

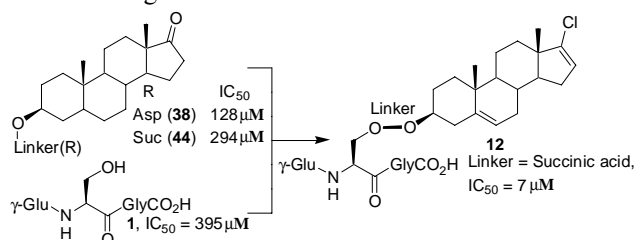
## Contents

### ARTICLES

#### Design of potent inhibitors for *Schistosoma japonica* glutathione *S*-transferase

pp 304–318

Shu-Chuan Jao, Jessica Chen, Kelvin Yang and Wen-Shan Li\*



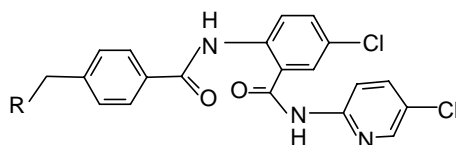
This figure shows design of the potent *Schistosoma japonicum* glutathione *S*-transferase inhibitors.



#### QSAR studies of *N*<sub>1</sub>-(5-chloro-2-pyridyl)-2-[[4-(alkyl methyl)benzoyl]amino]-5-chlorobenzamide analogs

pp 319–325

N. Rameshwar,\* K. Krishna, B. Ashok Kumar and T. Parthasarathy\*

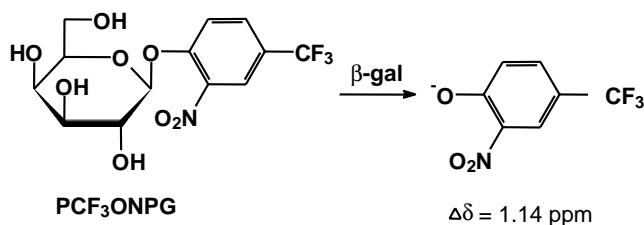


The paper deals with the quantitative structure–activity relationship study on an anthranilamide-based factor X<sub>a</sub> inhibitory activity as a function of physico-chemical parameters and predicts the best factor X<sub>a</sub> inhibitory compound. The predictive power of the proposed models is discussed on the basis of regression analysis and cross-validation parameters.

#### Synthesis and evaluation of novel enhanced gene reporter molecules: Detection of β-galactosidase activity using <sup>19</sup>F NMR of trifluoromethylated aryl β-D-galactopyranosides

pp 326–333

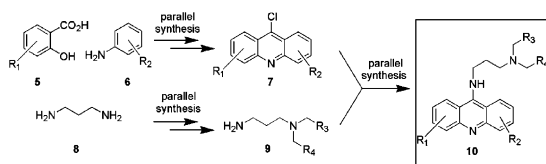
Jianxin Yu, Li Liu, Vikram D. Kodibagkar, Weina Cui and Ralph P. Mason\*



### Parallel synthesis of 9-aminoacridines and their evaluation against chloroquine-resistant *Plasmodium falciparum*

pp 334–343

Marc O. Anderson, John Sherrill, Peter B. Madrid, Ally P. Liou,  
Jennifer L. Weisman, Joseph L. DeRisi and R. Kiplin Guy\*



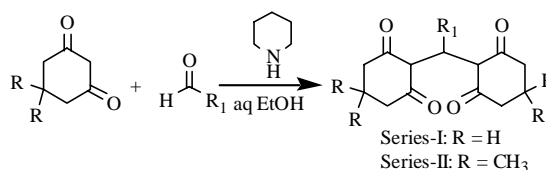
A parallel synthetic strategy to the 9-aminoacridine scaffold of the classical anti-malarial drug quinacrine (**2**) is presented



### Tetraketones: A new class of tyrosinase inhibitors

pp 344–351

Khalid Mohammed Khan,\* Ghulam Murtaza Maharvi, Mahmud Tareq Hassan Khan,  
Ahson Jabbar Shaikh, Shahnaz Perveen, Saeedan Begum and Mohammad Iqbal Choudhary



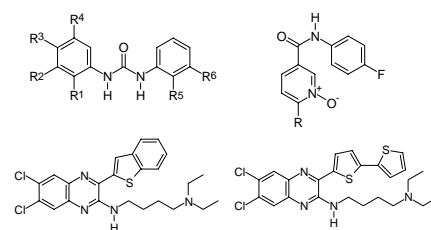
Twenty-eight tetraketones with variable substituents at C-7 were synthesized and evaluated as tyrosinase inhibitors.

### Quantitative structure–activity relationships for small non-peptide antagonists of CXCR2: Indirect 3D approach using the frontal polygon method

pp 352–365

Andrei I. Khlebnikov,\* Igor A. Schepetkin and Mark T. Quinn\*

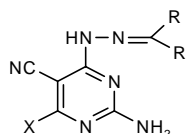
QSAR analysis of 59 nonpeptide antagonists of CXCR2 using a partial 3D comparison of the antagonists with local fingerprints obtained from rigid and flexible fragments of the molecules.



### Synthesis and in vitro antitumoral activity of new hydrazinopyrimidine-5-carbonitrile derivatives

pp 366–372

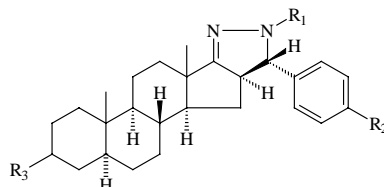
Maria T. Cocco, Cenzo Congiu, Valentina Lilliu and Valentina Onnis\*



Hydrazinopyrimidine-5-carbonitrile derivatives demonstrated inhibitory effects on the growth of a wide range of cancer cell lines generally at  $10^{-5}$  M level and in some cases at  $10^{-7}$  M concentrations.

## Synthesis and antiandrogenic activity of some new 3-substituted androstano[17,16-*c*]-5'-aryl-pyrazoline and their derivatives pp 373–384

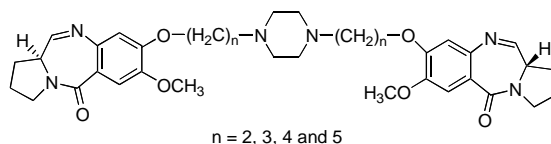
Abd El-Galil E. Amr,\* Nehad A. Abdel-Latif and Mohamed M. Abdalla



A series of androstano[17,16-*c*]pyrazolines and their oxidized derivatives were synthesized by using 3 $\beta$ -hydroxyandrostan-17-one as starting material.

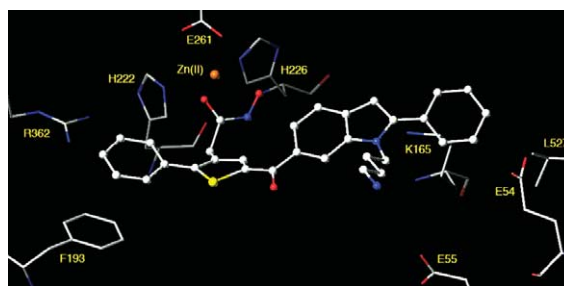
## DNA binding potential and cytotoxicity of newly designed pyrrolobenzodiazepine dimers linked through a piperazine side-armed-alkane spacer pp 385–394

Ahmed Kamal,\* P. S. Murali Mohan Reddy, D. Rajasekhar Reddy and E. Laxman



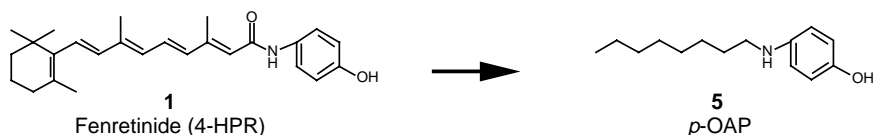
## Serotype-selective, small-molecule inhibitors of the zinc endopeptidase of botulinum neurotoxin serotype A pp 395–408

Jewn Giew Park, Peter C. Sill, Edward F. Makiyi, Alfonso T. Garcia-Sosa, Charles B. Millard, James J. Schmidt\* and Yuan-Ping Pang\*



## Anticancer and superoxide scavenging activities of *p*-alkylaminophenols having various length alkyl chains pp 409–417

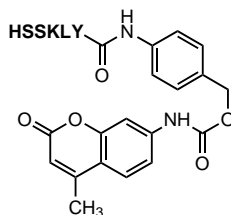
Noriko Takahashi,\* Toshio Honda and Toshihiro Ohba



### An image contrast agent selectively activated by prostate specific antigen

pp 418–425

Graham B. Jones,\* Curtis F. Crasto, Jude E. Mathews, Longfei Xie, Miguel O. Mitchell, Ahmed El-Shafey, Anthony V. D'Amico and Glenn J. Bubley

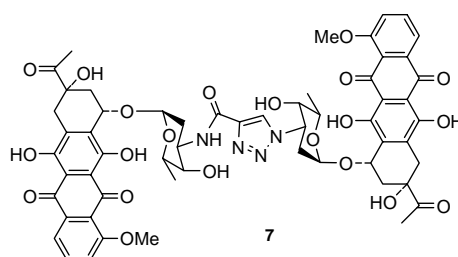


A three-component enzyme activated image contrast system was demonstrated using a family of tyrosine–chromophore conjugates linked by an inert spacer. A selective substrate for PSA was discovered, which releases free fluorophore on exposure to this key biomarker.

### Syntheses and biological activity of bisdaunorubicins

pp 426–434

Guisheng Zhang, Lanyan Fang, Lizhi Zhu, Duxin Sun\* and Peng George Wang\*

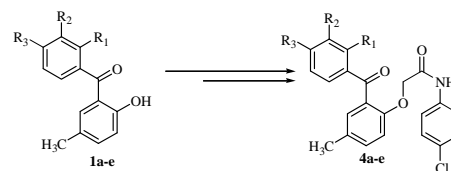


### Anti-tumor and proapoptotic effect of novel synthetic benzophenone analogues in Ehrlich ascites tumor cells

pp 435–446

B. T. Prabhakar, Shaukath Ara Khanum, K. Jayashree, Bharathi P. Salimath and S. Shashikanth\*

A series of substituted benzophenone analogues, (2-aroyl-4-methylphenoxy)acetamides **4a–e**, have been synthesized via the three-step synthesis sequence beginning with the 2-hydroxybenzophenones **1a–e** in excellent yield. Treatment of Ehrlich ascites tumor (EAT) cells with benzophenones in vivo resulted in inhibition of cell proliferation and ascites formation. Further, we demonstrate that induction of apoptosis in EAT cells is mediated via caspase-3 activation. These results suggest possible use of these compounds as potent anti-tumor and proapoptotic agents.

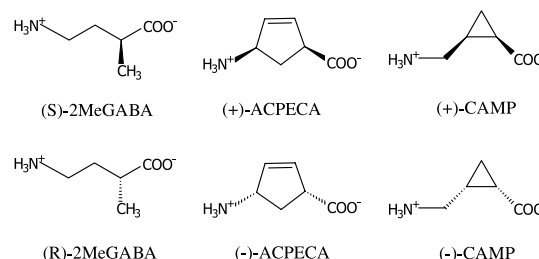


### Enantiomers of *cis*-constrained and flexible 2-substituted GABA analogues exert opposite effects at recombinant GABA<sub>C</sub> receptors

pp 447–455

Deborah L. Crittenden, Anna Park, Jian Qiu, Richard B. Silverman, Rujee K. Duke, Graham A. R. Johnston, Meredith J. T. Jordan and Mary Chebib\*

The effects of the enantiomers of a number of flexible and *cis*-constrained GABA analogues are tested on GABA<sub>C</sub> receptors expressed in *Xenopus Laevis* oocytes using two-electrode voltage-clamp electrophysiology. Different enantiomers are found to have opposite biological activities, with the (*S*) and (+) enantiomers possessing antagonist activity and the (*R*) and (–) enantiomers possessing antagonist activity. A novel stereoselective binding mechanism is proposed to explain this effect.

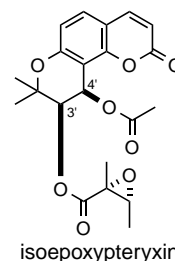


### Inhibitory effects of coumarin and acetylene constituents from the roots of *Angelica furcijuga* on D-galactosamine/lipopolysaccharide-induced liver injury in mice and on nitric oxide production in lipopolysaccharide-activated mouse peritoneal macrophages

Masayuki Yoshikawa,\* Norihisa Nishida, Kiyofumi Ninomiya, Teruki Ohgushi, Mizuho Kubo, Toshio Morikawa and Hisashi Matsuda

The methanolic extract, principal coumarin constituents (isoeopoxypteryxin, anomalin, and praeroside IV), and a polyacetylene constituent (faltarindiol) from the roots of *Angelica furcijuga* protected the liver injury induced by D-galactosamine (D-GalN)/lipopolysaccharide (LPS) in mice. In in vitro experiments, coumarin constituents (hyuganins A–D, anomalin, pteryxin, isopteryxin, and suksdorfin) and polyacetylene constituents [(–)-faltarinol and faltarindiol] substantially inhibited LPS-induced NO and/or TNF- $\alpha$  production in mouse peritoneal macrophages, and isoeopoxypteryxin inhibited D-GalN-induced cytotoxicity in primary cultured rat hepatocytes. Furthermore, hyuganin A, anomalin, and isopteryxin inhibited the decrease in cell viability by TNF- $\alpha$  in L929 cells.

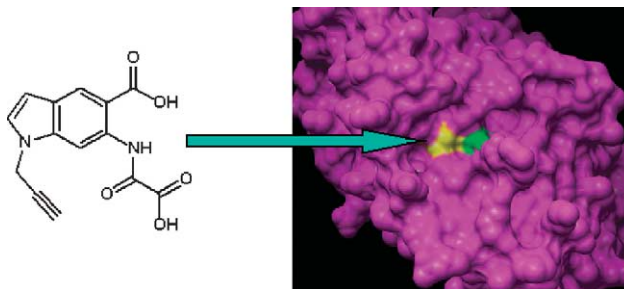
pp 456–463



### Engineering non-natural inhibitor sensitivity in protein tyrosine phosphatase H1

Elizabeth R. Blair, Hillary E. Hoffman and Anthony C. Bishop\*

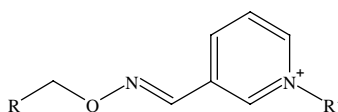
pp 464–471



### Search for dual function inhibitors for Alzheimer's disease: Synthesis and biological activity of acetylcholinesterase inhibitors of pyridinium-type and their A $\beta$ fibril formation inhibition capacity

Petra Kapková, Vildan Alptüzün, Peter Frey, Ercin Erciyas and Ulrike Holzgrabe\*

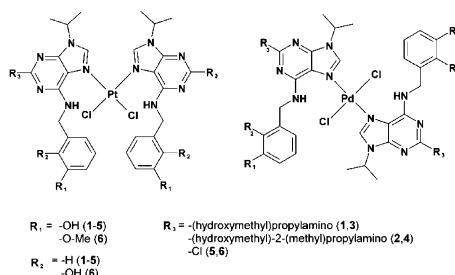
pp 472–478



### Novel platinum(II) and palladium(II) complexes with cyclin-dependent kinase inhibitors: Synthesis, characterization and antitumour activity

Lucie Szčová, Zdeněk Trávníček,\* Marek Zatloukal and Igor Popa

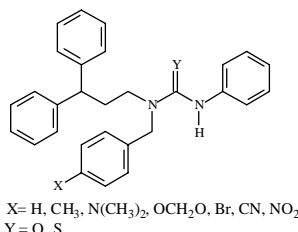
pp 479–491



### Synthesis, cytotoxicity, and DNA-topoisomerase inhibitory activity of new asymmetric ureas and thioureas

pp 492–499

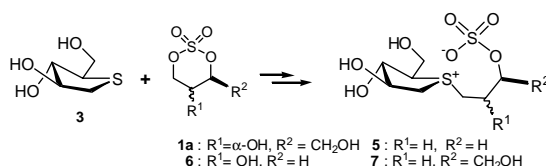
Andressa Esteves-Souza, Kenia Pissinate, Maria da Graça Nascimento, Noema Faiga Grynberg and Aurea Echevarria\*



### Synthesis and biological evaluation of deoxy salacinols, the role of polar substituents in the side chain on the $\alpha$ -glucosidase inhibitory activity

pp 500–509

Osamu Muraoka,\* Kazuya Yoshikai, Hideo Takahashi, Toshie Minematsu, Guangxin Lu, Genzoh Tanabe, Tao Wang, Hisashi Matsuda and Masayuki Yoshikawa

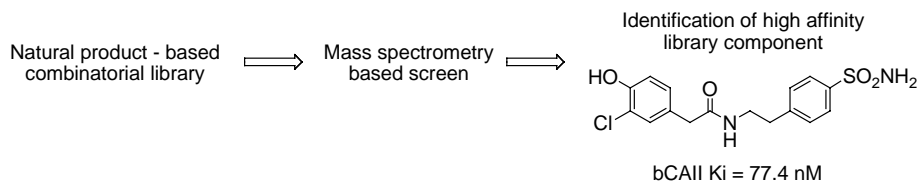


Three analogs (**5**, **6**, and **7**) lacking polar substituents in the side chain of salacinol (**1a**) were synthesized and their  $\alpha$ -glucosidase inhibitory activities were examined. The evaluation indicated the importance of the cooperative role of the polar substituents for the  $\alpha$ -glucosidase inhibitory activity. A practical synthetic route to **3** starting from D-xylose is also described.

### Screening a natural product-based combinatorial library using FTICR mass spectrometry

pp 510–515

Sally-Ann Poulsen,\* Rohan A. Davis and Timothy G. Keys

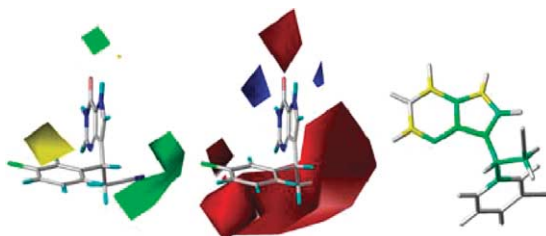


FTICR mass spectrometry was utilised to screen a natural product-based combinatorial library for bovine carbonic anhydrase II binders. One high-affinity ligand was identified in a single mass spectrometry experiment and this result was validated by a competitive bCAII enzyme binding assay.

### Two- and three-dimensional quantitative structure–activity relationships for a series of purine nucleoside phosphorylase inhibitors

pp 516–527

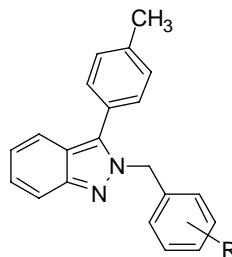
Marcelo S. Castilho, Matheus P. Postigo, Caroline B. V. de Paula, Carlos A. Montanari, Glaucius Oliva and Adriano D. Andricopulo\*



**Synthesis of *N*<sup>2</sup>-(substituted benzyl)-3-(4-methylphenyl)indazoles as novel anti-angiogenic agents**

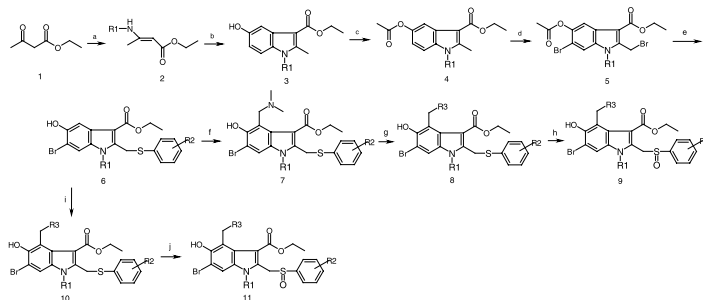
pp 528–536

Li-Jiau Huang, Mei-Ling Shih, Hua-Sin Chen, Shio-Lin Pan, Che-Ming Teng, Fang-Yu Lee and Sheng-Chu Kuo\*

**Synthesis and in vitro anti-hepatitis B virus activities of some ethyl 6-bromo-5-hydroxy-1*H*-indole-3-carboxylates**

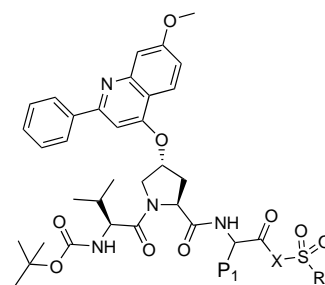
pp 537–543

Huifang Chai, Yanfang Zhao, Chunshen Zhao and Ping Gong\*

**Exploration of acyl sulfonamides as carboxylic acid replacements in protease inhibitors of the hepatitis C virus full-length NS3**

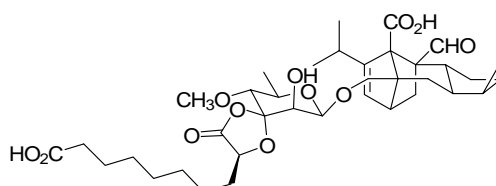
pp 544–559

Robert Rönn, Yogesh A. Sabnis, Thomas Gossas, Eva Åkerblom, U. Helena Danielson, Anders Hallberg and Anja Johansson\*

X = NH, NMe or CH<sub>2</sub>**The discovery of moriniafungin, a novel sordarin derivative produced by *Morinia pestalozzioides***

pp 560–566

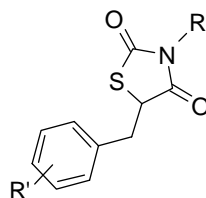
A. Basilio, M. Justice, G. Harris, G. Bills, J. Collado, M. de la Cruz, M. T. Diez, P. Hernandez, P. Liberator, J. Nielsen kahn, F. Pelaez, G. Platas, D. Schmatz, M. Shastry, J. R. Tormo, G. R. Andersen and F. Vicente\*



**In vitro aldose reductase inhibitory activity of 5-benzyl-2,4-thiazolidinediones**

pp 567–574

Dietmar Rakowitz, Rosanna Maccari,\* Rosaria Ottanà and Maria Gabriella Vigorita

**Acetoxy drug: Protein transacetylase catalyzed activation of human platelet nitric oxide synthase by polyphenolic peracetates**

pp 575–583

Pulkit Khurana, Ranju Kumari, Parag Vohra, Ajit Kumar, Seema, Garima Gupta, Hanumantharao G. Raj,\* Bilikere S. Dwarakanath, Virinder S. Parmar, Daman Saluja, Mridula Bose, Anjana Vij, Nabo K. Chaudhary, Jawahar S. Adhikari, Yogesh K. Tyagi and Ekta Kohli



Control



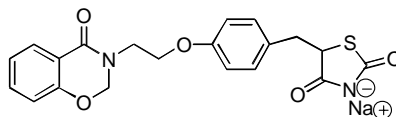
7,8-Diacetoxy-4-methylcoumarin

Polyphenolic acetates are the novel potent enhancers of intracellular nitric oxide.

**Dual PPAR- $\alpha$  and - $\gamma$  activators derived from novel benzoxazinone containing thiazolidinediones having antidiabetic and hypolipidemic potential**

pp 584–591

Gurram R. Madhavan,\* Ranjan Chakrabarti,\* K. Anantha Reddy, B. M. Rajesh, V. Balraju, P. Bheema Rao, R. Rajagopalan and Javed Iqbal



Synthesis, SAR study, and biological evaluation of a new series of 1,3-4(3*H*)benzoxazinone derivatives of thiazolidinedione are reported.

**OTHER CONTENTS**

Summary of instructions to authors

p I

\*Corresponding author

Supplementary data available via ScienceDirect



**COVER**

Structure of the novel sordarin analog moriniafungin superimposed on a colony of mycelia from the producing fungus, *Morinia pestalozzioides* (right). Illustration of the characteristic asexual spores of *Morinia pestalozzioides* (lower left). Inflorescences of *Sedum sediforme*, a host of the fungus (upper left). A. Basilio, M. Justice, G. Harris, G. Bills, J. Collado, M. de la Cruz, M. T. Diez, P. Hernandez, P. Liberator, J. Nielsen kahn, F. Pelaez, G. Platas, D. Schmatz, M. Shastry, J. R. Tormo, G. R. Andersen and F. Vicente. © 2005 Elsevier Ltd.



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