

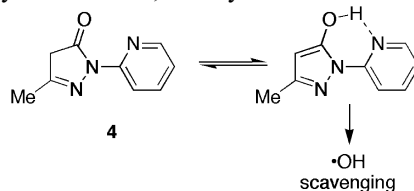
Contents

ARTICLES

Hydroxyl radical scavenging by edaravone derivatives: Efficient scavenging by 3-methyl-1-(pyridin-2-yl)-5-pyrazolone with an intramolecular base

pp 5939–5942

Hidehiko Nakagawa,* Ryo Ohyama, Ayako Kimata, Takayoshi Suzuki and Naoki Miyata*



The hydroxyl radical scavenging by pyrazolone derivatives was evaluated, and it was found that **4** was a more efficient derivative than edaravone. It was assumed to be due to the increase of an active form by a hydrogen-bonded intramolecular base.

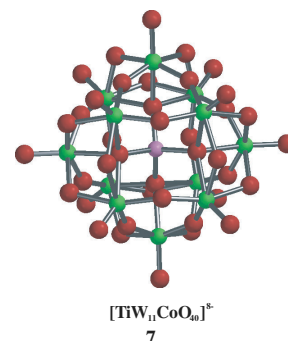
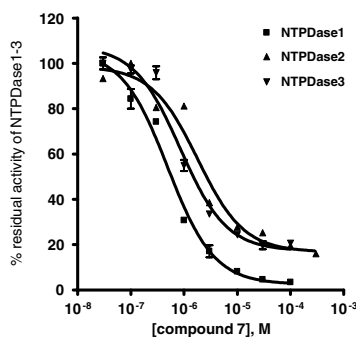


Polyoxometalates—a new class of potent ecto-nucleoside triphosphate diphosphohydrolase (NTPDase) inhibitors

pp 5943–5947

Christa E. Müller,* Jamshed Iqbal, Younis Baqi, Herbert Zimmermann, Anita Röllich and Holger Stephan

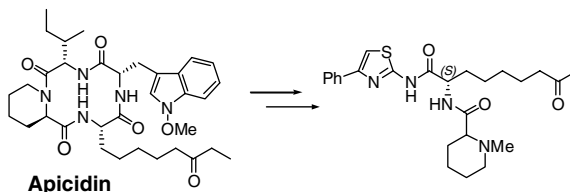
Polyoxotungstates were identified as novel potent inhibitors of ecto-NTPDases. $[\text{TiW}_{11}\text{CoO}_{40}]^{8-}$ (**7**) exhibited a K_i value of 140 nM at rat E-NTPDase1.



A series of novel, potent, and selective histone deacetylase inhibitors

pp 5948–5952

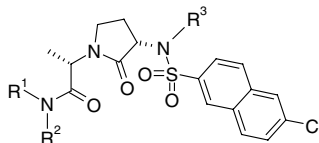
Philip Jones,* Sergio Altamura, Prasun K. Chakravarty, Ottavia Cecchetti, Raffaele De Francesco, Paola Gallinari, Raffaele Ingenito, Peter T. Meinke, Alessia Petrocchi, Michael Rowley, Rita Scarpelli, Sergio Serafini and Christian Steinkühler



The evolution of a novel series of HDAC inhibitors containing an unusual ketone zinc binding group is described. SAR studies resulted in optimization to potent, low molecular weight, selective, non-hydroxamic acid HDAC inhibitors.

Structure- and property-based design of factor Xa inhibitors: Pyrrolidin-2-ones with acyclic alanyl amides as P4 motifs pp 5953–5957

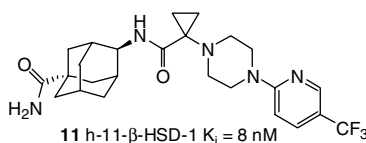
Robert J. Young,* Matthew Campbell, Alan D. Borthwick, David Brown, Cynthia L. Burns-Kurtis, Chuen Chan, Máire A. Convery, Miriam C. Crowe, Satish Dayal, Hawa Diallo, Henry A. Kelly, N. Paul King, Savvas Kleanthous, Andrew M. Mason, Jackie E. Mordaunt, Champa Patel, Anthony J. Pateman, Stefan Senger, Gita P. Shah, Paul W. Smith, Nigel S. Watson, Helen E. Weston and Ping Zhou



The synthesis and profiles of a series of fXa inhibitors with acyclic alanyl amide P4 motifs is described, which includes potent examples showing highly encouraging anticoagulant activity.

Adamantane 11-β-HSD-1 inhibitors: Application of an isocyanide multicomponent reaction pp 5958–5962

Bryan Sorensen, Jeff Rohde, Jiahong Wang, Steven Fung, Katina Monzon, William Chiou, Liping Pan, Xiaoqing Deng, DeAnne Stolarik, Ernst U. Frevert, Peer Jacobson and J. T. Link*

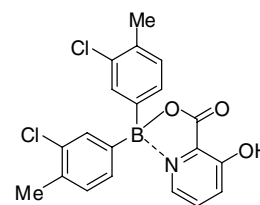


The synthesis of the potent and selective h-11-β-HSD-1 inhibitor **11** ($K_i = 8$ nM) is reported.

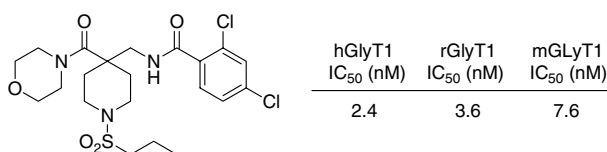
Identification of a novel boron-containing antibacterial agent (AN0128) with anti-inflammatory activity, for the potential treatment of cutaneous diseases pp 5963–5967

Stephen J. Baker,* Tsutomu Akama, Yong-Kang Zhang, Vittorio Sauro, Chetan Pandit, Rajeshwar Singh, Maureen Kully, Jehangir Khan, Jacob J. Plattner, Stephen J. Benkovic, Ving Lee and Kirk R. Maples

A series of borinic acid picolinate esters were synthesized and screened for antibacterial and anti-inflammatory activities. From these studies, we selected 3-hydroxypyridine-2-carboxyloxy-bis(3-chloro-4-methylphenyl)borane (**AN0128**) as a clinical candidate for dermatological diseases.


Synthesis and SAR of GlyT1 inhibitors derived from a series of N-((4-(morpholine-4-carbonyl)-1-(propylsulfonyl)piperidin-4-yl)methyl)benzamides pp 5968–5972

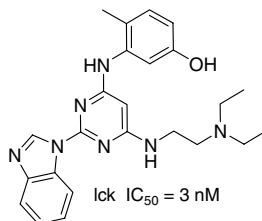
Zhijian Zhao,* Julie A. O'Brien, Wei Lemaire, David L. Williams, Jr., Marlene A. Jacobson, Cyrille Sur, Doug J. Pettibone, Philip R. Tiller, Sheri Smith, George D. Hartman, Scott E. Wolkenberg and Craig W. Lindsley



The development of 2-benzimidazole substituted pyrimidine based inhibitors of lymphocyte specific kinase (Lck)

pp 5973–5977

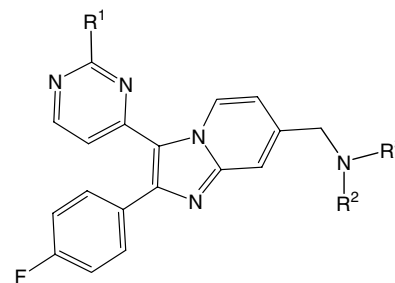
Mark Sabat,* John C. VanRens, Matthew J. Laufersweiler, Todd A. Brugel, Jennifer Maier, Adam Golebiowski, Biswanath De, Vijayasurian Easwaran, Lily C. Hsieh, Richard L. Walter, Marlene J. Mekel, Artem Evdokimov and Michael J. Janusz

**Synthesis and SAR of 2-(4-fluorophenyl)-3-pyrimidin-4-ylimidazo[1,2-a]pyridine derivatives as anticoccidial agents**

pp 5978–5981

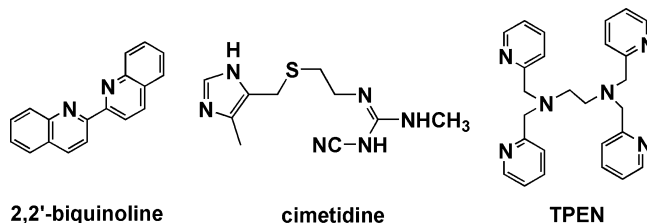
Dennis Feng,* Michael Fisher, Gui-Bai Liang, Xiaoxia Qian, Chris Brown, Anne Gurnett, Penny Sue Leavitt, Paul A. Liberator, John Mathew, Andrew Misura, Samantha Samaras, Tamas Tamas, Dennis M. Schmatz, Matthew Wyvratt and Tesfaye Biftu

The imidazopyridine derivatives are discovered as potent inhibitors of the *Eimeria tenella* cGMP-dependent protein kinase.

**Metal complexes with superoxide dismutase-like activity as candidates for anti-prion drug**

pp 5982–5987

Tomoko Fukuuchi,* Katsumi Doh-ura, Shin'ichi Yoshihara and Shigeru Ohta



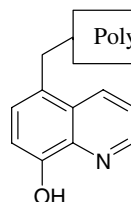
The compounds whose metal complexes had high SOD-like activity, 2,2'-biquinoline, cimetidine, and TPEN, had values of 50%-inhibitory concentration for PrP-res formation (IC_{50}) of <10 nM in ScN2a cells.

Synthesis and anti-HIV properties of new hydroxyquinoline–polyamine conjugates on cells infected by HIV-1 LAV and HIV-1 BaL viral strains

pp 5988–5992

Vincent Moret, Nathalie Dereudre-Bosquet, Pascal Clayette, Younes Laras, Nicolas Pietrancosta, Amandine Rolland, Clement Weck, Sylvain Marc and Jean-Louis Kraus*

General structure of the new synthesized hydroxyquinoline–polyamine conjugates monocyclam and bicyclam–hydroxyquinoline conjugates **7**, **8**, and **10**, respectively, found to be potent against HIV-1 LAV and HIV-1 BaL strains.



Polyamine linker structures:

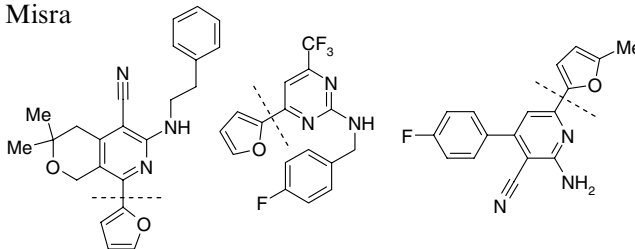
- linear
- polyazamacrocycles
- bis-polyazamacrocycles



Identification of non-furan containing A_{2A} antagonists using database mining and molecular similarity approaches

pp 5993–5997

Christine M. Richardson,* Roger J. Gillespie, Douglas S. Williamson,
Allan M. Jordan, Alexandra Fink, Antony R. Knight,
Daniel M. Sellwood and Anil Misra

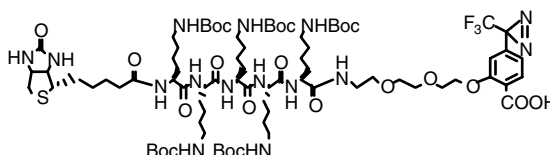


Identification of potent, non-furan containing A_{2A} antagonists using database mining.

Positively coded photoaffinity label for altering isoelectric points of proteins

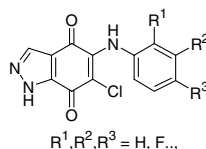
pp 5998–6000

Makoto Hashimoto* and Yasumaru Hatanaka


Synthesis and biological evaluation of 5-aryl-amino-6-chloro-1*H*-indazole-4,7-diones as inhibitors of protein kinase B/Akt

pp 6001–6005

Jong Hee Ko, Seung Woo Yeon, Jung Su Ryu, Tae-Yong Kim,
Eun-Ha Song, Hea-Jung You, Rae-Eun Park and Chung-Kyu Ryu*

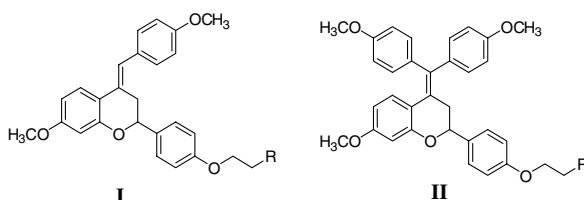


5-Arylamino-6-chloro-1*H*-indazole-4,7-diones were synthesized and evaluated for their inhibitory activity on protein kinase B/AKT. The 5-arylamino-6-chloro-1*H*-indazole-4,7-diones exhibited a potent Akt1 inhibitory activity.

Rapid synthesis of 4-benzylidene and 4-[bis-(4-methoxyphenyl)-methylene-2-substituted phenyl]-benzopyrans as potential selective estrogen receptor modulators (SERMs) using McMurry coupling reaction

pp 6006–6012

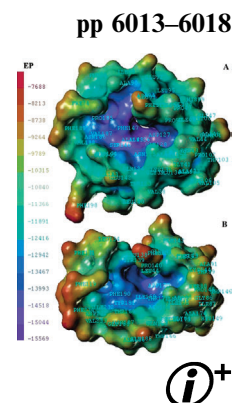
Atul Gupta,* Anila Dwivedy, Govind Keshri, Ramesh Sharma, Anil Kumar Balapure, Man Mohan Singh and Suprabhat Ray*



Comparative protein modeling and surface analysis of Leishmania sirtuin: A potential target for antileishmanial drug discovery

Rameshwar U. Kadam, Kiran V. M. and Nilanjan Roy*

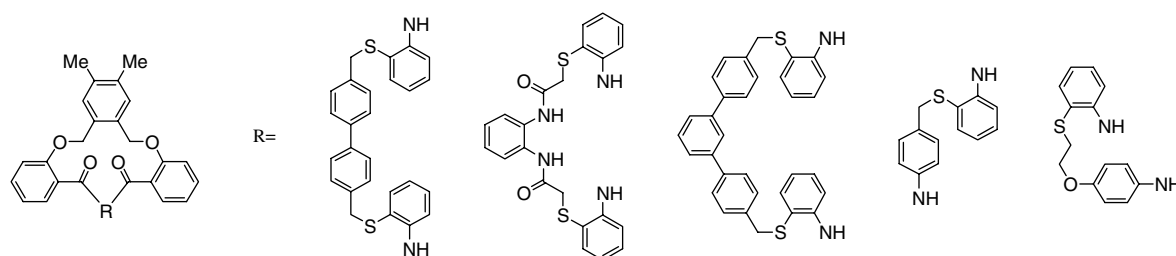
Comparative protein modeling and surface analysis of LmSIR2 and hSIRT2 provide sufficient evidences that selective LmSIR2 inhibitors can be designed using structure based drug design approaches.



Synthesis and study of anti-inflammatory activity of some novel cyclophane amides

Perumal Rajakumar,* A. Mohammed Abdul Rasheed, A. Iman Rabia and D. Chamundeeswari

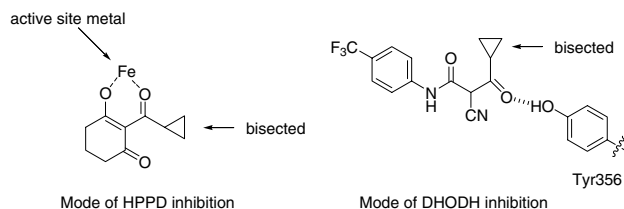
pp 6019–6023



Enzyme inhibition potency enhancement by active site metal chelating and hydrogen bonding induced conformation-restricted cyclopropanecarbonyl derivatives

Pei-Yu Kuo, Tien-Lan Shie, You-Sheng Chen, Jiun-Ting Lai and Ding-Yah Yang*

pp 6024–6027

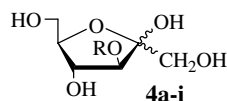


The enhancement by one order of magnitude of inhibition potency exhibited by cyclopropanecarbonyl derivatives relative to the corresponding isopropylcarbonyl analogs is probably caused by metal chelating and hydrogen bonding interactions at the ligand–receptor binding site.

Synthesis and antihyperlipidemic activity of novel glycosyl fructose derivatives

Pallavi Tiwari, Anju Puri, Ramesh Chander, Geetika Bhatia and Anup Kumar Misra*

pp 6028–6033



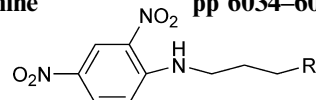
R = D-Galp, D-Manp, L-Rhap, D-Arap, D-Xylp, D-Ribp, D-lactose, D-cellobiose, D-maltose.

Synthesis, aerobic cytotoxicity, and radiosensitizing activity of novel 2,4-dinitrophenylamine tethered 5-fluorouracil and hydroxyurea

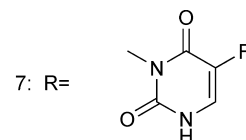
pp 6034–6038

Ali Khalaj,* Ali Reza Doroudi, Seyed Nasser Ostad, Mohammad Reza Khoshayand, Mohammad Babai and Neda Adibpour

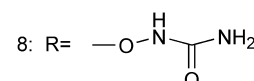
Two novel *N*-(2,4-dinitrophenylamine) derivatives containing 5-fluorouracil and hydroxyurea moieties were synthesized and their aerobic cytotoxicities toward HT-29 adenocarcinoma cell line with and without radiation in comparison to their components were evaluated.



4: R= H



7: R=



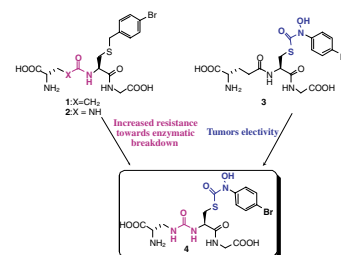
8: R=

A metabolically stable tight-binding transition-state inhibitor of glyoxalase-I

pp 6039–6042

Swati S. More and Robert Vince*

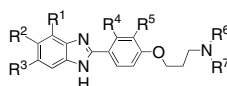
The design, synthesis, and enzyme kinetics evaluation of a transition-state inhibitor of glyoxalase-I is described. The union of the hydroxamic acid zinc-chelator with a urea isostere for the glu-cys amide bond led to a glutathione analog which retained inhibitory potency toward glyoxalase-I while possessing resistance toward γ -glutamyltranspeptidase mediated breakdown. This compound is viewed as a potential lead for the development of second-generation glyoxalase-I inhibitors wherein, the problems pertaining to metabolism and selectivity are overcome.



Identification of 2-arylbenzimidazoles as potent human histamine H₄ receptor ligands

pp 6043–6048

Alice Lee-Dutra,* Kristen L. Arienti, Daniel J. Buzard, Michael D. Hack, Haripada Khatuya, Pragnya J. Desai, Steven Nguyen, Robin L. Thurmond, Lars Karlsson, James P. Edwards and J. Guy Breitenbucher



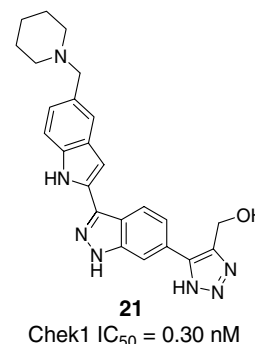
A series of 2-arylbenzimidazoles was synthesized and found to bind with high affinity to the human histamine H₄ receptor.

3-(Indol-2-yl)indazoles as Chek1 kinase inhibitors: Optimization of potency and selectivity via substitution at C6

pp 6049–6053

Mark E. Fraley,* Justin T. Steen, Edward J. Brnardic, Kenneth L. Arrington, Keith L. Spencer, Barbara A. Hanney, Yuntae Kim, George D. Hartman, Steven M. Stirdivant, Bob A. Drakas, Keith Rickert, Eileen S. Walsh, Kelly Hamilton, Carolyn A. Buser, James Hardwick, Weikang Tao, Stephen C. Beck, Xianzhi Mao, Robert B. Lobell, Laura Sepp-Lorenzino, Youwei Yan, Mari Ikuta, Sanjeev K. Munshi, Lawrence C. Kuo and Constantine Kretsoulas

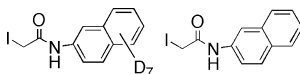
The optimization of potency and selectivity for a 3-(indol-2-yl)indazole class of Chek1 kinase inhibitors is described.



Synthesis of D-labeled naphthylidoacetamide and application to quantitative peptide analysis by isotope differential mass spectrometry

pp 6054–6057

Satomi Niwayama,* Sadamu Kurono, Hanjoung Cho and Hiroyuki Matsumoto



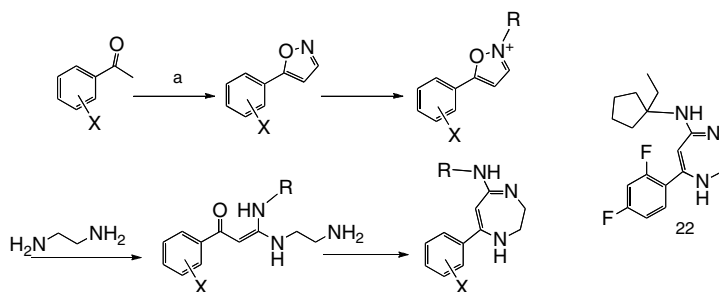
D-labeled and unlabeled *N*- β -naphthylidoacetamides that covalently react with cysteine residues have been synthesized and applied to quantitative analysis of peptides.

Identification and optimisation of 5-amino-7-aryldihydro-1,4-diazepines as 5-HT_{2A} ligands

pp 6058–6062

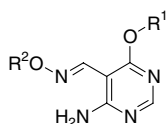
Christopher J. Swain,* Ana Teran, Marta Maroto and Angeles Cabello

A series of low molecular weight 5-HT_{2A} leads were identified from an analysis of HTS data, the exploration of SAR and optimisation one series using parallel synthesis is described affording compound **22** (5-HT_{2A} IC₅₀ 1.1 nM).

**Synthesis and biological study of 4-aminopyrimidine-5-carboxaldehyde oximes as antiproliferative VEGFR-2 inhibitors**

pp 6063–6066

Shenlin Huang,* Ronghua Li, Peter J. Connolly, Guozhang Xu, Michael D. Gaul, Stuart L. Emanuel, Kenneth R. LaMontagne and Lee M. Greenberger



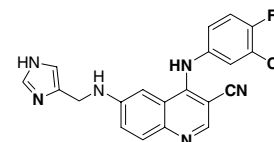
A novel 4-aminopyrimidine-5-carboxaldehyde oxime scaffold with inhibitory activity against VEGFR-2 kinase has been identified. With a 4-fluoro-2-methylindol-5-yloxy group at the 6-position and alkyl groups as the oxime side chains, many analogues showed good potency for VEGFR-2. This series also exhibited antiproliferative activity against cancer cells, causing cell accumulation at the G2/M phase of the cell cycle and preventing cells from entering mitosis.

Inhibition of Tpl2 kinase and TNF α production with quinoline-3-carbonitriles for the treatment of rheumatoid arthritis

pp 6067–6072

Yonghan Hu,* Neal Green, Lori K. Gavrin, Kristin Janz, Neelu Kaila, Huan-Qiu Li, Jennifer R. Thomason, John W. Cuzzo, J. Perry Hall, Sang Hsu, Cheryl Nickerson-Nutter, Jean-Baptiste Telliez, Lih-Ling Lin and Steve Tam

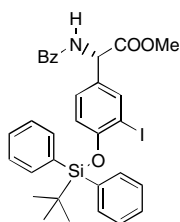
The synthesis and structure–activity studies of a series of quinoline-3-carbonitriles as inhibitors of Tpl2 kinase are described. Potent inhibitors of Tpl2 kinase with selectivity against a panel of selected kinases in enzymatic assays and specificity in cell-based phosphorylation assays in LPS-treated human monocytes were identified. Selected inhibitors with moderate activity in human whole blood assay effectively inhibited LPS/D-Gal induced TNF α release when administered intraperitoneally in mice.



Genotoxic activity of halogenated phenylglycine derivatives

pp 6073–6077

Alicia Boto,* Juan A. Gallardo, Rosendo Hernández,* Francisco Ledo, Ana Muñoz, José R. Murguía, Mauricio Menacho-Márquez, Aurelio Orjales* and Carlos J. Saavedra

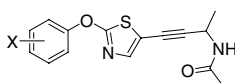


The discovery and synthesis of genotoxic (haloaryl)glycines is reported.

**Structure–activity relationships for a novel series of thiazolyl phenyl ether derivatives exhibiting potent and selective acetyl-CoA carboxylase 2 inhibitory activity**

pp 6078–6081

Richard F. Clark,* Tianyuan Zhang, Zhili Xin, Gang Liu, Ying Wang, T. Matthew Hansen, Xiaojun Wang, Rongqi Wang, Xiaolin Zhang, Ernst U. Frevert, Heidi S. Camp, Bruce A. Beutel, Hing L. Sham and Yu Gui Gu

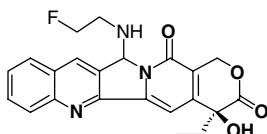


The SAR for a novel series of acetyl-CoA carboxylase inhibitors are described. Optimization of distal aryl ring substitution in the lead scaffold resulted in the identification of compounds displaying low-nanomolar potency and high isozyme-selectivity for acetyl-CoA carboxylase 2.

Microwave expedited synthesis of 5-aminocamptothecin analogs: Inhibitors of hypoxia inducible factor HIF-1 α

pp 6082–6085

Joelle Torregrossa, Glenn J. Bublely and Graham B. Jones*



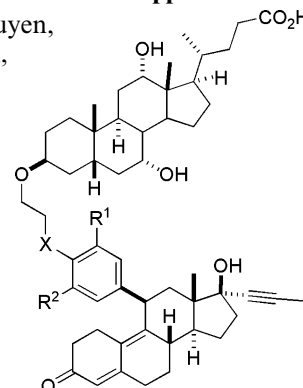
A series of 5-aminosubstituted camptothecin analogs were prepared using microwave accelerated synthesis. A fluoroethyl derivative showed superior inhibitory activity to camptothecin against the hypoxia inducible factor HIF-1 α .

Synthesis and activity of novel bile-acid conjugated glucocorticoid receptor antagonists

pp 6086–6090

Steven J. Richards,* Thomas W. von Geldern, Peer Jacobson, Denise Wilcox, Phong Nguyen, Lars Öhman, Marie Österlund, Birgitta Gelius, Marlena Grynfarb, Annika Goos-Nilsson, Jiahong Wang, Steven Fung and Masha Kalmanovich

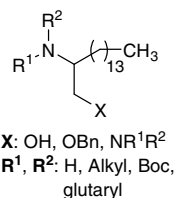
A series of potent steroidal glucocorticoid receptor antagonists has been discovered. After conjugation to cholic acid, the compounds retained an affinity for GR in vitro and had modest in vivo efficacy.



Synthesis and evaluation of some lipidic aminoalcohols and diamines as immunomodulators

pp 6091–6095

Esther del Olmo,* Alvaro Plaza, Antonio Muro,* Antonio R. Martínez-Fernández,
Juan J. Nogal-Ruiz, José L. López-Pérez and Arturo San Feliciano

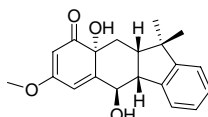


Lymphoproliferation inhibition and delayed hypersensitivity assays have served to select primarily the compounds to be evaluated further, through Graft-*vs*-Host reaction, NO production and other assays, in order to determine the potential of the title compounds for being used as immunomodulators.

Distachyasins: A new antioxidant metabolite from the leaves of *Carex distachya*

pp 6096–6101

Antonio Fiorentino,* Brigida D'Abrosca, Severina Pacifico, Rosa Iacovino,
Claudio Mastellone, Benedetto Di Blasio and Pietro Monaco

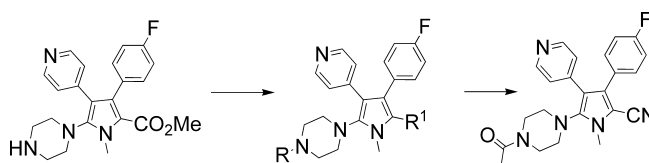


The elucidation and the antioxidant activities of a new prenyl stilbenoid are reported.

**Inhibitors of unactivated p38 MAP kinase**

pp 6102–6106

James Bullington,* Dennis Argentieri, Kristin Averill, Demetrius Carter,
Druie Cavender, Bohumila Fahmy, Xiaodong Fan, Daniel Hall,
Geoffrey Heintzelman, Paul Jackson, Wai-Ping Leung, Xun Li, Ping Ling,
Gilbert Olini, Thomas Razler, Michael Reuman, Kenneth Rupert, Ronald Russell,
John Siekierka, Scott Wadsworth, Russell Wolff, Bangping Xiang and Yue-Mei Zhang

**Synthesis and antiviral activity against tobacco mosaic virus and 3D-QSAR of α -substituted-1,2,3-thiadiazoleacetamides**

pp 6107–6111

Wei-Guang Zhao,* Jian-Guo Wang, Zheng-Ming Li and Zhao Yang

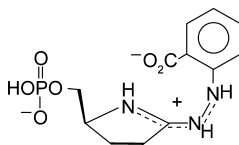


A series of α -substituted-1,2,3-thiadiazoleacetamides were prepared and tested in vitro against tobacco mosaic virus. The preliminary bioassays indicated that some of the new compounds are good as compared to the commercial pesticide Virus A at 500 mg/L, and the activity was influenced by the nature of the substituents. 3D-QSAR models were established based on the antiviral activity of the compounds. It has also been found that some of the new compounds also exhibit significant anti-HBV activity in human hepatoblastoma-derived liver Hep-G2 cells.

'Irreversible' slow-onset inhibition of orotate phosphoribosyltransferase by an amidrazone phosphate transition-state mimic

pp 6112–6115

John F. Witte, Kathryn E. Bray, Chelsea K. Thornburg and Ronald W. McClard*

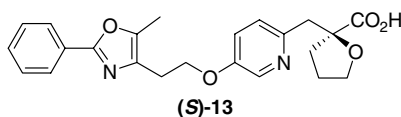


A mimic of the putative transition-state intermediate has been synthesized and found to be a very slow-onset inhibitor of yeast orotate phosphoribosyltransferase. The mechanism of inhibition may involve a rate-determining isomerization of the enzyme to a form receptive to the inhibitor, which then remains tightly bound.

**Pyridine-2-propanoic acids: Discovery of dual PPAR α / γ agonists as antidiabetic agents**

pp 6116–6119

Paul S. Humphries,* Jonathon V. Almaden, Sandra J. Barnum, Thomas J. Carlson, Quyen-Quyen T. Do, James D. Fraser, Mary Hess, Young H. Kim, Kathleen M. Ogilvie and Shaoxian Sun



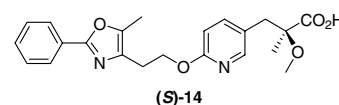
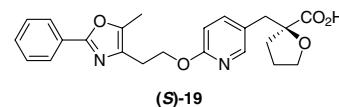
A novel series of potent dual PPAR α / γ agonists was identified. SAR studies led to the identification of a multitude of compounds with varied isoform selectivity.

Pyridine-3-propanoic acids: Discovery of dual PPAR α / γ agonists as antidiabetic agents

pp 6120–6123

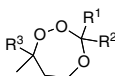
Paul S. Humphries,* Simon Bailey,* Jonathon V. Almaden, Sandra J. Barnum, Thomas J. Carlson, Lance C. Christie, Quyen-Quyen T. Do, James D. Fraser, Mary Hess, Jack Kellum, Young H. Kim, Guy A. McClellan, Kathleen M. Ogilvie, Brett H. Simmons, Donald Skalitzky, Shaoxian Sun, David Wilhite and Luke R. Zehnder

A novel series of potent dual PPAR α / γ agonists was identified. SAR studies led to the identification of a multitude of compounds with varied isoform selectivity.

**Synthesis of 1,2,4-trioxepanes via application of thiol-olefin Co-oxygenation methodology**

pp 6124–6130

Richard Amewu, Andrew V. Stachulski, Neil G. Berry, Stephen A. Ward, Jill Davies, Gael Labat, Jean-Francois Rossignol and Paul M. O'Neill*



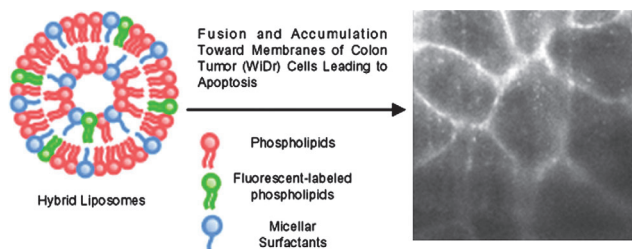
$R^1, R^2 = (CH_2)_4$ or $(CH_2)_5$ or Adamantylidene
 $R^3 = CH_2-SAr$, $Ar = p\text{-Cl-Ph}$
 or $R^3 = CH=CHCONEt_2$
 or $R^3 = CH=CHCO_2Me$

Thiol-olefin co-oxygenation (TOCO) of substituted allylic alcohols generates β -hydroxy peroxides that can be condensed in situ with various ketones, to afford a series of functionalised 1,2,4-trioxepanes in good yields. Manipulation of the phenylsulfenyl group in **8a–8c** allows for convenient modification to the spiro-trioxepane substituents.

Membrane targeted chemotherapy with hybrid liposomes for colon tumor cells leading to apoptosis

pp 6131–6134

Yuji Komizu, Yoko Matsumoto and Ryuichi Ueoka*

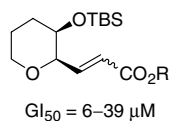


A good correlation between 50% inhibitory concentration of hybrid liposomes (HL) on the growth of human colon tumor cells and membrane fluidity of HL was obtained.

Synthesis and antiproliferative activity of (2*R*,3*R*)-disubstituted tetrahydropyrans

pp 6135–6138

Romen Carrillo, Leticia G. León, Tomás Martín,* Víctor S. Martín and José M. Padrón*

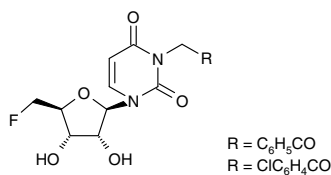


The synthesis and in vitro antitumor activity of a series of enantiomerically pure (2*R*,3*R*)-disubstituted tetrahydropyrans against human solid tumor cells are reported.

Rapid microwave-assisted fluorination yielding novel 5'-deoxy-5'-fluorouridine derivatives

pp 6139–6142

H. Phuoc Le* and Christa E. Müller



A rapid fluorination at the 5'-position of nucleosides derivatives is achieved within 45 min providing yields of 75–92% by application of microwave.

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*Corresponding author

📄⁺ Supplementary data available via ScienceDirect

COVER

View of the crystal structure of the DB819-d(CGCGAATTCGCG)₂ complex, looking down the minor groove of the DNA (see Campbell, N.H.; Evans, D.A.; Lee, M.P.H.; Parkinson, G.N.; Neidle, S. *Bioorg. Med. Chem. Lett.* **2006**, 16, 15). The DB819 molecule is shown in space-filling mode. Visualisation produced with the VMD program. [Humphrey, W.; Dalke, A.; Schulten, K. *J. Mol. Graphics* **1996**, 14, 33.]

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