

Contents

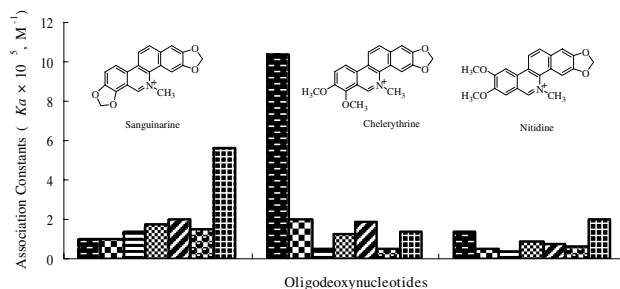
ARTICLES

DNA-binding affinities and sequence selectivity of quaternary benzophenanthridine alkaloids sanguinarine, chelerythrine, and nitidine

pp 5439–5445

Li-Ping Bai, Zhong-Zhen Zhao, Zongwei Cai and Zhi-Hong Jiang*

A comparative study on sequence selectivity of sanguinarine, chelerythrine, and nitidine with seven double-stranded GC-rich oligodeoxynucleotides was performed.

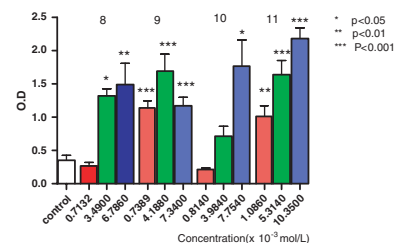


8-Hydroxyquinoline derivatives induce the proliferation of rat mesenchymal stem cells (rMSCs)

pp 5446–5450

He-Ping Zeng,* Ting-Ting Wang, Xin-Hua Ouyang, Ya-Dong Zhou, Hui-Lian Jing, Guo-Zan Yuan, Dong-Feng Chen, Shao-Hui Du, Hui Li and Jian-Hong Zhou

Effects of compounds **8–11** on the proliferation of rMSCs by MTT assay. Each bar represents means \pm SD from five independent experiments. * denotes values that are statistically significantly higher than control group.

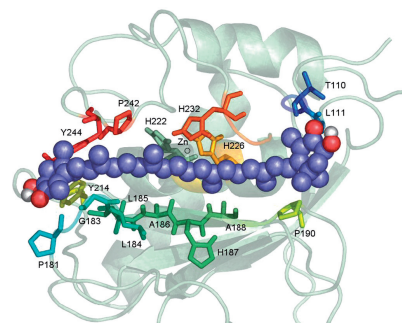


Molecular modeling of non-covalent binding of homochiral (3*S*,3'*S*)-astaxanthin to matrix metalloproteinase-13 (MMP-13)

pp 5451–5458

Zsolt Bikádi, Eszter Hazai, Ferenc Zsila and Samuel F. Lockwood*

Homochiral astaxanthin (3*S*,3'*S*-AST) bound at the 'groove' binding site of MMP-13, as revealed by molecular docking calculations using the published 1EUB X-ray structure.

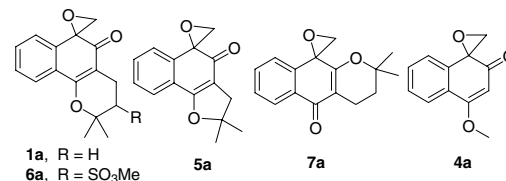


Trypanocidal agents with low cytotoxicity to mammalian cell line: A comparison of the theoretical and biological features of lapachone derivatives

pp 5459–5466

Vitor F. Ferreira,* Alessandra Jorqueira, Alessandra M. T. Souza, Milton N. da Silva, Maria C. B. V. de Souza, Robson M. Gouvêa, Carlos R. Rodrigues,* Antonio V. Pinto, Helena C. Castro, Dilvani O. Santos, Humberto P. Araújo and Saulo C. Bourguignon

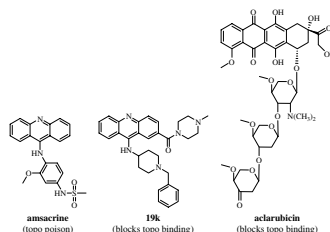
Trypanocidal effects against *Trypanosoma cruzi* and cytotoxicity to mammalian cells of several oxyrans structurally related to β -lapachone, nor- β -lapachone, α -lapachone, and 4-methoxy-1,2-naphthoquinone are described. It was found that the compound **7a** derived from α -lapachone (**7**) exhibits higher trypanocidal activity than β -lapachone with less cytotoxicity. A theoretical study was performed in order to determine structural and stereoelectronic effects that are related with the trypanocidal activity.



Synthesis and evaluation of acridine- and acridone-based anti-herpes agents with topoisomerase activity

pp 5467–5480

John R. Goodell, Avni A. Madhok, Hiroshi Hiasa and David M. Ferguson*

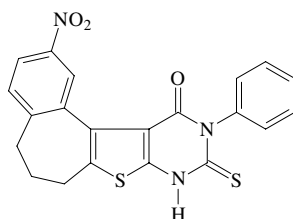


A series of substituted 9-amino acridines inhibit topoisomerase II relaxation of DNA suggesting a mechanism similar to that of the anticancer drug aclarubicin.

Anticancer activities of some newly synthesized pyridine, pyrane, and pyrimidine derivatives

pp 5481–5488

Abdel-Galil E. Amr,* Ashraf M. Mohamed, Salwa F. Mohamed, Nagla A. Abdel-Hafez and Abu El-Fotooh G. Hammam

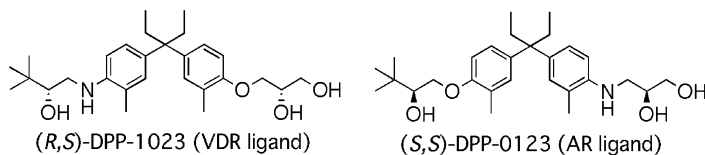


A series of pyridine, pyrane, and pyrimidine derivatives were synthesized by using nitrobenzosuberone **1** as starting material. The synthesized compounds **2–11** were evaluated for their antitumor activity.

Ligands with a 3,3-diphenylpentane skeleton for nuclear vitamin D and androgen receptors: Dual activities and metabolic activation

pp 5489–5502

Shinnosuke Hosoda,* Aya Tanatani, Ken-ichi Wakabayashi, Makoto Makishima, Keisuke Imai, Hiroyuki Miyachi, Kazuo Nagasawa and Yuichi Hashimoto*



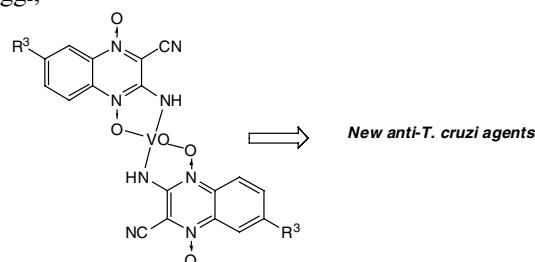
Ligands possessing dual vitamin D₃-agonistic and androgen-antagonistic activities with various activity spectra were prepared based on a substituted 3,3-diphenylpentane skeleton.

Improving anti-trypanosomal activity of 3-aminoquinoxaline-2-carbonitrile N^1,N^4 -dioxide derivatives by complexation with vanadium

pp 5503–5509

Carolina Urquiola, Marisol Vieites, Gabriela Aguirre, Adoración Marín, Beatriz Solano, Gabriel Arrambide, Pabla Noblía, María Laura Lavaggi, María H. Torre, Mercedes González, Antonio Monge, Dinorah Gambino* and Hugo Cerecetto*

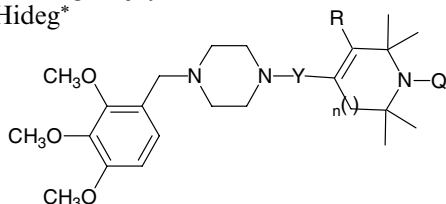
New vanadium complexes of the type $[V^{IV}O(L)_2]$, where L are 3-aminoquinoxaline-2-carbonitrile N^1,N^4 -dioxide derivatives, are described. Complexation to vanadium of the quinoxaline ligands leads to excellent antiprotozoal agents. Anti-*Trypanosoma cruzi* activity is explained on the basis of lipophilicity and electronic properties of quinoxaline substituents.



Structure–activity studies on the protection of Trimetazidine derivatives modified with nitroxides and their precursors from myocardial ischemia–reperfusion injury

pp 5510–5516

Tamás Kálai, Mahmood Khan, Mária Balog, Vijay Kumar Kutala, Periannan Kuppusamy and Kálmán Hideg*



$n = 0, 1$ $Y = CH_2, CO$ $R = H, Ph$ $Q = H, OH, O^*$

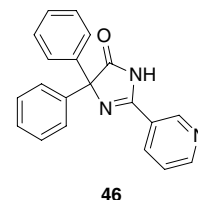
New Trimetazidine derivatives were synthesized with enhanced antioxidant activity.

Synthesis and evaluation of 5,5-diphenylimidazolones as potent human neuropeptide Y5 receptor antagonists

pp 5517–5526

Kevin W. Gillman,* Mendi A. Higgins, Graham S. Poindexter, Marc Browning, Wendy J. Clarke, Sharon Flowers, James E. Grace, John B. Hogan, Rachel T. McGovern, Lawrence G. Iben, Gail K. Mattson, Astrid Ortiz, Stefanie Rassnick, John W. Russell and Ildiko Antal-Zimanyi

A series of novel 5,5-diphenylimidazolones was synthesized and evaluated for activity against the human neuropeptide Y5 receptor. The 3-pyridyl analog **46** demonstrated an IC_{50} of 8.3 nM with a favorable pharmacokinetic profile in rats, but was ineffective in reducing food intake.

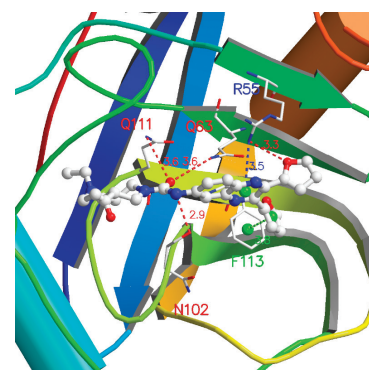


One novel quinoxaline derivative as a potent human cyclophilin A inhibitor shows highly inhibitory activity against mouse spleen cell proliferation

pp 5527–5534

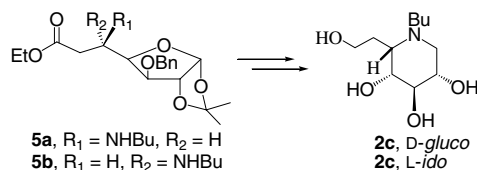
Jian Li, Jing Chen, Li Zhang, Feng Wang, Chunshan Gui, Li Zhang, Yu Qin, Qiang Xu, Hong Liu, Fajun Nan, Jingkang Shen, Donglu Bai, Kaixian Chen, Xu Shen* and Hualiang Jiang*

DC838 demonstrated highly inhibitory activity against CypA PPIase and the proliferation of spleen cells, demonstrating that this compound may be a good lead for discovering immunosuppressor based on CypA inhibitor.



Synthesis and evaluation of glycosidase inhibitory activity of *N*-butyl 1-deoxy-*D*-gluco-homonojirimycin and *N*-butyl 1-deoxy-*L*-ido-homonojirimycin pp 5535–5539

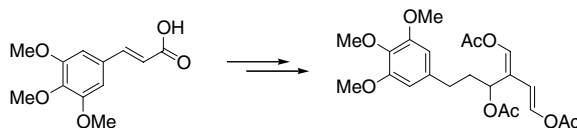
Shankar D. Markad, Narayan S. Karanjule, Tarun Sharma,
Sushma G. Sabharwal and Dilip D. Dhavale*



Caulerpenyne–colchicine hybrid: Synthesis and biological evaluation

pp 5540–5548

Julien Bourdron, Laurent Commeiras,* Pascale Barbier, Véronique Bourgarel-Rey,
Eddy Pasquier, Nicolas Vanthuyne, Jean-Claude Hubaud, Vincent Peyrot* and
Jean-Luc Parrain*

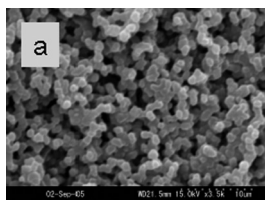


An easy preparation of ‘monolithic type’ hydrophilic solid phase:

pp 5549–5554

Capability for affinity resin to isolate target proteins

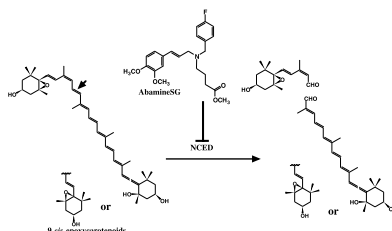
Tomoko Mori, Teruki Takahashi, Takaaki Shiyama, Akito Tanaka,
Natsuki Hira, Nobuo Tanaka and Ken Hosoya*



A 9-*cis*-epoxycarotenoid dioxygenase inhibitor for use in the elucidation of abscisic acid action mechanisms

pp 5555–5561

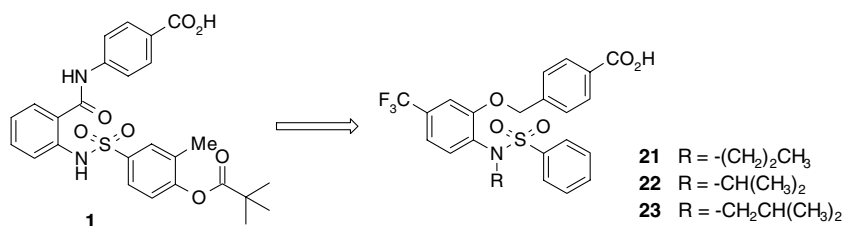
Nobutaka Kitahata, Sun-Young Han, Natsumi Noji, Tamio Saito,
Masatomo Kobayashi, Takeshi Nakano, Kazuyuki Kuchitsu, Kazuo Shinozaki,
Shigeo Yoshida, Shogo Matsumoto, Masafumi Tsujimoto and Tadao Asami*



Discovery of new chemical leads for selective EP1 receptor antagonists

pp 5562–5577

Atsushi Naganawa,* Tetsuji Saito, Yuuki Nagao, Hiromu Egashira, Maki Iwahashi, Tohru Kambe, Masatoshi Koketsu, Hiroshi Yamamoto, Michiyoshi Kobayashi, Takayuki Maruyama, Shuichi Ohuchida, Hisao Nakai, Kigen Kondo and Masaaki Toda

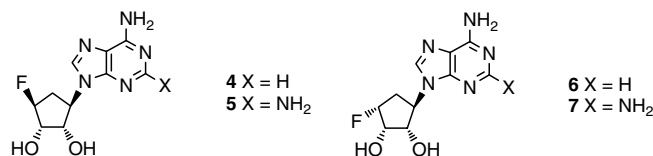


Discovery process of new selective EP1 receptor antagonists **21–23** starting from **1**.

4'-Fluorinated carbocyclic nucleosides: Synthesis and inhibitory activity against S-adenosyl-L-homocysteine hydrolase

pp 5578–5583

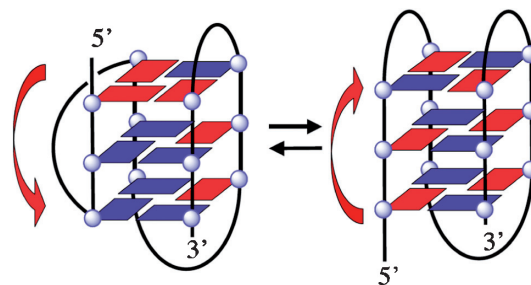
Yukio Kitade,* Takayuki Ando, Tsuyoshi Yamaguchi, Ayumi Hori, Masayuki Nakanishi and Yoshihito Ueno


The new models of the human telomere d[AGGG(TTAGGG)₃] in K⁺ solution

pp 5584–5591

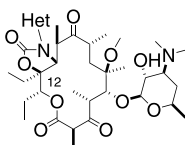
Yan Xu, Yuki Noguchi and Hiroshi Sugiyama*

We substituted the Gs in the sequence with 8-bromoguanine and examined the resultant structures and thermal stabilities by circular dichroism (CD) spectroscopy. The results suggest that the 22 nt in K⁺ solution exists as a mixture of mixed-parallel/antiparallel and chair-type G-quadruplex.


Synthesis and antibacterial activity of novel C₁₂ ethyl ketolides

pp 5592–5604

Matthew T. Burger,* Christy Hiebert, Mehran Seid, Daniel T. Chu, Lynn Barker, Mike Langhorne, Ribhi Shawar, Jolene Kidney, Manoj C. Desai and Jacob J. Plattner

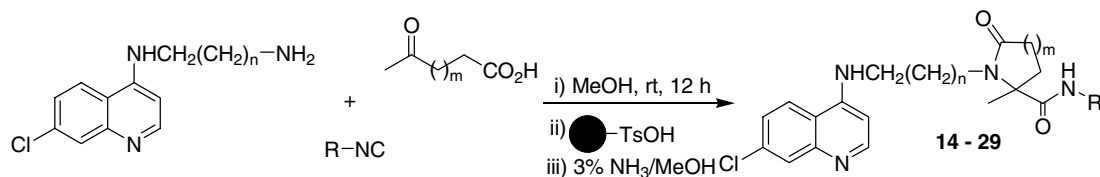


A novel series of C₁₂ ethyl erythromycin ketolide derivatives have been prepared which exhibit in vitro and in vivo potency against key respiratory pathogens, including those resistant to erythromycin.



Application of multicomponent reactions to antimalarial drug discovery. Part 2: New antiplasmodial and antitrypanosomal 4-aminoquinoline γ - and δ -lactams via a 'catch and release' protocol pp 5605–5615

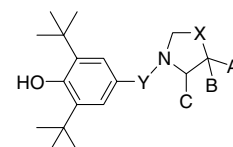
Chitalu C. Musonda, Jiri Gut, Philip J. Rosenthal, Vanessa Yardley, Renata C. Carvalho de Souza and Kelly Chibale*



New analogues of butylated hydroxytoluene as anti-inflammatory and antioxidant agents pp 5616–5624

George N. Ziakas, Eleni A. Rekka,* Antonios M. Gavalas, Phaedra T. Eleftheriou and Panos N. Kourounakis

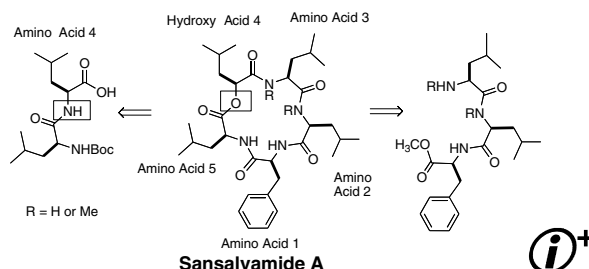
Amine or amide derivatives of substituted thiomorpholine, morpholine and proline bearing the 2,6-di-*tert*-butyl phenol moiety have been synthesised and found to acquire anti-inflammatory and antioxidant activity.



Y: CH_2 , X: CH_2S , A, B, C: H
 Y: $\text{C}=\text{O}$, X: CH_2S , A, B, C: H
 Y: CH_2 , X: CH_2S , A, B: H, C: Ph
 Y: CH_2 , X: CH_2O , A: Ph, B: OCH_2CH_3 , C: H
 Y: $\text{C}=\text{O}$, X: CH_2O , A: Ph, B: OCH_2CH_3 , C: H
 Y: CH_2 , X: CH_2 , A, B: H, C: COOCH_3
 Y: $\text{C}=\text{O}$, X: CH_2 , A, B: H, C: COOCH_3

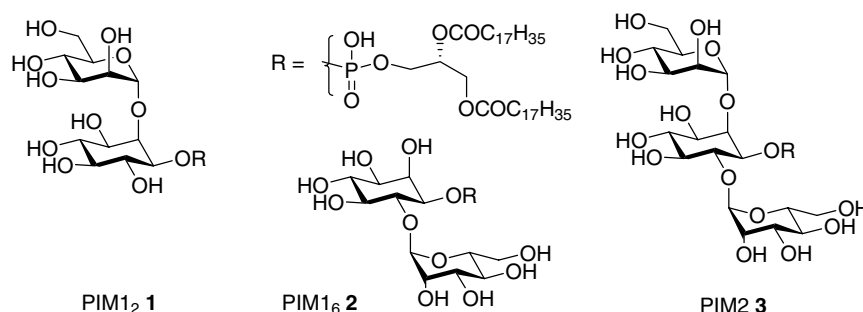
Synthesis of Sansalvamide A derivatives and their cytotoxicity in the MSS colon cancer cell line HT-29 pp 5625–5631

Thomas J. Styers, Ahmet Kecec, Rodrigo Rodriguez, Joseph D. Brown, Julia Cajica, Po-Shen Pan, Emily Parry, Chris L. Carroll, Irene Medina, Ricardo Corral, Stephanie Lopera, Katerina Otrubova, Chung-Mao Pan, Kathleen L. McGuire* and Shelli R. McAlpine*



Phosphatidylinositol mannosides: Synthesis and suppression of allergic airway disease pp 5632–5642

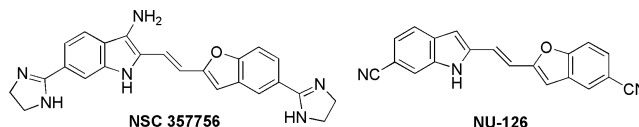
Gary D. Ainge, Jennifer Hudson, David S. Larsen,* Gavin F. Painter, Gurmit Singh Gill and Jacquie L. Harper



Novel benzofuran inhibitors of human mitogen-activated protein kinase phosphatase-1

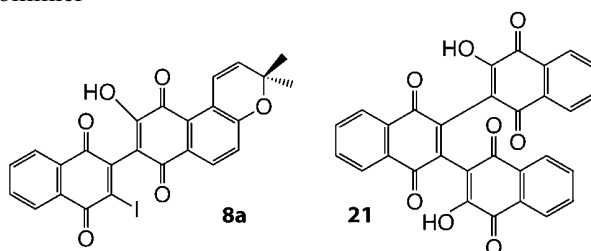
pp 5643–5650

John S. Lazo,* Ruth Nunes, John J. Skoko, Pierre E. Queiroz de Oliveira, Andreas Vogt and Peter Wipf

**Regiocontrolled synthesis and HIV inhibitory activity of unsymmetrical binaphthoquinone and trimeric naphthoquinone derivatives of conocurvone**

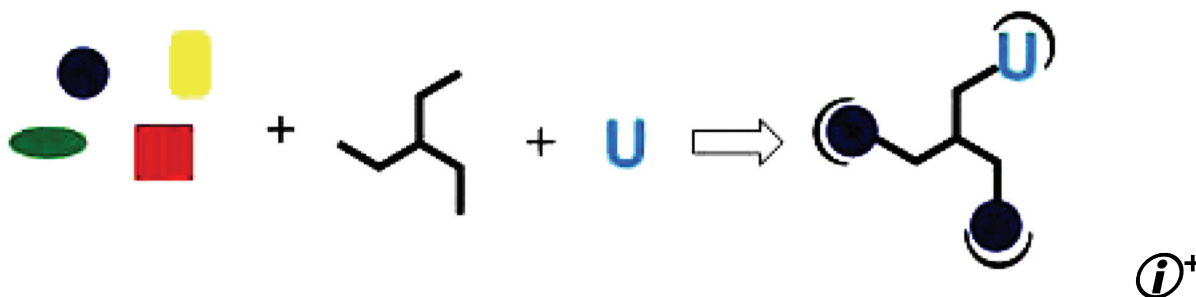
pp 5651–5665

Kenneth W. Stagliano, Ashkan Emadi, Zhenhai Lu, Helena C. Malinakova, Barry Twenter, Min Yu, Louis E. Holland, Amanda M. Rom, John S. Harwood, Ronak Amin, Allison A. Johnson and Yves Pommier*

**Synthesis and high-throughput evaluation of triskelion uracil libraries for inhibition of human dUTPase and UNG2**

pp 5666–5672

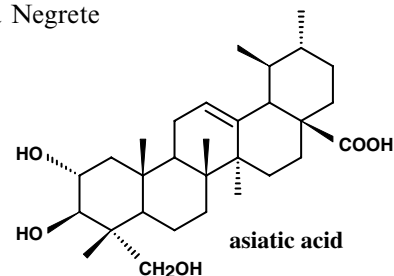
Yu Lin Jiang, Suhman Chung, Daniel J. Krosky and James T. Stivers*

**Topical anti-inflammatory activity of 2 α -hydroxy pentacyclic triterpene acids from the leaves of *Ugni molinae***

pp 5673–5677

María C. Aguirre,* Carla Delporte, Nadine Backhouse, Silvia Erazo, María Eugenia Letelier, Bruce K. Cassels, Ximena Silva, Sergio Alegría and Rosa Negrete

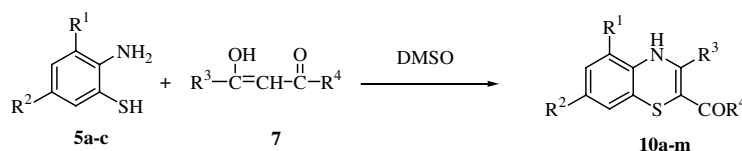
The leaves of *Ugni molinae*, Myrtaceae, showed potent anti-inflammatory activities due mainly to the presence of several pentacyclic triterpene acids, including the 2- α -hydroxy derivatives asiatic, corosolic, and alphitolic acids.



Synthesis of 7-chloro-5-trifluoromethyl/7-fluoro/7-trifluoromethyl-4*H*-1,4-benzothiazines as antimicrobial agents

pp 5678–5682

Bhawani Singh Rathore* and M. Kumar

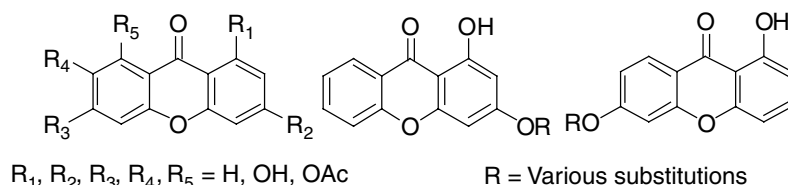


7-Chloro-5-trifluoromethyl/7-fluoro/7-trifluoromethyl-4*H*-1,4-benzothiazines have been synthesized by 2-amino-5-fluoro/5-trifluoromethyl/5-chloro-3-trifluoromethyl benzenethiols condensed with β-diketone/β-ketoesters in the presence of DMSO involving oxidative cyclization. Antimicrobial activities of synthesized compounds have also been included.

Synthesis and pharmacological activities of xanthone derivatives as α-glucosidase inhibitors

pp 5683–5690

Yan Liu, Lan Zou, Lin Ma, Wen-Hua Chen, Bo Wang* and Zun-Le Xu

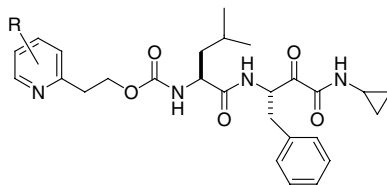


A series of hydroxyxanthenes and their acetoxy and alkoxy derivatives were synthesized and evaluated as α-glucosidase inhibitors, aimed at clarifying the structure–activity correlation. The results indicated that these xanthone derivatives were capable of inhibiting *in vitro* α-glucosidase.

Exploration of orally available calpain inhibitors. Part 3: Dipeptidyl α-ketoamide derivatives containing pyridine moiety

pp 5691–5698

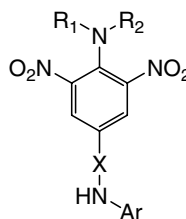
Yoshihisa Shirasaki,* Hiroyuki Miyashita and Masazumi Yamaguchi



Antikinetoplastid antimitotic activity and metabolic stability of dinitroaniline sulfonamides and benzamides

pp 5699–5710

Tesmol G. George, Jayaseharan Johnsamuel, Dawn A. Delfin, Adam Yakovich, Mitali Mukherjee, Mitch A. Phelps, James T. Dalton, Dan L. Sackett, Marcel Kaiser, Reto Brun and Karl A. Werbovetz*



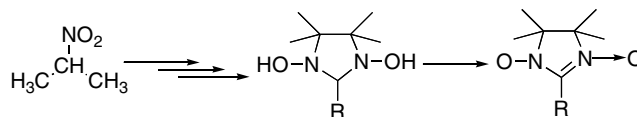
Seventeen new dinitroaniline sulfonamides and eleven dinitroaniline benzamides are reported. Nine of the sulfonamides display *in vitro* IC₅₀ values under 500 nM against African trypanosomes.



Novel 2-substituted nitronyl nitroxides as free radical scavengers: Synthesis, biological evaluation and structure–activity relationship

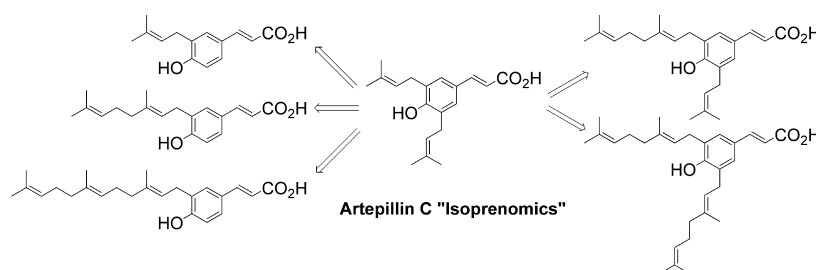
pp 5711–5720

Yihui Wu, Lanrong Bi, Wei Bi, Zeng Li, Ming Zhao,* Chao Wang, Jingfang Ju* and Shiqi Peng*


Artepillin C isoprenomics: Design and synthesis of artepillin C isoprene analogues as lipid peroxidation inhibitor having low mitochondrial toxicity

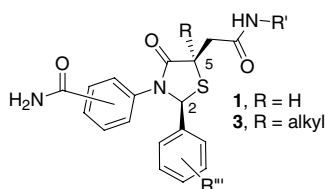
pp 5721–5728

Yoshihiro Uto, Shutaro Ae, Daisuke Koyama, Mitsutoshi Sakakibara, Naoki Otomo, Mamoru Otsuki, Hideko Nagasawa, Kenneth L. Kirk and Hitoshi Hori*


5-Alkylated thiazolidinones as follicle-stimulating hormone (FSH) receptor agonists

pp 5729–5741

Jay Wrobel,* James Jetter, Wenling Kao, John Rogers, Li Di, Jamin Chi, M. Claudia Pérez, Gi-Chung Chen and Emily S. Shen

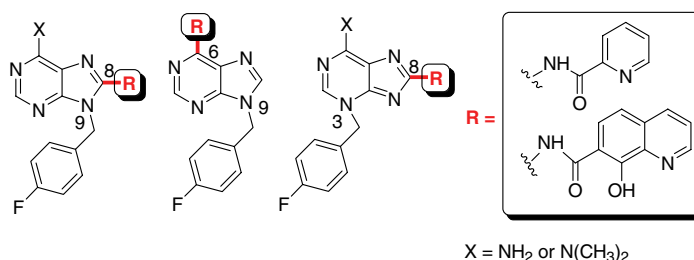


5-Alkylated thiazolidine analogs (3) potent FSH agonists 1 were prepared and evaluated for FSH activity.

Synthesis and biological evaluation of purine derivatives incorporating metal chelating ligands as HIV integrase inhibitors

pp 5742–5755

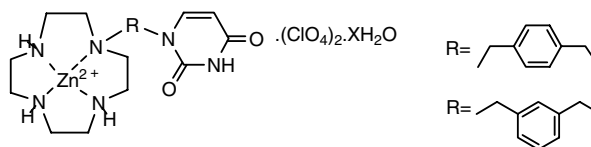
Xingnan Li and Robert Vince*



The conjugates of uracil–cyclen Zn(II) complexes: Synthesis, characterization, and their interaction with plasmid DNA

pp 5756–5764

Chuan-Qin Xia, Ning Jiang, Ji Zhang, Shan-Yong Chen,
Hong-Hui Lin,* Xin-Yu Tan, Yang Yue and Xiao-Qi Yu*

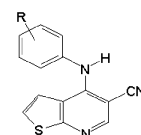


Design, synthesis, SAR, and biological evaluation of new 4-(phenylamino)thieno[2,3-*b*]pyridine derivatives

pp 5765–5770

Alice Maria Rolim Bernardino,* Luiz Carlos da Silva Pinheiro, Carlos Rangel Rodrigues, Natália Izabel Loureiro, Helena Carla Castro,* Adriana Lanfredi-Rangel, Juliano Sabatini-Lopes, Júlio César Borges, Jane Maria Carvalho, Gilberto Alves Romeiro, Vitor Francisco Ferreira, Izabel C. P. P. Frugulhetti and Marcos André Vannier-Santos

We performed the design, synthesis, and the structure–activity relationship studies of 13 new derivatives of thieno[2,3-*b*]pyridine system pointing the *p*-methoxy derivative as a leading compound for antiparasite development.



R = H, *m*-CH₃, *p*-CH₃, *m*-OCH₃, *p*-OCH₃, *m*-NO₂, *p*-NO₂, *m*-F, *p*-F, *m*-Cl, *p*-Cl, *m*-Br, *p*-Br

OTHER CONTENTS

Summary of instructions to authors

p I

*Corresponding author

Supplementary data available via ScienceDirect

COVER

2006: The cover figure shows a synthetic multifunctional pore that is composed of rigid-rod staves (para-octiphenyls, tan) and beta-sheet hoops (arrows) and can be activated with external ligands (fullerenes, golden spheres) and closed with internal blockers (alpha-helix, red ribbon) [Gorteau, V.; Bollot, G.; Mareda, J.; Pasini, D.; Tran, D.-H.; Lazar, A. N.; Coleman, A. W.; Sakai, N.; Matile, S. *Bioorg. Med. Chem.* **2005**, *13*, 5171–5180].

Indexed/Abstracted in: Beilstein, Biochemistry & Biophysics Citation Index, CANCERLIT, Chemical Abstracts, Chemistry Citation Index, Current Awareness in Biological Sciences/BIODISE, Current Contents: Life Sciences, EMBASE/Excerpta Medica, MEDLINE, PASCAL, Research Alert, Science Citation Index, SciSearch, TOXFILE



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