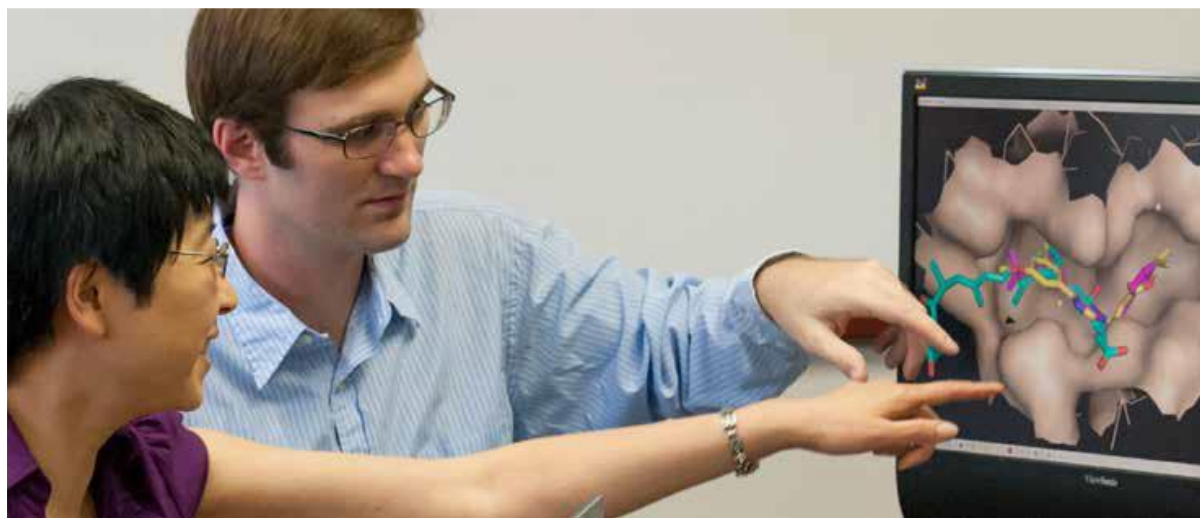


## Chronological list of medicinal chemistry articles authored or co-authored by SRI Biosciences Scientists (names in bold)



### 2014

#### Scaffold hopping towards potent and selective JAK3 inhibitors: Discovery of novel C-5 substituted pyrrolopyrazines

de Vicente, Javier; **Lemoine, Remy**; Bartlett, Mark; Hermann, Johannes C.; Hekmat-Nejad, Mohammad; Henningsen, Robert; Jin, Sue; Kuglstatler, Andreas; Li, Hongju; Lovey, Allen J.; et al Bioorganic & Medicinal Chemistry Letters (2014), Ahead of Print.  
DOI:10.1016/j.bmcl.2014.09.031

#### Structure-Based Drug Design of RN486, a Potent and Selective Bruton's Tyrosine Kinase (BTK) Inhibitor, for the Treatment of Rheumatoid Arthritis

Lou, Yan; Han, Xiaochun; Kuglstatler, Andreas; Kondru, Rama K.; Sweeney, Zachary K.; Soth, Michael; McIntosh, Joel; Litman, Renee; Suh, Judy; Kocer, Buelent; Davis, Dana; **Park, Jaehyeon**; et al Journal of Medicinal Chemistry (2014), Ahead of Print. DOI:10.1021/jm500305p

#### Discovery of N [4-[6-tert-Butyl-5-methoxy-8-(6-methoxy-2-oxo-1H-pyridin-3-yl)-3-quinolyl]phenyl]-methanesulfonamide (RG7109), a Potent Inhibitor of the Hepatitis C Virus NS5B Polymerase

Talamas, F.; Abbot, S.; Anand, S.; Brameld, K.; Carter, D.; Chen, J.; Davis, D.; de Vicente, J.; Fung, A.; **Gong, L.**; Harris, S.; Inbar, P.; Labadie, S.; Lee, E.; **Lemoine, R.**; Le Pogam, S.; Leveque, V.; Li, J.; McIntosh, J.; Najera, I.; Park, J.; Railkar, A.; Rajyaguru, S.; Sangi, M.; Schoenfeld, R.; Staben, L.; Tan, Y.; Taygerly, J.; Villasenor, A.; Weller, P.  
Journal of Medicinal Chemistry (2014), 57(5), 1914-1931.  
DOI:10.1021/jm401329s

#### Design of a Peptide Inhibitor of Tyrosine Kinase 2

Works, Melissa G.; Song, Benben; Kibler, Patrick; **Tanga, Mary J.**; Galande, Amit K.; D'Andrea, Annalisa  
Protein & Peptide Letters (2014), 21(5), 419-425.  
DOI:10.2174/0929866520666131203101841

### Design and synthesis of molecular probes for the determination of the target of the anthelmintic drug praziquantel

Sharma, Lalit Kumar; Cupit, Pauline M.; Goronga, Tino; **Webb, Thomas R.**; Cunningham, Charles  
Bioorganic & Medicinal Chemistry Letters (2014), 24(11), 2469-2472.  
DOI:10.1016/j.bmcl.2014.04.014

### Natural products as anti-infective agents

Chopra, Sidharth; Beaulieu, Ellen D.; **Malerich, Jeremiah P.**  
Frontiers in Anti-Infective Drug Discovery (2014), 2, 159-223.  
DOI:10.2174/9781608058600114020005

### Comparative molecular field analysis of fenoterol derivatives interacting with an agonist-stabilized form of the $\beta$ 2-adrenergic receptor

Plazinska, Anita; Pajak, Karolina; Rutkowska, Ewelina; Jimenez, Lucita; **Kozocas, Joseph**; Koolpe, Gary; **Tanga, Mary**; Toll, Lawrence; Wainer, Irving W.; Jozwiak, Krzysztof  
Bioorganic & Medicinal Chemistry (2014), 22(1), 234-246.  
DOI:10.1016/j.bmc.2013.11.030

## 2013

### Development of indole/indazole-aminopyrimidines as inhibitors of c-Jun N-terminal kinase (JNK): Optimization for JNK potency and physicochemical properties

**Gong, Leyi**; Han, Xiaochun; Silva, Tania; Tan, Yun-Chou; Goyal, Bindu; Tivitmahaisoon, Parch; Trejo, Alejandra; Palmer, Wylie; Hogg, Heather; Jahagir, Alam; et al  
Bioorganic & Medicinal Chemistry Letters (2013), 23(12), 3565-3569.  
DOI:10.1016/j.bmcl.2013.04.029

### Development of amino-pyrimidine inhibitors of c-Jun N-terminal kinase (JNK): Kinase profiling guided optimization of a 1,2,3-benzotriazole lead

Palmer, Wylie S.; Alam, Muzaffar; Arzeno, Humberto B.; Chang, Kung-Ching; Dunn, James P.; Goldstein, David M.; **Gong, Leyi**; Goyal, Bindu; Hermann, Johannes C.; Hogg, J. Heather; et al  
Bioorganic & Medicinal Chemistry Letters (2013), 23(5), 1486-1492.  
DOI:10.1016/j.bmcl.2012.12.047

### A systematic screen of FDA-approved drugs for inhibitors of biological threat agents

**Madrid, Peter B.**; Chopra, Sidharth; Manger, Ian D.; Gilfillan, Lynne; Keepers, Tiffany R.; Shurtleff, Amy C.; Green, Carol E.; Iyer, Lalitha V.; Hutcheson Dilks, Holli; Davey, Robert A.; et al  
PLoS One (2013), 8(4), e60579.  
DOI:10.1371/journal.pone.0060579

### Antileishmanial Activity of Naphthoquinones

**Malerich, Jeremiah P.**; Li, Jinfang; Joder, Dallas; Viera, Erica L. M.; Keesen, Tatjana S. L.; Vaidyanathan, Rajeev; Gollob, Kenneth J.; **Tanga, Mary J.**  
Drug Development Research (2013), 74(4), 237-241.  
DOI:10.1002/ddr.21067

### Optimization of Antitumor Modulators of Pre-mRNA Splicing

Lagiseti, Chandraiah; Palacios, Gustavo; Goronga, Tinopiwa; Freeman, Burgess; Caufield, William; **Webb, Thomas R.**  
Journal of Medicinal Chemistry (2013), 56(24), 10033-10044.  
DOI:10.1021/jm401370h

## The development and application of small molecule modulators of SF3b as therapeutic agents for cancer

**Webb, Thomas R.;** Joyner, Amanda S.; Potter, Philip M.  
Drug Discovery Today (2013), 18(1-2), 43-49.  
DOI:10.1016/j.drudis.2012.07.013

## 2012

### Discovery of a novel series of 4-quinolone JNK inhibitors

**Gong, Leyi;** Tan, Yun-Chou; Boice, Genevieve; Abbot, Sarah; McCaleb, Kristen; Iyer, Pravin; Zuo, Fengrong; Dal Porto, Joseph; Wong, Brian; Jin, Sue; et al  
Bioorganic & Medicinal Chemistry Letters (2012), 22(24), 7381-7387.  
DOI:10.1016/j.bmcl.2012.10.066

### Systematic discovery of synergistic novel antibiotic combinations targeting multidrug-resistant *Acinetobacter baumannii*

Chopra, Sidharth; Matsuyama, Karen; Tran, Tran; **Madrid, Peter**  
International Journal of Antimicrobial Agents (2012), 40(4), 377-379.  
DOI:10.1016/j.ijantimicag.2012.06.008

### Discovery and Optimization of Benzotriazine Di-N-Oxides Targeting Replicating and Nonreplicating *Mycobacterium tuberculosis*

Chopra, Sidharth; Koolpe, Gary A.; Tambo-ong, Arlyn A.; Matsuyama, Karen N.; Ryan, Kenneth J.; Tran, Tran B.; Doppalapudi, Rupa S.; Riccio, Edward S.; Iyer, Lalitha V.; Green, Carol E.; Wan, Baojie; Franzblau, Scott G.; **Madrid, Peter B.**  
Journal of Medicinal Chemistry (2012), 55(13), 6047-6060.  
DOI:10.1021/jm300123s

### Combining Cheminformatics Methods and Pathway Analysis to Identify Molecules with Whole-Cell Activity Against *Mycobacterium tuberculosis*

Sarker, Malabika; Talcott, Carolyn; **Madrid, Peter;** Chopra, Sidharth; Bunin, Barry A.; Lamichhane, Gyanu; Freundlich, Joel S.; Ekins, Sean  
Pharmaceutical Research (2012), 29(8), 2115-2127.  
DOI:10.1007/s11095-012-0741-5

### Evaluation of gyrase B as a drug target in *Mycobacterium tuberculosis*

Chopra, Sidharth; Matsuyama, Karen; Tran, Tran; **Malerich, Jeremiah P.;** Wan, Baojie; Franzblau, Scott G.; Lun, Shichun; Guo, Haidan; Maiga, Mariama C.; Bishai, William R.; et al  
Journal of Antimicrobial Chemotherapy (2012), 67(2), 415-421.  
DOI:10.1093/jac/dkr449

### Structural and biochemical basis for development of influenza virus inhibitors targeting the PA endonuclease

DuBois, Rebecca M.; Slavish, P. Jake; Baughman, Brandi M.; Yun, Mi-Kyung; Bao, Ju; Webby, Richard J.; **Webb, Thomas R.;** White, Stephen W.  
PLoS Pathogens (2012), 8(8), e1002830.  
DOI:10.1371/journal.ppat.1002830

### Identification of Influenza Endonuclease Inhibitors Using a Novel Fluorescence Polarization Assay

Baughman, Brandi M.; Jake Slavish, P.; DuBois, Rebecca M.; Boyd, Vincent A.; White, Stephen W.; **Webb, Thomas R.**  
ACS Chemical Biology (2012), 7(3), 526-534.  
DOI:10.1021/cb200439z

### Thermodynamics and docking of agonists to the $\beta$ 2-adrenoceptor determined using [3H](R,R')-4-methoxyfenoterol as the marker ligand

Toll, Lawrence; Pajak, Karolina; Plazinska, Anita; Jozwiak, Krzysztof; Jimenez, Lucita; **Kozocas, Joseph A.**; **Tanga, Mary J.**; Bupp, James E.; Wainer, Irving W.  
Molecular Pharmacology (2012), 81(6), 846-854.  
DOI:10.1124/mol.111.077347

## 2011

### SR16388: a steroidal antiangiogenic agent with potent inhibitory effect on tumor growth in vivo

Chao, Wan-Ru; Amin, Khalid; Shi, Yihui; Hobbs, Peter; Tanabe, Mas; **Tanga, Mary**; **Jong, Ling**; **Collins, Nathan**; Peters, Richard; Laderoute, Keith; et al  
Angiogenesis (2011), 14(1), 1-16.  
DOI:10.1007/s10456-010-9191-z

### Identification of antimicrobial activity among FDA-approved drugs for combating Mycobacterium abscessus and Mycobacterium chelonae

Chopra, Sidharth; Matsuyama, Karen; Hutson, Christopher; **Madrid, Peter**  
Journal of Antimicrobial Chemotherapy (2011), 66(7), 533-1536.  
DOI:10.1093/jac/dkr154

### Synthesis of an aryloxy oxo pyrimidinone library that displays ALK-selective inhibition

Slavish, P. Jake; Price, Jeanine E.; Jiang, Qin; Cui, Xiaoli; Morris, Stephan W.; **Webb, Thomas R.**  
Bioorganic & Medicinal Chemistry Letters (2011), 21(15), 4592-4596.  
DOI:10.1016/j.bmcl.2011.05.103

### 3-Amino-pyrazolo[3,4-d]pyrimidines as p38 $\alpha$ kinase inhibitors: Design and development to a highly selective lead

Soth, Michael; Abbot, Sarah; Abubakari, Allassan; Arora, Nidhi; Arzeno, Humberto; Billedeau, Roland; Dewdney, Nolan; Durkin, Kieran; Frauchiger, Sandra; Ghate, Manjiri; Goldstein, David M.; Hill, Ronald J.; Kuglstatler, Andreas; Li, Fujun; Loe, Brad; McCaleb, Kristen; McIntosh, Joel; Papp, Eva; **Park, Jaehyeon**; et al  
Bioorganic & Medicinal Chemistry Letters (2011), 21(11), 3452-3456.  
DOI:10.1016/j.bmcl.2011.03.098

### Acylideneoxindoles: A new class of reversible inhibitors of human transglutaminase 2

Kloeck, Cornelius; Jin, Xi; Choi, Kihang; Khosla, Chaitan; **Madrid, Peter B.**; Spencer, Andrew; Raimundo, Brian C.; Boardman, Paul; Lanza, Guido; Griffin, John H.  
Bioorganic & Medicinal Chemistry Letters (2011), 21(9), 2692-2696.  
DOI:10.1016/j.bmcl.2010.12.037

### Design, synthesis and initial biological evaluation of a novel pladienolide analog scaffold

Gundluru, Mahesh Kumar; Pourpak, Alan; Cui, Xiaoli; Morris, Stephan W.; **Webb, Thomas R.**  
MedChemComm (2011), 2(9), 904-908.  
DOI:10.1039/c1md00040c

### Sudemycins, Novel Small Molecule Analogues of FR901464, Induce Alternative Gene Splicing

Fan, Liying; Lagiseti, Chandraiah; Edwards, Carol C.; **Webb, Thomas R.**; Potter, Philip M.  
ACS Chemical Biology (2011), 6(6), 582-589.  
DOI:10.1021/cb100356k

### Synthesis and biological evaluation of a peptide-paclitaxel conjugate which targets the integrin $\alpha v\beta 6$

Li, Shunzi; Gray, Bethany Powell; McGuire, Michael J.; **Brown, Kathlynn C.**  
Bioorganic & Medicinal Chemistry (2011), 19(18), 5480-5489.  
DOI:10.1016/j.bmc.2011.07.046

### Discovery of 6-(2,4-Difluorophenoxy)-2-[3-hydroxy-1-(2-hydroxyethyl)propylamino]-8-methyl-8H-pyrido[2,3-d]pyrimidin-7-one (Pamapimod) and 6-(2,4-Difluorophenoxy)-8-methyl-2-(tetrahydro-2H-pyran-4-ylamino)pyrido[2,3-d]pyrimidin-7(8H)-one (R1487) as Orally Bioavailable and Highly Selective Inhibitors of p38 $\alpha$ Mitogen-Activated Protein Kinase

Goldstein, David M.; Soth, Michael; Gabriel, Tobias; Dewdney, Nolan; Kuglstatler, Andreas; Arzeno, Humberto; Chen, Jeffrey; Bingenheimer, William; Dalrymple, Stacie A.; Dunn, James; **Park, Jaeyeon**; et al  
Journal of Medicinal Chemistry (2011), 54(7), 2255-2265.  
DOI:10.1021/jm101423y

### Improved oral bioavailability in rats of SR13668, a novel anti-cancer agent

Green, Carol E.; Swezey, Robert; Bakke, James; Shinn, Walter; Furimsky, Anna; Bejugam, Naveen; Shankar, Gita N.; **Jong, Ling**; Kapetanovic, Izet M.  
Cancer Chemotherapy and Pharmacology (2011), 67(5), 995-1006.  
DOI:10.1007/s00280-010-1395-9

## 2010

### Diamino-1,2,4-triazole derivatives are selective inhibitors of TYK2 and JAK1 over JAK2 and JAK3

**Malerich, Jeremiah P.**; Lam, Jennifer S.; Hart, Barry; Fine, Richard M.; Klebansky, Boris; **Tanga, Mary J.**; D'Andrea, Annalisa  
Bioorganic & Medicinal Chemistry Letters (2010), 20(24), 7454-7457.  
DOI:10.1016/j.bmcl.2010.10.026

### Evaluation of amide replacements in CCR5 antagonists as a means to increase intrinsic permeability. Part 2: SAR optimization and pharmacokinetic profile of a homologous azacycle series

Wanner, Jutta; Chen, Lijing; **Lemoine, Remy C.**; Kondru, Rama; Jekle, Andreas; Heilek, Gabrielle; de Rosier, Andre; Ji, Changhua; Berry, Pamela W.; Rotstein, David M.  
Bioorganic & Medicinal Chemistry Letters (2010), 20(22), 6802-6807.  
DOI:10.1016/j.bmcl.2010.08.118

### Exploration of a new series of CCR5 antagonists: Multi-dimensional optimization of a sub-series containing N-substituted pyrazoles

**Lemoine, Remy C.**; Petersen, Ann C.; Setti, Lina; Jekle, Andreas; Heilek, Gabrielle; de Rosier, Andre; Ji, Changhua; Berry, Pamela; Rotstein, David M.  
Bioorganic & Medicinal Chemistry Letters (2010), 20(16), 4753-4756.  
DOI:10.1016/j.bmcl.2010.06.135

### Novel hexahydropyrrolo[3,4-c]pyrrole CCR5 antagonists

Rotstein, David M.; Melville, Chris R.; Padilla, Fernando; Cournoyer, Dick; Lee, Eun K.; **Lemoine, Remy**; Petersen, Ann C.; Setti, Lina Q.; Wanner, Jutta; Chen, Lijing; et al

Bioorganic & Medicinal Chemistry Letters (2010), 20(10), 3116-3119.  
DOI:10.1016/j.bmcl.2010.03.095

#### Evaluation of a 4-aminopiperidine replacement in several series of CCR5 antagonists

**Lemoine, Remy C.**; Petersen, Ann C.; Setti, Lina; Chen, Lijing; Wanner, Jutta; Jekle, Andreas; Heilek, Gabrielle; de Rosier, Andre; Ji, Changhua; Rotstein, David M.  
Bioorganic & Medicinal Chemistry Letters (2010), 20(6), 1830-1833.  
DOI:10.1016/j.bmcl.2010.02.004

#### Discovery of potent and bioavailable GSK-3 $\beta$ inhibitors

**Gong, Leyi**; Hirschfeld, Don; Tan, Yun-Chou; Heather Hogg, J.; Peltz, Gary; Avnur, Zafrira; Dunten, Pete  
Bioorganic & Medicinal Chemistry Letters (2010), 20(5), 1693-1696.  
DOI:10.1016/j.bmcl.2010.01.038

#### Evaluation of a 3-amino-8-azabicyclo[3.2.1]octane replacement in the CCR5 antagonist maraviroc

**Lemoine, Remy C.**; Petersen, Ann C.; Setti, Lina; Baldinger, Thomas; Wanner, Jutta; Jekle, Andreas; Heilek, Gabrielle; de Rosier, Andre; Ji, Changhua; Rotstein, David M.  
Bioorganic & Medicinal Chemistry Letters (2010), 20(5), 1674-1676.  
DOI:10.1016/j.bmcl.2010.01.080

#### Evaluation of secondary amide replacements in a series of CCR5 antagonists as a means to increase intrinsic membrane permeability. Part 1: Optimization of gem-disubstituted azacycles

**Lemoine, Remy C.**; Petersen, Ann C.; Setti, Lina; Wanner, Jutta; Jekle, Andreas; Heilek, Gabrielle; deRosier, Andre; Ji, Changhua; Berry, Pamela; Rotstein, David  
Bioorganic & Medicinal Chemistry Letters (2010), 20(2), 704-708.  
DOI:10.1016/j.bmcl.2009.11.072

#### Small molecule antagonists of the chemokine receptor CCR5

**Lemoine, Remy C.**; Wanner, Jutta  
Current Topics in Medicinal Chemistry (Sharjah, United Arab Emirates) (2010), 10(13), 1299-1338.  
ISSN:1568-0266

#### Structure-Activity Relationships of Substituted 1-Pyridyl-2-phenyl-1,2-ethanediones: Potent, Selective Carboxylesterase Inhibitors

Young, Brandon M.; Hyatt, Janice L.; Bouck, David C.; Chen, Taosheng; Hanumesh, Parimala; Price, Jeanine; Boyd, Vincent A.; Potter, Philip M.; **Webb, Thomas R.**  
Journal of Medicinal Chemistry (2010), 53(24), 8709-8715.  
DOI:10.1021/jm101101q

#### Development of a New Generation of 4-Aminoquinoline Antimalarial Compounds Using Predictive Pharmacokinetic and Toxicology Models

Ray, Sunetra; **Madrid, Peter B.**; Catz, Paul; Le Valley, Susanna E.; Furniss, Michael J.; Rausch, Linda L.; Guy, R. Kiplin; De Risi, Joseph L.; Iyer, Lalitha V.; Green, Carol E.; et al  
Journal of Medicinal Chemistry (2010), 53(9), 3685-3695.  
DOI:10.1021/jm100057h

#### Peptidic tumor targeting agents: the road from phage display peptide selections to clinical applications

**Brown, Kathlynn C.**  
Current Pharmaceutical Design (2010), 16(9), 1040-1054.  
DOI:10.2174/138161210790963788



### Pharmacokinetics and enhanced bioavailability of candidate cancer preventative agent, SR13668 in dogs and monkeys

Kapetanovic, Izet M.; Muzzio, Miguel; Hu, Shu-Chieh; Crowell, James A.; Rajewski, Roger A.; Haslam, John L.; **Jong, Ling**; McCormick, David L.

Cancer Chemotherapy and Pharmacology (2010), 65(6), 1109-1116.

DOI:10.1007/s00280-009-1116-4

### A novel steroidal inhibitor of estrogen-related receptor $\alpha$ (ERR $\alpha$ )

Duellman, Sarah J.; Calaoagan, Joy M.; Sato, Barbara G.; Fine, Richard; Klebansky, Boris; Chao, Wan-Ru; Hobbs, Peter; **Collins, Nathan**; Sambucetti, Lidia; Laderoute, Keith R.

Biochemical Pharmacology (2010), 80(6), 819-826.

DOI:10.1016/j.bcp.2010.05.024

### Comparative molecular field analysis of fenoterol derivatives: A platform towards highly selective and effective $\beta$ 2-adrenergic receptor agonists

Jozwiak, Krzysztof; Woo, Anthony Yiu-Ho; **Tanga, Mary J.**; Toll, Lawrence; Jimenez, Lucita; **Kozocas, Joseph A.**; Plazinska, Anita; Xiao, Rui-Ping; Wainer, Irving W.

Bioorganic & Medicinal Chemistry (2010), 18(2), 728-736.

DOI:10.1016/j.bmc.2009.11.062

## 2009

### CCR3 antagonists: a survey of the patent literature

**Gong, Leyi**; Wilhelm, Robert S.

Expert Opinion on Therapeutic Patents (2009), 19(8), 1109-1132.

DOI:10.1517/13543770903008544

### Modulation of a Schistosoma mansoni multidrug transporter by the antischistosomal drug praziquantel

Kasinathan, Ravi S.; Goronga, Tinopiwa; Messerli, Shanta M.; **Webb, Thomas R.**; Greenberg, Robert M.

FASEB Journal (2009), Volume Date2009-2010, 24(1), 128-135

DOI:10.1096/fj.09-137091

### Synthetic mRNA Splicing Modulator Compounds with in Vivo Antitumor Activity

Lagiseti, Chandraiah; Pourpak, Alan; Goronga, Tinopiwa; Jiang, Qin; Cui, Xiaoli; Hyle, Judith; Lahti, Jill M.; Morris, Stephan W.; **Webb, Thomas R.**

Journal of Medicinal Chemistry (2009), 52(22), 6979-6990.

DOI:10.1021/jm901215m

### 2-Substituted-4,5-dihydropyrimidine-6-carboxamide antiviral targeted libraries

Boyd, Vincent A.; Mason, John; Hanumesh, Parimala; Price, Jeanine; Russell, Charles J.; **Webb, Thomas R.**

Journal of Combinatorial Chemistry (2009), 11(6), 1100-1104.

DOI:10.1021/cc900111u

### Combinatorial synthesis and biological evaluation of peptide-binding GPCR-targeted library

Lee, Ju Yeon; Im, Isak; **Webb, Thomas R.**; McGrath, Douglas; Song, Mi-Ryoung; Kim, Yong-Chul

Bioorganic Chemistry (2009), 37(3), 90-95.

DOI:10.1016/j.bioorg.2009.04.001

### Design and synthesis of a novel tyrosine kinase inhibitor template

Jake Slavish, P.; Jiang, Qin; Cui, Xiaoli; Morris, Stephan W.; **Webb, Thomas R.**  
Bioorganic & Medicinal Chemistry (2009), 17(9), 3308-3316.  
DOI:10.1016/j.bmc.2009.03.046

### Anaplastic lymphoma kinase: role in cancer pathogenesis and small-molecule inhibitor development for therapy

**Webb, Thomas R.**; Slavish, Jake; George, Rani E.; Look, A. Thomas; Xue, Liquan; Jiang, Qin; Cui, Xiaoli; Rentrop, Walter B.; Morris, Stephan W.  
Expert Review of Anticancer Therapy (2009), 9(3), 331-356.  
DOI:10.1586/14737140.9.3.331

### Synthesis and characterization of a high-affinity $\alpha\beta 6$ -specific ligand for in vitro and in vivo applications

Li, Shunzi; McGuire, Michael J.; Lin, Mai; Liu, Ying-Horng; Oyama, Tsukasa; Sun, Xiankai; **Brown, Kathlynn C.**  
Molecular Cancer Therapeutics (2009), 8(5), 1239-1249.  
DOI:10.1158/1535-7163.MCT-08-1098

## 2008

### Antitumor Compounds Based on a Natural Product Consensus Pharmacophore

Lagiseti, Chandraiah; Pourpak, Alan; Jiang, Qin; Cui, Xiaoli; Goronga, Tinopiwa; Morris, Stephan W.; **Webb, Thomas R.**  
Journal of Medicinal Chemistry (2008), 51(19), 6220-6224.  
DOI:10.1021/jm8006195

### Adamantyl-Substituted Retinoid-Derived Molecules That Interact with the Orphan Nuclear Receptor Small Heterodimer Partner: Effects of Replacing the 1-Adamantyl or Hydroxyl Group on Inhibition of Cancer Cell Growth, Induction of Cancer Cell Apoptosis, and Inhibition of Src Homology 2 Domain-Containing Protein Tyrosine Phosphatase-2 Activity

Dawson, Marcia I.; Xia, Zebin; Jiang, Tao; Ye, Mao; Fontana, Joseph A.; Farhana, Lulu; Patel, Bhaumik; Xue, Li Ping; Bhuiyan, Mohammad; Pellicciari, Roberto; **Jong, Ling**; et al  
Journal of Medicinal Chemistry (2008), 51(18), 5650-5662.  
DOI:10.1021/jm800456k

### Generation of New Synthetic Scaffolds Using Framework Libraries Selected and Refined via Medicinal Chemist Synthetic Expertise

**Webb, Thomas R.**; Venegas, Ruben E.; Wang, Jian; Deschenes, A.  
Journal of Chemical Information and Modeling (2008), 48(4), 882-888.  
DOI:10.1021/ci7001928

### Peptide-Targeted Polyglutamic Acid Doxorubicin Conjugates for the Treatment of $\alpha\beta 6$ -Positive Cancers

Guan, Huili; McGuire, Michael J.; Li, Shunzi; **Brown, Kathlynn C.**  
Bioconjugate Chemistry (2008), 19(9), 1813-1821.  
DOI:10.1021/bc800154f

## 2007

### Repurposing FDA-approved drugs to combat drug-resistant *Acinetobacter baumannii*

Chopra, Sidharth; Torres-Ortiz, Maria; Hokama, Leslie; **Madrid, Peter**; **Tanga, Mary**; Mortelmans, Kristien; Kodukula, Krishna; Galande, Amit K.



Journal of Antimicrobial Chemotherapy (2010), 65(12), 2598-2601.  
DOI:10.1093/jac/dkq353

#### Synthesis and antitubercular activity of phenothiazines with reduced binding to dopamine and serotonin receptors

**Madrid, Peter B.**; Polgar, Willma E.; Toll, Lawrence; **Tanga, Mary J.**  
Bioorganic & Medicinal Chemistry Letters (2007), 17(11), 3014-3017.  
DOI:10.1016/j.bmcl.2007.03.064

#### Activity of piperazine and other 4-aminoquinoline antiplasmodial drugs against chloroquine-sensitive and resistant blood-stages of Plasmodium falciparum

Warhurst, David C.; Craig, John C.; Adagu, Ipemida S.; Guy, R. Kiplin; **Madrid, Peter B.**; Fivelman, Quinton L.  
Biochemical Pharmacology (2007), 73(12), 1910-1926.  
DOI:10.1016/j.bcp.2007.03.011

#### Application of a Novel Design Paradigm to Generate General Nonpeptide Combinatorial Templates Mimicking $\beta$ -Turns: Synthesis of Ligands for Melanocortin Receptors

**Webb, Thomas R.**; Jiang, Luyong; Sviridov, Sergey; Venegas, Ruben E.; Vlaskina, Anna V.; McGrath, Douglas; Tucker, John; Wang, Jian; Deschenes, Alain; Li, Rongshi  
Journal of Combinatorial Chemistry (2007), 9(4), 704-710.  
DOI:10.1021/cc0601581

#### Nonprofit model for drug discovery and development

Frank, Gregory Daniel; **Jong, Ling**; **Collins, Nathan**; Spack, Edward G.  
Drug Development Research (2007), 68(4), 186-196.  
DOI:10.1002/ddr.20181

#### Computer-Aided Rational Drug Design: A Novel Agent (SR13668) Designed to Mimic the Unique Anticancer Mechanisms of Dietary Indole-3-Carbinol to Block Akt Signaling

Chao, Wan-Ru; Yean, Dawn; Amin, Khalid; Green, Carol; **Jong, Ling**  
Journal of Medicinal Chemistry (2007), 50(15), 3412-3415.  
DOI:10.1021/jm070040e

#### Comparative Molecular Field Analysis of the Binding of the Stereoisomers of Fenoterol and Fenoterol Derivatives to the $\beta_2$ Adrenergic Receptor

Jozwiak, Krzysztof; Khalid, Chakir; **Tanga, Mary J.**; Berzetei-Gurske, Ilona; Jimenez, Lucita; **Kozocas, Joseph A.**; Woo, Anthony; Zhu, Weizhong; Xiao, Rui-Ping; Abernethy, Darrell R.; et al  
Journal of Medicinal Chemistry (2007), 50(12), 2903-2915.  
DOI:10.1021/jm070030d

#### An Adamantyl-Substituted Retinoid-Derived Molecule That Inhibits Cancer Cell Growth and Angiogenesis by Inducing Apoptosis and Binds to Small Heterodimer Partner Nuclear Receptor: Effects of Modifying Its Carboxylate Group on Apoptosis, Proliferation, and Protein-Tyrosine Phosphatase Activity

Dawson, Marcia I.; Xia, Zebin; Liu, Gang; Fontana, Joseph A.; Farhana, Lulu; Patel, Bhamik B.; Arumugarajah, Sankari; Bhuiyan, Mohammad; Zhang, Xiao-Kun; Han, Young-Hoon; **Jong, Ling**; et al  
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**2006**

### Synthesis and Testing of a Focused Phenothiazine Library for Binding to HIV-1 TAR RNA

Mayer, Moriz; Lang, P. Therese; Gerber, Sabina; **Madrid, Peter B.**; Pinto, Irene Gomez; Guy, R. Kiplin; James, Thomas L.  
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### Structure-activity relationship study of 9-aminoacridine compounds in scrapie-infected neuroblastoma cells

May, Barnaby C. H.; Witkop, Juanita; Sherrill, John; Anderson, Marc O.; **Madrid, Peter B.**; Zorn, Julie A.; Prusiner, Stanley B.; Cohen, Fred E.; Guy, R. Kiplin  
Bioorganic & Medicinal Chemistry Letters (2006), 16(18), 4913-4916.  
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### Incorporation of an Intramolecular Hydrogen-Bonding Motif in the Side Chain of 4-Aminoquinolines Enhances Activity against Drug-Resistant *P. falciparum*

**Madrid, Peter B.**; Liou, Ally P.; DeRisi, Joseph L.; Guy, R. Kiplin  
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### Design and Synthesis of 5-Aryl-pyridone-carboxamides as Inhibitors of Anaplastic Lymphoma Kinase

Li, Rongshi; Xue, Liquan; Zhu, Tong; Jiang, Qin; Cui, Xiaoli; Yan, Zheng; McGee, Danny; Wang, Jian; Gantla, Vidyasagar Reddy; Pickens, Jason C.; **Webb, Thomas R.**; et al  
Journal of Medicinal Chemistry (2006), 49(3), 1006-1015.  
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### Parallel synthesis of 9-aminoacridines and their evaluation against chloroquine-resistant *Plasmodium falciparum*

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### Polymer-Supported Synthesis of Pyridone-Focused Libraries as Inhibitors of Anaplastic Lymphoma Kinase

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### Synthesis of ring-substituted 4-aminoquinolines and evaluation of their antimalarial activities

**Madrid, Peter B.**; Sherrill, John; Liou, Ally P.; Weisman, Jennifer L.; DeRisi, Joseph L.; Guy, R. Kiplin  
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### Small molecules that reactivate p53 in renal cell carcinoma reveal a NF- $\kappa$ B-dependent mechanism of p53 suppression in tumors

Gurova, Katerina V.; Hill, Jason E.; Guo, Canhui; Prokvolit, Anatoly; Burdelya, Lyudmila G.; Samoylova, Eugenia; Khodyakova, Anna V.; Ganapathi, Ram; Ganapathi, Mahrukh; Tararova, Natalia D.; **Webb, Thomas, R.**; et al

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### Quinazolinone fungal efflux pump inhibitors. Part 2: In vitro structure-activity relationships of (N-methylpiperazinyl)-containing derivatives

Watkins, William J.; **Lemoine, Remy C.**; Chong, Lee; Cho, Aesop; Renau, Thomas E.; Kuo, Bonnie; Wong, Vickie; Ludwikow, Maria; Garizi, Negar; Iqbal, Nadeem; et al  
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### Quinazolinone-based fungal efflux pump inhibitors. Part 1: Discovery of an (N-methylpiperazine)-containing derivative with activity in clinically relevant *Candida* spp.

**Lemoine, Remy C.**; Glinka, Tomasz W.; Watkins, William J.; Cho, Aesop; Yang, Jessie; Iqbal, Nadeem; Singh, Rajeshwar; Madsen, Deidre; Lolans, Karen; Lomovskaya, Olga; et al  
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### Synthesis of benzoylpyrimidines as antagonists of the corticotropin-releasing factor-1 receptor

**Webb, Thomas R.**; Moran, Terry; Huang, Charles Q.; McCarthy, James R.; Grigoriadis, Dimitri E.; Chen, Chen  
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### The design and synthesis of a novel quinolizidine template for potent opioid and opioid receptor-like (ORL1, NOP) receptor ligands

**Jong, Ling**; Zaveri, Nurulain; Toll, Lawrence  
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### Parallel Synthesis and Antimalarial Screening of a 4-Aminoquinoline Library

**Madrid, Peter B.**; Wilson, Nathan T.; DeRisi, Joseph L.; Guy, R. Kiplin  
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### Design of 2,5-dimethyl-3-(6-dimethyl-4-methylpyridin-3-yl)-7-dipropylaminopyrazolo[1,5-a]pyrimidine (NBI 30775/R121919) and structure-activity relationships of a series of potent and orally active corticotropin-releasing factor receptor antagonists

Chen, Chen; Wilcoxon, Keith M.; Huang, Charles Q.; Xie, Yun-Feng; McCarthy, James R.; **Webb, Thomas R.**; Zhu, Yun-Fei; Saunders, John; Liu, Xin-Jun; Chen, Ta-Kung; et al  
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### Antagonist analogue of 6-[3'-(1-adamantyl)-4'-hydroxyphenyl]-2-naphthalenecarboxylic acid (AHPN) family of apoptosis inducers that effectively blocks AHPN-induced apoptosis but not cell-cycle arrest

Dawson Marcia I; Harris Danni L; Liu Gang; Hobbs Peter D; Lange Christopher W; **Jong Ling**; Bruey-Sedano Nathalie; James Sharon Y; Zhang Xiao-Kun; Peterson Valerie J; et al  
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### Synthetic dihydropacidamycin antibiotics: a modified spectrum of activity for the pacidamycin class

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Dawson, Marcia I.; Park, Ju Hui; Chen, Guo-Quan; Chao, Wan-Ru; Dousman, Linda; Waleh, Nahid; Hobbs, Peter D.; **Jong, Ling**; Toll, Lawrence; Zhang, Xiao-Kun; et al  
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Dawson, Marcia I.; Hobbs, Peter D.; **Jong, Ling**; Xiao, Dongmei; Chao, Wan-Ru; Pan, Chin; Zhang, Xiao-Kun  
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**Webb, Thomas R.**; Melman, Neli; Lvovskiy, Dmitriy; Ji, Xiao-Duo; Jacobson, Kenneth A.  
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Shenderovich, Mark D.; Koeber, Katalin E.; Wilke, Susanne; **Collins, Nathan**; Hruby, Victor J.

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### **Design and Synthesis of a Series of Non-Peptide High-Affinity Human Corticotropin-Releasing Factor1 Receptor Antagonists**

Chen, Chen; Dagnino, Raymond, Jr.; De Souza, Errol B.; Grigoriadis, Dimitri E.; Huang, Charles Q.; Kim, Kyung-Il; Liu, Zhengyu; Moran, Terry; **Webb, Thomas R.**; et al.

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Lung, Feng-Di T.; **Collins, Nathan**; Stropova, Dagmar; Davis, Peg; Yamamura, Henry I.; Porreca, Frank; Hruby, Victor J.

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### **Conformational Determinants of Agonist versus Antagonist Properties of [D-Pen<sub>2</sub>,D-Pen<sub>5</sub>] Enkephalin (DPDPE) Analogs at Opioid Receptors. Comparison of X-ray Crystallographic Structure, Solution <sup>1</sup>H NMR Data, and Molecular Dynamic Simulations of [L-Ala<sub>3</sub>]DPDPE and [D-Ala<sub>3</sub>]DPDPE**

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