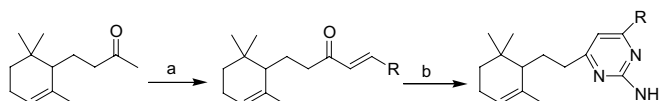


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2,4,6-Trisubstituted pyrimidine derivatives as pregnancy interceptive agents pp 1893–1899

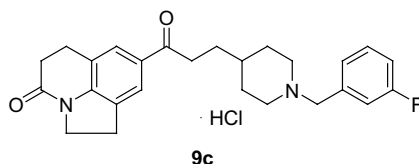
Anu Agarwal, Brijesh Kumar, Purshottam K. Mehrotra and Prem M. S. Chauhan*



A series of 2,4,6-trisubstituted-pyrimidine derivatives were synthesized and evaluated for their in vivo pregnancy interceptive activity.

Novel acetylcholinesterase inhibitor as increasing agent on rhythmic bladder contractions: SAR of 8-{3-[1-(3-fluorobenzyl)piperidin-4-yl]propanoyl}-1,2,5,6-tetrahydro-4H-pyrrolo[3,2,1-ij]-quinolin-4-one (TAK-802) and related compounds pp 1901–1911

Yuji Ishichi, Mitsuru Sasaki, Masaki Setoh, Tetsuya Tsukamoto, Seiji Miwatashi, Hiroshi Nagabukuro, Satoshi Okanishi, Shigemitsu Imai, Reiko Saikawa, Takayuki Doi and Yuji Ishihara*

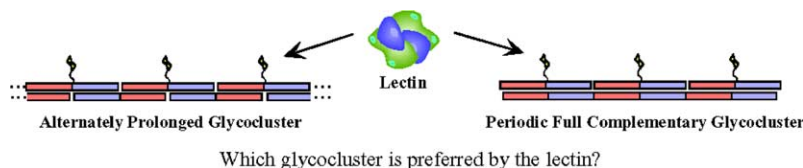


*h*AChE inhibition IC_{50} = 1.3 nM

The syntheses and structure–activity relationships of TAK-802 and related compounds are described.

Cooperative lectin recognition of periodical glycoclusters along DNA duplexes: alternate hybridization and full hybridization pp 1913–1922

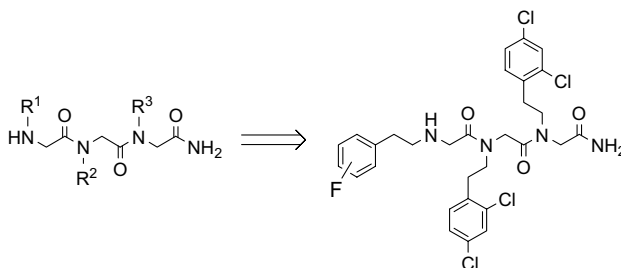
Yoshinao Yamada, Kazunori Matsuura and Kazukiyo Kobayashi*



Design and synthesis of an optimized positional scanning library of peptoids: identification of novel multidrug resistance reversal agents

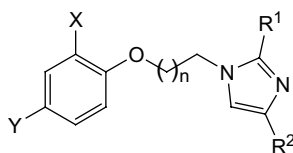
pp 1923–1929

Isabel Masip, Nuria Cortés, Maria-José Abad, Marisa Guardiola, Enrique Pérez-Payá, José Ferragut, Antonio Ferrer-Montiel and Angel Messeguer*


Design, synthesis, antibacterial and QSAR studies of benzimidazole and imidazole chloroaryloxyalkyl derivatives

pp 1931–1938

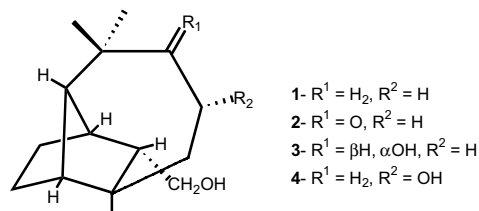
A. Khalafi-Nezhad,* M. N. Soltani Rad, H. Mohabatkar, Z. Asrari and B. Hemmateenejad


Microbial transformation of (–)-isolongifolol and butyrylcholinesterase inhibitory activity of transformed products

pp 1939–1944

M. Iqbal Choudhary,* Syed Ghulam Musharraf, Sarfraz Ahmad Nawaz, Shazia Anjum, Masood Parvez, Hoong-Kun Fun and Atta-ur-Rahman

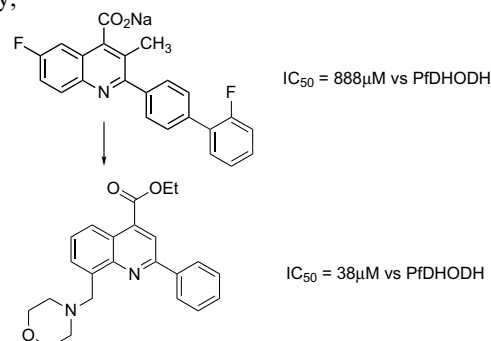
This paper describes the microbial transformation of (–)-isolongifolol (**1**) and butyrylcholinesterase inhibitory activity of the transformed products **2–4**. The structures of transformed products were determined by spectroscopic and single crystal X-ray diffraction techniques.


Synthesis of brequinar analogue inhibitors of malaria parasite dihydroorotate dehydrogenase

pp 1945–1967

Andrew N. Boa,* Shane P. Canavan, Paul R. Hirst, Christopher Ramsey, Andrew M. W. Stead and Glenn A. McConkey*

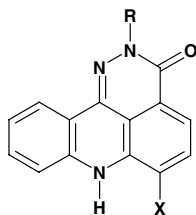
Starting from the human dihydroorotate dehydrogenase (DHODH) inhibitor brequinar, inhibitors of DHODH from *Plasmodium falciparum* have been discovered.



2,7-Dihydro-3H-pyridazino[5,4,3-*kl*]acridin-3-one derivatives, novel type of cytotoxic agents active on multidrug-resistant cell lines. Synthesis and biological evaluation

pp 1969–1975

Barbara Stefańska, Maria M. Bontemps-Gracz, Ippolito Antonini, Sante Martelli, Małgorzata Arciemiuk, Agnieszka Piwkowska, Dorota Rogacka and Edward Borowski*

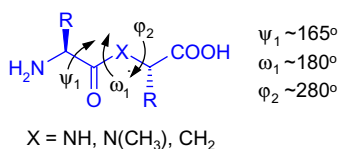


A series of pyridazinoacridin-3-one derivatives were synthesized and evaluated for their cytotoxic activity toward murine and human leukemia sensitive and resistant (MDR and MRP) cell lines.

Conformational restrictions in ligand binding to the human intestinal di-/tripeptide transporter: implications for design of hPEPT1 targeted prodrugs

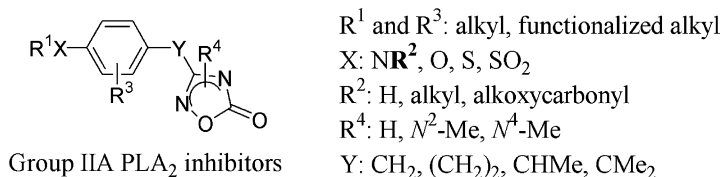
pp 1977–1988

Jon Våbenø, Carsten Uhd Nielsen, Bente Steffansen, Tore Lejon, Ingebrigt Sylte, Flemming Steen Jørgensen and Kristina Luthman*

**Inhibition of secretory phospholipase A₂. 2-Synthesis and structure–activity relationship studies of 4,5-dihydro-3-(4-tetradecyloxybenzyl)-1,2,4-oxadiazol-5-one (PMS1062) derivatives specific for group II enzyme**

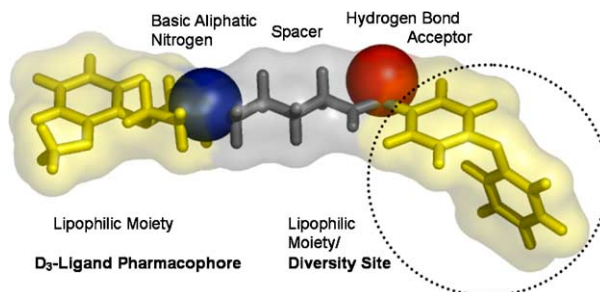
pp 1989–2007

Chang-Zhi Dong, Azali Ahamada-Himidi, Stéphanie Plocki, Darina Aoun, Mohamed Touaibia, Nadia Meddad-Bel Habich, Jack Huet, Catherine Redeuilh, Jean-Edouard Ombetta, Jean-Jacques Godfroid, France Massicot and Françoise Heymans*

**Parallel synthesis and dopamine D₃/D₂ receptor screening of novel {4-[4-(2-methoxyphenyl)piperazin-1-yl]butyl}carboxamides**

pp 2009–2014

Philipp Heidler, Vida Zohrabi-Kalantari, Thierry Calmels, Marc Capet, Isabelle Berrebi-Bertrand, Jean-Charles Schwartz, Holger Stark and Andreas Link*

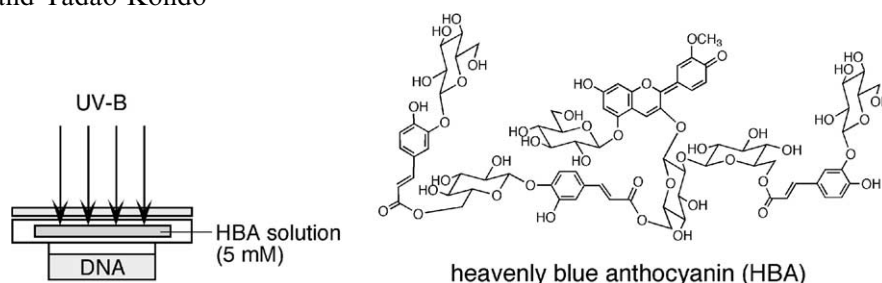


UV-B protective effect of a polyacylated anthocyanin, HBA, in flower petals of the blue morning glory, *Ipomoea tricolor* cv. Heavenly Blue

pp 2015–2020

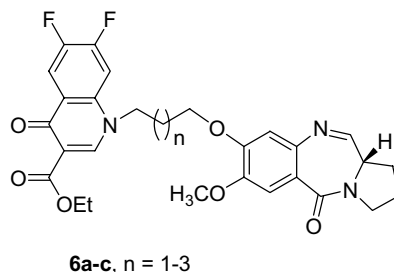
Mihoko Mori, Kumi Yoshida,* Yasuhito Ishigaki, Tsukasa Matsunaga, Osamu Nikaido, Kiyoshi Kameda and Tadao Kondo

HBA, a polyacylated anthocyanin of blue morning glory completely prevents UV-B induced DNA damage at a physiological concentration (5 mM).


Synthesis and biological activity of fluoroquinolone-pyrrolo[2,1-c][1,4]benzodiazepine conjugates

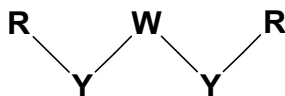
pp 2021–2029

Ahmed Kamal,* V. Devaiah, K. Laxma Reddy and M. Shiva Kumar


Synthesis and biological evaluation of new symmetrical derivatives as cytotoxic agents and apoptosis inducers

pp 2031–2044

Carmen Sanmartín, Mikel Echeverría, Beatriz Mendivil, Lucía Cordeu, Elena Cubedo, Jesús García-Foncillas, María Font and Juan Antonio Palop*

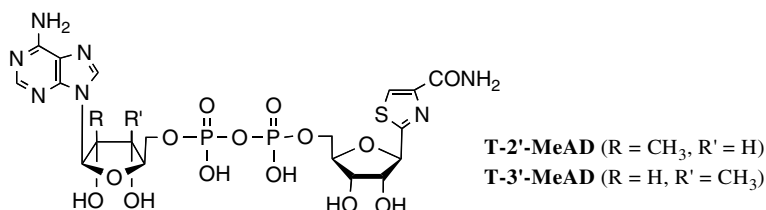


The synthesis and pharmacology of new symmetrical derivatives ($W = (CH_2)_n$; cyclohexane; piperazine; pyridopyrimidine; diphenylmethane. $Y =$ ether; amine; amide; carbamate; urea. $R =$ alkyl; aryl; heteroaryl; alkylaryl) is described. Compounds showing cytotoxic activity were subjected to an apoptosis assay. Some of the synthesized compounds provoked an increase in the level of caspase-3.

Synthesis, conformational analysis, and biological activity of new analogues of thiazole-4-carboxamide adenine dinucleotide (TAD) as IMP dehydrogenase inhibitors

pp 2045–2053

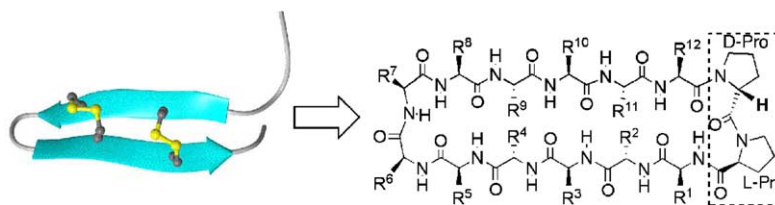
Palmarisa Franchetti, Loredana Cappellacci, Michela Pasqualini, Riccardo Petrelli, Vetrichelvan Jayaprakasan, Hiremagalur N. Jayaram, Donald B. Boyd, Manojkumar D. Jain and Mario Grifantini*



Properties and structure–activity studies of cyclic β -hairpin peptidomimetics based on the cationic antimicrobial peptide protegrin I

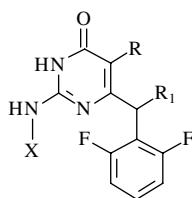
pp 2055–2064

John A. Robinson,* Sasalu C. Shankaramma, Peter Jetter, Ursula Kienzl,
Reto A. Schwendener, Jan W. Vrijbloed and Daniel Obrecht

**5-Alkyl-2-alkylamino-6-(2,6-difluorophenylalkyl)-3,4-dihydropyrimidin-4(3H)-ones, a new series of potent, broad-spectrum non-nucleoside reverse transcriptase inhibitors belonging to the DABO family**

pp 2065–2077

Antonello Mai,* Marino Artico, Rino Ragno, Gianluca Sbardella, Silvio Massa, Chiara Musiu,
Massimo Mura, Flavia Marturana, Alessandra Cadeddu, Giovanni Maga and Paolo La Colla*

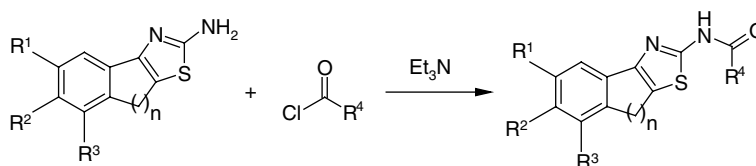


R = R₁ = H, Me; X = alkyl, aryl, arylalkyl

Synthesis and biological evaluation of 2-aminothiazoles and their amide derivatives on human adenosine receptors. Lack of effect of 2-aminothiazoles as allosteric enhancers

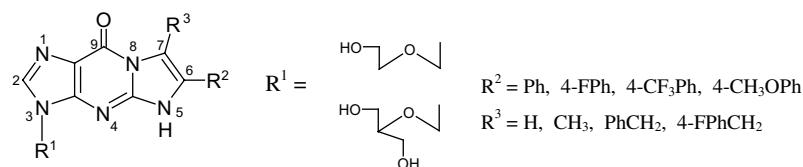
pp 2079–2087

Anikó Göblyös, Sabrina Neves Santiago, Daniele Pietra, Thea Mulder-Krieger,
Jacobien von Frijtag Drabbe Künzel, Johannes Brussee and Adriaan P. IJzerman*

**Fluorosubstitution and 7-alkylation as prospective modifications of biologically active 6-aryl derivatives of tricyclic acyclovir and ganciclovir analogues**

pp 2089–2096

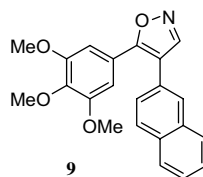
Tomasz Ostrowski, Bozena Golankiewicz,* Erik De Clercq and Jan Balzarini



New naphthylcombretastatins. Modifications on the ethylene bridge

pp 2097–2107

Ana B. Sánchez Maya, Concepción Pérez-Melero, Nélida Salvador, Rafael Peláez, Esther Caballero and Manuel Medarde*



The synthesis and biological evaluation of naphthylcombretastatins, modified on the ethylene bridge, are described.

A novel method of estimation of lipophilicity using distance-based topological indices: dominating role of equalized electronegativity

pp 2109–2120

Vijay K. Agrawal, Madhu Gupta, Jyoti Singh and Padmakar V. Khadikar*

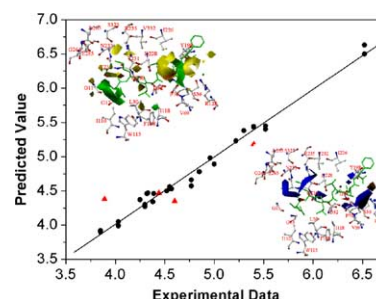
Attempt is made to propose yet another method for the estimation of lipophilicity of a heterogeneous set of 223 compounds. The method is based on the use of topological indices along with equalized electronegativity. The results have shown that excellent results are obtained in multiparametric regression upon introduction of indicator parameters.

Molecular docking and 3D-QSAR studies on the binding mechanism of statine-based peptidomimetics with β -secretase

pp 2121–2131

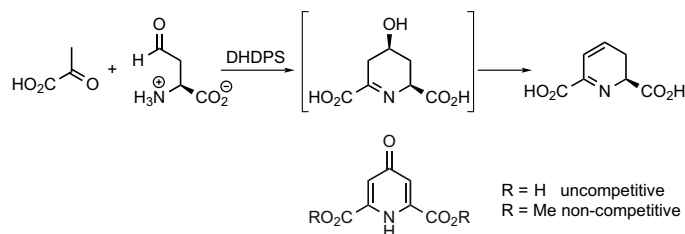
Zhili Zuo, Xiaomin Luo,* Weiliang Zhu,* Jianhua Shen, Xu Shen, Hualiang Jiang* and Kaixian Chen

The interaction mechanism of a series of statine-based peptidomimetics with human β -secretase was studied using molecular docking and 3D-QSAR approaches. A good correlation between predicted binding free energy and experimental pIC_{50} was discovered, and CoMFA and CoMSIA models with strong predictive capabilities were successfully constructed, providing clear guidelines for designing novel inhibitors as drug leads against Alzheimer's disease.

**Heterocyclic inhibitors of dihydrodipicolinate synthase are not competitive**

pp 2133–2140

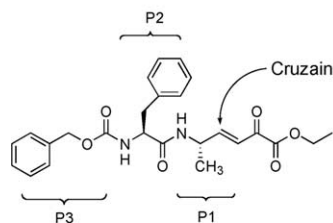
Jennifer J. Turner, Juliet A. Gerrard and Craig A. Hutton*



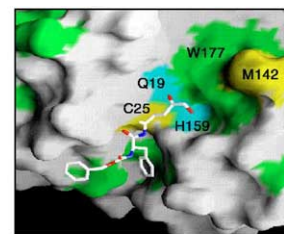
Development of α -keto-based inhibitors of cruzain, a cysteine protease implicated in Chagas disease pp 2141–2156

Youngchool Choe, Linda S. Brinen, Mark S. Price, Juan C. Engel, Meinolf Lange, Corinna Grisostomi, Scott G. Weston, Peter V. Pallai, Hong Cheng, Larry W. Hardy, David S. Hartsough, Marsha McMakin, Robert F. Tilton, Carmen M. Baldino and Charles S. Craik*

A series of novel α -keto based inhibitors has been developed that covalently binds to the active site of cruzain, a cysteine protease crucial for the life cycle of *Trypanosoma cruzi*, the causative agent for Chagas disease.



AQ581332

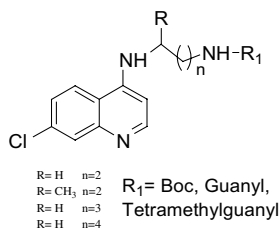


X-ray Structure of AQ581332 bound to Cruzain

Design and synthesis of new antimalarial agents from 4-aminoquinoline

pp 2157–2165

V. Raja Solomon, Sunil K. Puri, Kumkum Srivastava and S. B. Katti*

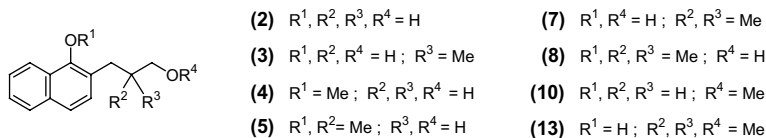


In the present study, synthesis of a new series of 4-aminoquinoline derivatives and evaluation of their activity against a chloroquine sensitive strain of *P. falciparum* in vitro and chloroquine resistant N-67 strain of *P. yoelii* in vivo studies are described.

Inhibitory effects of 2-substituted-1-naphthol derivatives on cyclooxygenase I and II

pp 2167–2175

Boonsong Kongkathip, Chak Sangma,* Kanyawim Kirtikara, Suwaporn Luangkamin, Komkrit Hasitapan, Nipa Jongkon, Supa Hannongbua and Ngampong Kongkathip*

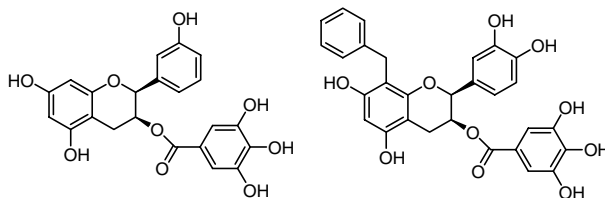


Naphthols **2**, **3**, **7** and their methyl ethers **10** and **13** showed inhibitory activity with preferential inhibition of COX-2 over COX-1 whereas the methyl ether of naphthols **4**, **5** and **8** showed no activity.

Structure–activity study of *epi*-gallicocatechin gallate (EGCG) analogs as proteasome inhibitors

pp 2177–2185

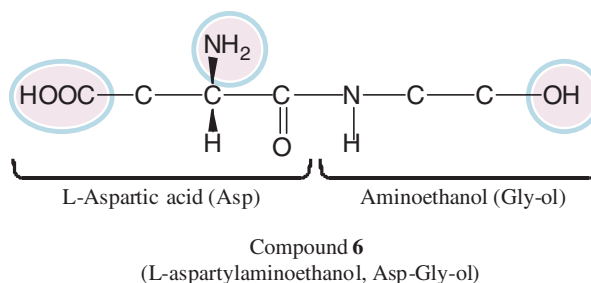
Sheng Biao Wan, Kristin R. Landis-Piowar, Deborah J. Kuhn, Di Chen, Q. Ping Dou and Tak Hang Chan*



Dipeptide alcohol-based inhibitors of eukaryotic DNA polymerase α

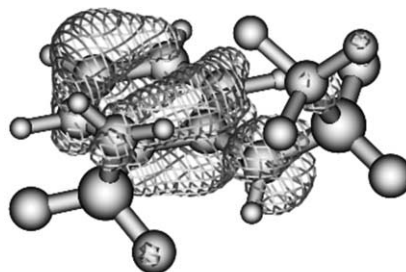
pp 2187–2196

Isoko Kuriyama, Naoki Asano, Ikuo Kato, Kyoko Ikeda, Masaharu Takemura, Hiromi Yoshida, Kengo Sakaguchi and Yoshiyuki Mizushima*

**A physically interpretable quantum-theoretic QSAR for some carbonic anhydrase inhibitors with diverse aromatic rings, obtained by a new QSAR procedure**

pp 2197–2211

Brian W. Clare* and Claudiu T. Supuran

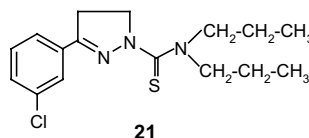


HOPO of Trifluoromethanesulfonylorthanilamide

**Synthesis and antiamoebic activities of 1-*N*-substituted cyclised pyrazoline analogues of thiosemicarbazones**

pp 2213–2220

Mohammad Abid and Amir Azam*

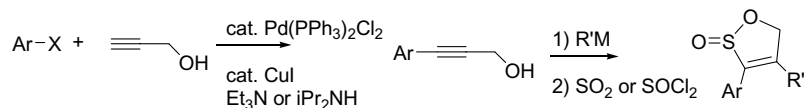


A series of 21 new 1-*N*-substituted cyclised pyrazoline analogues of thiosemicarbazones were synthesised by cyclisation of Mannich bases with thiosemicarbazides of variegated nature. The antiamoebic activities of these compounds were evaluated by microdilution method against *HMI:IMSS* strain of *Entamoeba histolytica*. Compounds **15**, **17**, **18**, **20** and **21** showed less IC_{50} value than metronidazole. Moreover, compound **21** have shown the most promising antiamoebic activity ($IC_{50} = 0.6 \mu M$ vs $IC_{50} = 1.8 \mu M$ of metronidazole).

Oxathiolene oxide synthesis via chelation-controlled addition of organometallic reagents to alkynols followed by addition of sulfur electrophiles and evaluation of oxathiolene oxides as anticarcinogenic enzyme inducers

pp 2221–2233

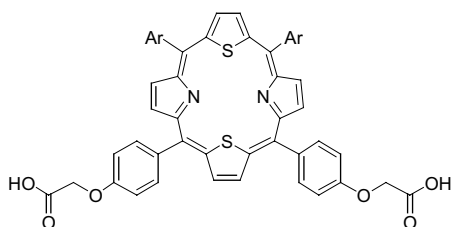
Marion A. Franks, Edward A. Schrader, E. Christine Pietsch, Daniel R. Pennella, Suzy V. Torti* and Mark E. Welker*



A number of alkynols have been prepared by Sonogashira coupling of propargyl alcohol to aromatic halides. Chelation-controlled addition of organometallic nucleophiles to these alkynols was then effected followed by the addition of the sulfur electrophiles, sulfur dioxide or thionyl chloride. This methodology was used to prepare a number of oxathiolene oxides, which have been screened as NQO1 (quinone oxidoreductase) inducers.

Core-modified porphyrins. Part 4: Steric effects on photophysical and biological properties in vitro
 Youngjae You,* Scott L. Gibson, Russell Hilf, Tymish Y. Ohulchanskyy and Michael R. Detty*

pp 2235–2251

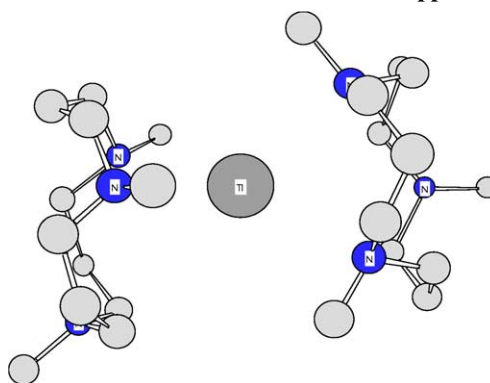


^1H NMR studies of homo and mixed ligand complexes of Ti^+ ion with several polyazamacrocycles

Maryam Bordbar, Mojtaba Shamsipur and Naader Alizadeh*

pp 2253–2262

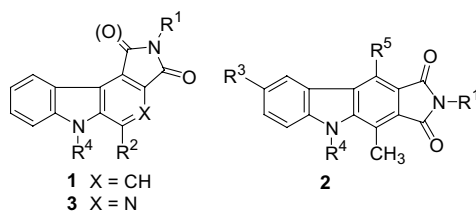
The formation of homo and mixed ligand sandwich complexes of Ti^+ ion with N_3 series such as [9]ane N_3 , [12]ane N_3 , and Me_3 [12]ane N_3 , the N_4 and N_6 series containing [12]ane N_4 , [14]ane N_4 , and [18]ane N_6 (HCY), and Me_6 [18]ane N_6 (HMHCY) was observed at 300 K.



Synthesis and anticancer activity of new pyrrolocarbazoles and pyrrolo- β -carbolines

M. Laronze,* M. Boisbrun, S. Léonce, B. Pfeiffer, P. Renard, O. Lozach, L. Meijer, A. Lansiaux, C. Bailly, J. Sapi and J.-Y. Laronze*

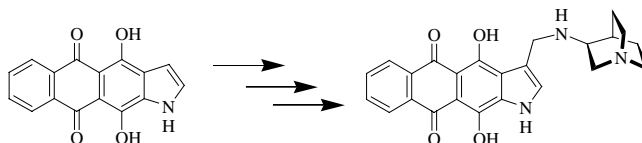
pp 2263–2283



3-Aminomethyl derivatives of 4,11-dihydroxynaphtho[2,3-*f*]indole-5,10-dione for circumvention of anticancer drug resistance

Andrey E. Shchekotikhin,* Alexander A. Shtil, Yuri N. Luzikov, Tatyana V. Bobrysheva, Vladimir N. Buyanov and Maria N. Preobrazhenskaya

pp 2285–2291

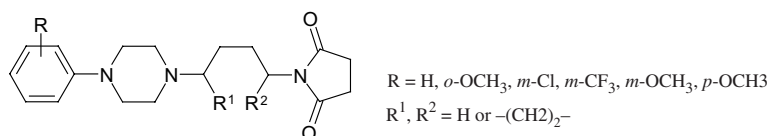


A series of 3-aminomethyl derivatives of 4,11-dihydroxynaphtho[2,3-*f*]indole-5,10-dione was synthesized. Mannich derivatives of 4,11-dihydroxynaphtho[2,3-*f*]indole-5,10-dione with cyclic diamine in their side chain were cytotoxic against cell lines resistant to adriamycin (MDR cell lines).

1-Aryl-4-(4-succinimidobutyl)piperazines and their conformationally constrained analogues: synthesis, binding to serotonin (5-HT_{1A}, 5-HT_{2A}, 5-HT₇), α_1 -adrenergic, and dopaminergic D₂ receptors, and in vivo 5-HT_{1A} functional characteristics

pp 2293–2303

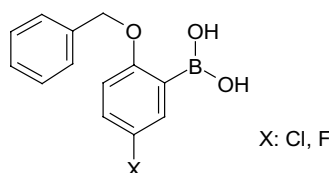
Andrzej J. Bojarski,* Maria H. Paluchowska, Beata Duszyńska, Aleksandra Kłodzińska, Ewa Tatarczyńska and Ewa Chojnacka-Wójcik



Structure–activity relationship for aryl and heteroaryl boronic acid inhibitors of hormone-sensitive lipase

pp 2305–2312

Søren Ebdrup,* Poul Jacobsen, Anupma Dhanda Farrington and Per Vedsø

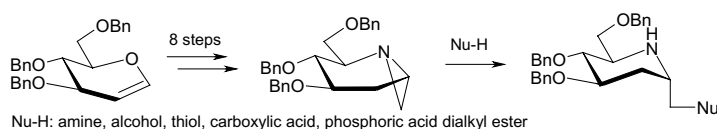


A range of aryl and heteroaryl boronic acids were tested for their in vitro hormone-sensitive lipase inhibitory properties. (2-Benzyloxy-5-fluorophenyl)boronic acid, (2-benzyloxy-5-chlorophenyl)boronic acid and 5-bromothiophene-2-boronic acid were found to be the most potent HSL inhibitors with IC₅₀ values of 140, 17 and 350 nM, respectively.

General synthesis and biological evaluation of α -1-C-substituted derivatives of fagomine (2-deoxynojirimycin- α -C-glycosides)

pp 2313–2324

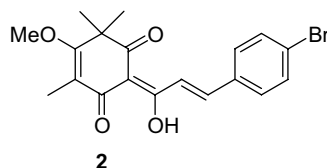
Jean-Yves Goujon, David Gueyrard, Philippe Compain,* Olivier R. Martin,* Kyoko Ikeda, Atsushi Kato and Naoki Asano



Antitumor agents 243. Syntheses and cytotoxicity of desmosdumotin C derivatives

pp 2325–2330

Kyoko Nakagawa-Goto, Jiu-Hong Wu, Kenneth F. Bastow, Chin-Chung Wu and Kuo-Hsiung Lee*



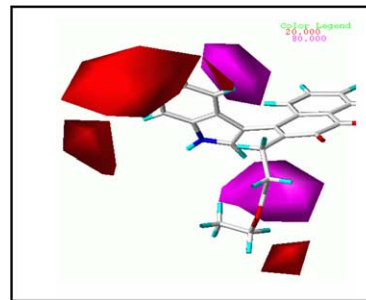
New analogs of desmosdumotin C, in which other aromatic rings replaced the terminal phenyl group and the A-ring was modified, were synthesized. The 4-bromophenyl analog (**2**) showed potent cytotoxic activity in four different tumor cell lines.

Comparative molecular similarity indices analysis (CoMSIA) studies of 1,2-naphthoquinone derivatives as PTP1B inhibitors

pp 2331–2338

M. Elizabeth Sobhia* and Prasad V. Bharatam

A correlation between the 1,2-naphthoquinone derivatives and the molecular fields has been developed using CoMSIA method by employing pre-screened data.

**OTHER CONTENTS**

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Instructions to contributors

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pp III–VII

*Corresponding author

①⁺ Supplementary data available via ScienceDirect**COVER**

Protegrin I is a naturally occurring antimicrobial peptide, whose backbone is constrained into a hairpin conformation by two disulfide bridges. The family of β -hairpin mimetics described, rely on the hairpin inducing properties of a template to achieve the same backbone conformation. The mimetics can be modified synthetically to optimize antimicrobial activity and reduce toxicity, and may provide access to novel antibiotics to combat the ever growing threat posed by resistant microorganisms [Robinson, J. A.; Shankaramma, S. C.; Jetter, P.; Kienzl, U.; Schwendener, R. A.; Vrijbloed, J. W.; Obrecht, D. *Bioorg. Med. Chem.* **2005**, *13*, 2055–2064].

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