

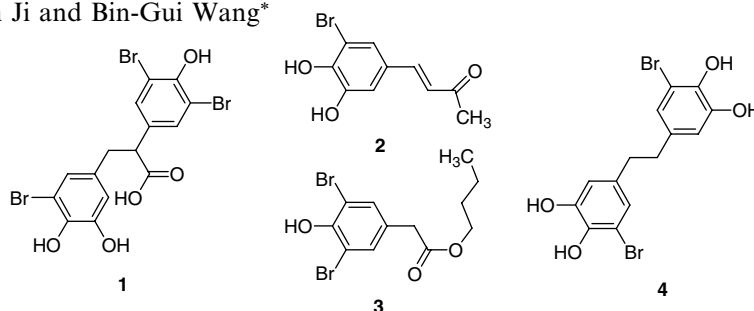
Contents

ARTICLES

Natural bromophenols from the marine red alga *Polysiphonia urceolata* (Rhodomelaceae): Structural elucidation and DPPH radical-scavenging activity

pp 6627–6631

Ke Li, Xiao-Ming Li,* Nai-Yun Ji and Bin-Gui Wang*

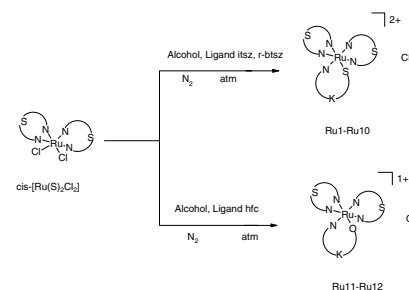


Synthesis, anticancer, and cytotoxic activities of some mononuclear Ru(II) compounds

pp 6632–6641

Subhas S. Karki,* Sreekanth Thota, Satyanarayana Y. Darj, Jan Balzarini and Erik De Clercq

The synthesis and characterization of ruthenium compounds (Ru1–Ru12) of the type *cis*-[Ru(S)₂(K)] (Ru1–Ru12) are described. These ligands form bidentate octahedral ruthenium complexes. Treatment with these compounds prolonged the life span of mice bearing EAC tumor by 10–43%. In vitro evaluation of these ruthenium compounds revealed cytotoxic activity from 0.24 to 27 μ M against Molt 4/C8, 0.27 to 48 μ M against CEM/0, and 0.94 to 248 μ M against L1210. Their ligands alone failed to show cytotoxic activity at the concentrations tested (68–405 μ M).

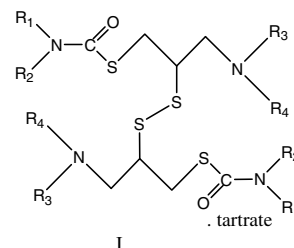


Synthesis of disulfide esters of dialkylaminocarbothioic acid as potent, non-detergent spermicidal agents

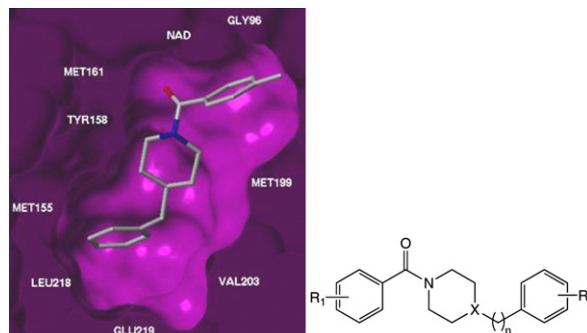
pp 6642–6648

Anil Kumar Dwivedi,* Vishnu Lal Sharma, Niharika Kumaria,
S. T. V. S. Kiran Kumar, Pradeep Kumar Srivastava, Abdul Haq Ansari,
Jagdamba Prasad Maikhuri, Gopal Gupta, Janak Dulari Dhar, Raja Roy,
Bhawani Shankar Joshi, Praveen Kumar Shukla, Manish Kumar and Satyawar Singh

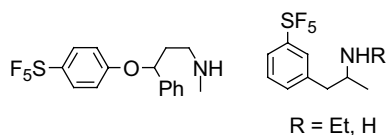
Disulfide esters of dialkylaminocarbothioic acid (**I**; **14–31**) were prepared and evaluated for the spermicidal activity and antifungal activity. Two compounds (**20**, **21**) were 25 times more active than nonoxynol-9 (N-9), the spermicide currently in the market.



Inhibition of the *Mycobacterium tuberculosis* enoyl acyl carrier protein reductase InhA by arylamides pp 6649–6658
Xin He, Akram Alian and Paul R. Ortiz de Montellano*

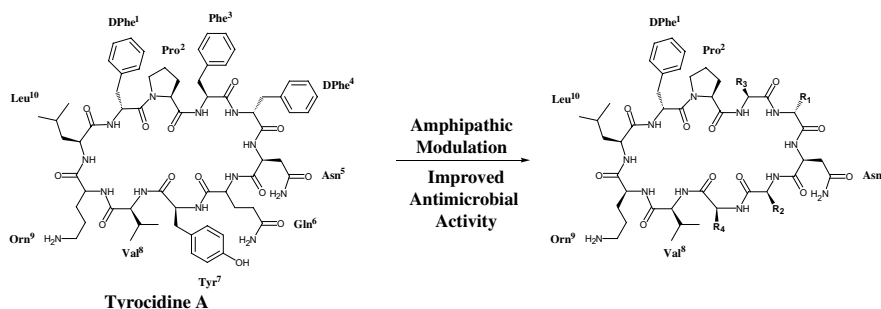


The synthesis and biological activity of pentafluorosulfanyl analogs of fluoxetine, fenfluramine, and norfenfluramine pp 6659–6666
John T. Welch* and Dong Sung Lim



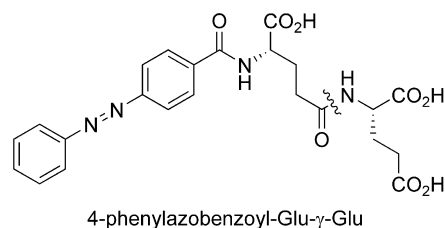
The affinity of the pentafluorosulfanyl analogs of fluoxetine, fenfluramine, and norfenfluramine for a panel of 5-HT receptors has been determined. The affinity of the analogs is compared and contrasted with that of the parent compounds.

Development of Tyrocidine A analogues with improved antibacterial activity pp 6667–6677
Michael A. Marques, Diane M. Citron and Clay C. Wang*



Substrate specificity of prostate-specific membrane antigen pp 6678–6686
Marc O. Anderson, Lisa Y. Wu, Nicholas M. Santiago, Jamie M. Moser, Jennifer A. Rowley, Erin S. D. Bolstad and Clifford E. Berkman*

A series of potential PSMA substrates was prepared that explored acidic residues at the P1 position and various chromophores at the P2 position, while keeping the P1' residue constant as L-Glu. The substrate 4-phenylazobenzoyl-Glu- γ -Glu was found to be proteolyzed most efficiently.



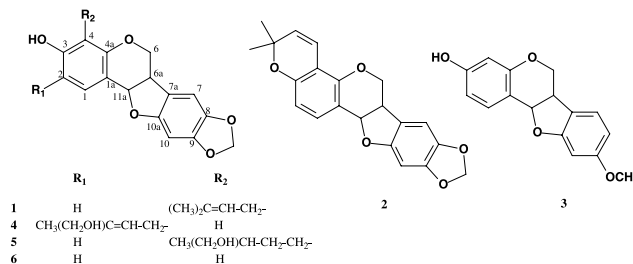
4-phenylazobenzoyl-Glu- γ -Glu

Bioassay-guided fractionation of pterocarpanes from roots of *Harpalyce brasiliensis* Benth

pp 6687–6691

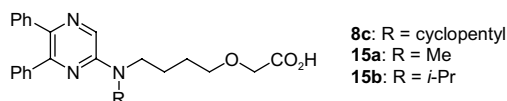
Gardenia C. G. Militão, Sávio M. Pinheiro, Ivana N. F. Dantas, Cláudia Pessoa, Manoel Odorico de Moraes, Leticia V. Costa-Lotufo,* Mary Anne S. Lima and Edilberto R. Silveira

A bioassay-guided fractionation of antimitotic pterocarpanes present in the EtOH extract from the roots of *Harpalyce brasiliensis*. Some initial studies on structure–activity relationship for these pterocarpanes are suggested.

**Structure–activity studies on diphenylpyrazine derivatives: A novel class of prostacyclin receptor agonists**

pp 6692–6704

Tetsuo Asaki,* Taisuke Hamamoto, Yukiteru Sugiyama, Keiichi Kuwano and Kenji Kuwabara

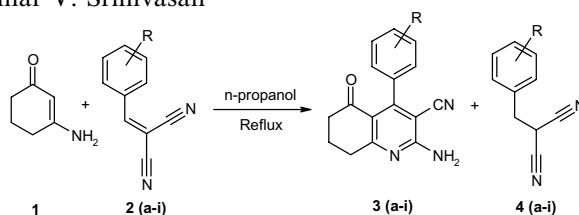


To develop new IP receptor agonists, a novel series of diphenylpyrazine derivatives was synthesized and evaluated for their inhibition of ADP-induced human platelet aggregation. This study led to the discovery of 2-amino-5,6-diphenylpyrazine derivatives **8c**, **15a**, and **15b**.

Synthesis and evaluation of antifungal properties of a series of the novel 2-amino-5-oxo-4-phenyl-5,6,7,8-tetrahydroquinoline-3-carbonitrile and its analogues

pp 6705–6715

Atul R. Gholap, Kiran S. Toti, Fazal Shirazi, Ratna Kumari, Manoj Kumar Bhat, Mukund V. Deshpande and Kumar V. Srinivasan*

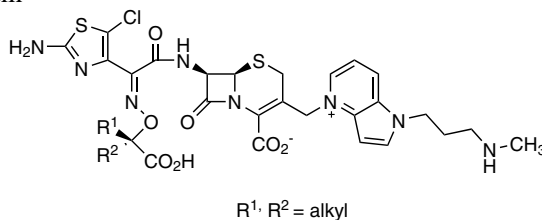


A series of 2-amino-5-oxo-4-phenyl-5,6,7,8-tetrahydroquinoline-3-carbonitrile and various analogues have been synthesized and screened for their antifungal activity.

**A novel series of parenteral cephalosporins exhibiting potent activities against *Pseudomonas aeruginosa* and other Gram-negative pathogens: Synthesis and structure–activity relationships**

pp 6716–6732

Kenji Yamawaki,* Takashi Nomura, Tatsuro Yasukata, Koichi Uotani, Hideaki Miwa, Kei Takeda and Yasuhiro Nishitani

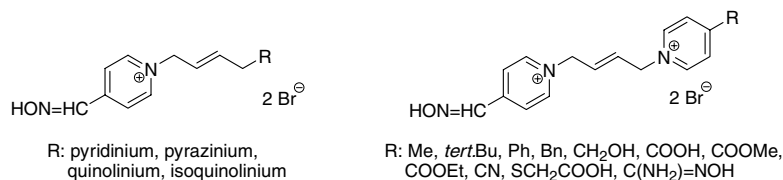


A novel series of cephalosporins bearing a chlorominothiazole and a carboxymethoxyimino moiety at the C-7 side chain was prepared, and their antibacterial activities were evaluated.

Monooxime reactivators of acetylcholinesterase with (*E*)-but-2-ene linker—Preparation and reactivation of tabun- and paraoxon-inhibited acetylcholinesterase

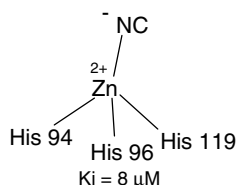
pp 6733–6741

Kamil Musilek, Ondrej Holas, Daniel Jun, Vlastimil Dohnal, Frank Gunn-Moore, Veronika Opletalova, Martin Dolezal and Kamil Kuca*


Carbonic anhydrase inhibitors: The inhibition profiles of the human mitochondrial isoforms VA and VB with anions are very different

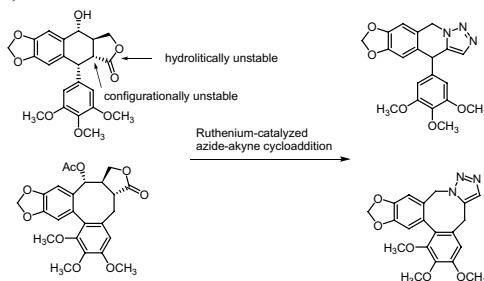
pp 6742–6747

Isao Nishimori, Alessio Innocenti, Daniela Vullo, Andrea Scozzafava and Claudiu T. Supuran*


Replacement of the lactone moiety on podophyllotoxin and steganacin analogues with a 1,5-disubstituted 1,2,3-triazole via ruthenium-catalyzed click chemistry

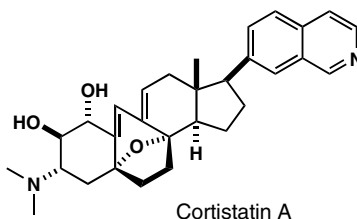
pp 6748–6757

Daniela Imperio, Tracey Pirali, Ubaldina Galli, Francesca Pagliai, Laura Cafici, Pier Luigi Canonico, Giovanni Sorba, Armando A. Genazzani and Gian Cesare Tron*


Structure–activity relationship and biological property of cortistatins, anti-angiogenic spongian steroidal alkaloids

pp 6758–6762

Shunji Aoki, Yasuo Watanabe, Daiki Tanabe, Masayoshi Arai, Hideaki Suna, Katsushiro Miyamoto, Hiroshi Tsujibo, Kazutake Tsujikawa, Hiroshi Yamamoto and Motomasa Kobayashi*

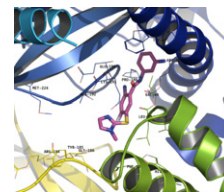
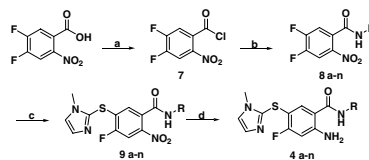

 Eleven steroidal alkaloids named cortistatins were isolated from the marine sponge *Corticium simplex* as anti-angiogenic agents. The detailed structure–activity relationship and biological property of these cortistatins are presented.

Discovering benzamide derivatives as glycogen phosphorylase inhibitors and their binding site at the enzyme

pp 6763–6774

Ling Chen, Honglin Li,* Jun Liu, Luyong Zhang, Hong Liu* and Hualiang Jiang

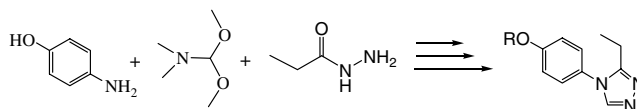
A series of novel benzamide derivatives was designed, synthesized, and their inhibitory activities against glycogen phosphorylase (GP) were also evaluated. Within these compounds, **4m** is the most potent GP inhibitor ($IC_{50} = 2.68 \mu M$). Analysis of mapping between pharmacophores of different binding sites and each compound demonstrated that these benzamide derivatives bind at the dimer interface of the rabbit muscle enzyme, and possible docking modes of compound **4m** were explored by molecular docking simulation.



Synthesis and anticonvulsant evaluation of 4-(4-alkoxyphenyl)-3-ethyl-4H-1,2,4-triazoles as open-chain analogues of 7-alkoxy-4,5-dihydro[1,2,4]triazolo[4,3-a]quinolines

pp 6775–6781

Jing Chen, Xian-Yu Sun, Kyu-Yun Chai, Jin-Seok Lee, Mi-Sun Song and Zhe-Shan Quan*



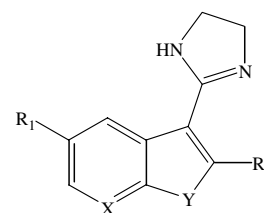
A series of 4-(4-alkoxyphenyl)-3-ethyl-4H-1,2,4-triazole derivatives was synthesized as open-chain analogues of 7-alkoxy-4,5-dihydro[1,2,4]triazolo[4,3-a]quinolines. Their anticonvulsant activities were evaluated by the maximal electroshock test (MES test) and their neurotoxicity was evaluated by the rotarod neurotoxicity test (Tox).

Synthesis and antidiabetic activity of 2,5-disubstituted-3-imidazol-2-yl-pyrrolo[2,3-b]pyridines and thieno[2,3-b]pyridines

pp 6782–6795

Rajesh H. Bahekar,* Mukul R. Jain, Pradip A. Jadav, Vijay M. Prajapati, Dipam N. Patel, Arun A. Gupta, Ajay Sharma, Robby Tom, Debdutta Bandyopadhyaya, Honey Modi and Pankaj R. Patel

Two series of aryl-imidazolines (**2a–l** and **3a–l**), were designed as analogs of BL 11282 and their in vitro and in vivo antidiabetic activities were evaluated.

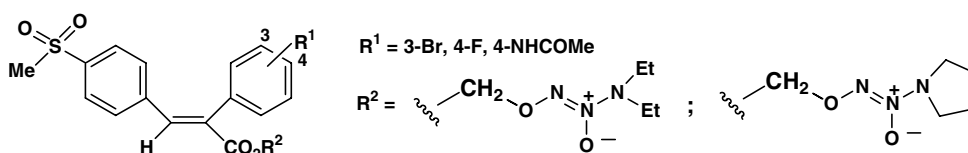


2a-l (X=N; Y=NH); 3a-l (X=N; Y=S)

Novel (E)-2-(aryl)-3-(4-methanesulfonylphenyl)acrylic ester prodrugs possessing a diazen-1-ium-1,2-diolate moiety: Design, synthesis, cyclooxygenase inhibition, and nitric oxide release studies

pp 6796–6801

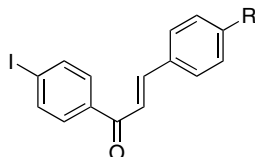
Khaled R. A. Abdellatif, Ying Dong, Qiao-Hong Chen, Morshed Alam Chowdhury and Edward E. Knaus*



Novel chalcones as probes for in vivo imaging of β -amyloid plaques in Alzheimer's brains

pp 6802–6809

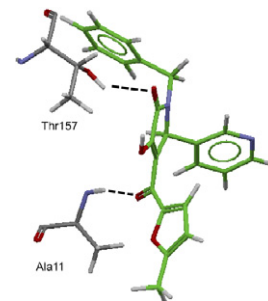
Masahiro Ono,* Mamoru Haratake, Hiroshi Mori and Morio Nakayama

R = NH₂, NHCH₃, N(CH₃)₂, OCH₃, OH**Identification of novel chemical inhibitors for ubiquitin C-terminal hydrolase-L3 by virtual screening**

pp 6810–6818

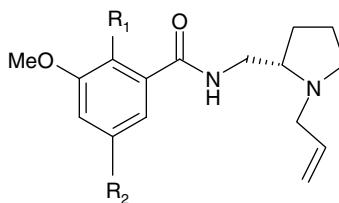
Kazunori Hirayama, Shunsuke Aoki,* Kaori Nishikawa, Takashi Matsumoto and Keiji Wada

A UCH-L3 inhibitor (1-benzyl-3-hydroxy-4-(5-methyl-2-furoyl)-5-(3-pyridinyl)-1,5-dihydro-2H-pyrrol-2-one) identified by virtual screening is shown.

**In vitro affinities of various halogenated benzamide derivatives as potential radioligands for non-invasive quantification of D₂-like dopamine receptors**

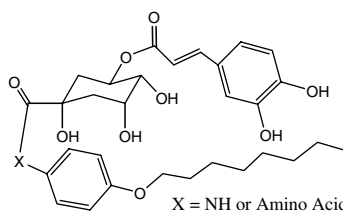
pp 6819–6829

Daniela Stark, Markus Piel, Harald Hübner, Peter Gmeiner, Gerhard Gründer and Frank Rösch*

**Synthesis of chlorogenic acid derivatives with promising antifungal activity**

pp 6830–6833

Chao-Mei Ma, Maureen Kully, Jehangir K. Khan, Masao Hattori and Mohsen Daneshtalab*



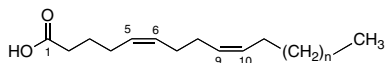
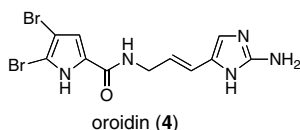
The synthesis of the chlorogenic acid derivatives with in vitro antifungal activity is reported.



Marine natural products from the Turkish sponge *Agelas oroides* that inhibit the enoyl reductases from *Plasmodium falciparum*, *Mycobacterium tuberculosis* and *Escherichia coli*

pp 6834–6845

Deniz Tasdemir,* Bülent Topaloglu, Remo Perozzo, Reto Brun, Rosann O'Neill, Néstor M. Carballeira, Xujie Zhang, Peter J. Tonge, Anthony Linden and Peter Rüedi



7 n: 11 (5Z,9Z)-5,9-tricosadienoic acid, 23:2)

8 n: 12 (5Z,9Z)-5,9-tetracosadienoic acid, 24:2)

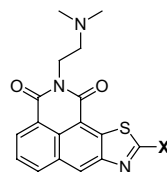
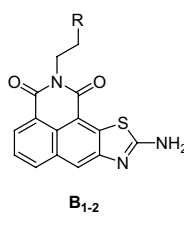
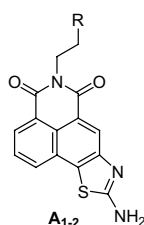
9 n: 13 (5Z,9Z)-5,9-pentacosadienoic acid, 25:2)

10 n: 14 (5Z,9Z)-5,9-hexacosadienoic acid, 26:2)

**Highly efficient antitumor agents of heterocycles containing sulfur atom: Linear and angular thiazonaphthalimides against human lung cancer cell in vitro**

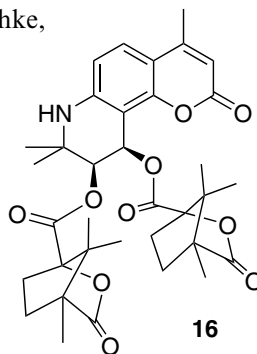
pp 6846–6851

Xuhong Qian,* Zhigang Li and Qing Yang*

A₁, B₁: R=N(CH₃)₂
A₂, B₂: R=CH₂N(CH₃)₂C: X=H
D: X=OH
E: X=Cl
F: X=NH(CH₂)₂N(CH₃)₂**Anti-AIDS agents 66: Syntheses and anti-HIV activity of phenolic and aza 3',4'-di-O(-)-camphanoyl-(+)-cis-khellactone (DCK) derivatives**

pp 6852–6858

Madoka Suzuki, Donglei Yu, Susan L. Morris-Natschke, Philip C. Smith and Kuo-Hsiung Lee*

**OTHER CONTENTS**

Summary of instructions to authors

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*Corresponding author

Supplementary data available via ScienceDirect

COVER

Terfenadine (an antihistamine pulled from the market in 1997) bound to a model of an open form of the homo-tetrameric pore domain of hERG, produced using Schrödinger's "Induced Fit Docking" technology [Farid, R.; Day, T.; Friesner, R. A.; Pearlstein, R. A. *Bioorg. Med. Chem.* **2006**, *14*, 3160–3173].

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