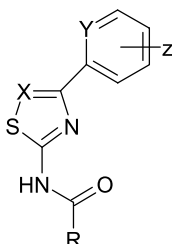


## Contents

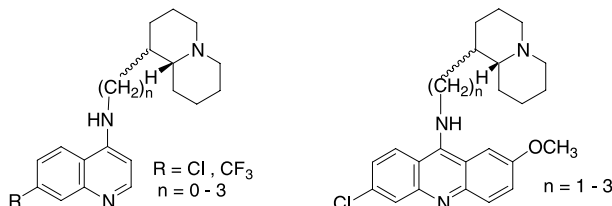
### ARTICLES

- QSAR study on thiazole and thiadiazole analogues as antagonists for the adenosine A<sub>1</sub> and A<sub>3</sub> receptors** pp 5330–5337  
Alice Borghini, Daniele Pietra, Patrick Domenichelli and Anna Maria Bianucci\*

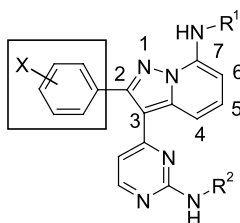


A QSAR study was carried out on thiazole and thiadiazole analogues on adenosine A<sub>1</sub> and A<sub>3</sub> receptors.

- 4-Aminoquinoline quinolizidinyl- and quinolizidinylalkyl-derivatives with antimalarial activity** pp 5338–5345  
Anna Sparatore,\* Nicoletta Basilio, Silvia Parapini, Sergio Romeo, Federica Novelli,  
Fabio Sparatore and Donatella Taramelli



- Synthesis of novel substituted 2-phenylpyrazolopyridines with potent activity against herpesviruses** pp 5346–5361  
Kristjan S. Gudmundsson,\* Brian A. Johns, Zhicheng Wang, Elizabeth M. Turner,  
Scott H. Allen, George A. Freeman, F. Leslie Boyd, Jr., Connie J. Sexton, Dean W. Selleseth,  
Kelly R. Moniri and Katrina L. Creech

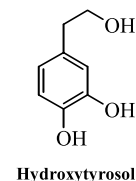
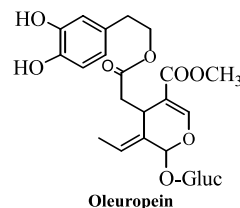


### Hypocholesterolemic effects of phenolic-rich extracts of *Chemlali* olive cultivar in rats fed a cholesterol-rich diet

pp 5362–5370

Ines Fki, Mohamed Bouaziz, Zouhair Sahnoun and Sami Sayadi\*

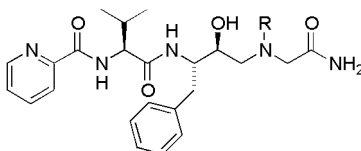
This study examined the lipid-lowering effect of *Chemlali* green and black olive extracts with high concentrations of oleuropein and hydroxytyrosol in high-cholesterol-fed rats. The supplementation of these extracts was effective in lowering the plasma cholesterol level and enhancing the antioxidant defence system.



### Synthesis, biological evaluation, and modeling studies of inhibitors aimed at the malarial proteases plasmepsins I and II

pp 5371–5390

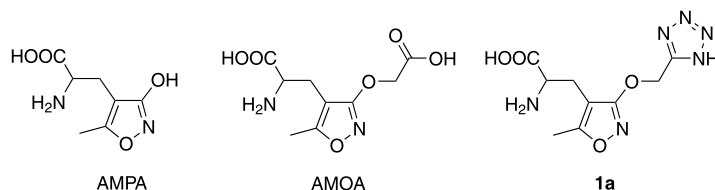
Daniel Muthas, Daniel Nöteberg, Yogesh A. Sabnis, Elizabeth Hamelink, Lotta Vrang, Bertil Samuelsson, Anders Karlén and Anders Hallberg\*



### Tetrazolyl isoxazole amino acids as ionotropic glutamate receptor antagonists: Synthesis, modelling and molecular pharmacology

pp 5391–5398

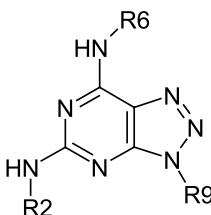
Bente Frølund,\* Jeremy R. Greenwood, Mai M. Holm, Jan Egebjerg, Ulf Madsen, Birgitte Nielsen, Hans Bräuner-Osborne, Tine B. Stensbøl and Povl Krogsgaard-Larsen



### 8-Azapurines as new inhibitors of cyclin-dependent kinases

pp 5399–5407

Libor Havlicek, Kveta Fuksova, Vladimir Krystof, Martin Orsag, Borivoj Vojtesek and Miroslav Strnad\*

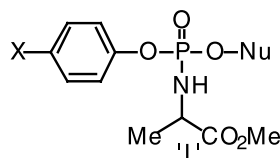


2,6,9-Trisubstituted 8-azapurines as new inhibitors of cyclin-dependent kinase 2 were synthesized and their biochemical properties were evaluated.

**Effect of change in nucleoside structure on the activation and antiviral activity of phosphoramidate derivatives**

pp 5408–5423

T. K. Venkatachalam, P. Samuel, S. Qazi and F. M. Uckun\*



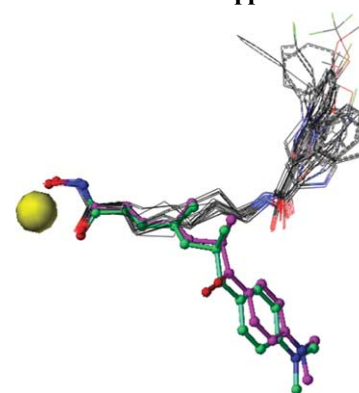
Changing the nucleoside group of a series of phosphoramidate derivatives affects the enzyme mediated hydrolysis rate of the compounds. d4T and AZT-substituted analogs were activated by enzymes such as lipases, esterases, and proteases. On the other hand, 3dT-substituted derivatives were comparatively less prone to hydrolysis under similar experimental conditions. Also, we show that d4T derivatives were more active compared to the AZT and 3dT derivatives.

**Exploration of a binding mode of indole amide analogues as potent histone deacetylase inhibitors and 3D-QSAR analyses**

pp 5424–5434

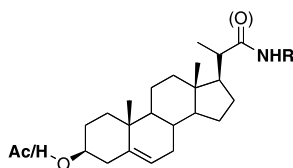
Yanshen Guo, Jingfa Xiao, Zongru Guo,\* Fengming Chu, Yonghao Cheng and Song Wu

Docking simulations and 3D-QSAR analyses were conducted on a series of indole amide analogues as potent HDAC inhibitors. Based on the docking results, a novel binding mode in the human HDAC1 catalytic core is presented, and enzyme/inhibitor interactions and discussed. Based on the binding mode, predictive 3D-QSAR models were established.

**Preparation of transition-state analogues of sterol 24-methyl transferase as potential anti-parasitics**

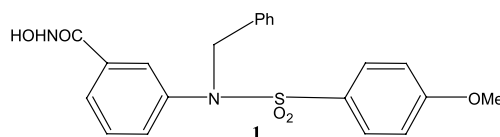
pp 5435–5453

Silvia Orenes Lorente, Carmen Jimenez Jimenez, Ludovic Gros, Vanessa Yardley, Kate de Luca-Fradley, Simon L. Croft, Julio A. Urbina, Luis M. Ruiz-Perez, Dolores Gonzalez Pacanowska and Ian H. Gilbert\*

**A quantitative structure–activity relationship study on some series of anthranilic acid-based matrix metalloproteinase inhibitors**

pp 5454–5462

S. P. Gupta\* and S. Kumaran

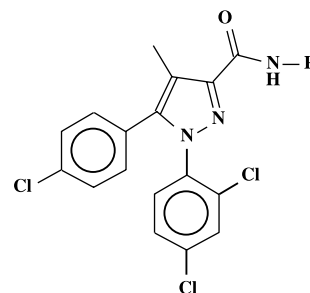


A QSAR study has been made on four different series of anthranilic acid-based matrix metalloproteinase inhibitors as represented by **1** to find that the sulfonamide group plays a very important role in the inhibition activity of these inhibitors.

**Synthesis of long-chain amide analogs of the cannabinoid CB1 receptor antagonist  
*N*-(piperidinyl)-5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-4-methyl-1*H*-pyrazole-3-carboxamide  
 (SR141716) with unique binding selectivities and pharmacological activities**

pp 5463–5474

Brian F. Thomas,\* Ma. Elena Y. Francisco, Herbert H. Seltzman, James B. Thomas,  
 Scott E. Fix, Anne-Kathrin Schulz, Anne F. Gilliam, Roger G. Pertwee and  
 Leslie A. Stevenson

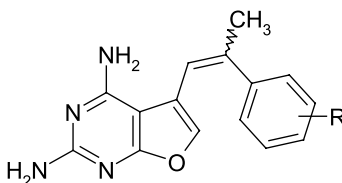


Cannabinoid receptor antagonists/inverse agonists.

**Novel 5-substituted, 2,4-diaminofuro[2,3-*d*]pyrimidines as multireceptor tyrosine kinase  
 and dihydrofolate reductase inhibitors with antiangiogenic and antitumor activity**

pp 5475–5491

Aleem Gangjee,\* Yibin Zeng, Michael Ihnat, Linda A. Warnke, Dixy W. Green,  
 Roy L. Kisliuk and Fu-Tyan Lin

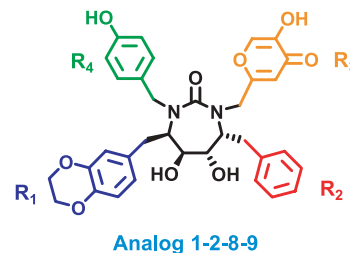


**Combinatorial design of nonsymmetrical cyclic urea inhibitors of aspartic protease of HIV-1**

pp 5492–5501

Vladimir Frecer, Enrico Burello and Stanislav Miertus\*

We have designed a focused virtual library of fully nonsymmetrical cyclic urea inhibitors of aspartic protease of HIV-1. Target-specific scoring function, parameterized for a QSAR training set of known inhibitors, was used to predict the inhibition constants. The library contains virtual hits with predicted  $K_i$ s in low picomolar range endowed with a wide range of pharmacokinetic properties that may allow discovery of a potent bioavailable antiviral drug.



## OTHER CONTENTS

Corrigendum

p 5502

Contributors to this issue

p I

Summary of instructions to authors 2005

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