

Contents

Publisher's Announcement

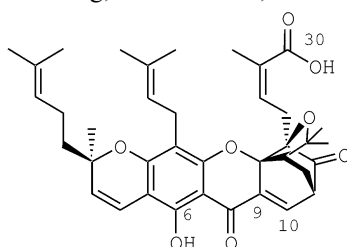
p 307

ARTICLES

Discovery, characterization and SAR of gambogic acid as a potent apoptosis inducer by a HTS assay

pp 309–317

Han-Zhong Zhang, Shailaja Kasibhatla, Yan Wang, John Herich, John Guastella, Ben Tseng, John Drewe and Sui Xiong Cai*

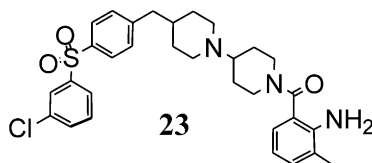


The discovery of gambogic acid as a potent inducer of apoptosis using a cell- and caspase-based HTS assay, as well as the characterization and SAR studies of gambogic acid as inducer of apoptosis, are reported.

Muscarinic M2 antagonists: anthranilamide derivatives with exceptional selectivity and in vivo activity

pp 319–326

John W. Clader,* William Billard, Herbert Binch, III, Lian-Yong Chen, Gordon Crosby, Jr., Ruth A. Duffy, Jennifer Ford, Joseph A. Kozlowski, Jean E. Lachowicz, Shengjian Li, Charles Liu, Stuart W. McCombie, Susan Vice, Gwei Zhou and William J. Greenlee

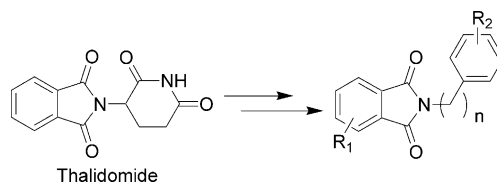


Anthranilamide analogues such as **23** are potent and highly selective muscarinic M2 antagonists that also show good oral bioavailability and in vivo activity.

Thalidomide analogues demonstrate dual inhibition of both angiogenesis and prostate cancer

pp 327–336

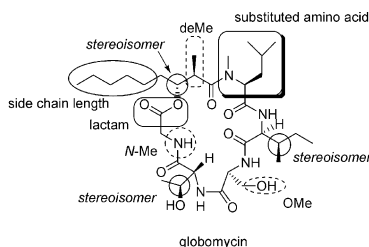
Scott M. Capitosti, Todd P. Hansen and Milton L. Brown*



Structure–activity relationships of globomycin analogues as antibiotics

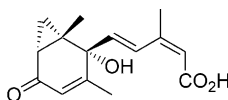
pp 337–361

Toshihiro Kiho, Mizuka Nakayama, Kayo Yasuda, Shunichi Miyakoshi, Masatoshi Inukai and Hiroshi Kogen*

**Metabolism of 5'α,8'-cycloabscisic acid, a highly potent and long-lasting abscisic acid analogue, in radish seedlings**

pp 363–370

Yasushi Todoroki,* Masao Sawada, Miyuki Matsumoto, Shigeko Tsukada, Kotomi Ueno, Masatoshi Isaka, Mariko Owaki and Nobuhiro Hirai

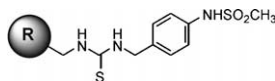


The highly potent and long-lasting activity of 5'α,8'-cycloabscisic acid is caused by resistance to abscisic acid 8'-hydroxylase, and it is partially metabolized to the glucose conjugate.

N-[4-(Methylsulfonylamino)benzyl]thiourea analogues as vanilloid receptor antagonists: analysis of structure–activity relationships for the 'C-Region'

pp 371–385

Jeewoo Lee,* Sang-Uk Kang, Ju-Ok Lim, Hyun-Kyung Choi, Mi-kyung Jin, Attila Toth, Larry V. Pearce, Richard Tran, Yun Wang, Tamas Szabo and Peter M. Blumberg

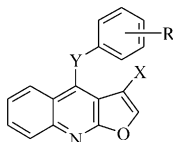


Analysis of structure–activity relationships in the 'C-Region' of N-[4-(methylsulfonylamino)benzyl]thiourea analogues is described as vanilloid receptor antagonists.

Synthesis and anti-inflammatory evaluation of 4-anilinofuro[2,3-b]quinoline and 4-phenoxyfuro[2,3-b]quinoline derivatives. Part 3

pp 387–392

Yeh-Long Chen,* I-Li Chen, Chih-Ming Lu, Cherng-Chyi Tzeng, Lo-Ti Tsao and Jih-Pyang Wang

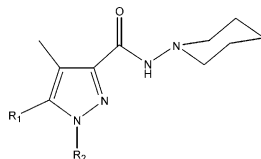


X = H, Cl
Y = O, NH
R = CHO, COMe, C(=NOH)Me,
C(=NOMe)Me, CH=CHCOMe,
CH₂CH₂COMe, CH₂CH₂CH(OH)Me

Synthesis, biological evaluation, and structural studies on N1 and C5 substituted cycloalkyl analogues of the pyrazole class of CB1 and CB2 ligands

pp 393–404

Mathangi Krishnamurthy, Wei Li and Bob M. Moore, II*

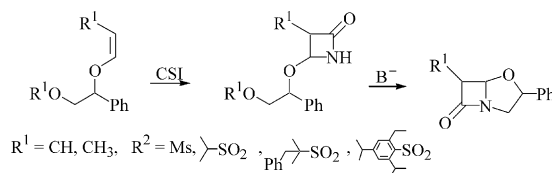


R_1 = 4-chlorophenyl, R_2 = cyclopentyl
 R_1 = 4-chlorophenyl, R_2 = cyclohexyl
 R_1 = 4-chlorophenyl, R_2 = cycloheptyl
 R_1 = 4-chlorophenyl, R_2 = 3-methylcyclohexyl
 R_1 = 4-chlorophenyl, R_2 = 4-methylcyclohexyl
 R_1 = 4-chlorophenyl, R_2 = 4-methylphenyl
 R_1 = cyclohexyl, R_2 = 4-chlorophenyl
 R_1 = cycloheptyl, R_2 = 4-chlorophenyl
 R_1 = cyclohexyl, R_2 = cyclohexyl

Synthesis, biological, and chiroptical activity of 3-phenyl-clavams

pp 405–416

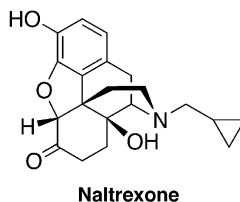
Maciej Cierpucha, Jolanta Solecka, Jadwiga Frelek, Patrycja Szczukiewicz and Marek Chmielewski*



Syntheses and receptor-binding studies of derivatives of the opioid antagonist naltrexone

pp 417–421

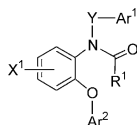
Koji Uwai, Hiroko Uchiyama, Shinobu Sakurada, Chizuko Kabuto and Mitsuhiro Takeshita*



Design, synthesis and structure–affinity relationships of aryloxyanilide derivatives as novel peripheral benzodiazepine receptor ligands

pp 423–438

Taketoshi Okubo, Ryoko Yoshikawa, Shigeyuki Chaki, Shigeru Okuyama and Atsuro Nakazato*



The design, synthesis and structure–affinity relationships of aryloxyanilide derivatives as novel peripheral benzodiazepine receptor ligands are described.

The alkaloids and other constituents from the root and stem of *Aristolochia elegans*

pp 439–446

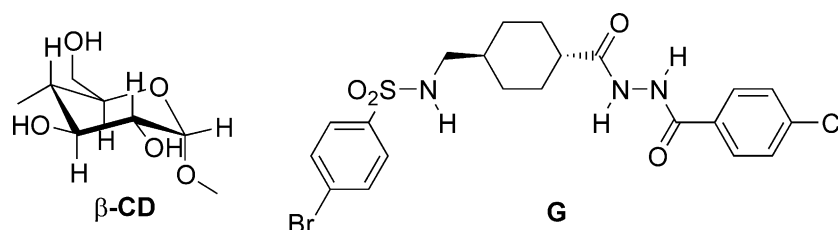
Li-Shian Shi, Ping-Chung Kuo, Yao-Lung Tsai, Amooru Gangaiah Damu and Tian-Shung Wu*

Two new aristolactams, aristolactam E (**1**) and aristolactam-AIIIa-6-*O*- β -D-glucoside (**2**), three novel benzoyl benzyltetrahydroisoquinoline ether *N*-oxide alkaloids, aristoquinoline A (**3**), aristoquinoline B (**4**), and aristoquinoline C (**5**), and a new biphenyl ether, aristogin F (**6**), together with sixty-two known compounds have been isolated from the root and stem of *Aristolochia elegans* Mast. Occurrence of the isoquinolones, biphenyl ethers, and benzoyl benzyltetrahydroisoquinoline ether alkaloids in the same plant indicated the definite possibility of these metabolites as biotransformation intermediates of bisbenzyltetrahydroisoquinoline alkaloids.

Combining NMR and molecular modelling in a drug delivery context: investigation of the multi-mode inclusion of a new NPY-5 antagonist bromobenzenesulfonamide into β -cyclodextrin

pp 447–458

Gloria Uccello-Barretta,* Federica Balzano, Giuseppe Sicoli, Carmen Friglola, Ignacio Aldana, Antonio Monge, Donatella Paolino and Salvatore Guccione*

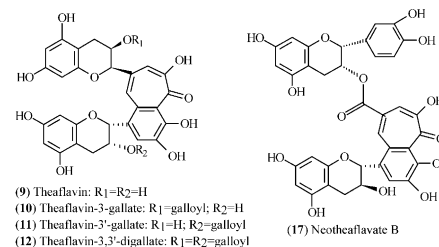


Enzymatic synthesis of tea theaflavin derivatives and their anti-inflammatory and cytotoxic activities

pp 459–467

Shengmin Sang,* Joshua D. Lambert, Shiyong Tian, Jungil Hong, Zhe Hou, Jae-He Ryu, Ruth E. Stark, Robert T. Rosen, Mou-Tuan Huang, Chung S. Yang and Chi-Tang Ho

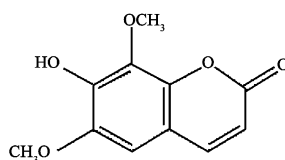
Derivatives based on a benzotropolone skeleton (**9–26**) have been prepared by the enzymatic coupling (horseradish peroxidase/ H_2O_2) of selected pairs of compounds (**1–8**), one with a *vic*-trihydroxyphenyl moiety, and the other with an *ortho*-dihydroxyphenyl structure. Some of these compounds have been found to inhibit TPA-induced mice ear edema, nitric oxide (NO) synthesis, and arachidonic acid release by LPS-stimulated RAW 264.7 cells. Their cytotoxic activities against KYSE 150 and 510 human esophageal squamous cell carcinoma and HT 29 human colon cancer cells were also evaluated.



Interaction of isofraxidin with human serum albumin

pp 469–474

Jiaqin Liu, Jianniao Tian, Xuan Tian, Zhide Hu* and Xingguo Chen

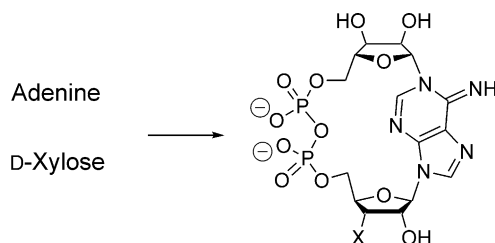


We studied firstly the binding of isofraxidin to human serum albumin (HSA) under physiological conditions utilizing fluorescence method in combination with FT-IR and CD technique.

***Aplysia californica* mediated cyclisation of novel 3'-modified NAD⁺ analogues:
a role for hydrogen bonding in the recognition of cyclic adenosine 5'-diphosphate ribose**

pp 475–487

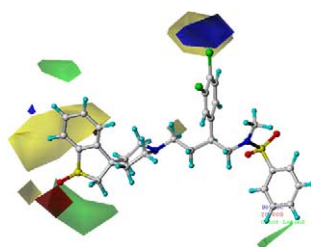
Christopher J. W. Mort, Marie E. Migaud, Antony Galione and Barry V. L. Potter*



Three-dimensional quantitative structure–activity relationship analyses of piperidine-based CCR5 receptor antagonists

pp 489–499

Minghu Song, Curt M. Breneman* and N. Sukumar

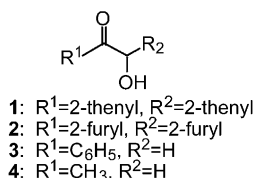


3D-QSAR models have been built for a series of piperidine-based CCR5 antagonists using CoMFA and CoMSIA approaches. The derived 3D-QSAR models showed predictive capabilities and a high level of internal consistency. The resulting contour maps can be used to identify structural features relevant to binding affinity, and can aid in the future development of potential anti-HIV agents.

α -Hydroxyketones as inhibitors of urease

pp 501–505

Toru Tanaka, Masami Kawase* and Satoru Tani



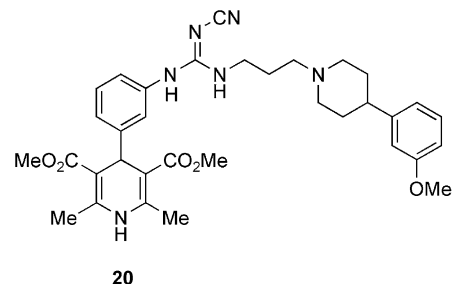
A variety of hydroxyketones and diketones were evaluated for their effect on the jack bean urease. 2,2-Thenoin (1), furoin (2), 2-hydroxy-1-phenylethanone (3) and acetol (4) showed potent inhibitory activity against the enzyme, comparable with hydroxyurea. However, the corresponding-diketones exhibited little or no ability to inhibit the urease.

Dihydropyridine neuropeptide Y Y₁ receptor antagonists 2: bioisosteric urea replacements

pp 507–521

Graham S. Poindexter,* Marc A. Bruce, J. Guy Breitenbucher, Mendi A. Higgins, S.-Y. Sit, Jeffrey L. Romine, Scott W. Martin, Sally A. Ward, Rachel T. McGovern, Wendy Clarke, John Russell and Ildiko Antal-Zimanyi

Structure–activity studies around the urea linkage in BMS-193885 identified the cyanoguanidine moiety (as represented by **20**) as an effective urea replacement in a series of dihydropyridine NPY Y₁ receptor antagonists.



OTHER CONTENTS

Contributors to this issue
Instructions to contributors

I
III–VI

*Corresponding author

COVER

2004: Overlaps of the eight known aldolase alpha-beta barrels in 2-Deoxyribose-5-phosphate aldolase (DERA). Ribbon model for DERA is shown in green, with key Lys residues capable of Schiff base formation highlighted in stick figure. Reactive Lys167 is shown in yellow. DeSantis, G.; Liu, J.; Clark, D. P.; Heine, A.; Wilson, I. A.; and Wong, C.-H. *Bioorganic & Medical Chemistry* **2003**, *11*, 43–52.



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CONTENTS
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ISSN 0968-0896