

European Journal of Medicinal Chemistry Vol 43, No 8, 2008

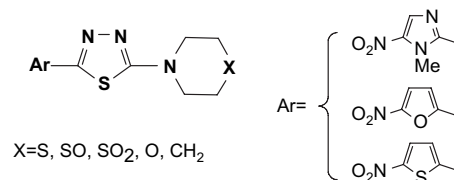
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ORIGINAL ARTICLES

- Synthesis and in vitro anti-*Helicobacter pylori* activity of *N*-[5-(5-nitro-2-heteroaryl)-1,3,4-thiadiazol-2-yl]thiomorpholines and related compounds** pp. 1575–1580

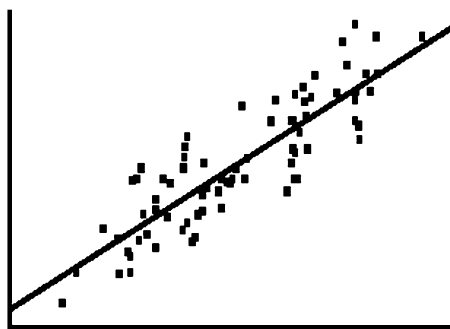
Javad Mirzaei, Farideh Siavoshi, Saeed Emami, Fatemeh Safari,
Mohammad Reza Khoshayand, Abbas Shafiee and Alireza Foroumadi*

Synthesis and in vitro anti-*Helicobacter pylori* activity of *N*-[5-(5-nitro-2-heteroaryl)-1,3,4-thiadiazol-2-yl]thiomorpholines and some related compounds **8a–c** and **9a–c** were described.



- In silico* prediction of brain and CSF permeation of small molecules using PLS regression models** pp. 1581–1592

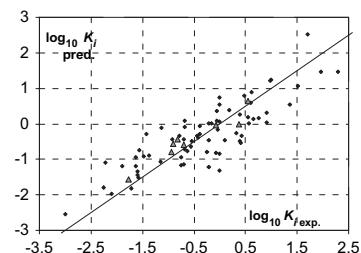
Stefanie Bendels*, Manfred Kansy, Björn Wagner and Jörg Huwyler



- QSAR modeling of the interaction of flavonoids with GABA(A) receptor** pp. 1593–1602

Pablo R. Duchowicz*, Martín G. Vitale, Eduardo A. Castro, Juan C. Autino,
Gustavo P. Romanelli and Daniel O. Bennardi

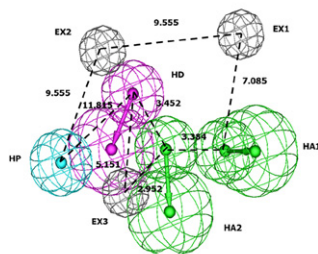
QSAR analysis for the interaction of 78 flavone derivatives based on linear combinations of Dragon molecular descriptors. Results are compared with previously reported ones.



A three-dimensional pharmacophore model for dipeptidyl peptidase IV inhibitors

pp. 1603–1611

I-Lin Lu, Keng-Chang Tsai, Yi-Kun Chiang, Weir-Torn Jiaang, Ssu-Hui Wu,
Neeraj Mahindroo, Chia-Hui Chien, Shiow-Ju Lee, Xin Chen, Yu-Sheng Chao and Su-Ying Wu*

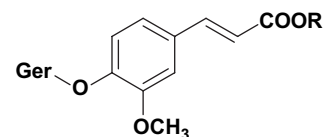


Effects of 3-(4'-geranyloxy-3'-methoxyphenyl)-2-trans propenoic acid and its ester derivatives on biofilm formation by two oral pathogens, *Porphyromonas gingivalis* and *Streptococcus mutans*

pp. 1612–1620

Charles Bodet, Francesco Epifano, Salvatore Genovese, Massimo Curini and Daniel Grenier*

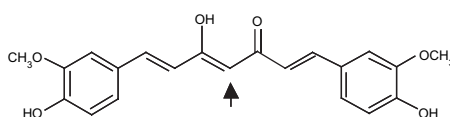
The synthesis of esters between 3-(4'-geranyloxy-3'-methoxyphenyl)-2-trans propenoic acid and natural alcohols and phenols exerting inhibition on biofilm formation by *Porphyromonas gingivalis* and *Streptococcus mutans* is reported.



Structure–activity relationships for the inhibition of recombinant human cytochromes P450 by curcumin analogues

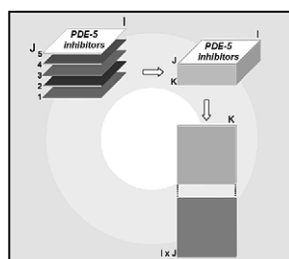
pp. 1621–1631

Regina Appiah-Opong, Iwan de Esch, Jan N.M. Commandeur, Mayagustina Andarini and Nico P.E. Vermeulen*

**Bioactivities of a series of phosphodiesterase type 5 (PDE-5) inhibitors as modelled by MIA-QSAR**

pp. 1632–1638

João E. Antunes, Matheus P. Freitas* and Roberto Rittner

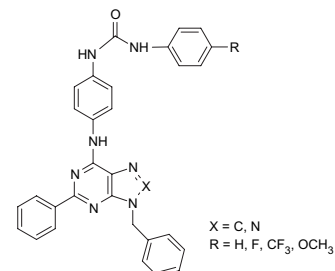


N⁶-1,3-Diphenylurea derivatives of 2-phenyl-9-benzyladenines and 8-azaadenines: Synthesis and biological evaluation as allosteric modulators of A_{2A} adenosine receptors

pp. 1639–1647

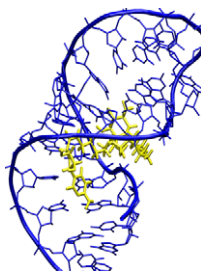
Irene Giorgi*, Giuliana Biagi, Anna Maria Bianucci, Alice Borghini, Oreste Livi, Michele Leonardi, Daniele Pietra, Vincenzo Calderone and Alma Martelli

It was found that some of these compounds can act as positive enhancers of agonist and antagonist radioligands for A_{2A} adenosine receptors; other compounds can act as negative modulators.

**Flexible computational docking studies of new aminoglycosides targeting RNA 16S bacterial ribosome site**

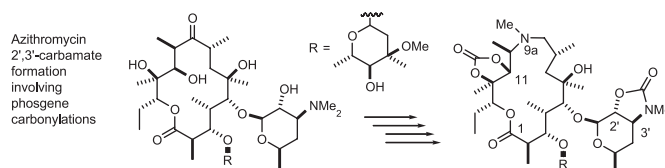
pp. 1648–1656

Florent Barbault*, Bo Ren, Joseph Rebehmed, Catia Teixeira, Yun Luo, Ornella Smila-Castro, François Maurel, BoTao Fan, Liangren Zhang** and Lihe Zhang

**Preparation and antibacterial activity of cyclic 2',3'-carbamate derivatives of azithromycin**

pp. 1657–1664

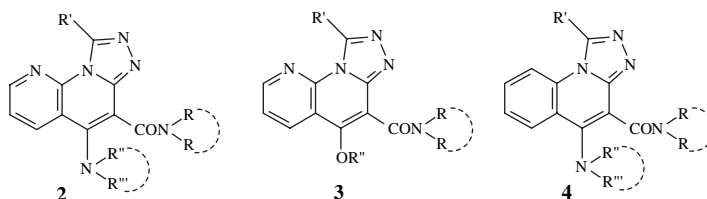
Audun Heggelund, Christian Rømming and Kjell Undheim*

**1,8-Naphthyridines VII. New substituted 5-amino[1,2,4]triazolo[4,3-a][1,8]naphthyridine-6-carboxamides and their isosteric analogues, exhibiting notable anti-inflammatory and/or analgesic activities, but no acute gastrolesivity**

pp. 1665–1680

Giorgio Roma*, Giancarlo Grossi, Mario Di Braccio, Daniela Piras, Vigilio Ballabeni, Massimiliano Tognolini, Simona Bertoni and Elisabetta Barocelli

A number of new substituted 5-amino[1,2,4]triazolo[4,3-a][1,8]naphthyridine-6-carboxamides **2** and some of their isosteric analogues **3** and **4** were synthesized. Many compounds **2** showed notable analgesic and/or potent anti-inflammatory activities. Lower but interesting activities were exhibited by compounds **4**, whereas the 5-alkoxy substituted compounds **3** were clearly less active.

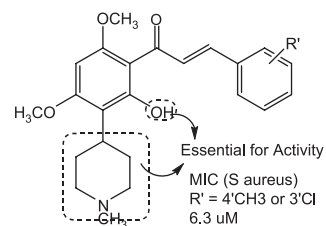


Functionalized chalcones with basic functionalities have antibacterial activity against drug sensitive *Staphylococcus aureus*

pp. 1681–1687

X.L. Liu, Y.J. Xu and M.L. Go*

Chalcones with phenolic OH and basic heterocyclic rings had antibacterial activities comparable to lico-chalcone A (MIC 6.3 μ M *S. aureus*) and protected erythrocytes from hemolysis at 100 μ M.



Synthesis, characterization, antioxidant activity and DNA-binding studies of two rare earth(III) complexes with naringenin-2-hydroxy benzoyl hydrazone ligand

pp. 1688–1695

Tian-Rong Li, Zheng-Yin Yang*, Bao-Dui Wang and Dong-Dong Qin

Two novel rare earth complexes were synthesized and characterized. DNA-binding studies show that the metal complexes and the ligand can strongly bind to calf thymus DNA via an intercalation mechanism.

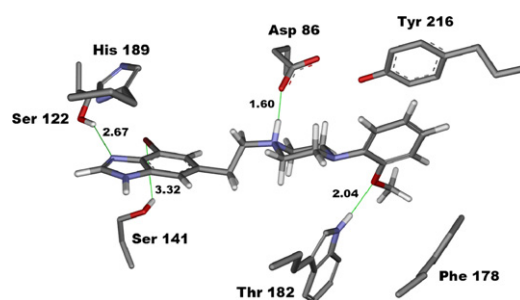


Synthesis, binding properties and receptor docking of 4-halo-6-[2-(4-arylpiperazin-1-yl)ethyl]-1H-benzimidazoles, mixed ligands of D₂ and 5-HT_{1A} receptors

pp. 1696–1705

Deana Andrić, Goran Roglić, Vladimir Šukalović, Vukić Šoškić* and Sladjana Kostić-Rajačić

4-Halo-6-[2-(4-arylpiperazin-1-yl)ethyl]-1H-benzimidazoles tested in this study have moderate to high affinity for serotonin 5-HT_{1A} and D₂-like dopamine receptors. *In silico* docking analysis of selected ligands was performed in order to explain obtained results.

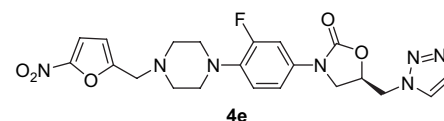


Synthesis and biological evaluation of new N-linked 5-triazolylmethyl oxazolidinones

pp. 1706–1714

Houxing Fan, Yilang Chen, Zhiteng Jiang, Shuhua Zhang, Dafang Zhong, Ruyun Ji and Yushe Yang*

A new series of oxazolidinones bearing N-linked 5-triazolylmethyl group are disclosed. The selected compounds of this series display *in vitro* and *in vivo* activities comparable to linezolid. Compound **4e** shows excellent activity against Gram-positive organisms.

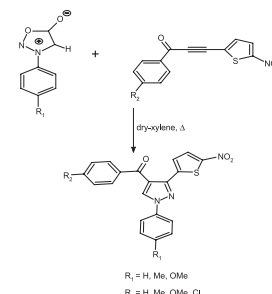


Convenient access to 1,3,4-trisubstituted pyrazoles carrying 5-nitrothiophene moiety via 1,3-dipolar cycloaddition of sydnone with acetylenic ketones and their antimicrobial evaluation

pp. 1715–1720

N. Satheesha Rai, Balakrishna Kalluraya*, B. Lingappa, Shaliny Shenoy and Vedavati G. Puranic

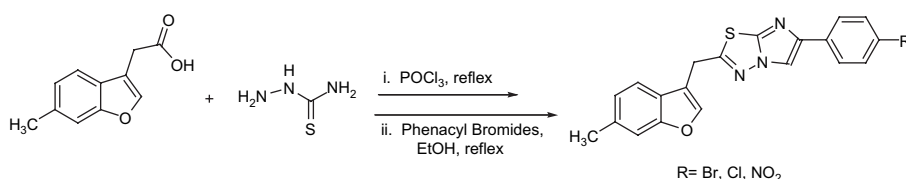
Novel 1-aryl-4-aryl-3-(5-nitro-2-thienyl) pyrazoles have been synthesized by the 1,3-dipolar cycloaddition of 3-aryl sydnone with 1-aryl-3-(5-nitro-2-thienyl)-2-propyne-1-ones.



Synthesis and anti-inflammatory evaluation of methylene bridged benzofuranyl imidazo [2,1-*b*][1,3,4]thiadiazoles

pp. 1721–1729

V.B. Jadhav, M.V. Kulkarni*, V.P. Rasal, S.S. Biradar and M.D. Vinay



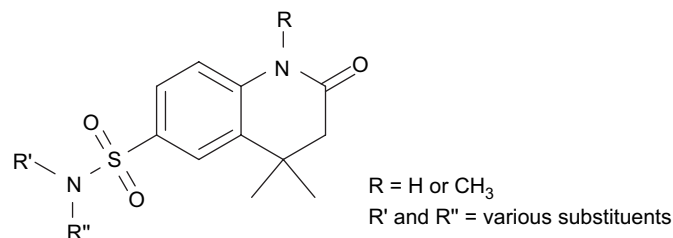
SHORT COMMUNICATIONS

Synthesis of potential Rho-kinase inhibitors based on the chemistry of an original heterocycle: 4,4-Dimethyl-3,4-dihydro-1*H*-quinolin-2-one

pp. 1730–1736

Marie-Anne Letellier, Jérôme Guillard, Daniel-Henri Caignard, Gilles Ferry, Jean A. Boutin and Marie-Claude Viaud-Massuard*

A new series of substituted 4,4-dimethyl-3,4-dihydro-1*H*-quinolin-2-one have been synthesized. The seven compounds obtained were tested in the inhibition of the Rho-kinase enzyme known to be of major importance in the cascade reactions leading to arterial hypertension.

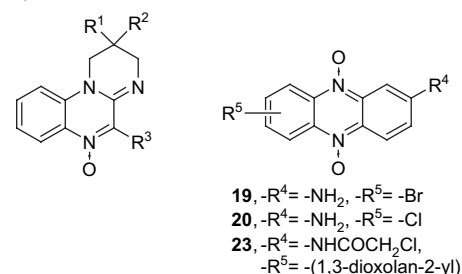


Pyrimido[1,2-*a*]quinoxaline 6-oxide and phenazine 5,10-dioxide derivatives and related compounds as growth inhibitors of *Trypanosoma cruzi*

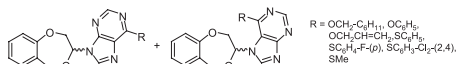
pp. 1737–1741

María Laura Lavaggi, Gabriela Aguirre, Lucía Boiani, Liliana Orelli, Beatriz García**, Hugo Cerecetto* and Mercedes González**

Two series of *N*-oxide containing heterocycles were studied as anti-*T. cruzi* agents. Phenazine 5,10-dioxide derivatives with relevant *in vitro* activity were identified.

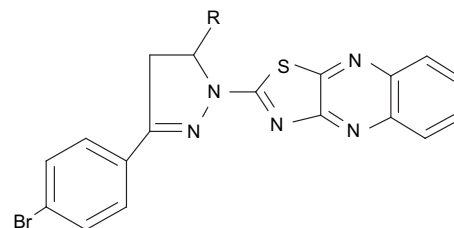


Ana Conejo-García, María C. Núñez, Juan A. Marchal, Fernando Rodríguez-Serrano, Antonia Aránega, Miguel A. Gallo, Antonio Espinosa and Joaquín M. Campos*



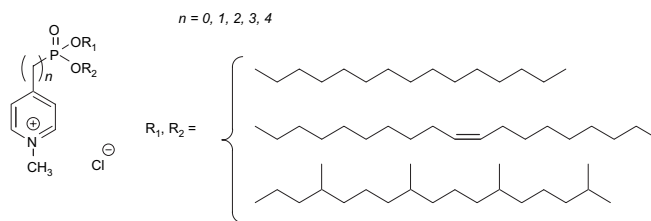
Asha Budakoti, Abdul R. Bhat, Fareeda Athar and Amir Azam*

A variety of 3-(3-bromo phenyl)-5-phenyl-1-(thiazolo [4,5-*b*] quinoxaline-2-yl)-2-pyrazoline were obtained by the refluxing of 1-*N*-thiocarbamoyl 3,5-diphenyl-2-pyrazoline with 2,3-dichloroquinoxaline. The antiamebic activity of these compounds was evaluated against *Entamoeba histolytica*. Some of the quinoxaline derivatives showed less IC₅₀ values than metronidazole. To elucidate the toxic effect, MTT assay was performed using kidney epithelial cell line. The compound **18** has lowest toxicity and highest antiamebic activity.



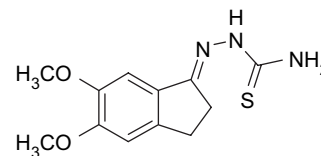
Angélique Durand Dal-Maso, Jérôme Dellacasagrande,
Frédéric Legendre, Gérard Tiraby, Casimir Blonski and Pascal Hoffmann*

A series of cationic lipids containing phosphonate esters were prepared. Lipids were assessed as vectors for transfecting DNA to various cell lines, under different conditions, in a 96-well format.



Liliana M. Finkielstein, Eliana F. Castro, Lucas E. Fabián, Graciela Y. Moltrasio*,
Rodolfo H. Campos, Lucía V. Cavallaro and Albertina G. Moglioni

The synthesis of thiosemicarbazones derived from 1-indanones active against BVDV is reported.

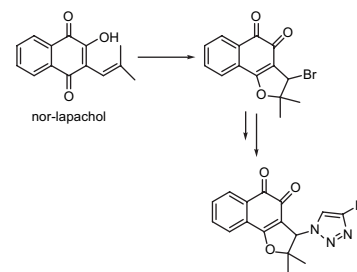


Naphthoquinoidal [1,2,3]-triazole, a new structural moiety active against *Trypanosoma cruzi*

pp. 1774–1780

Eufrânio N. da Silva, Jr., Rubem F.S. Menna-Barreto, Maria do Carmo F.R. Pinto, Raphael S.F. Silva, Daniel V. Teixeira, Maria Cecília B.V. de Souza, Carlos Alberto De Simone, Solange L. De Castro*, Vitor F. Ferreira and Antônio V. Pinto

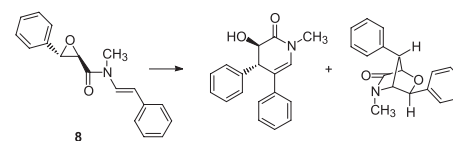
Several [1,2,3]-triazole derivatives of nor- β -lapachone were synthesized and found to display potent activity *in vitro* against *Trypanosoma cruzi*. These naphthoquinoidal triazoles emerge as interesting new lead compounds in drug development for Chagas disease.

**LABORATORY NOTES**
Study of the intramolecular cyclization of *N*-methyl-3-phenyl-*N*-(2-(*E*)-phenylethenyl)-*trans*(*cis*)-oxiranecarboxamide — Syntheses of Homoclausenamide and Dehydroclausenamide

pp. 1781–1784

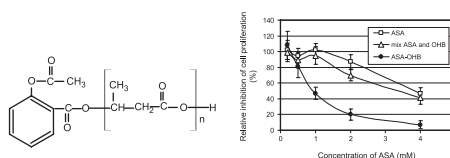
Nianchun Ma*, Kemei Wu and Liang Huang

Under Lewis acid condition, compound **8** undergoes cyclizations to give Homoclausenamide and Dehydroclausenamide.

**Oligo(3-hydroxybutanoate) conjugates with acetylsalicylic acid and their antitumour activity**

pp. 1785–1790

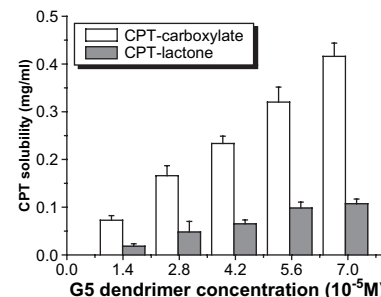
Maria Juzwa, Aleksandra Rusin, Barbara Zawidlak-Węgrzyńska, Zdzisław Krawczyk*, Ilona Obara and Zbigniew Jedliński**


Potential of poly(amidoamine) dendrimers as drug carriers of camptothecin based on encapsulation studies

pp. 1791–1795

Yiyun Cheng*, Mingzhong Li and Tongwen Xu**

Solubility of CPT (CPT-lactone and CPT-carboxylate) in the presence of G5 PAMAM dendrimers.



COVER

Overlay of the experimental and docked conformations of the ligand fluorescein in complex with an anti-fluorescein 4-4-20 Fab fragment (PDB code 1flr, 1.85 Å). The top-scoring conformation (purple) selected by the HINT force field, among the 255 poses generated by AutoDock, nearly overlays the crystallographic structure (yellow), while the conformation selected by the AutoDock scoring function (green) reverses the positions of the carbonyl and hydroxyl groups.

Image provided by Francesca Spyraakis, Alessio Amadasi, Micaela Fornabaio, Donald J. Abraham, Andrea Mozzarelli, Glen E. Kellogg, Pietro Cozzini. © 2008. Published by Elsevier Masson SAS

* Corresponding authors.

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ISSN 0223-5234