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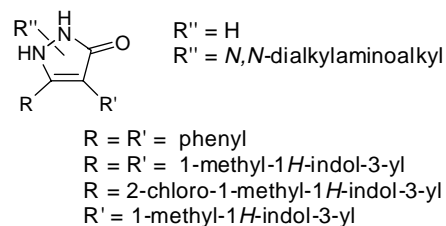
ARTICLES

Synthesis and biological activity of *N,N*-dialkylaminoalkyl-substituted bisindolyl and diphenyl pyrazolone derivatives

pp 9–16

Miguel F. Braña,* Ana Gradillas,* Angel G. Ovalles, Berta López, Nuria Acero, Francisco Llinares and Dolores Muñoz Mingarro

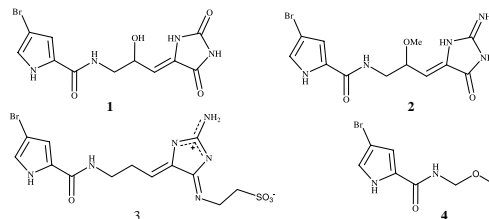
The synthesis of new bisindolyl and diphenylpyrazolone derivatives are reported. Many showed inhibition against TPA induced TNF- α production in HL-60 cells. Several of these analogues also showed apoptotic activity.



Novel bioactive bromopyrrole alkaloids from the Mediterranean sponge *Axinella verrucosa*

pp 17–24

Anna Aiello, Monica D'Esposito, Ernesto Fattorusso,* Marialuisa Menna, Werner E. G. Müller, Sanja Perović-Ottstadt and Heinz C. Schröder



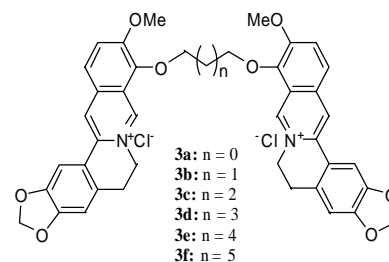
Four novel bromopyrrole alkaloids (compounds **1–4**) have been isolated from the sponge *Axinella verrucosa* and their structures established through spectroscopic methods. Compounds **1–4** exhibited a neuroprotective effect in vitro against the agonists serotonin and glutamate.

Synthesis, DNA-binding affinities, and binding mode of berberine dimers

pp 25–32

Yong Qin, Ji-Yan Pang, Wen-Hua Chen,* Zongwei Cai and Zhi-Hong Jiang*

Berberine dimers were synthesized in moderate to high yield and showed remarkably enhanced affinities toward double-stranded DNA. The binding mode was determined to be intercalation based on UV titration and ethidium bromide displacement experiments.

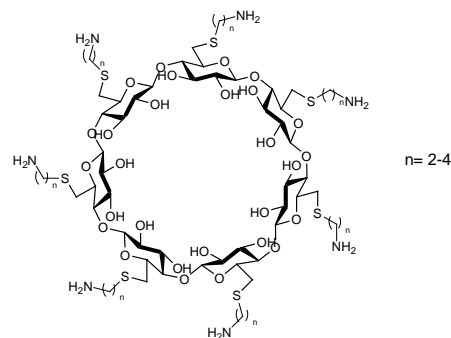


β -Cyclodextrin derivatives that inhibit anthrax lethal toxin

pp 33–40

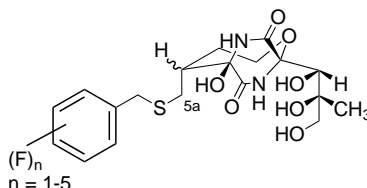
Vladimir A. Karginov,* Adiamseged Yohannes, Tanisha M. Robinson,
Nour Eddine Fahmi, Kenneth Alibek and Sidney M. Hecht

Positively charged β -cyclodextrin derivatives designed to block the pore formed by protective antigen inhibit the action of anthrax toxin.

**Fluorine-substituted dihydrobicyclomycins: Synthesis and biochemical and biological properties**

pp 41–61

Boon-Saeng Park, William Widger and Harold Kohn*



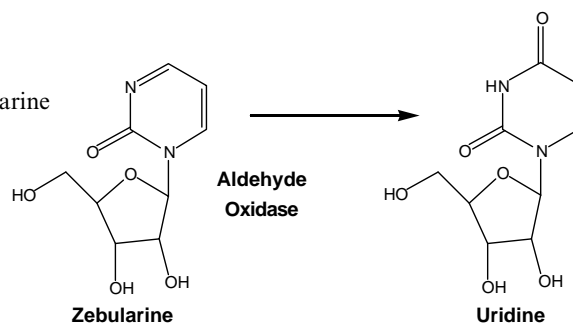
The correlation of the effect of fluorine substitution of 5a-(benzylsulfanyl)-dihydrobicyclomycin with *Escherichia coli* rho inhibitory activity permits the rational prediction of potent inhibitors.

Zebularine metabolism by aldehyde oxidase in hepatic cytosol from humans, monkeys, dogs, rats, and mice: Influence of sex and inhibitors

pp 62–66

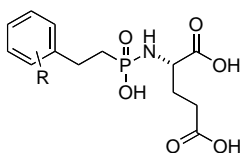
Raymond W. Klecker,* Richard L. Cysyk and Jerry M. Collins

Activity and inhibition of aldehyde oxidase on the metabolism of zebularine varied between species. Inhibitors: raloxifene and 5-benzylacetyluridine.

**Optimizing phenylethylphosphonamidates for the inhibition of prostate-specific membrane antigen**

pp 67–76

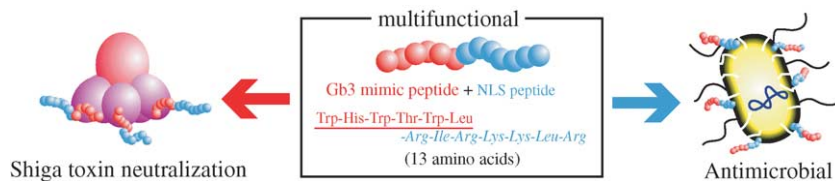
David W. G. Wone, Jennifer A. Rowley, Albert W. Garofalo and Clifford E. Berkman*



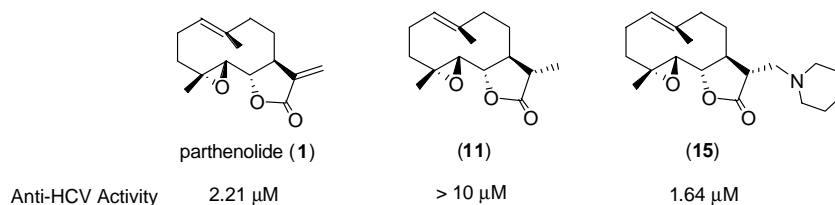
The Topliss batchwise approach successfully led to an *N*-2-phenylethylphosphonyl derivative of glutamic acid with enhanced inhibitory potency against PSMA.

Design of multifunctional peptides expressing both antimicrobial activity and shiga toxin neutralization activity

pp 77–82

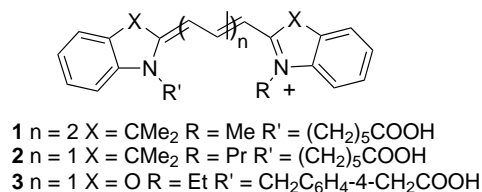
Yoshinao Yamada, Yoshiko Miura, Akio Sakaki,
Tetsuhiko Yoshida and Kazukiyo Kobayashi***Synthesis and anti-viral activity of a series of sesquiterpene lactones and analogues in the subgenomic HCV replicon system**

pp 83–91

Der-Ren Hwang, Yu-Shan Wu, Chun-Wei Chang, Tzu-Wen Lien, Wei-Cheng Chen,
Uan-Kang Tan, John T. A. Hsu* and Hsing-Pang Hsieh***Practical syntheses of dyes for difference gel electrophoresis**

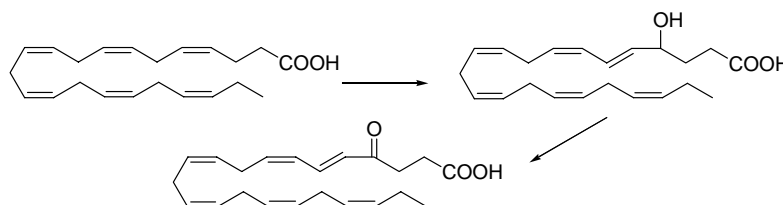
pp 92–97

Michael E. Jung* and Wan-Joong Kim

**Synthesis of docosahexaenoic acid derivatives designed as novel PPAR γ agonists and antidiabetic agents**

pp 98–108

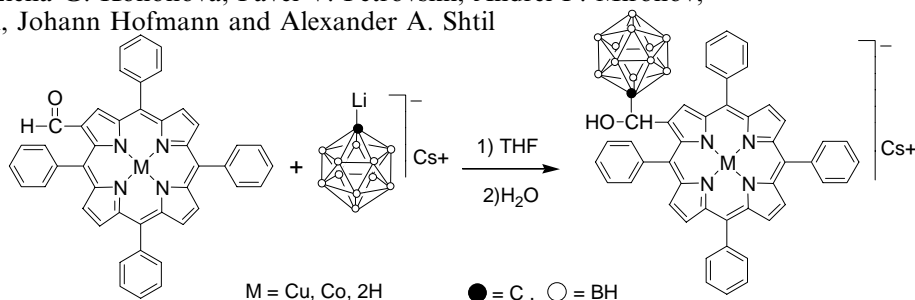
Toshimasa Itoh, Itsuki Murota, Kazuyoshi Yoshikai, Sachiko Yamada and Keiko Yamamoto*



Novel boronated derivatives of 5,10,15,20-tetraphenylporphyrin: Synthesis and toxicity for drug-resistant tumor cells

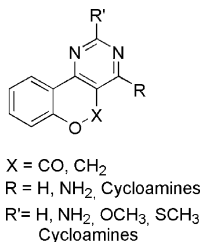
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Valentina A. Ol'shevskaya,* Andrei V. Zaitsev, Valentina N. Luzgina, Tatyana T. Kondratieva, Oleg G. Ivanov, Elena G. Kononova, Pavel V. Petrovskii, Andrei F. Mironov, Valery N. Kalinin, Johann Hofmann and Alexander A. Shtil


Synthesis, antiplatelet and antithrombotic activities of new 2-substituted benzopyrano[4,3-*d*]pyrimidin-4-cycloamines and 4-amino/cycloamino-benzopyrano[4,3-*d*]pyrimidin-5-ones

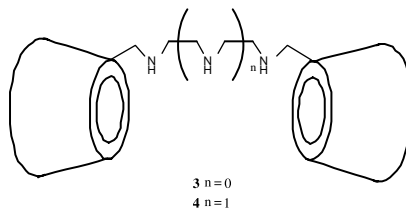
pp 121–130

Olga Bruno,* Chiara Brullo, Silvia Schenone, Francesco Bondavalli, Angelo Ranise, Massimiliano Tognolini, Mariannina Impicciatore, Vigilio Ballabeni and Elisabetta Barocelli


Interactions of some modified mono- and bis-β-cyclodextrins with bovine serum albumin

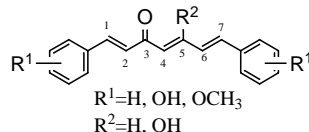
pp 131–137

Hui Gao, Yi-Nong Wang, Yun-Ge Fan and Jian-Biao Ma*


Inhibitors from the rhizomes of *Alpinia officinarum* on production of nitric oxide in lipopolysaccharide-activated macrophages and the structural requirements of diarylheptanoids for the activity

pp 138–142

Hisashi Matsuda, Shin Ando, Tomoko Kato, Toshio Morikawa and Masayuki Yoshikawa*

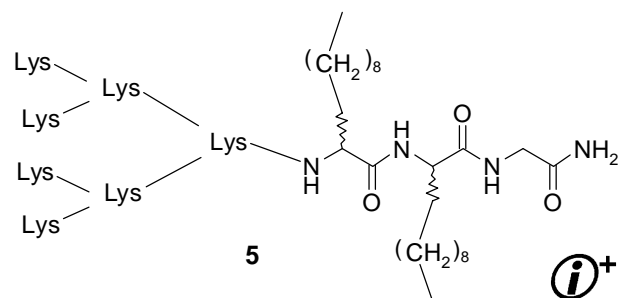


The 80% aqueous acetone extract from the rhizomes of *Alpinia officinarum*, a Chinese medicinal herb, were found to inhibit nitric oxide (NO) production in lipopolysaccharide (LPS)-activated mouse peritoneal macrophages. Through bioassay-guided separation, two diarylheptanoids [7-(4'-hydroxy-3'-methoxyphenyl)-1-phenylhept-4-en-3-one and 3,5-dihydroxy-1,7-diphenylheptane] and a flavonol constituent (galangin) substantially inhibited LPS-induced NO production with IC₅₀ values of 33–62 μM. To clarify structure–activity relationships of diarylheptanoids, related diarylheptanoids from *Curcuma zedoaria* were examined. Results indicate that the double bond or enone moiety at the 1–7 positions is important for the activity.

Polycationic lipophilic-core dendrons as penetration enhancers for the oral administration of low molecular weight heparin

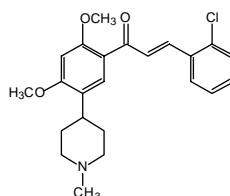
Patricia Y. Hayes, Benjamin P. Ross, Bradley G. Thomas and Istvan Toth*

Polycationic lipophilic-core dendrons were tested in rats as penetration enhancers for the oral delivery of low molecular weight heparin (LMWH). A significant anti-factor Xa activity was obtained when LMWH was coadministered with dendron **5**.



Antiproliferative properties of piperidinylchalcones

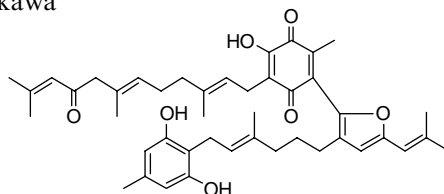
Xiaoling Liu and Mei-Lin Go*



N-Methylpiperidinylchalcones were investigated for antiproliferative activity against human tumour cell lines. The role of the piperidinyl ring in activity was explored in structure–activity relationship investigations.

Grifolin derivatives from *Albatrellus caeruleoporus*, new inhibitors of nitric oxide production in RAW 264.7 cells

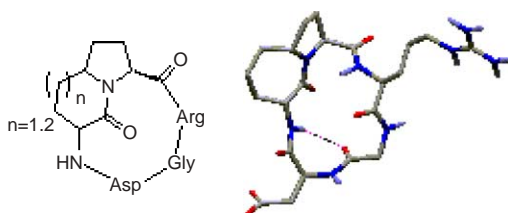
Dang Ngoc Quang, Toshihiro Hashimoto, Yuuki Arakawa, Chie Kohchi, Takashi Nishizawa, Gen-Ichiro Soma* and Yoshinori Asakawa*



Two new farnesyl phenols named grifolinones A and B, together with known grifolin and neogrifolin which exhibited the inhibitory activity of nitric oxide production stimulated by lipopolysaccharide in RAW 264.7 cells, were isolated from the fungus *Albatrellus caeruleoporus*.

Targeting integrins: Insights into structure and activity of cyclic RGD pentapeptide mimics containing azabicycloalkane amino acids

Laura Belvisi, Anna Bernardi, Matteo Colombo, Leonardo Manzoni, Donatella Potenza, Carlo Scolastico,* Giuseppe Giannini, Marcella Marcellini, Teresa Riccioni, Massimo Castorina, Pietro LoGiudice and Claudio Pisano*

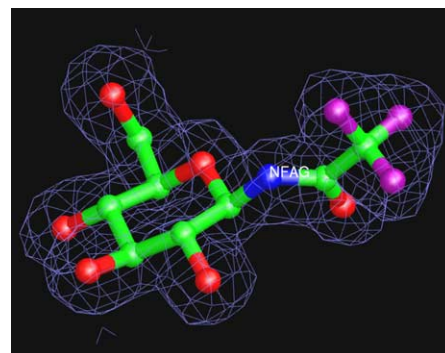


Crystallographic studies on two bioisosteric analogues, *N*-acetyl- β -D-glucopyranosylamine and *N*-trifluoroacetyl- β -D-glucopyranosylamine, potent inhibitors of muscle glycogen phosphorylase

pp 181–189

Eleni Anagnostou, Magda N. Kosmopoulou, Evangelia D. Chrysina, Demetres D. Leonidas, Theodoros Hadjiloi, Costantinos Tiraidis, Spyros E. Zographos, Zoltán Györgydeák, László Somsák, Tibor Docsa, Pál Gergely, Fragiskos N. Kolisis and Nikos G. Oikonomakos*

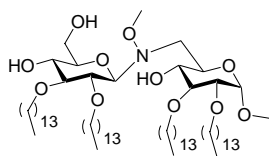
Two bioisosteric analogues *N*-acetyl- β -D-glucopyranosylamine (NAG) and *N*-trifluoroacetyl- β -D-glucopyranosylamine (NFAG), were tested for inhibition of and binding to glycogen phosphorylase b. The structural basis of inhibition is presented by analyzing the crystal structures of the enzyme in complex with both inhibitors at 1.9 and 1.8 Å resolution, respectively.



Synthesis and biological evaluation of novel lipid A antagonists

pp 190–199

Francesco Peri,* Chiara Marinzi, Marek Barath, Francesca Granucci, Matteo Urbano and Francesco Nicotra



A novel lipid A mimetic with a methoxyamino glycosidic linkage presents antagonist activity against bacterial LPS.

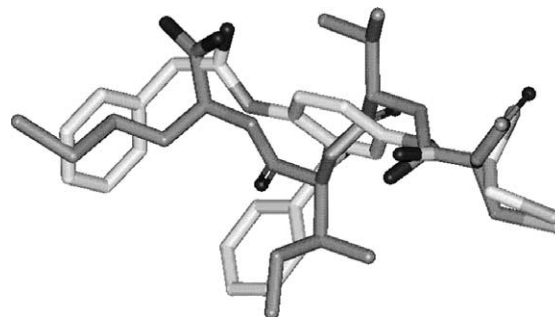


Modeling of farnesyltransferase inhibition by some thiol and non-thiol peptidomimetic inhibitors using genetic neural networks and RDF approaches

pp 200–213

Maykel Pérez González, Julio Caballero, Alain Tundidor-Camba, Aliuska Morales Helguera and Michael Fernández*

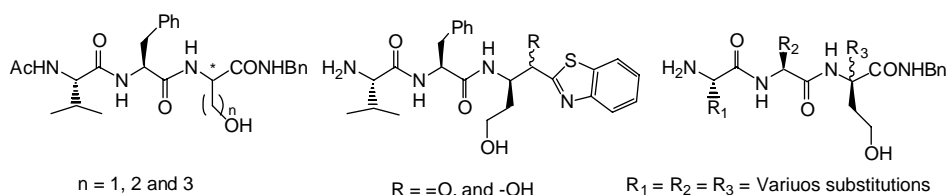
Alignment between a peptidomimetic farnesyltransferase inhibitor and the enzyme-bound conformation of *N*-acetyl-Cys-Val-Ile-selenoMetOH (PDB 1QBQ)



Engineering D-amino acid containing novel protease inhibitors using catalytic site architecture

pp 214–236

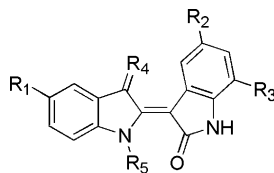
Subhash C. Annedi, Farooq Biabani, Ewa Poduch, Baskar M. Mannargudi, Kanchana Majumder, Lianhu Wei, Reza Khayat, Liang Tong and Lakshmi P. Kotra*



Synthesis and structure–activity relationships of novel indirubin derivatives as potent anti-proliferative agents with CDK2 inhibitory activities

pp 237–246

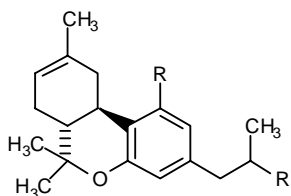
Myoung Ju Moon, Sang Kook Lee, Jong-Won Lee, Woo Keun Song, Si Wouk Kim, Jae Il Kim, Chunghee Cho, Soo Jeong Choi and Yong-Chul Kim*



Enantioselective synthesis of 1-methoxy- and 1-deoxy-2'-methyl- Δ^8 -tetrahydrocannabinols: New selective ligands for the CB₂ receptor

pp 247–262

John W. Huffman,* Simon M. Bushell, Sudhir N. Joshi, Jenny L. Wiley and Billy R. Martin

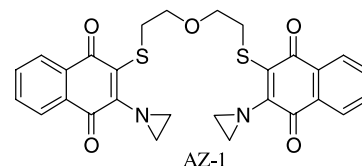


The enantioselective synthesis and pharmacology of two series of (2'*R*)- and (2'*S*)-methyl- Δ^8 -THC ligands are described. R = H, OCH₃; R' = methyl to *n*-pentyl.

The lethal effect of bis-type azridinylnaphthoquinone derivative on oral cancer cells (OEC-M1) associated with anti-apoptotic protein bcl-2

pp 263–272

Yi-Chen Peng, Hsien-Shou Kuo, Hsin-Da Tsai, Yu-Ping Yang and Yuh-Ling Lin*

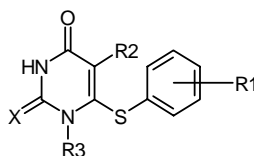


Bis-type bioreductive compound AZ-1 was synthesized to study the mechanism of death effect in oral cancer cell (OEC-M1). The AZ-1 compound induced two of oral cancer cells, with LC₅₀ = 0.72 μ M in OEC-M1 cell and with LC₅₀ = 1.02 μ M in KB cell, and with less cytotoxicity to normal fibroblast cell (SF with LC₅₀ = 5.6 μ M) which was still with over 90% of survival rate as high as 2 μ M of AZ-1. There is significant difference between oral cancer cells (OEC-M1 and KB cells) and normal fibroblasts. The AZ-1 compound induced the cell death of OEC-M1 that was mediated through the G2/M phase arrest of cell cycle first at 24 h and into apoptosis pathway at 48 h which might be associated with p53 protein and bcl-2 protein expression.

A 4D-QSAR study on anti-HIV HEPT analogues

pp 273–279

Andrzej Bak and Jaroslaw Polanski*



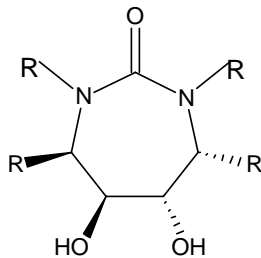
4D QSAR method has been used for the investigation of the HEPT series.



Modeling of activity of cyclic urea HIV-1 protease inhibitors using regularized-artificial neural networks

pp 280–294

Michael Fernández and Julio Caballero*

**OTHER CONTENTS**

Summary of instructions to authors

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*Corresponding author

i+ Supplementary data available via ScienceDirect

COVER

Schematic diagram of the target enzyme showing the position of the catalytic site with bound inhibitor *N*-trifluoroacetyl- β -D-glucopyranosylamine, in ball-and-stick representation. Close-up: Details of the interactions of the inhibitor, well defined in the $2F_o - F_c$ electron density (blue) by X-ray crystallography at 1.8 Å resolution, with protein residues. E. Anagnostou, M. N. Kosmopoulou, E. D. Chrysina, D. D. Leonidas, T. Hadjiloi, C. Tiraidis, S. E. Zographos, Z. Gyorgydeak, L. Somsak, T. Docsa, P. Gergely, F. N. Kolisis and N. G. Oikonomakos. © 2005 Elsevier Ltd.



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