

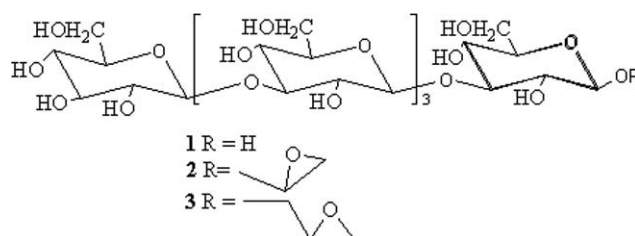
## Contents

### ARTICLES

**Synthesis, immunological activities, and scavenging ability toward superoxide anion of (1→3)-β-D-pentagluconide and its epoxyalkyl derivatives**

pp 3873–3877

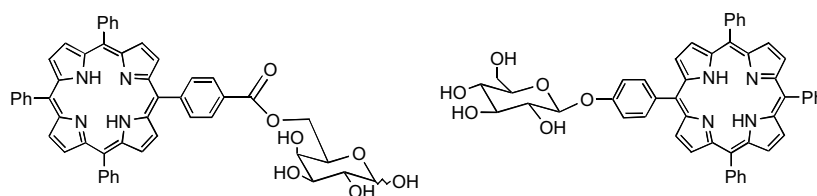
Gang-Liang Huang,\* Man-Xi Liu, Xin-Ya Mei and Ying Wang



**Synthesis of glycoporphyrin derivatives and their antiviral activity against herpes simplex virus types 1 and 2**

pp 3878–3888

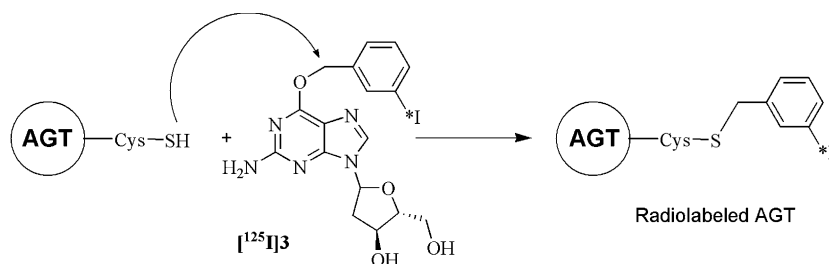
João P. C. Tomé, Maria G. P. M. S. Neves, Augusto C. Tomé, José A. S. Cavaleiro,\* Ana F. Mendonça, Inês N. Pegado, Ricardo Duarte and Maria L. Valdeira



***O*<sup>6</sup>-3-[<sup>125</sup>I]iodobenzyl-2'-deoxyguanosine ([<sup>125</sup>I]IBdG): synthesis and evaluation of its usefulness as an agent for quantification of alkylguanine-DNA alkyltransferase (AGT)**

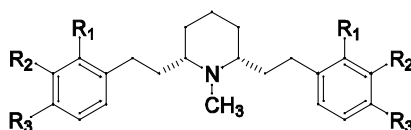
pp 3889–3898

Sriram Shankar, Michael R. Zalutsky and Ganesan Vaidyanathan\*



**Lobeline analogues as novel ligands for the vesicular monoamine transporter-2**

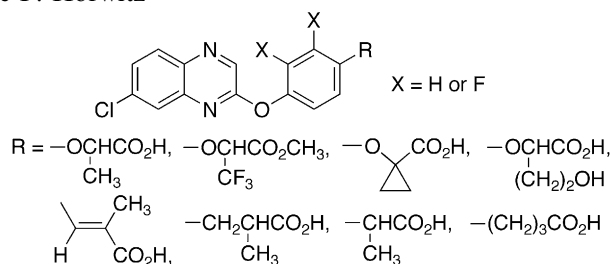
pp 3899–3909

Guangrong Zheng, Linda P. Dwoskin, Agripina G. Deaciuc, Jun Zhu,  
Marlon D. Jones and Peter A. Crooks\*

A series of lobeline analogues has been synthesized and their structure–activity relationships at the vesicular monoamine transporter-2 (VMAT2) have been evaluated. The most potent analogues in this series were the *cis*-2,6-piperidino analogues, **25b**, **27b**, **28b**, and **30b**, with  $K_i$  values ranging from 430 to 580 nM.

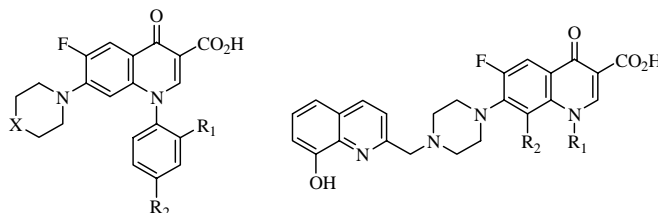
**Synthetic modification of the 2-oxypropionic acid moiety in 2-{4-[(7-chloro-2-quinoxalinyloxy]phenoxy}propionic acid (XK469), and consequent antitumor effects. Part 4**

pp 3910–3920

Stuart T. Hazeldine, Lisa Polin, Juiwanna Kushner, Kathryn White,  
Thomas H. Corbett and Jerome P. Horwitz\***Synthesis and antimycobacterial evaluation of certain fluoroquinolone derivatives**

pp 3921–3926

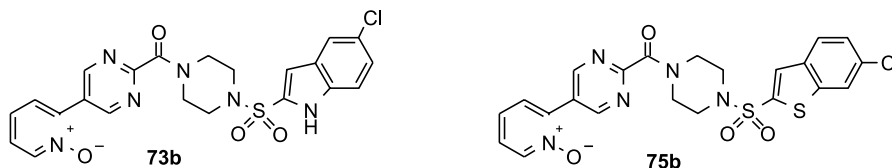
Yue-Ling Zhao, Yeh-Long Chen, Jia-Yuh Sheu, I-Li Chen, Tai-Chi Wang and Cherng-Chyi Tzeng\*



A number of 1-(4-nitrophenyl)quinolones, 1-(4-aminophenyl)quinolones and bifunctional fluoroquinolone–hydroxyquinoline complexes were synthesized and evaluated for antimycobacterial activity.

**Design, synthesis, and biological activity of non-basic compounds as factor Xa inhibitors: SAR study of S1 and aryl binding sites**

pp 3927–3954

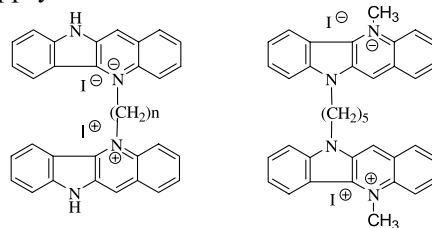
Satoshi Komoriya,\* Noriyasu Haginoya, Shozo Kobayashi, Tsutomu Nagata,  
Akiyoshi Mochizuki, Masanori Suzuki, Toshiharu Yoshino, Haruhiko Horino,  
Takayasu Nagahara, Makoto Suzuki, Yumiko Isobe and Taketoshi Furugoori

The optimized compounds **73b** and **75b** showed sub to one digit micromolar anticoagulant activity (PTCT2). Particularly, anti-fXa activity was detected in plasma of rats orally administered with 1mg/kg of compound **75b**.

**Identification of bis-quindolines as new anti-infective agents**

pp 3955–3963

Leroy G. Mardenborough, Xue Y. Zhu, Pincheng Fan, Melissa R. Jacob, Shabana I. Khan, Larry A. Walker and Seth Y. Ablordeppey\*

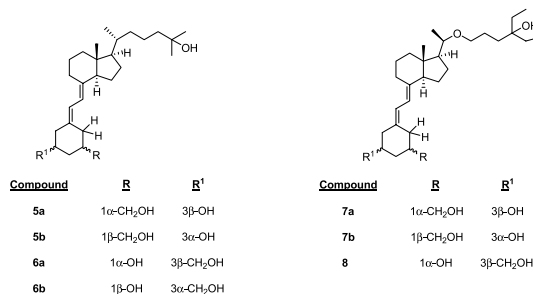


Novel bis-quindolines with alkylated positively charged N-atoms constitute novel agents with expanded antimicrobial/antiparasitic spectra and lower cytotoxicity.

**A-ring hydroxymethyl 19-nor analogs of the natural hormone 1 $\alpha$ ,25-dihydroxyvitamin D<sub>3</sub>: synthesis and preliminary biological evaluation**

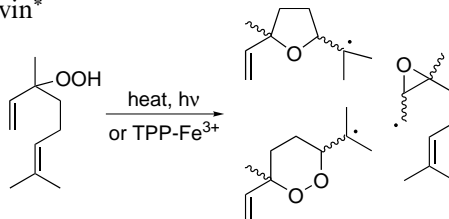
pp 3964–3976

Mark A. Hatcher, Sara Peleg, Patrick Dolan, Thomas W. Kensler, Amy Sarjeant and Gary H. Posner\*

**Identification of carbon-centred radicals derived from linalyl hydroperoxide, a strong skin sensitizer: a possible route for protein modifications**

pp 3977–3986

Michael Bezard, Elena Giménez-Arnau, Bernard Meurer, Loris Grossi and Jean-Pierre Lepoittevin\*



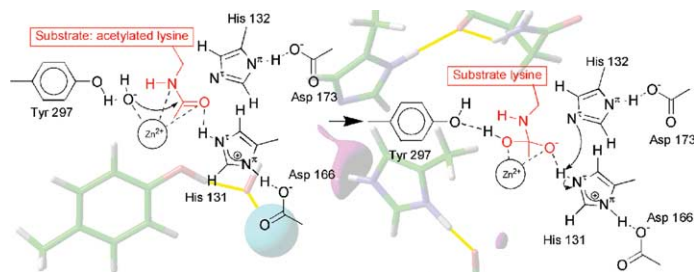
The formation of carbon-centred radicals derived from linalyl hydroperoxide is described using radical trapping and EPR studies. These radicals are suspected to play an important role for the binding of the hydroperoxide with skin proteins to form antigenic structures, the first step of the skin sensitization mechanism.

**Theoretical study revealing the functioning of a novel combination of catalytic motifs in histone deacetylase**

pp 3987–3992

K. Vanommeslaeghe,\* F. De Proft, S. Loverix, D. Tourwé and P. Geerlings

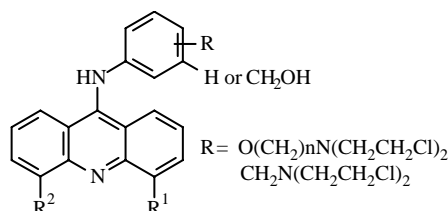
Computational study of the active site of HDAC at a high level of theory, yielding evidence for a novel catalytic mechanism that differs from a previous proposal in the native protonation state of the enzyme, and in the deprotonation of water as a distinct step in the mechanism.



**Potent antitumor 9-anilinoacridines bearing an alkylating N-mustard residue on the anilino ring: synthesis and biological activity**

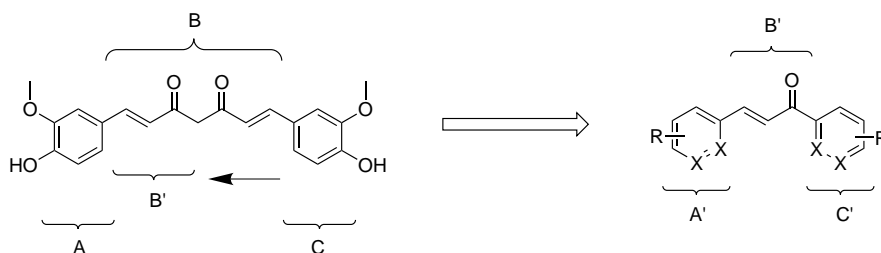
pp 3993–4006

Valeriy A. Bacherikov, Ting-Chao Chou, Hua-Jin Dong, Xiuguo Zhang, Ching-Huang Chen, Yi-Wen Lin, Tsong-Jen Tsai, Rong-Zau Lee, Leroy F. Liu and Tsann-Long Su\*

**Synthesis and biological evaluation of aromatic enones related to curcumin**

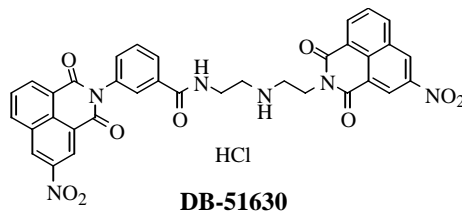
pp 4007–4013

Thomas Philip Robinson, Richard B. Hubbard IV, Tedman J. Ehlers, Jack L. Arbiser, David J. Goldsmith and J. Phillip Bowen\*

**Napthalimidobenzamide DB-51630: a novel DNA binding agent inducing p300 gene expression and exerting a potent anti-cancer activity**

pp 4014–4021

Kenji Suzuki, Hideko Nagasawa, Yoshihiro Uto, Yoshikazu Sugimoto, Kazuharu Noguchi, Motoji Wakida, Konstanty Wierzba, Tadafumi Terada, Tetsuji Asao, Yuji Yamada, Kenji Kitazato and Hitoshi Hori\*

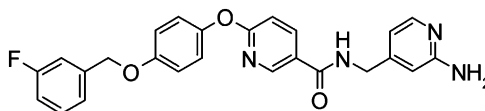


DB-51630 specifically induced p300 gene expression in cancer cells and showed a potent anti-cancer activity both in vitro and in vivo.

**Discovery of an *N*-(2-aminopyridin-4-ylmethyl)nicotinamide derivative: a potent and orally bioavailable NCX inhibitor**

pp 4022–4036

Takahiro Kuramochi,\* Akio Kakefuda, Hiroyoshi Yamada, Issei Tsukamoto, Taku Taguchi and Shuichi Sakamoto

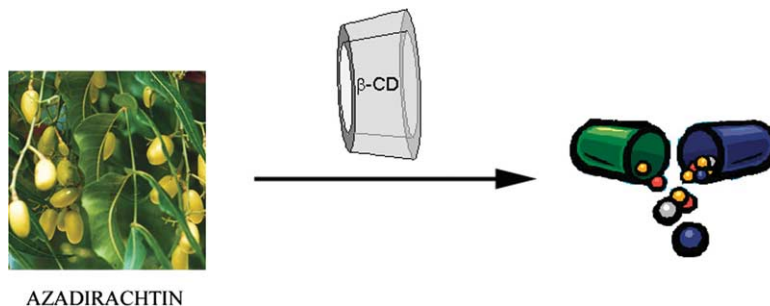


A series of 2-aminopyridine derivatives were prepared and evaluated for their inhibitory activities against the reverse and forward modes of the sodium–calcium exchanger (NCX). The structure–activity relationships of these compounds and their inhibitory activities against NCX are discussed. *N*-[(2-Aminopyridin-4-yl)methyl]-6-[4-[(3-fluorobenzyl)oxy]phenoxy]nicotinamide was evaluated for its effect in a heart failure model.

**Inclusion complexes of azadirachtin with native and methylated cyclodextrins: solubilization and binding ability**

pp 4037–4042

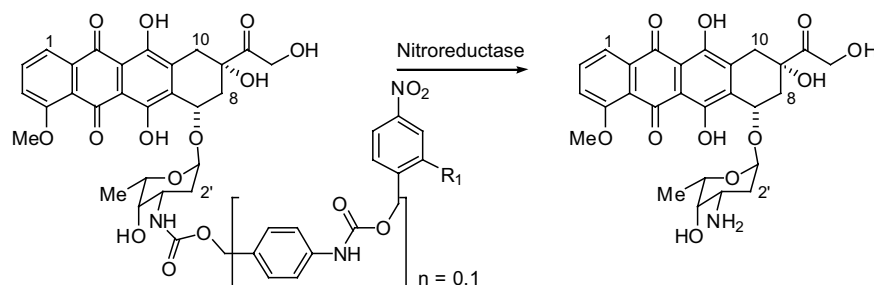
Yu Liu,\* Guo-Song Chen, Yong Chen and Jun Lin

**Nitroarylmethylcarbamate prodrugs of doxorubicin for use with nitroreductase gene-directed enzyme prodrug therapy**

pp 4043–4055

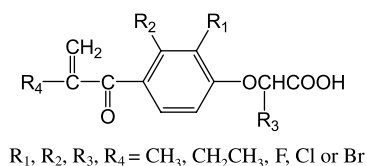
Michael P. Hay,\* William R. Wilson and William A. Denny

A series of nitrobenzyl and nitroimidazolylmethyl carbamate prodrugs of doxorubicin were synthesized and evaluated as substrates for nitroreductase-mediated gene-directed enzyme prodrug therapy.

**Synthesis and structure–activity relationship of ethacrynic acid analogues on glutathione-s-transferase P1-1 activity inhibition**

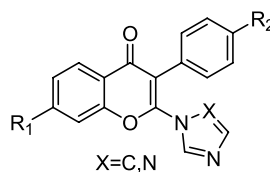
pp 4056–4062

Guisen Zhao, Tao Yu, Rui Wang, Xiaobing Wang and Yongkui Jing\*

**Synthesis and characterization of azole isoflavone inhibitors of aromatase**

pp 4063–4070

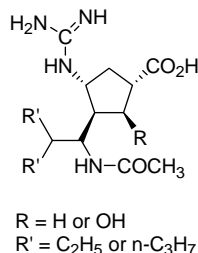
John C Hackett, Young-Woo Kim, Bin Su and Robert W. Brueggemeier\*



**Comparison of the anti-influenza virus activity of cyclopentane derivatives with oseltamivir and zanamivir in vivo**

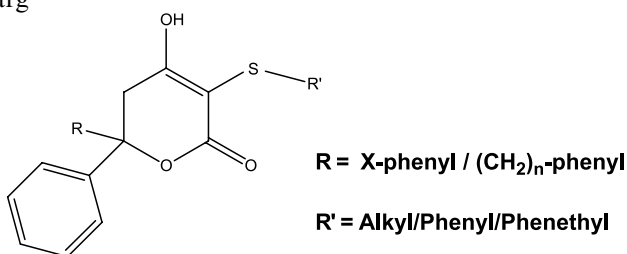
pp 4071–4077

Pooran Chand,\* Shanta Bantia, Pravin L. Kotian, Yahya El-Kattan, Tsu-Hsing Lin and Yarlagadda S. Babu


**From SAR to comparative QSAR: role of hydrophobicity in the design of 4-hydroxy-5,6-dihydropyran-2-ones HIV-1 protease inhibitors**

pp 4078–4084

Barun Bhattacharai and Rajni Garg\*

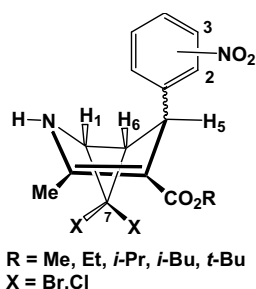


In the present study, the role of hydrophobicity in the design of 4-hydroxy-5,6-dihydropyran-2-ones HIV-1 protease inhibitors is discussed. It has been found that a sufficient spread in the data is required to observe the optimum value of Clog *P* for these inhibitors.

**Design and synthesis of alkyl 7,7-dihalo-3-methyl-5-(nitrophenyl)-2-azabicyclo-[4.1.0]hept-3-ene-4-carboxylates with calcium channel antagonist activity**

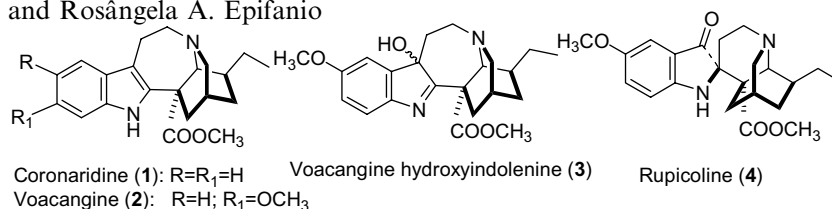
pp 4085–4091

Javid S. Mojarad, Dean Vo, Carlos Velázquez and Edward E. Knaus\*


**Indole alkaloids from *Tabernaemontana australis* (Müell. Arg) Miers that inhibit acetylcholinesterase enzyme**

pp 4092–4095

Marcelo T. Andrade, Josélia A. Lima, Angelo C. Pinto, Claudia M. Rezende,\* Meriane P. Carvalho and Rosângela A. Epifanio

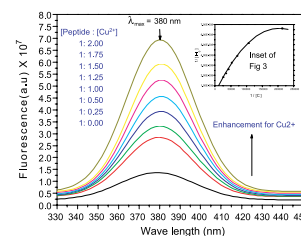
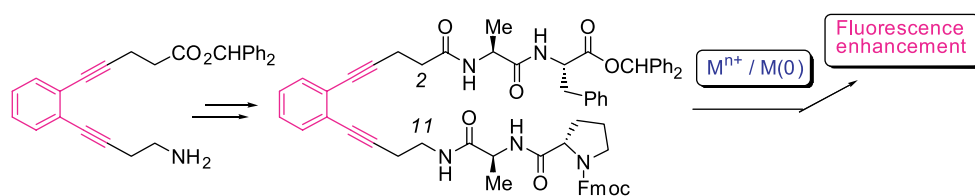


In an enzymatic TLC survey, among the 10 alkaloids identified in *Tabernaemontana australis*, 1–4 inhibited the acetylcholinesterase enzyme at the same detection limit concentration of the reference compounds physostigmine and galanthamine, showing that iboga alkaloids are promising anti-Alzheimer agents.

## Design and synthesis of a novel enediynyl pentapeptide with predominantly $\beta$ -turn structural motif and its potential as a fluorescence-based chemosensor

pp 4096–4102

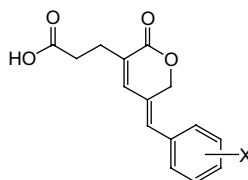
Amit Basak,\* Subhendu Sekhar Bag and Ajoy Basak



## Synthesis of arylidene-substituted gelastatin analogues and their screening for MMP-2 inhibitory activity

pp 4103–4112

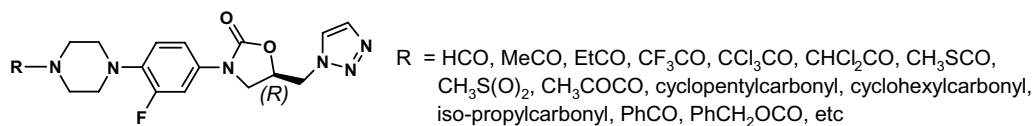
Eun Jin Kim and Soo Y. Ko\*



## Synthesis and antibacterial activity of new N-linked 5-triazolylmethyl oxazolidinones

pp 4113–4123

Oludotun A. Phillips,\* Edet E. Udo, Ahmed A. M. Ali and Santhosh M. Samuel

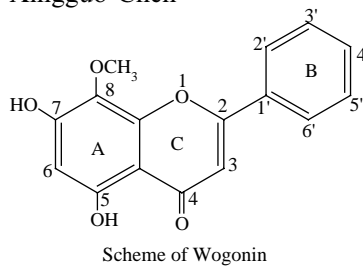


Synthesis and structure–antibacterial activity of new N-linked-5-triazolylmethyl oxazolidinones are presented.

## Interaction of wogonin with bovine serum albumin

pp 4124–4129

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



The binding of wogonin with bovine serum albumin (BSA) was investigated at different temperatures by fluorescence, circular dichroism (CD) and Fourier transform infrared spectroscopy (FT-IR) at pH7.40.


**CORRIGENDUM**

Corrigendum to “Studies on the cytochrome P450 catalyzed oxidation of  $^{13}\text{C}$  labeled 1-cyclopropyl-4-phenyl-1,2,3,6-tetrahydropyridine by  $^{13}\text{C}$  NMR”. [*Bioorg. Med. Chem.* 13 (2005) 2975] pp 4130  
Philippe Bissel, Neal Castagnoli, Jr. and Sarah Penich

**OTHER CONTENTS**

Contributors to this issue p I  
Instructions to contributors pp III–VII

\*Corresponding author

\* Supplementary data available via ScienceDirect

**COVER**

2005: Human liver glycogen phosphorylase A (HLGPa) is an attractive target enzyme for discovering anti-type 2 diabetes drugs. This picture shows the interaction model for a series of indole-2-carboxamides to HLGPa derived from molecular docking simulations [Liu, G.; Zhang, Z.; Luo, X.; Shen, J.; Liu, H.; Shen, X.; Chen, K.; Jiang, H. *Bioorg. Med. Chem.* **2004**, 12, 4147–4157].



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