# MEDI

## DIVISION OF MEDICINAL CHEMISTRY

### Final Program, 229th ACS National Meeting, San Diego, CA, March 13-17, 2005

D. L. Flynn, *Program Chair*

**SOCIAL EVENTS:**
**Sci-Mix:** Mon
**Social Hour:** Sun

**BUSINESS MEETING:** Sun

### SUNDAY MORNING

Section A

Unknown Site -- Unknown Room

**Cannabinoid Receptors**

D. G. Brown and W. K. Hagmann, *Organizers*

**8:00 —1.** Cannabinoid receptors as therapeutic targets. **F. Barth**

**8:45 —2.** Role of endocannabinoid system in brain reward. **B. R. Martin**

**9:25 —3.** Identification of potent cannabinoid-1 receptor inverse agonists. **W. K. Hagmann**

**10:05 —4.** Identification of triaryl bis-sulfones as novel, orally active cannabinoid-2 (CB2) receptor inverse agonists. **B. J. Lavey**, G. Zhou, J. Spitler, J. Wu, B. Shankar, R. Rizvi, D -Y. Yang, J. Kozlowski, R. W. Hipkin, W. Gonsiorek, L. Bober, J. Fine, A. Rojas-Triana, J. V. Jackson, J. Fossetta, L. Heimark, N. Clarke, R. Wolin, D. Lundell, N -Y. Shih, J. J. Piwinski, S. Narula, C. A. Lunn

**10:45 —5.** Novel pyrimidine CB2 receptor agonists for inflammatory pain. **G. M. P. Giblin**, C. O'Shaughnessy, A. Naylor, W. L. Mitchell, A. Eatherton, K. Jandu, T. Rawlings, B. Slingsby, J. Sweeting, I. Wall, P. Goldsmith, A. J. Brown, C. Haslam, A. Wilson, N. Clayton, A. Whittington, R. Green (Late)

**11:25 —6.** Enzymatic regulation of endogenous cannabinoid signaling. **B. F. Cravatt**

Unknown Site -- Unknown Room

**General Oral Session I**

D. L. Flynn, *Organizer*
B. S. J. Blagg, *Presiding*

**9:00 —7.** Allosteric enhancers of A1 adenosine receptors. **M. D. Chordia**, H. Figler, R. A. Olsson, J. Linden

**9:20 —8.** Discovery and efficacy of the first orally administered derivatives of B-type natriuretic peptide. **K. D. James**, M. A. Miller, N. B. Malkar, D. Severynse-Stevens, K. G. Yarbrough, K. Polowy, M. J. Bednarcik, R. E. Dugdell, A. Cataliotti, J. A. Schirger, R. Krishnan, M. E. Puskas, D. Surguladze, J. L. Boyer, N. N. Ekwuribe, J. C. Burnett Jr.

**9:40 —9.** Design and synthesis of orally efficacious Melanin Concentrating Hormone (MCH) receptor antagonists as antiobesity therapeutics. **M. D. McBriar**, H. Guzik, R. Xu, J. Paruchova, S. Li, A. Palani, S. Shapiro, J. W. Clader, W. J. Greenlee, B. E. Hawes, T. J. Kowalski, K. O'Neill, B. Spar, B. Weig

**10:00 —10.** Over 100 peptide-activated GPCRs recognize turn motifs in ligands. **D. P. Fairlie**, J. D. A. Tyndall, G. Abbenante, B. Pfeiffer

**10:20 —11.** Novel Benzoxazocine Analogues as Potent Analgesic Agents. **A. D. Baxter**, M. Lyne, S. Brown

**10:40 —12.** Opioid Receptor Like (ORL1/NOP) agonists as novel analgesics. **P. D. Ratcliffe**

**11:00 —13.** A Chemical Genetics Approach for the Discovery of Novel Anti-cancer Agents and Targets: Identification of Transferrin Receptor as the Molecular Target of Gambogic Acid, a Rapid and Potent Apoptosis-Inducer. **S. X. Cai**, H -Z. Zhang, K. Jessen, S. Maliartchouk, J. Y. Wang, N. English, L. Qiu, N. Sirisoma, S. Jiang, J. Kuemerle, J. Drewe, K. Gehlsen, B. Tseng, S. Kasibhatla

**11:20 —14.** A chemogenomic approach for ion channel and transport modulators. **H. Heitsch**

**11:40 —15.** Clofibrate-induced changes in the lipid metabolome. **C. E. Wheelock**, J. W. Newman, S. M. Watkins, B. D. Hammock

**12:00 —16.** Rational Design of Multiple Ligands - Risks and Benefits. **J. R. Morphy**

Section C

Unknown Site -- Unknown Room

**MEDI Business meeting**

D. L. Flynn, *Presiding*

**8:30 —17.** Medi Division Business Meeting. **D. L. Flynn**

## SUNDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

**First Time Disclosure of Clinical Candidates: Sponsored by Biotage**

B. Balasubramanian and J. C. Barrish, *Organizers*

**1:30 —18.** Design and synthesis of thrombin receptor (PAR-1) antagonists - Alfred Burger Award Address. **W. J. Greenlee**

**2:20 —19.** Discovery of potent, selective and orally active 5-HT1A agonist, PRX-00023, for the treatment of anxiety, depression and attention deficit hyperactivity disorder. **D. S. Dhanoa**

**3:00 —20.** Design, synthesis and evaluation of novel phosphonates as potent and selective FBPase inhibitors with oral efficacy in rodent models of type 2 diabetes. **Q. Dang**, M. D. Erion, K. R. Reddy, S. R. Kasibhatla, M. R. Reddy, P. D. van Poelje

**3:40 —21.** BMS-599626: A novel dual inhibitor of HER1 and HER2 protein tyrosine kinases. **A. V. Gavai**, B. E. Fink, J. S. Tokarski, D. Fairfax, G. Martin, L. Grubb, Z. Fu, S -H. Kim, K. Leavitt, H. Mastalerz, T. Mitt, J. T. Hunt, J. F. Kadow, K. Du, W -C. Han, D. Norris, B. Goyal, D. M. Vyas, C. Yu, S. Oppenheimer, H. Zhang, F. Y. Lee, T. W. Wong, G. D. Vite

**4:20 —22.** The Discovery of Imidazo[1,2-b][1,2,4]triazines as GABA-Aa2/3 Binding Site Agonists for the Treatment of Anxiety. **L. J. Street**

**Current Aspects of Synthetic Organic Chemistry**

*Cosponsored with ORGN*

## SUNDAY EVENING

Section A

Unknown Site -- Unknown Room

**Poster Session I and Social Hour**

**Sponsored by Eli Lilly & Company**

D. L. Flynn, *Organizer*

**6:00 - 8:00**

**23.** Probing the ligand binding pocket of the cannabinoid receptors - Synthesis, biological evaluation and structure activity relationship studies of novel classical cannabinoid analogs. **M. Krishnamurthy**

**24.** QSAR models for potent CB1/CB2 selective Cannabinoids. **H. Bhattacharjee**, B. M. Moore

**25.** Synthesis and SAR of CB1 Selective Classical/Non-classical Hybrid Cannabinoids. **G. A. Thakur**, A. Makriyannis

**26.** Synthesis and testing of a new series of cannabinoid ligands for positron emission tomography (PET). **P. G. Willis**, A. G. Horti, A. G. Mukhin, O. A. Pavlova, S. I. Chefer

**27.** Discovery and optimization of novel 4,4-disubstituted piperidine derivatives as potent and selective Melanocortin-4 receptor antagonists for the treatment of cancer cachexia. **M. Soeberdt**, R. Bolliger, P. Dunant, M. Henneböhle, K. Hofbauer, S. Leuzinger, J. Magyar, J. Nicholson, F. Schärer, F. Schnüriger, M. Stebler, A. von Sprecher, P. Weyermann

**28.** Discovery of (2S)-N-[(1R)-2-[4-cyclohexyl-4-[[(1,1-dimethylethyl)amino]carbonyl]-1-piperidinyl]-1-[(4-fluorophenyl)methyl]-2-oxoethyl]-4-methyl-2-piperazinecarboxamide (MB243), a potent and selective melanocortin subtype-4 receptor agonist. **B. L. Palucki**, M. K. Park, R. P. Nargund, Z. Ye, I. K. Sebhat, P. G. Pollard, R. N. Kalyani, R. Tang, T. MacNeil, D. H. Weinberg, A. Vongs, C. I. Rosenblum, G. A. Doss, R. R. Miller, R. A. Stearns, Q. Peng, C. Tamvakopoulos, E. McGowan, W. J. Martin, J. M. Metzger, C. A. Shepherd, A. M. Strack, D. E. MacIntyre, L. H. T. Van der Ploeg, A. A. Patchett

**29.** Novel and highly selective antagonist scaffold for human melanocortin 3 receptor:

Computer-aided design and biological evaluation. **A. V. Mayorov**, M. Cai, A. R. Van Scoy, Z. Yu, K. B. Chandler, R. R. Petrov, D. Trivedi, V. J. Hruby

**30.** Synthesis and SAR of novel 4-phenylpiperidine derivatives as potent and selective Melanocortin subtype-4 receptor (MC4-R) antagonists. **P. Weyermann**, R. Bolliger, M. Henneböhle, S. Leuzinger, J. Magyar, F. Schärer, F. Schnüriger, M. Soeberdt, M. Stebler, A. von Sprecher

**31.** Discovery of 2-biaryl-1,4-diaminobutane and 4-biaryl-4-aminomethylpiperidine derivatives as melanin concentrating hormone receptor 1 antagonists through combinatorial chemistry. **D. W. Hobbs**, T. Guo, R. C. Hunter, H. Gu, Y. Shao, G. Qian, S. D. Babu, L. L. Rokosz, T. M. Stauffer

**32.** MCHR-1 Antagonists Incorporating the Phenoxypyridine Motif Showing Subnanomolar Functional Activity. J. Choi, **T -A. Tran**, **S. Han**, B. Kramer, D. Hsu, M. Casper, N. Zou, P. Vallar, J. Xu, B. Thomsen, C. Testa, G. Semple

**33.** Novel Series of 4-(Dimethylamino)quinazoline Containing Heterocylic Ethers as Potent Antagonists of hMCH-R1. J. Choi, T -A. Tran, **B. Kramer**, S. Han, D. Hsu, M. Casper, N. Zou, P. Vallar, J. Xu, B. Thomsen, C. Testa, G. Semple

**34.** 2-{2-[3-(Pyridin-3-yloxy)phenyl]-2H-tetrazol-5-yl}pyridine: A Highly Potent, Orally Active, Metabotropic Glutamate Subtype 5 (mGlu5) Receptor Antagonist. **D. Huang**, S. F. Poon, D. F. Chapman, J. Chung, M. Cramer, T. S. Reger, J. Roppe, L. Tehrani, N. D. P. Cosford, N. D. Smith

**35.** 3-(2-Ethoxy-4-{4-[3-hydroxy-2-methyl-4-(3-methylbutanoyl)phenoxy]butoxy}phenyl)propanoic acid: A Brain Penetrant Allosteric Potentiator at the Metabotropic Glutamate Receptor 2 (mGluR2). **R. V. Cube**, J -M. Vernier, J. H. Hutchinson, M. F. Gardner, J. K. James, B. A. Rowe, H. Schaffhauser, L. Daggett, A. B. Pinkerton

**36.** Benzazoles as allosteric potentiators of metabatropic glutamate receptor 2. **S. P. Govek**, C. Bonnefous, U. C. Campbell, L. Daggett, M. F. Gardner, J. H. Hutchinson, J. K. James, J. McQuiston, R. Pracitto, D. E. Rodriguez, B. A. Rowe, H. Schaffhauser, J -M. Vernier, X. Zhao, T. Kamenecka

**37.** Phenyl-carboxylic indanones: Discovery of positive allosteric potentiatiors of the metabotropic glutamate subtype 2 (mGlu2) receptor. **C. Bonnefous**, J -M. Vernier, J. H. Hutchinson, M. F. Gardner, B. A. Rowe, H. Schaffhauser, U. C. Campbell, D. E. Rodriguez, J. K. James, L. J. Bristow, L. Daggett, T. Kamenecka

**38.** Substituted acetophenones as selective and potent allosteric potentiators of the metabotropic glutamate receptor 2 (mglur2). **A. B. Pinkerton**, R. V. Cube, J. H. Hutchinson, M. F. Gardner, J. K. James, B. A. Rowe, H. Schaffhauser, D. E. Rodriguez, U. C. Campbell, C. S. Baccei, D. S. Lorrain, L. Daggett, J -M. Vernier

**39.** Synthesis and evaluation of 3-benzyloxyaspartate derivatives as EAAT2 inhibitor. **A. Hiratate**, M. Kawamura, M. Nishiguchi, M. Nakamura, N. Kawashima

**40.** The occurrence of D-aspartate and N-methyl-D-aspartate in the serum, liver and brain of chicken (*Gallus domesticus*). **J -J. Poisson**, R. A. Mirza, G. Ferrandino, P. Spinelli, A. D'Aniello, G. Fisher

**41.** Aminoalkoxy indoles: Potent and selective 5ht6 receptor ligands. **R. V. S. Nirogi**, A. V. Daulatabad, S. A. Daulatabad, S. B. Bhosale, N. V. Gaddiraju, R. Dwivedi, M. A. Deshpande, R. S. Kambhampati, V. S. Shirsath

**42.** Bioisosteric modifications of urea derivatives as 5-$HT_{2A}$ inverse-agonists. **S. Strah-Pleynet**, B. R. Teegarden, S. D. Selaya, H. Jayakumar, R. R. Webb, N. R. A. Beeley, W. Thomsen, H. Reyes

**43.** Conformationally restricted aminoalkyl indoles : A new chemical class of selective 5ht6 receptor ligands with drug like properties. **R. S. Kambhampati**, P. Kothmirkar, J. B. Konda, R. F. Kurangi, T. R. Bandyala, S. Kota, S. P. Chinthapalli, V. S. Shirsath, R. V. S. Nirogi

**44.** Construction of Indole Library for Serotonin Related Drugs in Solid-Phase Reaction. H -S. Mun, K -T. Lee, **J -H. Jeong**

**45.** Dialkyl piperazines: A new chemical class of selective 5ht6 receptor ligands. **V. S. Shirsath**, A. D. Deshpande, A. R. Dwarampudi, S. M. Patel, R. K. Badange, V. R. Bhatta, D. Chinthapalli, R. S. Kambhampati, R. V. S. Nirogi

**46.** Evaluation of Selective 5-$HT_{2C}$ Phenylpiperazine Agonists for the Treatment of Obesity. **J. H. Tsai**, B. M. Smith, R. Chen, E. Prieto, D. Park, J. Smith, J. A. Schultz, C. Gallardo, S. Estrada, S. Fang, C. Gilson, W. Thomsen, H. Saldana, C. Bjenning, K. Creehan, L. Gonzalez, K. Whelan, R. R. Webb, N. Beeley

**47.** Molecular modelling of the binding of [18F]-MPPF, a PET radiotracer, on the 5-HT1A cerebral receptors in the rat. L. Montreuil, **R. Terreux**, M. Domard, L. Zimmer

**48.** Synthesis and SAR of Substituted Benzazepines as Selective 5-$HT_{2C}$ Agonists. **J. A. Schultz**, B. M. Smith, J. Smith, J. H. Tsai, C. Gilson, S. Estrada, R. Chen, D. Park, E. Prieto, C. Gallardo, D. Sengupta, W. Thomsen, H. Saldana, C. Bjenning, K. Creehan, L. Gonzalez, K. Whelan, R. R. Webb, N. Beeley

**49.** Synthesis and SAR of substituted diphenylamines as 5-$HT_{2A}$ inverse-agonists. **H. Jayakumar**, B. R. Teegarden, S. Strah-Pleynet, S. D. Selaya, N. Kato, K. Elwell, J. Davidson, Y -J. Shin, R. R. Webb, N. R. A. Beeley, W. Thomsen, H. Reyes, F. Menzaghi, K. Whelan

**50.** Synthesis of (*E*)-4, 3, 2-[$^{11}$C]methoxy-*N*-(4-(4-(2-methoxyphenyl)piperazin-1-yl)butyl)-cinnamoylamides and (*E*)-4, 3, 2-[$^{18}$F]fluoro-*N*-(4-(4-(2-methoxyphenyl)piperazin-1-yl)butyl)-cinnamoylamides as new potential PET dopamine $D_2$ and $D_3$ receptor ligands. **M. Gao**, J -Q. Wang, Q -H. Zheng

**51.** Aplysamine-1 and related analogs as Histamine $H_3$ receptor antagonists. **D. M. Swanson**, S. J. Wilson, J. D. Boggs, A. J. Barbier, W. Xiao, R. Apodaca, T. W. Lovenberg, N. I. Carruthers

**52.** Development of benzimidazoles as ligands for the H4 receptor. **A. Lee**, K. L. Arienti, J. G. Breitenbucher, D. J. Buzard, P. Desai, J. P. Edwards, M. D. Hack, L. Karlsson, H. Khatuya, D. E. Kindrachuk, R. L. Thurmond, J. D. Venable

**53.** Preparation of Benzimidazole Carboxamides as Potent Human Histamine H4 Antagonists. **J. D. Venable**, B. Pio, C. A. Dvorak, C. A. Grice, K. S. Ly, C. R. Shah, J. Wei, P. J. Desai, W. Jiang, S. Nguyen, S. J. Wilson, P. J. Dunford, R. L. Thurmond, T. W. Lovenberg, L. Karlsson, N. I. Carruthers, J. P. Edwards

**54.** Derivatives of cis-1,2,3,6-tetrahydrophthalimide as alpha1A – selective adrenergic receptor antagonists. **P. K. S. Sarma**, S. Jain, N. Sinha, L. G. Hegde, K. Nanda, A. Chugh, J. B. Gupta, N. Anand

**55.** Chiral synthesis of (+)-(S,S)-reboxetine via a new (S)-2-(hydroxymethyl)morpholine preparation: application for the development of new norepinephrine reuptake inhibitors. E. Brenner, R. M. Baldwin, F. tarazi, R. J. Baldessarini, **G. D. Tamagnan**

**56.** Development of polyfluorotropanes for 19F magnetic resonance imaging (MRI) and spectroscopic analysis (MRS) at the dopamine transporter. **A. Zhang**, J. L. Neumeyer, N. S. Kula, K. Zhang, R. J. Baldessarini

**57.** Synthesis and biological activity at monoamine transporters of 3-{2-(diarylmethoxy-ethylidene)}-8-substituted-8-azabicyclo[3.2.1]octane analogues. **S. A. Cararas**, S. Izenwasser, M. L. Trudell

**58.** Synthesis and discovery of novel small molecule inhibitors of the norepinephrine re-uptake 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

**59.** Synthesis and monoamine transporter affinity of GBR12909-benztropine hybrid analogues. **S. Zhang**, S. Izenwasser, M. L. Trudell

**60.** Ab initio conformational studies of imine and ketone analogs: Implications for ChAT inhibitors. **J. P. Bowen**, H. Zhong, E. L. Stewart, M. Kontoyianni

**61.** Synthesis of Some Novel Compounds as Muscarinic Receptor Antagonists. **N. Kumar**, K. Kaur, A. Mehta, S. Arundutt, S. Aeron, S. Dharamarajan, S. Gupta, A. Chugh, J. Gupta

**62.** Endorphins: Biousian glycopeptides cross the BBB due to surfactant properties. **D. R. Polt**, M. Dhanasekaran, R. D. Egleton, E. J. Bilsky, H. I. Yamamura, F. Porreca, I. Alves, G. Tollin

**63.** Mu-selective opioid glycopeptide that crosses the blood-brain barrier. **L. Yeomans**, D. Muthu, C. M. Keyari, N. E. Jacobsen, P. Davis, F. Porreca, J. M. Bidlack, E. J. Bilsky, R. L. Polt

**64.** New benzhydrylpiperazines as potent kappa opioid receptor agonists. **J. Lehmann**, A. Wong, C. Xing, H. Otlik, D. Unett, A. Grottick, J. Gatlin, G. Semple, R. M. Jones

**65.** Novel N-substituted trans-3,4-dimethyl-4-(3-hydroxyphenyl)piperidines as mu selective opioid antagonists. **B. Le Bourdonnec**, W. M. Barker, S. Belanger, J. A. Cassel, R. N. DeHaven, R. E. Dolle

**66.** Rapid optimization of delta selective peptides. **T. O. Schrader**, P. D. Boatman, P. Vallar, D. Unett, B. Thomsen, J. Frazer, J. Adams, D. Connolly, G. Semple

**67.** Syntheses of kappa-opioid receptor ligands: Salvinorin A analogs with modification at C-4 position. **M. He**, D. Y. W. Lee, L -Y. Liu-Chen, Z. Ma, Y. Wang, Y. Chen, W. A. Carlezon Jr., C. Beguin, B. M. Cohen

**68.** Synthesis and binding assay of new dimeric ligands containing the naltrexone pharmacophore for mu and kappa opioid receptors. **Y. Bu**, M. P. Wentland, Q. Lu, J. M. Bidlack

**69.** Synthesis and evaluation of salvinorin A analogues as kappa-opioid receptor ligands for the treatment of mood disorders. **C. Beguin**, M. R. Richards, L -Y. Liu-Chen, D. Y. W. Lee, W. A. Carlezon Jr., B. M. Cohen

**70.** Synthesis and opioid receptor binding properties of conformation-rigidified analogues of 8-carboxamidocyclazocine and 8-formamidocyclazocine. **X. Sun**, M. P. Wentland, R. J. Kucejko, J. M. Bidlack

**71.** Synthesis and structure activity relationship of a series of 2- and 6-substituted trans-3,4-dimethyl-4-(3-hydroxyphenyl)piperidine opioid antagonists. **A. J. Goodman**, B. Le Bourdonnec, M. Michaut, H. F. Ye, S. Belanger, J. A. Cassel, R. N. DeHaven, R. E. Dolle

**72.** Synthesis and evaluation of orally active NK-1 antagonists: C-5 position SAR of the 1,2,3-triazole core. **A. K. Amegadzie**, K. M. Gardinier, J. W. Cramer, D. A. Gehlert, E. J. Hembre, S. Iyengar, L. N. Jungheim, D. L. Li, K. A. Savin, D. A. Schober

**73.** Synthesis and evaluation of orally active NK1 antagonists: Replacement of pyrrolidine with oxazole. **K. M. Gardinier**, A. K. Amegadzie, J. W. Cramer, D. A. Gehlert, E. J. Hembre, S. Iyengar, L. N. Jungheim, D. L. Li, K. A. Savin, D. A. Schober

**74.** Synthesis of 1-[2-(3,5-bis-trifluoromethyl-benzyloxy)-1-phenyl-ethyl]-4-[$^{11}$C]methyl-piperazine and {4-[2-(3,5-bis-trifluoromethyl-benzyloxy)-1-phenyl-ethyl]-piperazine-1-yl}-acetic acid [$^{11}$C]methyl ester as new potential PET $NK_1$ receptor ligands. **M. Gao**, J -Q. Wang, Q -H. Zheng

**75.** Design and synthesis of bradykinin B1 receptor antagonists: Aryl piperidines as potent and selective replacements for biphenyl scaffolds. **C. Ng**, S. D. Kuduk, R. K. Chang, K. L. Murphy, R. W. Ransom, C. Tang, T. Prueksaritanont, R. M. Freidinger, D. J. Pettibone, M. G. Bock

**76.** Design and synthesis of bradykinin B1 receptor antagonists: Development of potent and selective ligands with modified biphenyl motifs. **R. K. Chang**, S. D. Kuduk, C. Ng, K. L. Murphy, R. W. Ransom, C. Tang, T. Prueksaritanont, R. M. Freidinger, D. J. Pettibone, M. G. Bock

**77.** Focused library sets in discovery of dual $AT_1/ET_A$ antagonists. **A. Kiselyov**

**78.** INS50589, a potent, selective, and reversible inhibitor of $P2Y_{12}$ mediated platelet aggregation. **J. G. Douglass**, R. I. Patel, M. C. Cowlen, B. R. Yerxa, S. R. Shaver, S. Mahanty, P. Watson, J. L. Boyer

**79.** Molecular recognition of 3'-modified adenosine neoligands to the human A3 adenosine receptor and its neoceptor. **S -K. Kim**, Z -G. Gao, H. T. Duong, L. S. Jeong, K. A. Jacobson

**80.** Novel pyrazolidine-3,5-dione derivatives are P2Y12 receptor antagonists and inhibit ADP-triggered blood platelet aggregation. **H. Fretz**, O. Houille, K. Hilpert, O. Peter, V. Breu, T. Giller, O. Valdenaire, M. Riederer

**81.** Selective A2B adenosine receptor antagonists: New mono-N-1 alkyl 8-(pyrazol-4-yl) xanthines. **R. Kalla**, E. Elzein, T. Perry, X. Li, T. Maa, A. Gimbel, D. Zeng, J. Zablocki

**82.** Synthesis and binding affinity of 3'-Ureidoadenosine Analogues at the A3 adenosine receptor. **L. S. Jeong**, M. J. Kim, A. Y. Kim, J. A. Lee, K. A. Jacobson, Z -G. Gao, S -K. Kim, M. W. Chun

**83.** Discovery of novel human glucagon receptor antagonists. **D -M. Shen**, F. Zhang, E. J. Brady, M. R. Candelore, V. D. -H.Ding, G. Jiang, S. Mock, S. A. Qureshi, R. Saperstein, C. Tamvakopoulos, X. Tong, L. M. Tota, M. Wright, S. Zheng, K. T. Chapman, B. B. Zhang, J. R. Tata, E. Parmee

**84.** Peptide-directed delivery of small molecule agonists of GLP-1R. **M. B. Scobee**, D. R. Haines, C. I. Worrall, M. Beinborn

**85.** Structure-activity studies of the interaction of GLP-1 with GLP-1R. **K. A. Moy**, D. R. Haines, A. Weight, C. I. Worrall, M. Beinborn

**86.** Design and synthesis of type-II' Î²-turn constrained somatostatin analogues selective for receptor subtype hsst2. **A. Kelleman**, H. Huang, G. Melacini, M. Grant, U. Kumar, M. S. VanNieuwenhze, M. Goodman

**87.** Darmstoff analogues: Subtype-selective agonists and antagonists of LPA receptors. **V. Gududuru**, M. D. Walker, R. Tsukahara, Y. Fujiwara, S. Yasuda, G. Tigyi, D. D. Miller

**88.** Synthesis of Novel Alkyl Thiophosphate Lysophosphatidic Acid (Lpa) Analogues as Receptor (Ant)Agonists. Y. Xu, L. Qian, T. Simper, **G. D. Prestwich**

**89.** Discovery of a highly potent and orally active CCR5 antagonist TAK-652 as an anti-HIV-1 agent: Synthesis and biological activities of 1-benzazocine derivatives containing a sulfoxide moiety. **M. Seto**, K. Aikawa, Y. Aramaki, N. Miyamoto, N. Kanzaki, Y. kuze, K. Takashima, M. Baba, M. Shiraishi

**90.** Discovery of the piperidine-4-carboxamide derivative TAK-220, a highly potent CCR5 antagonist anti-HIV-1 agent. **S. Imamura**, T. Ichikawa, Y. Nishikawa, S. Hashiguchi, N. Kanzaki, K. Takashima, S. Niwa, Y. Yamamoto, M. Baba, Y. Sugihara

**91.** ISO-1, an inhibitor of MIF, protects in endotoxemia and sepsis. **Y. Al-Abed**, K. F. Cheng, D. Dabideen, M. Ochani, B. Aljabari, V. Pavlov, E. Miller, K. Tracey

**92.** Design, synthesis and evaluation of alkyl and aryl substituted N-hydroxyethyl pyrrolidines targeting α-7 nicotinic acetylcholine receptor. **M. G. Puppali**, J. J. Buccafusco, J. W. Beach

**93.** Docking studies involving a homology model of an alpha-7 human neuronal nicotinic receptor. **M. Shelley**, P. S. Hammond, T. Minehardt, J. D. Schmitt

**94.** Homologated monovalent ligands for nicotinic receptors based on polyethylene glycol tethers. **R. W. Fitch**, B. C. Chastain, A. M. Clay, F. M. Bedi, B. T. Elliott

**95.** Human alpha-7 neuronal nicotinic receptor docking studies as an alignment method for Comparative Molecular Field Analysis (CoMFA). **P. S. Hammond**, M. Y. Shelley, T. Minehardt, Y -D. Xiao, J. Klucik, J. D. Schmitt

**96.** Nicotine analogs protect in septic shock and sepsis. **Y. Al-Abed**, H. wang, L. Ulloa, C. A. Amella, M. Tanovic, M. Ochani, K. Tracey

**97.** Structure-activity relationships for cytotoxicity of nicotinic acid ester prodrugs for pulmonary delivery. **L. Xu**, S. M. Vyas, H -J. Lehmler, G. Ludewig

**98.** Synthesis of *N*-[$^{11}$C]methyl-3-[[(dimethylamino)carbonyl]oxy]-2-(2',2'-diphenylpropionoxymethyl)pyridinium as a new potential PET tracer for imaging heart acetylcholinesterase. J -Q. Wang, **M. Gao**, Q -H. Zheng

**99.** Synthetic studies toward Epiquinamide and Analogs. **R. W. Fitch**, S. R. Patel, K. J. Lipscomb

**100.** Unexpected nicotinic effects of nicotinic acid amides. **P. Iturriaga-Vásquez**, J. L. Ulloa, B. K. Cassels, S. Peraccio, I. Bermúdez

**101.** Conformational Analyses of N-Aryl Cinnamides as TRPV1 Antagonists. **J. Zhu**, V. Viswanadhan, V. Ognyanov, Y. Bo, N. Chen, P. P. Chakrabarti, E. Doherty, C. Fotsch, N. Gavva, N. Han, L. Klionski, Q. Liu, R. Tamir, X. Wang, Y. Sun, J. J. S. Treanor, M. H. Norman

**102.** Efforts to circumvent major metabolic pathways of oxidation and glucuronidation in arylurea-based vanilloid (TRPV1) series. **M. E. McDonnell**, J. J. McNally, S -P. Zhang, A. Dubin, S. L. Dax

**103.** N-Pyridin-3-yl- and N-quinolin-3-yl- benzamides: modulators of human vanilloid receptor 1 (VR1). **J. J. McNally**, A. Dubin, M. A. Youngman, M. C. Jetter, S -P. Zhang, M. E. McDonnell, E. E. Codd, R. W. Colburn, D. J. Stone, N. Nasser, C. M. Flores, S. L. Dax

**104.** Analogs of bastadin 5 and structure activity relationships of modulation of the RyR-1 calcium channel. **M. N. Masuno**, I. N. Pessah, T. F. Molinski

**105.** Design, synthesis and SAR of novel and selective T-type calcium channel antagonists containing a biaryl sulfonamide core. J. J. Hangeland, **T. J. Friends**, D. L. Cheney, P. C. Levesque, A. J. Rich, L. Sun, T. R. Bridal, L. P. Adam, D. E. Normandin

**106.** Benzofuroindole analogues as potent $Ca^{+2}$ independent $BK_{Ca}$ channel openers. A. E. Gormemis, T. S. Ha, C -S. Park, **Y -C. Kim**

**107.** Design of a selective small molecule Kv1.3 blocker. **A. Sankaranarayanan**, A. Schmitz, K. Schmidt-Lassen, D. Homerick, W. Hänsel, H. Wulff

**108.** Novel cyclopentane dicarboxamide sodium channel blockers as a potential treatment for chronic pain. **P. Shao**, M. H. Fisher, M. L. Garcia, G. J. kaczorowski, K. Lyons, W. J. Martin, P. T. Meinke, B. T. Priest, M. M. Smith, M. J. Wyvratt, F. Ye, W. H. Parsons

**109.** Pyrazoles as modulators of the cystic fibrosis transmembrane conductance regulator. **M. T. Miller**, F. Chambers III, C. Decker, A. Galue, P. D. J. Grootenhuis, S. S. Hadida,

L. Jiang, Y. Liu, L. R. Makings, P. Negulescu, E. Olson, J. Rader, A. K. Singh, R. D. Tung, F. Van Goor

**110.** Screening for ion channel activity in human T lymphocytes for diagnosis and therapeutic monitoring of multiple sclerosis. **M. Mayer**, S. Memarsadeghi

**111.** Synthesis and evaluation of 5-tert-butyl-trans-2-[F-18]fluoropropynylphenyl-2-methyl-1,1-dioxo-1,3-dithiane (FPMDD) and 5-tert-butyl-trans-2-[F-18]fluoropropynylphenyl-2-methyl-1,1',3-trioxo-1,3-dithiane (FPMTrD) as GABAA-gated chloride ion channel ligands. **X. Li**, Y -W. Jung, S. E. Snyder, P. S. Sherman, M. R. Kilbourn

**112. Novel 5-substituted, 2,4-diaminofuro[2,3-*d*]pyrimidines as potential multi–receptors Tyrosine kinase and Dihydrofolate reductase inhibitors**. **A. Gangjee**, **W. Li**, M. Ihnat, D. Green, W. T. Miller, R. L. Kisliuk

**113.** Immobilization of small-molecule probes for kinase profiling assays. H. K. Patel, **R. M. Grotzfeld**, Z. V. Milanov, S. A. Mehta, A. G. Lai, M. A. Fabian, T. A. Carter, P. T. Edeen, A. M. Velasco, J. M. Ford, M. Floyd, P. Ciceri, D. E. Insko, S. Herrgard, C. E. Atteridge, L. M. Wodicka, W. H. Biggs III, D. K. Treiber, P. P. Zarrinkar, D. J. Lockhart

**114.** Design, synthesis and biological activities of 2-Amino-4-anilino substituted-6-arylethyl pyrrolo[2,3-*d*]pyrimidines as Receptor Tyrosine Kinase inhibitors and Antiangiogenic agents. A. Gangjee, **O. A. Namjoshi**, M. Ihnat, D. Green, W. T. Miller

**115.** Novel 2-amino-4-anilino substituted -7-arylmethyl pyrrolo[2,3-*d*]pyrimidines as Receptor Tyrosine Kinase inhibitors and Antiangiogenic agents. A. Gangjee, **N. Zaware**, M. Ihnat, D. Green, W. T. Miller

**116.** Synthesis and biological evaluation of potential dual ErbB-2/EGFR tyrosine kinase inhibitors: 3,3-Bis(coumarinsulfonyl) methanes. **V. R. Pallela**, M. R. Mallireddigari, K. Gumireddy, S. C. Cosenza, S. C. Bell, E. P. Reddy, M. V. R. Reddy

**117.** Synthesis of 5-[5-[$^{18}$F]fluoro-2-oxo-1,2-dihydroindol-(3*Z*)-ylidenemethyl]-2,4-dimethyl-1*H*-pyrrole-3-carboxylic acid (2-diethylaminoethyl)amide as a new potential PET tracer for imaging cancer tyrosine kinase. J -Q. Wang, **M. Gao**, Q -H. Zheng

**118.** Dihydropyrrolo pyrazole TGF-beta RI inhibitors: a novel benzimidazole series and their selectivity versus TGF-beta R II and MLK7. **Y. Wang**, H. li, S. R. Mundla, L. Yan, R. M. Campbell, B. D. Anderson, J. R. Wagner, J. M. Y. Yingling

**119.** Down Regulation of Erk 1/2 and Stat 3/5 Phosphorylation in Tumor Cells by Novel Styryl Benzylsulfones. **M. V. R. Reddy**, M. R. Mallireddigari, V. R. Pallela, S. C. Cosenza, K. A. Robell, K. Gumireddy, S. C. Bell, E. P. Reddy

**120.** SAR of a series of 3-[6-(4-substituted-piperazin-1-yl)-4-methyl-1H-benzimidazol-2-

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**122.** Successful treatment of diabetic peripheral facial paralysis by injection of Batroxobin: A report of four cases. **Q. Liu**, J. Fan, H. Jiang, J. Liu

**123.** Discovery of potent and specific FLT3 kinase inhibitors. H. K. Patel, Z. V. Milanov, **S. A. Mehta**, R. M. Grotzfeld, A. G. Lai, M. A. Fabian, T. A. Carter, P. T. Edeen, A. M. Velasco, J. M. Ford, P. Ciceri, D. E. Insko, M. Floyd, S. Herrgard, C. E. Atteridge, L. M. Wodicka, W. H. Biggs III, D. K. Treiber, P. P. Zarrinkar, D. J. Lockhart

**124.** Structure-activity relationship of C4-substituted pyrimidopyrimidines; Dual KDR/FGFR tyrosine kinase inhibitors. **P. Rossman**, K. Luk, Y. Chen, L. Garafalo, B. Graves, N. Jackson, M. Kabat, F. Konzelmann, J. -J.Liu, C. Lukacs, L. McDermott, C. Michoud, L. Portland, J. Roberts, A. Schutt, M. Simcox, S. -S.So, B. Tamborini, H. Yang

**125.** Synthesis and Structure-Activity Relationships of Pyrazine-Pyridine Biheteroaryls as Novel, Potent and Selective Vascular Endothelial Growth Factor Receptor-2 (VEGFR-2) Inhibitors. G. H. Kuo, **C. Prouty**, A. Wang, S. Emanuel, A. DeAngelis, Y. Zhang, F. Song, P. J. Connolly, P. Karnachi, X. Chen, R. H. Gruninger, J. Sechler, F -P. Angel, S. A. Middleton, L. Jolliffe, W. V. Murray

**126.** Protein-ligand binding free energy estimation using linear interaction energy method: Application to Grb2 SH2 domain binding ligands. **R. Karki**, S. Oishi, Z -D. Shi, S -U. Kang, K. Lee, C -Q. Wei, K. M. Worthy, L. Bindu, R. J. Fisher, T. R. Burke Jr., M. C. Nicklaus

**127.** Synthesis and SAR of 3-(quinolin-2-yl)indolin-2-ones as kinase inhibitors: Crystallographic evidence for an unique binding conformation. **A. R. Gangloff**, K. Williams, B. R. Paraselli, H. Wijesekera, J. C. Bressi, J. W. Brown, P. H. Vu, A. J. Jennings, M. Tennant, J. Nowakowski, D. Vaughn, C. Caster, J. A. Stafford

**128.** Synthetic approach to compound 48/80 and its analogues. **M. G. Numbere**, H. C. Hailes, E. Rosivatz, R. Byrne, R. Woscholski

**129.** C7-substituted Quinazolinone and Dihydroquinazolinone Inhibitors of p38 MAP Kinase. **J. Bao**, S. Miao, K. M. Rupprech, J. V. Pivnichny, D. M. Zaller, W. L. Shoop, E. A. O'Neill, S. J. O'Keefe, C. M. Thompson, R. M. Cubbon, R. Wang, W. X. Zhang, J. E. Thompson, J. B. Doherty

**130.** Highly selective triazole-based inhibitors of p38-alpha map kinase: progress towards

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**131.** Novel inhibitor of p38 MAP kinase as an anti-TNF-&alpha drug: Discovery of *N*-[4-[2-ethyl-4-(3-methylphenyl)-1,3-thiazol-5-yl]-2-pyridyl]benzamide (TAK-715) as a potent and orally active anti-rheumatic agent. **S. Miwatashi**, Y. Arikawa, E. Kotani, M. Miyamoto, K -I. Naruo, H. Kimura, T. Tanaka, S. Asahi, S. Ohkawa

**132.** Discovery of Pyrrolo[1,2-a]pyrazine analogues as JNK Inhibitors. **S. Thurairatnam**, C. Adams, D. J. Aldous, S. Amendola, D. Chatterjee, N. Hopkins, S. King, J -P. Letallec, T. Majid, N. Moorcroft, A. Ratcliffe, R. Petheram, J. Souness, A. Timm, R. Walsh, R. Walsh

**133.** Development of potent inhibitors for Imatinib (Gleevec) resistant ABL and KIT kinase mutants. **R. M. Grotzfeld**, H. K. Patel, S. A. Mehta, Z. V. Milanov, A. G. Lai, M. A. Fabian, T. A. Carter, P. T. Edeen, A. M. Velasco, J. M. Ford, M. Floyd, P. Ciceri, D. E. Insko, S. Herrgard, C. E. Atteridge, L. M. Wodicka, W. H. Biggs III, D. K. Treiber, P. P. Zarrinkar, D. J. Lockhart

**134.** Design and synthesis of amino-1H-pyrazolo[3,4-d]pyrimidines as novel and selective inhibitors of Tie2 Kinase. **J. Kasparec**, N. W. Johnson, C. Yuan, J. H. Murray, J. L. Adams

**135.** Design and Synthesis of 3,4-dihydroquinazolin-2(1H)-ones as CDK5 inhibitors. **R. M. Rzasa**, M. R. Kaller, E. Magal, G. Liu, T. T. Nguyen, T. Osslund, D. Powers, H -L. Wang, X. Xiong, J. Zhang, W. Zhong, M. H. Norman

**136.** Design and synthesis of benzodiazepinone derivatives as CDK5 inhibitors. **H -L. Wang**, X. Xiong, D. Powers, E. Magal, M. H. Norman

**137.** Design and synthesis of pyridones as CDK5 inhibitors. **M. R. Kaller**, W. Zhong, T. T. Nguyen, R. M. Rzasa, H -L. Wang, M. H. Norman, X. Xiong, D. Powers, W. Wang, C. Henley, E. Magal, J. Zhang, T. Osslund

**138.** Design, synthesis, and biological evaluation of aminothiazoles as selective inhibitors of Cyclin-Dependent Kinase 4 (CDK4). **A. Lovey**, W. Depinto, Q. Ding, N. Jiang, K. Kim, X. Yin, X -J. Chu, D. Bartkovitz, B. Desai, M. Smith, J. Mullin, W. Mccomas, B. Graves, C. Lukacs, S -S. So, Y. Chen, Q. Xiang

**139.** Quinolin-2(1H)-one derivatives as CDK5 inhibitors. **W. Zhong**, H. Liu, M. R. Kaller, T. T. Nguyen, R. M. Rzasa, H -L. Wang, M. H. Norman, X. Xiong, D. Powers, W. Wang, C. Henley, E. Magal, J. Zhang, T. Osslund

**140.** Synthesis of N-acyl sulfonamides as prodrugs of a cyclin-dependent kinase inhibitor. **S. Huang**, R. Lin, P. J. Connolly, S. Emanuel, S. A. Middleton, S. K. Wetter

**141.** Synthesis and evaluation of pyridothienopyrrimidine as potent and selective cdc7 inhibitor. **C. Zhao**, L. Chen, Q. Xu, C. Tovar, L. T. Vassilev

**142.** Protein kinase B/Akt antagonists as antitumor agents Part 1: Discovery of novel, potent and highly selective pyridine-isoquinoline Akt Inhibitors. **J. Gong**, K. W. Woods, T. Li, J. Fisher, G. Packard, V. B. Gandhi, A. Claibone, Y. Luo, Y. Shi, X. Liu, V. Klinghofer, J. Bouska, A. Shoemaker, A. Oleksijew, K. Jarvis, V. S. Stoll, C. Hutchins, R. De Jong, T. Oltersdorf, Q. Li, S. H. Rosenberg, V. L. Giranda, G -D. Zhu

**143.** Protein kinase B/Akt antagonists as antitumor agents Part 2: Rational approach to the identification of oxyindole-pyridine based Akt inhibitors. **V. B. Gandhi**, J. Gong, T. Li, K. W. Woods, J. Fisher, G. Packard, X. Song, Y. Luo, Y. Shi, X. Liu, V. Klinghofer, J. Bouska, A. Shoemaker, A. Oleksijew, K. Jarvis, V. S. Stoll, C. Park, R. De Jong, T. Oltersdorf, Q. Li, S. H. Rosenberg, V. Giranda, G -D. Zhu

**144.** Protein kinase B/Akt antagonists as antitumor agents Part 4: Syntheses of potent, highly selective and orally bioavailable Akt inhibitors with reduced toxicity. **J. Gong**, V. B. Gandhi, T. Li, Y. Luo, Y. Shi, X. Liu, V. Klinghofer, J. Bouska, A. Olson, A. Shoemaker, V. S. Stoll, N. L. Lubbers, J. Polakowski, S. Ballaron, T. J. Campbell, R. De Jong, T. Oltersdorf, Q. Li, S. H. Rosenberg, V. Giranda, G -D. Zhu

**145.** Pyrazyl Phenyl Ureas as Potent and Selective Chk 1 Inhibitors: The Exploration of C6-Position of Pyrazyl Ring and SAR Studies at C4-Position of Phenyl Ring. **Z -F. Tao**, G. Li, G. T. Wang, P. Kovar, H. Zhang, C. Park, K. Stewart, H. L. Sham, T. Sowin, S. H. Rosenberg, N -H. Lin

**146.** Synthesis and biological evaluation of 3-Ethylidene-1,3-dihydro-indol-2-one as novel checkpoint 1 kinase inhibitors. **N -H. Lin**, P. Xia, P. Kovar, C. Park, Z. Chen, H. Zhang, S. Rosenberg, H. L. Sham

**147.** Synthesis and Biological Evaluation of 4-Amino Derivatives of Benzimidazoquinoxaline, Benzimidazoquinoline and Benzopyrazoloquinazoline as Potent IKK Inhibitors. **C. Ouellet**, F. Beaulieu, E. H. Ruediger, M. Belema, J. Banville, J. R. Burke, K. R. Gregor, J. F. MacMaster, A. Martel, K. W. McIntyre, M. A. Pattoli, Y. Qiu, D. Vyas, X. Yang, F. C. Zusi

**148.** Unprecedented olefin-dependent histidine-kinase inhibitory of zerumbone ring opening material. **T. Kitayama**, R. Iwabuchi, S. Minagawa, F. Shiomi, J. Cappiello, S. Sawada, R. Utsumi, T. Okamoto

**149.** Discovery of a novel lead for Protein Tyrosine Phosphatase 1b inhibition. Y -L. Zhang, **E. Binnun**, S. Kirincich, W. Xu, D. Joseph-McCarthy, M. Markus, M. Tam, D. Erbe, D. P. Wilson, Z -K. Wan, B. Follows, J. Wu, A. Moretto, R. Hotchandani, S. Tam, J. Tobin, J. Lee

**150.** Sesterterpenoids and an alkaloid from a Thorectandra sp. as inhibitors of the phosphatase Cdc25B. **S. Cao**, J. S. Lazo, C. Foster, D. G. I. Kingston

**151.** Synthesis and screening of a library of bidentate protein tyrosine phosphatase inhibitors. **J. Xie**, C. T. Seto

**152.** Three new diterpenoids inhibitors of the phosphatase Cdc25B from a marine organism. **S. Cao**, J. S. Lazo, C. Foster, D. G. I. Kingston

**153.** Towards the synthesis of truncated analogues of okadaic acid and their in vitro influence on PP1 activity. **K. K. Sweimeh**, A. R. Chamberlin

**154.** Design and Synthesis of 1-Benzyl-4-phenyl-1H-quinazolin-2-one Derivatives as Selective Phosphodiesterase Inhibitors. **S -Y. Lai**

**155.** Fused pyrimidine based inhibitors of Phosphodiesterase 7 (PDE7) : Synthesis and structure-activity relationships. **J. Kempson**, A. Marinier, M. Dodier, C. A. Quesnelle, P. Gill, J. Barbosa, J. Guo, M. Carlsen, A. Watson, K. Stebbins, D. Lee, G. Starling, A. Martel, W. J. Pitts, J. H. Dodd, P. Kiener, J. Barrish, M. McKinnon

**156.** Substituted pyrimidines as potent and selective inhibitors of phosphodiesterase 7 (PDE7). **A. Marinier**, M. Dodier, C. A. Quesnelle, P. Gill, J. Barbosa, J. Guo, J. Kempson, M. Carlsen, A. J. Watson, K. L. Stebbins, D. Lee, G. C. Starling, A. Martel, W. J. Pitts, J. H. Dodd, P. A. Kiener, J. C. Barrish, M. Mckinnon

**157.** Synthesis and biological evaluation of dihydrobenzofurans as PDE4 inhibitors. **K. Yanagawa**, T. Kawakita, H. Manabe, M. Ichimura, R. Hirose, E. Ohshima

**158.** Aza-bicyclic amino acid amides as a4b1/a4b7 integrin receptor antagonists. **A. B. Dyatkin**, Y. Gong, T. A. Miskowski, B. E. Maryanoff, W. A. Kinney, E. S. Kimball, R. Santulli, M. C. Fisher, P. J. Hornby, W. He

**159.** Integrin $\alpha_v\beta_3$-targeted optical imaging probes. **C. A. Burnett**, J. Xie, J. Quijano, F. Hunter, H. Sun, M. Bur, K. C. P. Li, S. N. Danthi

**160.** Synthesis and Evaluation of 2-Aza-bicyclo[2.2.2]octane-Containing α4β1 Integrin Antagonists in Animal Models of Asthma. **E. C. Lawson**, W. M. Abraham, B. P. Damiano, A. B. Dyatkin, L. De Garavilla, W. A. Kinney, B. E. Maryanoff, C. Page, S. Rudman, R. Santulli

**161.** Betamethasone 17α-carbamates as potent, dissociated glucocorticoid receptor agonists. **G. G. Weingarten**, K. Biggadike, T. I. Jack, P. S. Jones, A. J. Harker, S. J. Taylor

**162.** Conformational analysis of 17alpha-(phenylvinyl) estradiol conjugates using 1D and 2D NMR and computational methods. **E. Y. Hua**, E. McCaskill, D. A. Forsyth, R. N.

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**163.** Discovery and synthesis of novel selective estrogen receptor alpha modulators (SERAMS). **K. D. Dykstra**, L. Guo, E. Birzin, W. Chan, Y. T. Yang, L. Colwell, R. Mosley, B. Kraker, J. Dahllund, F. DiNinno, S. P. Rohrer, J. M. Schaeffer, M. Hammond

**164.** Identification and synthesis of the metabolites M1 and M17 of an ER alpha-selective antagonist for Osteoporosis. **J. Y. Wu**, S. Kim, Z. Zhang, W. Tang, G. Doss, B. Dean, F. DiNinno, M. L. Hammond

**165.** Molecular dynamics studies of (17alpha,20E)-21-(2-/3-/4-substituted phenyl)-19-norpregna-1,3,5(10),20-tetraene-3,17beta-diols as ligands for the estrogen receptor-alpha-ligand binding domain (ERalpha-LBD). **R. N. Hanson**, R. Dilis

**166.** New synthesis of potent apoptotic steroidal 17-alpha-[(4-amino)phenyl]-(Z)-vinyl estradiol. **P. Tongcharoensirikul**, J. A. Mobley, J. O. L'Esperance, S -M. Ho, R. N. Hanson

**167.** Newly discovered orally active pure antiestrogens. **Y. Kanbe**, M -H. Kim, M. Nishimoto, Y. Ohtake, N. Kato, S -I. Kaiho, I. Ohizumi, T. Yoneya, T. Tsunenari, K. Taniguchi, H. Araya, S. Kawata, Y. Nabuchi, K. Morikawa, J -C. Jo, H -A. Kwon, H -S. Lim, H -Y. Kim

**168.** Preparation of heteroarylvinyl estradiols: Comparison of Suzuki and Stille coupling reactions. **K. Gandiaga**, P. Tongcharoensirikul, R. N. Hanson

**169.** Synthesis and applications of tether-containing indole estrogens. **B. G. Trogden**, S. H. Kim, J. A. Katzenellenbogen

**170.** Synthesis and evaluation of a new series of 17alpha-(phenylvinyl) estradiol conjugates as probes for the estrogen receptor-alpha ligand binding domain (ERalpha-LBD). **R. N. Hanson**, E. McCaskill

**171.** Synthesis and evaluation of isomeric (17alpha,20E)-11beta-methoxy-21-(trifluoromethylphenyl)-19-norpregna-1,3,5(10),20-tetraene-3,17beta-diols as ERalpha-hormone binding domain ligands: Effect of the methoxy group on receptor binding and uterotrophic growth. **R. N. Hanson**, P. Tongcharoensirikul, R. Dilis, A. Hughes, E. R. DeSombre

**172.** Identification of a Selective Inverse-Agonist for the Orphan Nuclear Receptor ERRa. **B. B. Busch**

**173.** Synthesis and Androgen Receptor Affinity of Several Linkages of 1,3-Disubstituted-2-hydroxy-2-methylpropionamide Selective Androgen Receptor Modulators (SARMs). **D. J. Hwang**, J. Kim, J. T. Dalton, D. D. Miller

**174.** Synthesis and biological evaluation of N-arylpiperazine 1-carboxamides as novel peripherally selective androgen receptor antagonists. **E. Kawaminami**, I. Kinoyama, E. Nozawa, T. Kamikubo, M. Imamura, A. Toyoshima, K. Samizu, N. Taniguchi, H. Koutoku, T. Furutani, M. Okada, M. Ohta

**175.** Synthesis and biological evaluation of potent, efficacious androgen antagonists based on pyridono[5,6-*g*]quinolines. **R. I. Higuchi**, K. L. Arienti, L. G. Hamann, F. J. Lopez, D. E. Mais, B. A. Pio, T. K. Jones, B. Risek, K. B. Marschke, W. T. Schrader

**176.** Synthesis and Biological Testing of (2S)-Multi-Halogenated B-ring 2-Hydroxy-2-methylpropionamide Selective Androgen Receptor Modulators (SARMs): Probing the B-ring Pocket. **D. J. Hwang**, J. Chen, J. Kim, J. T. Dalton, D. D. Miller

**177.** Synthesis of Isothiocyanate Derivatives of Irreversible Selective Androgen Receptor Modulators (SARMs) and Biological Testing in Prostate Cancer Cell Lines. **D. J. Hwang**, J. Chen, H. Xu, S. M. Mustafa, J. T. Dalton, D. D. Miller

**178.** Synthesis of New Steroidal 5-Alpha-Reductase Inhibitors. **E. Bratoeff**, M. Cabeza, M. Ochoa, N. Teran, E. Ramirez, V. Perez, D. Valdez

**179.** Chromone and Flavone based ligands for Retinoic Acid Receptors. **S. Desai**, S. Nantogmah, D. Soprano, J. L. Gabriel, D. J. Canney

**180.** Conformationally defined retinoic acid analogs: Synthesis and structure-activity relationships for ring-substituted analogs of 9cUAB30. **A. M. Deshpande**, V. R. Atigadda, K. K. Vines, M. Xia, X -K. Zhang, D. D. Muccio, W. J. Brouillette

**181.** Design and structure-activity relationships of novel indole-based PPAR agonists as antidiabetic agents. **H. P. Hsieh**, N. Mahindroo, C -C. Wang, C -F. Huang, T -W. Lien, C -H. Tsai, Y -H. Peng, L -H. Lee, E. Prakash, W -C. Chen, Y -W. Chang, T -A. Hsu, X. Chen, S -Y. Wu, C -T. Chen, S -J. Lan, Y -S. Chao

**182.** Design, synthesis and SAR of indole-based PPAR agonists. H. P. Hsieh, N. Mahindroo, **M. S. Coumar**, C -C. Wang, C -F. Huang, T -W. Lien, C -H. Tsai, Y -T. Lin, L -H. Lee, E. Prakash, T -A. Hsu, X. Chen, S -Y. Wu, C -T. Chen, Y -S. Chao

**183.** Fluorescence based high throughput assays for identification of PPARγ modulators. **M. S. Shekhani**, **H. C. Eliason**, D. A. Lasky, N. Qadir, S. R. Duff, K. L. Vedvik, L. J. Aston, S. Hayes, K. W. Vogel

**184.** Novel dual activators of PPAR- α and γderived from Benzoxazinone containing thiazolidine diones having antidiabetic and hypolipidemic potential. **G. R. Madhavan**, R. Chakrabarti, K. A. Reddy, P. B. Rao, V. Balraju, B. M. Rajesh, R. Rajagopalan

**185.** Troglitazone and Its Derivatives Induce Degradation of Cyclin D1 through A Peroxisome Proliferator-Activated Receptor gamma-Independent Mechanism in Breast

Cancer Cells. **J -W. Huang**, **C -W. Shiau**, Y -T. Yang, K -F. Chen, S. K. Kulp, C -S. Chen

**186.** Fluorometric and LC-MS investigation on prooxidant and antioxidant activities of NO. **Q. Li**, A. C. Nicolescu, G. R. J. Thatcher

**187.** Non-*seco*-steroidal vitamin $D_3$ analogs bearing a dicarba-*closo*-dodecaborane. **H. Kagechika**, K. Yaguchi, C. Songkram, A. Tanatani, Y. Taoda, T. Yoshimi, E. Kawachi, Y. Endo

**188.** Phenylacetamides as LXR Agonists. **G. X. Yang**, Z. Hu, H. Koyama, L. Mitnaul, J. Chin, C. Sparrow, J. P. Berger, T. E. Akiyama, S. P. Sahoo

**189.** SAR of highly potent full-range modulators of the farnesoid X receptor. **B. T. Flatt**, J. D. Kahl, B. B. Busch, E. Boman, A. Liu, P. Ordentlich, G. Yan, R. Mohan, R. Martin

**190.** Electrospun Polyethylenimine diazeniumdiolates for the controlled delivery of nitric oxide. **M. bhide**, W. Flores-Santana, D. D. J. Smith

**191.** Mechanism studies of nitric oxide synthase inactivation by amidines. Implications for nitric oxide synthase and heme oxygenase mechanisms. **Y. Zhu**, R. B. Silverman

**192.** Metabolism of a liver-selective nitric oxide-releasing agent, V-PYRRO/NO, by human microsomal cytochromes P450. **K. Inami**, R. W. Nims, A. Srinivasan, M. L. Citro, J. E. Saavedra, A. Cederbaum, L. K. Keefer

**193.** Synthesis of new sugar-NO donor conjugates. **T. B. Cai**, X. Tang, P. G. Wang

**194.** Structure–based modification of indomethacin as cyclooxygenase–2 inhibiting nitric oxide donor. **S. -J.Wey**, M. E. Augustyniak, E. D. Cochran, J. L. Ellis, X. -Q.Fang, D. S. Garvey, D. R. Janero, L. G. Letts, A. M. Martino, T. L. Melim, M. G. Murty, S. K. Richardson, J. D. Schroeder, W. M. Selig, A. M. Trocha, D. V. Young, I. S. Zemtseva

**195.** Design and synthesis of functionalized cyclodextrins as inhibitors of amyloid-β-peptide derived toxins. **Z. Wang**, P. A. Fernandez, L. Chang, W. L. Klein, D. L. Venton, G. R. J. Thatcher

**196.** The synthesis and structure activity relationship of substituted isoindoline analogs as amyloid aggregation inhibitors. **A. T. Sakkab-Tan**, C. E. Augelli-Szafran, C. Choi, Y. Lai, H. Levine III, J. Milbank, P. Orahovats, T. Yasunaga, Y. Ye

**197.** Genistein, a natural product from soy, is a potent inhibitor of transthyretin amyloidosis. **N. S. Green**, T. Foss, J. W. Kelly

**198.** Identification of γ-Secretase inhibitors derived from 2,4,6-trisubstituted triazine scaffolds. **D. G. Brown**, F. M. McLaren, R. W. Smith, J. Cacciola, A. B. Shenvi, M. J.

Schooler, J. B. Campbell, B. D. Greenberg, C. D. Sobotka-Briner, M. P. DeMartino, R. T. Jacobs

**199.** Structure-activity relationship study of novel tissue transglutaminase (TGase 2) inhibitors. E. Duval, A. Case, R. L. Stein, **G. D. Cuny**

**200.** Syntheses and properties of the major hydroxy metabolites in humans of blonanserin (AD-5423, a novel antipsychotic agent). **T. Ochi**, M. Sakamoto, A. Minamida, H. Toda, T. Ueda, K. Suzuki, T. Une, K. Matsumoto, Y. Terauchi

**201.** Synthesis and In Vivo Evaluation of Selenoflavanone : A New Class of Neuroprotective Agent. D -M. Kim, J -H. Ryu, **J -H. Jeong**

**202.** Synthesis and Neuroprotective Effect of Neu2000 against Rat Transient Ischemic Stroke Models. S -H. Yoon, **H. Park**, J. Lee, B. Gwag, Y. Lee

**203.** Alpha- LIPOIC ACID-BASED PPAR gamma-AGONISTS FOR TREATING TYPE II DIABETES. **C. S. Mizuno**, A. G. Chittiboyna, M. S. Venkatraman, M. A. Avery, J. Meingassner, C. Ho, S. C. Benson, J. Varani, C. N. Ellis, T. W. Kurtz, H. A. Pershadsingh

**204.** Design, synthesis and biological evaluation of Lisofylline (LSF) analogs as a possible treatment for Type 1 diabetes. **P. Cui**, T. L. Macdonald, M. Chen, Z. Yang, J. Nadler

**205.** Discovery of dipeptidyl peptidase IV (DPP-IV) inhibitors by structure-based de novo design. **L. Qiao**, C. Baumann, C. Crysler, N. Ninan, M. Abad, J. Spurlino, R. DesJarlais, J. Kervinen, M. Neeper, S. Bayoumy, R. Williams, I. Deckman, B. Tomczuk, K. Moriarty

**206.** Discovery of potent, selective and orally bioavailable phenylalanine based dipeptidyl peptidase IV inhibitors. **J. Xu**, L. wei, R. Mathvink, J. He, Y. J. Park, H. He, B. Leiting, K. A. Lyons, F. Marsilio, R. A. Patel, J. K. Wu, N. A. Thornberry, A. E. Weber

**207.** Potent and selective azetidine-based Dipeptidyl Peptidase IV (DPP IV) inhibitors. **W. Li**, E. Oliver, C. Rojas, S. Lauter, B. Thomas, S. Belyakov

**208.** Heteroaryl-O-glucosides as novel sodium glucose co-transporter 2 (SGLT2) inhibitors. X. Zhang, M. Urbanski, M. Patel, **R. Zeck**, G. Cox, H. Bian, B. R. Conway, M. P. Beavers, P. Rybczynski, K. Demarest

**209.** Indole-glucosides as novel sodium glucose co-transporter 2 (SGLT2) inhibitors. X. Zhang, M. Urbanski, M. Patel, **G. Cox**, H. Bian, R. Zeck, B. R. Conway, M. P. Beavers, P. Rybczynski, K. Demarest

**210.** Novel route to site-specific chemical modification of insulin via proinsulin. **M. E. Puskas**, D. Aggarwal, B. R. Krishnan

**211.** Synthesis and biological evaluation of sulfonamidooxazoles as selective inhibitors of the 11b-HSD1, a potential treatment for diabetes. **J. S. Xiang**, I. Manus, W. Massefski, V. Suri, M. Tam, Y. Xin, J. Tobin, X. Xu, J. McKew, S. Tam

**212.** Type 2 Diabetes Management using Aegle marmelos Seeds. **A. N. Kesari**, R. K. Gupta, G. Watal

**213.** Spacer based selectivity in the binding of two-prong ligands to recombinant human carbonic anhydrase-I. A. L. Banerjee, **D. R. Eiler**, B. C. Roy, S. Mallik, D. K. Srivastava

**214.** Two-Prong Inhibitors for Human Carbonic Anhydrase II. S. Mallik, D. K. Srivastava, B. C. Roy, M. Haldar, **X. Jia**, A. L. Banerjee, M. Swanson

**215.** 2-dimensional Electrophoresis Analysis Software Packages Causes Increased Variance in Quantitative Proteomics Studies. **Å. M. Wheelock**, A. R. Buckpitt

**216.** A fluorescent internal protein standard for quantitative 2-dimensional electrophoresis. **Å. M. Wheelock**, D. Morin, M. Bartosiewicz, A. R. Buckpit

**217.** A highly efficient approach for the synthesis of cationic lipid DOSPA. **Y. Li**, T. Heath

**218.** Computational and statistical analysis of microarray analyzed FAC sorted calvarial osteoblast differentiation. **R. R. Gupta**, L. E. K. Achenie, I. Kalajzic, D. W. Rowe

**219.** Novel chemogenomics approach to design selective enzyme inhibitors. **L. Urge**, F. Darvas, G. Dorman, Á. Papp, T. Szommer

**220.** A new 1,5-diarylheterocycles for selective COX-2 inhibitors: Synthesis of 1,5-diarylhydantoins by one-pot reaction. **M -S. Park**, S -K. Kwon, H -S. Park, E -H. Park

**221.** Inhibition of COX1/COX2 activity by substituted chalcones and flavones. **N. N. Mateeva**, C. J. Mills, K. K. Redda

**222.** Synthesis and Biological Evaluation of Salicylic Acid Analogues of Celecoxib as a New Class of Selective Cyclooxygenase-1 Inhibitor. **S -H. Yoon**, **J. Lee**, J -Y. Park, Y. Lee, B. Gwag

**223.** Synthesis of a heteroaryl modified, 1, 5-disubstituted pyrazole cyclooxygenase-2 (COX-2) selective inhibitor. **M. Ezawa**, D. S. Garvey, D. R. Janero, S. P. Khanapure, L. G. Letts, A. M. Martino, R. R. Ranatunge, D. J. Schwalb, D. V. Young

**224.** Synthesis of an iodine-123 labeled COX-2 inhibitor as a potential SPECT agent. G.

W. Kabalka, **A. R. Mereddy**, H. Schuller

**225.** Synthesis of substituted flavonoids and evaluation of their COX-1/COX-2 inhibitory activity. **C. J. Mills**, N. N. Mateeva, K. K. Redda

**226.** Asymmetric Synthesis of Analogues of Phosphatidylinositol 3-Phosphate. Y. Xu, **G. D. Prestwich**

**227.** Efficient synthesis of sulfonamide analogs of indole cPLA2a inhibitors: Chemistry and SAR. **W. Wang**, L. Chen, K. L. Lee, M. Shen, J. L. Wu, W. Zhang, X. Xu, S. Tam, J. D. Clark, J. C. McKew

**228.** INDOLE-BASED INHIBITORS OF CPLA2a: PHENYLSULFONAMIDES. **J. Nunez**, M. Behnke, L. Chen, M. Foley, K. L. Lee, R. Vargas, W. Wang, E. Murphy, M. Shen, W. Zhang, S. Tam, J. D. Clark, J. C. McKew

**229.** Structure-based design of secretory and cytosolic phospholipase A2 inhibitors. **B. P. Smart**, M. H. Gelb

**230.** Development of a novel high-throughput screening assay for rapid discovery of lipoxygenase inhibitors. **J. D. Deschamps**, R. R. Shah, T. R. Holman

**231.** Development of a Potent and Selective Inhibitor of Leukotriene A4 Hydrolase. **J. Wei**, K. Tays

**232.** Activation of NF-κB is inhibited by curcumin and related enones. **W. M. Weber**, C. N. Roybal, E. V. Bobrovnikova-Marjon, L. A. Hunsaker, S. F. Abcouwer, L. M. Deck, D. L. Vander Jagt

**233.** Degradation study of curcumin analog UBS 109. **S. M. Malick**, S. Trotman-Pruett, U. Sunay, M. Herold, J. P. Snyder, D. C. Liotta

**234.** Design and development of high affinity ligands that bind to HLA-DR10. **F. C. Lightstone**, J. Perkins, M. Cosman, A. Zemla, M. H. Corzett, C. Valdez, J. L. Herberg, G. L. DeNardo, R. Balhorn

**235.** Discovery of KRP-203, a potent and orally active new type of immunosuppressant, sphingosine-1-phosphate receptor agonist. **Y. Kohno**, N. Ando, T. Tanase, T. Sawada, K. Tanaka, K. Yumoto, S. Tanioka

**236.** Folate-targeted immunotherapy to activated macrophages in rheumatoid arthritis. **B. Varghese**, C. M. Paulos, G. J. Breur, W. R. Widmer, P. S. Low

**237.** Highly Efficient Synthesis of α O-Galactosyl Ceramides. **W. Du**, J. Gervay-Hague

**238.** Orally active small molecule IL-12 production inhibitors. **Z. Demko**, D.

Chimmanamada, D. James, E. Kostik, K. Koya, H. Li, G. Liang, T. Przewloka, L. Sun, N. Tatsuta, Y. Wada, Q. Wang, Y. Wu, S. Zhang, D. Zhou

**239.** Squarate based peptidic inhibitors of matrix metalloproteinase-1 (MMP-1). **M. B. Onaran**, A. B. Comeau, C. T. Seto

**240.** Synthesis and evaluation of novel pyridine-based MMP inhibitors. G. R. Cook, **R. Hayashi**

**241.** Synthesis of piperidine phenyl sulfone hydroxamates as TACE (TNF-α Converting Enzyme) inhibitors. **K. Park**, J. I. Levin, A. Aplasca, M. Du, F. E. Lovering, J. S. Condon, Y. Zhang, L. Sun, Y. Zhu, W. Xu

**242.** Structure determination of APAZA, a small, novel, diazo molecule currently being developed for treatment of inflammatory bowel disease (IBD). **M. Ferro**, S. Donaldson, R. Krishnan

**243.** Novel Orally Bioavailable Thrombin Inhibitors: Cyanofluorophenylacetic Acid Derivatives. **K. D. Kreutter**, L. Lee, T. Lu, V. Mohan, S. Patel, H. Huang, G. Xu, M. Fitzgerald, C. Crysler, M. R. Player, E. C. Giardino, B. E. Maryanoff, B. P. Damiano, B. E. Tomczuk, N. D. Huebert, S. Eisennagel, M. Dasgupta, J. C. Spurlino, M. McMillan

**244.** Potent Small Molecule, Non-Peptidic Chlorophenyl Acetamide Thrombin Inhibitors. **L. Lee**, K. D. Kreutter, W. Pan, T. Lu, C. Crysler, S. Eisennagel, M. MacMillan, J. Spurlino, B. Tomczuk, M. Player, V. Mohan

**245.** Structure-based design, structure-conformation and structure-activity relationships of DPhe(D/L-Tic)-Pro-DArg-P1'-CONH2 tetrapeptides with inhibitory activity for thrombin. **C. Clement**, M. Philipp

**246.** Anthranilamide inhibitors of factor Xa. **D. Mendel**, A. L. Marquart, S. Joseph, P. Waid, Y. K. Yee, A. L. Tebbe, D. K. Herron, T. Goodson, J. J. Masters, J. B. Franciskovich, J. M. Tinsley, M. R. Wiley, L. C. Weir, J. A. Kyle, V. J. Klimkowski, G. F. Smith, R. D. Towner, L. L. Froelich, J. Buben, T. J. Craft

**247.** Design, Synthesis and Biological Evaluation of Peptidomimetic FXIa Inhibitors. **J. Lin**, H. Deng, L. Jin, P. Pandey, M. Rynkiewicz, F. Bibbins, S. Cantin, J. Quinn, S. Magee, J. Gorga, C. Celatka, P. Nagafuji, T. Bannister, H. V. Meyers, R. Babine, N. Hayward, S. S. Abdel-Meguid, J. Strickler

**248.** SAR exploration of alpha-ketothiazole arginine derived factor XIa inhibitors. **H. Deng**, T. D. Bannister, L. Jin, P. Nagafuji, C. A. Celatka, J. Lin, T. I. Lazarova, M. J. Rynkiewicz, F. Bibbins, J. E. Strickler, R. E. Babine, H. V. Meyers, S. S. Abdel-Meguid

**249.** Synthesis and biological evaluation of aryl boronic acids as inhibitors of factor XIa. **T. I. Lazarova**, L. Jin, M. Rynkiewicz, J. Gorga, F. Bibbins, H. V. Meyers, R. Babine, J.

Strickler, S. S. Abdel-Meguid

**250.** Development of Factor VIIa inhibitors: Addressing pharmacokinetic parameters. A. Kolesnikov, **R. Rai**, W. B. Young, S. Torkelson, W. D. Shrader, E. M. Leahy, B. A. Katz, P. A. Sprengeler, L. Liu, J. Mordenti, E. Gjerstad, J. Janc

**251.** Development of Factor VIIa inhibitors: Selectivity in Trypsin family proteases. **W. D. Shrader**, J. Costerison, J. Hendrix, H. Hu, A. Kolesnikov, V. Kumar, E. Leahy, R. Rai, M. Shaghafi, T. Ton, S. Torkelson, K. Wesson, W. B. Young, B. A. Katz, P. A. Sprengeler, C. Yu, R. Cabuslay, E. Gjerstad, J. Janc, E. Sanford

**252.** Discovery of potent and selective biaryl derivatives as tissue factor/factor VIIa inhibitors through structure-based drug design. **P. Chand**, P. L. Kotian, A. Dehghani, Y. El-Kattan, T -H. Lin, M. Wu, R. S. Rowland, K. Raman, S. Bantia, S. Arnold, Y. S. Babu

**253.** Noncovalent Inhibition of the Serine Proteases, alpha-Chymotrypsin and Trypsin by Trifluoro(organo)borates. **R. Smoum**

**254.** Discovery of novel inhibitors of kallikrein. **M. M. Staveski**, S. F. Sneddon, F. J. Vinick, J. S. Gregory, C. Yee, A. D. Janjigian, S. Nahill, A. Napper, M. Leonard

**255.** Development of new hemostatic drugs on the basis of labdane diterpenoids isolated from Central Asian *Lagochilus* plant species. U. N. Zainutdinov, **M. A. Turabekova**, S. I. Salikhov

**256.** Molecular docking of the highly hypolipidemic agent α-asarone with the catalytic portion of HMG-CoA reductase. **J. L. Medina-Franco**, F. López-Vallejo, S. Rodríguez-Morales, R. Castillo, G. Chamorro, J. Tamariz

## MONDAY MORNING

Section A

Unknown Site -- Unknown Room

**Biological Tools in Drug Discovery: Sponsored by Bentham Science Publishers Ltd**

L. McQuire and M. D. Shultz, *Organizers, Presiding*

**9:00 —** Introductory Remarks.

**9:05 —257.** RNA Interference: An enabling tool for target identification and validation. **C. P. Miller**

**9:40 —258.** Genetic modeling of chemical antagonists: genome-scale discovery of drug

targets by in vivo functional analysis. **B. P. Zambrowicz**

**10:15 —259.** Protease substrate profiling. **J. Harris**

**10:50 —260.** Benzopyrans are selective estrogen receptor beta agonists for use in the treatment of prostatic diseases. **B. H. Norman**, T. I. Richardson, V. Krishnan, J. A. Dodge, C. W. Lugar, Y. Wang, K. Chen, G. L. Durst, R. J. Barr, C. Montrose-Rafizadeh, H. E. Osborne, H. Mo

**11:25 —261.** Overcoming IKr issues in the search for a CCR5 antagonist for the treatment of HIV. **D. A. Price**

Section B

Unknown Site -- Unknown Room

**P-glycoprotein - Structure and Function**

K. A. Jacobson, *Presiding*
G. F. Ecker, *Organizer, Presiding*

**9:00 —262.** Targeting P-glycoprotein - a continuing challenge. **G. F. Ecker**

**9:40 —263.** Structural studies of P-glycoprotein and multidrug resistance protein 1. **M. Rosenberg**

**10:20 —264.** Functional aspects of multidrug transport. **P. Chiba**, G. F. Ecker, K. Pleban, S. Kopp, W. N. Konings

**11:00 —265.** A pharmacophore hypothesis for P-Glycoprotein substrate recognition. **V. Roy**, G. Cianchetta, R. W. Singleton, M. Zhang

**11:40 —266.** Progress in computational modeling of P-glycoprotein. **S. Ekins**

**Current Aspects of Synthetic Organic Chemistry**

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**Frontiers in Bio-organic Chemistry and Chemical Biology**

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## MONDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

**Gene Expression and Medicinal Chemistry: Sponsored by Elsevier**

S. Pikul, *Organizer*

**1:30 —267.** Transcriptional profiling for small molecule drug discovery. **K. Chan**

**2:10 —268.** Tuning the specificity and potency of artificial transcriptional activators. **A. K. Mapp**

**2:50 —269.** Gene expression driven drug discovery. **S. Pikul**

**3:30 —270.** Genomics applied to drug candidate prioritization and for identification of novel therapeutically useful properties of existing drugs. **K. Jarnagin**, A. Roter, A. Tolley, M. Lee, C. G. Natsoulis

Section B

Unknown Site -- Unknown Room

**Druggable Targets in Functional Lipidomics**

L. Feng and G. D. Prestwich, *Organizers*

**1:30 —271.** High-Throughput Parallel Analysis of Multiple Cellular Lipids by Esi Mass Spectrometry. S. B. Milne, J. S. Forrester, **H. A. Brown**

**2:10 —272.** Lipid-Based Inhibitors of Icmt and other Prenylated Protein Processing Enzymes. **R. A. Gibbs**, B. S. Henriksen, J. L. Donelson, S. K. De, J. L. Anderson, S. Hudon, C. A. Hrycyna

**2:50 —273.** Discovery of Potent, Orally Bioavailable, Immunosuppressive N-Benzyl Pyrrolidine and Azetidine Carboxylate $S1P_1$ Receptor Agonists. **J. J. Hale**

**3:30 —274.** Phosphoinositide recognition domains: targeting of proteins to membranes. **T. G. Kutateladze**, S. Lee, M. Cheever, M. Overduin, C. Burd

**4:10 —275.** Probing lipid-protein interactions by lipidomics approaches. **L. Feng**

**Frontiers in Bio-organic Chemistry and Chemical Biology**

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**Undergraduate Research Poster Session: Medicinal Chemistry**

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## MONDAY EVENING

Section A

Unknown Site -- Unknown Room

**Sci-Mix**

D. L. Flynn, *Presiding*

**8:00 - 10:00**

**23, 25, 31, 37, 41, 55, 63, 86, 103-104, 121, 123, 127, 133, 141, 149, 160, 172, 185, 189, 195, 208, 219, 232, 238-239, 251.** See previous listings.

**319, 327-328, 335, 350, 354, 366, 370, 373, 377, 380, 383, 403, 407, 417, 429, 431, 464, 472, 474, 485, 487, 499, 503, 517, 521, 523, 534.** See subsequent listings.

## TUESDAY MORNING

Section A

Unknown Site -- Unknown Room

**E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances**

K. A. Jacobson, *Organizer*

**9:00 —276.** Promiscuous drugs: Superior efficacy of one pill on many targets. **M. D. Miller**

**9:40 —277.** Mapping bioactivity space for fragment-based lead discovery. **T. I. Oprea**,

M. Olah, M. Mracec, R. Rad, L. Ostopovici, A. Bora, N. Hadaruga, C. G. Bologa

**10:20 —278.** Finding drugs within chemistry space: Impact of the clinical development process. **J. F. Blake**

**11:00 —279.** The discovery of nitroimidazopyrans and PA824: Novel therapeutics for the treatment of tuberculosis. **W. R. Baker**

**11:40 —** Introduction of E.B. Hershberg Award Winner by Daniel L. Flynn.

**11:50 —280.** Medicinal chemistry and the innovation gap. **C. A. Lipinski**

**ADME/tox Informatics**

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**Informatics and High Throughput Experimentation**

**Part I**

*Cosponsored with CINF*

## TUESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

**5HT2C and Higher Order Serotonin Receptors: Sponsored by Arena Pharmaceuticals, Inc**

J. Gross and D. Rotella, *Organizers*

**1:30 —** Introductory Remarks.

**1:35 —281.** 10-Benzyl-4-piperazinyldibenzoxazepin-11-one: A new molecular scaffold for refining the pharmacophore characteristics for 5-$HT_6$ antagonism. **R. N. Harris III**, D. B. Repke, J. M. Kress, R. S. Stabler, J. Berger, L. Zhang, J. M. Brothers

**2:15 —282.** Discovery and SAR studies of 2,6-difluorobenzenesulfonic acid 1-methyl-3-(1-methylpiperidin-4-yl)-1H-indol-5-yl ester, a novel and potent 5-HT6 antagonist for the

treatment of cognitive deficit. **M. M. Piñeiro-Núñez**, D. D. Bauzon, F. P. Bymaster, Z. Chen, E. Chernet, M. P. Clay, R. Crile, N. W. DeLapp, C. P. Denny, J. F. Falcone, M. E. Flaugh, L. J. Heinz, A. D. Kiefer Jr., D. J. Koch, J. H. Krushinski Jr., J. D. Leander, T. D. Lindstrom, B. Liu, D. L. McKinzie, D. L. Nelson, L. A. Phebus, V. P. Rocco, J. M. Schaus, M. C. Wolff, J. S. Ward

**2:55 —283.** Synthesis and biological evaluation of novel, selective 5-HT2C receptor agonists for obesity. **T. Lee**, A. J. Robichaud, W. Chen, Y. Lu, S. Dowdell, K. E. Boyle, I. S. Mitchell, J. M. Fevig, R. R. Wexler, K. J. Miller, B. L. Largent, K. W. Rohrbach, J. J. Devenny, J. F. McElroy

**3:35 —284.** Potential therapeutics for the treatment of psychiatric disorders: design and synthesis of potent, selective, bioavailable 5HT2C receptor agonists. **A. L. Sabb**, R. L. Vogel, G. S. Welmaker, J. Sabalski, J. Nelson, G. Stack, M. Antane, H. Mazandarani, J. Zhang, J. Dunlop, S. Rosenzweig-Lipson, K. Marquis, S. Grauer, B. L. Harrison

**4:15 —285.** Discovery, SAR and biology of 5-HT2C receptors for the treatment of obesity. **B. M. Smith**, J. Smith, J. H. Tsai, J. A. Schultz, C. Gilson, R. Chen, S. Estrada, D. Park, E. Prieto, D. Sengupta, H. Saldana, W. Thomsen, W. Kevin, K. Creehan, L. Gonzalez, F. Menzaghi, C. Bjenning, N. Beeley, R. R. Webb, D. Behan

Section B

Unknown Site -- Unknown Room

**General Oral Session II**

J. A. Zablocki, *Organizer, Presiding*

**1:30 —286.** Design and synthesis of noncovalent inhibitors of cathepsin S. **H. Liu**, P. Alper, D. Tully, R. Epple, A. Chatterjee, J. Harris, J. Li, B. Bursulaya, J. William, K. Nguyen, D. Mutnick, D. Woodmansee, M. Roberts, R. Russo, B. Masick, Y. He, D. S. Karanewsky

**1:50 —287.** Bioavailable Cathepsin S Inhibitors. **S. Thurairatnam**, D. J. Aldous, J. Aguiar, C. Bryant, M. Graupe, S. King, J. Lai, V. Leroy, J -P. Letallec, J. Link, V. Martichonok, J. Patterson, A. Timm, S. Zipfel

**2:10 —288.** Pyrrolo[3,4-c]quinoline-1,3-diones as a novel chemotype of potent nonpeptide caspase-3 inhibitors. D. Kravchenko, V. Kysil, A. P. Ilyin, A. Khvat, S. Tkachenko, I. Okun, S. Maliartchouk, **A. Ivachtchenko**

**2:30 —289.** Design and Synthesis of Highly Potent and Selective Protein Geranylgeranyltransferase-I Inhibitors. **E. E. Pusateri**, D. Carrico, H. Peng, S. Sebti, A. D. Hamilton

**2:50 —290.** 4-Heterocyclohexanone-based inhibitors of serine protease plasmin. **F. Xue**

**3:10 —291.** Design, synthesis, and bioactivity of simplified paclitaxel analogs based on the T-taxol bioactive conformation. **T. Ganesh**, A. Norris, S. Sharma, S. Bane, A. S. Lakdawala, J. P. Snyder, D. G. I. Kingston

**3:30 —292.** Quantum mechanics studies on the DNA sequence preference of camptothecin. **X. Xiao**, M. Cushman

**3:50 —293.** Synthesis and evaluation of retinoic acid metabolism blocking agents (RAMBAs) as indirect differentiating agents for cancer therapeutics. **S. W. Yee**, L. Jarno, C. Simons, A. Brancale, R. I. Nicholson

**4:10 —294.** Synthesis and SAR of Novel Tricyclic Indanopyrazoles with Dual Anti-angiogenesis and Tumor Cell Anti-proliferative Activity. **C. Y. Ho**, J. Mei, R. Tuman, D. Ludovici, U. Maharoof, E. Strobel, L. Andraka, J. Yen, A. De Vine, R. Tomminovich, H. Lu, J. Baker, C. Burns, J. Sechler, D. Johnson, R. Galemmo

**4:30 —295.** Withanolides: A new class of angiogenesis inhibitors. P. Bargagna-Mohan, R. Gambaro, **R. Mohan**

**ADME/tox Informatics**

**New Methodologies**

*Cosponsored with CINF*

**Informatics and High Throughput Experimentation**

**Part II**

*Cosponsored with CINF*

## WEDNESDAY MORNING

Section A

Unknown Site -- Unknown Room

**Kinase Inhibitors as Anti-Inflammatory Agents: Sponsored by Biotage**

D. M. Goldstein and J. Barrish, *Organizers*

**9:00 —296.** Discovery and development of orally active p38 kinase inhibitors as anti-TNF agents. **R. V. Devraj**

**9:40 —297.** Small molecule modulators of nuclear factor-kB. **M. E. Hepperle**, P. Raman, J. Liu, J. Little, F. Soucy, H. Mazdiyasni, R. Murray, Y. Ye, G. Harriman, Y. Xu, D. Wen, L. Schopf, B. Jaffee, T. Ocain

**10:20 —298.** Development of aniline amides containing alternative cores as orally active p38 MAP kinase inhibitors. **K. Leftheris**, J. Hynes Jr, A. Dyckman, T. Li, S. Lin, S. T. Wrobleski, H. Wu, R. Zhang, K. M. Gillooly, D. Loo, K. W. McIntyre, S. Pitt, D. R. Shen, D. J. Shuster, A. Doweyko, J. Sack, J. C. Barrish, J. Dodd, G. L. Schieven

**11:00 —299.** Discovery of JNK inhibitors based on an indazole template. **Y. Satoh**, S. Sakata, A. Kois, V. Plantevin, K. Sahasrabudhe, Q. Chao, C. Buhr, W. Lew, G. Shevlin, R. Albers, L. Nadolny, N. D'Sidocky, J. Sapienza, R. Ferri, A. Motiwala, J. Muir, C. Grimshaw, L. Xu, S. Pai, O. Khatsenko, M. A. Shirley, E. O'Leary, H. Raymon, P. Omholt, J. Leisten, S. Bhagwat, A. C. Manning, J. Wright, B. Bennett

**11:40 —300.** p38 α MAP kinase inhibitors: From discovery to the clinic. **S. Dugar**, B. Mavunkel, S. Chakravarty, J. Perumattam, G. Luedtke, Q. Lu, Z. Chen, Y -J. Xu, A. Protter, G. Schreiner, R. Almirez, B. Scott, M. Laney, M. Henson, J. Lewicki, A. Moore, S. Lee, E. Brahn, D. Liu

Section B

Unknown Site -- Unknown Room

**Histone Deacetylase Inhibitors as Anticancer Agents**

S. Ananthan, *Organizer*

**9:00 —301.** Histone deacetylase inhibitors. **T. A. Miller**

**9:35 —302.** Novel hydroxamate and non-hydroxamate histone deacetylase inhibitors. **M. L. Curtin**

**10:10 —303.** Discovery and development of histone deacetylase inhibitors. **M. Yoshida**, N. Nishino

**10:45 —304.** Computer aided molecular design of HDAC inhibitors. **O. Wiest**, D -F. Wang, P. Helquist, N. Wiech, S. Roy, M. Tenniswood

**11:20 —305.** Crystal structure of human HDAC8 provides insights into the class I histone deacetylases. **J. R. Somoza**, R. J. Skene, B. A. Katz, C. Mol, J. Ho, A. J. Jennings, C. Luong, A. Arvai, J. J. Buggy, E. Chi, J. Tang, B -C. Sang, E. Verner, R. Wynands, E. M. Leahy, D. R. Dougan, G. Snell, M. Navre, K. Mark W, R. V. Swanson, D. E. McRee, L. W. Tari

**ADME/tox Informatics**

**Applications**

*Cosponsored with CINF*

## WEDNESDAY AFTERNOON

Section A

Unknown Site -- Unknown Room

**Kinase Inhibitors as Anti-Cancer Agents: Sponsored by Novartis**

R. Doll and P. W. Manley, *Organizers*
A. B. Cooper, *Organizer, Presiding*

**1:30 —306.** Inhibitors of protein kinase signaling pathways: Emerging targets and agents. **J. E. Dancey**

**2:10 —307.** "Perspectives on the discovery of VX-680, a selective inhibitor of the Aurora kinases". **J. M. C. Golec**

**2:50 —308.** Discovery of BMS-536924, a small molecule inhibitor of IGF-1R with broad spectrum in vivo activity. **M. D. Wittman**, J. Carboni, F. Y. Lee, B. Balasubramanian, F. Beaulieu, F. David, S. Krishnanathan, L. Peiying, C. Ouellet, X. Sang, M. G. Saulnier, K. Stoffan, U. Velaparthi, D. M. Vyas, H. S. Wong, K. Zimmermann

**3:30 —309.** Structural biology guided optimization of tyrosine kinase inhibitors: AMN107 a selective and potent Bcr-Abl inhibitor. **P. W. Manley**, W. Breitenstein, J. Brüggen, S. W. Cowan-Jacob, P. Furet, J. D. Griffin, J. Mestan, T. Meyer, E. Weisberg

**4:10 —310.** Evolution of the MEK Inhibitor PD 0325901: From Discovery to Clinical Development. **J. S. Leopold**

Section B

Unknown Site -- Unknown Room

**Drug Resistant Tuberculosis**

I. Ojima, *Organizer*

**1:30 —** Introductory Remarks.

**1:35 —311.** Development of new tuberculosis drug candidates. **B. E. Laughon**

**2:05 —312.** Development of nitrofuranylamides as antituberculosis agents. **R. E. Lee**, R. P. Tangallapally, R. Yendapally, R. E. B. Lee, A. J. Daniels, K. Hevener

**2:35 —313.** Screening novel anti-tuberculosis agents effective against MDR-TB. **M. Matsumoto**

**3:05 —314.** Why does multidrug chemotherapy still allow the emergence of drug resistance during tuberculosis treatment? **C. E. Barry III**

**3:35 —315.** Novel inhibitors of InhA, the enoyl reductase from Mycobacterium tuberculosis. **P. J. Tonge**, T. J. Sullivan, P. Novichenok, J. J. Truglio, C. Kisker, F. Johnson, R. A. Slayden

**4:05 —316.** Cell Wall of Mycobacterium tuberculosis and Drug Discovery. **P. J. Brennan**

## WEDNESDAY EVENING

Section A

Unknown Site -- Unknown Room

**Poster Session II**

D. L. Flynn, *Organizer*

**6:00 - 8:00**

**317.** Solid phase synthesis of vancomycin-bis(8-amido-3,6-dioxaoctanoyl)-amidopropylsiloxy-titanium implants that inhibit proliferation of *Staphylococcus aureus*. **B. Jose**, S. J. King, A. R. Zeiger, C. J. Adams, N. J. Hickok, E. Wickstrom

**318.** Development of gene probes: Synthesis of radioiodo and radioiodovinyl arabinosyl uridine analog. **C -S. Yu**, L -W. Chiang, C -H. Wu, R -T. Wang, H -Y. Wang, C -H. Yeh

**319.** 5-(5,6)-Dihydrouracil substituted 8-hydroxy-[1,6]naphthyridine-7-carboxylic acid 4-fluorobenzylamide inhibitors of HIV-1 integrase and viral replication in cells. **M. W. Embrey**, J. S. Wai, T. W. Funk, C. F. Homnick, D. S. Perlow, S. D. Young, J. P. Vacca, D. J. Hazuda, P. J. Felock, K. A. Stillmock, M. V. Witmer, G. Moyer, W. A. Schleif, L. J. Gabryelski, L. Jin, I -W. Chen, J. D. Ellis, B. K. Wong, J. H. Lin, Y. M. Leonard, N. N. Tsou, L. Zhuang

**320. Synthesis and SAR analysis of novel anthrax lethal factor inhibitors**. **C. Tang**, G -S. Jiao, S. Millis, L. Cregar, D. Nguyen, M. Goldman

**321.** An efficient synthesis of 3'-deoxy-3'beta-fluoro and 3'-deoxy-3'alpha-fluoro -5'-Noraristeromycin and their antiviral activities. **A. Roy**, T. Serbessa, S. W. Schneller

**322.** Design and synthesis of pyranobenzothiophenes as inhibitors of HCV RNA dependent RNA polymerase. A. Gopalsamy, **G. M. Ciszewski**, A. Aplasca, J. W. Ellingboe, B. Feld, M. Orlowski, A. Y. M. Howe

**323.** Design, synthesis and metabolic stabilities of alkenyldiarylmethanes (ADAMs) having nonidentical aromatic substituents as NNRTIs. **B -L. Deng**, M. Cushman

**324.** Design, synthesis, and evaluation of dioxane antiviral agents targeted against the hydrophobic binding pocket of Syndbis virus capsid protein. **H. Y. Kim**, R. Warrier, C. Patkar, R. Kuhn, M. Cushman

**325.** Discovery of potent and selective fucosidase inhibitors by rational and combinatorial approach. **C -W. Ho**, **C -F. Chang**, **C -Y. Wu**, **C -H. Lin**

**326.** Identification of carbazole and cyclopentaindole derivatives as inhibitors of HCV RNA dependent RNA polymerase. A. Gopalsamy, **M. shi**, G. M. Ciszewski, K. Park, J. W. Ellingboe, B. Feld, M. Orlowski, A. Y. M. Howe

**327.** Importance of backbone hydrogen bonds in binding a tetrapeptide scaffold to the HCV NS3-4A protease. **R. B. Perni**, K. C. Cottrell, J. J. Court, L. J. Farmer, C. A. Gates, C. Lin, K. Lin, Y -P. Luong, J. Pitlik, B. G. Rao, W. Schairer, Y. Wei, J. H. Van Drie

**328.** NMR-based design of CD4-binding peptide mimetics as HIV entry inhibitors. **H. M. Möller**, J. Wülfken, B. Hünnefeld, A. Çoksezen, B. Meyer

**329.** Novel 8-substituted dipyridodiazepinone derivatives as HIV NNRTIs with broad antiviral potency. **S. Landry**, P. R. Bonneau, J. Bordeleau, L. Doyon, J. Duan, I. Guse, E. Malenfant, J. Naud, J. A. O'Meara, B. Thavonekham, C. Yoakim, B. Simoneau, M. Bös, M. G. Cordingley

**330.** Novel C-terminal functionalities in hepatitis C virus NS3 protease inhibitors. **R. Rönn**, T. Gossas, Y. A. Sabnis, E. Åkerblom, U. H. Danielson, B. Samuelsson, A.

Hallberg, A. Johansson

**331.** Pharmacophore modeling and computational analysis of a key protein-protein interaction in herpes simplex virus. **M. J. Grubisha**, S. M. Firestine

**332.** Synthesis and evaluation of [$^{18}$F]-2'-Deoxy-2'-fluoro-1-beta-D-arabinofuranosyluracil derivatives as PET probes for imaging HSV1-tk gene expression in vivo. **N. Pillarsetty**, S. Cai, D. Mikhail, L. Ageyeva, R. D. Finn, R. G. Blasberg

**333.** Prediction of HIV-1 protease inhibitors through molecular modeling and statistical analysis. **C. J. Collar**, L. Fabry-Asztalos

**334.** Prodrugs of 1-(β-D-dioxolane)thymine (DOT): Synthesis, anti-HIV-1 activity and stability study. **Y. Z. Liang**, V. Yadav, R. F. Schinazi, C. K. Chu

**335.** Promazine analogues as potential anti SARS-CoV drugs. H. P. Hsieh, **Y -S. Wu**, P -H. Lu, C -M. Chen, Y -C. Chao, J -T. Jan, H -R. Lo, S -H. Ma, Y -S. Chao, T -A. Hsu

**336.** Pyrazolo [1,5-a] pyridine antiherpetics. **J. G. Weatherhead**, B. A. Johns, S. H. Allen, K. S. Gudmundsson, F. L. Boyd Jr., G. A. Freeman

**337.** Pyrazolopyrimidines as inhibitors of HCV RNA polymerase. **J. V. Popovici-Müller**, G. W. Shipps Jr., K. E. Rosner, Y. Deng, T. Wang, P. Curran, M. A. Brown, A. B. Cooper, M. Cable, N. Butkiewicz, V. Girijavallabhan

**338.** Structure Activity Relationship of Disulfone-Containing HIV-1 Integrase Inhibitors. **D. C. Meadows**, J. Gervay-Hague, T. B. Matthews, T. W. North

**339.** Structure activity relationship of substituted pyranoindoles as HCV RNA dependent RNA polymerase inhibitors. A. Gopalsamy, **G. M. Ciszewski**, K. Lim, K. Park, M. Shi, J. Bloom, R. Chopra, A. Agarwal, G. Krishnamurthy, J. W. Ellingboe, J. Upeslacis, T. S. Mansour, S. M. Condon, M. G. LaPorte, L. M. Miller, C. J. Burns, A. Y. M. Howe, B. Feld, M. Orlowski, M. van Zeijl, J. O'Connell

**340.** Substituted 4H-pyrazolo[1,5-a]pyrimidin-7-ones as hepatitis C virus polymerase inhibitors. **Y. Deng**, J. V. Popovici-Müller, G. W. Shipps Jr., K. E. Rosner, T. Wang, P. Curran, A. B. Cooper, V. Girijavallabhan, N. Butkiewicz, M. Cable

**341.** Syntheses and anti-viral properties of N-6 substituted derivatives of L-like 4'-deoxy-5'-noraristeromycin and oxyamino and hydroxylamino carbanucleosides. **T. Serbessa**, A. Roy, M. Yang, S. W. Schneller

**342.** Syntheses and Antiviral Properties of Carbocyclic Formycins. **J. Zhou**, M. Yang, S. W. Schneller

**343.** Synthesis and antiviral activity studies of 5'-deoxy-5', 5', 5'-trifluoro Neplanocin A.

**A. Roy**, S. W. Schneller

**344.** Synthesis and antiviral properties of 6'-â-F-5'-NororIsteromicin. **X. Yin**, S. W. Schneller

**345.** Synthesis and biological properties of 2′-C-modified analogues of 5′-methyl aristeromycin analogues. **W. Ye**, S. W. Schneller

**346.** A Versatile Synthetic Route to 6'-β-F-Aristeromycin, Aristeromycin, 2',3'-Dideoxydidehydroaristeromycin and the Antiviral Activity of 6'-β-F-Aristeromycin. **X. Yin**, S. W. Schneller

**347.** Synthesis of N3,5'-Cyclo-4-(beta-D-ribofuranosyl)-vic-triazolo[4,5-b]pyridin-5-one Analogues with improved Anti-Hepatitis C Activity in vitro. **P. Wang**, J. Du, S. Rachakonda, B -K. Chun, L. J. Stuyver, M. J. Otto, R. F. Schinazi, K. A. Watanabe

**348.** Synthesis of novel pyrazolopyridine antiherpetics: SAR of the C2 phenyl substituent. **E. M. Turner**, K. S. Gudmundsson, B. A. Johns, Z. Wang, S. H. Allen, G. A. Freeman, C. J. Sexton, D. W. Selleseth, K. L. Creech, K. R. Moniri

**349.** The Chemical Synthesis of Poly(ethylene oxide)-Based Biomimetic SDF-1 Materials for Anti-HIV-1 Study. **M -H. Chen**, C -P. Chen

**350.** Toward smaller HCV NS3-4A protease inhibitors: 3-Substituted proline-based tripeptide scaffolds. **R. B. Perni**, K. C. Cottrell, J. J. Court, L. J. Farmer, C. A. Gates, Y -P. Luong, J. Pitlik, B. G. Rao

**351.** 2'-Substituted penicillin-derived inhibitors of β-lactamase. **J. D. Buynak**, L. Vogeti, V. R. Gadhachanda, A. Sheri

**352.** 3-Amino-1H-quinazoline-2,4-diones: A novel class of antibacterial agents. **T. P. Tran**, E. L. Ellsworth, J. P. Sanchez, M. A. Stier, B. M. Watson, S. A. Powell, K. M. Hutchings, H. D. H. Showalter, J. M. Domagala, M. A. Shapiro, M. D. Huband, J. W. Gage, T. E. Joannides, S. J. Gracheck, P. Bird, D. Q. Nguyen, J. Yip, T. Li, J. Tailor, R. Singh

**353.**

Synthesis and design of 2,4-diamino-6-substituted-pyrido[3,2-*d*]pyrimidines as dihydrofolate reductase inhibitors from opportunistic pathogens

. A. Gangjee, **Z. Ye**, R. L. Kisliuk, S. F. Queener

**354.** Design and Synthesis of a Ser-Phe-Phe Ketomethylene Isostere for Inhibitors of Botulinum Neurotoxin B. **B. M. Bax**, D. H. Rich

**355.** Design, Parallel Synthesis and SAR for Tethered Dimer Inhibitors of NAD Synthethase. W. J. Brouillette, **L. Mou**, S. E. Velu, C. G. Brouillette, C -H. Luan, L. J. DeLucas

**356.** Molecular recognition in the adenine-binding region of an aminoglycoside antibiotic kinase. **D. D. Boehr**, A. R. Farley, F. J. LaRonde, T. R. Murdock, A. Al-Mestarihi, G. D. Wright, J. R. Cox

**357.** New insights into the use of ß-chloro-alanine in the tryptophan synthase kinetic assay. **A. L. Looney**, J. O. Boles, C. Harrington

**358.** New Laspartomycin-based semi-synthetic lipopeptide antibiotics. **D. R. Cameron**, Y. Chen, D. Dugourd, J. Sun, L. Wang, D. B. Borders, W. V. Curran, R. A. Leese

**359.** Novel antibacterial tripeptides. **B. E. Haug**, J. S. M. Svendsen

**360.** Polypeptide Deformylase Inhibitors: Design, Synthesis and Evaluation of a Novel Benzamide Scaffold. **J. M. Karpinski**, S. B. Christensen, K. M. Aubart, G. S. Van Aller, P. L. DeMarsh, T. F. Lewandowski, S. Rittenhouse, S. G. Kulkarni, T. A. McIntyre, L. C. Woods, M. A. Lonetto, S. C. Pearson, K. J. Smith, A. Bhat, M. Cummings, K. Saylers

**361.** Post-polyketide tailoring oxygenases of the landomycin biosynthesis. **L. Zhu**, J. Rohr

**362.** Rapid method to synthesis of 2,3-dihydro-2-phenyl-4-quinolone derivatives as new antibacterial agents. **M -S. Park**, J -H. Kim, J -I. Lee

**363.** Structure guided design, synthesis and in vitro characterization of aqueous soluble inhibitors of staphylococcal enoyl-ACP reductase. **J. Berman**

**364.** Structure-Activity Relationship of Mansonone F, a Potent Anti-MRSA Sesquiterpenoid Quinone: SAR Studies on C6 and C9 Analogues. Y -G. Suh, **S. N. Kim**, D -Y. Shin, S -S. Hyun, K -H. Min, Y -S. Lee, S -H. Kim, S -M. Paek, J -W. Jung

**365.** Sub-cloning and Purification of the Lid Sub-domain of DnaK. **N. Bahr**, N. Steede, S. Landry

**366.** Synthesis and antibacterial activities of multivalent vancomycins based on 8-hydroxyquinoline platforms. **L. Li**, P. L. Ho, B. Xu

**367.** Synthesis and structure-activity relationship (SAR) studies on Dab-9 substitutions of the lipopeptide antibiotic Amphomycin. **S. A. Wacowich-Sgarbi**, V. A. Boyd, D. R. Cameron, Y. Chen, D. Dugourd, Q. Jia, M. Nodwell, P. W. M. Sgarbi, J. Sun, L. Wang, D. B. Borders, W. V. Curran, R. A. Leese

**368.** Synthesis and structure-activity relationship (SAR) studies on the lipophilic tail of

the lipopeptide antibiotic Amphomycin. **P. W. M. Sgarbi**, V. A. Boyd, D. R. Cameron, Y. Chen, Q. Jia, M. Nodwell, R. Siu, J. Sun, S. A. Wacowich-Sgarbi, L. Wang, D. B. Borders, W. V. Curran, R. A. Leese

**369.** Synthesis of biologically active phosphonate oxazolidinone derivatives. **K -Y. Jung**, J -M. Hwang, U -I. Kim

**370.** Synthesis of potential Holliday Junction inhibitors. **I. Medina**, C. Carroll, S. R. McAlpine

**371.** Synthesis, antibiotic activity, and antiangiogenic activity of calixarene derivatives that are topological mimetics of amphipathic peptides. **X. Chen**, T. R. Hoye, K. H. Mayo

**372.** Volsurf studies of 5-nitro-2-thiophylidene derivatives with antimicrobial activity against multidrug-resistant strain of *Staphylococcus aureus*. A. Masunari, L. D. Rezende, A. T. D. Amaral, **L. C. Tavares**

**373.** Anti-tuberculosis structure-activity relationship of macrolides. **Z. Zhu**, K. Falzari, D. Pan, O. Krasnykh, S. G. Franzblau

**374.** Synthesis and evaluation of substituted benzyl nitrofuranyl amides as novel antituberculosis agents. **R. P. Tangallapally**, R. E. B. Lee, A. J. M. Lenaerts, R. E. Lee

**375.** Competitive induction of anti-mycobacterial activity in marine bacteria. **J. A. Trischman**, R. E. Oeffner, R. Nelson, T. Cook, P. Rascoe

**376.** Design, synthesis, and biological evaluation of nitrofuranyl amides, diamides and amines with enhanced activity against *Mycobacterium tuberculosis*. **R. Yendapally**, R. P. Tangallapally, R. E. B. Lee, R. E. Lee

**377.** Developing novel inhibitors of the enoyl reductase from Mycobacterium tuberculosis (InhA) : SAR studies of triclosan congeners. **T. J. Sullivan**, P. Novichenok, J. J. Truglio, C. Kisker, F. Johnson, R. A. Slayden, P. J. Tonge

**378.** Docking and 3D QSAR models of hydroxyethylamine based plasmepsin II inhibitors. **D. Muthas**, Y. A. Sabnis, D. Nöteberg, E. Hamelink, J. Hultén, L. Vrang, B. Samuelsson, A. Hallberg, A. Karlén

**379.** Design, synthesis and antimalarial activity of novel peptidomimetics based on Michael acceptor core. **O. V. Miroshnikova**, S. Zhu, T. H. Hudson, L. Gerena, A. J. Lin

**380.** Inhibition of M. tuberculosis fatty acid synthetase I isolated from M. smegmatis by 5-Cl-pyrazinamide and analogs. **S. C. Ngo**, O. Zimhony, H. Sayahi, W. R. Jacobs Jr., J. T. Welch

**381.** Microbial transformation of Artemisinin to 5-Hydroxyartemisinin. I. A. Parshikov,

**B. Miriyala**, M. A. Avery, J. Williamson

**382.** Predicting antimycobacterial activity of quinolone derivatives using theoretical molecular descriptors. **D. Mills**, M. C. Bagchi, B. C. Maiti, S. C. Basak

**383.** Protein Farnesyltransferase Inhibitors Exhibit Potent Anti-Malarial Activity. **L. Nallan**, K. Bauer, P. M. Bendale, K. Yokayama, O. Hucke, C. L. M. J. Verlinde, D. Floyd, L. J. Lombardo, D. Williams, W. C. Van Voorhis, M. H. Gelb

**384.** Synthesis and prophylactic antimalarial activities of 2-guanidinylimidazolidinedione derivatives. **Q. Zhang**, J. Guan, G. Montipa, W. Y. Ellis, A. Ager, W. K. Milhlous, D. R. Skillman, A. J. Lin

**385.** Synthesis of methylhemigossypol for biological studies. **J. Wei**, L. A. Hunsaker, D. L. Vander Jagt, R. E. Royer, L. M. Deck

**386.** Targeting FtsZ for anti-tuberculosis drug discovery: non-cytotoxic taxanes as novel anti-TB agents. **Q. Huang**, A. Pepe, I. Zanardi, P. J. Tonge, R. A. Slayden, F. Kirikae, T. Kirikae, I. Ojima

**387.** 3D-QSAR study of heterocyclic quinone compounds with antifungal activity by CoMFA. **H -Y. P. Choo**, S -Y. Choi, C -K. Ryu

**388.** Exploring the mechanism of quorum-sensing in *Candida albicans* with synthetic farnesol analogs. **R. Shchepin**, P. H. Dussault, K. W. Nickerson, R. Dumitru, A. Atkin

**389.** Antiparasitic compounds from *Psorothamnus arborescens*. **M. M. Salem**, K. A. Werbovetz

**390.** Design, synthesis and evaluation of novel inhibitors of T. cruzi dUTPase as potential anti-parasitic drugs. **O. K. Mc Carthy**, I. H. Gilbert, D. González Pacanowska, R. Brun

**391.** DNA binding properties of an antitrypanosomal agent. **B. Nguyen**, J. Stanek, R. Brun, W. D. Wilson

**392.** Identification of novel parasitic cysteine protease inhibitors using virtual screening. **P. V. Desai**, A. Patny, Y. A. Sabnis, B. L. Tekwani, J. Gut, P. J. Rosenthal, A. Srivastava, M. A. Avery

**393.** Rational design of inhibitors of the Cryptosporidium parvum ATP-Binding Cassette 3 protein. **R. Terreux**, P. lawton, S. radix, D. Deruaz, M. Lussignol, J. Reynaud, C. Marminon, P. Nebois, Z. Bouaziz, N. Walchshofer

**394.** Synthesis and Antiplasmodial Activities of 4-Amino-7-chloroquinolines with Terminal N-Substitutions on the Side Chain. **H. Liu**, F. M. Krogstad, H. Deng, D. J. Krogstad

**395.** Amino acid content of propolis, worked out in Uzbekistan. **B. N. Khodjakulov**

**396.** Characterization of medicinal plants of southwest desert by GC/MS analysis. **K. Zarrabi**, E. Gebrekidane, L. Harizanova, J. Smigel, H. Fels, J. Fietzke, P. Leary

**397.** Twenty high-grade Traditional Chinese Medicines: Their anti-HIV, antibacterial, and anticancer biological screening. **J -F. Hu**, K. Kuhen, D. Hafenbradl, J. Li, T. Chen, J. Harris, N. Gray, P. G. Schultz

**398.** Synthesis of Some Alkenol Analogs of 1-Octen-3-Ol for Use as Mosquito Attractants. **C. O. Ikediobi**

**399.** Synthesis of some cis & trans-alkenol analogs of 1-octen-3-ol for use as mosquito attractants. **T. K. Mazu**, C. O. Ikediobi, L. M. Latinwo, L. Ayuk-Takem, J. E. Cilek

**400.** Synthesis and insecticidal activity of fluorinated 2-(2,6-dichloro-4-trifluoromethyl-phenyl)-2,4,5,6-tetrahydrocyclopentapyrazoles. **S. K. Meegalla**, D. Doller, R. Liu, D. Sha, Y. Lee, R. M. Soll, N. Wisnewski, G. M. Silver, D. Dhanoa

**401.** Do marine mollusks possess aphrodisiacal properties? **R. A. Mirza**, J -J. Poisson, G. H. Fisher, A. D'Aniello, P. Spinelli, G. Ferrandino

**402.** Synthesis, SAR, in vivo, and clinical data of the deoxyarbutin class of tyrosinase inhibitors. **M. A. deLong**, R. E. Boissy, M. Visscher

**403.** 4-Aryl-4H-chromenes as a new series of apoptosis inducers using a cell- and caspase-based high throughput screening assay. Structure-activity relationships of the 7- and 5-, 6-, 8-positions. **W. Kemnitzer**, S. Kasibhatla, S. Jiang, H. Zhang, J. Zhao, S. Jia, R. Rej, R. Denis, S. Lamothe, H. Gourdeau, B. Tseng, J. Drewe, S. X. Cai

**404.** 4-Substituted 2-(2-acethyloxyethyl)-8-(morpholine-4-sulfonyl)-pyrrolo[3,4-c]quinoline-1,3-diones as potent caspase-3 inhibitors. D. Kravchenko, Y. A. Kuzovkova, V. Kysil, S. Tkachenko, S. Maliartchouk, I. Okun, **A. Ivachtchenko**

**405.** A facile synthesis of 2-substituted 4-(morpholin-4-ium-4-methyl)-1,3-dioxo-2,3-dihydro-1H-pyrrolo[3,4-c]quinolin-8-sulfonates as potent caspase-3 inhibitors. D. Kravchenko, Y. A. Kuzovkova, V. Kysil, S. Tkachenko, S. Maliartchouk, I. Okun, **A. Ivachtchenko**

**406.** Design, synthesis and biochemical evaluation of cysteine protease inhibitors: Novel compounds for chagas treatment. **R. Siles**, M. Zhou, S -E. Chen, K. G. Pinney, M. L. Trawick

**407.** Design, synthesis and biological evaluation of small-molecule inhibitors of XIAP. **J. Chen**, N -C. Zaneta, C -Y. Yang, G. Wang, Q. Su, L. Xu, S. Wang

**408.** 3-R-7-(phenylmethylene)-s-triazolo[3,4-b][1,3,4]-thiadiazines as anticancer agents. **H. Malik**, N. Heindel, C. Guillon, L. O'Keiffe, P. DeMatteo, J. Laskin

**409.** 4-X-Catechols-Tyrosinase Interactions: A QSAR Study. **R. P. Verma**, A. Z. Tan, C. D. Selassie

**410.** $O^6$-{4-(3-[$^{18}$F]fluoropropyl)-benzyl}-2'-deoxyguanosine ([$^{18}$F]FPBdG) – synthesis and evaluation of a potential DNA repair protein $O^6$-alkyguanine-DNA alkyltransferase (AGT) imaging agent. G. Vaidyanathan, **K. Base**, M. R. Zalutsky

**411.** An Efficient Formal Total Synthesis of (-)-Kazusamycin A, A Potential Antitumor Agent. S. Zhou, H. Chen, **W. Liao**, S. Chen, G. Li, R. Ando, I. Kuwajima

**412.** An SAR study of conjugated indole-imidazole derivatives displaying substantial *in vitro* antiproliferative activities against cancer cell lines. **D. James**, H. Li, S. Chen, Z. Xia, W. Ying, Y. Wu, L. Sun, K. Koya

**413.** Design and synthesis of bio-oxidatively activated prodrugs based upon the duocarmycins: Routes to Boc-CI and CI-MI prodrugs. **N. Ortuzar Kerr**, S. S. Grewel, B. Garcia-Ochoa Martin, K. Karu, L. H. Patterson, M. Searcey

**414.** Prodrug analogs of the duocarmycins activated by CYP-oxidation. **M. Searcey**, K. Karu, S. S. Grewal, N. Ortuzar Kerr, W. Griffith, L. H. Patterson

**415.** Design, synthesis and biological evaluation of potential anticancer agents based on the azinomycins. **M. A. Casely-Hayford**, K. Pors, L. H. Patterson, M. Searcey

**416.** Design, synthesis and cytotoxicity of discodermolide analogues. **M. A. Burlingame**, S. J. Shaw, K. F. Sundermann, D. Zhang, J. Petryka, E. Mendoza, F. Liu, D. C. Myles, M. J. LaMarche, T. Hirose, B. S. Freeze, A. B. Smith III

**417.** SAR and structural minimization of the C1-C8 region of (+)-Discodermolide. **K. F. Sundermann**, S. J. Shaw, M. A. Burlingame, D. C. Myles, B. S. Freeze, M. Xian, I. Brouard, A. B. Smith III

**418.** Further studies of adverse events relating Echinacea angustifolia and cancer chemotherapy. **E. D. Huntimer**, F. T. Halaweish

**419.** Inhibition of urokinase by substituted chloroisocoumarins: Potential therapeutics for breast cancer metastasis. **J. J. Heynekamp**, T. A. Vander Jagt, L. A. Hunsaker, L. M. Deck, D. L. Vander Jagt

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**421.** New Cucurbitacin derivatives: Potential anticancer candidates. **A. J. Young**, F. T. Halaweish

**422.** Nitroimidazole derivatives as a new class of anticancer compounds. **I. Weidlich**, D. Nevozhay, A. Opolski, S. Sobiak

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**424.** Novel synthetic analogs of Betulinic acid and their Biological activity. **P. K. Gupta**, B. Kaskar

**425.** Poly(sebacic acid-co-ricinoleic acid) biodegradable carrier for anti -tumor drugs. **A. Shikanov**, A. J. Domb

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**429.** Structure based design, synthesis and evaluation of boronic acid bioisosteres of combretastatin A-4. **Y. Kong**, J. Grembecka, M. C. Edler, E. Hamel, S. L. Mooberry, M. Sabat, **M. L. Brown**

**430.** Synthesis and cytotoxicity studies of epoxide and pyrazole analogs of combretastatins. T. Brown, R. LeBlanc, J. Dickson, H. Holt Jr., **M. Lee**

**431.** Synthetic Mono and Difluoro Combretastatin as Powerful Antitumoral Agents. **M. Marzi**, G. Giannini, M. marcellini, D. Alloatti, T. riccioni, M. castorina, C. pisano

**432.** Synthesis, biological evaluation and structure-activity relationship analysis of (–)-dictyostatin-1 and analogues. **C. Madiraju**, B. S. Raccor, Y. Shin, R. Balachandran, M. C. Edler, E. Hamel, K. A. Giuliano, A. Vogt, D. P. Curran, B. W. Day

**433.** Structure-Activity Relationship Study of (-)-Epicatechin Analogues as DNA Methyltransferase Inhibitors. **Y -J. Shaw**, C -S. Chen

**434.** Synthesis and biological evaluation of 3,6-dioxa-[3,2,0]bicyclonucleosides. **X. Fang**, R. F. Schinazi, D. C. Liotta

**435.** Synthesis and biological evaluation of 5-(alkyn-1-yl)-1-(p-toluenesulfonyl)uracil

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**436.** Synthesis and cellular uptake of novel nuclear targeted carborane peptides for Boron Neutron Capture Therapy. **P. Dozzo**, S. B. Kahl, E. A. Blakely, K. A. Bjornstad

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**438.** Synthesis of 1-/ 2-substituted-[1,2,3]triazolo[4,5-g]phthalazine-4,9-diones and evaluation of their cytotoxicity. **H -Y. P. Choo**, J. Kim, H. Park, S. Lee

**439.** Synthesis of controlled-release chemotherapeutic agents using Carboxymethylcellulose. **M. N. Nollenberger**, C. Martey-Ochola

**440.** Synthesis of novel cyclobutyl nucleoside analogs. **Y. Li**, S. Mao, M. W. Hager, D. C. Liotta, R. F. Schinazi

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**442.** Tumor-specific delivery of novel maytansinoids: Synthesis and biological evaluation. **S. D. Wilhelm**, W. C. Widdison, K. R. Whiteman, E. E. Roller, E. E. Cavanaugh, R. M. Steeves, R. J. Lutz, M. F. Mayo, H. Xie, R. V. J. Chari

**443.** Virginiamycin M1 Conformation in Aqueous Systems. **R. P. Metzger**, J. Dang, C. A. Ng, R. T. C. Brownlee, M. Bergdahl, F. Separovic

**444.** Anthracyclines affect calcium ion binding to calsequestrin. **W. K. Mercer**, N. Cantone, D. J. Muhlestein, H. A. Charlier Jr., S. E. Shadle

**445.** Sugar derivatives of polyamine anthraquinones; synthesis and preclinical evaluation. **D. R. I. Ishmael**

**446.** Hepatic effects of novel selenazolidine prodrugs of selenocysteine developed as potential cancer chemopreventive agents. **T. Aboul-Fadl**, W. M. El-Sayed, T. Schofield, J. Constance, J. G. Lamb, J. C. Roberts, M. R. Franklin

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**448.** Liposomal loading of water-soluble iron(III) porphyrins as anticancer drugs based on superoxide reactions. **M. Yuasa**, K. Oyaizu, A. Ogata, T. Hatsugai, A. Yamaguchi, H. Kawakami

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**451.** Effect of the Bridging Groups of Dirhodium(II,II) Complexes on the Efficiency of Transcription Inhibition in Vitro. **H. Chifotides**, K. R. Dunbar, C. Turro

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**454.** Insight into the CisPlatin mediated apoptosis in CHO cells by nuclear magnetic resonance spectroscopy and phase contrast light microscopy. **L. Maurmann**, M. Dasgupta, L. A. Joudah, J. Stalvey, R. N. Bose

**455.** Multiple Molecular Dynamics Crystal Simulations of DNA/Polyamide Complexes. **A. Loccisano**, S. A. Mueller-Stein, S. M. Firestine, J. D. Evanseck

**456.** Reading the language of pyrrole– and imidazole–containing polyamides that recognize specific DNA sequences. **K. Buchmueller**, P. Uthe, C. Howard, M. Le, K. Cox, S. Bailey, D. Matthews, J. Register, C. Bruce, B. Nguyen, C. O'Hare, J. Hartley, W. D. Wilson, M. Lee

**457.** Regulation of transcription by synthetic DNA bending agents. **S. M. Firestine**, D. Bednarski

**458.** Synthesis and biological studies of NCS-Chrom metabolite isosteres: Binding agents for bulged DNA microenvironments. **Y. Lin**, G. B. Jones, G -S. Hwang, I. H. Goldberg

**459.** Thermodynamic and structural bases for the binding of the better-than-nature triheterocyclic polyamide f-ImPyIm to its cognate sequence, ACGCGT. **K. Buchmueller**, P. Uthe, S. Bailey, D. Matthews, K. Cox, J. Register, C. Bruce, B. Nguyen, W. D. Wilson, M. Lee

**460.** Anthranilate based analogues of farnesyl pyrophosphate. **M. A. Maalouf**, A. J. Wiemer, R. J. Hohl, D. F. Wiemer

**461.** Chemical tools to induce altered protein farnesyl transferase specificity. **S. A. Reigard**, D. S. Rawat, R. A. Gibbs

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**463.** Solid-phase synthesis of lipidated peptides on chlorotrityl resin: Potential inhibitors of Ras-converting enzyme 1 (Rce1). **J. L. Donelson**, S. Hudon, C. A. Hrycyna, R. A. Gibbs

**464.** Sonogashira Coupling of Isoprenoid Triflates with Alkynes: Synthesis and Biological Evaluation of Isoprenoid- based Icmt Inhibitors. **S. K. De**, C. A. Hrycyna, R. A. Gibbs

**465.** Substrate analogues modulate protein farnesyl transferase activity. **A. J. Krzysiak**, S. A. Reigard, D. S. Rawat, R. A. Gibbs

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**470.** Electrocoating of stainless steel stents for the extended release of paclitaxel. **R. Okner**, I. Danziger, R. Slivniak, A. J. Domb

**471.** Evaluation of the bioactive tubulin-binding paclitaxel conformation: Synthesis and biological evaluation of C4 to C3'-phenyl bridged paclitaxel analogs. **T. Ganesh**, S. Bane, R. Ravindra, N. Shanker, A. S. Lakdawala, J. P. Snyder, A. Norris, D. G. I. Kingston

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**478.** Cytotoxic activities of imido-substituted 2-chloro-1,4-naphthoquinone derivatives on three human prostate cancer cell lines. **O. Bakare**, R. L. Copeland Jr., Y. Kanaan, L. H. Zalkow

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**481.** Optimizing the Potency of Phenethylphosphonamidate Inhibitors of Prostate-Specific Membrane Antigen. **D. W. G. Wone**, J. A. Rowley, J. Maung, A. W. Garofalo, C. E. Berkman

**482.** Polymer supported reagents and diagnostics for biomedical imaging: Applications in prostate cancer. **J. Li**, G. B. Jones

**483.** Radioimaging and radiotherapy of prostate and bladder cancer. **A. E. Tedesco**, Z. Keller, P. Y. Yan, A. Jain

**484.** Database searching and pharmacophore studies for inhibitors of hMDM2: A promising approach for drug discovery? **H. Zhong**, J. P. Bowen, H. A. Carlson

**485.** Design, Synthesis and Biological Evaluation of Novel Small-Molecule Inhibitors of Bcl-2 and Bcl-xL Proteins. **K. Ding**, Z. Nikolovska-Coleska, R. Wang, M. Zhang, M. L. Liu, D. Yang, Y. Tomita, S. Wang

**486.** Induction of apoptosis in cancer cells with small molecule inhibitors of Bcl-xL and Bcl-2. **C -W. Shiau**, C -C. Yang, K -F. Chen, J -W. Huang, C. Chen, C -S. Chen

**487.** Preliminary SAR study on a novel inhibitor of the apoptosis suppressor Bcl proteins. **L. Bélec**, K. Daïri, L. Dumas, G. G. Gonzalez, J -F. Lavallée, M. Lemay, V. Perron, É. Rioux, S. Tripathy, A. Babineau, S. Bailly, H. Chan, G. Chen, G. Gagnon, A. Jang, A. Khadir, M. Madiraju, R. Marcellus, D. Paquette, A. Roulston, N. Steenaart, M. Watson, Z. Zhang, G. Attardo, P. Beauparlant, G. Shore

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**489.** Thiazolyl hydrazones as novel inhibitors of eIF4E/eIF4G interaction for cancer therapy. **H. Chen**, N. Moerke, F. Harbinski, H. Aktas, G. Wagner, M. Chorev, J. A. Halperin

**490.** Transcription activation by a synthetic molecule in living mammalian cells. **P. Yu**, B. Liu, T. J. Kodadek

**491.** Design and synthesis of N-[4-(2,4-diamino-5-propyl-7H-pyrrolo[2,3-*d*]pyrimidin-6-ylsulfanyl)-benzoyl]-L-glutamic acid as a potent inhibitor of dihydrofolate reductase and as an antitumor agent. A. Gangjee, **H. Jain**, S. F. Queener, R. L. Kisliuk

**492.** Folate targeted chemotherapeutics and their size-dependent penetration into solid tumor mass. **E. Vlashi**, **W. A. Henne Jr.**, **D. Doorneweerd**, **A. R. Hilgenbrink**, P. S. Low

**493.** Prodrug strategy for intracellular Inhibition of folylpolyglutamate synthetase. **Y. Feng**, J. K. Coward

**494.** Design, synthesis and HDAC inhibitory activity of cyclic tetrapeptides with modifications at the Tyr residue. **B. Jose**, T. Kato, N. Nishino, Y. Sumida, M. Yoshida

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**496.** Sulfonamides of 5,6-disubstituted anthranilic acids as potent inhibitors of methionine aminopeptidase-2 (MetAP2). **R. Mantei**, G. T. Wang, G. S. Sheppard, M. Kawai, J. S. Tedrow, D. M. Barnes, C. Park, J. Wang, Q. Zhang, P. Lou, L. A. Garcia, M. S. Yates, J. J. Bouska, R. L. Bell

**497.** Molecular modeling of asparagine synthetase. **R. Humkey**, Y. Ding, N. G. J. Richards

**498.** Novel inhibitors of carbonyl reductase. **B. Williams**, C. L. Larson, A. Slupe, K. Olson, S. Begic, L. Lee, H. A. Charlier Jr.

**499.** Investigation of polyamine analogs on the growth of MCF-7 breast cancer cell lines. M. Piel, **K. Thornburg**, C. Higgins, F. C. Mayville Jr., P. Leonard

**500.** Polyamine conjugates of serine, 4-thiazolidinone and thiazolidine-4-carboxylic acid: Synthesis and growth inhibitory effects on human prostate cancer cell lines. **V. Gududuru**, E. Hurh, J. T. Dalton, D. D. Miller

**501.** Polyamino-heterocycle chelating agents with cytotoxic activity in tumor cells: Structure-activity relationship of imidazole, thiazole and pyridyl donor groups. **R. P. Planalp**, M. Childers, D. P. Kennedy, A. Lindell, G. Broker, R. D. Rogers, M. W. Brechbiel, R. Ma, F. M. Torti, S. V. Torti

**502.** Synthesis and biological evaluation of Dihydromotuporamine derivatives in cells containing active polyamine transporters. **N. Kaur**, F. Breitbeil III, O. Phanstiel IV

**503.** New indenoisoquinolinium salts, *N*-6-desalkylindenoisoquinolines, and 5,11-diketoindenoisoquinolines: Design and synthesis of topoisomerase I inhibitors as anticancer agents. **A. S. Ioanoviciu**, S. Antony, G. Kohlhagen, Y. Pommier, B. Staker, L. Stewart, M. Cushman

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**506.** Synthesis and evaluation of multisubstrate bicyclic pyrimidine nucleoside inhibitors of human Thymidine Phosphorylase. **A. L. Allan**, P. L. Gladstone, M. L. P. Price, S. A. Hopkins, J. C. Juarez, F. Doñate, R. J. Ternansky, B. Ganem, Y. Li, W. Wang, S. E. Ealick

**507.** Three-dimensional QSAR studies on human thymidine kinase-1 substrates. **A. K. Bandyopadhyaya**, J. Johnsamuel, Y. Byun, A. S. Al-Madhoun, S. Eriksson, W. Tjarks

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**513.** Screening for drug-membrane interactions using arrays of supported lipid bilayers with varying lipid compositions. **M. Mayer**, S. Majd

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**515.** Cell-selective drug delivery using the polyamine transporter. **O. Phanstiel IV**, N. Kaur, J -G. Delcros

**516.** GC/MS analysis of hydroxyurea metabolism to hydroxylamine by rat liver. **M. Yakubu**, J. Huang, D. B. Kim-Shapiro, S. B. King

**517.** hERG mutant panel for lead optimization of compounds with hERG liability. M. W. Nowak, **N. M. Zacharias**, A. A. Kulkarni, J. B. Nicholas, S. D. Sahba, B. S. Lally, H. P. Lesso, S. J. Reyes, E. D. Mackey, N. W. Shiva, P. B. Bennett

**518.** Novel drug delivery vehicles: Synthesis and biological evaluation of dendrimers based on melamine. **H -T. Chen**, M. F. Neerman, A. R. Parrish, E. E. Simanek

**519.** Prevalence of Scaffolds in P450 Inhibitors. **R. Kho**, K. Koch, M. R. Hansen, J. Hodges, C. Sanglimsuwan

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**524.** Base-Catalyzed Deuterium and Tritium Labeling of Aryl Methyl Sulfones and Aryl Methyl Ketones. Applications to Drug Development. **J. Scheigetz**, C. Berthelette, C. Li, R. Zamboni

**525.** Characterization and antioxidative activities of agar-derived oligosaccharides. **W. Mao**, L. Wu

**526.** Effect of 2',5'-linked nucleic acid on siRNA activity. **T. P. Prakash**, B. Kraynack, B. Baker, M. Manoharan, E. E. Swayze, R. H. Griffey, B. Bhat

**527.** Effect of sulfur oxidation state and hydrophobicity on the binding kinetics of trifluoromethyl ketone-containing carboxylesterase inhibitors. **C. E. Wheelock**, Z. Ying, P. D. Jones, M. E. Colvin, M. M. Olmstead, B. D. Hammock

**528.** MIF imbalance in the seminal fluid is predictive of male infertility: Development of

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**529.** Modified polyelectrolyte capsules as smart antioxidant systems for drug and enzyme encapsulation. T. Shutava, D. Shchukin, **Z. Zheng**, Y. Lvov

**530.** MtmOIV, a key baeyer-villiger type oxygenase of the Mithramycin biosynthetic pathway. **M. P. Gibson**, M. Nur-e-alam, C. Wang, J. Rohr

**531.** Peripheral sequence elements key to self-cleavage activity of natural Hammerhead ribozymes by forming tertiary contacts. **M. R. Saha**, S. Roychowdhury, D. H. Burke

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**533.** Protease inhibition by novel fluoropeptidomimetics: A mechanism-based design strategy. **L. P. Kotra**, S. C. Annedi, K. Majumder, S. Samson

**534.** Rapid Diversity-Oriented Synthesis of Five-menbered Iminocyclitols in Microtiter Plates for In Situ Screening of Glucosidase Inhibitors. **P -H. Liang**, C -Y. Wu, C -H. Wong

**535.** Rapid discovery of potent inhibitors using diversity-oriented synthesis followed by in situ screening. **A. Brik**, C -H. Wong

**536.** Silver/dendrimer nanocomposites as biomarkers: fabrication, characterization, in vitro toxicity and intracellular detection. W. Lesniak, X. Shi, A. Bielinska, K. Janczak, K. Sun, J. R. Baker Jr., **L. P. Balogh**

**537.** Triggered release of liposome contents by MMP-9. **A. Krueger**, N. Sarkar, A. L. Banerjee, K. Benton, S. Mallik, D. K. Srivastava

**538.** Construction of classification models for the virtual screening. **N. Grinevich**

**539.** Effect of vapor phase pre-minimization versus MD simulations on docking calculation performance. **I. G. Welsford**, M. J. McManus

**540.** New computational tool for medicinal chemists that uses design “Rules-of-Thumb”. **K. D. Stewart**, C. A. James

**541.** Selection of a diverse set of drugs based on multivariate design. **C. Sköld**, S. Winiwarter, J. Wernevik, F. Bergström, H. Lennernäs, T. Lundstedt, A. Hallberg, A. Karlén

**542.** Useful cycloalkylamine pharmacophor building blocks. **J. Havel**, J. Solomon, C. Guillon, N. Heindel

**543.** Comparison of Scaffolds Found in Screening Libraries. **M. R. Hansen**, R.

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**544.** A Circular Dichroism Spectroscopy Study: Secondary Structure of Organophosphorus Acid Anhydrolase (OPAA) in Solution and in Langmuir-Blodgett Film. **L. Zhao**, X. Ji, J. Xu, T. C. Cheng, R. M. Leblanc

**545.** Detection of carbon-fluorine bonds by raman spectroscopy in selected fluorine-containing blood substitutes. **D. F. Shellhamer**, O. Sharts, M. O'Hagan, L. P. Avakyants, S. Sarkisyan, V. Contreras, R. P. Metzger

**546.** Fluoro-Raman for drug discovery and pharmaceutical analysis. **O. Sharts**, L. P. Avakyants

**547.** Site-selective fluorescent probes for cells and organelles. **K. A. McNitt**, **G. J. Sormunen**, L. L. Scardino, E. M. Ott, S. C. Hartsel, D. E. Lewis

**548.** Small molecule vs genetically encoded FRET sensors: Pros and cons. **C. Schultz**, O. Wichmann, A. Schleifenbaum, J. Brumbaugh

**549.** A New Method for Macrodiolide Formation Using Selenol Ester. L. Shen, H -S. Mun, **J -H. Jeong**

**550.** An efficient strategy for the synthesis of Sparse Matrix Libraries using integrated robotics. **M. El-Araby**, A. Vergnon, E. Arvanitis, R. Pottorf, D. J. Hlasta

**551.** C-Lithiation / Alkylation of Trimethylamine Cyanoborane. **K. J. Takrouri**, J. katzhendler, M. Srebnik

**552.** Deamidation of peptides in aerobic nitric oxide solution. **L. Kong**, B. M. Showalter, J. E. Saavedra, G. S. Buzard, L. K. Keefer

**553.** Design and synthesis of new bicyclic diketopiperazines as scaffolds for receptor probes of structurally diverse functionality. **P. Besada**, L. Mamedova, C. J. Thomas, S. Costanzi, K. A. Jacobson

**554.** Efficient method for the solid-phase synthesis of trisubstitued guanidines. **J. Urban**, V. J. Huber

**555.** Epoxidation and nucleophilic addition to 4, 4a, 5, 6-tertrahydronaphthalen-2-one: a convenient stereoselective synthesis strategy. **Z. Li**

**556.** Macrolactones and polyesters from ricinoleic acid. **R. Slivniak**, A. J. Domb

**557.** New Substrates for Ugi Three-Component Condensation. **Q. J. Yu**, F. Wei, J. Wang, L. Huang, Z. Fang, W. Ma

**558.** Redox Reactions of Bioactive Phenazines: Voltammetric and Spectrophotometric Study. **D. Vukomanovic**

**559.** Synthesis of 1,5-Benzothiazepines and 1,5-Benzooxazepines via Cyclization of trans-3-Benzylidenechroman-4-ones and 2-Aminothiophenols. **E. R. Biehl**, H. Zhang, R. Sathunuru

**560.** Synthesis of cyclic anilines by reductive rearrangement of O-silylated ketoximes using borane / boron trifluoride. **M. Ortiz-Marciales**, S. Espinosa, L. D. Rivera, M. De Jesús, O. E. Casanova, J. A. Benjamin, S. E. Rodriguez, W. Correa

**561.** Synthesis of prenylated aromatic compounds. **S. I. Odejinmi**, D. F. Wiemer

**562.** Synthesis of Side-chain Modified Derivatives of (-)-Laulimalide. **J. Fan**, S. G. Nelson

**563.** A Study on Flash Chromatography Performance Using Different Sample Loading Methods. **J. Liu**

**564.** Use of Isco's RediSep specialty media columns for the separation of low-solubility compounds. **V. D. Thomason**

**565.** C18 Flash columns in rapid isolation of organic compounds. **S. Ghassemi**

**566.** Determination of Modafinil in plasma and urine by reversed phase liquid chromatography. H. A. Schwertner, **S. B. Kong**

**567.** New method extracting salicylic acid from plasma and for its analysis by high performance liquid chromatography. H. A. Schwertner, **S. B. Kong**, E. L. Richter

**568.** Super Critical Fluid (SFC) and HPLC for the analysis of chiral pharmaceuticals. **A. L. Jenkins**, **M. A. Burns**

**569.** Supercritical fluid chromatography of ionic analytes. **J. Zheng**, L. Taylor, J. D. Pinkston

**570.** The removal of TFA from organic solutions using polymeric SPE devices. **P. A. Boguszewski**, A. F. Coffey, J. W. Davies, A. A. MacDonald, **A. J. Mendonca**, F. P. Warner

**571.** Investigation of the effect that different drying methods have on the mechanism of theophylline release from microcrystalline cellulose beads. **P. Cruz**, **K. Kurek**, F. C. Mayville Jr., R. J. Wigent

**572.** Methods for Producing Polymeric Drug Loaded Ultrasound Contrast Agents. **O. Mualem Burstein**, M. A. Wheatley

## THURSDAY MORNING

Section A

Unknown Site -- Unknown Room

**From Bench to Pilot Plant: Sponsored by Teledyne Isco, Inc**

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L. McQuire, *Organizer*

**9:00 —** Introductory Remarks.

**9:05 —573.** Practical asymmetric synthesis of a potent PDE4 inhibitor via stereoselective enolate alkylation of a chiral aryl-heteroaryl secondary tosylate. **C -Y. Chen**, P. D. O'Shea, W. Chen, P. Dagneau, L. F. Frey, E. J. J. Grabowski, K. M. Marcantonio, R. A. Reamer, L. Tan, R. D. Tillyer, A. Roy, X. Wang, D. Zhao

**9:40 —574.** Application of new technologies in pharmaceutical process research and development. **J. L. Rutherford**

**10:15 —575.** Enzymatic synthesis of pharmaceutical intermediates. **B. Morgan**, G. DeSantis, N. Barton, D. P. Weiner, W. A. Greenberg, M. J. Burk

**10:50 —576.** Evolution of a manufacturing route for a highly potent drug candidate. **A. K. Singh**

**11:25 —577.** From deep-sea sponge to pilot plant: The large scale total synthesis of the marine natural product (+)-Discodermolide. **S. J. Mickel**

Section B

Unknown Site -- Unknown Room

**General Oral Session III**

D. L. Flynn, *Organizer*

**9:00 —578.** Design, synthesis and SAR of novel phosphonates as potent and selective FBPase inhibitors with oral efficacy in rodent models of type 2 diabetes. **Q. Dang**, M. D. Erion, K. R. Reddy, S. R. Kasibhatla, M. R. Reddy, P. D. van Poelje

**9:20 —579.** Discovery of novel PTP1b inhibitors from a non-HTS hit. **S. Kirincich**, B. Follows, A. Moretto, Z -K. Wan, D. P. Wilson, M. J. Smith, D. Erbe, J. Tobin, Y -L. Zhang, M. Tam, W -X. Xu, D. Joseph-McCarthy, K. Foreman, S. Tam, J. Lee

**9:40 —580.** Discovery of potent and selective orally bioavailable β-substituted phenylalanine derived dipeptidyl peptidase IV inhibitors. **S. D. Edmondson**, A. Mastracchio, J. L. Duffy, G. J. Eiermann, H. He, B. Leiting, J. F. Leone, K. A. Lyons, A. M. Makarewicz, R. A. Patel, A. Petrov, J. K. Wu, N. A. Thornberry, A. E. Weber

**10:00 —581.** MIF knockout mice are resistant to the development of type 1 diabetes. **Y. Al-Abed**, I. Cvetkovic, D. Miljkovic, C. Metz, F. Nicoletti, S. Stosic-Grujicic

**10:20 —582.** Clustering of Beta-lactam antibiotics to predict cross-reactivities in allergic patients. **R. Terreux**, O. preaud, A. roziere, M. Domard, J. F. Nicolas

**10:40 —583.** Evaluation of DPD and synthetic analogs in AI-2 based quorum sensing. **M. M. Meijler**, K. M. McKenzie, C. A. Lowery, L. Qi, K. D. Janda

**11:00 —584.** Stereochemical preferences of autoinducer analogs of Pseudomonas aeruginosa quorum sensing regulators LasR and RhlR. **G. J. Jog**, H -A. Suga

**11:20 —585.** Structure-based design of nonpeptidic inhibitors for the malarial protease plasmepsin II. **F. Hof**, A. Schütz, D. Bur, F. Diederich

**11:40 —586.** Drug Guru: A new tool for medicinal chemists. **K. D. Stewart**, C. A. James

**12:00 —587.** Discovery of novel carboxylated, heteroaryl-substituted chalcones as inhibitors of VCAM-1 expression for use in chronic inflammatory diseases. **C. Q. Meng**, L. Ni, K. J. Worsencroft, Z. Ye, M. D. Weingarten, J. E. Simpson, J. W. Skudlarek, E. M. Marino, K -L. Suen, C. Kunsch, R. B. Howard, C. L. Sundell, M. A. Wasserman, J. A. Sikorski