



European Journal of Medicinal Chemistry Vol 52, 2012

Contents

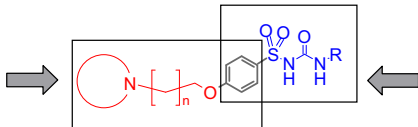
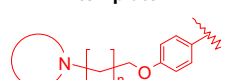
ORIGINAL ARTICLES

Novel sulfonylurea derivatives as H₃ receptor antagonists. Preliminary SAR studies

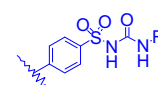
pp. 1–13

Javier Ceras, Nuria Cirauqui, Silvia Pérez-Silanes, Ignacio Aldana, Antonio Monge and Silvia Galiano*

Forty-four new sulfonylurea derivatives were designed and synthesized as an approach to finding new dual therapeutic agents for the treatment of type 2 diabetes associated with obesity. Preliminary SAR was performed.

H₃ receptor antagonism template

proposed general structure for compounds with dual activity as H₃ receptor antagonists and K_{ATP} blockers

sulfonylurea moiety for anti-diabetic drugs**Synthesis, vasorelaxant activity, and molecular modeling study of some new phthalazine derivatives**

pp. 14–21

Fadi M. Awadallah*, Wafaa I. El-Eraky and Dalia O. Saleh

Phthalazine derivatives were designed and tested for their vasorelaxant activities. Compound **8d** had an IC₅₀ = 0.10 mM. Molecular modeling, including 3D-pharmacophore and homology model as α_1 -AR antagonists was performed.

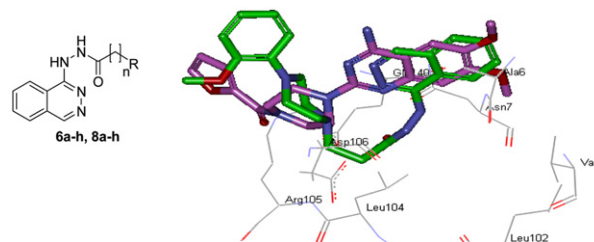
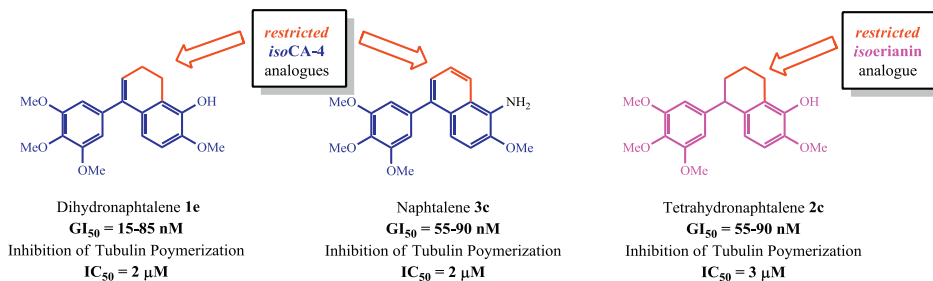


Figure 4.a. Alignment of compound **8d** (green) and prazosin (violet) in the binding site of α_1 -AR homology model.

Conformationally restricted naphthalene derivatives type isocombretastatin A-4 and isoerianin analogues: Synthesis, cytotoxicity and antitubulin activity

pp. 22–32

Evelia Rasolofonjatovo, Olivier Provot*, Abdallah Hamze, Jordi Rodrigo, Jérôme Bignon, Joanna Wdzieczak-Bakala, Déborah Desravines, Joëlle Dubois, Jean-Daniel Brion and Mouad Alami*

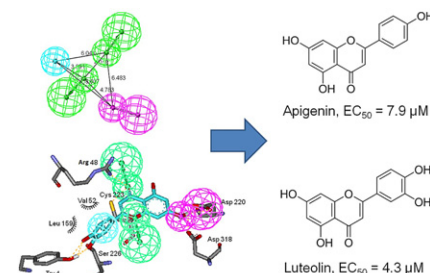


Discovery of flavonoid derivatives as anti-HCV agents via pharmacophore search combining molecular docking strategy

pp. 33–43

Ming-Ming Liu, Lu Zhou, Pei-Lan He, Yi-Nan Zhang, Jia-Yi Zhou, Qing Shen, Xin-Wen Chen, Jian-Ping Zuo^{**}, Wei Li^{*} and De-Yong Ye^{*}

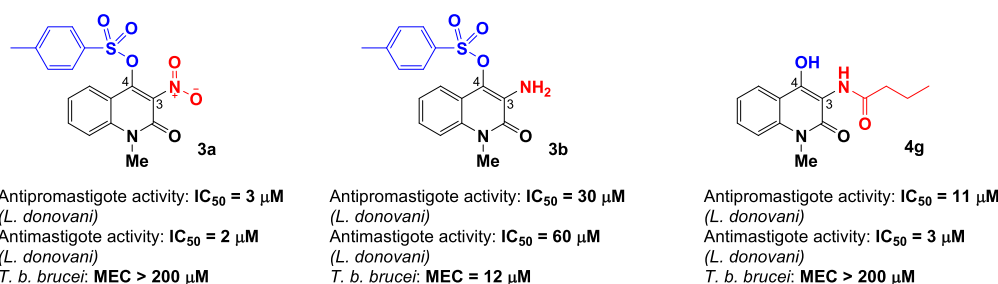
Combined pharmacophore and structure-based approaches were employed in screening novel anti-HCV candidates and 20 compounds were found to be active *in vitro* including two naturally occurring flavones.



Synthesis and antikinetoplastid activities of 3-substituted quinolinones derivatives

pp. 44–50

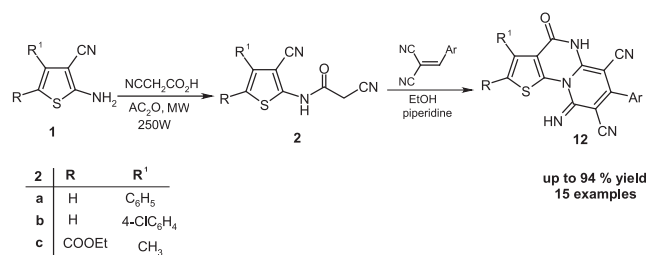
Davide Audisio, Samir Messaoudi^{*}, Sandrine Cojean^{*}, Jean-François Peyrat, Jean-Daniel Brion, Christian Bories, Françoise Huteau, Philippe M. Loiseau and Mouad Alami



2-Aminothiophenes as building blocks in heterocyclic synthesis: Synthesis and antimicrobial evaluation of a new class of pyrido[1,2-a]thieno[3,2-e]pyrimidine, quinoline and pyridin-2-one derivatives

pp. 51–65

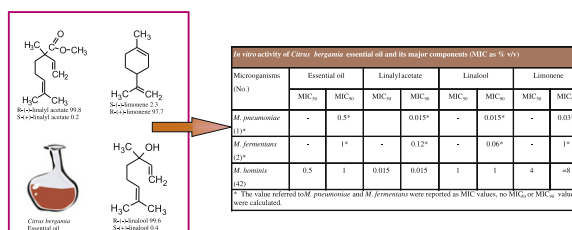
Haider Behbehani^{*}, Hamada Mohamed Ibrahim, Saad Makhseed, Mohamed H. Elnagdi and Huda Mahmoud



In vitro antimycoplasmal activity of citrus bergamia essential oil and its major components

pp. 66–69

Pio Maria Furneri^{*}, Luigi Mondello, Giuseppina Mandalari, Donatella Paolino, Paola Dugo, Adriana Garozzo and Giuseppe Bisignano

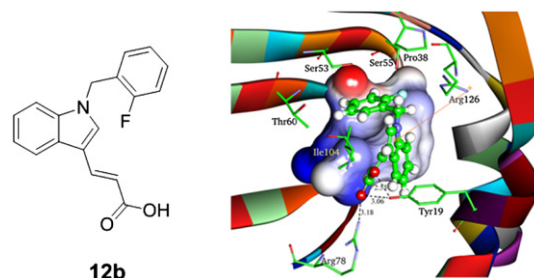


Design, synthesis and biological evaluation of thiazole- and indole-based derivatives for the treatment of type II diabetes

pp. 70–81

Qinyuan Xu, Li Huang, Juan Liu, Liang Ma, Tao Chen, Jinying Chen, Fei Peng, Dong Cao, Zhuang Yang, Neng Qiu, Jingxiang Qiu, Guangcheng Wang, Xiaolin Liang, Aihua Peng, Mingli Xiang, Yuquan Wei and Lijuan Chen*

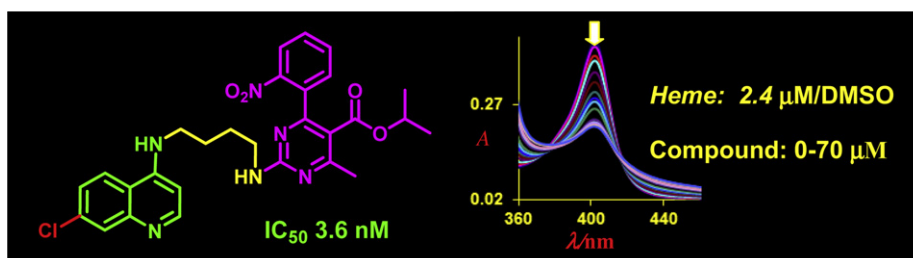
The docking **12b** to the protein of ap2 showed that it specifically binds to endogenous fatty acids include Tyr 19 and Arg 78.



2-Aminopyrimidine based 4-aminoquinoline anti-plasmodial agents. Synthesis, biological activity, structure–activity relationship and mode of action studies

pp. 82–97

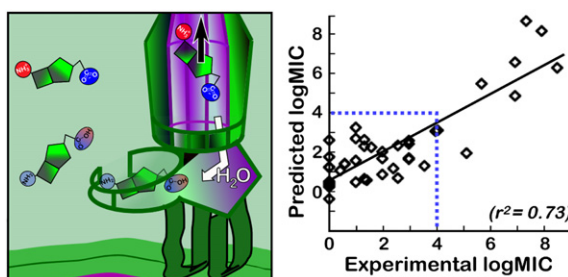
Kamaljit Singh*, Hardeep Kaur, Kelly Chibale, Jan Balzarini, Susan Little and Prasad V. Bharatam



Computational analysis of structure-based interactions and ligand properties can predict efflux effects on antibiotics

pp. 98–110

Aurijit Sarkar, Kelcey C. Anderson and Glen E. Kellogg*

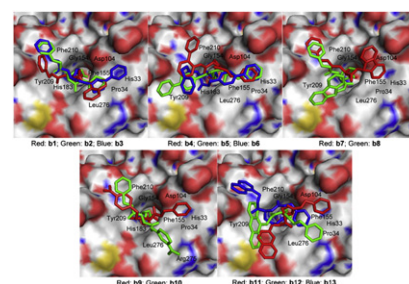


A novel series of L-2-benzoyloxycarbonylamino-8-(2-pyridyl)-disulfidylactanoic acid derivatives as histone deacetylase inhibitors: Design, synthesis and molecular modeling study

pp. 111–122

Dawei Huang, Xiaohui Li*, Yingdong Wei and Zhilong Xiu

A series of L-2-benzoyloxycarbonylamino-8-(2-pyridyl)-disulfidylactanoic acid derivatives were designed and synthesized as novel potent HDACIs, and the interactions between all compounds and HDAC2 were investigated by molecular modeling study.

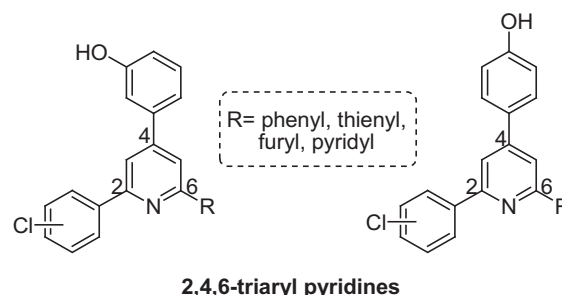


Design, synthesis, and antitumor evaluation of 2,4,6-triaryl pyridines containing chlorophenyl and phenolic moiety

pp. 123–136

Pritam Thapa, Radha Karki, Minh Yun, Tara Man Kadayat, Eunyoung Lee, Han Byeol Kwon, Younghwa Na, Won-Jea Cho, Nam Doo Kim, Byeong-Seon Jeong^{**}, Youngjoo Kwon and Eung-Seok Lee^{*}

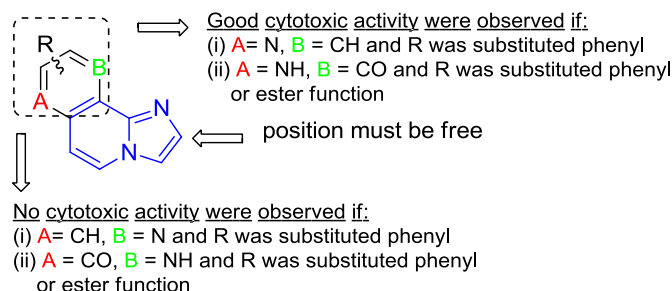
2,4,6-Triaryl pyridine derivatives with chlorophenyl and phenolic moiety at 2-, and 4-position of the central pyridine were synthesized and evaluated their antitumor activities.



Imidazonaphthyridine systems (part 2): Functionalization of the phenyl ring linked to the pyridine pharmacophore and its replacement by a pyridinone ring produces intriguing differences in cytotoxic activity

pp. 137–150

Nicolas Masurier, Eric Debiton, Alicia Jacquemet, Antoine Bussière, Jean-Michel Chezal, Anthony Ollivier, Daté Tétégan, Mounir Andaloussi, Marie-Joseph Galmier, Jacques Lacroix, Damien Canitrot, Jean-Claude Teulade, René C. Gaudreault, Olivier Chavignon and Emmanuel Moreau*

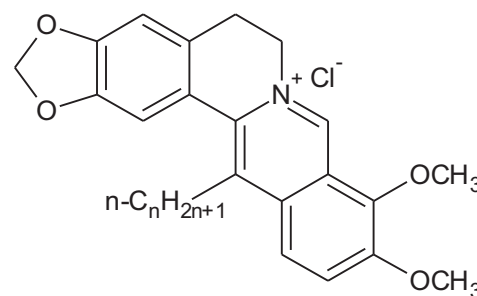


Synthesis, structure–activity relationship and in vitro anti-mycobacterial evaluation of 13-n-octylberberine derivatives

pp. 151–158

Yan-Xin Liu, Chun-Ling Xiao, Yan-Xiang Wang, Ying-Hong Li, Yan-Hui Yang, Yang-Biao Li, Chong-Wen Bi, Li-Mei Gao, Jian-Dong Jiang** and Dan-Qing Song*

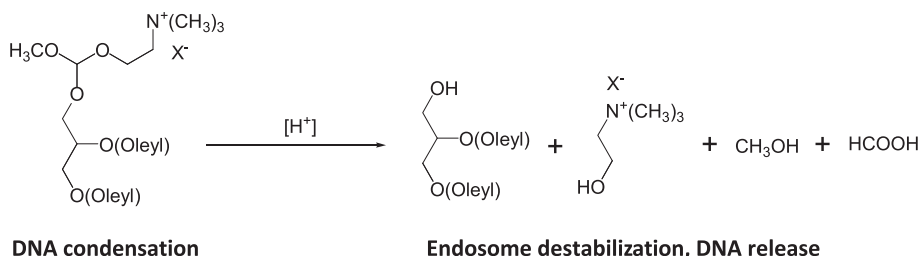
A novel series of 13-substituted berberine derivatives have been identified as potent antimicrobial agents against both drug-susceptible and MDR strains of *Mycobacterium tuberculosis*.



Novel pH-sensitive cationic lipids with linear ortho ester linkers for gene delivery

pp. 159–172

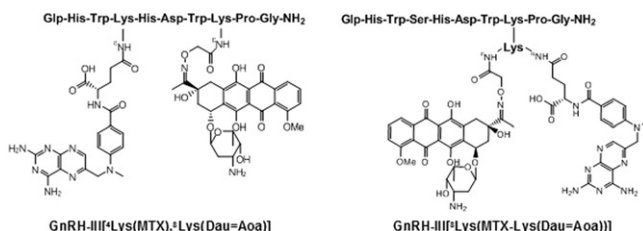
Haigang Chen, Huizhen Zhang, Der Thor, Roshanak Rahimian and Xin Guo*



GnRH-III based multifunctional drug delivery systems containing daunorubicin and methotrexate

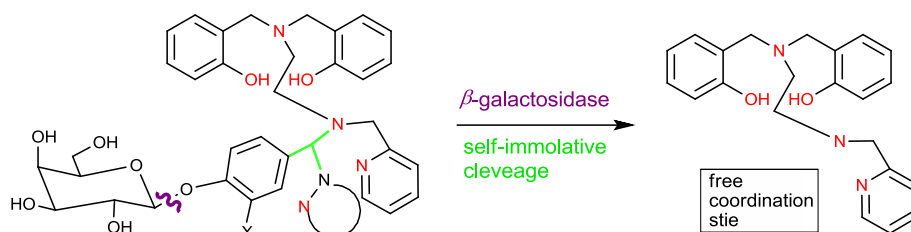
pp. 173–183

Ulrike Leurs, Eszter Lajkó, Gábor Mező, Erika Orbán, Peter Öhlschlager, Andreas Marquardt, László Kóhidai** and Marilena Manea*

**A new class of bioactivable self-immolative *N,O*-ligands**

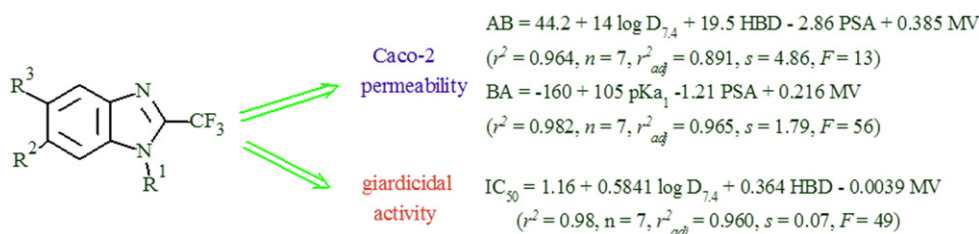
pp. 184–192

Nikodem Kuźnik*, Arkadiusz Chrobaczyński, Małgorzata Mika, Patrycja Miler, Roman Komor and Maciej Kubicki

**Exploring the interplay of physicochemical properties, membrane permeability and giardicidal activity of some benzimidazole derivatives**

pp. 193–204

Carlos Hernández-Covarrubias, Miguel A. Vilchis-Reyes, Lilian Yépez-Mulia, Remedios Sánchez-Díaz, Gabriel Navarrete-Vázquez, Alicia Hernández-Campos, Rafael Castillo and Francisco Hernández-Luis*

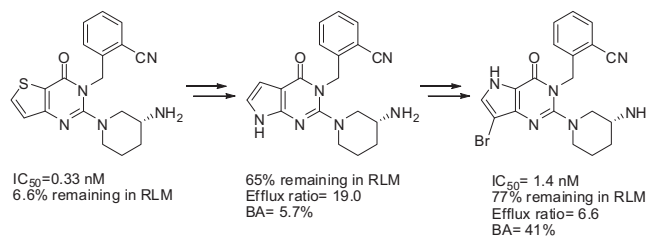


Study of giardicidal activity and Caco-2 permeability relationship of benzimidazole derivatives

Novel pyrrolopyrimidine analogues as potent dipeptidyl peptidase IV inhibitors based on pharmacokinetic property-driven optimization

pp. 205–212

Hui Xie, Lili Zeng, Shaogao Zeng, Xin Lu, Guicheng Zhang, Xin Zhao, Na Cheng, Zhengchao Tu, Zhiyuan Li, Hongjiang Xu, Ling Yang, Xiquan Zhang, Min Huang, Junling Zhao* and Wenhui Hu*

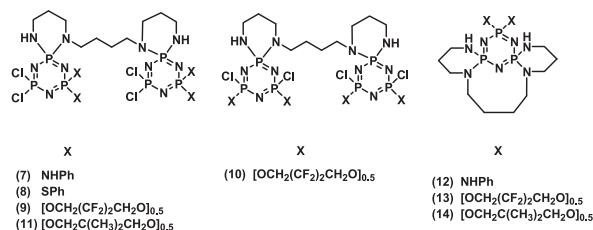


Synthesis, cytotoxicity and apoptosis of cyclotriphosphazene compounds as anti-cancer agents

pp. 213–220

Tuba Yıldırım*, Kemal Bilgin, Gönül Yenilmez Çiftçi, Esra Tanrıverdi Eçik, Elif Şenkuytu, Yıldız Uludağ, Leman Tomak and Adem Kılıç

Dispirobino and dispiroansa spermine derivatives of cyclotriphosphazenes.

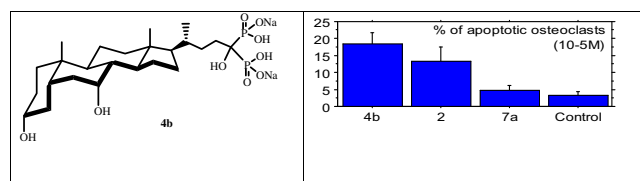


Synthesis, characterization and biological activity of hydroxyl-bisphosphonic analogs of bile acids

pp. 221–229

Olga Bortolini*, Giancarlo Fantin*, Marco Fogagnolo, Stefano Rossetti, Loredana Maiuolo, Gemma Di Pompo, Sofia Avnet and Donatella Granchi**

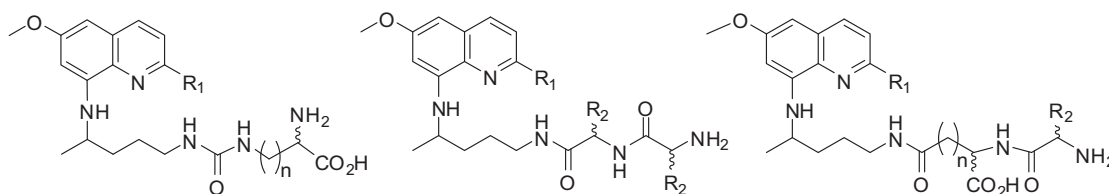
A simple and efficient synthesis of bile acid-derived hydroxyl-bisphosphonates is described. The hydroxy-bisphosphonate salt containing the chenodeoxycholic acid structure **4b** exhibited a high affinity toward hydroxyapatite and a remarkable biological activity in a comparison with bisphosphonate drug references. In the inhibition of osteoclastogenesis, **4b** was found to be more active than neridronate **2** or other bisphosphonates of established activity.



Amino acid, dipeptide and pseudodipeptide conjugates of ring-substituted 8-aminoquinolines: Synthesis and evaluation of anti-infective, β -haematin inhibition and cytotoxic activities

pp. 230–241

Kirandeep Kaur, Meenakshi Jain, Shabana I. Khan, Melissa R. Jacob, Babu L. Tekwani, Savita Singh, Prati Pal Singh and Rahul Jain*

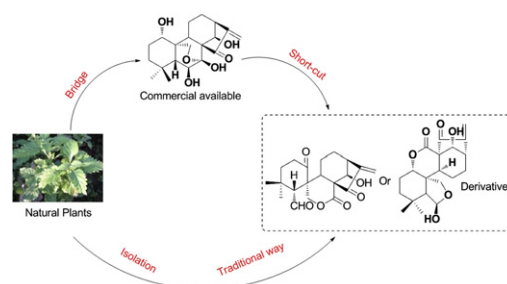


The conversion of oridonin to spirolactone-type or enmein-type diterpenoid: Synthesis and biological evaluation of *ent*-6,7-*seco*-oridonin derivatives as novel potential anticancer agents

pp. 242–250

Lei Wang, Dahong Li, Shengtao Xu, Hao Cai, Hequan Yao, Yihua Zhang*, Jieyun Jiang and Jinyi Xu*

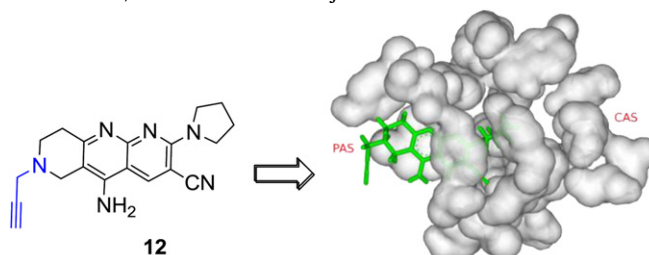
The conversion of oridonin to spirolactone-type or enmein-type diterpenoid were accomplished, and a series of 14-*O*-derivatives of *ent*-6,7-*seco*-oridonin were synthesized and evaluated as novel potential anticancer agents.



Multipotent MAO and cholinesterase inhibitors for the treatment of Alzheimer's disease: Synthesis, pharmacological analysis and molecular modeling of heterocyclic substituted alkyl and cycloalkyl propargyl amine

pp. 251–262

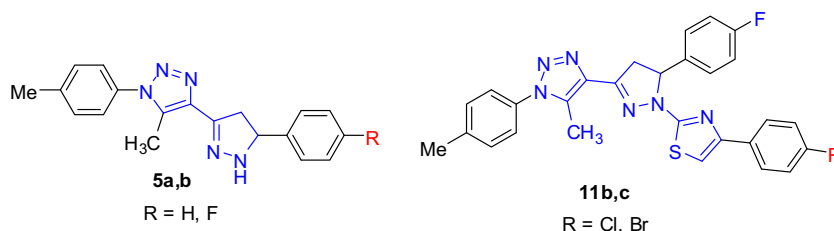
Abdelouahid Samadi*, Cristóbal de los Ríos, Irene Bolea, Mourad Chioua, Isabel Iriepa, Ignacio Moraleda, Manuela Bartolini, Vincenza Andrisano, Enrique Gálvez, Carolina Valderas, Mercedes Unzeta and José Marco-Contelles*

**Design and synthesis of new 4-pyrazolin-3-yl-1,2,3-triazoles and 1,2,3-triazol-4-yl-pyrazolin-1-ylthiazoles as potential antimicrobial agents**

pp. 263–268

Bakr F. Abdel-Wahab*, Ehab Abdel-Latif, Hanan A. Mohamed and Ghada E.A. Awad

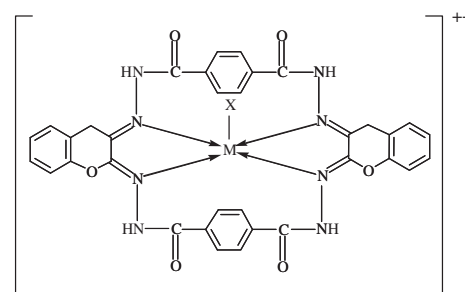
New pyrazolyl-1,2,3-triazoles and 1,2,3-triazol-4-yl-pyrazolylthiazoles, showing excellent antimicrobial activities, were synthesized through multi step reactions using 1-tolyl-4-acetyl-5-methyl-1,2,3-triazole as a precursor.

**Synthesis, spectral characterization and antimicrobial evaluation of Schiff base Cr (III), Mn (III) and Fe (III) macrocyclic complexes**

pp. 269–274

Gajendra Kumar*, Shoma Devi, Rajeev Johari and Dharmendra Kumar

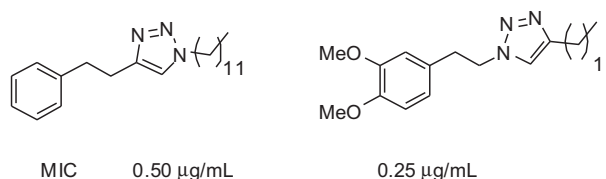
Schiff base M (III) complexes were synthesized and evaluated for antimicrobial activity. Complex 3 [Cr(C₃₄H₂₄N₈O₆)OAc]OAc₂ exhibited best antimicrobial activity.

**Chemical synthesis and biological evaluation of triazole derivatives as inhibitors of InhA and antituberculosis agents**

pp. 275–283

Christophe Menendez, Aurélien Chollet, Frédéric Rodriguez, Cyril Inard, Maria Rosalia Pasca, Christian Lherbet* and Michel Baltas*

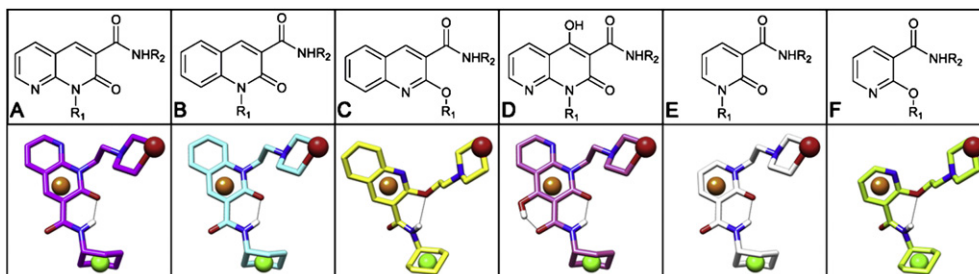
A series of 1,4-disubstituted triazole derivatives were synthesized and evaluated against InhA and *Mycobacterium tuberculosis* H₃₇R_v. Two compounds show antimycobacterial activities with MIC values in the low micromolar range.



Rational design, synthesis and anti-proliferative properties of new CB2 selective cannabinoid receptor ligands: An investigation of the 1,8-naphthyridin-2(1H)-one scaffold

pp. 284–294

Clementina Manera*, Giuseppe Saccomanni, Anna Maria Malfitano, Simone Bertini, Francesca Castelli, Chiara Laezza, Alessia Ligresti, Valentina Lucchesi, Tiziano Tuccinardi, Flavio Rizzolio, Maurizio Bifulco, Vincenzo Di Marzo, Antonio Giordano, Marco Macchia and Adriano Martinelli



Olean-18-ene triterpenoids from Celastraceae species inhibit HIV replication targeting NF-κB and Sp1 dependent transcription

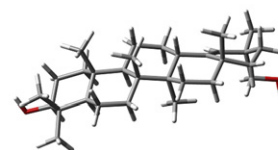
pp. 295–303

Alex A. Osorio, Alejandro Muñoz, David Torres-Romero, Luis M. Bedoya, Nayra R. Perestelo, Ignacio A. Jiménez, José Alcamí and Isabel L. Bazzocchi*

A new series of olean-18-ene triterpenoids isolated from Celastraceae species, were able to successfully inhibit HIV transcription.



Cassine xylocarpa

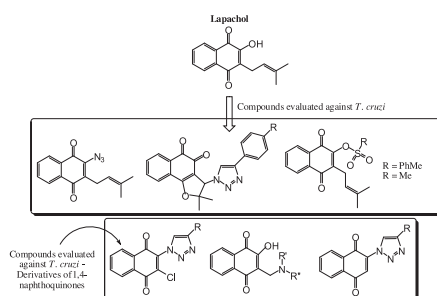


3β,29-dihydroxy-olean-18-ene

On the search for potential anti-*Trypanosoma cruzi* drugs: Synthesis and biological evaluation of 2-hydroxy-3-methylamino and 1,2,3-triazolic naphthoquinoidal compounds obtained by click chemistry reactions

pp. 304–312

Eufrânio N. da Silva, Júnior*, Isadora M.M. de Melo, Emílly B.T. Diogo, Verenice A. Costa, José D. de Souza Filho, Wagner O. Valença, Celso A. Camara, Ronaldo N. de Oliveira, Alexandre S. de Araujo, Flávio S. Emery, Marcelo R. dos Santos, Carlos A. de Simone, Rubem F.S. Menna-Barreto and Solange L. de Castro



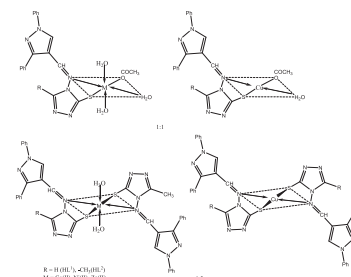
SHORT COMMUNICATION

Cobalt, nickel, copper and zinc complexes with 1,3-diphenyl-1H-pyrazole-4-carboxaldehyde Schiff bases: Antimicrobial, spectroscopic, thermal and fluorescence studies

pp. 313–321

Kiran Singh*, Yogender Kumar, Parvesh Puri, Mahender Kumar and Chetan Sharma

Two new Schiff bases of 1,3-diphenyl-1H-pyrazole-4-carboxaldehyde and 4-amino-5-mercapto-3-methyl/H-1,2,4-triazole [H1¹⁻²] and their Cobalt, Nickel, Copper and Zinc complexes have been synthesized, characterized and tested as antimicrobial agents.

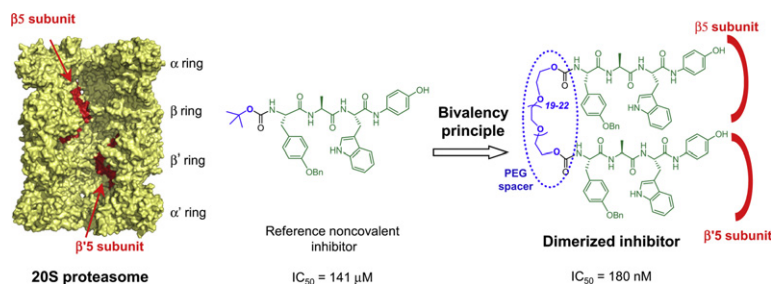


PRELIMINARY COMMUNICATION

Noncovalent inhibition of 20S proteasome by pegylated dimerized inhibitors

pp. 322–327

Xavier Maréchal, Anaïs Pujol, Nicolas Richy, Emilie Genin, Nicolas Basse, Michèle Reboud-Ravaux** and Joëlle Vidal*



COVER

This picture is taken from the review published in: European Journal of Medicinal Chemistry, 2010, Volume 45, Pages 2095–2116. The review is focused on the binding of inhibitors to the catalytic site of histone deacetylase © 2010 Published by Elsevier Masson SAS

* Corresponding authors.

SciVerse ScienceDirect

Full text of this journal is available online from **ScienceDirect**. Visit www.sciencedirect.com for more information.

Cited/Abstracted in : Biological Abstracts, Chemical Abstracts, CABS, CNRS/Pascal, Current Contents (Life Sciences), EMbase, Index Medicus/Medline, Science Citation Index. Also covered in the abstract and citation database SciVerse SCOPUS®. Full text available on SciVerse ScienceDirect®.



ISSN 0223-5234