

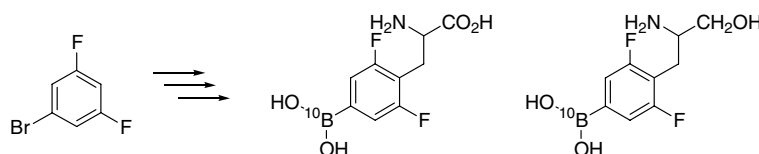
## Contents

### ARTICLES

**Study on the compounds containing  $^{19}\text{F}$  and  $^{10}\text{B}$  atoms in a single molecule for the application to MRI and BNCT**

pp 3258–3262

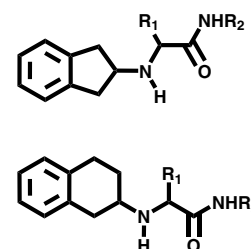
Yoshihide Hattori, Tomoyuki Asano, Yoko Niki, Hirofumi Kondoh, Mitsunori Kiriha, Yoshihiro Yamaguchi and Tateaki Wakamiya\*



**Synthesis and anticonvulsant activity of a class of 2-amino 3-hydroxypropanamide and 2-aminoacetamide derivatives**

pp 3263–3274

Eleonora Ghidini,\* Maurizio Delcanale, Renato De Fanti, Andrea Rizzi, Manuela Mazzuferi, Donata Rodi, Michele Simonato, Milco Lipreri, Franco Bassani, Loredana Battipaglia, Marco Bergamaschi and Gino Villetti

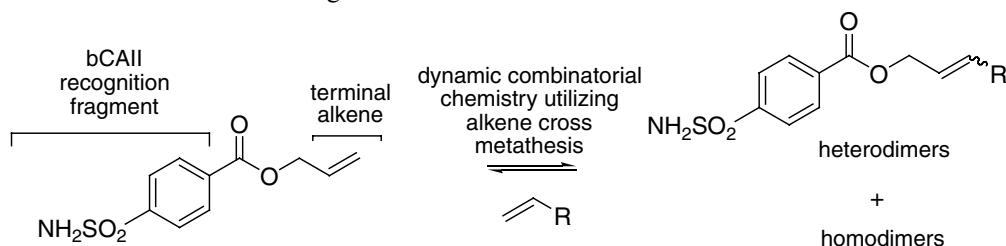


R1= CH<sub>2</sub>OH, CH<sub>3</sub>, H, Cyclopropyl, Cyclopentyl  
R2= H, CH<sub>3</sub>

**Fragment-based drug discovery of carbonic anhydrase II inhibitors by dynamic combinatorial chemistry utilizing alkene cross metathesis**

pp 3275–3284

Sally-Ann Poulsen\* and Laurent F. Bornaghi

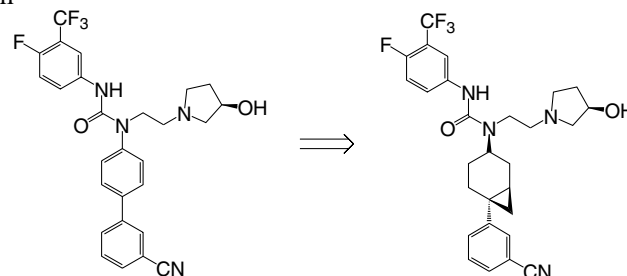


A fragment-based drug discovery approach to the synthesis of inhibitors of bovine carbonic anhydrase II (bCAII) is described. Dynamic combinatorial chemistry utilizing alkene cross metathesis was employed in this study.

**Bicyclic[4.1.0]heptanes as phenyl replacements for melanin concentrating hormone receptor antagonists** pp 3285–3299

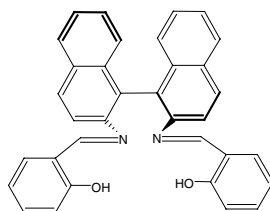
Ruo Xu,\* Shengjian Li, Jaroslava Paruchova, Mark D. McBriar, Henry Guzik, Anandan Palani, John W. Clader, Kathleen Cox, William J. Greenlee, Brian E. Hawes, Timothy J. Kowalski, Kim O'Neill, Brian D. Spar, Blair Weig and Daniel J. Weston

Bicyclic[4.1.0]heptanes were discovered as replacements for the middle phenyl ring of the biphenylamine moiety in order to eliminate its potential mutagenic liability.

**Interaction of chromium(III) complex of chiral binaphthyl tetradentate ligand with DNA**

pp 3300–3306

Rajamanickam Vijayalakshmi, Mookandi Kanthimathi, Ramakrishnan Parthasarathi and Balachandran Unni Nair\*

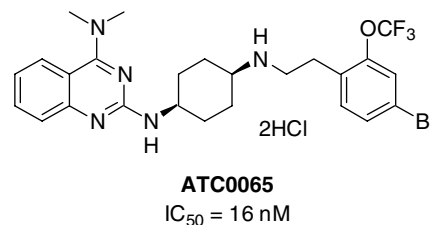


The influence of ligand chirality of Cr(III) Schiff base complex on its DNA binding properties has been investigated.

**Identification of 4-amino-2-cyclohexylaminoquinazolines as metabolically stable melanin-concentrating hormone receptor 1 antagonists** pp 3307–3319

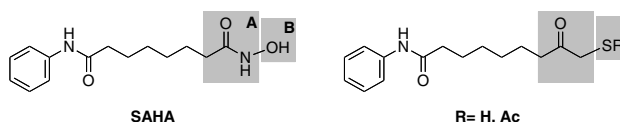
Kosuke Kanuma, Katsunori Omodera, Mariko Nishiguchi, Takeo Funakoshi, Shigeyuki Chaki, Yasuko Nagase, Izumi Iida, Jun-ichi Yamaguchi, Graeme Semple, Thuy-Anh Tran and Yoshinori Sekiguchi\*

Through an optimization of the distance between two key pharmacophore features, 4-amino-2-cyclohexylaminoquinazolines were identified as potent melanin-concentrating hormone receptor 1 (MCH-R1) antagonists, leading to the discovery of ATC0065.

**Carbonyl- and sulfur-containing analogs of suberoylanilide hydroxamic acid: Potent inhibition of histone deacetylases**

pp 3320–3329

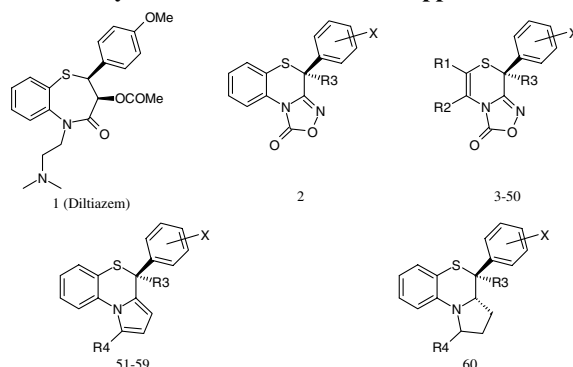
Wenxin Gu, Inna Nusinzon, Ronald D. Smith, Jr., Curt M. Horvath and Richard B. Silverman\*



## 2D Autocorrelation modeling of the negative inotropic activity of calcium entry blockers using Bayesian-regularized genetic neural networks

Julio Caballero, Miguel Garriga and Michael Fernández\*

Basic structures of the 60 Diltiazem-like calcium entry blockers used for modeling negative inotropic activity.

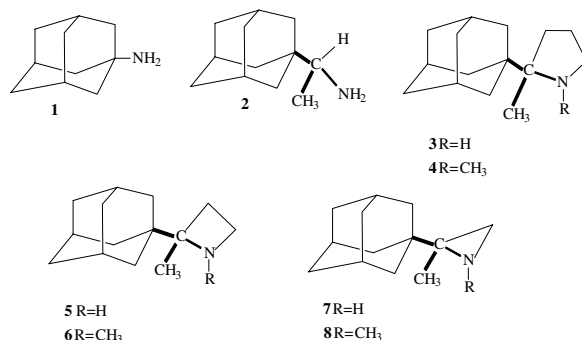


pp 3330–3340

## Heterocyclic rimantadine analogues with antiviral activity

Grigoris Zoidis, Christos Fytas, Ioannis Papanastasiou, George B. Foscolos, George Fytas, Elizaveta Padalko, Erik De Clercq, Lieve Naesens, Johan Neyts and Nicolas Kolocouris\*

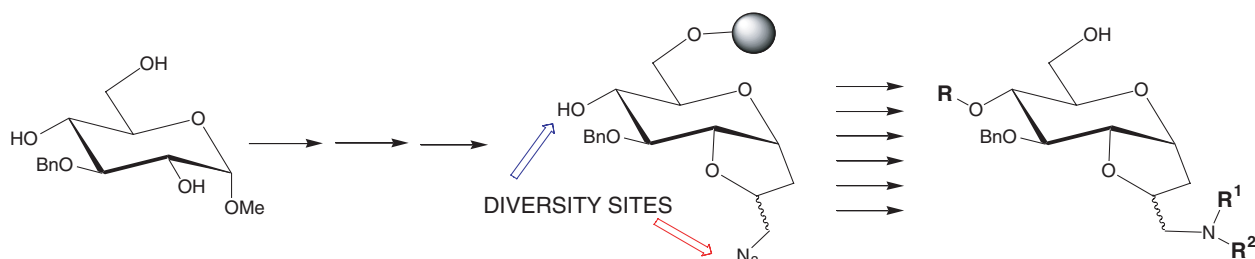
The prime target of this study was to synthesize and examine the anti-influenza A virus activity of rimantadine analogues **3**, **5**, and **7** and to correlate their potency to the size of the heterocyclic ring they bear in their skeleton.



pp 3341–3348

## Bicyclic carbohydrate-derived scaffolds for combinatorial libraries

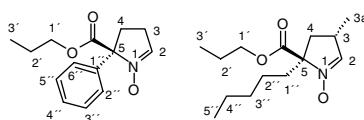
Giovanni Cervi, Francesco Peri, Carlo Battistini, Cesare Gennari and Francesco Nicotra\*



pp 3349–3367

## Spin trapping of C- and O-centered radicals with methyl-, ethyl-, pentyl-, and phenyl-substituted EMPO derivatives

Klaus Stolze,\* Natascha Rohr-Udilova, Thomas Rosenau, Andreas Hofinger, Daniel Kolarich and Hans Nohl\*



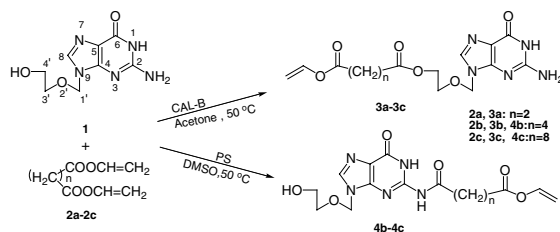
pp 3368–3376

Synthesis and spin trapping properties of a series of EMPO-derived nitrones are reported.

### Controllable synthesis of polymerizable ester and amide prodrugs of acyclovir by enzyme in organic solvent

pp 3377–3382

Xia Li, Qi Wu, De-shui Lv and Xian-fu Lin\*

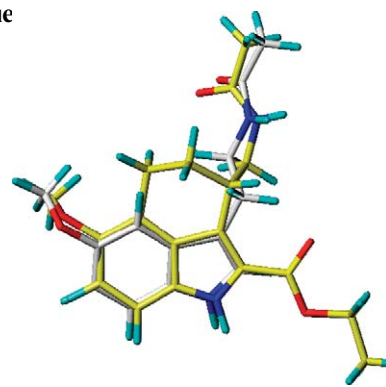


A facile control of the acylation position at the primary hydroxyl and amino of acyclovir to obtain polymerizable 2-*N*-acyl and 4'-*O*-acyl acyclovir vinyl derivatives, respectively, was achieved.

### Reassessing the melatonin pharmacophore—Enantiomeric resolution, pharmacological activity, structure analysis, and molecular modeling of a constrained chiral melatonin analogue

pp 3383–3391

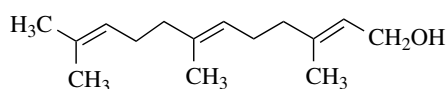
Silvia Rivara, Giuseppe Diamantini, Barbara Di Giacomo,\* Doriano Lamba, Giuseppe Gatti, Valeria Lucini, Marilou Pannacci, Marco Mor, Gilberto Spadoni and Giorgio Tarzia



### Isolation and characterization of a monoamine oxidase B selective inhibitor from tobacco smoke

pp 3392–3398

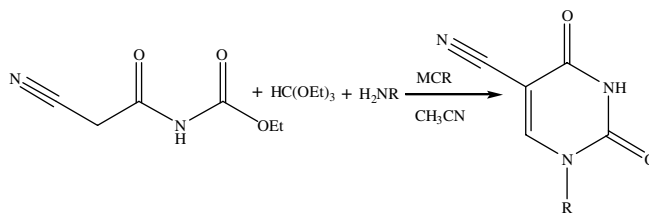
Ashraf A. Khalil, Bruce Davies and Neal Castagnoli, Jr.\*



### A multi-component reaction to 5-cyanouracils: Synthesis and mechanistic study

pp 3399–3404

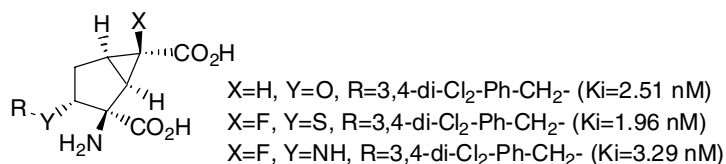
Bo-Ren Zhuang, Gien-Jow Hsu and Kuangsen Sung\*



### Synthesis, in vitro pharmacology, and structure–activity relationships of 2-aminobicyclo[3.1.0]hexane-2,6-dicarboxylic acid derivatives as mGluR2 antagonists

pp 3405–3420

Akito Yasuhara,\* Kazunari Sakagami, Ryoko Yoshikawa, Shigeyuki Chaki, Masato Nakamura and Atsuro Nakazato



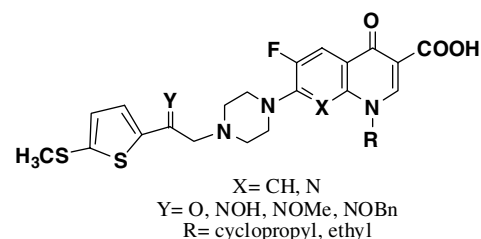
2-Aminobicyclo[3.1.0]hexane-2,6-dicarboxylic acids showed high affinity for the mGluR2 receptor and potent antagonist activities for mGluR2.

### Synthesis and antibacterial activity of *N*-[2-[5-(methylthio)thiophen-2-yl]-2-oxoethyl] and *N*-[2-[5-(methylthio)thiophen-2-yl]-2-(oxymino)ethyl]piperazinylquinolone derivatives

pp 3421–3427

Alireza Foroumadi, Mehdi Oboudiat, Saeed Emami, Alireza Karimollah, Lotfollah Saghaee, Mohammad Hassan Moshafi and Abbas Shafiee\*

A number of *N*-substituted piperazinylquinolone derivatives were synthesized and evaluated for antibacterial activity against Gram-positive and Gram-negative bacteria. Most compounds demonstrated comparable or better activity against *Staphylococcus aureus* and *Staphylococcus epidermidis* than their parent piperazinylquinolones. Among these derivatives, ciprofloxacin derivative **5a**, containing *N*-[2-[5-(methylthio)thiophen-2-yl]-2-oxoethyl] residue, showed significant improvement of potency against staphylococci, maintaining Gram-negative coverage.

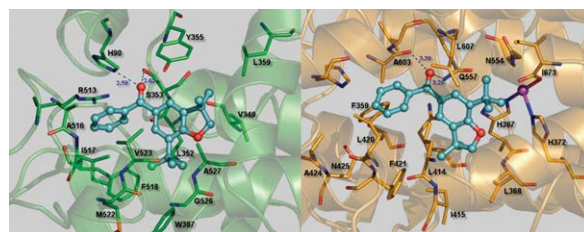


### Essential structural profile of a dual functional inhibitor against cyclooxygenase-2 (COX-2) and 5-lipoxygenase (5-LOX): Molecular docking and 3D-QSAR analyses on DHDMBF analogues

pp 3428–3437

Mingyue Zheng, Zhenshan Zhang, Weiliang Zhu,\* Hong Liu,\* Xiaomin Luo, Kaixian Chen and Hualiang Jiang\*

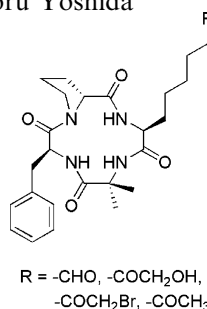
A series of COX-2/5-LOX inhibitors of DHDMBF analogues were studied with molecular docking and 3D-QSAR approaches to provide guidance on designing potent dual functional inhibitors for developing anti-inflammation drugs with favorable safety profile.



### Chlamydocin analogs bearing carbonyl group as possible ligand toward zinc atom in histone deacetylases

pp 3438–3446

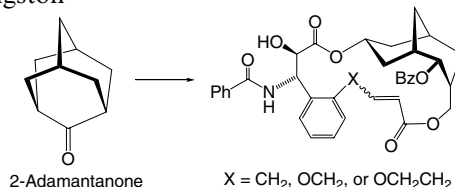
Mohammed P. I. Bhuiyan, Tamaki Kato, Tatsuo Okauchi, Norikazu Nishino,\* Satoko Maeda, Tomonori G. Nishino and Minoru Yoshida



### Design, synthesis, and bioactivity of simplified paclitaxel analogs based on the T-Taxol bioactive conformation

pp 3447–3454

Thota Ganesh, Andrew Norris, Shubhada Sharma, Susan Bane, Ana A. Alcaraz, James P. Snyder and David G. I. Kingston\*



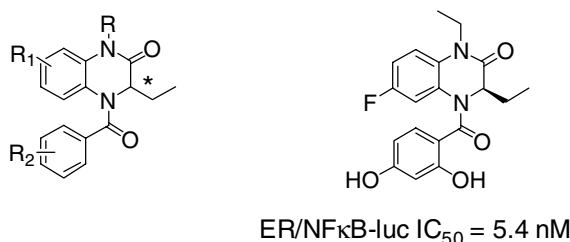
A strategy for the design and synthesis of simplified paclitaxel analogs based on the T-Taxol conformation is presented. The resulting compounds have both cytotoxic and tubulin polymerization activities, although less so than those of paclitaxel itself.



### Synthesis and activity of a new class of pathway-selective estrogen receptor ligands: Hydroxybenzoyl-3,4-dihydroquinoxalin-2(1H)-ones

pp 3455–3466

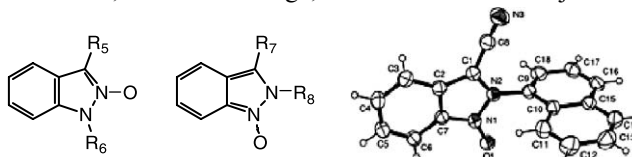
Paige E. Mahaney,\* Michael B. Webb, Fei Ye, Joseph P. Sabatucci, Robert J. Steffan, Christopher C. Chadwick, Douglas C. Harnish and Eugene J. Trybulski



### Indazole *N*-oxide derivatives as antiprotozoal agents: Synthesis, biological evaluation and mechanism of action studies

pp 3467–3480

Alejandra Gerpe, Gabriela Aguirre, Lucía Boiani, Hugo Cerecetto,\* Mercedes González,\* Claudio Olea-Azar, Carolina Rigol, Juan D. Maya, Antonio Morello, Oscar E. Piro, Vicente J. Arán, Amaia Azqueta, Adela López de Ceráin, Antonio Monge, Maria Antonieta Rojas and Gloria Yaluff



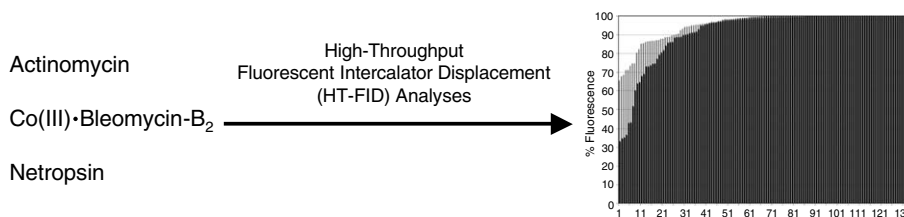
Indazole *N*-oxide derivatives as antitrypanosomal and leishmanocidal compounds are described. Electrochemical studies, ESR experiments, inhibition of parasitic respiration and QSAR studies are presented in order to understand the mechanism of action.



### Fluorescent intercalator displacement analyses of DNA binding by the peptide-derived natural products netropsin, actinomycin, and bleomycin

pp 3481–3490

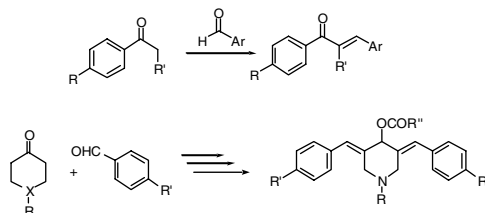
Mark A. Lewis and Eric C. Long\*



**Anticancer activities of novel chalcone and bis-chalcone derivatives**

pp 3491–3495

Aneta Modzelewska, Catherine Pettit, Geetha Achanta, Nancy E. Davidson, Peng Huang and Saeed R. Khan\*



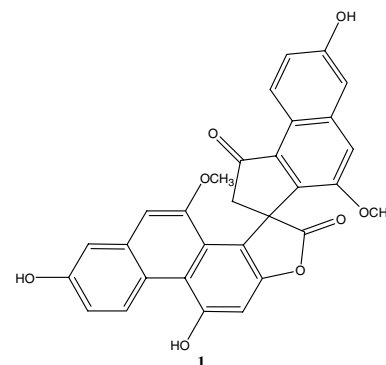
Novel chalcone and bis-chalcone derivatives have been synthesized and evaluated for antitumor activity. These molecules inhibited the growth of the human breast cancer cell lines at low micromolar to nanomolar concentrations, with five of them (**1–4, 9**) showing preferential inhibition of the human breast cancer cell lines.

**A new phenanthrene with a spirolactone from *Dendrobium chrysanthum* and its anti-inflammatory activities**

pp 3496–3501

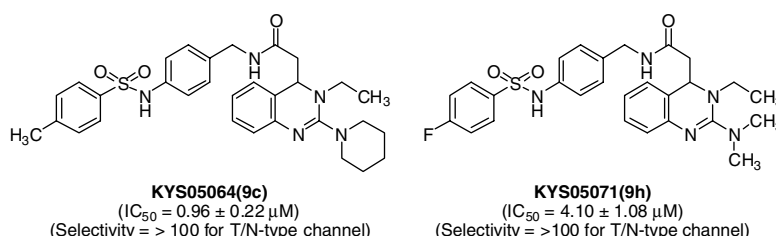
Li Yang, Lin-Hua Qin, S. W. Annie Bligh, A. Bashall, Chao-Feng Zhang, Mian Zhang, Zheng-Tao Wang\* and Luo-Shan Xu

Investigation of phenolic patterns from the stems of *Dendrobium chrysanthum* by HPLC–PDA–MS has led to the isolation of a new phenanthrene derivative with a spirolactone ring, dendrochrysanene (**1**), that proved to suppress the mRNA level of TNF- $\alpha$ , IL8, IL10, and iNOS in murine peritoneal macrophages.

**Synthesis and SAR studies of a novel series of T-type calcium channel blockers**

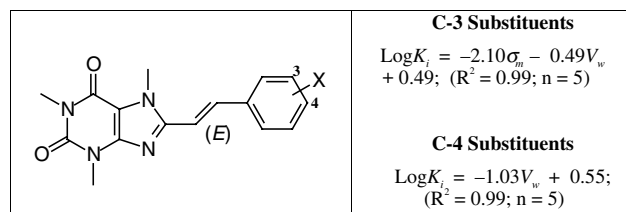
pp 3502–3511

Seong Jun Park, Sung Jun Park, Min Joo Lee, Hyewhon Rhim, Yoonjee Kim, Jung-Ha Lee, Bong Young Chung and Jae Yeol Lee\*

**Inhibition of monoamine oxidase B by analogues of the adenosine A<sub>2A</sub> receptor antagonist (*E*)-8-(3-chlorostyryl)caffeine (CSC)**

pp 3512–3521

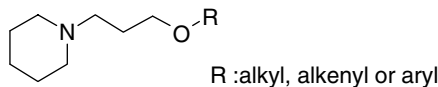
Nevil Vlok, Sarel F. Malan, Neal Castagnoli, Jr., Jacobus J. Bergh and Jacobus P. Petzer\*



**Ether derivatives of 3-piperidinopropan-1-ol as non-imidazole histamine H<sub>3</sub> receptor antagonists**

pp 3522–3529

Dorota Łażewska, Xavier Ligneau, Jean-Charles Schwartz, Walter Schunack, Holger Stark and Katarzyna Kieć-Kononowicz\*

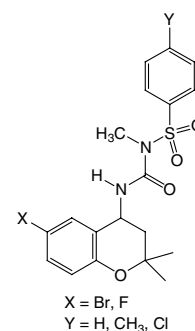


A series of asymmetrically ether derivatives of 3-piperidino-1-ol was prepared and evaluated as histamine H<sub>3</sub> receptor antagonists. The most potent compounds were in vitro **19** ( $hK_i = 8.4$  nM) and in vivo **2** (ED<sub>50</sub> = 1.0 mg/kg).

**Synthesis and pharmacological evaluation of some *N*-arylsulfonyl-*N*'-methyl-*N*'-(2,2-dimethyl-2*H*-1-benzopyran-4-yl)ureas structurally related to cromakalim**

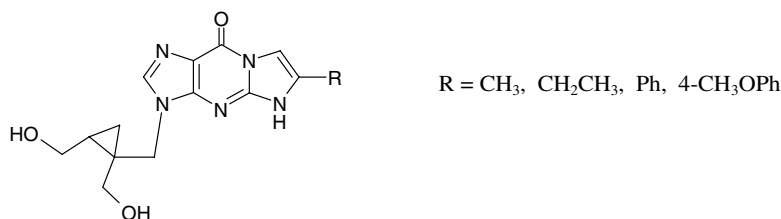
pp 3530–3534

Smail Khelili, Philippe Lebrun, Pascal de Tullio and Bernard Pirotte\*

**Synthesis and biological activity of tricyclic analogues of 9-*[(cis-1',2'-bis(hydroxymethyl)cycloprop-1'-yl)methyl]guanine***

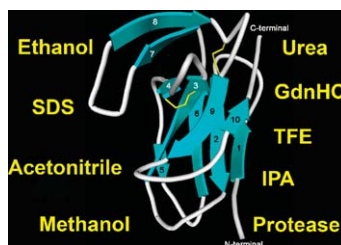
pp 3535–3542

Tomasz Ostrowski, Bożenna Golankiewicz,\* Erik De Clercq and Jan Balzarini

**Aponeocarinostatin—A superior drug carrier exhibiting unusually high endurance against denaturants**

pp 3543–3552

Christopher G. Sudhahar and Der-Hang Chin\*



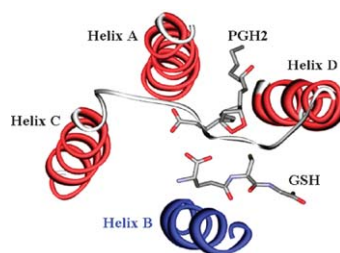
Stability of apoNCS is discerned via its resistance against denaturants in comparison to proteins known to be stable. Its unusual structural stability suggests its inherent superiority as a drug delivery system.



**Structural and functional characterization of human microsomal prostaglandin E synthase-1 by computational modeling and site-directed mutagenesis**

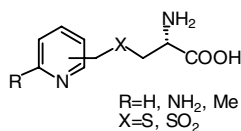
pp 3553–3562

Xiaoqin Huang, Weili Yan, Daquan Gao, Min Tong, Hsin-Hsiung Tai\* and Chang-Guo Zhan\*

**Design, synthesis, and evaluation of new type of L-amino acids containing pyridine moiety as nitric oxide synthase inhibitor**

pp 3563–3570

Ryosuke Ijuin, Naoki Umezawa and Tsunehiko Higuchi\*

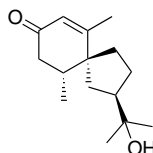


We designed and synthesized a new class of nitric oxide synthase (NOS) inhibitors incorporating a picolyl group at the sulfur atom of cysteine and evaluated their structure–activity relationship.

**New sesquiterpene from Vietnamese agarwood and its induction effect on brain-derived neurotrophic factor mRNA expression in vitro**

pp 3571–3574

Jun-ya Ueda, Lisa Imamura, Yasuhiro Tezuka, Quan L. Tran, Masaaki Tsuda and Shigetoshi Kadota\*

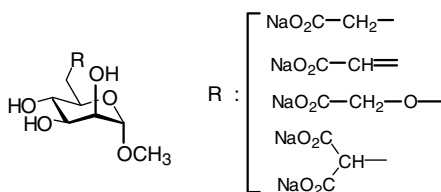


The new sesquiterpenoid, (4*R*,5*R*,7*R*)-1(10)-spirovetiven-11-ol-2-one, isolated from agarwood significantly induced brain-derived neurotrophic factor (BDNF) exon III–V mRNA expression.

**Synthesis and receptor binding affinity of carboxylate analogues of the mannose 6-phosphate recognition marker**

pp 3575–3582

Audrey Jeanjean, Marcel Garcia, Alain Leydet, Jean-Louis Montero and Alain Morère\*

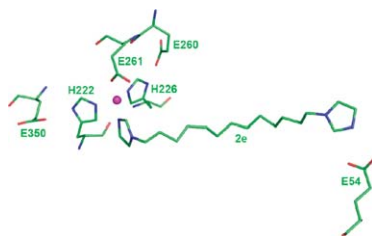


Four analogues of M6P have been prepared and their binding affinity for the M6P/IGF2 receptor evaluated.

### Bis-imidazoles as molecular probes for peripheral sites of the zinc endopeptidase of botulinum neurotoxin serotype A

pp 3583–3591

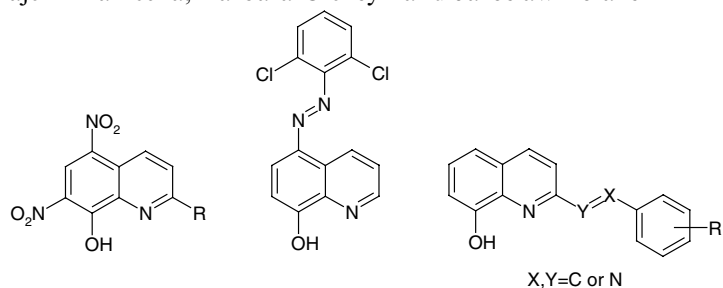
Isidro Merino, Jason D. Thompson, Charles B. Millard, James J. Schmidt\* and Yuan-Ping Pang\*



### Antifungal properties of new series of quinoline derivatives

pp 3592–3598

Robert Musiol, Josef Jampilek, Vladimir Buchta, Luis Silva, Halina Niedbala, Barbara Podeszwa, Anna Palka, Katarzyna Majerz-Maniecka, Barbara Oleksyn and Jaroslaw Polanski\*

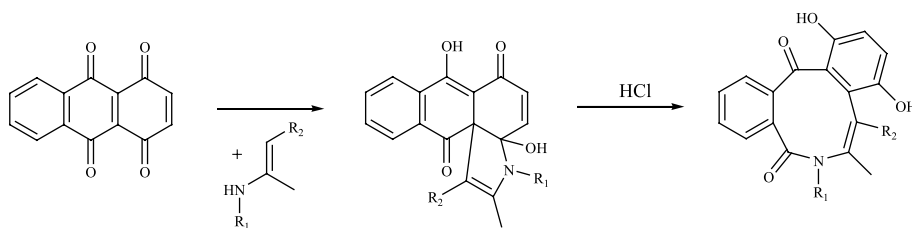


The synthesis and antifungal activity for a new series of quinoline derivatives are reported.

### 1,4,9,10-Anthradiquinone as precursor for antitumor compounds

pp 3599–3614

Lothar Werner Schenck, Krystina Kuna, Walter Frank, Antje Albert, Christian Asche and Uwe Kucklaender\*



## OTHER CONTENTS

Summary of instructions to authors

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\*Corresponding author

①\* 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].



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