

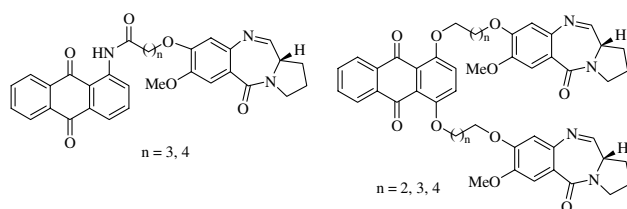
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Synthesis, DNA binding, and cytotoxicity studies of pyrrolo[2,1-c][1,4]benzodiazepine-anthraquinone conjugates

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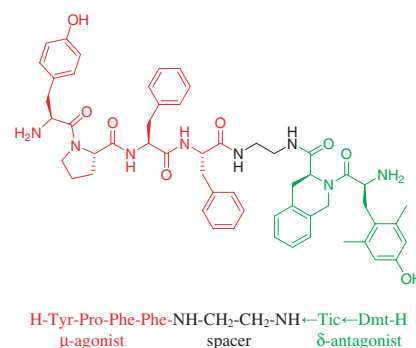
Ahmed Kamal,* R. Ramu, Venkatesh Tekumalla, G. B. Ramesh Khanna,
Madan S. Barkume, Aarti S. Juvekar and Surekha M. Zingde



A new opioid designed multiple ligand derived from the μ opioid agonist endomorphin-2 and the δ opioid antagonist pharmacophore Dmt-Tic

pp 6876–6881

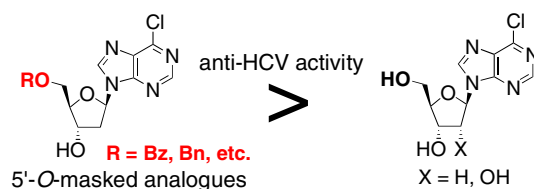
Severo Salvadori, Claudio Trapella, Stella Fiorini,
Lucia Negri, Roberta Lattanzi, Sharon D. Bryant,
Yunden Jinsmaa, Lawrence H. Lazarus and Gianfranco Balboni*



5'-O-Masked 2'-deoxyadenosine analogues as lead compounds for hepatitis C virus (HCV) therapeutic agents

pp 6882–6892

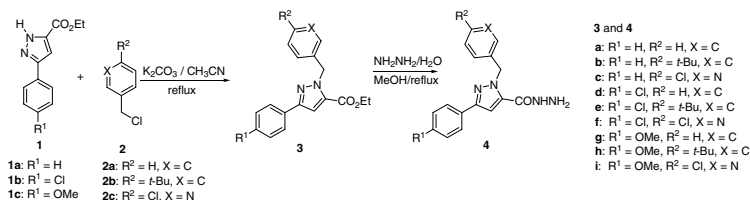
Masahiro Ikejiri, Takayuki Ohshima, Keizo Kato, Masaaki Toyama,
Takayuki Murata, Kunitada Shimotohno and Tokumi Maruyama*



Synthesis and structure–activity relationships of novel 1-arylmethyl-3-aryl-1*H*-pyrazole-5-carbohydrazide derivatives as potential agents against A549 lung cancer cells

pp 6893–6899

Yong Xia, Zhi-Wu Dong, Bao-Xiang Zhao,* Xiao Ge, Ning Meng, Dong-Soo Shin* and Jun-Ying Miao*

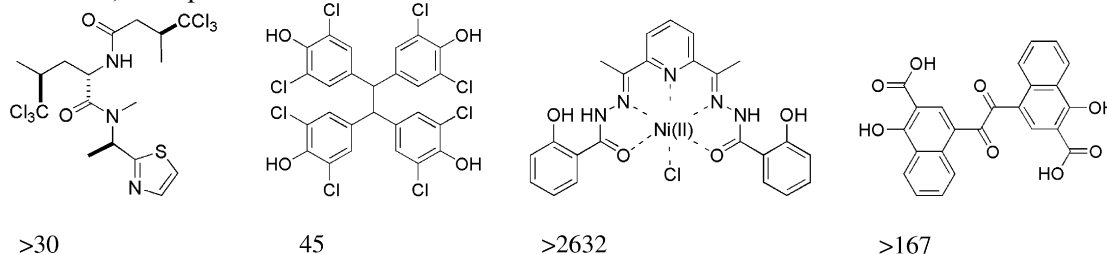


1-Arylmethyl-3-aryl-1*H*-pyrazole-5-carbohydrazide derivatives were synthesized, and their effects on A549 cell growth and apoptosis were evaluated. The structure–activity relationships and prediction of lipophilicity of compounds were studied.

Discovery of platelet-type 12-human lipoxygenase selective inhibitors by high-throughput screening of structurally diverse libraries

pp 6900–6908

Joshua D. Deschamps, Jeffrey T. Gautschi, Stephanie Whitman, Tyler A. Johnson, Nadine C. Gassner, Phillip Crews and Theodore R. Holman*

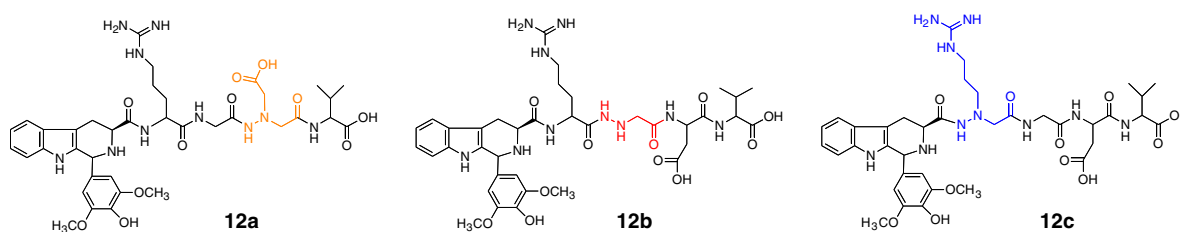


15-hLO-1/12-hLO Inhibition ratios of selective inhibitors against platelet 12-hLO.

Design, synthesis and cardioprotective effect of a new class of dual-acting agents: Phenolic tetrahydro- β -carboline RGD peptidomimetic conjugates

pp 6909–6919

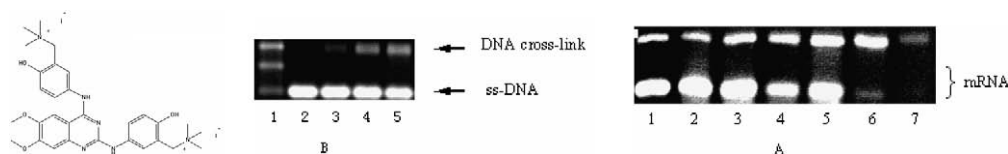
Wei Bi,* Jianhui Cai, Sanguang Liu, Michèle Baudy-Floc'h and Lanrong Bi*



Synthesis and biological activities of quinazoline derivatives with *ortho*-phenol-quaternary ammonium salt groups

pp 6920–6926

Lixia Zhang, Lige Ren, Minghui Bai, Liwei Weng, Jing Huang, Lin Wu, Minggang Deng and Xiang Zhou*



One phenol-quaternary ammonium salt derivative with a flexible linker and three derivatives with a quinazoline moiety were present. Their binding affinities for DNA were discussed and it is clearly demonstrated that this class of phenol-quaternary ammonium salt derivatives could inhibit DNA transcription effectively.

α -Diaminobutyric acid-linked hairpin polyamides

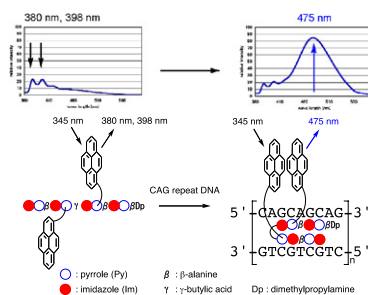
pp 6927–6936

Michelle E. Farkas, Sherry M. Tsai and Peter B. Dervan*

**Detection of CAG repeat DNA sequences by pyrene-functionalized pyrrole-imidazole polyamides**

pp 6937–6942

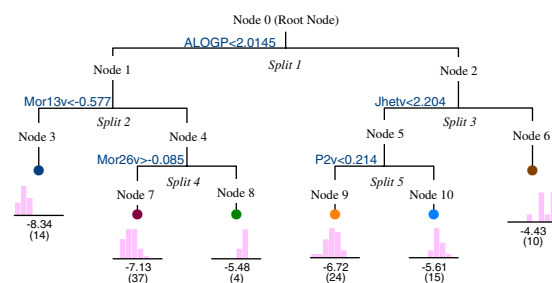
Toshikazu Bando,* Jun Fujimoto, Masafumi Minoshima, Ken-ichi Shinohara, Shunta Sasaki, Gengo Kashiwazaki, Masatoshi Mizumura and Hiroshi Sugiyama*

**Transdermal penetration behaviour of drugs: CART-clustering, QSPR and selection of model compounds**

pp 6943–6955

Bram Baert, Eric Deconinck, Mireille Van Gele, Marian Slodicka, Paul Stoppie, Samuel Bodé, Guido Slegers, Yvan Vander Heyden, Jo Lambert, Johan Beetens and Bart De Spiegeleer*

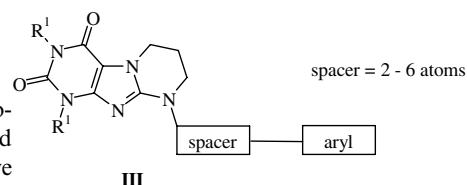
Transdermal penetration was studied as a function of selected descriptors in QSPR using CART, boosted CART and MLR models.

**Phenylethyl-substituted pyrimido[2,1-f]purinediones and related compounds: Structure–activity relationships as adenosine A₁ and A_{2A} receptor ligands**

pp 6956–6974

Anna Drabczyńska, Christa E. Müller, Anke Schiedel, Britta Schumacher, Janina Karolak-Wojciechowska, Andrzej Fruziński, Weronika Zobnina, Olga Yuzlenko and Katarzyna Kieć-Kononowicz*

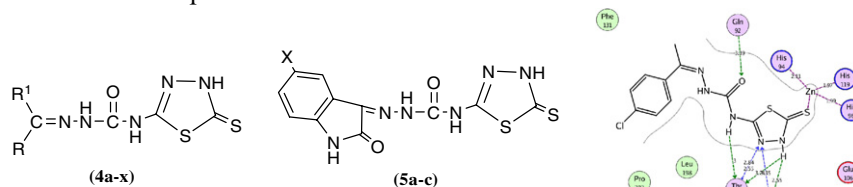
A series of arylpyrimido[2,1-f]purinediones containing varied (with carbon and heteroatoms) spacer between tricyclic scaffold and (un)substituted aryl was synthesized and evaluated for their adenosine receptor affinity and anticonvulsant activity. Mainly selective adenosine A_{2A} receptor antagonists were identified especially among structures with 2–3 carbon atoms spacer. Ligands for A₁ AR were found as well, however without selectivity towards A_{2A}AR. Investigated compounds were devoid of anticonvulsant activity.



Design, synthesis, and docking studies of new 1,3,4-thiadiazole-2-thione derivatives with carbonic anhydrase inhibitory activity

pp 6975–6984

Mohammed K. Abdel-Hamid,* Atef A. Abdel-Hafez, Nawal A. El-Koussi, Nadia M. Mahfouz, Alessio Innocenti and Claudiu T. Supuran



New series of 1,3,4-thiadiazole-thione derivatives was synthesized and tested for their carbonic anhydrase (CA) inhibitory activities. The tested compounds were docked into the CA II active site using MOE software.

Synthesis and evaluation of chloromethyl sulfoxides as a new class of selective irreversible cysteine protease inhibitors

pp 6985–6993

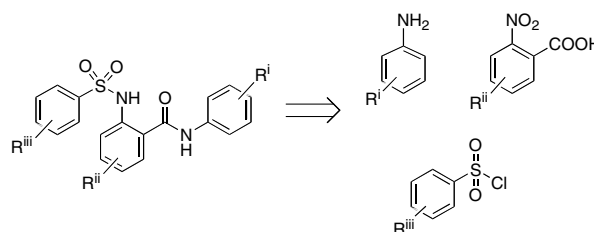
Arwin J. Brouwer, Anton Bunschoten and Rob M. J. Liskamp*



Inhibitors of type III secretion in *Yersinia*: Design, synthesis and multivariate QSAR of 2-arylsulfonylamino-benzanilides

pp 6994–7011

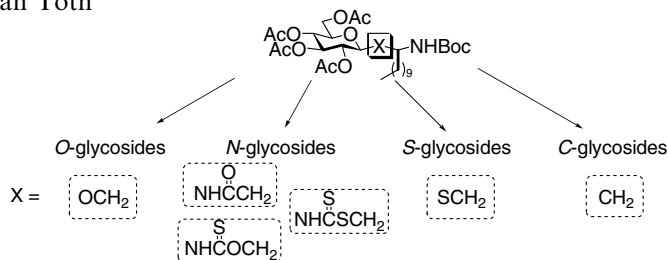
Anna M. Kauppi, C. David Andersson, Henrik A. Norberg, Charlotta Sundin, Anna Linusson and Mikael Elofsson*



Design, synthesis and biological evaluation of novel lipoamino acid-based glycolipids for oral drug delivery

pp 7012–7020

Robert A. Falconer and Istvan Toth*



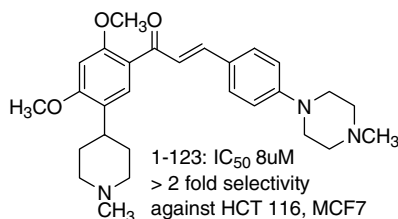
The design and synthesis of a series of lipoamino acid-based glycolipids is described.



Antiproliferative activity of chalcones with basic functionalities

pp 7021–7034

Xiaoling Liu and Mei-Lin Go*



Basic groups on the chalcone template influenced key physicochemical parameters for antiproliferative activity and possibly, the mode of antiproliferative activity.

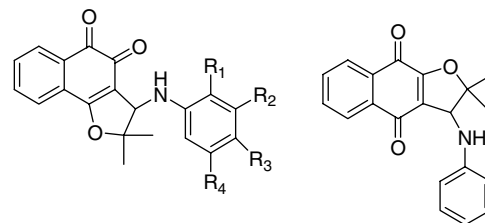


Synthesis and potent antitumor activity of new arylamino derivatives of nor-β-lapachone and nor-α-lapachone

pp 7035–7041

Eufrânio N. da Silva Júnior, Maria Cecília B. V. de Souza, Antônio V. Pinto, Maria do Carmo F. R. Pinto, Marília O. F. Goulart, Francisco W. A. Barros, Claudia Pessoa, Leticia V. Costa-Lotufo, Raquel C. Montenegro, Manoel O. de Moraes and Vitor F. Ferreira*

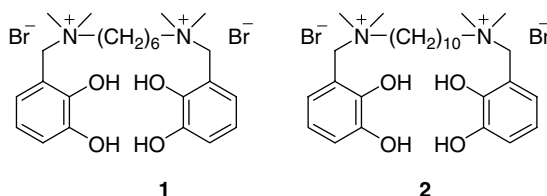
Several arylamino derivatives of nor-β-lapachone and one derivative of nor-α-lapachone were synthesized in moderate to high yields and found to show very potent cytotoxicity against six neoplastic cancer cells: SF-295 (central nervous system), HCT-8 (colon), MDAMB-435 (breast), HL-60 (leukemia), PC-3 (prostate) and B-16 (murine melanoma), with IC₅₀ below 1 μg/mL.



Inhibition of choline transport by redox-active cholinomimetic bis-catechol reagents

pp 7042–7047

Shuang Cai, Jhingan Mukherjee, L. M. Viranga Tillekeratne, Richard A. Hudson and Jon R. Kirchhoff*

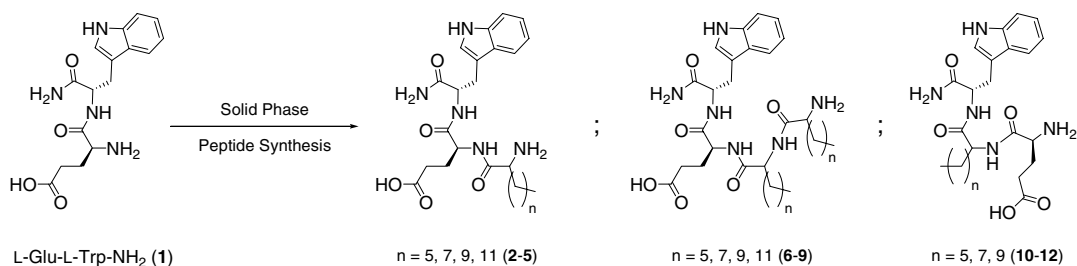


Two symmetrical bis-catechol substituted hexamethonium and decamethonium analogues were found to inhibit high-affinity choline transport in mouse brain synaptosomes. Inhibition parameters were evaluated and compared with known mono-catechol derivatives.

Enhancement of oral drug absorption—Effect of lipid conjugation on the enzymatic stability and intestinal permeability of L-Glu-L-Trp-NH₂

pp 7048–7057

Julie A. Bergeon and Istvan Toth*

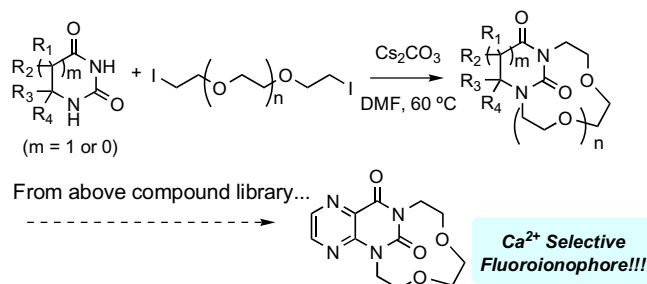


A versatile strategy for the synthesis of crown ether-bearing heterocycles: Discovery of calcium-selective fluoroionophore

pp 7108–7115

Yuko Aoki, Naoki Umezawa, Yuko Asano, Keiichiro Hatano, Yuki Yano, Nobuki Kato and Tsunehiko Higuchi*

A simple and versatile synthesis of crown ether-bearing heterocycles was achieved. Among the molecules synthesized, we found a Ca^{2+} -selective fluoroionophore.

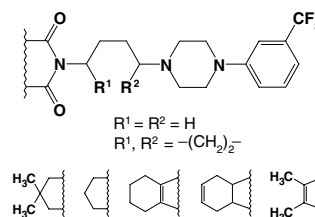


The influence of modifications in imide fragment structure on 5-HT_{1A} and 5-HT₇ receptor affinity and in vivo pharmacological properties of some new 1-(*m*-trifluoromethylphenyl)piperazines

pp 7116–7125

Maria H. Paluchowska,* Ryszard Bugno, Beata Duszyńska, Ewa Tatarczyńska, Agnieszka Nikiforuk, Tomasz Lenda and Ewa Chojnacka-Wójcik

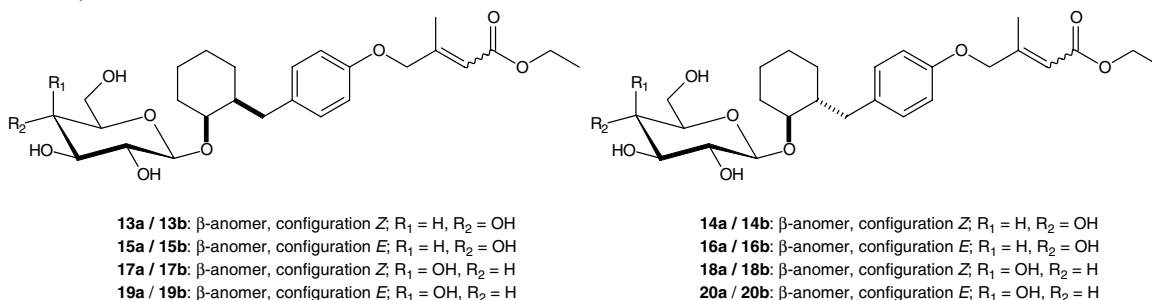
New, flexible and rigid 1-(*m*-trifluorophenyl)piperazines with very high affinity and agonistic in vivo activity for 5-HT_{1A} receptors were synthesized. Flexible compounds also bound to 5-HT₇ receptors. Two of tested glutarimides demonstrated anxiolytic- and antidepressant-like activity in the pharmacological tests.



Glycosidic juvenogens: Derivatives bearing α,β -unsaturated ester functionalities

pp 7126–7137

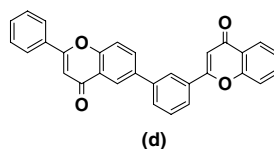
Zdeněk Wimmer,* Lucie Pechová, Laura Sile, David Šaman, Pavel Jedlička, Martina Wimmerová and Erkki Kolehmainen



Inhibitory effect of synthetic C–C biflavones on various phospholipase A₂s activity

pp 7138–7143

Tae Chul Moon, Zhejiu Quan, Jeongsoo Kim, Hyun Pyo Kim, Ichiro Kudo, Makodo Murakami, Haeil Park* and Hyeun Wook Chang*

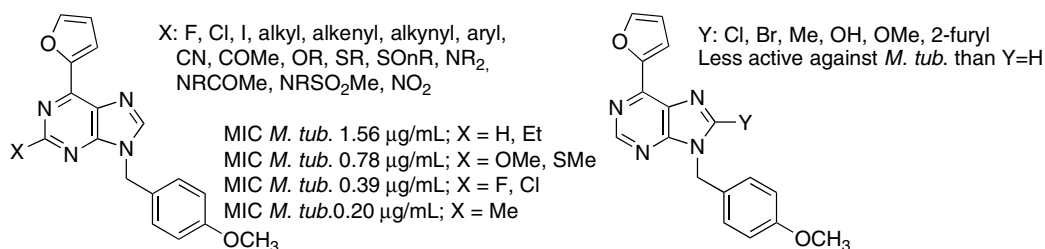


Several C–C biflavones (**a–f**) were synthesized and evaluated for their inhibitory activity against phospholipase A₂s (PLA₂s) activity. The synthetic C–C biflavones showed rather different inhibitory activity against various sPLA₂s. Most synthetic C–C biflavonoids exhibited potent and broad inhibitory activity against various PLA₂s tested regardless of their structural array. In particular, of natural and synthetic biflavonoids tested, the synthetic C–C biflavonoid (**d**) only showed inhibitory activity against sPLA₂ X. None of the natural and synthetic biflavonoids tested showed inhibitory activity against sPLA₂ IB.

Synthesis, biological activity, and SAR of antimycobacterial 2-and 8-substituted 6-(2-furyl)-9-(*p*-methoxybenzyl)purines

pp 7144–7165

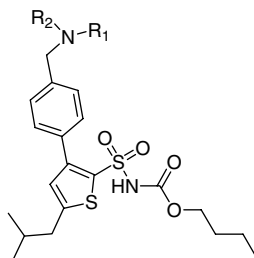
Morten Brændvang and Lise-Lotte Gundersen*



Selective angiotensin II AT₂ receptor agonists devoid of the imidazole ring system

pp 7166–7183

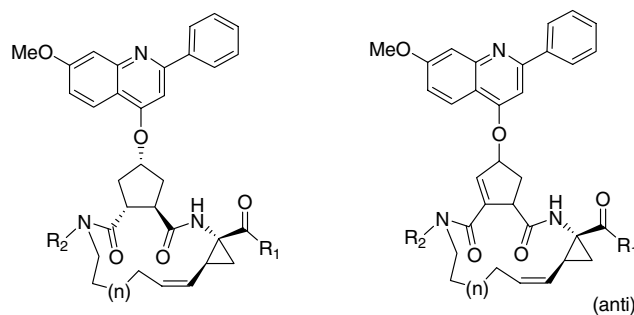
A. M. S. Murugaiah, Chalotta Wallinder, A. K. Mahalingam, Xiongyu Wu, Yiqian Wan, Bianca Plouffe, Milad Botros, Anders Karlén, Mathias Hallberg, Nicole Gallo-Payet and Mathias Alterman*



Novel potent macrocyclic inhibitors of the hepatitis C virus NS3 protease: Use of cyclopentane and cyclopentene P2-motifs

pp 7184–7202

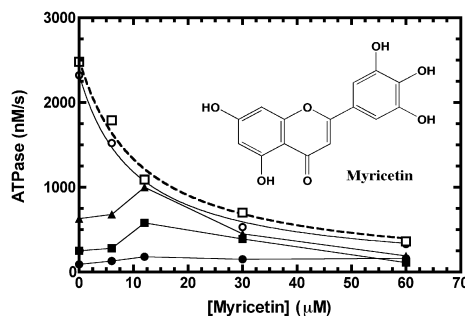
Marcus Bäck, Per-Ola Johansson, Fredrik Wängsell, Fredrik Thorstensson, Ingemar Kvarnström, Susana Ayesa, Horst Wähling, Mikael Pelcman, Katarina Jansson, Stefan Lindström, Hans Wallberg, Björn Classon, Christina Rydberg, Lotta Vrang, Elizabeth Hamelink, Anders Hallberg, Asa Rosenquist* and Bertil Samuelsson*



Myricetin inhibits *Escherichia coli* DnaB helicase but not primase

pp 7203–7208

Mark A. Griep,* Sheldon Blood, Marilyn A. Larson, Scott A. Koepsell and Steven H. Hinrichs

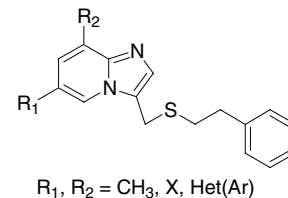


Influence of 6 or 8-substitution on the antiviral activity of 3-phenethylthiomethylimidazo[1,2-*a*]pyridine against human cytomegalovirus (HCMV) and varicella-zoster virus (VZV)

pp 7209–7219

Jean-Baptiste Véron, Cécile Enguehard-Gueiffier, Robert Snoeck, Graciela Andrei, Erik De Clercq and Alain Gueiffier*

From the synthesized compounds, the 6-halogeno and 6-phenylimidazo[1,2-*a*]pyridine derivatives emerged as the most potent inhibitors of HCMV and VZV replication; these compounds showed the same range of activities against TK⁺ and TK⁻ VZV strains, demonstrating a mechanism of action independent of the viral thymidine kinase.

**OTHER CONTENTS**

Summary of instructions to authors

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*Corresponding author

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

Terfenadine (an antihistamine pulled from the market in 1997) bound to a model of an open form of the homo-tetrameric pore domain of hERG, produced using Schrödinger's "Induced Fit Docking" technology [Farid, R.; Day, T.; Friesner, R. A.; Pearlstein, R. A. *Bioorg. Med. Chem.* **2006**, *14*, 3160–3173].

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