. Oppenheimer, H. Zhang, F. Lee, T. W. Wong, G. D. Vite

3:30 —18. The discovery of MK-0812, a potent and selective CCR2 antagonist. **L. Yang**, R. X. Jiao, C. Moyes, G. Morriello, G. Butora, K. Shankaran, A. Pasternak, S. Goble, C. Zhou, M. MacCoss, A -M. Cumiskey, L. Peterson, M. Forrest, J. M. Ayala, H. Jin, J. DeMartino, S. G. Mills

4:10 —19. Discovery of PF-184298, a dual serotonin/noradrenaline reuptake inhibitor. **G. A. Whitlock**, F. Wakenhut, A. Stobie, P. V. Fish, M. J. Fray

4:50 —20. Discovery of MK-0974: A potent, orally bioavailable calcitonin gene-related peptide (CGRP) receptor antagonist for the treatment of migraine. **D. V. Paone**, A. Shaw, D. Nguyen, C. Burgey, J. Deng, C. Stump, A. Quigley, J. DeSolms, S. Kane, K. Koblan, R. Bednar, J. Mallee, S. Mosser, C. Salvatore, D. McMasters, J. Hershey, H. Corcoran, B. Lyle, B. Wong, S. Roller, C. Miller-Stein, J. Rowe, S. Yu, S. Graham, J. Vacca, T. Williams

Claude S. Hudson Award in Carbohydrate Chemistry: Symposium in Honor of Pierre Sinay

Sponsored by CARB, Cosponsored with HIST, MEDI, and ORGN

SUNDAY EVENING

Section A

Unknown Site -- Unknown Room

General Poster Session

Cosponsored with Eli Lilly
D. P. Rotella, *Organizer*
7:00 - 9:00
21. Synthesis of 4',4'-C-diaminomethyl nucleoside derivative as a building block for constructing libraries via amide bond formation. **C -S. Yu**, R -T. Wang, L -W. Chiang, K. Pei, H -L. Huang, M -H. Lee

22. An improved method for synthesis of ceramide for constructing alpha-galactosyl ceramide analogs. **C -S. Yu**, C -H. Yeh, L -W. Chiang, S -D. Pan, K -H. Chang

23. Synthesis of rhamnosyl trisaccharide repeating unit to mimic the antigen determinant of Pseudomonas syringae lipopolysaccharide. **C -S. Yu**, H -Y. Wang, L -W. Chiang, S -W. Chen, C -T. Pan

24. Preparation and screening of novel inhibitors of MurG. **A. E. Trunkfield**, T. D. H. Bugg

25. Inhibitors for the aminoacyl tRNA: lipid 2 ligase MurM from *S. pneumoniae*. **E. Cressina**, T. D. H. Bugg, A. J. Lloyd, C. Dowson, D. Roper

26. Total synthesis of IKD-8344. **W. H. Kim**

27. Novel diphenyl ethers: Design, docking studies and inhibition of enoyl ACP reductase from *Plasmodium falciparum* and *Escherichia coli* and their structure activity relationship. **G. Kumar**, M. Chhibber, P. Parasuraman, R. T. N. Chakravarthy, N. Surolia, A. Surolia

28. Mechanism of antimicrobial peptides studied by controlling the topology of peptide assembly. **A. W. Young**, Z. Liu, C. Zhou, N. R. Kallenbach

29. Molecular template for designing de novo antimicrobial peptide mimetics. **C. Zhou**,

Z. Liu, J. Min, A. W. Young, Y -T. Chang, N. R. Kallenbach

30. De novo multivalent antimicrobial peptides as therapeutics against multidrug-resistant bacterial strain. Z. Liu, **C. Zhou**, A. W. Young, N. R. Kallenbach

31. Characterization of a small ribozyme with splicing activity: A step forward in the development of a molecular machine to treat pathogens. **L. B. Harris**, S. O. Rogers

32. Annulation route to kinamycin precursors. **Y. Yuan**, G. A. Kraus, A. J. Schuster

33. Minor groove binding agents as antibacterials. **S. K. Vooturi**, C. Cheung, M. Rybak, J. Baltz

34. Substrate mimics as novel inhibitors of the PlsX/PlsY pathway in S. pneumoniae. **K. D. Grimes**

35. Cloning, expression, and characterization of a *K. pneumoniae* acetyltransferase involved in virulence. **A. E. Zercher**, J. L. DuBois

36. Novel preparation of nano-silver particles for bacteriostat drug and antimicrobial test. **H. Feng**, M. D. Wang, Z. L. Fu

37. Screening of a peptide library for protein-protein interaction inhibitors of LpxA. **N. Ciminillo**, G. D. Dotson

38. Expression, purification, and characterization of *Enterococcus faecalis* phosphopantothenoylcysteine synthetase. **J. Yao**, G. D. Dotson

39. Synthesis and evaluation of catalytic intermediate-based inhibitors of phosphopantothenoylcysteine synthetase. **J. Patrone**, G. D. Dotson

40. Structure activity relationship study of para-substituted phenol derivatives, with comparison of minimum inhibition concentration and zone of inhibition. **J. St. Denis**, W. W. Steiner, R. Priefer

41. Pseudans, a synthetic approach to HAQs found in *Pseudomonas aeruginosa*. **W. M. Stalick**, R. V. Honeychuck, R. R. Pant, M. Rogers

42. Systems biology solutions on bacterial infections: Optimization of the concentration of a generic quorum sensing inhibitor in *Escherichia coli* and *Pseudomonas aeruginosa* based on stochastic modeling. **A. F. Gonzalez Barrios Sr.**, L. E. K. Achenie

43. Investigation of the methionine salvage pathway as a possible target for antimicrobial

drugs. **C. A. Isom**

44. Chemical and antimicrobial properties of anise essential oil. **E. H. Hudson II**, B. Woodard, K. Casmire, F. Abdel-Rahman, W. Zhang, M. A. Saleh

45. Chemical and antimicrobial properties of Chinese star anise essential oil. **K. Casmire**, B. Woodard, E. H. Hudson II, F. Abdel-Rahman, W. Zhang, M. A. Saleh

46. Synthesis and potency of PA-824 and metronidazole analogs as probes for anaerobic vs. aerobic activity against mycobacterium tuberculosis. **P. Kim**, U. Manjunatha, C. E. Barry III, C. S. Dowd

47. Small molecule inhibitors of mycothiol production from mycobacterium tuberculosis. **B. B. Metaferia**, S. S. U. Hussan, C. A. Bewley

48. Synthesis and antimycobacterial activity of 4-(5-substituted-1,3,4-oxadiazol-2-yl)pyridines. **G. Navarrete-Vazquez**, G. Molina-Salínas, Z. V. Duarte-Fajardo, J. Vargas-Villarreal, F. González-Salazar, H. Tlahuext, S. Said-Fernández, S. Estrada-Soto

49. Inhibitors of Trypanosoma cruzi DHFR: Potential chemotherapeutic agents for Chaga's disease. B. A. Shinkre, O. Senkovich, A. Desai, **S. E. Velu**, D. Chattopadhyay

50. DNA binding properties of anti-parasitic agents. **B. Nguyen**, F. A. Tanious, A. Kumar, D. W. Boykin, W. D. Wilson

51. Development of Quantitative Structure-Activity Relationship (QSAR) Models for a Series of Isoflavones As Novel Antigiardial Agents. **N. S. Telang**, P. Mukherjee, M. A. Avery

52. Design, synthesis, and biological evaluation of tetramic acids as antibacterial agents. **R. Yendapally**, E. I. Carson, R. E. B. Lee, R. E. Lee

53. Structure-activity relationships of novel pyrimidine derivatives as Plasmodial ODCase inhibitors. **A. M. Bello**, E. Poduch, I. Crandall, L. Wei, K. C. Kain, E. F. Pai, L. P. Kotra

54. Characterization of novel inhibitors of orotidine 5'-monophosphate decarboxylase (ODCase) using isothermal calorimetry. E. Poduch, A. M. Bello, M. Fujihashi, E. F. Pai, **L. P. Kotra**

55. Covalent inhibitor of orotidine 5'-monophosphate decarboxylase with antimalarial activity. A. M. Bello, E. Poduch, M. Fujihashi, Y. Li, I. Crandall, P. I. Lee, K. C. Kain, E. F. Pai, **L. P. Kotra**

56. Synthesis of cyclic disulfides as possible antimalarial agents. **S. Espinosa**, G. A. McConkey, T. Heikkilä, C. P. Vlaar

57. The synthesis of novel 5- and 6-substituted quinazoline antimalarial compounds. **V. E. Kokai**, T. Vilaivan

58. New analogs of the natural antifungals cleistopholine and sampangine. O. Marcq, **D. Sail**, N. Chauhan

59. Design, synthesis and evaluation of 1-(D-ribityl)-1,7-dihydro-pyrazolo[3,4-d]pyrimidine-4,6-diones bearing alkyl phosphate substituents as inhibitors of lumazine synthase. **Y. Zhang**, A. Bacher, M. Fisher, B. Illarionov, M. Cushman

60. Synthesis and antifungal activities of modified fluconazole derivatives. N. H. Nam, S. Sardari, **K. Parang**

61. Optmizing the synthesis of N-methanocarbathymidine, a potent and selective antiviral agent. V. E. Marquez, **O. R. Ludek**

62. Synthesis and evaluation of a group of selective inhibitors of Ebola cell entry. **M. V. Yermolina**, J. Wang, D. J. Wardrop, L. Wang

63. Synthesis and antiviral activity of Abyssinone II analogs. R. M. Moriarty, **B. C. Surve**, R. Naithani, S. N. Chandersekera, V. Tiwari, D. Shukla

64. Synthesis and antiviral activity of Sulforamate derivatives. R. M. Moriarty, **R. Naithani**, B. C. Surve, V. Tiwari, D. Shukla

65. Synthesis and nuclear magnetic resonance characterization of nelfinavir. J. Yan, **G. Yao**, L. Yang

66. Discovery of potent and orally bioavailable CCR5 antagonists: Part I. **R. G. Wei**, B. Chen, L. Dunning, E. Ho, S. Jaroch, W. Lee, J. Onuffer, B. Subramanyam, J. Shen, J -L. Tseng, B. Ye, P. Gary

67. Quinolyl amide derivatives as CCR5 antagonists. **S -F. Lu**, L. Dunning, S. Jaroch, T. Kirkland, J. Onuffer, G. Phillips, B. Subramanyam, J -L. Tseng, M. Wei, H. Ye, B. Ye

68. 8-Hydroxy-5-(1-H or 1-alkyl-5-oxopyrrolidin-3-yl)-1,6-naphthyridine-7-carboxamide inhibitors of HIV-1 integrase. **J. Y. Melamed**, M. Egbertson, S. Varga, J. P. Vacca, P. A. Ciecko, G. Moyer, L. Gabryelski, P. J. Felock, K. A. Stillmock, M. V. Witmer, D. Hazuda, W. A. Schleif, Y. Leonard, L. Jin, J. D. Ellis, S. D. Young

69. Binding specificity of HIV-fusion blocking protein (MVL) determined by NMR techniques. **S. S. U. Hussan**, C. A. Bewley

70. Comparing the conformational behavior of a series of HIV-1 protease inhibitor drugs using the Low Mode:Monte Carlo conformational search method. **J. Lee**, C. A. Parish

71. How can (-)-epigallocatechin gallate from green tea prevent HIV-1 virus infection? Mechanistic insights from computational modeling and the implication for rational design of anti-HIV-1 entry inhibitors. **A. Hamza**, C -G. Zhan

72. Synthesis and biological evaluation of alkenyldiarylmethane HIV-1 non-nucleoside reverse transcriptase inhibitors that possess increased hydrolytic stability. **M. D. Cullen**, E. De Clercq, C. Pannecouque, T. L. Hartman, R. W. Buckheit Jr., B. L. Deng, M. Cushman

73. 3'-Fluoro-2', 3'-unsaturated carbocyclic nucleosides: Synthesis, anti-HIV activity and molecular modeling studies. **J. Wang**, Y. Jin, K. L. Rapp, R. F. Schinazi, C. K. Chu

74. Stereoselective, de novo synthetic route to a combinatorial library of peptide-linked nucleosides. **K. W. C. Poon**, A. Datta

75. Screening anti-viral agents based on yeast killer system model. L. Pan, **Y -W. Huang**, Y. Yanrui

76. Total synthesis of carbocyclic sinefungin. **X. Yin**, G -X. Zhao, S. W. Schneller

77. Synthesis and biological properties of carbocyclic 6'-deaminosinefungin and related compounds. **W. Ye**, Q. Chen, S. W. Schneller

78. Design and synthesis of carbaformycin, carbaneplanicin and their 3-deaza analogs. **H. Wang**, Y. Zhang, S. W. Schneller

79. 5'-Fluoro-5'-deoxyaristeromycin. **W. Li**, X. Yin, S. W. Schneller

80. 4'-Fluoro analog of 5'-noraristeromycin. **W. Li**, X. Yin, S. W. Schneller

81. Enatioselective synthesis of carbocyclic 5'-norformycin. **M. He**, X. Yin, J. Zhou, S. W. Schneller

82. Synthesis and the antiviral activity of 3-methyl-3-deaza-5'-noraristeromycin. **C. Liu**, S. W. Schneller

83. Benzofuran inhibitors of hepatitis-C RNA polymerase: Synthesis of lead molecules including clinical candidate HCV-796. A. K. Saha, T. H. Faitg, **B. A. Kulkarni**, C. Blackledge, S. Masterson, Y. Deng, S. Rippin, D. Rys, T. Lessen, C. Cebula, L. Leister, J. Swestock, T. J. Nitz, H. Feng, C. J. Burns, D. C. Young, S. Chunduru

84. Optimization of N-alkyl indole allosteric inhibitors of the HCV NS5B polymerase enzyme. **B. Pacini**, S. Altamura, S. Avolio, M. Bisbocci, M. DiFilippo, S. DiMarco, O. Gonzalez Paz, R. Laufer, F. Narjes, G. Paonessa, M. Rowley, S. Harper

85. Docking and 3-D-QSAR analysis of HCV NS5B RNA-dependent RNA polymerase inhibitors based on a common benzothiadiazine scaffold. **S. Odde**, P. Sivaprakasam, R. J. Doerksen

86. Structure-activity relationship of a series of P2 proline arylether inhibitors of the HCV NS3•4A protease. **J. J. Court**, C. A. Gates, C. Lin, K. Lin, Y -P. Luong, J. H. van Drie, R. B. Perni

87. Tetrahydrocarbazoles as potential therapeutic agents for human papillomavirus infection. **P. R. Sebahar**, K. W. Brown, K. S. Gudmundsson, R. Harvey, L. Richardson, P. Sethna

88. Tetrahydrocarbazole-amides as potential agents for treatment of papillomavirus infection. **K. S. Gudmundsson**, S. Boggs, B. A. Johns, L. Richardson, P. R. Sebahar, J. G. Weatherhead, D. Haigh, K. W. Brown, R. Harvey, P. Sethna, Q. Zhang, P. Golden, S. Xie

89. 2-Substituted tetrahydrocarbazoles as potential therapeutic agents for human papillomavirus infection. **L. D. Richardson**, K. W. Brown, R. Harvey, K. S. Gudmundsson, P. R. Sebahar, P. Sethna

90. Studies toward a new foot-and-mouth disease antiviral agent. **N. Roqué-Rosell**, S. Curry, R. J. Leatherbarrow

91. Synthesis of imidazolyl substituted heterosteroidal derivatives as potent aromatase inhibitors. **R. Bansal**, S. Guleria, R. W. Hartmann, A. Palusczak

92. Synthesis of 8-[4-(aminoethoxy)-3-methoxyphenyltheophylline derivatives as potent adenosine receptor antagonists. **R. Bansal**, G. Kumar, A. L. Harvey, L. Young

93. Synthesis, SAR and biological evaluation of racemic abyssinone II and analogs as potential aromatase inhibitors for prevention of breast cancer. **A. Maiti**, M. Cuendet, V. L. Croy, D. C. Endringer, J. M. Pezzuto, M. Cushman

94. Identification of a novel small molecule antagonist of anti-apoptotic Bcl-2 proteins: Bcl-2 protein binding, in vitro cytotoxicity, and synergism. C. Xing, **J. M. Doshi**

95. Design and evaluation of novel smac mimetics as potent inhibitors of XIAP. **Y. Peng**, H. Sun, Z. Nikolovska-Coleska, S. Qiu, C -Y. Yang, S. Wang

96. Novel, simplified α-helix mimetics targeted to Bcl-x_L. **J. M. Rodriguez**, G -I. Lee, D. Dhar, A. D. Hamilton

97. Discovery and optimization of substituted N-Aryl-1H-pyrazolo[3,4-b]quinolin-4-amines as potent apoptosis inducers using a cell-based high throughput assay. **H -Z. Zhang**, G. Claassen, C. Crogan-Grundy, J. Drewe, S. Kasibhatla, B. Tseng, S. X. Cai

98. 4-Aryl-4*H*-chromenes as a new series of apoptosis inducers using a cell- and caspase-based high throughput screening assay: Structure-activity relationships of *N*-substituted pyrrole fused at the 7, 8-positions. **W. Kemnitzer**, S. Kasibhatla, S. Jiang, H. Zhang, R. Denis, S. Lamothe, H. Gourdeau, B. Tseng, J. Drewe, S. X. Cai

99. Drug-ability case study: Exploration of structural modifications and their impact on oral bioavailability of novel radio-sensitization agents (A): Z-(±)-2-(1-Benzylindole-3-yl-methylene)azabicyclo[2.2.2]octane-3-ol, (B): Z-(±)-2-(1-Benzylindole-3-yl-methylene)azabicyclo[2.2.2]octane-3-one and (C): Z-(±)-2-[1-(4-chlorobenzyl)indole-3-yl-methylene]azabicyclo[2.2.2]octane-3-ol. **A. M. Al-Ghananeem**, Z. Al-Beyati, A. H. Malkawi, V. N. Sonar, M. Freeman, P. A. Crooks

100. Synthesis of carbon-11 labeled cyclofenil derivatives as new potential PET agents for imaging breast cancer estrogen receptors. M. Gao, **M. Wang**, Q -H. Zheng

101. Generation of new chelates for targeted MRI and radioimmunotherapy. X. Ma, H. Song, H. Lee, S. Mhaske, S. Bhuniya, **H -S. Chong**

102. Fluorine-substituted 6-Aryl-1,4-dihydrobenzo[d][1,3]oxazine-2-thiones for breast tumor imaging and radiotherapy: Synthesis and receptor binding affinity. **H -B. Zhou**, K. E. Carlson, **J. A. Katzenellenbogen**

103. Synthesis and evaluation of carrier linked small molecules as targeted chemo and binary radiotherapeutic agents. V. J. Reddy, **V. R. Mereddy**

104. Radiosynthesis of 18F-fluro-BMS-354825 for PET imaging of SRC expression in tumors. **Y. Ying**, U. Mukhopadhyay, M. M. Alauddin, W. Bornmann, J. Gelovani

105. Synthesis of [^{124}I]Iodo-ABT-737, a PET imageable tracer for BCl-2 expression in tumors. **D. Han**, L. Guo, D. S. Maxwell, D. J. Yang, S. T. Lim, I. Samudio, M. Andreeff,

W. G. Bornmann, J. G. Gelovani

106. Improved synthesis of 17β-hydroxy-16α-[^{124}I]iodowortmannin for molecular imaging of PI-3 kinases expression with PET. **D. Han**, L. Guo, D. J. Yang, H. Kurihara, H. H. Yeh, W. G. Bornmann, J. G. Gelovani

107. Synthesis toward the active side chains of avicins and their analogs. **D. Han**, W. G. Bornmann, J. U. Gutterman

108. An improved synthesis of beta-D-galactopyranosyl-(1,4')-2'-deoxy-2'-[18F]-fluoro-beta-D-glucopyranoside for PET imaging of lactose-binding protein expression. **Y. Ying**, L. Guo, P. Ghosh, M. M. Alauddin, W. Bornmann, J. Gelovani

109. STI571 Analogs: 18F- STI571 as potential agents for PET imaging of c-kit expression at a kinase level. **Z. Peng**, W. Bornmann, A. Pal, P. Ghosh, S. T. Lim, J. Gelovani, D. Maxwell, M. M. Alauddin

110. Activity of novel sulfonium-containing bisphosphonates in tumor cell lines: A QSAR analysis. **M. P. Hudock**, Y. Zhang, A. Leon, K. Krysiak, E. Oldfield

111. Development of novel cucurbitacin derivatives through QSAR studies as anticancer candidates. **A. J. Young**, F. T. Halaweish

112. Functionalized bionanocomposites for guided hyperthermic ablation of brain tumors. **E. A. Rozhkova**, X. Liu, T. Rajh, V. Novosad, S. D. Bader, A. J. Rosengart

113. Synthesis and biological activity of 2-amino-4-substitutedanilino-6-substituted phenylmethyl pyrrolo[2,3-*d*]pyrimidines as inhibitors of multiple receptor tyrosine kinases. A. Gangjee, **S. Kurup**, M. Ihnat, D. Green

114. Structure-based drug design of c-kit inhibitors for use in the treatment of acute myeloid leukemia. **D. S. Maxwell**, A. Pal, Z. Peng, A. Shavrin, S. Faderl, D. Harris, Q. Van, Z. Liu, S. Verstovsek, T. Manshouri, A. Ferrajoli, H. Kantarjian, Z. Estrov, W. G. Bornmann

115. Structure-based drug design of c-met inhibitors for use in the treatment of multiple myeloma. **D. S. Maxwell**, Y. Ying, D. Han, Z. Peng, H. Kantarjian, C. Stellrecht, V. Gandhi, W. G. Bornmann

116. 3-Cyclohexylindoles: A new class of inhibitors of 3-phosphoinositide-dependent kinase 1 (PDK1). **K. M. K. Kutterer**, Z. Tang, A. Aplasca, A. Malana, B. Guo, X. Han, K. Arndt, A. Gopalsamy, J. W. Ellingboe

117. SAR of a series of 1H- and 3H-imidazo[4,5]pyridin-2-yl-pyridin-2(1H)-one and 9H-purin-8-yl-pyridin-2(1H)-one inhibitors of IGF-1R Kinase. **C. Ouellet**, F. Beaulieu, M. D. Wittman, K. Zimmermann, J. Carboni, F. Y. Lee, P. Balimane, L. Discenza, A. Greer, A. Li, Z. Yang, J. Banville, A. Martel, R. Attar, M. Gottartis, D. M. Vyas

118. A novel series of low nM JAK2 selective inhibitors exhibit potent in vitro activities with favorable preclinical properties. **C. C. Mak**, J. Cao, C. Chow, R. Fine, J. Hood, X. Kang, B. Klebansky, D. Lohse, A. McPherson, G. Noronha, V. P. Pathak, J. Renick, R. Soll, B. Zeng

119. Design, syntheses and SAR of low nM inhibitors targeting JAK2. **J. Cao**, C. Chow, R. Fine, J. Hood, X. Kang, B. Klebansky, D. Lohse, C. C. Mak, A. McPherson, G. Noronha, V. P. Pathak, J. Renick, R. Soll, B. Zeng

120. Development of novel and potent inhibitors of JAK2: Structure activity relationship studies for optimiziation of JAK2 potency while minimizing JAK3 activity. **A. McPherson**, J. Cao, C. Chow, R. Fine, J. Hood, X. Kang, B. Klebansky, D. Lohse, C. C. Mak, G. Noronha, V. P. Pathak, J. Renick, R. Soll, B. Zeng

121. Development of highly selective Chk-1 inhibitors with low nanomolar cellular activity. **F. A. Diaz**, R. Holcomb, F. Farouz, G. Thorsett

122. Investigation of novel 7,8-disubstituted-5,10-dihydro-dibenzo[b,e][1,4]diazepin-11-ones as potent and selective Chk1 inhibitors. **L. A. Hasvold**, L. Wang, G. M. Sullivan, M. Przytulinska, L. Hexamer, Z. Xiao, Z. Chen, W -Z. Gu, P. Merta, J. Xue, P. Kovar, H. Zhang, J. Bouska, C. Park, T. Sowin, S. Rosenberg, N -H. Lin

123. Investigation of novel 7-substituted and 8-substituted-5,10-dihydro-dibenzo[b,e][1,4]diazepin-11-one based potent, and selective Chk-1 inhibitors. **L. Hexamer**, L. Wang, G. M. Sullivan, M. Przytulinska, Z. Chen, Z. Xiao, W -Z. Gu, J. Xue, M -H. Bui, P. Merta, P. Kovar, J. Bouska, J. Bauch, K. C. Marsh, H. Zhang, T. Sowin, S. H. Rosenberg, N -H. Lin

124. Aza-rebeccamycin analogs as potent Checkpoint kinase 1 inhibitors. **M. Prudhomme**, S. Messaoudi, F. Anizon, B. Pfeiffer, R. M. Golsteyn

125. Synthesis of novel macrocyclic bioreductive alkylating agents. **J. M. Wilson**, D. J. Robins, A. Sutherland

126. Synthesis of bis and trisbenzamidoximes. **J. E. Johnson**, C. Carvallo, N. Sanchez, V. Garza, D. C. Canseco, D. D. Dolliver, G. L. Eggleton, F. R. Fronczek

127. The synthesis of the stable substrate for imaging HSV1-TK expression and its

biological study. **G. An**, K. Lee, H. Rhee

128. Utilization of HPLC to determine a potential interaction between O^6-benzylguanine and cisplatin. **C. A. Rabik**, M. E. Dolan

129. Synthesis of sansalvamide A derivatives: Novel templates as potent anti-tumor agents. **E. K. Singh**, R. Rodriguez, T. J. Styers, P -S. Pan, C -M. Pan, S. Ravula, S. Lapera, J. Cajica, J. D. Brown, E. Parry, S. McAlpine

130. Synthesis of FR235222 derivatives: Novel templates as potent anti-cancer agents. **C -M. Pan**, E. K. Singh, S. Ravula, S. McAlpine

131. The synthesis and structure-activity evaluation of deguelin analogs. Z. Peng, **W. Bornmann**, L. Gao, W -Y. Kim, H -Y. Lee

132. Molecularly engineered specificity in anti-cancer activity. A. Fernández, **Z. Peng**, W. Bornmann, L -B. Gabriel, D. Maxwell

133. Synthesis, in vitro tubulin inhibition and cell cytotoxicity of cyclohexenone derivatives of combretastatin-A4. J. Ruprich, A. Prout, J. Dickson, B. Younglove, H. Mackay, K. Baxi, R. LeBlanc, L. Forrest, H. Holt Jr., P. Hills, S. Mooberry, T. Brown, **M. Lee**

134. Binding of f-PIP and JH-37 to the inverted CCAAT box-2 of the topoisomerase IIα promoter. A. Sielaff, A. Cooper, H. Mackay, T. Brown, C. O'Hare, J. Kluza, M. Kotecha, M. Le, D. Hochhauser, J. A. Hartley, **M. Lee**

135. Discovery of potent EDG4 antagonists as potential anticancer agents. **H. P. Beck**, K. Dai, B. Frank, K. Hasslinger, C. Hedberg, R. Hungate, J. Jaen, T. Kohn, C. Li, L. Liang, J. Medina, S. Rubenstein, R. Schwandner, W. Shen, H. Wesche

136. Synthesis and CYP26A1 inhibitory activity of 1-[benzofuran-2-yl-(4-alkyl/aryl-phenyl)-methyl]-1H-triazoles and amino-benzooxazole derivatives. **S. Pautus**, M. P. Coogan, C. Simons

137. Synthesis of substituted stilbenes and benzanilides as therapeutics for cancer. **M. I. Noce**, J. J. Heynekamp, L. A. Hunsaker, L. M. Deck, D. L. Vander Jagt

138. Design and synthesis of PEG-containing CC-1065 analogs for targeted therapy of cancer. **R. Y. Zhao**, D. Sun, E. Cavanagh, M. Miller, B. Leece, H. Erickson, R. Singh, Y. Kovtun, V. Goldmacher, R. Chari

139. Synthesis and biological evaluation of novel T-type calcium channel blockers. **H. N.**

Seo, J. Y. Choi, H. Rhim, A. N. Pae, D. J. Choo, J. Y. Lee

140. Anti-cancer activities of 3,4-dihydroquinazoline derivatives as T-type calcium channel blockers. **J. Y. Choi**, H. N. Seo, M. J. Lee, H. Rhim, D. J. Choo, J. Y. Lee

141. Enhancement of the anticancer activity of cladribine by application of the phosphoramidate protide approach. **R. Valente**, C. Congiatu, E. Walsby, K. Mills, C. McGuigan

142. Synthesis of isoprenoid bisphosphonate isomers and their impact on protein geranylgeranylation. **J. S. Yu**, A. J. Wiemer, K. M. Lamb, R. J. Hohl, D. F. Wiemer

143. A new versatile photoactivable probe designed to investigate the diphosphate binding site of enzymes using isoprenoid diphosphates as substrates. **O. Henry**, M. D. Distefano

144. Synthesis of deuterium-labeled isoprenoids. **M. W. Amolins**, R. A. Gibbs, A. Placzek

145. Synthesis and evaluation of peptide analogs designed to disrupt the interaction between Cdc42 and RhoGDI. **J. W. Wollack**, D. G. Mullen, N. A. Zeliadt, E. V. Wattenberg, M. D. Distefano

146. Insight into the structural requirements of farnesyltransferase inhibitors based on 3-D QSAR CoMFA and CoMSIA models. **D. S. Puntambekar**, R. Giridhar, M. R. Yadav

147. Imidazole-containing farnesyltransferase inhibitors: 3-D quantitative structure-activity relationship and molecular docking studies. **A. Xie**, S. Odde, P. Sivaprakasam, R. J. Doerksen

148. Development of peptide signaling pathway..antagonists and agonists of the TGF-β **L. Li**, A. P. Hinck, F. M. Hoffmann, L. L. Kiessling

149. Discovery and SAR of A-620223, a potent and efficacious inhibitor of poly(ADP-ribose) polymerase for the treatment of cancer. **G -D. Zhu**, V. B. Gandhi, J. Gong, S. Thomas, W. Lubisch, R. Grandel, W. Wernet, Y. Luo, X. Liu, Y. Shi, V. Klinghofer, E. F. Johnson, D. Frost, J. Bouska, K. C. Marsh, C. Park, S. H. Rosenberg, V. L. Giranda, T. D. Penning

150. Synthesis and SAR of novel, potent and orally bioavailable benzimidazole inhibitors of Poly(ADP-ribose) Polymerase (PARP) with a quaternary methylene-amino substituent. **V. B. Gandhi**, J. Gong, S. Thomas, Y. Luo, X. Liu, Y. Shi, V. Klinghofer, E. F. Johnson, D. Frost, C. Donawho, J. Bouska, C. Park, S. H. Rosenberg, V. Giranda, T.

D. Penning, G -D. Zhu

151. Mutual prodrugs of all-trans retinoic acid and histone deacetylase inhibitors: Potent anticancer agents. **L. K. Gediya**, A. Khandelwal, J. Mehta, P. Purushottamachar, V. C. O. Njar

152. In vitro characterization of cryptophycin epoxidase. **Y. Ding**, Z. Q. Beck, W. H. Seufert, D. H. Sherman

153. G-quadruplex binding agents: 2-Carboxy-4-hydroxybenzo-(h)-quinoline derivatives. **H. Paritala**, S. M. Firestine

154. Structure-activity relationships of mono-methyl derivatives of quercetin on HSP70 production and HSP27 phosphorylation. **R. Wang**, C. Hunt, J -S. Taylor

155. Chimeric macrocycles as novel Hsp90 inhibitors. **N. Ortuzar**, B. S. J. Blagg

156. Structure-activity relationships of conformationally-biased chimeric inhibitors of Hsp90. **M. K. Hadden**, S. Apte, B. S. J. Blagg

157. Novobiocin: A bidirectional approach toward cytotoxic inhibitors of Hsp90. **J. A. Burlison**, D. J. Lubbers, C. Avila, J. Holzbeierlein, B. Blagg

158. Semi-synthesis and biologically activity of camptothecin tripartate conjugates. **C. Samorì**, A. Battaglia, A. Guerrini, G. Varchi, G. L. Beretta, F. Zunino, G. Fontana, E. Bombardelli

159. Semi-synthesis and biologically activity studies of 16a-thio-camptothecins. **G. Fontana**, C. Samorì, A. Battaglia, G. Varchi, G. L. Beretta, F. Zunino, G. Bifulco, E. Bombardelli

160. Semi-synthesis and biologically activity studies of C-ring modified camptothecins and 16a-thio-camptothecins. **G. Varchi**, A. Battaglia, C. Samorì, A. Guerrini, G. L. Beretta, F. Zunino, G. Fontana, E. Bombardelli

161. Psoralen conjugates for visualization of localized genomic interstrand crosslinks. **A. Kalliat Thazhathveetil**, S -T. Liu, F. E. Indig, M. M. Seidman

162. Synthesis and anticancer properties of novel pyranopyridones. **J. D. Bettale**, M. A. Ogasawara, M. Manpadi, E. M. Elias, S. Rogelj, S. T. Shors, P. Y. Uglinskii, N. M. Evdokimov, I. V. Magedov, A. Kornienko

163. Synthesis and radiolabeling of SAHA analog for radio Imaging of HDAC expression-

occupancy in tumors during molecular-targeted therapy of cancer. **A. Pal**, H. Kurihara, Z. Peng, D. J. Yang, W. Bornmann, J. Gelovani

164. Net charge is not the primary determinant of onconase cytotoxicity. **R. F. Turcotte**, R. T. Raines

165. Natural defense against cancer: Computational analysis of the role of the key residues of formamido-pyrimidine DNA glycosylase in lesion recognition. **K. Song**, C. De los santos, A. P. Grollman, C. Simmerling

166. 1-Azolyl-4-phenyl-2-butanones as heme oxygenase inhibitors: Probing for various azoles as pharmacophores. **G. Roman**, R. T. Kinobe, K. Nakatsu, W. A. Szarek

167. Structure-based design and evaluation of peptide and peptido-mimetic antagonists of Survivin. **S. A. Kawamoto**

168. Targeted degradation of aryl hydrocarbon receptor via the PROTAC approach: A chemical genetic tool for AHR biology. **H. Lee**, D. Puppala, E -Y. Choi, H. I. Swanson, K -B. Kim

169. 2-Amino-4-methyl-5-phenylethyl substituted-7-*N*-benzyl-pyrrolo[2,3-*d*]pyrimidines as novel antitumor antimitotic agents that also reverse tumor resistance. A. Gangjee, **O. A. Namjoshi**, S. N. Keller, C. D. Smith

170. Cytotoxicity of Parthenolide Analogs against Leukemia Cells in vitro. **S. Nasim**, P. A. Crooks

171. Polyamine/transition metal complexes as potential antitumor agents. **H. Amunugama**, A. Hirata, F. Hirata, R. A. Casero, A. M. Angeles-Boza, K. R. Dunbar, J -G. Delcros, P. M. Woster

172. Probing the mechanism of 3-deoxyschweinfurthin B anticancer activity via fluorescence microscopy. **J. D. Neighbors**, C. H. Kuder, R. J. Hohl, D. F. Wiemer

173. Effects of C-ring substitution on the pharmacophore of the schweinfurthins. **M. P. Callahan**, J. D. Neighbors, D. F. Wiemer

174. Differential thermal denaturation profiles of structurally diverse DNA aptamers. **B. D. Jeanfreau**, G. R. Bishop

175. Correlating temperature-dependent fluorescence emission and circular dichroism spectra. **J. A. James**, G. R. Bishop

176. Statistical mechanical models for analyzing the stabilities of drug-DNA complexes. **A. C. Holley**, G. R. Bishop

177. Method development for the determination of the molar absorbance properties of DNA aptamers. **H. K. Goel**, G. R. Bishop

178. Effects of ion binding and solution pH on the molar absorbance properties of DNA aptamers. **S. O. Gibson**, G. R. Bishop

179. Energetic signatures for induced-fit binding modes in structurally diverse DNA aptamers. **B. C. Polander**, G. R. Bishop

180. Highly regioselective synthesis of 5-fluorouridine ester derivatives catalyzed by Lipozyme TL IM in organic media. H. Wang, W -Y. Lou, H. Wu, **M -H. Zong**

181. Novel analogs of Atiprimod for targeting multiple myeloma. **A. Kazimierski**, K. Shailubhai, D. Picker, W. Priebe

182. Synthesis of ageladine A, analogs and their biological screening. **S. R. Shengule**, P. Karuso

183. Tandem enzymatic syntheses of TDP-deoxysugars and spinosyn analogs by in vitro recombination of natural product biosynthetic pathways. **H -T. Chiu**, Y -L. Chen, C. C. Wu

184. Free radical chemistry of tobacco-specific nitrosamines. **C. R. Cox**, J. J. Kiddle, S. P. Mezyk

185. Reaction of nitrosamines with biologically important free radicals under anaerobic and aerobic conditions. **J. J. Kiddle**, S. P. Mezyk, K. P. Madden

186. *In silico* design of effective inhibitors for α-tubulin. **K. Diraviyam**, D. Sept

187. A combinatorial study of group 3 and lanthanide based polymer supported Lewis acids. **P. A. Boguszewski**

188. A scaleable route to a polymer supported hypervalent iodine (V) oxidant. **P. A. Boguszewski**, M. J. I. Williamson

189. Advanced topics for use of RediSep® specialty media columns in flash chromatography. **V. D. Thomason**, V. Williams

190. Analytical automation batch design for pharmacokinetic studies. **B -L. Wan**, K. D.

Anderson

191. Novel approach for drug delivery: "Trojan" dendrimers. **J. A. Valencia-Gallegos**, M. M. Alvarez, P. Arce

192. Approaches to precision-guided nanoparticles: Focus on linker and targeting molecule design and synthesis. **R. N. Hanson**, J. A. Hendricks, K. Bailey

193. Asymmetric reduction of ketones with the spiroborate ester derived from diphenyl prolinol and ethylene glycol. **M. De Jesus**, W. Correa, V. Stepanenko, I. Guzman, W. de la Cruz, M. Ortiz, L. Ortiz, C. Vazquez

194. Biological implications of the environmental effects on tryptophan-singlet oxygen interaction. C. L. Jones, **K. N. Grier**

195. Chemical constituents of Calorhyllum membranaceum Gardn. **X. Song**, C. Han

196. Chemical constituents of the stem of Artabotrys hainanensis. C. Han, **X. Song**

197. Computational investigation on the reductive amination of pharmacologically important triquinanes. **W. J. Geldenhuys**, L -M. Bezuidenhout, S. F. Malan, C. J. Van der Schyf

198. Conformational features of substituted cyclopropanes in drug-like molecules: A brief guide for medicinal chemists. **D. L. Cheney**, J. X. Qiao

199. Controlled rate drug delivery systems: Effect of non-Fick diffusion - response to a pulse injection. **K. R. Sharma**

200. Design and synthesis of novel Xylosides as glycosaminoglycan primers. **M. Ethirajan**, X. Victor, V. Tran, K. Nguyen, K. Balagurunathan

201. Design and synthesis of ä-sugar amino acids as inhibitors of protein-protein interactions. **S. K. Mamidyala**, J. Baltz, D. Coen, S. M. Firestine

202. Synthesis and bioactivity of sulfonamide chalcones. D. H. Murray, **L. Lange**, **A. Matak**

203. 17-Arylcarbamidomethyl-4-azasteroids as selective androgen receptor modulators. **W. P. Dankulich**, H. J. Mitchell, G. D. Hartman, R. S. Meissner

MONDAY MORNING

Section A

Unknown Site -- Unknown Room

Drugs from Academia: Marketed Drugs Discovered in Academic Labs

J. E. Macor, *Organizer, Presiding*
9:00 —204. Invention of SAHA, the first HDAC inhibitor approved by the FDA. **R. Breslow**

9:40 —205. Darunavir, a new protease inhibitor to combat drug-resistance: Structure-based design targeting protein backbone. **A. K. Ghosh**

10:20 —206. The discovery and development of 3'-heteranucleosides. **D. C. Liotta**

11:00 —207. Discovery of Alimta, a broadly effective new antitumor agent. **E. C. Taylor**

11:40 —208. The taxol story. **R. A. Holton**

Section B

Unknown Site -- Unknown Room

Kinesin Spindle Protein Inhibitors

C. Cox and R. M. Garbaccio, *Organizers, Presiding*
9:00 — Introductory Remarks.

9:05 —209. Targeting kinesin spindle protein (KSP) for the treatment of cancer. **K. W. Wood**

9:40 —210. Examining the chemical inhibition and microscopic properties of kinesin-5. **T. M. Kapoor**

10:15 —211. Discovery and optimization of kinesin spindle protein (KSP) inhibitors. **C. D. Cox**, P. J. Coleman, M. E. Fraley, R. M. Garbaccio, M. J. Breslin, D. B. Whitman, J. D. Schreier, G. D. Hartman, M. Torrent, R. Lobell, C. Buser, W. Tao, H. Huber, N. E. Kohl, Y. Yan, L. C. Kuo

10:50 —212. Discovery of novel heterocyclic inhibitors of kinesin spindle protein (KSP). **X. S. Qian**, A. I. McDonald, H -J. Zhou, B. Yao, L. W. Ashcraft, J. K. Huang, M. V. Marin, C. E. Aroyan, K. W. Wood, D. J. Morgans Jr., G. Bergnes

11:25 —213. Dihydropyrimidones induce mitotic arrest and a monoastral phenotype consistent with inhibition of the mitotic kinesin Eg5 in cultured cells. **L. J. Lombardo**

MONDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Ligands for the Glucocorticoid Receptor

S. McDonald and R. P. Trump, *Organizers, Presiding*
1:30 —214. Introduction to the glucocorticoid receptor and modeling studies. **E. L. Stewart**, K. Biggadike

1:50 —215. Nonsteroidal glucocorticoid receptor modulators for use in inflammation and oncology. **R. I. Higuchi**, R. J. Ardecky, S. L. Roach, A. R. Hudson, D. P. Phillips, J. S. Tyhonas, D. S. Karanewsky, K. B. Marschke, F. J. López, E. G. Vajda, D. K. Rungta, E. A. Kallel, R. P. Bissonette, W. W. Lamph, J. Rosen, L. Zhi, A. Negro-Vilar, J. N. Miner

2:20 —216. Non-steroidal GR agonists: Improving the established drugs? **H. Rehwinkel**, H. Schaecke, K. Asadullah, S. Baeurle, M. Berger, W -D. Doecke, H. Hennekes, S. Jaroch, K. Krolikiewicz, M. Lehmann, A. Mengel, R. Neuhaus, D. Nguyen, L. Roese, A. Rotgeri, N. Schmees, A. Schottelius, W. Skuballa, P. Strehlke

2:50 —217. Identification and optimization of non-steroidal glucocorticoid receptor agonists. **D. S. Thomson**

3:20 —218. A design and iterative approach to non-steroidal and steroidal agonists. K. Biggadike, **D. M. Coe**, I. M. Mclay

4:00 —219. Discovery of novel, selective glucocorticoid receptor modulators. **A. Ali**, C. F. Thompson, J. Balkovec, D. Graham, M. Greenlee, M. L. Hammond, N. Quraishi, G. Rouen, C. Smith, J. R. Tata, G. Taylor, M. Einstein, L. Ge, G. Harris, T. M. Kelly, P. Mazur, S. Pandit, J. Santoro, A. Sitlani, C. Wang, J. Williamson, D. F. Miller, E. A. O'Neill, C. M. Thompson, D. M. Zaller, M. J. Forrest, E. Carballo-Jane, S. Luell, D. Visco, C. Rasa, K. Lowitz

4:30 —220. Azadecalin as a scaffold for selective glucocorticoid receptor antagonists. R. D. Clark, N. C. Ray, **H. J. Hunt**, D. E. Clark, K. Williams, P. Blaney, C. Hurley, R. Devos, M. Wong, J. K. Belanoff

Undergraduate Research Poster Session: Medicinal

Sponsored by CHED, Cosponsored with SOCED, and MEDI

MONDAY EVENING

Section A

Unknown Site -- Unknown Room

Sci-Mix

D. P. Rotella, *Presiding*
7:00 - 9:00
27, 35-36, 44, 53, 59, 66, 73, 76, 85, 89, 99, 103, 105, 113, 118, 127, 129, 138, 142, 146, 151, 156, 159, 162, 167, 180, 183, 186, 189, 192, 198. See previous listings.
287-288, 304-305, 311, 321, 328, 332, 334, 338, 347, 349, 356, 360, 366, 368-369, 372-374, 378, 395, 397, 407-408, 416-417, 425, 430, 433, 440, 443. See subsequent listings.

TUESDAY MORNING

Section B

Unknown Site -- Unknown Room

Mechanistic Approaches to Increasing High Density Lipoprotein Cholesterol

Cosponsored with Wyeth Research
H. Elokdah and S. D. Larsen, *Organizers, Presiding*
8:30 —221. Introduction to mechanistic approaches to increasing high density lipoprotein cholesterol. **G. P. Vlasuk**

8:45 —222. Azepine inhibitors of plasma cholesteryl ester transfer protein. **N. B. Mantlo**, T. Fields, X. Wang, M -C. Fernandez, A. I. Mateo, A. Escribano, E. M. M. de la Nava, S. Parthasarathy, M. W. Giese, M. Carson, T. P. Beyer, S. L. Cockerham, G. Cao, K. Kovach, S. Sweetana, A. Borel, T. M. Jones, E. A. Cannady, C. Cioffe, X. Chen, S. Dinn

9:25 —223. Inhibitors of endothelial and hepatic lipases: Development and challenges. **M. Mosior**, H -S. Lin, P. Eacho, P. Foxworthy, M. E. Richett, R. W. Harper, J. E. Lopez, B. Chao, M. L. Chouinard

10:05 —224. Niacin receptor agonists. **G. Semple**

10:45 —225. New steroidal mimetics as novel LXR modulators. **M. M. Abelman**, R. H. Jiang, B. Joshi, J. Chisholm, J. Hao, N. Chu, N. Mollova, K. Leung, R. Lawn, J. A. Zablocki

11:25 —226. Structure based design of nuclear receptor hormone ligands: Potent quinoline-based liver X receptor (LXR) agonists. **R. L. Magolda**

TUESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Emerging Targets for the Treatment of Type-2 Diabetes

G. Bebernitz and P. T. Cheng, *Organizers, Presiding*

1:30 —227. Discovery and biological evaluation of a novel, potent and selective series of ACC2 inhibitors. **Y. G. Gu**, M. Weitzberg, R. F. Clark, X. Xu, Q. Li, T. Zhang, T. M. Hansen, R. F. Keyes, G. Liu, Z. Xin, X. Wang, R. Wang, T. McNally, B. A. Zinker, B. W. Dickinson, N. L. Lubbers, Y. Yang, D. W. A. Beno, D. L. Widomski, J. F. Waring, S. L. Carroll, C. H. Healan-Greenberg, E. A. Blomme, E. U. Frevert, B. A. Beutel, H. L. Sham, H. S. Camp

2:05 —228. Discovery of potent and selective 11ß-HSD-1 inhibitors. **W. Yao**, J. Zhuo, C. Zhang, M. Xu, D. Qian, D. Burns, C. He, Y. Li, E. Shi, Q. Lin, L. Chen, C. Agrios, L. Weng, Y. Li, R. Huber, P. Scherle, S. Diamond, D. Hunter, M. Covington, C. Marando, R. Wynn, K. Katiyar, N. Contel, K. Vaddi, S. Yeleswaram, G. Hollis, S. Friedman, B. Metcalf

2:40 —229. Bicyclo[2.2.2]octyltriazole inhibitors of 11beta-HSD1 are efficacious in animal models of metabolic disease. **S. T. Waddell**, M. Maletic, G. Santorelli, A. Leeman, D. Graham, J. M. Balkovec

3:15 —230. Design and synthesis of novel glucokinase activators as potential treatments for type 2 diabetes. **D. McKerrecher**, J. V. Allen, P. W. R. Caulkett, C. S. Donald, M. L. Fenwick, E. Grange, K. M. Johnson, C. Johnstone, C. D. Jones, K. G. Pike, J. W. Rayner, R. P. Walker

3:50 —231. Discovery and SAR studies of thienopyridones: A class of small molecule AMPK activators. **R. R. Iyengar**, G. Zhao, A. S. Judd, L. Kifle, N. Cao, W. J. Chiou, B. L. Cool, H. S. Camp, E. U. Frevert, T. M. Turner, K. C. Marsh, J. Liu, A. Mika, M. A. Perham, B. A. Zinker, H. L. Sham, P. R. Kym

4:25 —232. Stearoyl-CoA desaturase-1 inhibitors: Discovery and in vivo evaluation. **G. Liu**, Z. Xin, H. Zhao, M. D. Serby, H. T. Smith, N. Cao, T. K. Surowy, A. Adler, A. Mika, T. B. Farb, C. Keegan, K. Landschulz, M. Brune, C. A. Collins, H. L. Sham, H. S. Camp

Section B

Unknown Site -- Unknown Room

General Oral Session

Cosponsored with Advanced Chemistry Development
D. P. Rotella, *Organizer, Presiding*
1:30 —233. SSA-426: A combined SSRI/5-HT1A antagonist for the treatment of depression. **G. Stack**, M. Tran, B. Harrison, J. Gross, G. E. M. Husbands, D. A. Evrard, S. Rosenzweig-Lipson, L. A. Dawson, H. Q. Nguyen, T. Spangler, D. Smith, G. Hornby, R. Scerni, H. Gao, S. Kalgaonkar, G. Zhang, M. Abou-Gharbia, C. Kim, L. Schechter, T. Andree

1:50 —234. Aminohydantoins as highly potent, selective and orally active BACE1 inhibitors. **M. S. Malamas**, J. Erdei, I. Gunawan, N. Pawel, M. Chlenov, A. J. Robichaud, J. Turner, Y. Hu, E. Wagner, S. Aschmies, T. Comery, L. Di, K. Fan, R. Chopra, A. Oganesian, C. Huselton, J. Bard

2:10 —235. Gamma-lactam diaminopropane inhibitors of BACE. **K. M. Boy**, J. M. Guernon, J. Shi, C. Zheng, A. Liauw, J. J. Bronson, J. E. Macor, A. P. Combs, G. Trainor, C. P. Decicco, A. Good, A. J. Tebben, J. H. Toyn, C. R. Burton, D. M. Barten, J. Marcinkeviciene, R. A. Copeland, J. K. Muckelbauer, P. E. Morin, K. Lentz, C. Albright, L. A. Thompson III

2:30 —236. DG-051: A novel leukotriene A4 hydrolase inhibitor for the treatment of myocardial infarction and stroke. **V. Sandanayaka**, B. Mamat, P. Yu, L. Zhao, L. Bedell, N. Bhagat, J. Winger, M. Keyvan, B. Bock, M. Krohn, P. Chandrasekar, X. Mo, L -M. Zhou, R. Mishra, E. Onua, J. Zhang, M. Þorsteinsdóttir, G. Halldórsdóttir, H. Sigþórsdóttir, M. Friedman, D. Zembower, Þ. Andrésson, J. Singh, M. Gurney

2:50 —237. Discovery of peliglitazar, a potent oxybenzylglycine dual PPARα/γ activator with \efficacious glucose and lipid-lowering activities. **S. Chen**, F. Qu, P. Devasthale, Z. Lai, C. Shao, W. Wang, S. Wu, H. Zhang, D. Farrelly, L. Moore, L. Gu, W. Sun, N. Flynn, T. Harrity, M. Cap, L. Kunselman, A. Peters, K. Locke, J. Lippy, L. Zhang, G. Chandrasena, V. Hosagrahara, P. Kadiyala, J. Muckelbauer, C. Chen, Y. An, A. Doweyko, D. Ryono, S. A. Biller, J. Wetterau, N. Hariharan, P. T. W. Cheng

3:10 —238. Discovery of HCV-796: A potent and orally bioavailable hepatitis-C polymerase inhibitor under clinical development. **A. K. Saha**, C. Young, A. M. Del Vecchio, T. A. Bailey, J. A. Reinhardt, B. A. Kulkarni, T. H. Faitg, H. Feng, S. R. Rippin, C. W. Blackledge, D. J. Rys, T. A. Lessen, J. Swestock, Y. Deng, T. J. Nitz, S. Chunduru, R. Chopra, M. Collett, D. Pevear, A. Y. M. Howe, J. O'Connell, T. Mansour, C. J. Burns

3:30 —239. Discovery and SAR of ABT-888, an inhibitor of poly(ADP-ribose) polymerase (PARP) for the treatment of cancer. **G -D. Zhu**, J. Gong, V. B. Gandhi, Y. Luo, X. Liu, Y. Shi, V. Klinghofer, E. F. Johnson, D. Frost, C. Donawho, L. Rodriguez, G. Bukofzer, K. Jarvis, J. Bouska, A. Olson, K. C. Marsh, C. Park, S. Rosenberg, V. L. Giranda, T. D. Penning

3:50 —240. SAR of 3-(6-(piperidin-4-yl)-1H-benzo[d]imidazol-2-yl)pyridin-2(1H)-ones as inhibitors of the insulin-like growth factor-1-receptor (IGF-1R) with broad spectrum in vivo activity. **U. Velaparthi**, M. D. Wittman, P. Liu, M. G. Saulnier, K. Zimmermann, J. Carboni, F. Y. Lee, Z. Yang, D. B. Frennesson, X. Sang, L. Aixin, P. Balimane, D. R. Langley, R. Attar, M. Gottardis, D. M. Vyas

4:10 —241. Discovery of trisubstituted cyclohexanes as a new class of CCR2 antagonists. **R. J. Cherney**, R. Mo, D. T. Meyer, D. J. Nelson, Y. C. Lo, G. Yang, P. A. Scherle, S. Mandlekar, Z. R. Wasserman, H. Jezak, K. A. Solomon, A. J. Tebben, P. H. Carter, C. P. Decicco

4:30 —242. Neohexyl derivatives of B-ring alkylaminobenzothiadiazine inhibitors of HCV NS5B polymerase. **J. T. Randolph**, P. P. Huang, D. K. Hutchinson, L. L. Klein, D. A. Montgomery, S. V. Masse, W. M. Kati, D. Beno, D. J. Kempf

WEDNESDAY MORNING

Section A

Unknown Site -- Unknown Room

E. B. Hershberg Award for Important Discoveries in Medicinally Active Products: Estrogen Receptor Beta Symposium in Honor of John A. Katzenellenbogen

Cosponsored with Eli Lilly
B. H. Norman, *Organizer, Presiding*
9:00 — Introductory Remarks.

9:10 —243. Award Address (E. B. Hershberg Award for Important Discoveries in Medicinally Active Products, sponsored by Schering-Plough Corporation). Estrogen receptors: Tools, travails, and triumphs in estrogen receptor biology, pharmacology and imaging. **J. A. Katzenellenbogen**

9:50 —244. Structure-based design, synthesis, and evaluation of benzopyrans as selective estrogen receptor-beta agonists for the treatment of benign prostatic hyperplasia. **T. I. Richardson**, J. Shah, B. H. Norman, J. S. Kroin, E. M. Thomas, J. A. Dodge, C. W. Lugar, S. A. Jones, L. A. Pfeifer, P. S. Borromeo, G. L. Durst, Y. Y. Wang, J. D. Durbin, C. Montrose-Rafizadeh, R. J. Barr, H. E. Osborne, R. M. Amos, K. Chen, V. Krishnan

10:25 —245. Estrogen receptor-beta in the central nervous system. **I. Merchenthaler**

11:00 —246. 8β-Substituted estratrienes as ERβ selective ligands. **O. Peters**, N. Bräuer, P. Droescher, P. Muhn, K. Prelle, K -H. Fritzemeier

11:35 —247. Design and synthesis of selective estrogen receptor β agonists as potential anti-inflammatory agents. **R. E. Mewshaw**, M. S. Malamas, A. T. Vu, E. Manas, S. M. Opal, J. C. Keith Jr., H. A. Harris

Section B

Unknown Site -- Unknown Room

High Throughput Screening and Drug Discovery

Cosponsored with CINF
J. K. Padia, *Organizer, Presiding*
9:00 —248. Effective biological assay support for medicinal chemists. **Y. Li**

9:40 —249. Use of BacMam transient expression technology to support HTS and profiling of compounds targeting G protein-coupled receptors. **Z. Wu**

10:20 —250. Discovery of novel inhibitors of methionine aminopeptidase by HTS. **Q -Z. Ye**

11:00 —251. Application of a quantitative HTS approach for accelerating Hit-to-Lead process in discovery of glucocerebrosidase inhibitors. **W. Zheng**, J. K. Padia

11:40 —252. Molecular profiles in drug discovery: Using pathway signatures to indentify Inhibitors of the Beta-catenin and Aurora pathways. **S. K. Horrigan**

Advanced Mining and Use of Life Science Information

Sponsored by CINF, Cosponsored with CSA Trust, BIOT, BTEC, MEDI, and COMP

WEDNESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

ACS Award for Team Innovation: New Approaches to Confront Antibacterial Resistance Symposium in Honor of Steven J. Brickner, Michael R. Barbachyn, Douglas K. Hutchinson, and Peter R. Manninen

S. F. Singleton and B. S. J. Blagg, *Organizers, Presiding*
1:30 —253. Evolution and inhibition of antibiotic resistance. **F. Romesberg**

2:10 —254. Small molecule inhibitors of bacterial MarA (AraC) transcriptional factors which prevent bacterial infection. **O. K. Kim**, L. K. Garrity-Ryan, J. C. Mecsas, S. B. Levy

2:50 —255. Bacterial efflux pumps: Implications in antibiotic discovery and development of novel inhibitors as potentiators of existing antimicrobial agents. **M. N. Dudley**, O. Lomovskaya

3:30 —256. DNA repair, a novel target of antibiotics: Peptides and small molecules that bind Holliday junctions. **A. M. Segall**, J. L. Boldt, G. D. Cassell, C. W. Gunderson, K. V. Kepple, I. Naili, N. Patel, N. Radosevich, L. Su

4:10 —257. Award Address (ACS Award for Team Innovation, sponsored by ACS Corporation Associates). Zyvox® (linezolid), the first member of a completely new class of antibacterial agents for treatment of serious gram-positive infections. **S. J. Brickner**, M. R. Barbachyn, D. K. Hutchinson, P. R. Manninen

Section B

Unknown Site -- Unknown Room

Medicinal Chemistry of Ion Channels/Voltage-Gated Channels and Pain

N. Tamayo and M. L. Brown, *Organizers, Presiding*
1:30 —258. Regulation of N-type calcium channels in the pain pathway. **G. W. Zamponi**

2:05 —259. Ion channel assay technologies. **O. McManus**

2:40 —260. Structural dynamics of voltage-dependent ion channels. **E. Perozo**

3:15 —261. Piperazine surrogates, a novel class of calcium channel blockers. **H.**

Pajouhesh

3:50 —262. Voltage-gated sodium channel blockers for the treatment of neuropathic pain. **P. K. Chakravarty**

4:25 —263. Structure-activity relationships and in vivo profiles of amino acid ligands for the α2δ subunit of voltage-gated calcium channels. **K. H. Mortell**, D. J. Anderson, J. J. Lynch III, C -H. Lee, M. Gopalakrishnan

WEDNESDAY EVENING

Section A

Unknown Site -- Unknown Room

General Poster Session

Cosponsored with Nature Reviews Drug Discovery
D. P. Rotella, *Organizer*
7:00 - 9:00
264. Design, synthesis, and evaluation of novel peptidomimetics. **J. P. Cain**, A. V. Mayorov, M. Cai, E. S. Palmer, B. Tan, K. B. Chandler, T. Yamamoto, P. Nair, S. Wallace, G. N. Ortiz, H. Wang, G. Santarelli, Y. S. Lee, R. R. Petrov, J. M. Ndungu, D. Trivedi, V. J. Hruby

265. Modeling study of the binding modes of mono- and dinucleotides at the human $P2Y_2$ receptor. **A. A. Ivanov**, K. A. Jacobson

266. How does dopamine transporter (DAT) reuptake dopamine: Insights from molecular modeling and molecular dynamics simulations. **X. Huang**, C -G. Zhan

267. Synthesis and evaluation of quinuclidine incorporated lobelane analogs as vesicular monoamine transporter ligand. **G. Zheng**, L. P. Dwoskin, A. G. Deaciuc, P. A. Crooks

268. Design and synthesis of lobelane analogs targeting the vesicular monoamine transporter (VMAT2) as a potential treatment for methamphetamine abuse. **J. P. Culver**, A. G. Deaciuc, L. P. Dwoskin, P. A. Crooks

269. Computational neural network analysis of the affinity of lobeline and tetrabenazine analogs for the vesicular monoamine transporter-2. **F. Zheng**, G. Zheng, A. G. Deaciuc, C -G. Zhan, L. P. Dwoskin, P. A. Crooks

270. Synthesis and biological activity of meperidine analogs as selective serotonin reuptake inhibitors. **X. Gu**, S. Izenwasser, M. L. Trudell

271. Synthesis and biological evaluation of 3-aryl-3-arylmethoxytropane derivatives at monoamine transporters. **H. Kaur**, S. Izenwasser, M. L. Trudell

272. Synthesis and biological activity at monoamine transporters of 3-[2-(diarylmethoxyethylidenyl)]-N-substituted tropane and azetidine analogs. **S. A. Cararas**, S. Izenwasser, M. L. Trudell

273. Structure activity relationship study of cis-(6-benzhydryl-piperidin-3-yl)-benzyl-amine and its constrained counterpart 1,4-diazabicyclo[3.3.1]nonane derivatives: Study on influence of exocyclic hydroxyl function on affinity for monoamine transporters. **M. Mishra**, R. Kolhatkar, J. Zhen, M. Reith, A. Dutta

274. Synthesis and SAR evaluation of lactam-fused chroman derivatives having dual affinity at serotonin 5-HT1A receptor and serotonin transporter. **Z. Shen**, N. T. Hatzenbuhler, D. A. Evrard, M. Chlenov, B. L. Harrison, R. L. Magolda, M. Abou-Gharbia, G. Hornby, D. L. Smith, K. M. Sullivan, L. E. Schechter, T. H. Andree, P. S. Ramamoorthy

275. Exploring the structural requirements for potency and selectivity exhibited by novel asymmetric tetrahydropyran inhibitors of SERT and NET using 3-D QSAR CoMFA method. **P. S. Kharkar**, M. Reith, A. Dutta

276. Novel concept of chromatography applied to screen the interaction between drugs and monoamine oxidase. **P. Ma**, **S. Wang**, **F. Qu**, **Y. Deng**

277. A new discovery platform for novel CNS therapeutics with potential to alter disease progression. **H. A. Behanna**, S. M. Roy, L. Munoz, W. Hu, L. K. Wing, H. Ralay Ranaivo, L. Guo, L. Van Eldik, D. M. Watterson

278. Synthesis of heterocycle-based selective inhibitors of neuronal nitric oxide synthase with improved pharmacokinetic properties. **G. R. Lawton**, H. Ji, R. B. Silverman

279. Design and synthesis of propofol analogs as new anesthetic agents. **I. M. Maciagiewicz**, K. S. Bruzik, A. J. Hopfinger, A. Jenkins, N. Harrison

280. Sulfamides as new target for anconvulsant drugs: Design, synthesis and evaluation. **L. Gavernet**, I. A. Barrios, J. E. Elvira, M. Sella Cravero, G. A. Samaja, V. Pastore, L. E. Bruno Blanch

281. Block of cyclic nucleotide-gated channels by tetracaine derivatives: Role of apolar interactions at two distinct locations. **S. R. Kirk**, T. Strassmaier, J. W. Karpen

282. Synthesis of cyclopropanated carbohydrates for employment as antiepileptic drugs. **J. Talisman**, C. H. Marzabadi

283. Modeling evolution of hydrogen bonding and stabilization of transition states in the process of cocaine hydrolysis catalyzed by human butyrylcholinesterase. **D. Gao**, C -G. Zhan

284. Synthesis and pharmacological evaluation of some quinoline derivatives as potential antiamnesic agents. **P. Piplani**, A. Rani, R. Sandhir, S. K. Kulkarni

285. Synthesis of a carbon-11 labeled conformationally restricted rivastigmine analog for PET imaging of heart enzymes AChE and BChE. **M. Wang**, J -Q. Wang, M. Gao, Q -H. Zheng

286. Discovery of long acting inhaled muscarinic M3 receptor antagonists. **U. Baettig**, S. Collingwood, D. Janus, N. Devereux, E. Stanley, B. Cox, C. McCarthy, S. Charlton, J. Leighton-Davis, J. R. Fozard, F. Baur, D. Farr, L. Mazzoni, V. Patel

287. The effect of anesthetic molecule binding on neuronal nicotinic and GABA receptor model dynamics, gating mechanisms and open receptor states. **R. J. Law**, F. C. Lightstone

288. The mechanism of K+ ion pumping and double gating elucidated by simulations and mutagenesis experiments on the gastric H,K-ATPase. **R. J. Law**, K. Munson, G. Sachs, F. C. Lightstone

289. Synthesis and initial evaluation of novel dipyridyl derivatives as potential radioligands for imaging of the nicotinic acetylcholine receptors by positron-emission tomography (PET). **Y. Gao**, H. T. Ravert, D. P. Holt, J. Hilton, C. Endres, M. Alexander, A. Kumar, M. G. Pomper, A. Rahmim, H. Kuwabara, D. F. Wong, R. F. Dannals, A. G. Horti

290. Subtype-selective agonists binding with a4b2 and a7 nicotinic acetylcholine receptors: From microscopic binding to phenomenological binding affinity. **C -G. Zhan**

291. PEG-ligand analogs for nicotinic acetylcholine receptors. **B. A. Scates**, N. J. Theising, T. G. Baker, B. C. Chastain, K. Tominaga, B. T. Elliott, R. W. Fitch

292. Development of the first predictive pharmacophore models for sigma-1 and sigma-2 receptor antagonists. **N. Singh**, C. Mesangeau, S. Narayanan, J. Shaikh, R. R. Matsumoto, C. R. McCurdy

293. Preparation of piperazine derivatives as 5-HT7 receptor active agents. **H -Y. P. Choo**, A. N. Pae, H. Rhim, E. Yoo

294. Identification of enantiomerically pure 5-HT_6 receptor antagonists by chiral resolution. **C. M. Park**, S. Kang, W. Park, N. Park, C. Seong

295. *trans*-2,3-Dihydroxy-6a,7,8,12b-tetrahydro-6H-chromeno[3,4-*c*]isoquinoline: A novel β-phenyl-dopamine template for D_1 receptor activation. **J. P. Cueva**, B. R. Chemel, D. E. Nichols, V. J. Watts

296. Further structure activity relationship (SAR) study of novel hybrid 7-{[2-(4-Phenyl-piperazin-1-yl)-ethyl]-propyl-amino}-5,6,7,8-tetrahydro-naphthalen-2-ol analogs focusing on modification of the N-aromatic moiety: Development of a highly potent and selective lead molecule for the D3 dopamine receptor. **B. Ghosh**, J. Zhen, M. Reith, A. Dutta

297. Design, structure activity relationships and biological evaluation of novel D3 receptor preferring agonists: A potential neuroprotective treatment for Parkinson's disease. **S. Biswas**, S. Zhang, F. Fernandez, J. Zhen, M. Reith, A. Dutta

298. Optimization of a hit molecule derived from virtual high throughput screening for metabotropic glutamate receptor (group III) agonist activity. **C. Selvam**, N. Oueslati, I. Brabet, C. Goudet, N. Triballeau, H -O. Bertrand, J -P. Pin, F. Acher

299. Synthesis of subtype selective ligands for alpha 5-containing GABAA/Bz receptors to treat memory deficits. **T. Clayton**

300. Development of cyclopropylcarboxamide bradykinin B1 receptor antagonists with modified biphenyl motifs. **R. K. Chang**, C. N. Di Marco, K. L. Murphy, R. W. Ransom, D. R. Reiss, C. Tang, T. Prueksaritanont, D. J. Pettibone, M. G. Bock, S. D. Kuduk

301. 2-Aminobenzophenones as a novel class of BK-1 antagonists. **D -S. Su**

302. Design and synthesis of stereoenantiomeric benzodiazepine receptor ligands. S. Huang, M. Savic, R. Furtmüller, A. Duke, T. Clayton, W. Sieghart, J. K. Rowlett, **J. M. Cook**

303. Computational approaches to the prediction of blood-brain barrier permeability: Comparative analysis of CNS drugs vs. the secretase inhibitors for Alzheimer's disease. **G. M. Rishton**, K. LaBonte, A. J. Williams, K. Kassam, E. Kolovanov

304. New aids for molecular chaperones in combating ß-amyloid formation. J. E. Gestwicki, **A. J. Turbiak**

305. CNI-1493 inhibits Aß production and prevents plaque formation in an animal model

of Alzheimet's disease. **Y. Al-Abed**, R. Dodel, B. Aljabari, K. Keyvani, P. Marambaud, R. Kayed, R. Glabe, N. Goertz, S. Schnell, M. Bacher

306. Synthesis of small molecule gamma-secretase inhibitors for Alzheimer's disease. **J. Pu**, L. Resnick, S. Aschmies, K. Atchison, J. Berkowitz, T. J. Caggiano, M. Chlenov, G. Diamantidis, B. Harrison, Y. Hu, D. Huryn, J. S. Jacobsen, M. Jin, A. Kreft, P. Lu, R. Martone, K. M. Morris, J. Sonnenberg-Reines, D. Riddell, J. E. Sabalski, S -C. Sun, E. Wagner, E. Wang, Z. Xu, H. Zhou

307. Hit-to-lead optimization of aminohydantoins as b-Secretase inhibitors. **P. Nowak**, A. Aulabaugh, J. Chen, D. C. Cole, R. Chopra, R. Cowling, M. Dar, J. W. Ellingboe, K. Y. Fan, B. Hu, S. Jacobsen, M. Jani, G. Jin, M -C. Lo, M. S. Malamas, E. S. Manas, R. Narasimhan, A. Robichaud, C. Sabus, J. R. Stock, M. Tischler, J. Turner, E. Wagner, P. Zhou, J. Bard

308. Carbocyclic substituted aminohydantoins as BACE1 inhibitors. **J. Erdei**, I. Gunawan, M. S. Malamas, P. Novak, J. Turner, A. J. Robichaud, J. Bard, Y. Hu, E. Wagner, L. Di, K. Fan, R. Chopra, A. Oganesian, C. Huselton

309. Piperidinyl-2-aminohydantoin derivatives for the inhibition of beta-secretase. **Y. Yan**, P. Zhou, M. S. Malamas, Y. Li, S. Aschmies, J. Bard, R. C. Bernotas, R. Chopra, T. Comery, K. Y. Fan, Y. Hu, A. Oganesian, J. Turner, E. Wagner, Z. Wang, P. Reinhart, A. J. Robichaud

310. Fragment based lead generation approaches for inhibitors of beta-secretase: Development of a novel series of dihydroisocytosine-based inhibitors. **J. S. Albert**, P. D. Edwards, D. Andisik, J. B. Campbell, R. Carr, G. Chessari, M. S. Congreve, G. M. Koether, R. C. Mauger, C. W. Murray, S. Patel, M. A. Sylvester

311. Fragment based lead generation approaches for inhibitors of beta-secretase: Development of a novel series of isocytosine-based inhibitors. **J. S. Albert**, P. D. Edwards, D. Andisik, J. B. Campbell, M. S. Congreve, R. Carr, G. Chessari, F. Edfeldt, R. H. Folmer, G. M. Koether, K. Kolmodin, C. W. Murray, L -L. Olsson, S. Patel, T. DeBeer

312. Synthesis of bifunctional small molecules for imaging β-amyloid aggregation. **A. H. Negussie**, A. O. Akinola, S. Fung, K. C. Li, N. S. Danthi

313. Substituted biaryl imidazoles, oxazoles and thiazoles as sodium channel blockers. **S. Tyagarajan**, B. Zhou, W. H. Parsons, M. H. Fisher, M. J. Wyvratt, K. A. Lyons, T. Klatt, X. Li, S. Kumar, B. Williams, J. Felix, B. T. Priest, R. M. Brochu, V. Warren, M. S. Smith, M. Garcia, G. J. Kaczorowski, W. J. Martin, C. Abbadie, E. McGowan, N. Jochnowitz, P. K. Chakravarty

314. Substituted biaryl pyrazoles as sodium channel blockers. **S. Tyagarajan**, B. Zhou, B. Taylor, W. H. Parsons, M. H. Fisher, M. J. Wyvratt, K. A. Lyons, T. Klatt, X. Li, S. Kumar, B. Williams, J. Felix, B. T. Priest, R. M. Brochu, V. Warren, M. Smith, M. Garcia, G. J. Kaczorowski, W. J. Martin, C. Abbadie, E. McGowan, N. Jochnowitz, P. K. Chakravarty

315. Synthesis of antagonists of acid sensing ion channels. **Z. Liu**, J. D. Rainier, R. W. Hughen, A. R. Light

316. Discovery and SAR of furan piperazines as sodium channel blockers for the treatment of neuropathic pain. **I. Drizin**, R. J. Gregg, M. J. C. Scanio, L. Shi, M. F. Gross, R. N. Atkinson, J. B. Thomas, M. S. Johnson, W. A. Carroll, B. E. Marron, M. L. Chapman, D. Liu, M. J. Krambis, C -C. Shieh, X. Zhang, G. Hernandez, D. M. Gauvin, J. P. Mikusa, C. Z. Zhu, S. Joshi, P. Honore, K. C. Marsh, R. Roeloffs, S. Werness, D. S. Krafte, M. F. Jarvis, C. R. Faltynek, M. E. Kort

317. Discovery and biological evaluation of 5-aryl-2-furfuramides, potent and selective blockers of the $Na_v1.8$ sodium channel with efficacy in models of neuropathic pain. **M. E. Kort**, I. Drizin, R. J. Gregg, M. J. C. Scanio, L. Shi, M. F. Gross, R. N. Atkinson, M. S. Johnson, G. F. Pacofsky, M. E. Secrest, J. B. Thomas, W. A. Carroll, B. E. Marron, M. L. Chapman, M. J. Krambis, D. Liu, C -C. Shieh, X. Zhang, G. Hernandez, J. P. Mikusa, C. Zhong, S. Joshi, P. Honore, R. Roeloffs, K. C. Marsh, B. P. Murray, J. Liu, S. Werness, C. R. Faltynek, D. S. Krafte, M. F. Jarvis

318. Improved synthesis of penciclovir. Y. Deng, **N. He**, **S. Li**

319. SAR development of potent, selective pyridine-based blockers of the Nav1.8 (PN3) sodium channel. **B. E. Marron**, R. N. Atkinson, J. B. Thomas, M. S. Johnson, G. J. Pacofsky, M. E. Secrest, L. Shi, M. E. Kort, I. Drizin, M. J. C. Scanio, R. J. Gregg, M. A. Matulenko, M. L. Chapman, D. Liu, M. J. Krambis, X. Su, C -C. Shieh, X. Zhang, G. Hernandez, S. Joshi, P. Honore, K. C. Marsh, A. Knox, R. Roeloffs, S. Werness, M. F. Jarvis, C. R. Faltynek, D. S. Krafte

320. The discovery of potent, selective pyridine-based blockers of the Nav1.8 (PN3) sodium channel. **R. N. Atkinson**, J. B. Thomas, M. S. Johnson, G. J. Pacofsky, M. E. Secrest, L. Shi, M. E. Kort, I. Drizin, R. J. Gregg, M. A. Matulenko, M. L. Chapman, D. Liu, M. J. Krambis, X. Su, C -C. Shieh, X. Zhang, G. Hernandez, S. Joshi, P. Honore, K. C. Marsh, A. Knox, R. Roeloffs, S. Werness, D. S. Krafte, M. F. Jarvis, C. R. Faltynek, B. E. Marron

321. Potent, selective pyrazine-based blockers of the $Na_v1.8$ (PN3) sodium channel. **M. J. C. Scanio**, L. Shi, M. E. Kort, I. Drizin, R. J. Gregg, J. B. Thomas, R. N. Atkinson, M.

S. Johnson, B. E. Marron, M. L. Chapman, D. Liu, M. J. Krambis, X. Su, C -C. Shieh, X. Zhang, G. Hernandez, S. Joshi, P. Honore, K. C. Marsh, A. Knox, S. Werness, D. S. Krafte, M. F. Jarvis, C. R. Faltynek

322. Development of imidazopyridine Nav1 blockers for the treatment of neuropathic pain. **S. B. Hoyt**, C. London, D. J. Gorin, W. H. Parsons, A. E. Weber, C. Abbadie, R. M. Brochu, J. P. Felix, M. L. Garcia, N. Jochnowitz, B. V. Karanam, S. Kumar, K. A. Lyons, X. Li, D. E. MacIntyre, E. McGowan, W. J. Martin, B. T. Priest, M. M. Smith, V. A. Warren, B. S. Williams, G. J. Kaczorowski, J. L. Duffy

323. Polycyclic amine derivatives: The synthesis of triquinylamines as calcium modulators. **L -M. Bezuidenhout**, W. Liebenberg, S. F. Malan, C. J. Van der Schyf

324. Synthesis and SAR of heterocyclic KCNQ2 potassium channel modulators based on the 1,4-diaminobenzene template. **A. Ritzén**, D. R. Greve, N. A. Khanzhin, M. B. Nørgaard, M. Rottländer, T. B. Stensbøl, L. Tagmose, C. W. Tornøe, W. P. Watson

325. Synthesis and SAR of trisubstituted anilines as novel KCNQ2 potassium channel modulators. **C. W. Tornøe**, D. R. Greve, N. A. Khanzhin, M. B. Nørgaard, A. Ritzén, M. Rottländer, T. B. Stensbøl, L. Tagmose, W. P. Watson

326. Synthesis and SAR of indolines as potent conformationally restricted KCNQ2 potassium channel openers. **N. A. Khanzhin**, D. R. Greve, M. B. Nørgaard, A. Ritzén, M. Rottländer, T. B. Stensbøl, L. Tagmose, C. W. Tornøe, W. P. Watson

327. Synthesis and evaluation of new cathepsin D inhibitors containing substituted hydroxyethyl piperazine isosteres. **P. Velusamy**, D. Driver, W. E. Godwin, R. M. McConnell

328. Full length zinc selective inhibitors of matrix metalloproteinase. **F. E. Jacobsen**, C. A. F. de Oliveira, J. A. McCammon, S. M. Cohen

329. Design and synthesis of tryptophan butynyloxy carboxylate derivatives as TACE inhibitors. **K. Park**, J. I. Levin, A. Aplasca, A. Gopalsamy, J. W. Ellingboe, Y. Zhang, L. Sun, W. Xu

330. Synthesis and properties of cyclocystine subunits (CCS): Application to thioredoxin reductase and hepcidin. **E. L. Ruggles**, R. J. Hondal, P. B. Deker

331. Identification of a contiguous binding site in PKC-zeta and the binding of ruboxistaurin to PKC-alpha, -beta and -zeta. S. Tang, V. Xiao, C. I. Whiteside, **L. P. Kotra**

332. Interactions of β-lactam antibiotics with proteases. P. M. Tschische, K. Majumder, S. Tang, E. Poduch, P. Dixit, **L. P. Kotra**

333. Design of N-Heteroaryl or N-Heteroarylmethyl-3-alkyl substituted piperazines as scaffolds for a Rho-kinase inhibition. **I -H. Paik**, W. H. Brooks, S. M. Sebti, A. D. Hamilton

334. Development of selective inhibitors of protein tyrosine phosphatases using combinatorial fluorogenic peptide substrates. **S. Mitra**, A. M. Barrios

335. Synthetic approaches to amino acid cyclobutanone derivatives. **P. Kataria**, N. Armoush, D. Becker

336. Progress toward amino acid cyclobutanone derivatives as potential serine protease inhibitors via a ketene [2+2] cycloaddition strategy. **M. R. Lutz Jr.**, P. Farid, A. Panagopoulos, D. Becker

337. Synthesis and evaluation of aeruginosin analogs as serine protease inhibitors. G. Wang, X. Nie, **B. Hopkinson**, S. Cheuk

338. Peptide libraries containing Phe analogs-reversible inhibitors of thrombin and potent inhibitors of platelets aggregation. **C. Clement**, A. Babinska, J. Gonzalez, M. Philipp

339. Synthesis and SAR study of 1*H*-pyrrole-2,5-dione and furan-2,5-dione derivatives as novel COX-2 inhibitors. **J. T. Moon**, J. H. Heo, J. Y. Jeon, J -Y. Kim, K -T. Lee, J. Y. Lee, D. J. Choo

340. Benzoxazole and pyridinothiazoles as 5-lipoxygenase inhibitors. **H -Y. P. Choo**, S -R. Oh, H -K. Lee, K. Ann, G. Han, J -H. Kim

341. Synthesis and SAR of pyrrolidine and piperidine aryl ethers as novel leukotriene A4 hydrolase inhibitors. **M. Keyvan**, V. Sandanayaka, B. Mamat, J. Winger, M. Krohn, G. Halldórsdóttir, H. Sigþórsdóttir, D. Zembower, Þ. Andrésson, J. Singh, M. Gurney

342. Discovery, synthesis, and SAR of novel arylpiperazine derivatives as leukotriene A4 hydrolase inhibitors. **L -M. Zhou**, V. Sandanayaka, B. Mamat, R. Mishra, G. Halldórsdóttir, H. Sigþórsdóttir, D. Zembower, Þ. Andrésson, J. Singh, M. Gurney

343. Discovery of novel pyrrolidine derivatives as potent leukotriene A4 hydrolase inhibitors. **P. Yu**, V. Sandanayaka, L. Zhao, B. Mamat, R. Mishra, G. Halldórsdóttir, H. Sigþórsdóttir, D. Zembower, Þ. Andrésson, J. Singh, M. Gurney

344. Preparation of non-urea inhibitors of soluble epoxide hydrolase. **A. S. Kumar**, D.

Chen, Z. N. Do, H. K. Webb, R. D. Gless

345. Synthesis and evaluation of conformationally restricted soluble epoxide hydrolase (sEH) inhibitors. **S. H. Hwang**, H -J. Tsai, C. Morisseau, Z. Do, B. D. Hammock

346. Preparation of sEH inhibitors with improved drug-like properties. P. A. Baecker, Z. N. Do, H. K. Webb, **R. D. Gless**, I -H. Kim, B. D. Hammock

347. Liposome mediated inhibition of carbonic anhydrase. **J. A. Kooren**, A. Elegbede, M. Haldar, S. Mallik, D. K. Srivastava

348. 3-D-QSAR and docking studies on 3-anilino-4-phenylmaleimides for glycogen synthase kinase-3α inhibition. **P. Sivaprakasam**, P. R. Daga, A. Xie, R. J. Doerksen

349. Characterization of a catalytic ligand bridging metal ions in phosphodiesterases 4 and 5 by molecular dynamics simulations and hybrid quantum mechanical/molecular mechanical calculations. **Y. Xiong**, H -T. Lu, C -G. Zhan

350. Microscopic modes and free energies of 3-phosphoinositide-dependent kinase-1 (PDK1) binding with celecoxib and other inhibitors. **M. D. M. AbdulHameed**, A. Hamza, C -G. Zhan

351. Effect of trifluoroethanol on the structure and function of mesophilic and thermophilic chorismate mutases. **E. Csuhai**, P. Kast, D. Hilvert

352. Understanding the rate-determining step in the kinetic pathway of eubacterial tRNA-guanine transglycosylase. **S. M. Chervin**, G. A. Garcia

353. Recognition of cognate tRNAs by the human tRNA-guanine transglycosylase. **Y -C. Chen**, G. A. Garcia

354. Regulation of human tRNA-guanine transglycosylase: Interactions of catalytic and regulatory subunits. **K -H. Lee**, G. A. Garcia

355. Modification of an mRNA involved in bacterial virulence by tRNA-guanine transglycosylase. **J. K. Cutcher**, G. A. Garcia

356. Progress toward the development of synthetic transcriptional activators. **R. J. Casey**, B. B. Brennan, C. A. Bates, A. K. Mapp

357. Design, synthesis and biological activities of novel PPAR α/γ dual agonist as potential antidiabetics. Y -G. Suh, **J -W. Jung**, J. Jang, F -N. Li, S. J. Lee, N -J. Kim, B. W. Koo, K -O. Lee, M -K. Kim, J -K. Kim, J -I. Lim

358. Design, synthesis and biological evaluation of novel PPARa/g dual agonist, lobeglitazone sulfate (CKD-501). **S. K. Kang**, H. W. Lee, S. K. Ahn, J. B. Ahn, D. J. Jeon, J. S. Shin, Y. M. Kwon, M. H. Ki

359. Novel pyrimidine-5-carboxylic acid as a potent and orally active PPARγ partial agonist. **S. Seto**, K. Okada, K. Kiyota

360. Synthesis and LXR activity of 4-(3-(phenylethynyl)phenyl quinolines. **J. W. Ullrich**, R. L. Morris, P. Nambi, E. Quinet, L. Chen, A. Halpern, Q -Y. Liu, D. Savio, M. Basso, R. Unwalla, A. Wilhelmsson, A. Goos Nilsson, C. Ursu, E. Arnelof, J. Sandberg, C. Enroth, J. Wrobel

361. Carboxylic acid based quinolines as liver x receptor (LXR) modulators. **B. Hu**, M. Collini, J. Jetter, R. Unwalla, E. Quinet, D. Savio, A. Halpern, I. Feingold, A. Goos-Nilsson, A. Wilhelmsson, P. Nambi, J. Wrobel

362. Selective silyl ether protection of hydroxyls in 3,11ß,17ß-estriols: A new approach to 11ß-methoxyestrogens. **M. G. C. Kahn**, R. M. Hoyte

363. Identification of peptides that bind to estrogen response elements: Using peptide phage display library. **M. Eshete**, Z. Ndegwa

364. Methylation of estrogen receptor-beta promoter 0N CpG sites in LNCaP cells. **J. B. Elston**, X. Zhang, Y -K. Leung, S -M. Ho

365. Estrogen receptor (ER) ligands that recruit FK506 binding proteins: A novel mechanism of ER antagonism? **T. W. Moore**, J. R. Gunther, J. A. Katzenellenbogen

366. Pyrimidine core small molecule inhibitors of estrogen and androgen receptor-coactivator binding. **A. A. Parent**, J. R. Gunther, J. P. Amin, J. A. Katzenellenbogen

367. Bioactive compounds with unusual elemental composition: Boron-nitrogen estrogen receptor ligands, structural features of partial agonists. **H -B. Zhou**, K. W. Nettles, K. E. Carlson, F. Stossi, G. L. Greene, **J. A. Katzenellenbogen**

368. Synthesis of a selective proteolysis inducer (PROTAC): Chemically knocking out estrogen receptor function. **M. K. Mann**, **J. A. Katzenellenbogen**

369. Dual interaction assay receptor-corpressor/receptor-coactivator binding. **M. Jeyakumar**, P. Webb, T. S. Scanlan, J. A. Katzenellenbogen

370. Applying computational tools in drug discovery: Oxidative susceptibility and

estrogen receptor interactions of arzoxifene analogs. **I. Kastrati**, Z. Qin, P. A. Petukhov, J. L. Bolton, G. R. J. Thatcher

371. Improved synthetic technology of chlorodehydromethyltestosterone. Y. Deng, **S. Li**, **N. He**

372. Identification of estrogen receptor ligands using a new multi-step computer-aided approach. **S. Dakshanamurthy**, E. Thembani, S. Divekar, M. B. Martin

373. Synthesis and evaluation of 17-alpha-heteroarylvinyl estradiols as ligands for the estrogen receptor ligand binding domain (ER-LBD). S. Olmsted, **R. N. Hanson**, P. Tongcharoensirikul, E. McCaskill, R. B. Hochberg, D. C. Labaree

374. Quantitation of estrogens in male plasma using liquid chromatography with an electrochemical detector. **A. Kallmerten**, B. Rowland, M. Pomerantz, W. Oh, J. Glick

375. 3-(2,4-Dimethyl-9H-pyrido[2,3-b]indol-3-yl)propanoic acid derivatives as potent and bioavailable microsomal triglyceride transfer protein(MTP) inhibitors with reduced cytochrome P450 3A4(CYP3A4) inhibitory activity. **A. Suga**, H. Kubota, M. Miura, N. Imanishi, D. Sasuga, H. Moritani, S. Naganuma, C. Kitada, M. Furutani, S. Sakamoto, S -I. Tsukamoto

376. Novel 4-phenyl-1,8-naphthyridin-2(1H)-on-3-yl ureas: Synthesis and inhibitory activity against acyl-CoA:cholesterol acyltransferase. **H. Ban**, M. Muraoka, S. Ohnuma, K. Ioriya, N. Ohashi

377. Synthesis and SAR of aryl and heteroaryl 11B-HSD-1 inhibitors. **H. Wang**, J. Li, L. Simpkins, J. Sutton, S. Wu, R. Smirk, D. Yoon, Z. Ruan, C. Cooper, K. V. Kirk, R. Hutchins, Y -X. Li, Z. Ma, R. Seethala, R. Golla, A. Nayeem, S. Krystek, D. Gordon, J. A. Robl, L. Hamann

378. Discovery of orally active butyrolactam 11b-HSD1 inhibitors for the treatment of metabolic syndrome. **V. S. C. Yeh**, R. Kurukulasuriya, D. Madar, F. A. Kerdesky, J. J. Rohde, M. Pliushchev, S. Fung, K. Monzon, W. J. Chiou, J. Wang, D. Stolarik, H. Imade, D. W. A. Beno, R. Shapiro, V. Knourek-Segel, E. N. Bush, D. M. Wilcox, P. Nguyen, M. Brune, P. B. Jacobson, J. T. Link

379. Structure-activity relationship study of stearoyl Co-A desaturase-1 (SCD1) inhibitors with privileged phenoxypiperidines. **B. Liu**, V. S. C. Yeh, J. Lynch, J. Freeman, Z. Xin, T. S. Suhar, N. Cao, H. T. Smith, H. S. Camp, C. A. Collins, H. L. Sham, G. Liu

380. Synthesis and structure-activity relationships of piperidine-1-carboxamides as stearoyl-CoA desaturase 1 inhibitors. **M. Liu**, Z. Xin, H. Zhao, M. D. Serby, H. T.

Smith, T. S. Suhar, N. Cao, T. K. Surowy, H. S. Camp, C. A. Collins, H. L. Sham, G. Liu

381. Novel urea-based stearoyl-CoA desaturase 1 inhibitors: Design, synthesis, and biological evaluation. **Z. Xin**, H. Zhao, M. D. Serby, B. Liu, M. Liu, B. G. Szczepankiewicz, L. T. Nelson, H. T. Smith, T. S. Suhar, N. Cao, T. K. Surowy, D. M. Wilcox, P. Nguyen, M. Voorbach, K. Landschulz, H. S. Camp, C. A. Collins, H. L. Sham, G. Liu

382. Discovery of potent stearoyl-CoA desaturase 1 (SCD1) inhibitors via scaffold hopping. **H. Zhao**, M. D. Serby, H. T. Smith, N. Cao, T. S. Suhar, T. K. Surowy, H. S. Camp, C. A. Collins, H. L. Sham, G. Liu

383. Discovery of phenoxypiperidines as novel stearoyl-CoA desaturase inhibitors: From assay validation to lead development. **J. C. Freeman**, J. K. Lynch, R. R. Iyengar, H. T. Smith, T. S. Suhar, L. E. Chovan, H. Xu, T. K. Surowy, C. A. Collins, P. R. Kym

384. Design and biological evaluation of small molecule ligands for the melanocortin-4 receptor: In vivo characterization of potent, selective MC4R agonists. **R. T. Backer**, K. Briner, M. P. Clay, I. Collado, L. S. Craft, P. J. Emmerson, M. J. Fisher, M. L. Heiman, J. L. Hertel, S. Husain, S. L. Kuklish, T. D. Lindstrom, A. I. Mateo, J. T. Mullaney, T. P. O'Brien, P. L. Ornstein, T. I. Richardson, J. A. Shah, T. M. Williams, J. M. Zgombick

385. First pharmacophore and 3-D QSAR model for selective 5-hydroxytryptamine2C (5-HT2C) receptor agonists. **T. Ramasamy**, P. A. Petukhov

386. Synthesis and SAR of heteroaryl-fused piperidines as novel cannabinoid-1 receptor antagonists. **C. Sun**, Y. Huang, R. Sulsky, Y. Zhu, L. Kang, Y. Yang, R. A. Baska, M. J. Cullen, W. Keim, M. A. Pelleymounter, P. Stetsko, O. Gudmunsson, S. Johnghar, S. Wu, K. Behnia, K. E. Carlson, W. R. Ewing

387. Design and synthesis of 2,5-substituted pyridines as novel anti-coagulant factor Xa inhibitors. **Y -L. Li**, K. A. Rossi, J. M. Luettgen, R. M. Knabb, R. R. Wexler, P. Y. S. Lam

388. Highly potent and selective Factor Xa inhibitors containing alpha-substituted arylcycloalkyl P4 residues: SAR studies of C3 substitution and the aryl binding site. **J. X. Qiao**, S. R. King, P. C. Wong, K. He, A. R. Rendina, J. M. Luettgen, R. M. Knabb, R. R. Wexler, P. Y. S. Lam

389. Novel sulfonylaminopiperidone derivatives as potent coagulation factor Xa inhibitors. **W. Han**, Z. Hu, A. Rendina, J. Luettgen, K. He, P. C. Wong, R. M. Knabb, R. R. Wexler, P. Y. S. Lam

390. Chemical modification of heparin with deoxycholic acid for improvement of oral bioavailability. **Y -K. Lee**, O. M. Kwon, H. T. Moon, Y. Byun

391. Heparinoid-active sulfated polysaccharides from marine green algae. **W. Mao**, H. Sun

392. VLA1 integrin inhibitors: Diaminopropionic acid derivatives. **A. A. Thomas**, R. Xu, S. C. Miller, S. A. Boyd, K. Condroski, I. Gunawardana, G. Zhang, M. L. Lupher Jr., F. Farouz, I. Jacobson, D. S. Staunton, E. D. Thorsett

393. VLA1 integrin inhibitors: Aminopiperidine amides. **A. A. Thomas**, S. C. Miller, S. A. Boyd, K. Condroski, J. De Meese, I. Gunawardana, R. Xu, G. Zhang, M. L. Lupher Jr., F. S. Farouz, I. Jacobson, D. S. Staunton, E. D. Thorsett

394. Acrylamide amido acid derivatives as potent and selective VLA-1 antagonists: Optimization of the amido acid region. **R. Xu**, I. Gunawardana, Y. Le Huerou, S. C. Miller, S. A. Boyd, K. Condroski, J. De Meese, A. A. Thomas, G. Zhang, M. L. Lupher Jr., L. Sui, F. Farouz, I. C. Jacobson, D. S. Staunton, E. D. Thorsett

395. Discovery of potent and selective VLA-1 antagonists for the treatment of inflammatory diseases: Modifications of B-ring portion of hit compound A-328282.0. **I. Gunawardana**, M. Yanik, R. Xu, S. C. Miller, S. Boyd, K. Condroski, M. L. Lupher Jr., L. Sui, I. C. Jacobson, D. S. Staunton, E. D. Thorsett

396. Synthesis and structure-activity relationship of novel phenylalanine derivatives as potent VLA-4 integrin antagonists. **T. Okuzumi**, S. Makino, K. Sagi, A. Chiba, Y. Satake, N. Suzuki, H. Izawa, T. Yoshimura, M. Murata, E. Nakanishi, T. Tsuji

397. Synthesis of bivalent beta2 adrenergic partial agonists. **P. Karellas**, P. Scammells, G. Krippner

398. Selective β_3 adrenergic receptor agonists with reduced rat atrial tachycardia. **F. C. Stevens**, D. B. Bennett, W. E. Bloomquist, M. L. Cohen, C. A. Droste, M. L. Heiman, A. V. Kriauciunas, D. J. Sall, F. C. Tinsley, C. D. Jesudason

399. A new flavone 5-O-diglycoside from the leaves of Cephalotaxus sinensis (Rehd et Wile) Li. W. Li, R. Dai, Y. Yu, L. Li, **Y. Deng**

400. A novel C- glycoside favanoid from leaves of Belamcanda chinensis. L. Li, Y. Yu, R. Dai, W. Li, W. Meng, **Y. Deng**

401. GLUT-4 translocation facilitating activity of flavonoids from Cephalotaxus sinensis on mice adipocytes. W. Li, **Y. Deng**, R. Dai, Y. Yu, L. Li

402. Fluorescence-based probe for the detection of hydroxyl radicals produced by γ-rays and $Na^{125}I$ in aqueous solution. **A. Singh**, S. J. Adelstein, A. I. Kassis

403. High-boiling solvents and morphology of crystals. **C. Acquah**, L. E. Achenie, A. T. Karunanithi, S. Sithambaram, S. L. Suib

404. In-silico fragment-based pharmacophore design and lead optimization. **S. Toba**, K. Poptodorov, J. Sutter, A. J. Maynard, C. keolmel

405. Amino acid esters of 3-(hydroxymethyl)phenyl guanidine: Affinity to PEPT 1 transporter. **J. Sun**, G. L. Amidon

406. Novel synthesis of 4-carboxy-4-pyridylpiperidines. **Y. Wang**, R. Nair

407. Predictive model of the inhibition of CYP3A4 by selected natural compounds. **S. Thotakura**, J. A. Darsey, K. Wang, J. T. Arnason, C. M. Compadre

408. Synthesis of fluorinated dihydropyrazolo-pyrimidine derivatives as potential biologically active compounds. **O. O. Fadeyi**, K. Wash, C. O. Okoro

409. Synthesis of some alkenol and alkynol analogs of 1-octen-3-ol and investigation of their mosquito attractant properties. **S. M. Farah**, C. Ikediobi, L. M. Latinwo, L. Ayuk-Takem, J. Cilek, **O. Okungbowa**

410. Synthetic small molecule ligands for bulged RNA secondary structure. **S. T. Meyer**, P. J. Hergenrother

411. Structural characterization of unknown impurities in muraglitazar using LC/MS/MS and advanced NMR techniques. **Q. Ye**, Y. Huang, A. Rusowicz, T. Raglione, V. Palaniswamy

412. Benzindene prostacyclin prodrugs: Synthesis, characterization and biological activity. **R. M. Moriarty**, A. Hirtopeanu, I. Dragutan, R. Naithani, K. Gao, K. R. Phares

413. Tackling barbiturates: Making a Phenobarbital chemiluminescent tracer. **B. M. Bax**, Z. Lin, Y. Pan, R. E. Reddy, B. T. Merchant, R. J. Himmelsbach

414. Designed synthetic spirocyclic helical compounds as binding agents for bulged DNA and RNA microenvironments. **D. Ma**, Y. Lin, G. B. Jones, N. Zhang, Z. Xiao, I. H. Goldberg

415. Enantioselective synthesis and biological evaluation of stereoisomers of 1-octen-3-ol and its analogs. **A. O. Adesunloro**, C. Ikediobi, L. M. Latinwo, L. Ayuk-Takem, J. Cilek

416. Synthesis and evaluation of functionalized carboranes as potential anticancer agents. A. V. Reddy, P. V. K. Reddy, **S. C. Jonnalagadda**, V. R. Mereddy

417. Extraction and fractionation of polyphenols from chinese medicinal plant torreya grandis and their antioxidant activity against ferric reducing ability, DPPH and reducing power activity. **M. K. Saeed IV**, Y. Deng, R -J. Dai

418. Feigrisolide C: Structural revision and synthesis. **J. H. Jung**

419. FVP of steroid oxalate dimers for synthesis of androst-16-enes. **A. B. Turner**, L. Nahar

420. Genomic screening of Juzen-Taiho-to. **T. H. Hasson**, A. Kawamura

421. Improved synthesis of 1-O-acetyl-2,3,5-tri-O-benzoyl-beta-D-ribofuranose from inosine. Y. Deng, D. Tao, **N. He**, **S. Li**

422. Interactions among the polymer components of cartilage matrix. **F. Horkay**, D. C. Lin, E. K. Dimitriadis, I. Horkayne-Szakaly, P. J. Basser

423. New synthetic methodology for the formation of quaternary carbon centers: A concise, microwave-assisted synthesis of cuparene in zeolite HY. T. Poon, **L. Young**

424. Novel inhibitors of cellular wound healing and cytokinesis. **A. G. Clark**, W. M. Bement

425. Novel local drug delivery utilizing 1,8-naphthalimide derivatives. **P. D. Youso**, R. E. Utecht

426. Predicting drug absorption from permeability measurements across a lipid-coated membrane using a diffusion cell and a UV spectrophotometer. **A. Kraft**, N. M. Howarth, H. N. Sheppard, H. Perston, J. Fouquet

427. Prodrugs of PROLI/NO, a nitric oxide donor. **H. Chakrapani**, J. E. Saavedra, B. M. Showalter, L. K. Keefer

428. Quantitative analysis and isolation of shikimic acid from *Liquidambar styraciflua*. T. Poon, **L. Enrich**, **A. Mohadjer**

429. Rapid DMSO labeling for high yield radioiodinated pharmaceutical. **K. W. S. J. A. A. A. I. Kassis**

430. Screening of disulfide induced protein refolding intermediates by capillary isoelectric focusing. **H. P. Gunawardena**, J. Fredlin, K. van der Drift, K. Wee

431. Silica based metal scavengers for the purification of pharmaceutical active ingredients. **F. Béland**, A. Michaud, M. Morin

432. Structural basis for substrate flexibility and product diversity of cytochrome P450 PikC from Streptomyces venezuelae. **S. Li**, D. H. Sherman, L. M. Podust

433. Surface-functionalizable drug-conjugated polymer nanoparticles via ring-opening metathesis polymerization. **D. Smith**, P. J. Endres, K. W. Macrenaris, H. Cheng, S. M. Raja, T. R. Holden, P. A. Bertin, C. K -F. Shen, V. Band, H. Band, T. J. Meade, S. T. Nguyen

434. Synthesis of (Z)-2-acetamido-3- (1H-indol-3-yl) acrylic acid derivatives as tryptophan precursors from relatively inexpensive 2-nitrobenzaldehydes and ethyl diazoacetate. **R. C. Todd**, M. E. Dudley, M. M. Hossain, N. Uddin, M. S. Islam

435. Synthesis of 6-(4'-N,N-dimethylamino)pyrid-2'-yl-7-amino-4-methylcoumarin (DAMC) as a novel fluorophore. **X. Wu**, L. Hu

436. Synthesis of highly enantiopure primary amines by the catalytic reduction of benzyl oxime ethers using the novel spiroborate ester/borane system. **F. G. Merced Ortiz**, A. Ayala, Z. Oquendo, M. Ortiz, X. Huang

437. Synthesis, characterization, and evaluation of novel bioconjugation linkers. **C. Y. Lee**, **M. R. Shepard**, **N. T. Zalenski**, J. A. Muller II, D. W. Ki

438. Synthesis, resolution, and diastereoselectivity of the chiral auxiliary trans-2-(9H-fluoren-9-yl)cyclohexanol. **M. A. Cheney**, J. M. Salvador

439. Two new tetraoxygenated xanthones from the branch of Calophyllum membranaceum. **X. Song**, **C. Han**

440. Understanding the biosynthetic capability of marine cyanobacteria: Enzymatic study of the curacin A pathway. **L. Gu**, D. Sherman

441. Wittig reactions and rearrangements leading to benzophenone- and chromone-based ligands for evaluation as potential retinoids. **S. Desai**, W. Sun, P. J. Carroll, J. L. Gabriel, D. Soprano, D. J. Canney

442. Zirconium Nitrate: A mild, efficient catalyst for the synthesis of 4 (3H)-quinazolinones under solvent free conditions. **S. Gowravaram**, N. Mallikarjuna Reddy,

M. Nagendra Prasad, G. Santosh, J. S. Yadav

443. Toward achieving non-protein based selective retrieval of crosslinked peptides in mass spectrometric analysis of protein complexes. **F. Yan**, R. H. Angeletti, B. P. C. AECOM

THURSDAY MORNING

Section A

Unknown Site -- Unknown Room

General Oral Session

D. P. Rotella, *Organizer*
9:00 —444. Neutron activation analysis determination of self-assembled monolayer (SAM) disruption in a bioelectrode: Kinetics of release of antiinflammatory Au thiolate. **M. Ovadia**, D. Zavitz, H. A. Chou, D. J. Vanderah

9:20 —445. Synthesis of a new prodrug linker system used for selective delivery of drugs to prostate cancer. **G. A. Suaifan**, M. D. Threadgill

9:40 —446. Pyrrolotriazine dual EGFR/HER2 protein tyrosine kinase inhibitors with solubilizing groups at C-5. **H. Mastalerz**, M. Chang, P. Chen, D. Cook, P. Dextraze, B. E. Fink, A. Gavai, B. Goyal, W -C. Han, W. Johnson, S -H. Kim, D. Langley, F. Lee, K. Leavitt, D. Norris, P. Marathe, A. Mathur, S. Oppenheimer, E. Ruediger, J. Tarrant, J. Tokarski, G. Vite, D. Vyas, H. Wong, T. Wong, H. Zhang, G. Zhang

10:00 —447. Design of class selective HDAC inhibitors. **G. Estiu**, C. Harrison, O. Wiest, R. Mazitschek, J. Bradner

10:20 —448. Structural insights into the binding sites of histone deacetylase isoforms HDAC1 and HDAC6: Implications in drug design. **H. Yuan**, Y. Chen, A. M. Gaysin, A. P. Kozikowski, P. A. Petukhov

10:40 —449. Studies on the stability of HA 14-1, a small molecule antagonist for anti-apoptotic Bcl-2 protein. C. Xing, **J. M. Doshi**

11:00 —450. Design, synthesis, and biochemical evaluation of Lumazine synthase inhibitors as potential antimicrobial agents. **A. Talukdar**, A. Bacher, M. Fisher, B. Illarionov, M. Cushman

11:20 —451. Antitubercular nucleosides that inhibit siderophore biosynthesis. **R. V.**

Somu, D. Wilson, C. Qiao, J. Vannada, E. Bennett, H. Boshoff, C. E. Barry III, C. C. Aldrich

11:40 —452. Antibiotic microarrays to study resistance. M. D. Disney, **O. J. Barrett**

12:00 —453. Design, synthesis and SAR of novel inhibitors for glutamate racemase (RacE2) from *Bacillus anthracis*. **K. Gao**, Z. Wang, D. C. Mulhearn, H. Yu, G. R. J. Thatcher, M. E. Johnson

THURSDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

General Oral Session

D. P. Rotella, *Organizer, Presiding*

1:30 —454. Design, synthesis and pharmacological evaluation of novel analogs of the anti-addiction alkaloid, lobeline. **A. P. Vartak**, A. G. Deaciuc, L. P. Dwoskin, P. A. Crooks

1:50 —455. 3-D-QSAR studies of Salvinorin A analogs as kappa opioid receptor agonists. **D. Pandit**, W. Harding, K. Tidgewell, M. Schmidt, A. Lozama, C. M. Dersch, W. J. Skawinski, R. B. Rothman, T. Prisinzano, C. A. Venanzi

2:10 —456. Development of benzazepinone Nav1 blockers for the treatment of neuropathic pain. **S. B. Hoyt**, C. London, D. J. Gorin, W. H. Parsons, A. E. Weber, C. Abbadie, R. M. Brochu, J. P. Felix, M. L. Garcia, N. Jochnowitz, B. V. Karanam, S. Kumar, K. A. Lyons, X. Li, D. E. MacIntyre, E. McGowan, W. J. Martin, B. T. Priest, M. M. Smith, V. A. Warren, B. S. Williams, G. J. Kaczorowski, J. L. Duffy

2:30 —457. Prediction of the 3-D structure for FMRF-amide peptides bound to the mouse MrgC11 GPCR and experimental validation. **J. Heo**, S -K. Han, N. Vaidehi, J. Wendel, P. M. Kekenes-Huskey, W. A. Goddard III

2:50 —458. Discovery of novel small molecule regulators of the integrin CD11b/CD18. J. Y. Park, M. A. Arnaout, **V. Gupta**

3:10 —459. Why are we still doing drug *discovery*? **M. D. Segall**

3:30 —460. Developing magic bullets: Advances in heterocyclic ligands for activated $\alpha_4\beta_1$ integrin. **R. D. Carpenter**, K. S. Lam, M. J. Kurth

3:50 —461. Synthesis and characterization of unnatural peptide inhibitors of thrombin activated platelet aggregation. **F. M. Burke**, M. Warnock, A. H. Schmaier, J. Hilfinger, H. I. Mosberg

4:10 —462. Synthesis of 1,4-disubstituted piperazine analogs with moderate to high sigma subtype affinity and selectivity. **R. Xu**, J. R. Lever, S. Z. Lever

4:30 —463. Medicinal chemistry vs. hERG. **Z. Rankovic**