

MEDI

DIVISION OF MEDICINAL CHEMISTRY

Final Program, 228th ACS National Meeting, Philadelphia, PA, August 22-26, 2004

D. L. Flynn, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Arthur C. Cope Award and Arthur C. Cope Scholar Awards (see *ORGN*, Tue)

Combinatorial, Parallel and Solid-Phase Chemistry (see *ORGN*, Thu)

Peptides, Enzymes, Lipids, and Nucleotides (see *ORGN*, Thu)

Proteins, Peptides, and Amino Acids (see *ORGN*, Thu)

Tetrahedron Prize for Creativity in Organic Chemistry (see *ORGN*, Mon)

SOCIAL EVENT:

Social Hour: Sun

BUSINESS MEETING: Sun

SUNDAY MORNING

Section A

Unknown Site -- Unknown Room

Amino Acid Neurotransporters

Sponsored by Bentham Science Publishers Ltd

W. J. Porter, *Organizer*

9:00 —1. Amino acid transporters as targets for therapeutic intervention. **B. J. Hoffman**

9:40 —2. Combining fluorescence and electrophysiology to probe glutamate transporter structure and function. **G. Leary**, J. B. Ross, M. P. Kavanaugh

10:20 —**3.** Pharmacophore development for the glutamate vesicular transporter (VGLUT1). **C. M. Thompson**, R. J. Bridges, J. M. Gerdes

11:00 —**4.** Discovery and SAR of selective inhibitors of the hGlyT-1b transporter. **S. Gibson**, R. Gilfillan, D. Jaap, D. Miller, G. Walker, G. Wishart

11:40 —**5.** Synthesis and Structure Activity Relationship of Novel Chiral Ligands for the Glycine-Reuptake Transporter Type-2 (GlyT-2). **M. Isaac**

Section B

Unknown Site -- Unknown Room

General Oral Session I

B. S. J. blagg, *Presiding*

8:30 —**6.** 4-Piperidiny-Substituted β -Aryl Butyric Acids: A New Class of Potent $\alpha\beta3/\alpha\beta5$ Integrin Antagonists. **B. L. De Corte**, W. A. Kinney, L. Liu, S. Ghosh, L. Brunner, W. J. Hoekstra, R. Santulli, J. C. Proost, B. P. Damiano, B. E. Maryanoff, D. L. Johnson, R. A. Galemno

8:50 —**7.** Identification and biological activity of a new series of antagonists of hMCH-R1. **G. Semple**, B. Kramer, D. Hsu, M. Casper, S.-S. Pleyne, B. Thomsen, T.-A. Tran, C. Bjenning, K. Whelan, K. Kanuma, K. Omodera, M. Nishiguchi, T. Funakoshi, S. Chaki, Y. Sekiguchi

9:10 —**8.** Synthesis and structure-activity relationships of substituted 5-aryl-6-methyluracils as human GnRH receptor antagonists. **M. W. Rowbottom**, F. Tucci, Y.-F. Zhu, Z. Guo, T. Gross, G. Reinhart, Q. Xie, R. S. Struthers, J. Saunders, C. Chen

9:30 —**9.** Discovery of a novel class of thiophene-derived antagonists of the human glucagon receptor. **J. L. Duffy**, B. A. Kirk, Z. Konteatis, E. Campbell, R. Liang, N. J. Kevin, J. R. Tata, K. T. Chapman, A. Bansal, S. Tong, S. Zheng, S. M. Cohen, C. Miller, M. R. Candelore, V. Ding, R. Saperstein, E. J. Brady, G. Jiang, D. Xie, X. Yang, S. A. Qureshi, B. B. Zhang

9:50 —**10.** Immunoconjugates comprised of drugs with impaired cellular permeability: a new approach to targeted therapy. **S. Doronina**, B. Mendelsohn, B. Toki, S. Alley, D. Meyer, K. Hamblett, J. Francisco, C. Cerveny, A. Wahl, P. Senter

10:10 —**11.** Diazaspirocyclic Compounds as Selective Ligands for the $\alpha4\beta2$ Nicotinic Acetylcholine Receptor: Synthesis and Pharmacological Studies. **B. S. Bhatti**, G. D. Hawkins, S. R. Breining, T. Y. Phillips, A. Mazurov, C. Miller

10:30 —12. Development of substituted indoles as ionotropic glutamate receptor ligands. **X. Shou**, A. R. Chamberlin

10:50 —13. Discovery, design, synthesis and SAR of VR1 antagonists. **S. L. Dax**, M. C. Jetter, M. McDonnell, M. A. Youngman, J. J. McNally, S.-P. Zhang, A. Dubin, L. Moser, N. Nasser, E. E. Codd, C. M. Flores

11:10 —14. Chemical biology and mechanism of action studies on the antitumour agent, (-)-agelastatin A. K. J. Hale, **M. M. Domostoj**, E. Irving, F. Scheinmann, M. El-Tanani, C. Mason, C. Campbell

11:30 —15. Discovery of inhibitors of the core binding factor β -smooth muscle myosin heavy chain fusion protein as a treatment of acute myeloid leukemia. **M. J. Gorczynski**

11:50 —16. Wrench-shaped synthetic molecules that modulate gene transcription. **Y. Kwon**, H. Shimogawa, Q. Mao, Y. Kawazoe, Y. Choi, H. Kigoshi, M. Uesugi

SUNDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Transporters in Drug Discovery

Sponsored by Biotage

M. R. Myers, *Organizer*

1:30 —17. Membrane Transporters and Prodrug Activating Enzymes: Modern Molecular Pharmaceutics. **G. L. Amidon**

2:10 —18. Chemical approaches to overcoming multidrug resistance at the blood-brain barrier. **K. L. Audus**, A. Rice, Y. Liu, M. Michaelis, R. H. Himes, G. I. Georg

2:50 —19. New strategies in medicinal chemistry: Harnessing nutrient transport mechanisms to optimize drug absorption and disposition *in vivo*. **M. A. Gallop**

3:30 —20. Peptide prodrug design for improving oral absorption. **C. Pedregal**

4:10 —21. Guanidinium-Rich Molecular Transporters: Mechanisms and Applications. **P. A. Wender**, J. Rothbard, T. Jessop

Section B

Unknown Site -- Unknown Room

Nicotinic ACH Receptors

Sponsored by Bentham Science Publishers Ltd

S. Ananthan, *Organizer*

1:00 —22. Adventures in the rational design of nicotinic acetylcholine receptor therapeutics. **J. D. Schmitt**, B. S. Bhatti, S. R. Breining, P. S. Hammond, R. Harris, G. D. Hawkins, J. Klucik, L. Miao, C. H. Miller, Y.-D. Xiao, T. Y. Phillips, A. Seamans, W. S. Caldwell

1:35 —23. Design, synthesis and pharmacological characterization of selective ligands for neuronal nAChRs. **A. P. Kozikowski**, Z.-L. Wei, J. Lei, Y. Xiao, K. J. Kellar

2:10 —24. $\alpha 7$ -Selective compounds as novel potential therapeutics for CNS diseases. **E. Phillips**

2:45 —25. Subtype selective nicotinic acetylcholine receptor agonists. **P. C. Astles**

3:20 —26. Development of subtype-selective nicotinic receptor ligands as receptor antagonists at the dopamine-releasing receptor subtype. **P. A. Crooks**

3:55 —27. Development of neuronal nicotinic receptor (NNR) agonists as novel analgesics. **W. H. Bunnelle**

SUNDAY EVENING

Section A

Unknown Site -- Unknown Room

Poster Session I

Sponsored by John Wiley & Sons Inc

D. L. Flynn, *Presiding*

6:00 - 8:00

28. Novel Isoxazole Carboxamides as Growth Hormone Secretagogue Receptor (GHS-R) Antagonists. B. Liu, **G. Liu**, Z. Xin, M. D. Serby, H. Zhao, D. H. Falls, C. A. Collins, H. Sham, W. Kaszubska, V. G. Schaefer

29. Discovery of potent biaryl diketopiperazine FSH receptor agonists: rapid lead optimization through parallel synthesis. T. Guo, **G. Dong**, D. Fitzpatrick, P. Geng, K.-K. Ho, C. H. Jibilian, S. G. Kultgen, R. Liu, E. McDonald, K. W. Saionz, K. J. Valenzano, D. Xie, A. E. P. Adang, N. C. R. van Straten, M. L. Webb

30. 3-Phenyl-2-indolylcarbohydrazide and their azo analogues as potent antagonists for the GalR3 receptor. <. **P.** <. **Topiwala**, <. **Chen**, H. Jimenez, M. Reitman, J. M. Wetzel, M. Walker, K. Han, N. Boyle, G. Caputo, G. Muske, M. J. Konkel

31. Discovery of 3-Phenyl-2-indolylcarbohydrazides as Antagonists of the GalR3 Receptor. <. **Chen**, <. **P.** <. **Topiwala**, L. W. Boteju, E. Eldemenky, H. Jimenez, M. Reitman, M. W. Walker, K. Han, N. Boyle, G. Caputo, G. Muske, J. Yang, M. J. Konkel, J. M. Wetzel

32. Pyrazole-based series as selective CCK1-receptor antagonists. **L. Gomez**, J. G. Breitenbucher, K. McClure, N. Shankley, M. Morton, T. Barrett, L. Li, M. Hack, N. Mani, J. Liang, M. Rabinowitz, M. Pippel, C. Sehon, L. Huang

33. Synthesis and SAR studies with a first in class series of non-peptide motilin receptor antagonists. **M. A. Xiang**, **P. Rybczynski**, R. H. K. Chen, M. P. Beavers, D. W. Combs, J. W. Gunnet, W. Hageman, J. B. Moore, L. Zhou, M. Urbanski, K. T. Demarest

34. Synthesis of agomelatonin and biological activity on the rat duodenum motility and crayfish photoreceptors. **A. Lira-Rocha**, V. H. Pérez Castillo, E. B. Naranjo-Rodríguez, O. Espejo González, B. Fuentes-Pardo, A. De la O Martínez

35. Towards a potent small molecule Glucagon receptor antagonist. **R. Kurukulasuriya**, B. K. Sorensen, J. T. Link

36. Antagonists of Glucagon Receptor for Type 2 Diabetes Treatment. **H.-S. Jae**, M. Winn, B. K. Sorensen, J. T. Link, A. L. Alder, N. D. Grihalde, C. W. Lin, S. Hing

37. [11C]-SN003: A potential PET ligand for in vivo imaging of CRF1 receptors. **J. S. D. Kumar**, V. J. Majo, R. V. Parsey, V. Arango, M. D. Underwood, N. R. Simpson, S. Kassir, J. Prabhakaran, J. Arcement, R. L. Van Heertum, J. J. Mann

38. 1,4,5,6-Tetrahydroimidazo[4,5-d][1]benzazepine derivatives 2: Oral active non-peptide antagonists of arginine vasopressin receptors. **H. Koshio**, A. Kakefuda, I. Sato, R. Wakayama, M. Sanagi, J. Tsukada, T. Yatsu, S. Sakamoto, S.-I. Tsukamoto

39. Potent, selective, orally active, nonpeptide vasopressin receptor antagonists. **J. M. Matthews**, A. B. Dyatkin, L. Hecker, D. J. Hlasta, W. J. Hoekstra, B. Poulter, P. Andrade-Gordon, L. de Garavilla, K. Demarest, E. Ericson, J. Gunnet, W. Hageman, R. Look, J. Moore, C. H. Reynolds, B. E. Maryanoff

- 40.** Design, synthesis and pharmacological evaluation of a novel class of potent, selective oxytocin receptor antagonists. **A. Quattropani**, J. Dorbais, D. Covini, S. Halazy, A. Scheer, M. Missotten, G. Ayala, A.-M. De Raemy-Schenk, A. Nichols, R. Cirillo, E. Gillio Tos, L. Golzio, P. Marinelli, C. Giachetti, C. Barberis, A. Chollet, M. K. Schwarz
- 41.** Oral hBNP conjugates Part 1: Design, synthesis and characterization. **N. B. Malkar**, M. A. Miller, M. J. Bednarcik, M. E. Puskas, K. D. James, N. N. Ekwuribe
- 42.** Oral hBNP conjugates Part 2: In vitro activity and bioavailability in rats. **M. A. Miller**, N. B. Malkar, K. G. Yarbrough, D. Surguladze, J. L. Boyer, K. Polowy, K. D. James, N. Ekwuribe
- 43.** 2,3-Diaminopyridine Bradykinin B1 receptor antagonists. **S. D. Kuduk**, C. Ng, D.-M. feng, J. Wai, R. S. L. Chang, C. M. Harrell, K. L. Murphy, R. W. Ransom, D. Reiss, T. Prueksaritanont, C. Tang, G. Mason, S. Boyce, R. M. Freidinger, D. Pettibone, M. Bock
- 44.** C-terminal truncation study of the novel CXCR4 chemokine receptor ligand vMIP-II-(1-21)NH₂. S. C. Vigil-Cruz, **C. Amela-Cortés**, M. M. Rezende, X. Wang, E. M. Perchellet, J.-P. H. Perchellet
- 45.** 4-(9-Aryltropanylidene)methyl)benzamides as Opioid Agonists. **P. M. Pitis**, J. R. Carson, S. J. Coats, E. E. Codd, S. L. Dax, J. Lee, R. P. Martinez, L. A. McKnown, W.-N. Wu, S.-P. Zhang, L. A. Neilson
- 46.** Arylacetamide κ agonists with reduced cytochrome P450 2D6 activity. **C. W. Ajello**, B. Le Bourdonnec, J. A. Cassel, G. Stabley, S. Belanger, R. N. DeHaven, R. E. Dolle
- 47.** Modeling studies of cytochrome P450 2D6 activity of arylacetamide κ agonists. **P. R. Seida**, R. G. Susnow, C. W. Ajello, B. Le Bourdonnec, J. A. Cassel, R. N. DeHaven, R. E. Dolle
- 48.** Novel N-Phenylamino Acetamide Derivatives as Potent and Selective Kappa Opioid Receptor Agonists. **G.-H. Chu**, M. Gu, R. E. Dolle, J. A. Cassel, S. Belanger, T. M. Graczyk, R. N. DeHaven
- 49.** Parallel methods for the preparation of *N*-ethyl-4-[(8-alkyl-8-aza-bicyclo[3.2.1]oct-3-ylidene)-aryl-methyl]-benzamides, powerful mu and delta opioid agonists. **S. J. Coats**, M. J. Schulz, J. R. Carson, E. E. Codd, D. J. Hlasta, P. M. Pitis, D. J. Stone, S.-P. Zhang, S. L. Dax
- 50.** Functionalization of the Ethano Bridge of Orvinols via an Intramolecular Benzyl Transfer. **H. Wu**, W. Chen, D. Bernard, A. D. MacKerell Jr., J. R. Deschamps, A. Coop
- 51.** Discovery of MCH-R1 antagonists from GPCR-directed libraries. **T.-A. Tran**, N. Beeley, B. Thomsen, I.-L. Lin, Y. Sekiguchi

- 52.** Identification of ATC0065 as a potent antagonist of hMCH-R1. **K. Kanuma**, Y. Sekiguchi, K. Omodera, M. Nishiguchi, T. Funakoshi, S. Chaki, B. Kramer, D. Hsu, M. Casper, S.-S. Pleyne, G. Semple, N. Beeley, B. Thomsen, I.-L. Lin, T.-A. Tran
- 53.** Identification of ATC0175 (AR224349) as a potent antagonist of hMCH-R1. **Y. Sekiguchi**, K. Kanuma, K. Omodera, M. Nishiguchi, T. Funakoshi, S. Chaki, B. Kramer, D. Hsu, M. Casper, S.-S. Pleyne, G. Semple, B. Thomsen, I.-L. Lin, T.-A. Tran
- 54.** SAR of a series of 2-substituted 4-amino-quinazolines: Antagonists of hMCH-R1. **B. Kramer**, T.-A. Tran, D. Hsu, M. Casper, S.-S. Pleyne, N. Beeley, B. Thomsen, I.-L. Lin, K. Kanuma, K. Omodera, M. Nishiguchi, T. Funakoshi, S. Chaki, Y. Sekiguchi
- 55.** Synthesis and SARs of Novel Piperazine Derivatives as Melanocortin-4 Receptor Antagonists. **A. Nakazato**, T. Ishii, T. Okubo, D. Nozawa, S. Chaki, T. Ueki, S. Okuyama
- 56.** Discovery of Potent Prostaglandin EP₂ and EP₄ Receptors Agonists that Inhibit Bronchomuscle Constriction in Guinea Pigs. **Z. Zhao**, B. Bao, N. Brugger, D. Fischer, C. Giachetti, L. Golzio, S. Karra, P. Marinelli, S. McKenna, E. Palmer, A. Reddy, Y. Xiao, G. L. Araldi
- 57.** Design, synthesis and biological evaluation of novel aza-prostaglandin derivatives analogs of PGE₂ as selective EP₂ and EP₂ receptors agonists. **G. L. Araldi**, H. Majgier-Baranowska, N. Brugger, D. Fischer, Y. Liao, E. Palmer, Y. Xiao, Z. Zhao
- 58.** Effect of hydroxylation and fluorination of aryloxy phenylpropanamine serotonin and norepinephrine reuptake inhibitors on CYP450 2D6 dependant metabolism. **S. L. Boulet**, B. M. Mathes, K. J. Hudziak, J. R. Boot, A.-H. Clugery, J. D. Findlay, A. A. Lavis, S. Mahadevan, L. Wallace, S. A. Filla
- 59.** Synthesis and discovery of novel small molecule inhibitors of the norepinephrine reuptake transporter. M. Cases, G. Campbell, L. Haughton, **J. J. Masters**, M. W. Walter, P. T. Gallagher, D. R. Dobson, T. Finn, B. Bonnier, C. White, J. D. Findlay, L. Hayhurst, A.-H. Kluge, S. Mahadevan, F. J. Brunelle, C. L. Delatour, A. A. Lavis, N. A. Dezutter, V. N. Vervaeke, J. Y. Liénard, J. R. Boot
- 60.** Synthesis and selectivity studies of yohimbine and its monomeric analogs on α 2c-adrenergic receptors. **S. M. Mustafa**, S. A. Bavadekar, B. M. .. Moore, S. B. Liggett, D. R. Feller, D. D. Miller
- 61.** Synthesis of pipercolic acid based spiro bicyclic peptidomimetic modulators of the dopamine receptor. **R. V. Somu**, R. L. Johnson
- 62.** Design, Synthesis and Evaluation of Enantiomerically Pure Substituted Hexahydropyrazinoquinolines As Potent and Highly Selective Dopamine 3 Receptor Ligands. **K. Ding**, J. Chen, M. Ji, X. Wu, J. Varady, B. Levant, S. Wang

- 63.** Synthesis and SAR of Benzofuran-based H3 Receptor Antagonists. **M. Sun**, C. Zhao, M. Curtis, R. Faghih, G. Gfesser, T. R. Miller, K. Marsh, J. Wetter, T. A. Esbenshade, A. A. Hancock, M. Cowart
- 64.** Probing the ligand-binding pocket of the cannabinoid receptors-Synthesis and testing of novel phenyl substituted side-chain analogs of Δ^8 -THC. **M. Krishnamurthy**, A. M. Ferreira, B. M. Moore
- 65.** Synthesis and structure activity relationship of biaryl cannabinoid mimetics. **K. Worm**, Q. J. Zhou, R. E. Dolle, G. Stabley, R. N. DeHaven
- 66.** Synthesis and biological evaluation of adenosine A_{2a} receptor antagonists. **J. Caldwell**, J. Matasi, D. Tulshian, L. Arik, A. Fawzi, C. Foster, L. K. Isaac, J. Lachowicz, H. Zhang
- 67.** Syntheses of Novel Fluorinated Phencyclidine Analogs: Variation of Ring Sizes. A. Adejare, **S. Sun**
- 68.** Synthesis and evaluation of potential inhibitors and inactivators of γ -aminobutyric acid aminotransferase (GABA-AT). **Z. Wang**, R. B. Silverman
- 69.** 1-(3-Nitro-pyrid-2-yl)-piperazine analog as potent metabotropic Glutamate receptor Inhibitor. **J. Yang**, J. Yao, A. Patel, M. Hachicha, P. Gharagozloo
- 70.** Synthesis of novel metabotropic glutamate receptor ligands. **C. Grube Jørgensen**, J. Kehler, H. Bräuner-Osborne, P. Krogsgaard-Larsen, U. Madsen
- 71.** Library design and synthesis of ionotropic glutamate receptor ligands. **X. Shou**, A. R. Chamberlin
- 72.** Asymmetric synthesis and study of glutamate analogues. **J. K. Nelson**, D. J. Burkhart, A. R. McKenzie, K. I. Myers, X. Zhao, K. R. Magnusson, N. R. Natale
- 73.** Design and synthesis of novel potent aryl substituted benzimidazoles sodium channel blockers. **X. Zhou**, Q. Sun, D. J. Kyle, V. Ilyin, J. Limberis
- 74.** Development of novel sodium channel blockers based on an amitriptyline scaffold, towards the treatment of pain. **D. P. Hudgens**, P. J. Griffith, M. K. Patel, M. L. Brown
- 75.** Quinazolinones and benzothiazinones as novel sodium channel blockers. **S. F. Victory**, Q. Sun, J. Limberis, D. J. Kyle
- 76.** Cinnamoylimidazolidine-2,4-dione derivatives as potent voltage-gated potassium channel modulators for use as anticonvulsants. **C. Y. Kim**, W. Childers, M. Abou-Gharbia, B. Harrison, D. Hurn, K. Mason, M. Bowlby, K. Rhodes, M. Monaghan, H.

Zhang, F. Jow, S. Lin, Q. Wang, T. Lee

77. Design, synthesis and structure-activity relationships of a series of 3-benzoylimidazolidine-2,4-dione derivatives as a Kv1.1/ β 1 potassium channel disinactivator. **C. Y. Kim**, W. Childers, M. Abou-Gharbia, B. Harrison, D. Huryn, M. Bowlby, K. Rhodes, M. Monaghan, H. Zhang, F. Jow, S. Lin, Q. Wang, T. Lee

78. Fused bicyclic dione derivatives as Kv1.1/Kv β 1 potassium channel disinactivators with anticonvulsant activity. **L. Greenblatt**, J. Wu, B. Harrison, D. Huryn, M. Abou-Gharbia, A. Katz, M. Bowlby, F. Jow, Y. Lee, S. Lin, M. Monaghan, K. Rhodes, Q. Wang, H. Zhang

79. Substituted heterocyclicdione amide derivatives as potent voltage-gated potassium channel disinactivators. **J. Wu**, G. Zhang, A. Katz, W. E. Childers Jr., B. Harrison, D. Huryn, M. Abou-Gharbia, M. Bowlby, F. Jow, Y. Lee, S. Lin, M. Monaghan, K. Rhodes, Q. Wang, H. Zhang

80. Synthesis and SAR of a series of cyclic 1,3-diones as Kv1.1/Kv β 1 potassium channel disinactivators possessing anticonvulsant activity. **J. J. Bicksler**, D. Sarantakis, J. Wu, W. E. Childers Jr., B. Harrison, D. Huryn, M. Abou-Gharbia, A. H. Katz, M. Bowlby, F. Jow, Y. Lee, S. Lin, M. Monaghan, K. Rhodes, Q. Wang, H. Zhang

81. Synthesis and structure-activity relationships of a series of bicyclic-1,3-dione derivatives as Kv1.1/Kv β 1 potassium channel disinactivators. **W. E. Childers Jr.**, J. Wu, C. Y. Kim, E. Podlesny, B. Harrison, D. Huryn, M. Abou-Gharbia, A. Katz, M. Bowlby, F. Jow, Y. Lee, S. Lin, M. Monaghan, K. Rhodes, Q. Wang, H. Zhang

82. Enantiospecific Synthesis of nAChR ligands, (R) and (S)-2-(3-pyridyl)-1-azabicyclo[3.2.2]nonane dihydrochloride. B. S. Bhatti, **G. D. Hawkins**

83. Selective α 7 nicotinic receptor ligands. **A. Mazurov**, J. Klucik, L. Miao, T. Y. Phillips, A. Seamans, J. D. Schmitt, C. Miller

84. Structure activity studies of multiple ring analogues of methyllycaconitine. Synthesis of antagonists to the nicotinic acetylcholine receptors. **S. C. Bergmeier**, J. Huang, D. D. Reed, S. McKay, D. B. McKay

85. Structure activity studies of ring E analogues of methyllycaconitine. Synthesis of antagonists to the α 3 β 4* nicotinic acetylcholine receptors. **S. C. Bergmeier**, J. Huang, A. Pulipaka, P. Pulanikat, K. M. Arason, K. Ismail, D. L. Bryant, S. McKay, D. B. McKay

86. Synthesis and SAR evaluation of 3-Amino-5-cyano pyridines as novel α 4 β 2 neuronal nicotinic receptor (NNR) agents. **T. Li**, D. J. Anderson, A. Basha, W. H. Bunnelle, P. Curzon, J. Ji, J. M. Pace, K. Sippy, M. R. Schrimpf, K. Tietje, M. D. Meyer

- 87.** Synthesis and evaluation of 1,2,5-thiadiazolylpiperazines as vanilloid receptor 1 antagonists. **S. F. Victory**, L. Tafesse, B. Shao, L. A. Schmid, E. Gross, K. Islam, Q. Sun, K. J. Valenzano, D. J. Kyle
- 88.** β -Aminotetralin ureas as novel VR1 antagonists: Synthesis, *in vitro* and *in vivo* activity. **M. C. Jetter**, M. A. Youngman, J. J. McNally, M. McDonnell, S. L. Dax, E. E. Codd, R. W. Colburn, D. J. Stone, S.-P. Zhang, C. M. Flores, N. Nasser, A. Dubin
- 89.** Synthesis and evaluation of 4-(2-pyridazine)piperazine-1-carboxamides as Vanilloid Receptor 1 Antagonists. **L. Tafesse**, L. A. Schmid, Q. Sun, Y. Rotshteyn, K. J. Valenzano, D. J. Kyle
- 90.** Synthesis and pharmacology of iodohomovanillic amides as vanilloid (VR1) antagonists. **M. McDonnell**, S. L. Dax, S.-P. Zhang, A. Dubin
- 91.** Anti-tumor and anti-angiogenic activity of heterocycle-bridged fused pyrroloindencarbazoles. **T. L. Underiner**, B. A. Ruggeri, L. Aimone, T. S. Angeles, G. Gessner, E. Hellriegel, C. Robinson, J. Singh, S. X. Yang
- 92.** Benzenesulfonamide derivatives as novel antimicrotubule agents. **J.-W. Chern**, G. S. Chen, K.-Y. Chen, P.-Y. Chen, F.-Y. Chen
- 93.** SU-5416 analogs with anti-proliferative, anti-microtubule and apoptosis inducing properties. **B. Pandit**, P.-K. Li, Z. Hu, D. L. Sackett, Z. Xiao, C. Cheah
- 94.** The discovery of STA-5312 – A Novel microtubule inhibitor demonstrating potent *in vitro* and *in vivo* antitumor activities against MDR cancers. **L. Sun**, K. Koya, H. Li, T. Przewloka, D. James, S. Chen, Z. Xia, G. Liang, N. Tatsuta, Y. Wu, D. Zhou, T. Korbut, Z. Du, M. Ono
- 95.** Concise synthesis and structure-activity relationships of combretastatin A-4 analogues, 1-aryloindoles and 3-aryloindoles, as novel classes of potent antitubulin agents. **H.-P. Hsieh**, J.-P. Liou, Y.-L. Chang, S.-J. Lee
- 96.** Synthesis and SAR studies of novel C-seco-taxoids. **A. Pepe**, I. Zanardi, P. J. Pera, R. Bernacki, C. Ferlini, G. Scambia, G. Fontana, A. Riva, E. Bombardelli, I. Ojima
- 97.** Rational design, synthesis and evaluation of conformationally restrained novel paclitaxel analogs. **L. Sun**, R. Geney, X. Geng, I. Ojima
- 98.** Taxol specificity: yeast vs. mammalian tubulin. **P. Thepchatrri**, J. Nettles, J. P. Snyder, D. Liotta
- 99.** SAR of 14-substituted Taxanes. **G. Fontana**, A. Battaglia, M. L. Gelmi, E. Baldelli, G. Carenzi, E. Bombardelli, C. Manzotti, R. J. Bernacki

- 100.** Synthesis of new polyamine- β -lactam conjugates as potential anti-cancer agents. **I. Zanardi**, G. Varchi, A. Battaglia, I. Ojima
- 101.** Design and synthesis of N-[4-[(2,4-diamino-5-methylfuro[2,3-*d*]pyrimidin-6-yl)thio]benzoyl]-L-glutamic acid as a classical dual inhibitor of TS and DHFR. A. Gangjee, **H. D. Jain**, S. F. Queener, R. L. Kisliuk
- 102.** Design, synthesis and biological evaluation of novel small-molecule inhibitors of Bcl-2 and Bcl-xL proteins based upon gossypol. **G. Tang**, Z. Nikolovska-Coleska, R. Wang, L. Xu, M.-L. Liu, M. zhang, D. yang, Y. Tomita, S. Wang
- 103.** Design, Synthesis and Testing of Novel and Highly Potent Bcl-2 Inhibitors as New Anti-Cancer Agents. **G. Wang**, Z. Nikolovska-Coleska, R. Wang, L. Xu, W.-H. Tang, M.-L. Liu, M. Zhang, D. Yang, M. E. Lippman, Y. Tomita, S. Wang
- 104.** Exploration of analogs of RWJ-540973/JNJ-10198409: Separation of anti-angiogenic and anti-proliferative activities. **U. S. M. Maharroof**, C. Y. Ho, D. W. Ludovici, E. D. Strobel, L. Andracka, H. Lu, R. Tominovich, J. Baker, J. Sechler, C. Burns, T. Garrabrant, J. Mei, R. Tuman, D. L. Johnson, R. A. Galemno Jr.
- 105.** Interference of *Echinacea angustifolia* with cancer chemotherapy. **E. D. Huntimer**
- 106.** Novel anti-proliferatives for Inhibition of Angiogenesis and Cancer. **M. Kawai**, N. Y. BaMaung, R. Craig, M. K. Verzal, P. Lou, J. Wang, P. Tapang, D. H. Albert, Z. Chen, I. Joseph, M. R. Michaelides, J. Henkin, G. Sheppard, Y. Dai, A. Vasudevan, J. Bouska, T. Magoc, S. Anderson, Y.-C. Wang, D. Frost, R. Lesniewski
- 107.** PhosphoSer-cis-Pro isostere inhibits Pin1 23-fold better than the trans-Pro isostere. F. A. Etzkorn, **X. J. Wang**, B. Xu, F. K. Neiler, A. B. Mullins
- 108.** Smac Peptido-mimetics As XIAP Inhibitors. **J. Chen**, N.-C. Zaneta, L. Xu, S. Wang
- 109.** Structure-based design, synthesis and evaluation of conformationally constrained Smac mimetics that target XIAP/caspase-9 interaction site. **H. Sun**, Z. Nikolovska-Coleska, C.-Y. Yang, L. Xu, Y. tomita, K. Krajewski, P. P. Roller, S. Wang
- 110.** 2-Amino- O^4 -benzylpteridines and O^4 -benzylfolic acid: Potent inactivators of O^6 -alkylguanine-DNA alkyltransferase and potential chemotherapy adjuvants. **M. E. Nelson**, N. Loktionova, A. E. Pegg, R. C. Moschel
- 111.** Synthesis and anticancer activity of bis(styrylsulfonyl)methanes. **V. R. Pallela**, M. R. Mallireddigari, S. C. Bell, S. Cosenza, E. P. Reddy, M. V. R. Reddy
- 112.** Synthesis and Biological evaluation of novel cytotoxic thiazolo[5,4-*b*]quinolines derivatives. **M. A. Loza-Mejía**, A. Quintero, J. D. Solano, S. Olvera-Vázquez, A. Lira-Rocha

- 113.** Synthesis and biological evaluation of novel sphingosine analogs. **R. L. Moore**, A. M. Dougherty, D. C. Liotta, F. E. McDonald, A. H. Merrill Jr.
- 114.** Synthesis and biological evaluation of phosphate isosteres as metabolically stable agonists or antagonists of S1P receptors. **F. W. Foss Jr.**, J. J. Clemens, M. D. Davis, K. R. Lynch, T. L. Macdonald
- 115.** Peptide beacons as novel photodynamic therapy (PDT) agents. **J. Chen**, K. Stefflova, S. Kim, M. Niedre, B. Wilson, J. Glickson, G. Zheng
- 116.** Photodynamic therapy (PDT) agent with a built-in apoptosis sensor. **K. Stefflova**, J. Chen, G. Zheng
- 117.** Phthalocyanine-based tumor imaging and photodynamic therapy agents targeting LDL receptors. **H. Li**, S. Kim, D. Marotta, U. Sunar, T. Busch, B. Chance, J. Glickson, G. Zheng
- 118.** Synthesis and utilization of LDL receptor-targeted MRI contrast agent. **I. Corbin**, H. Li, J. Chen, J. D. Glickson, G. Zheng
- 119.** Synthesis of novel bacteriochlorophyll analogs as targeted contrast agents for cancer detection and treatment. **S. Kim**, C. Qi, Y. Chen, H. Li, B. Chance, J. Glickson, G. Zheng
- 120.** Synthesis and Topo I Inhibition of 5-Substituted Camptothecins. **L.-M. Zhou**, Y. Zhou, A. Burgin, X. Mo, D. Zembower, Y. Xie
- 121.** Benzo[*i*]phenanthridines and 6H-Dibenzo[*c,h*][2,6]naphthyridin-5-ones with Potent Topoisomerase I-targeting Activity and Cytotoxicity. A. L. Ruchelman, **S. Zhu**, N. Zhou, A. Liu, L. F. Liu, E. J. LaVoie
- 122.** Synthesis of new coumarin 3-(N-phenyl) sulfonamides and their anticancer activity. **N. S. Reddy**, M. R. Mallireddigari, S. C. Bell, E. P. Reddy, M. V. R. Reddy
- 123.** 3-Aminophenyldihydroindenopyrazole anti-tumor agents with a dual mode of action. **C. Y. Ho**, D. Ludovici, U. Maharroof, E. Strobel, L. Andraka, J. Yen, R. W. Tuman, J. Mei, A. DeVine, R. Tominovich, H. Lu, J. Baker, C. Burns, J. Sechler, D. Johnson, R. A. Galemno
- 124.** Synthesis of novel Chloromethylphenyl purine nucleoside analogues and related compounds. **N. R. Kode**, A. Dare, S. Phadtare
- 125.** Synthesis of novel cyclobutyl nucleosides. **S. Mao**, M. W. Hager, D. C. Liotta
- 126.** Synthesis of phosphoramidate prodrugs of antitumor and antiviral nucleoside analogues. **W. Wu**, R. F. Borch

- 127.** Synthesis of potential tumor vasculature targeting agents. **A. Hannan**, N. J. Lawrence, A. T. McGown, S. Ducki
- 128.** Synthesis of Symmetrical Bis-Alkynyl or Alkyl Pyridine and Thiophene Derivatives and Their Antiangiogenic Activities. **C. M. Ahn**, W.-S. Shin, S. Lee, H.-W. Lee, H. B. Woo
- 129.** Novel 8-substituted dipyrindodiazepinone inhibitors with broad-spectrum of activity against NNRTI-resistant HIV-1. C. Yoakim, P. R. Bonneau, R. Déziel, L. Doyon, J. Duan, I. Guse, B. Haché, S. Landry, E. Malenfant, J. Naud, W. W. Ogilvie, J. A. O'Meara, R. Plante, **B. Thavonekham**, B. Simoneau, M. Boes, M. G. Cordingley
- 130.** Novel inhibitors of respiratory syncytial virus RNA-dependent RNA polymerase. **J. Bordeleau**, M. Liuzzi, S. Mason, G. Bolger, N. Dansereau, G. Fazal, Y. Gaudette, L. Lagacé, S. Landry, J. Rancourt, B. Simoneau
- 131.** SAR of 5,10-dihydrobenzo[b][1,8]naphthyridine N-oxides as Non-Nucleoside Reverse Transcriptase inhibitors of HIV-1 with high potency against clinically relevant mutants variants. **B. L. Johnson**, C. M. Tarby, A. J. Cocuzza, A. Srivastava, D. M. Bilder, R. Bakthavatchalam, Q. Lin, J. D. Rodgers, G. L. Trainor, P. S. Anderson, L. T. Bacheler, S. Diamond, R. M. Klabe, B. C. Cordova, S. Garber, K. Logue, S. Jeffrey, S. Erickson-Viitanen
- 132.** The Synthesis of Pyranoindole Derivatives as HCV Polymerase Inhibitors. **K. Park**, A. Gopalsamy, J. W. Ellingboe, A. Howe, M. Orłowski
- 133.** Tripeptide inhibitors of the Hepatitis C virus serine protease. **E. Ghiro**, M. Bailey, V. Gorys, N. Goudreau, T. Halmos, M. Poirier, J. Rancourt, M. Llinàs-Brunet
- 134.** Design of potent nontoxic nonpeptide-based antimicrobial agents and heparin antidote. **S. Choi**, D. Liu, D. J. Clements, J. D. Winkler, W. F. DeGrado
- 135.** Expedient synthesis and antibacterial evaluation of a library of Kanamycin B analogs. **J. Li**, J. Wang, P. G. Czyryca, H. Chang, C.-W. T. Chang
- 136.** Microwave Synthesis of Biphenyl Hydroxy Furanones as Bacterial Cell Wall Inhibitors. **S. A. Antane**, K. M. Morris, C. Caufield, B. Rasmussen, D. Keeney, P. Petersen, P. Labthavikul, A. Severin
- 137.** Synthesis and Antibacterial Activity of 6-Carbamoyl-11, 12-Lactocethromycin Derivatives. **E. B. Grant**
- 138.** Structure-guided design of Pantothenate Kinase substrate analogues as potential inhibitors. **K. G. Virga**, K. Hevener, Y.-M. Zhang, C. O. Rock, S. Jackowski, H.-W. Park, R. Ivey, R. E. Lee

- 139.** Studies of L-pyranoses on ring III of pyranmycins. **J. Wang, J. Li, C.-W. T. Chang**
- 140.** Design, synthesis and SAR of taxane-based anti-tuberculosis agents. **Q. Huang, I. Zanardi, A. Pepe, P. A. Nair, P. J. Tonge, T. Kirikae, F. Kirikae, I. Ojima**
- 141.** Efforts to understand the uptake, localization and targets of artemisinin action using fluorescent probes. **K. M. Muraleedharan, A. Srivastava, B. L. Tekwani, M. A. Avery**
- 142.** Progress towards the total synthesis of Pseudolaric acid B: A novel antipneumocystic and antifungal natural product. **K. K. Vines, B. E. Watkins, M. A. Avery, D. R. Feller**
- 143.** Synthesis of two Sterol Hydrazone Derivative from 2-Hydrazine-2-imidazoline and their Antiproliferative Evaluation against *Leishmania mexicana*. **G. G. Visbal, A. Alvarez-Aular, R. Luna, D. Arrieche, E. Marchan**
- 144.** Synthesis and antigardial activity of 2-(Trifluoromethyl)benzimidazole derivatives. **F. Hernandez-Luis, M. A. Vilchis-Reyes, L. Yépez-Mulia, A. Hernandez-Campos, R. Castillo, A. Tapia**
- 145.** Synthesis and giardicidal activity of substituted benzoxazole derivatives. **R. Castillo, V. Arroyo-Sánchez, A. Luna-González, J. González- Aguilar, A. Hernandez-Campos, F. Hernandez-Luis, L. Yépez-Mulia, A. Tapia**
- 146.** Synthesis and antiparasitic activity of novel 2-(methylthio)benzimidazole derivatives. **A. Hernandez-Campos, R. Castillo, F. Hernandez-Luis, N. López-Balbiaux, Y. Islas-Fonseca, E. Sandoval-Rivera, L. Yépez-Mulia, A. Tapia**
- 147.** Synthesis and antiprotozoal activity of 1-H and 1-methylbenzimidazole 5(6)-carboxamides. **N. López-Balbiaux, P. Vargas-Benítez, A. Hernandez-Campos, F. Hernandez-Luis, L. Yépez-Mulia, A. Tapia, R. Castillo**
- 148.** Novel Dicationic Fused Ring System DNA-Minor Groove Binders and Antiparasitic Agents. **R. K. Arafa, B. Reto, F. A. Tanious, W. D. Wilson, D. W. Boykin**
- 149.** Synthesis of CAY-1, an antifungal steroidal saponin. **K. L. Bowdy, B. S. Jursic**
- 150.** Synthesis of Protein Farnesyltransferase Inhibitors as Anti-malarial Drugs. **L. Nallan, M. H. Gelb, W. C. Van Voorhis**
- 151.** Synthesis of substrate-mimic analogues of mycothiol as inhibitors of Rv1170 and Rv1082 of *Mycobacterium tuberculosis*. **B. B. Metaferia, C. A. Bewley**
- 152.** Synthesis of two new inhibitors of the sterol 24-methyltransferase and activity

against *Paracoccidioides brasiliensis*. **G. G. Visbal**, G. San-Blas, A. Alvarez-Aular, B. Moreno

MONDAY MORNING

Section A

Unknown Site -- Unknown Room

Alfred Burger Award Symposium - Recent Advances Towards Novel Cardiovascular Therapeutics

K. A. Jacobson, *Presiding*

R. R. Wexler, *Organizer, Presiding*

8:30 — Introductory Remarks.

8:35 —153. Orally efficacious renin inhibitors – New perspectives in a challenging field. **J. Maibaum**

9:10 —154. PPARpanTM Agonists—The Next Generation of PPAR Ligands. **P. L. Feldman**

9:45 —155. Zetia mechanism of action. **S. W. Altmann**

10:20 —156. Discovery of the novel antithrombotic agent BAY 59-7939, an orally active, direct Factor Xa inhibitor. **S. Roehrig**, A. Straub, J. Pohlmann, T. Lampe, J. Pernerstorfer, K.-H. Schlemmer, E. Perzborn

10:55 — Introduction of Alfred Burger Award recipient by Ken Jacobson.

11:05 —157. Design and synthesis of thrombin receptor (PAR-1) antagonists - Award Address. **W. J. Greenlee**

MONDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Diversity and Chemogenomics

Sponsored by Biotage

Cosponsored with ORGN

P. Wipf, *Organizer*

1:30 —158. Expanding chemical diversity using stereocontrolled synthesis. **J. A. Porco Jr.**

2:05 —159. Potentiation of apoptosis: Remarkably potent small molecule Smac replacements. **J. K. De Brabander**, R. M. Thomas, H. Suzuki, L. Li, X. Wang, P. G. Harran

2:40 —160. Identification of Potent, Selective VLA-4 Antagonists As Chemical Tools To Answer Biological Questions. **D. M. Huryn**, S. Ashwell, R. B. Baudy, D. B. ... Dressen, S. B. Freedman, F. S. Grant, J. Kennedy, A. W. Konradi, A. Kreft, L. J. Lombardo, M. A. Pleiss, D. Sarantakis, T. Yednock

3:15 —161. Using small molecule libraries to probe pharmacological space. **J. S. Lazo**

3:50 —162. Diversity-oriented synthesis and ChemBank. **S. L. Schreiber**

Section B

Unknown Site -- Unknown Room

Conventional and Non-Conventional Nucleosides

Sponsored by Idenix Pharmaceuticals

Cosponsored with CARB

V. E. Marquez, *Organizer*

1:30 — Introductory Remarks.

1:35 —163. Zebularine induces and sustains DNA cytosine demethylation in human cancer cells. **P. A. Jones**, J. C. Cheng, C. Yoo, G. Liang, V. E. Marquez

2:15 —164. Nucleoside analogues as agents for the treatment of hepatitis B and C. **R. Storer**

2:55 —165. Novel fluorinated antiviral nucleosides: Synthesis, molecular mechanism and resistance. **C. K. Chu**

3:35 —166. Methylene-cyclopropane analogues of purine nucleosides as agents against drug-resistant cytomegalovirus. **J. Zemlicka, J. C. Drach**

4:15 —167. Fixed conformation nucleoside analogs are effective against excision-proficient HIV-1 RTs. P. L. Boyer, V. E. Marquez, J. G. Julias, **S. H. Hughes**

Integration of Analytical and Experimental Data into Enterprise-Wide Systems

Cosponsored with CINF

Pharmacoproteomics: Tools For Drug Discovery And Drug Evaluation

Cosponsored with BTEC

MONDAY EVENING

Section A

Unknown Site -- Unknown Room

Sci-Mix Session

D. L. Flynn, *Presiding*

8:00 - 10:00

11, 33, 35, 62, 68, 74-75, 87-88, 96, 102-103, 108, 129-131, 150. See previous listings.

173, 216, 220, 225, 232, 236, 241, 244, 249, 253, 258, 266, 274-275, 281, 299, 301-302, 304-305, 312, 327, 329, 333. See subsequent listings.

TUESDAY MORNING

Section A

Unknown Site -- Unknown Room

Graduate Student Award Symposium

K. A. Jacobson, *Presiding*

9:00 —168. Envelope specific anti-hepatitis C agents. **M. L. Mohler**, C. E. Wagner, G. S. Kang, Y.-A. Chang, E. B. Fleischer, K. J. Shea, H. Tani, E. E. Geisert Jr., M. A. Whitt, D. D. Miller

9:20 —169. Thalidomide analogues: dual inhibitors of both angiogenesis and human

cancer cell proliferation. **S. M. Capitosti**, M. L. Brown

9:40 —170. Bicyclomycin Fluorescent Probes: Synthesis and Biochemical, Biophysical, and Biological Properties. **A. P. Brogan**, W. R. Widger, H. Kohn

10:00 —171. Discovery of potent, non-steroidal FXR agonists originating from natural product-like libraries. K. C. Nicolaou, R. M. Evans, **A. J. Roecker**, R. Hughes, M. Downes, J. A. Pfefferkorn

10:20 —172. Progress Toward the Total Synthesis of Amphidinolide B1. **J. S. Schneekloth Jr.**, A. Mandal, C. M. Crews

Section B

Unknown Site -- Unknown Room

General Oral Session II

D. Rotella, *Presiding*

8:30 —173. Combinatorial biosynthesis of novel mTOR inhibitors. **B. Wilkinson**, M. A. Gregory, S. Gaisser, R. E. Lill, R. M. Sheridan, H. Petkovic, A. J. Weston, I. Carletti, J. Staunton, P. F. Leadlay, M. Q. Zhang

8:50 —174. Rapid assembly of diverse and potent Akt inhibitors. **Z. Wu**, J. C. Hartnett, L. A. Neilson, M. T. Bilodeau, G. D. Hartman, S. F. Barnett, D. Defeo-Jones, S. Fu, R. Robinson, H. E. Huber

9:10 —175. Bisarylmaleimides as inhibitors of protein kinase C and glycogen synthase kinase-3. **H.-C. Zhang**, H. Ye, K. B. White, D. F. McComsey, C. K. Derian, B. R. Conway, M. F. Addo, A. J. Eckardt, D. R. Croll, J. Li, L. R. Hecker, L. Westover, J. Z. Xu, R. Look, S. Emanuel, P. Andrade-Gordon, B. P. Damiano, K. T. Demarest, G.-H. Kuo, B. E. Maryanoff

9:30 —176. Discovery and progression of a novel series of orally active p38 kinase inhibitors. **K. Leftheris**, G. Ahmed, R. Chan, A. Dyckman, J. Hynes, S. Lin, A. Metzger, K. Moriarty, Y. Shimshock, J. Wen, J. Wityak, S. Wroblewski, H. Wu, J. Wu, K. Behnia, A. M. Doweiko, K. Gillooly, T. Lin, D. Loo, K. McIntyre, S. Pitt, D. R. Shen, D. Shuster, H. Zhang, R. Zhang, J. Barrish, J. Dodd, I. Henderson, G. Schieven, M. Webb

9:50 —177. The Discovery of Protein Kinase C (PK-C) Isozyme – Specific Ligands Driven by a Solid-Phase Combinatorial Synthesis of Diacylglycerol-Lactones (DAG-lactones). **D. Duan**, M. L. Peach, C. C. Lai, N. E. Lewin, J. A. Kelley, P. M. Blumberg, V. E. Marquez

10:10 —178. Synthesis and SAR of novel, 6-aryl-1,4-dihydrobenzo[d][1,3]oxazine-2-thiones as progesterone receptor modulators leading to the potent and selective non-steroidal PR agonist Tanaproget. **A. Fensome**, R. Chopra, J. Cohen, M. A. Collins, V. Hudak, K. Malakian, A. Olland, K. Svenson, E. A. Terefenko, R. J. Unwalla, J. M. Wilhelm, S. Wolfrom, Y. Zhu, Z. Zhang, P. Zhang, R. C. Winneker, J. Wrobel

10:30 —179. Design and synthesis of ligands for mutated thyroid hormone receptor (R320H) : Tailor-made approach toward the genetic disease. **A. Hashimoto**, Y. Shi, J. T. Koh

10:50 —180. Design and synthesis of novel, potent, and selective PPAR delta agonists. **S. E. Conner**, G. Zhu, C. Montrose-Rafizadeh, R. J. Barr, D. Jett, R. W. Zink, N. Yumibe, N. B. Mantlo

11:10 —181. Discovery of a novel SERM that behaves as a potent Estrogen in CNS neurons but lacks nuclear ER activity. **S. C. Tobias**, J. Qiu, M. J. Kelly, T. S. Scanlan

11:30 —182. Identification of a novel thyroid hormone metabolite with potent physiological effects. **M. E. Hart**, K. L. Suchland, J. Bunzow, P. Kruzich, D. Grandy, G. Chiellini, R. Zucchi, Y. Huang, E. Lim, T. S. Scanlan

TUESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

David Robertson Memorial Symposium

B. K. Trivedi, *Organizer*

1:00 — Introductory Remarks.

1:10 —183. A chemical tag for the estrogen receptor: Affinity labels and the graduate work of David Robertson. **J. A. Katzenellenbogen**

1:50 —184. Testing the Amyloid Hypothesis: Optimization and characterization of a novel small molecule functional g-secretase inhibitor. **J. E. Audia**, J. S. Nissen, T. E. Mabry, S. McDaniel, W. J. Porter, S. S. Henry, T. C. Britton, J. K. Reel, J. J. Droste, D. Mitchell, L. A. Hay, Q. Shi, M. H. Bender, L. N. Boggs, J. W. Cramer, D. Czilli, D. K. Dieckman, C. O. Garner, B. Gitter, P. A. Hyslop, E. M. Johnstone, W. Y. Li, S. P. Little, C. McMillian, F. D. Miller, T. Yin, P. May, E. D. Thorsett, L. H. Lattimer, J. S. Tung, B. K. Folmer, L. Y. Fang, J. Neitz, J. Wu, H. F. Dovey, S. B. Freedman, D. B. Schenk

2:30 —185. Nuclear Receptors as Drug Targets for the Treatment of Metabolic Disease.

R. A. Heyman

3:10 —186. Orally active γ -secretase inhibitors. **R. E. Olson**

3:50 —187. Structure-activity relationships of amino acids that target the $\alpha 2\delta$ protein. **A. J. Thorpe**, T. Belliotti, I. V. Ekhatu, T. Capiris, J. Schwarz, J. Kinsora, M. Vartanian, L. Meltzer, C. Taylor, T.-Z. Su, M. Weber, D. Wustrow, M. Field, M. Dickerson, S. Donevan, Z. Li

WEDNESDAY MORNING

Section A

Unknown Site -- Unknown Room

Inflammation Part I, Emerging Small Molecule Inhibitors for Treatment of Autoimmune and Inflammatory Diseases

Sponsored by Bristol-Myers Squibb

Cosponsored with Inflammation Research Association

J. Kozlowski and D. Lundell, *Organizers*

8:30 — Introductory Remarks.

8:40 —188. Inflammation and the Revolution in the Treatment of Rheumatoid Arthritis. **S. B. Abramson**

9:15 —189. "p-38, MAP- kinase: An exciting target for the treatment of Inflammatory Diseases". **C. Dominguez**, L. Liu, D. Zhang, N. Tamayo, D. Powers, W. Min, F. Feige, R. Harris, S. Wild, S. Neervannan, S. Rashid, T. Harvey

9:50 —190. Selective estrogen receptor-beta agonists are potent antiinflammatory agents. **R. L. Magolda**, M. S. Malamas, R. E. Mewshaw, H. A. Harris, J. C. Keith Jr., B. McDevitt, I. Gunawan, C. P. Miller, L. M. Albert, Y. Leathurby, E. S. Manas

10:25 —191. Development of a potent, orally active antagonist of the human CCR5 receptor. **P. E. Finke**

11:00 —192. Small molecule antagonists for the CXCR2 chemokine receptor: N,N'-Diarylureas and related series. **J. Busch-Petersen**, Q. Jin, B. W. McClelland, H. Nie, M. R. Palovich, R. S. Davis, W. Fu, J. D. Elliott, M. Burman, J. J. Foley, D. B. Schmidt, P. Podolin, B. J. Bolognese, D. C. Underwood, R. R. Osborn, C. J. Dehaas, M. Salmon, D. C. Carpenter, D. J. Killian, H. M. Sarau, K. L. Widdowson

Section B

Unknown Site -- Unknown Room

Anti-Obesity Therapy

Sponsored by GlaxoSmithKline

M. J. Bishop, *Presiding*

9:00 — Introductory Remarks.

9:10 —193. Discovery of potent and selective MCH receptor-1 antagonists for the treatment of obesity. **A. L. Handlon**, K. A. Al-Barazanji, K. K. Barvian, E. C. Bigham, D. L. Carlton, A. J. Carpenter, J. P. cooper, A. J. Daniels, D. T. Garrison, A. S. Goetz, G. M. Green, M. K. Grizzle, Y. C. Guo, D. L. Hertzog, C. E. Hyman, D. M. Ignar, G. E. Peckham, J. D. Speake, C. Britt, W. R. Swain

9:50 —194. Design and synthesis of potent, selective melanocortin subtype-4 receptor agonists for the treatment of obesity. **N. Xi**, J. Adams, Y. Bo, N. Chen, M. Croghan, E. Doherty, N. Han, H. Liao, Q. Liu, M. Kelly, M. Norman, M. Stec, N. Tamayo, S. Xu, J. Cheetham, D. Smith, F. Hsieh, T. Bannon, C. Hale, J. Baumgartner, C. Fotsch

10:30 —195. Opioid receptor antagonists and obesity: non-clinical studies with antagonists of the phenylpiperidine structural class. **C. H. Mitch**, M. L. Heiman, F. C. Tinsley, P. J. Emmerson, D. K. Sindelar, M. A. Statnick

11:10 —196. CB1 antagonists. **J. Antel**

11:50 —197. Nipecotnic acid derivatives as potent, nonselective acetyl-CoA carboxylase inhibitors: A novel approach for obesity. **D. A. Perry**, H. J. Harwood Jr., M. R. Makowski, C. J. Coletta, J. Pyrke-Fairchild, S. F. Petras, L. D. Shelly, L. M. Zaccaro, D. M. Hargrove, K. A. Martin, D. Dalvie, V. Soliman, C. J. Mularski, R. T. Wester, S. A. Eisenbeis

Advances in Virtual High-Throughput Screening

Structure-Based Design Applications

Cosponsored with CINF

WEDNESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

Inflammation Part II, Emerging Small Molecule Inhibitors for Treatment of Autoimmune and Inflammatory Diseases

Sponsored by Novartis

Cosponsored with Inflammation Research Association

L. McQuire, R. J. Cherney, and P. H. Carter, *Organizers*

R. J. Cherney and P. H. Carter, *Presiding*

1:30 — Introductory Remarks.

1:40 —**198.** Cannabinoid receptors as potential therapeutic targets for inflammation. **A. Makriyannis**

2:15 —**199.** Allosteric inhibition of beta 2 integrins by low molecular weight compounds: The molecular basis. **G. Weitz-Schmidt**, K. Welzenbach, J. Dawson, S. Cottens, R. Albert, S. Wattanasin, U. Hommel, J. Kallen

2:50 —**200.** Orally-active ICE inhibitors for the treatment of inflammatory and autoimmune diseases. **J. C. R. Randle**

3:25 —**201.** Discovery and optimization of small molecule CCR2b antagonists. **J. G. Kettle**, D. H. Davies, A. W. Faull, M. A. Stone

4:00 —**202.** CCR3 Antagonists: Lead optimization and identification of a clinical candidate. **S. Hodgson**, C. Eldred, L. Harrison, P. Gore, C. Cook, S. Keeling, S. Swanson, M. Dowle, M. Johnson, E. Robinson, N. Trevedi, T. Redfern

4:35 —**203.** Selective Glucocorticoid Receptor Agonists (SEGRAs). **H. Rehwinkel**, H. Schaecke, K. Asadullah, S. Baeurle, M. Berger, H. Hennekes, S. Jaroch, K. Krolkiewicz, M. Lehmann, A. Mengel, D. Nguyen, A. Reichel, A. Rotgeri, N. Schmees, A. Schottelius, W. Skuballa, P. Strehlke

Section B

Unknown Site -- Unknown Room

Dipeptidyl Peptidase IV Inhibitors

Sponsored by Merck Research Labs, Cosponsored with the Women Chemists Committee (WCC)

A. E. Weber, *Presiding*

1:30 — Introductory Remarks.

1:35 —204. Dipeptidyl peptidase 4 (DPP-4) as a target for type 2 diabetes. **T. E. Hughes**

2:10 —205. Synthesis and biological evaluation of potent, selective, orally active 4-fluoro-2-cyanopyrrolidine inhibitors of DPP-IV. **C. D. Haffner**, D. L. McDougald, S. M. Reister, K. A. Dwornik, S. A. Randhawa, B. D. Thompson, D. J. Cowan, B. R. Henke, R. D. Caldwell, I. W. Kaldor, J. M. Lenhard, D. K. Croom, D. Clancy, D. J. McConn, K. M. Hedeem, K. J. Wells-Knecht, M. Secosky, W. Zhang

2:45 —206. Novel inhibitors of dipeptidyl-peptidase IV. **M. P. Boehringer**, M. Hennig, B. Kuhn, B. M. Loeffler, T. Luebbers, P. Mattei, R. Narquizian, J.-U. Peters, H. P. Wessel, P. Wyss

3:20 —207. Design, synthesis, and pharmacology of BMS-477118: a long-acting, orally active dipeptidyl peptidase IV inhibitor for the treatment of type II diabetes. **L. G. Hamann**, D. J. Augeri, D. A. Betebenner, J. Robl, D. Magnin, A. Khanna, J. G. Robertson, L. M. Simpkins, P. Taunk, D. Sitkoff, C. weigelt, Q. Huang, S.-P. Han, B. Abboa-Offei, A. Wang, M. Cap, L. xin, L. Tao, C. R. Dorso, M. S. Kirby, R. A. Parker

3:55 —208. MK-0431: A potent, orally active DP-IV inhibitor for the treatment of type 2 diabetes. **D. Kim**, L. Wang, J. Kowalchick, E. R. Parmee, L. L. Brockunier, J. He, J. Xu, S. Edmondson, M. Beconi, L. F. Colwell Jr., B. Habulihaz, H. He, B. Leiting, K. A. Lyons, F. Marsilio, R. A. Patel, R. Sinha Roy, Y. Teffera, G. Eiermann, J. K. Wu, M. J. Wyvratt, M. H. Fisher, B. B. Zhang, N. A. Thornberry, A. E. Weber

Advances in Virtual High-Throughput Screening

Property-Based Screening

Cosponsored with CINF

WEDNESDAY EVENING

Section A

Unknown Site -- Unknown Room

Poster Session II

D. L. Flynn, *Presiding*

6:00 - 8:00

- 209.** Comparing the Conformational Behavior of a Series of HIV-1 Protease Inhibitor Drugs using the Low Mode:Monte Carlo Conformational Search Method. **H. Castillo**, C. Parish
- 210.** Rationally designed orthogonal ligand-receptor pair: Implicated as a probe to understand thyroid hormone signaling pathways and associated diseases. **A. Q. Hassan**, J. T. Koh
- 211.** CoMFA and CoMSIA analyses of *Pneumocystis carinii*, *Toxoplasma gondii* and rat liver dihydrofolate reductase (DHFR) inhibitors. A. Gangjee, **X. Lin**
- 212.** Comparing the Conformational Behavior of a Series of Eneidyne Natural Product Anticancer Agents using the Low Mode:Monte Carlo Conformational Search Method. **R. Splain**, C. Parish
- 213.** Computational Study of Phenazine Antibiotics. **T. Su**, D. Vukomanovic, J. A. Stone
- 214.** Docking, CoMFA and CoMSIA studies of HIV-1 reverse transcriptase inhibitors of the pyridinone derivative type. **J. L. Medina-Franco**, S. Rodríguez-Morales, A. Hernandez, C. Juárez-Gordiano, R. Castillo
- 215.** Molecular mechanisms of adefovir resistance in rtN236T HBV polymerase mutant and its sensitivity in 3TC resistant HBV polymerase mutants: A molecular dynamics study. **V. Yadav**, C. K. Chu
- 216.** Highly selective p38-alpha inhibitors for treatment of inflammatory diseases: rapid identification and progression towards drug leads. **I. Popa-Burke**, J. Dickson, J. Mendoza, J. Clark, R. P. Mohny, J. L. Norris, P. Bernasconi, S. Galasinski, K. Williams, W. P. Janzen, C. N. Hodge
- 217.** Discovery & Biological Evaluation of p38 α MAP Kinase Inhibitor SX-011. **Q. Lu**, B. Mavunkel, S. Chakravarty, J. Perumattam, G. Luedtke, Z. Chen, Y.-J. Xu, S. Dugar, A. Protter, G. Schreiner, R. Almirez, B. Scott, M. Laney, M. Henson, J. Lewicki, A. Moore, S. Lee, E. Brahn, D. Liu
- 218.** Discovery and Design of Novel Benzimidazolone as Inhibitors of p38 MAP Kinase. **A. Hammach**, M. Ralph, F. Corbo, A. Barbosa, P. Liu, F. Soleymanzadeh, D. Goldberg, C. Sarko, B. Mckibben, N. Moss, M.-H. Hao, A. White, K. Qian, C. Pargellis, R. Kroe, J. Wildeson, R. Nelson, T. Fadra, A. Capolino, M. Kashem, L. Patnaude, J. Madwed, C. Torcellini, P. Kaplita, T. Farrel, H. Hu, M. Yazdania, K. Kavanaugh
- 219.** Novel Inhibitors of p38 MAP kinase. **R. Shetty**, K. K. Moffett, D. Nguyen, M. J. Kelly, E. L. Michelotti, B. D. Dorsey, E. Springman, M. Bukhtiyarova, K. Northrop, X. Chai, M. S. Saporito, A. R. Ochman, M. Karpusas
- 220.** 7-Aryl substituted-4-anilinoquinoline-3-carbonitriles as potent MEK-1 kinase

inhibitors. **D. M. Berger**, D. Cole, M. Dutia, E. Honores, D. W. Powell, L. Feldberg, D. Wojciechowicz, R. Mallon

221. The effect of linker group and heteroatom modification on a series of quinoline 3-carbonitrile MEK-1 inhibitors - an SAR study. **L. Abrous**, M. Dutia, D. W. Powell, D. M. Berger, K. Collins, D. Wojciechowicz, R. Mallon

222. Design and Synthesis of 2-amino-4-(3-bromoanilino)-6-substituted benzylthieno[2,3-*d*]pyrimidines as Inhibitors of Receptor Tyrosine Kinases. A. Gangjee, **Y. Qiu**, M. A. Ihnat Jr.

223. Development of 2,4,5 substituted pyridines as inhibitors of Akt kinase. **J. C. Hartnett**, Z. Wu, M. T. Bilodeau, G. D. Hartman, S. F. Barnett, D. Defeo-Jones, R. G. Robinson, A. M. Kral, R. E. Jones, H. E. Huber

224. Development of diaryl-naphthyridine inhibitors of Akt kinase. **A. E. Balitza**, S. F. Barnett, M. T. Bilodeau, D. Defeo-Jones, G. D. Hartman, J. M. Hoffman, H. E. Huber, R. E. Jones, A. M. Kral, P. J. Manley, R. G. Robinson, A. M. Smith

225. Discovery of pyrazinyl ureas as inhibitors of the cell-cycle checkpoint kinase Chk1. **E. A. Kesicki**, J. J. Gaudino, A. W. Cook, L. E. Burgess, R. J. Kaufman, B. J. Brandhuber, G. P. A. Vigers, M. L. Howard, M. F. Weidner, E. Dickinson, K. S. Keegan

226. Identification of a new class of Src kinase inhibitors. **D. H. Boschelli**, B. Wu, A. C. Barrios Sosa, H. Durutlic, F. Ye, Y. Raifeld, J. M. Golas, F. Boschelli

227. Optimization of a new class of Src kinase inhibitors. **A. C. Barrios Sosa**, D. H. Boschelli, B. Wu, H. Durutlic, J. M. Golas, F. Boschelli

228. Synthesis and SAR of 7,8-dialkoxy-4-anilinobenzo[*g*]quinoline-3-carbonitriles as potent Src kinase inhibitors. **M. Dutia**, G. H. Birnberg, Y. D. Wang, F. DeMorin, D. H. Boschelli, D. W. Powell, J. M. Golas, F. Boschelli

229. Hydrophobic ligand-protein interactions versus ligand-lipid Interactions of DAG-lactones with protein kinase C (PK-C). **D. M. Sigano**, H. Tamamura, N. E. Lewin, M. L. Peach, M. C. Nicklaus, P. M. Blumberg, V. E. Marquez

230. Synthesis of dequalinium analogues and their inhibitory potencies with protein kinase C. **C. Abeywickrama**, A. D. Baker, S. A. Rotenberg

231. Selective Itk Inhibitors.3. Optimization of the 2-Amino-5-(thioaryl)thiazoles. **J. Das**, J. Wityak, C. Liu, R. V. Moquin, J. A. Furch, J. Lin, S. H. Spergel, A. M. Doweyko, A. Kamath, H. Zhang, K. D. O'Day, B. Penhallow, C.-Y. Hung, S. Kanner, T.-A. Lin, J. H. Dodd, J. C. Barrish

232. Substituted aminobenzimidazole pyrimidines as cyclin-dependent kinase inhibitors.

S. K. Verma, S. Reddy, D. Nagarathnam, J. Shao, L. Zhang, J. Zhao, Y. Wang, T. Li, E. Mull, C. Wang, Q. Zhu, M. Altieri, T.-A. Dang, J. Jordan

233. Synthesis and Discovery of Pyrazine-Pyridine Biheteroaryl as a Novel Series of Potent Vascular Endothelial Growth Factor Receptor-2 (VEGFR-2) Inhibitors. **G.-H. Kuo**, A. Wang, S. Emanuel, A. DeAngelis, R. Zhang, P. J. Connolly, W. V. Murray, R. H. Gruninger, J. Sechler, A. Fuentes-Pesquera, D. Johnson, S. A. Middleton, L. Jolliffe, X. Chen

234. 4(3H)-quinazolinone library synthesis from virtual to reality: A kinase initiative project library. **T. L. Deegan**, R. A. Wildonger, J. W. Lee, R. J. Murphy, D. Yu, M. J. Duffield, K. Daniels, L. Schaffter

235. Structure-activity relationships of rationally designed Hsp90 Inhibitors. **R. C. Clevenger**, B. S. J. blagg, G. Shen

236. The Design and Synthesis of Novobiocin Analogues as Hsp90 C-terminal Inhibitors. **X. M. Yu**, B. S. J. blagg

237. Design and evaluation of mono-charged inhibitors of PTP1B. **D. A. Mareska**, R. D. Groneberg, X. Sun, E. Wallace, M. Rodriguez, A. Toro, D. Clarke, H. Suzuki, K. Ash, J. Yingling, J. Rizzi, G. Vigers, B. Brandhuber, L. E. Burgess, K. Koch, M. Norman, R. Lindberg, J. McCarter, M. Kelly

238. 2,3-Disubstituted pyridine derivatives as non-emetic phosphodiesterase type 4 inhibitors. **T. Nigo**, S. Nakamura, S. Yoshioka, Y. Teranishi, M. N. Itoh, M. Kawasaki

239. Antiasthmatic activity of OS-0217, a novel, orally active phosphodiesterase 4 inhibitor in the guinea pigs, mice and human eosinophils. **S. Nakamura**, S. Yoshioka, Y. Teranishi, T. Nigo, M. Kawasaki, M. N. Itoh

240. Synthesis of deuterium labeled Sildenafil, Tadalafil and Vardenafil. **H. Junga**, N. Weng

241. Identification and SAR of Potent Inhibitors of Phosphodiesterase 7 (PDE7). **J. Guo**, M. Carlsen, J. Barbosa, J. Kempson, C. A. Quesnelle, M. Dodier, A. Watson, K. Donaldson, D. Lee, G. Starling, W. J. Pitts, J. H. Dodd, P. Kiener, M. McKinnon, J. Barrish

242. Design and Synthesis Biotinylated Ligands Exhibiting High Grb2 SH2 Domain-Binding Affinity. **Z.-D. Shi**, H. Liu, M. Zhang, L. R. Roberts, R. J. Fisher, D. Yang, D. Bottaro, M. Linehan, T. R. Burke Jr.

243. A potent and highly selective cyclooxygenase-2 (COX-2) inhibitor from a novel, pyridyl metharyl series. **S. P. Khanapure**, M. E. Augustyniak, R. A. Earl, D. S. Garvey, L. G. Letts, A. M. Martino, M. G. Murty, D. S. Schwalb, M. J. Shumway, A. M. Trocha,

D. V. Young, I. S. Zemtseva, D. R. Janero

244. Synthesis of [¹¹C]-TMI: A potential PET tracer for imaging COX-2 expression. **J. S. D. Kumar**, M. D. Underwood, J. Prabhakaran, R. V. Parsey, V. Arango, V. J. Majo, N. R. Simpson, A. R. Cooper, J. Arcement, R. L. Van Heertum, J. J. Mann

245. Novel Benzimidazole, Carbolone, and Indole Derivatives as cPLA2 Inhibitors. **B. Hu**, A. Oliphant, J. Ellingboe, J. C. McKew, S. Tam, F. E. Lovering, M. Behnke, J. Thomason, M. Shen, W. Zhang, J. D. Clark

246. Synthesis and evaluation of carbocyclic-fused inhibitors of human nonpancreatic Secretory Phospholipase A2. **D. W. Beight**, D. G. Carlson, L. W. Hartley, J. S. Sawyer, E. C. R. Smith

247. The Synthesis and Anti-inflammatory Activity of a Series of N-Substituted Glycolamides of Naproxen: Nitric Oxide Donor Containing Naproxen Prodrugs. **R. R. Ranatunge**, M. E. Augustyniak, V. Dhawan, J. L. Ellis, D. S. Garvey, D. R. Janero, L. G. Letts, S. K. Richardson, M. J. Shumway, A. M. Trocha, D. V. Young, I. S. Zemtseva

248. Design and synthesis of inhibitors of human golgi α -mannosidase II based on the azasugar swainsonine. **S. Anand**, U. Das, D. A. Kuntz, D. R. Rose, J. M. Rimoldi, A. Siriwardena

249. Design and synthesis of potent small molecule inhibitors of α -amylase. **X. Li**, A. Nijjar, A. Mishra, M. Staveski, G. Asmussen, M. Booker, R. Burrier, A. Kloss, R. Holmes-Farley, H. Mandeville, P. Dhal

250. Design and synthesis of peptide hemiaminals as protease inhibitors. **T. M. Ross**, W. P. Malachowski

251. Design, synthesis and biological activities of new potent Factor Xa inhibitor. **H. Nishida**, T. Mukaihira, F. Saitoh, Y. Hosaka, T. Matsusue, I. Shiromizu, M. Kamiya, H. Naba, S. Ohnishi, H. Mochizuki, K. Yanagibashi

252. Non-aromatic D-amino acid-derived inhibitors of human fXa. M. R. Wiley, **S. M. Smith**, J. A. Bastian, N. Y. Chirgadze, T. J. Craft, R. S. Foster, J. B. Franciskovich, L. L. Froelich, P. R. Guzzo, J. Haynes, M. M. Hsia, V. J. Klimkowski, J. K. Kyle, M. J. Mayer, D. Gifford-Moore, C. W. Murray, J. W. Liebeschuetz, J. Marimuthu, J. J. Masters, J. E. Reilly, D. J. Sall, S. M. Sheehan, J. K. Smallwood, G. F. Smith, R. D. Towner, B. M. Watson, S. C. Young, E. F. Kogut

253. Novel solubilizing S4-residues for factor Xa inhibitors: Synthesis and structure-activity relationships of 1-aryl-2-imino-pyrrolidine and -piperidine derivatives. B. Cezanne, **D. Dorsch**, W. W. K. R. Mederski, C. Tsaklakidis, J. Gleitz, S. Anzali

254. SAR investigation of heteroatom containing non-arylglycine inhibitors of human fXa.

M. R. Wiley, **J. A. Bastian**, D. J. Sall, S. M. Smith, N. Y. Chirgadze, C. L. Cioffi, Y. Y. Cheung, T. J. Craft, R. S. Foster, L. L. Froelich, P. R. Guzzo, M. M. Hsia, J. W. Liebeschuetz, V. J. Klimkowski, J. A. Kyle, M. J. Mayer, D. S. Gifford-Moore, C. W. Murray, J. Pan, J. E. Reilly, J. K. Smallwood, G. F. Smith, R. D. Towner, S. C. Young

255. SBDD of novel FXa inhibitors: Using the crystal structures of human FXa complexed with our novel inhibitors and new pharmacophore. **T. Matsusue**, I. Shiromizu, H. Nishida, T. Mukaihira, F. Saitoh, Y. Hosaka, H. Morishita, H. Mochizuki, S. Ohnishi

256. Switching the configuration from L to D of P1' substituents is increasing inhibitory activity for thrombin of DPhe-Pro-DArg-P1'-CONH₂ peptides. **C. C. Clement**, M. Philipp

257. Development of potent inhibitors of thrombin derived by linking of fragments detected by screening using x-ray crystallography. **M. S. Congreve**, G. Chessari, D. J. Davis, S. Howard, R. L. M. Van Montfort, C. W. Murray, N. Howard, C. Abell

258. Discovery and optimization of 4-biphenyl sulfonyl thiophene amidines as a novel class of potent and selective complement C1s inhibitors. **E. M. Khalil**, N. Subasinghe, J. M. Travins, F. Ali, H. R. Hufnagel, S. K. Ballentine, M. D. Gaul, R. M. Soll, M. D. Cummings, R. L. DesJarlais, C. Crysler, R. Bone

259. Synthesis and SAR of some aryl- and heteroarylsulfonyl thiopheneamidines as inhibitors of the complement serine protease C1s. **J. M. Travins**, N. L. Subasinghe, E. M. Khalil, F. Ali, J. Gushue, H. R. Hufnagel, S. K. Ballentine, H. Huang, M. D. Gaul, R. Bone, R. M. Soll, C. Crysler, R. L. DesJarlais, M. D. Cummings

260. Design, Synthesis and SAR of Substituted Pyranoindoles as Inhibitors of Plasminogen Activator Inhibitor-1 (PAI-1) Useful in the Treatment of Atherothrombosis and Fibrinolytic Disorders. **D. Z. Li**, H. Elokdah, G. McFarlane, D. L. Crandall

261. Design, synthesis and SAR analysis of anthrax lethal factor protease inhibitors. C. Tang, **O. Simo**, M. Nagata, G.-S. Jiao, S. O'Malley, M. Goldman, L. Cregar, D. Nguyen, T. Hemscheidt

262. Development of a novel inhibitor of DPP-IV using a byproduct as the lead compound. **K. Kira**, R. S. J. Clark, H. Ikuta, S. Yoshikawa, N. Yasuda, K. Yamazaki, T. Nagakura, O. Takenaka, T. Uehara

263. Dipeptidyl peptidase IV inhibitors derived from β -aminoacylpiperidines bearing a fused thiazole, oxazole, isoxazole, or pyrazole. **W. T. Ashton**, R. M. Sisco, H. Dong, K. A. Lyons, H. He, G. A. Doss, B. Leiting, R. A. Patel, J. K. Wu, F. Marsilio, N. A. Thornberry, A. E. Weber

264. Fused tricyclic piperazine amides derivatives as novel dipeptidyl peptidase-IV

inhibitors. **A. Mastracchio**, S. D. Edmondson, E. R. Parmee, H. He, B. Leiting, K. A. Lyons, F. Marsilio, R. A. Patel, J. K. Wu, M. J. Wyvratt, M. H. Fisher, N. A. Thornberry, A. E. Weber

265. Novel piperazine-substituted, heterocyclic compounds as selective, competitive DPP-IV inhibitors. **R. S. J. Clark**, F. Matsuura, K. Kira, S. Yoshikawa, H. Ikuta, N. Yasuda, **T. Nagakura**, K. Yamazaki, O. Takenaka

266. Preparation and SAR of novel selective cathepsin S inhibitors. M. A. Ashwell, **Y. Liu**, B. Mekonnen, P. Roboissen, M. Cronin

267. Discovery of a novel caspase inhibitor and protection of liver damage in mouse models. **H. K. Chang**, M. Park, J. Park, S. Kim, Y. Oh

268. Synthesis and discovery of PGE-527667, an orally bioavailable Caspase-1 inhibitor. **D. L. Soper**, S. V. O'Neil, Y. Wang, K. A. Oppong, C. D. Ellis, M. C. Laufersweiler, T. P. Demuth Jr., A. N. Fancher, W. Lu, R. L. Wang, W. P. Schwecke, C. A. Cruze, M. Buchalova, M. Belkin, J. A. Wos

269. Development of novel amino-aryl-piperidine-based renin inhibitors. **W. L. Cody**, D. D. Holsworth, N. A. Powell, M. Jalaie, E. Zhang, W. Wang, B. Samas, J. Bryant, R. Ostroski, M. Ryan, J. J. Edmunds

270. Development of novel non-peptidic ketopiperazine-based renin enzyme antagonists. **D. D. Holsworth**, N. A. Powell, W. L. Cody, C. Cai, D. Downing, E. Clay, M. Jalaie, M. Ryan, J. Bryant, R. Ostroski, J. J. Edmunds

271. Ketopiperazine-based renin inhibitors 2. Optimization of the "C" ring. N. A. Powell, D. D. Holsworth, **W. L. Cody**, X.-M. Cheng, C. Lee, N. Erasga, D. M. Downing, C. Cai, E. Clay, M. Jalaie, E. Zhang, J. Bryant, M. Ryan, J. J. Edmunds, T. Li, A. Kasani, E. Hall, R. Subedi, M. Rahim, S. Maiti

272. Ketopiperazine-based renin inhibitors. 3. The S-enantiomer is also active. **N. A. Powell**, E. Clay, F. L. Ciske, D. D. Holsworth, C. Lee, M. Jalaie, J. Bryant, M. Ryan, J. J. Edmunds

273. Ketopiperazine-based renin inhibitors. 4. SAR of C ring benzyl ethers. **N. A. Powell**, E. Clay, D. D. Holsworth, M. Jalaie, J. Bryant, M. Ryan, T. Li, A. Karsana, S. Maiti, J. J. Edmunds

274. Discovery of novel hydantoins as selective non-hydroxamate inhibitors of TNF- α converting enzyme (TACE). **J. E. Sheppeck II**, J. L. Gilmore, A. Yang, C.-B. Xue, X. He, D. Chen, M. B. Covington, R. R. Liu, J. Giannaras, J. J.-W. Duan

275. Reverse hydroxamate derivatives as TNF α convertase inhibitors. **R. W. Wiethe**, M. W. Andersen, R. C. Andrews, J. D. Becherer, D. G. Bubacz, D. M. Bickett, J. H. Chan, J.

G. Conway, D. J. Cowan, M. D. Gaul, M. H. Lambert, M. A. Leesnitzer, D. L. McDougald, J. L. Mitchell, M. L. Moss, D. L. Musso, M. H. Rabinowitz, M. C. Rizzolio, T. K. Tippin, J. R. Warner, L. G. Whitesell

276. TACE inhibitors: discovery of 4-(2-methylquinolin-4-ylmethyl)phenyl as an effective P1' group. **X.-T. Chen**, R. L. Corbett, B. Ghavimi, C.-B. Xue, Z. R. Wasserman, R.-Q. Liu, M. B. Covington, M. Qian, K. G. Vaddi, D. D. Christ, K. D. Hardman, M. D. Ribadeneira, J. M. Trzaskos, R. C. Newton, J. J. -W.Duan, C. P. Decicco

277. Reverse hydroxamate-based selective TACE inhibitors. **M. Shimano**, N. Kamei, T. Tanaka, K. Kawai, K. Miyawaki, A. Okuyama, Y. Murakami, Y. Arakawa, M. Haino, T. Harada

278. Synthesis and evaluation of novel heterocyclic MMP inhibitors. G. R. Cook, **W. Xu**, E. Manivannan

279. 1,2,3,4-Tetrahydroquinolines: Potent, Orally Bioavailable $\alpha_v\beta_3/\alpha_v\beta_5$ Integrin Antagonists. **S. Ghosh**, W. A. Kinney, B. De Corte, L. Liu, J. C. Proost, A. S. Thompson, I. Chen, R. Kawahama, R. Santulli, R. Tuman, R. A. Galemme, D. L. Johnson, B. P. Damiano, B. E. Maryanoff

280. In Vitro and In Vivo Evaluation of a Ketone-Containing $\alpha_v\beta_3$ Integrin Antagonist for the Treatment for Osteoporosis. **R. Meissner**, J. J. Perkins, A. E. Zartman, L. T. Duong, J. E. Fisher, C. Fernandez-Metzler, M. A. Gentile, Y. Meng, G. D. Hartman, D. B. Kimmel, C.-T. Leu, K. Merkle, R. M. Nagy, B. L. Pennypacker, T. Prueksaritanont, G. A. Wesolowski, G. A. Rodan, S. B. Rodan, M. E. Duggan

281. Non-peptidic $\alpha_v\beta_3$ antagonist containing indol-1-yl propionic acids. **J. Gushue, K. Leonard**, W. Pan, B. Anaclerio, Z. Guo, R. L. DesJarlais, J. Lattanze, C. Carl, J. J. Marugan, C. Manthey, B. Tomczuk, T. Lu, T. Markotan, M. Chaikin, R. Donatelli, N. Hubert, S. Eisennagel, M. Desgupta, H. Fries

282. Second generation $\alpha_v\beta_3$ integrin antagonists. N. Danthi, **C. A. Burnett**, J. Xie, Z. Shen, K. C. P. Li

283. A novel microwave assisted synthesis of N-hydroxy, and N- methoxy imides as potential anticancer and antidepressant agents. Y. M. Hijji, **E. Benjamin**

284. A synthesis of dihydropyridones. M. Harmata, **D. R. Lee**

285. Automating TLC to Flash Purification Gradient Methods Containing Polar Solvents. **J. Liu**, S. K. Armentrout, P. Rahn

286. Increasing purification throughput using a new automated flash chromatographic system. **J. Liu**, P. Rahn

- 287.** Minimizing Solvent Impact on Purification of Nitrogen-containing Compounds. **J. Liu**, P. Rahn
- 288.** Solid phase syntheses of cyclophane libraries. **G. Bez**, B. S. J. blagg
- 289.** The Intramolecular Michael Addition as a Route to Five-membered Iminocyclitols. R. M. Moriarty, **H. Kaur**
- 290.** Solubility studies of amine salts: DMSO versus pH 7 buffer as stock solutions. **P. E. Mahaney**, L. M. Mallis, S. Brecker, C. Petucci, G. Stack, G. E. M. Husbands, E. J. Trybulski
- 291.** Prediction of Intestinal and Blood Brain Barrier Permeability Utilizing Immobilized Artificial Membrane Chromatography. A. Adejare, **A. El-Gendy**
- 292.** AEI-Novel Furanocoumarin Inhibitors of CYP3A4. **C. Jen**, C. J. Kelley, D. J. Greenblatt, L. L. von Moltke, J. L. Weemhoff, S. X. Duan, B. W. LeDuc
- 293.** Stability limitation on the use of phosphate promoieties with resonance-stabilized structures in prodrug design. **H. Remes**, J. Rautio, A. Mäntylä, T. Järvinen, J. Vepsäläinen
- 294.** Side chain SAR of dihydrobenzoxathiin SERAMs: bicyclic and heteroatom-substituted amine side chains. **T. A. Blizzard**, F. DiNinno, J. D. Morgan II, H. Y. Chen, J. Y. Wu, C. Gude, S. Kim, W. Chan, E. T. Birzin, Y. T. Yang, L.-Y. Pai, Z. Zhang, E. C. Hayes, C. DaSilva, W. Tang, S. P. Rohrer, J. M. Schaeffer, M. L. Hammond
- 295.** 4-Hydroxy-Phenyl Aryloximes as Estrogen Receptor-Beta (ER β) Selective Ligands. **S. Cohn**, H. Harris, E. Manas, R. E. Mewshaw
- 296.** Estrogen receptor β selective ligands: Exploiting different binding modes within the 6-H-Chromene[c,h] diol template. **R. J. Edsall Jr.**, R. E. Mewshaw, C. Yang, E. S. Manas, H. A. Harris, J. C. Keith Jr., Y. Leathurby, L. M. Albert
- 297.** Structure-based approach towards potent and selective ERR γ (estrogen-related receptor γ) chemical tools. **E. Y. Chao**, J. L. Collins, A. B. Miller, L. A. Orband-Miller, R. T. Nolte, L. Wang, W. Zuercher
- 298.** Synthesis and estrogen binding activity of substituted Naphthalenes: Potential selective estrogen receptor modulators (SERMs). **A. Akwabi-Ameyaw**, J. Fang, D. Heyer, S. R. Katamreddy, A. B. Miller, J. P. Peckham, **F. Navas III**, L. A. Orband-Miller, D. Gray, J. Shearin
- 299.** Indenones: Selective ER/NF- κ B inhibitors. **W. R. Solvibile**, M. A. Ashwell, D. Harnish, C. Chadwick, S. Chippari, T. Kenney, L. Shaw

- 300.** 1,4-Dihydro-benzo[d][1,3]oxazin-2-ones Containing a 6-(5'-Cyanopyrrol-2-yl) Group as Progesterone Receptor Modulators. **P. Zhang**, E. A. Terefenko, J. Kern, A. Fensome, M. A. Collins, V. Hudak, J. Wrobel, Y. Zhu, J. Cohen, R. Winneker, Z. Zhang
- 301.** Synthesis and SAR Studies of 6-Aryl-1,3-dihydro-benzoimidazol-2-ones as Progesterone Receptor Antagonists. **E. A. Terefenko**, J. Kern, A. Fensome, J. Wrobel, Z. Zhang, Y. Zhu, J. Cohen, R. Winneker, **P. Zhang**
- 302.** Human steroid sulfatase, a potential drug target for antiandrogen/antiestrogen therapy: from substrate derived inactivators to potent reversible inhibitors. **E. P. Schreiner**, P. Nussbaumer, P. Lehr, A. Horvath, B. Wolff, A. P. Winiski, A. Billich
- 303.** Synthesis and Structure Activity Relationships of Some Nonsteroidal Selective Androgen Receptor Modulators. **V. A. Nair**, S. M. Mustafa, M. L. Mohler, S. Fischer, J. T. Dalton, D. D. Miller
- 304.** Synthetic Neurosteroids : Synthesis of 3 β and 17-substituted androstan-3 α ols. R. S. Shetty, **L. Kondaveti**, L. Wang, D. Y. W. Lee
- 305.** Design, synthesis and in vivo evaluation of Gamendazole[®], a novel orally active male contraceptive agent. **R. Chakrasali**, **S. R. Jakkaraj**, J. S. Tash, S. A. Hild, B. Attardi, G. I. Georg
- 306.** Design and synthesis of 3-(2-methyl-4-{2-[3-methyl-5-(4-trifluoromethyl-phenyl)-thiophen-2-yl]-propoxy}-phenyl)-propionic acid as a potent selective PPAR delta agonist. **X. Wang**, G. Zhu, R. Barr, C. Montrose-Rafizadeh, J. J. Osborne, N. Yumibe, D. R. Jett, R. W. Zink, N. B. Mantlo
- 307.** Novel PPAR δ agonists via thiophene-assisted stereospecific 1,2-methyl migration. C. R. Schmid, R. Barr, **T. Braden**, C. Montrose-Rafizadeh, J. J. Osborne, R. W. Zink
- 308.** Design and synthesis of novel, potent, and selective PPAR delta agonists. **S. E. Conner**, G. Zhu, C. Montrose-Rafizadeh, R. Barr, D. Jett, R. Zink, N. Mantlo
- 309.** Synthesis and nuclear receptor activities for ring-expanded and -contracted homologs of (9Z)-UAB30, a chemopreventive RXR-selective retinoid. **A. M. Deshpande**, K. K. Vines, D. D. Muccio, W. J. Brouillette
- 310.** Discovery of novel orally efficacious small molecule IL-12 production inhibitors. **E. Kostik**, S. Zhang, T. Przewloka, M. Ono, L. Sun, Y. Wada, D. Cimmanamada, Z. Demko, N. Tatsuta, G. Liang, Q. Wang, D. Zhou, Y. Wu, K. Koya
- 311.** Structural Requirement of New Chalcones for the Inhibitory Activity of Interleukin-5. **S.-H. Jung**, C. Soo-Hyun, J.-H. Lee, J.-H. Ju, M.-K. Kim, S.-H. Lee, J.-C. Ryu, Y. Kim

- 312.** Antidiabetic activity of gallotannin. **Y. Ren**, K. Himmeldirk, Y. Li, J.-K. Kim, X. Chen
- 313.** Impact of terpenoid bisphosphonates on isoprenoid metabolism. **L. W. Shull**, A. J. Wiemer, R. J. Hohl, D. F. Wiemer
- 314.** Design and Syntheses of Benzodiazepine-derived Cyclic Malonamides and Aminoamides as Potent APP Inhibitors. **M. G. Yang**, J.-L. Shi, D. P. Modi, J. Wells, B. M. Cochran, M. A. Wolf, L. A. Thompson, M. Ramanjulu, C. M. Rominger, A. H. Roach, R. Zaczek, R. R. Wexler, R. E. Olson
- 315.** PD 0118057 and PD 0202091: Small molecule inhibitors of beta-amyloid peptide. **C. E. Augelli-Szafran**, F. Bian, M. J. Callahan, R. Feng, A. Iwai, Y. Lai, H. LeVine III, W. Lipinski, L. C. Walker, T. Yasunaga
- 316.** Small molecule modulation of read-through: Cyclic α -phenoxy-N-aryl amides as potential agents for the treatment of Duchenne muscular dystrophy and cystic fibrosis. **J. J. Takasugi**, A. R. Khan, R. G. Wilde, N. G. Almstead, E. M. Welch, J. Zhuo, M. L. Weetall
- 317.** Small molecule modulation of read-through: Hydantoin-substituted benzoic acids as potential agents for the treatment of Duchenne muscular dystrophy and cystic fibrosis. **H. Ren**, R. G. Wilde, S. Hwang, A. R. Khan, E. M. Welch, J. Zhuo, M. L. Weetall, N. G. Almstead
- 318.** Small molecule modulation of read-through: N,N'-Diaryl imidazolidinones as potential agents for the treatment of Duchenne muscular dystrophy and cystic fibrosis. **G.-M. Chen**, G. M. Karp, A. Turpoff, R. G. Wilde, S. W. Jones, N. G. Almstead, E. M. Welch, J. Zhuo, M. L. Weetall
- 319.** Succinoyl Benzazepinones as γ -Secretase Inhibitors. **R. E. Olson**, **N. Wang**, W. E. Fritze, W. Buckner, M. G. Yang, J.-L. Shi, B. M. Cochran, K. Zhao, T. Forsythe, L. Richardson, M. Decaire, M. A. Wolf, A. H. Roach, C. R. Burton, J. M. Meredith Jr., D. A. Seiffert, S. Ren, P. L. Golden, L. Richards, S. A. Grossman, R. Zaczek, D. W. Robertson, R. R. Wexler
- 320.** Design and Syntheses of Non-Peptide γ -Secretase Inhibitors. **A. Adejare**, R. M. Wells, T. E. Golde
- 321.** Synthesis and structure activity relationship of substituted N-phenyl anthranilic acid analogs as amyloid aggregation inhibitors. **L. J. Simons**, C. E. Augelli-Szafran, B. W. Caprathe, J. M. Graham, T. Kimura, Y. Lai, H. LeVine III, A. T. Sakkab, Y. Tasaki, T. Yasunaga, Y. Ye, N. Zhuang
- 322.** Biodistribution and Radiation Dosimetry of [11C]-6-OH-BTA-1 in Baboon. R. V.

Parsey, L. O. Sokol, M.-J. Bélanger, **J. S. D. Kumar**, N. R. Simpson, T. S. Wang, R. L. Van Heertum, J. J. Mann

323. Metabolism and structure activity relationships of the antiepileptic drug Felbamate. **W. F. McCalmont**, T. L. Macdonald

THURSDAY MORNING

Section A

Unknown Site -- Unknown Room

General Oral Session III

D. L. Flynn, *Presiding*

8:30 —324. Design, Synthesis and Evaluation of β -Benzamido Hydroxamic Acid Inhibitors of TNF- α Converting Enzyme (TACE). **G. R. Ott**, Z. Lu, N. Asakawa, M. B. Covington, M. Qian, R.-Q. Liu, R. C. Newton, D. D. Christ, C. P. Decicco, J. J.-W. Duan

8:50 —325. Sulfonamide analogs of indole cPLA2 alpha inhibitors: Are potent, water soluble inhibitors possible? **L. Chen**, W. Wang, K. Lee, M. Shen, J. L. Wu, W. Zhang, X. Xu, S. Tam, J. D. Clark, J. C. McKew

9:10 —326. Structure-based design of serine protease inhibitors: Discovery of cathepsin G and chymase inhibitors containing a novel β -ketophosphonic acid motif. **M. N. Greco**, M. J. Hawkins, E. T. Powell, H. A. Almond, T. Corcoran, L. de Garavilla, J. A. Kauffman, R. Recacha, D. Chattopadhyay, P. Andrade-Gordon, E. Giardino, B. E. Maryanoff

9:30 —327. Targeted Protein Degradation Induced by Small Molecules: A Novel Strategy in Chemical Genetics. **D. Zhang**, S.-H. Baek, K. B. Kim

9:50 —328. New melphalan prodrugs useful in antibody-directed enzyme prodrug therapy (ADEPT). **B. Toki**, C. Cervený, T. Bovee, P. Senter

10:10 —329. Caffeoyle-Based Affinity Acetylators of HIV-1 Integrase as Novel Pharmacological Tools. **S. S. Patil**, N. Shkriabai, X. Zhang, G. C. G. Pais, E. S. Svarovskaia, C. Merchand, V. K. Pathak, Y. Pommier, S. L. Grice, M. Kvaratskhelia, T. R. Burke Jr.

10:30 —330. D- & L-2'-fluoro-2', 3'-unsaturated carbocyclic nucleosides as potential antiviral agents. C. K. Chu, **J. Wang**, Y. Jin, R. F. Schinazi

10:50 —331. Discovery of a Potent Lethal Factor Inhibitor as an Adjunct Therapy of

Anthrax Infection. **Y. Xiong**, W. L. Shoop, J. Wiltsie, A. Woods, J. Guo, J. V. Pivnichny, T. Felcetto, B. F. Michael, A. Bansal, R. T. Cummings, B. R. Cunningham, A. M. Friedlander, C. M. Douglas, S. B. Patel, G. Scapin, S. Salowe, D. M. Zaller, K. T. Chapman, E. M. Scolnick, D. M. Schmatz, K. Bartizal, J. D. Hermes, M. MacCoss

11:10 —332. Discovery of cationic inhibitors of anthrax lethal factor protease. **C. Tang**, O. Simo, S. O'Malley, M. Nagata, M. Goldman, L. Cregar, D. Nguyen, P. Kuzmic, M. Moayeri, S. Leppla, R. Liddington, T. Hemscheidt, G.-S. Jiao

11:30 —333. Inhibition of the Measles Virus cell entry: Fusion blockade. **A. Sun**, R. K. Plemper, K. J. Erlandson, A. Lakdawala, A. Prussia, E. Akisener, I. Yalcin, I. Yildiz, O. Temiz-Arpaci, B. Tekiner, D. C. Liotta, R. W. Compans, J. P. Snyder

Section B

Unknown Site -- Unknown Room

Gamma-Secretase Inhibitors, Sponsored by Eli Lilly & Company

D. G. Brown and R. E. Olson, *Organizers*
M. S. Wolfe, *Presiding*

9:00 —334. Chemical probes for γ -secretase. **M. S. Wolfe**

9:40 —335. Gamma secretase inhibitors as potential Alzheimer's therapeutics. **I. Churcher**

10:20 —336. Inhibition of γ -secretase as an approach to disease-modifying treatment of alzheimer's disease. **R. T. Jacobs**, P. R. Bernstein, C. J. Ohnmacht, J. D. Rosamond, A. B. Shenvi, T. R. Simpson, P. Ciaccio, N. C. Ledonne, F. Liu, T. M. Piser, J. Stahl, G. Tian, B. D. Greenberg

11:00 —337. Arylsulfonamides as Inhibitors of A β Production. **D. W. Smith**, B. Munoz, J. Anderson, J. Arruda, D. Barten, P. Baskin, C. Bergstrom, J. Corsa, K. Felsenstein, V. Guss, G. Holtz, Y. Hu, M. Kounnas, W. Lau, A. Loo, J. Noonan, M. Parker, C. Polson, S. Roberts, J. Roope, C. Sloan, K. Srinivasan, R. Tomlinson, T. Tran, S. Wagner, O. Wallace, B. Wang, R. Wang, J. Wong, F. Yang

11:40 —338. Design, synthesis, and SAR of novel 1,5-benzodiazepine functional γ -secretase inhibitors. **W. J. Porter**, J. K. Reel, J. J. Droste, J. E. Audia, T. C. Britton, B. Gitter, S. S. Henry, P. A. Hyslop, S. P. Little, T. E. Mabry, P. May, S. McDaniel, J. S. Nissen, Q. Shi, L. H. Latimer, J. S. Tung, H. F. Dovey, S. B. Freedman, D. B. Schenk, E. D. Thorsett

Advances in Virtual High-Throughput Screening

Innovative Approaches

Cosponsored with CINF

THURSDAY AFTERNOON

Advances in Virtual High-Throughput Screening

Pharmacophore-Based Approaches

Cosponsored with CINF

[Submit Final Program](#)