

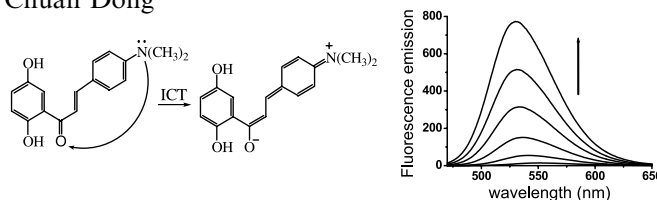
## Contents

### ARTICLES

**Studies on interaction of an intramolecular charge transfer fluorescence probe:  
4'-Dimethylamino-2,5-dihydroxychalcone with DNA**

pp 5694–5699

Zhicheng Xu, Guan Bai and Chuan Dong\*

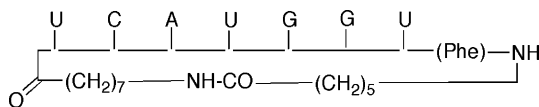


An intramolecular charge transfer fluorescence probe binding to DNA exhibited dramatic enhancement of fluorescence intensity accompanying blueshift of the emission maximum. Experimental results give evidence that this probe is inserted into the base-stacking domain of the DNA double helix.

**A cyclic PNA-based compound targeting domain IV of HCV IRES RNA inhibits in vitro IRES-dependent translation**

pp 5700–5709

Sergio A. Caldarelli, Mohamed Mehiri, Audrey Di Giorgio, Amaury Martin, Olivier Hantz, Fabien Zoulim, Raphael Terreux, Roger Condom and Nadia Patino\*

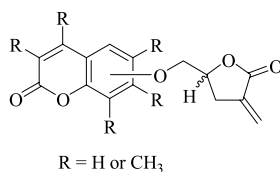


Synthesis of peptide nucleic acid (PNA) [UCAUGGU]Fc and in vitro antiviral properties are presented.

**Synthesis, antiproliferative, and vasorelaxing evaluations of coumarin  $\alpha$ -methylene- $\gamma$ -butyrolactones**

pp 5710–5716

Yeh-Long Chen,\* Chih-Ming Lu, Shoiw-Ju Lee, Daih-Huang Kuo, I-Li Chen, Tai-Chi Wang and Cherng-Chyi Tzeng

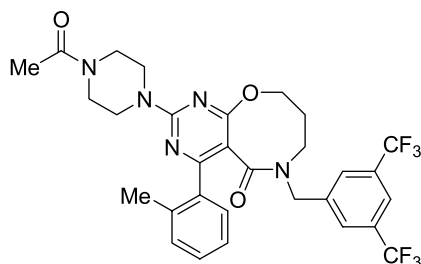


A number of  $\gamma$ -(2-oxo-2H-1-benzopyranyloxy)methyl]- $\alpha$ -methylene- $\gamma$ -butyrolactones were synthesized and evaluated for antiproliferative and vasorelaxing activities.

### Design, synthesis, and evaluation of novel 2-substituted-4-aryl-6,7,8,9-tetrahydro-5H-pyrimido[4,5-b][1,5]oxazocin-5-ones as NK<sub>1</sub> antagonists

pp 5717–5732

Shigeki Seto,\* Asao Tanioka, Makoto Ikeda and Shigeru Izawa

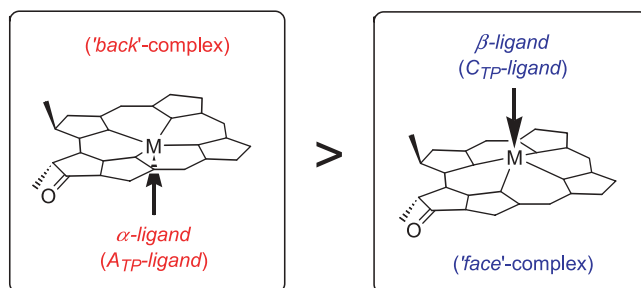


### Effects of peripheral substituents on diastereoselectivity of the fifth ligand-binding to chlorophylls, and nomenclature of the asymmetric axial coordination sites

pp 5733–5739

Toru Oba\* and Hitoshi Tamiaki

It was confirmed that in photosynthetic proteins (bacterio)chlorophylls prefer the fifth ligand-binding on the one side of the  $\pi$ -macrocycle.

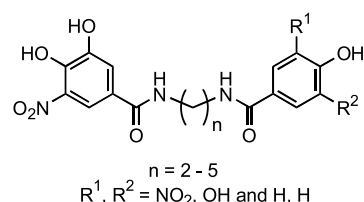


### Synthesis and evaluation of bifunctional nitrocatechol inhibitors of pig liver catechol-*O*-methyltransferase

pp 5740–5749

Karl Bailey and Eng Wui Tan\*

A series of bifunctional compounds were tested in vitro as potential inhibitors of pig liver catechol-*O*-methyltransferase (COMT). The bifunctional compounds were a composite of either two nitrocatechols or one nitrocatechol and one phenol, linked by amide bonds to a spacer unit comprising two to five methylene groups. The unsymmetrical compounds demonstrated strong inhibitory action against COMT with  $K_i$  values in the 100 nM range. In comparison, the monofunctional nitrocatechol analogues of these compounds had  $K_i$  values that were significantly higher.

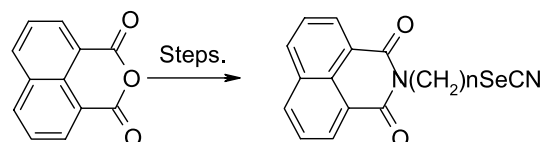


### Synthesis and evaluation of antioxidative properties of a series of organoselenium compounds

pp 5750–5758

Sk. Ugir Hossain, Sumitra Sengupta and Sudin Bhattacharya\*

A series of novel organoselenium compounds **4a–d** were synthesized and these compounds were evaluated for their antioxidative activities against DMBA–PMA-induced oxidative stress in Swiss albino mice. The levels of lipid-peroxidation and phase II detoxifying enzymes were measured 15 days after the first DMBA application. Compound **4d** was found to be the most active.

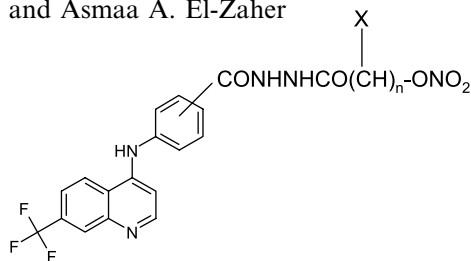


**4a**, n=2  
**4b**, n=3  
**4c**, n=4  
**4d**, n=5

**Synthesis of novel 4-substituted-7-trifluoromethylquinoline derivatives with nitric oxide releasing properties and their evaluation as analgesic and anti-inflammatory agents**

pp 5759–5765

Ashraf H. Abadi,\* Gehan H. Hegazy and Asmaa A. El-Zaher

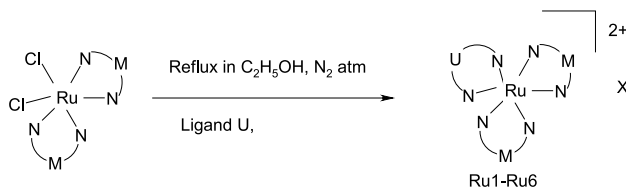


substitution only on position 2 and 4 of the anilino ring  
 $n = 1$ ,  $X = H$ ;  $n = 2$ ,  $X = CH_3$ ;  $n = 2$ ,  $X = H$

**Synthesis and pharmacological activities of some mononuclear Ru(II) complexes**

pp 5766–5773

Upal K. Mazumder,\* Malaya Gupta, Subhas S. Karki, Shiladitya Bhattacharya, Suresh Rathinasamy and Thangavel Sivakumar



Where  $U = \text{tpl}$ , 4-Cl-tpl, 4-MeO-tpl, 4-Me-tpl, 4-NO<sub>2</sub>-tpl, pai

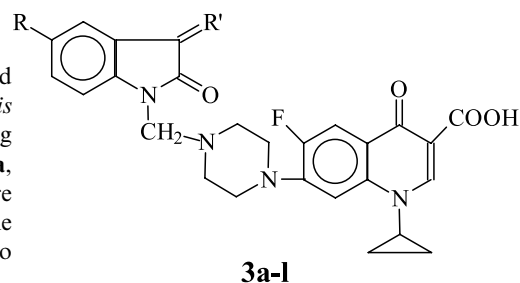
$M = 1,10\text{-phen}/2,2'\text{-bpy}$  and  $X = (\text{ClO}_4)_2$  Ru1-Ru5;  $X = \text{Cl}_2$  Ru6

**Synthesis and antimycobacterial evaluation of various 7-substituted ciprofloxacin derivatives**

pp 5774–5778

Dharmarajan Sriram,\* Perumal Yogeeswari, Jafar Sadik Basha, Deshpande R. Radha and Valakunja Nagaraja

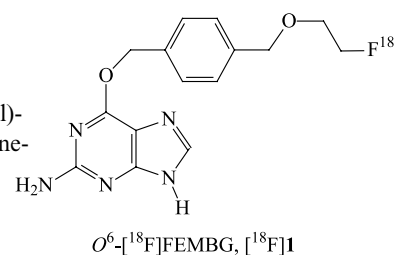
Various 7-substituted ciprofloxacin derivatives were synthesized and evaluated for antimycobacterial in vitro and in vivo against *Mycobacterium tuberculosis* and tested the ability of representative compounds to inhibit the supercoiling activity of DNA gyrase from *Mycobacterium smegmatis*. Five compounds (**3a**, **g-i**, and **k**) showed most promising activity with MIC<sub>90</sub> of 0.78 µg/mL and were more potent than parent compound ciprofloxacin. Compound **3h** decreased the bacterial load in spleen tissue with 0.76-log<sub>10</sub> protections and was considered to be moderately active in reducing bacterial count in spleen.

**Synthesis and preliminary biological evaluation of O<sup>6</sup>-[4-(2-[<sup>18</sup>F]fluoroethoxymethyl)benzyl]guanine as a novel potential PET probe for the DNA repair protein O<sup>6</sup>-alkylguanine-DNA alkyltransferase in cancer chemotherapy**

pp 5779–5786

Ji-Quan Wang, Emiko L. Kreklau, Barbara J. Bailey, Leonard C. Erickson and Qi-Huang Zheng\*

The synthesis and preliminary biological evaluation of O<sup>6</sup>-[4-(2-[<sup>18</sup>F]fluoroethoxymethyl)-benzyl]guanine, as a novel potential PET probe for the DNA repair protein O<sup>6</sup>-alkylguanine-DNA alkyltransferase in cancer chemotherapy, are reported.

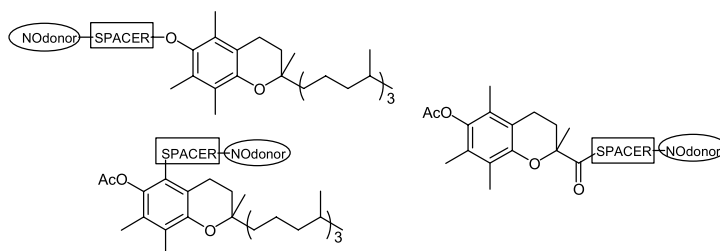


### Design, synthesis, and biological characterization of potential antiatherogenic nitric oxide releasing tocopherol analogs

pp 5787–5796

Gloria V. López, Carlos Batthyány, Fabiana Blanco, Horacio Botti, Andrés Trostchansky, Eduardo Migliaro, Rafael Radi, Mercedes González, Hugo Cerecetto\* and Homero Rubbo\*

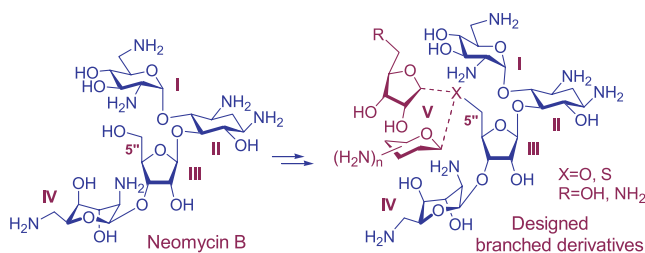
Synthesis and biological characterization of a series of products obtained by coupling  $\alpha$ -tocopherol or analogs through appropriate spacers with the NO-donor either nitrooxy or furoxan moieties.



### Branched aminoglycosides: Biochemical studies and antibacterial activity of neomycin B derivatives

pp 5797–5807

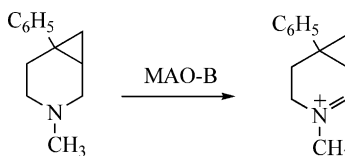
Mariana Hainrichson, Varvara Pokrovskaya, Dalia Shallom-Shezifi, Micha Fridman, Valery Belakhov, Dina Shachar, Sima Yaron and Timor Baasov\*



### A novel and selective monoamine oxidase B substrate

pp 5808–5813

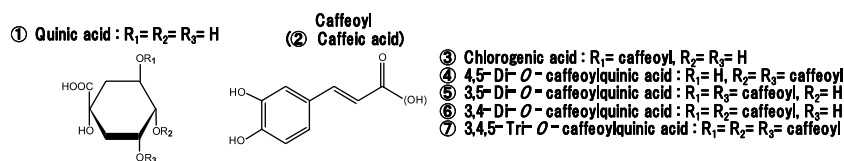
John M. Rimoldi,\* Satish G. Puppali, Emre Isin, Philippe Bissel, Ashraf Khalil and Neal Castagnoli, Jr.\*



### Identification of caffeoylquinic acid derivatives from Brazilian propolis as constituents involved in induction of granulocytic differentiation of HL-60 cells

pp 5814–5818

Satoshi Mishima, Yoshikazu Inoh, Yukio Narita, Shozo Ohta, Takashi Sakamoto, Yoko Araki, Kazu-Michi Suzuki,\* Yukihiro Akao and Yoshinori Nozawa

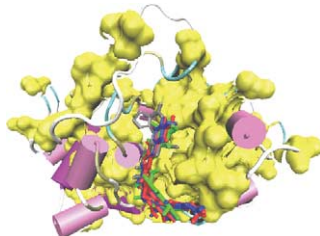


Caffeoylquinic acid derivatives (④–⑦) induced granulocytic differentiation of HL-60 cells.

**Amentoflavone and its derivatives as novel natural inhibitors of human Cathepsin B**

pp 5819–5825

Xulin Pan, Ninghua Tan,\* Guangzhi Zeng, Yumei Zhang and Ruirui Jia



The structure–activity relationship (SAR) and binding mechanism of three biflavones amentoflavone (AMF1), 4'''-methylamentoflavone (AMF2) and 7',4'''-dimethylamentoflavone (AMF3) were elucidated by density functional theory (DFT) method as well as FlexX methods.

**Calorimetric and computational study of enthalpy of formation of 3,6-dibutanoic-1,2,4,5-tetroxane**

pp 5826–5829

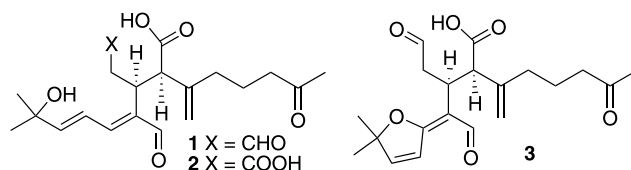
J. M. Romero, D. A. Ayala, N. L. Jorge, M. E. Gómez-Vara, E. A. Castro\* and A.H. Jubert

A thermochemical method, a rather simple experimental technique, is used to determine the enthalpy of the formation of 3,6-dibutanoic-1,2,4,5-tetroxane. The study is complemented with suitable theoretical calculations at the semiempirical and ab initio levels. A particular satisfactory agreement between both ways is found for the ab initio calculation at the 6-311G basis set level. Some possible extensions of the present procedure are pointed out.

**Four diterpenoid inhibitors of Cdc25B phosphatase from a marine anemone**

pp 5830–5834

Shugeng Cao, Caleb Foster, John S. Lazo and David G. I. Kingston\*

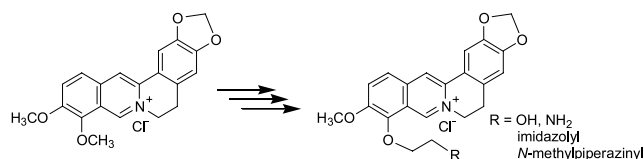


New diterpenoids from a sea anemone of the order Actiara are active against Cdc25B phosphate.

**Synthesis and DNA-binding affinities of monomodified berberines**

pp 5835–5840

Ji-Yan Pang, Yong Qin, Wen-Hua Chen,\* Guo-An Luo and Zhi-Hong Jiang\*

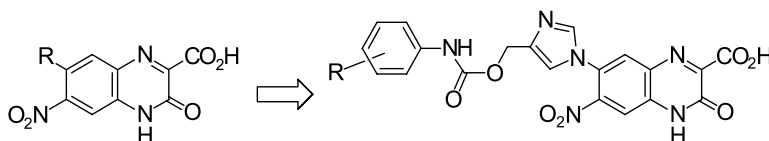


Four new monomodified berberine derivatives have been synthesized in moderate to good yields and have been shown to bind strongly to calf-thymus DNA, presumably via an intercalation mechanism.

**Design, synthesis, and AMPA receptor antagonistic activity of a novel 6-nitro-3-oxoquinoxaline-2-carboxylic acid with a substituted phenyl group at the 7 position**

pp 5841–5863

Yasuo Takano,\* Futoshi Shiga, Jun Asano, Naoki Ando, Hideharu Uchiki, Kazunori Fukuchi and Tsuyosi Anraku

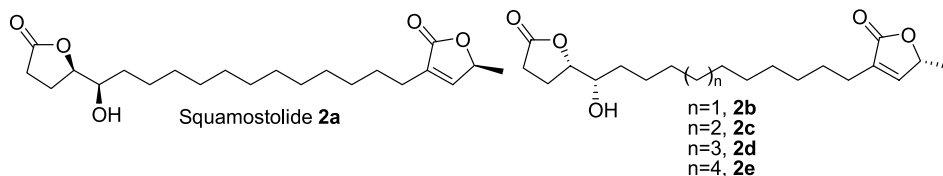


We describe the design, synthesis, and biological properties of a novel series of 6-nitro-3-oxoquinoxaline-2-carboxylic acids which bear a substituted phenyl group through a urethane linkage at the 7 position.

**Design, syntheses, and biological evaluations of squamostolide and its related analogs**

pp 5864–5872

Cheng-Lin Lee, Chi-Fong Lin, Wan-Ru Lin, Kun-Sheng Wang, Ya-her Chang, Shinne-Ren Lin, Yang-Chang Wu and Ming-Jung Wu\*

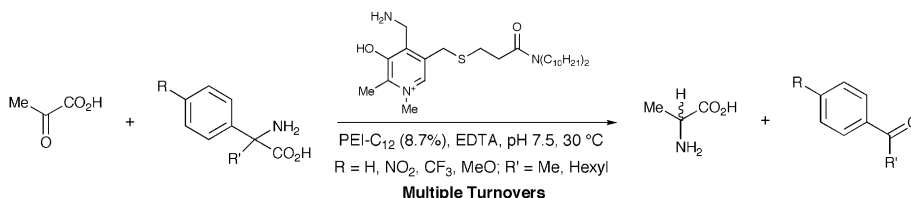


Squamostolide and its related analogs were designed and synthesized for biological evaluation. All these compounds were tested for growth inhibition activities against human tumor cell lines, in which one of the compounds showed the most potent cytotoxicity among these derivatives against a full panel of 60 human cancer cell lines. The same compound also showed G2/M phase arrest and a slightly apoptotic effect during flow cytometric analysis.

**Hydrophobic and electronic factors in the design of dialkylglycine decarboxylase mimics**

pp 5873–5883

Jason J. Chruma, Lei Liu, Wenjun Zhou and Ronald Breslow\*


**OTHER CONTENTS**

Corrigendum

Contributors to this issue

Summary of instructions to authors 2005

p 5884

p I

p II

\*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].



Full text of this journal is available, on-line from **ScienceDirect**. Visit [www.sciencedirect.com](http://www.sciencedirect.com) for more information.

---

**CONTENTS**  
**direct**

This journal is part of **ContentsDirect**, the *free* alerting service which sends tables of contents by e-mail for Elsevier books and journals. You can register for **ContentsDirect** online at: <http://contentsdirect.elsevier.com>

---

Indexed/Abstracted in: Beilstein, Biochemistry & Biophysics Citation Index, CANCERLIT, Chemical Abstracts, Chemistry Citation Index, Current Awareness in Biological Sciences/BIOBASE, Current Contents: Life Sciences, EMBASE/Excerpta Medica, MEDLINE, PASCAL, Research Alert, Science Citation Index, SciSearch, TOXFILE

---



ISSN 0968-0896