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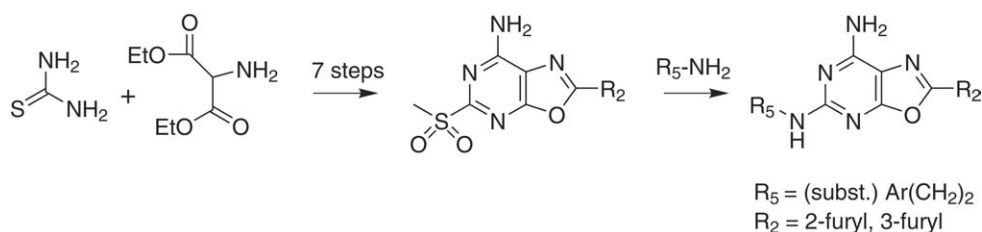
Contents

ORIGINAL ARTICLES

Synthesis and evaluation of 7-amino-2-(2(3-furyl)-5-phenylethylamino-oxazolo[5,4-*d*]pyrimidines as potential A_{2A} adenosine receptor antagonists for positron emission tomography (PET)

pp 7–15

Marcus H. Holschbach*, Dirk Bier, Stefan Stüsgen, Walter Wutz, Wiebke Sihver, Heinz H. Coenen and Ray A. Olsson

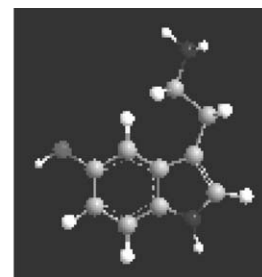
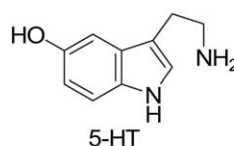


Optimization of a pharmacophore model for 5-HT₄ agonists using CoMFA and receptor based alignment

pp 16–26

Magdy N. Iskander*, Lok M. Leung, Trevor Buley, Fadi Ayad, Juliana Di Iulio, Yean Y. Tan and Ian M. Coupar

A refined model for 5-HT₄ agonist using CoMFA and receptor based alignment was produced. The predictive power of this model stems from far lower steric contribution and dominant electrostatic contribution.

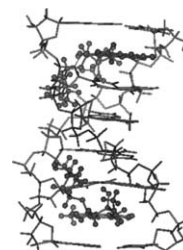


Structure of daunomycin complexed to d-TGATCA by two-dimensional nuclear magnetic resonance spectroscopy

pp 27–39

Ritu Barthwal*, Uma Sharma, Nandana Srivastava, Monica Jain, Pamita Awasthi, Manpreet Kaur, Sudhir Kumar Barthwal and Girjesh Govil

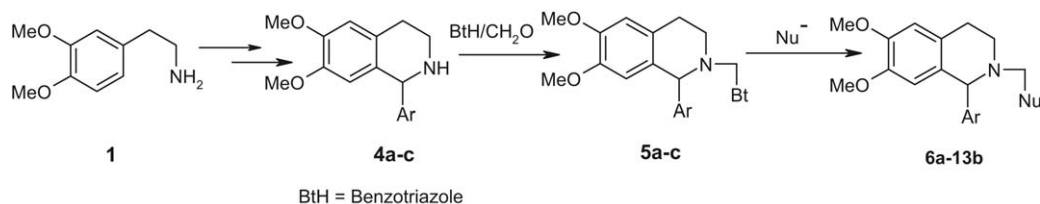
NOEs (nuclear Overhauser effect) in nuclear magnetic resonance data of 2:1 daunomycin-d(TGATCA)₂ complex show that drug chromophore intercalates at d-TpG/CpA sites and the conformation of DNA and drug change on binding.



Synthesis, antibacterial activity and QSAR studies of 1,2-disubstituted-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolines

pp 40–49

Rakesh Kumar Tiwari, Devender Singh, Jaspal Singh, Anil Kumar Chhillar, Ramesh Chandra and Akhilesh Kumar Verma*

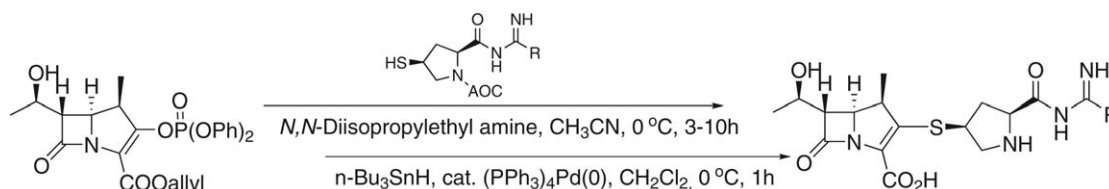


Synthesis, QSAR and *in vitro* antimicrobial activity of new substituted-tetrahydroisoquinoline derivatives were describe against the standard Gram positive and Gram negative strains and compounds **4a-c** were found to be most effective.

Synthesis and biological evaluation of 1 β -methylcarbapenems having guanidino moieties

pp 50–55

Chang-Hyun Oh* and Jung-Hyuck Cho

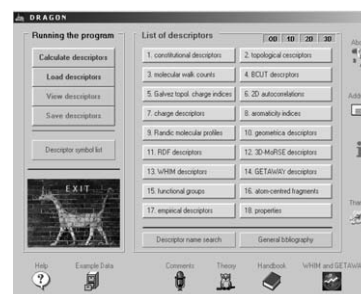


Radial distribution function descriptors: an alternative for predicting A_{2A} adenosine receptors agonists

pp 56–62

Maykel Pérez González*, Carmen Terán, Marta Teijeira and Aliuska Morales Helguera

The RDF approach has been applied to the study of the A_{2A} adenosine receptors agonist. A model able to describe around 85% of the variance in the experimental activity was developed. In contrast, no one of nine different approaches were able to explain more than 78% of the variance in the mentioned property.

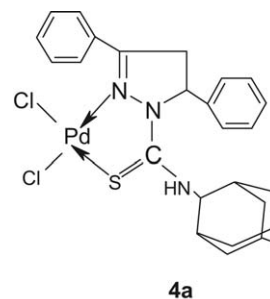


Synthesis and antiamoebic activity of new 1-*N*-substituted thiocarbamoyl-3,5-diphenyl-2-pyrazoline derivatives and their Pd(II) complexes

pp 63–70

Asha Budakoti, Mohammad Abid and Amir Azam*

Some 1-*N*-substituted thiocarbamoyl-3,5-diphenyl-2-pyrazoline derivatives and their palladium (II) complexes were synthesized. These compounds were evaluated for their *in vitro* anti-amoebic activity. Compound **4a** showed most promising activity.

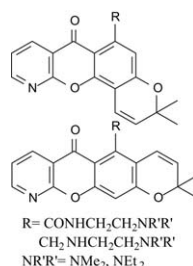


SHORT COMMUNICATIONS

Design, synthesis and antiproliferative activity of some new azapyranoxanthenone aminoderivatives

pp 71–79

George Kolokythas, Nicole Pouli, Panagiotis Marakos*, Harris Pratsinis and Dimitris Kletsas

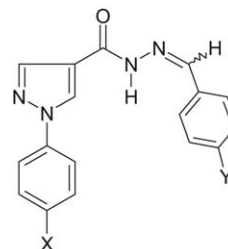
**Synthesis and leishmanicidal activities**

pp 80–87

of 1-(4-X-phenyl)-N'-[(4-Y-phenyl)methylene]-1H-pyrazole-4-carbohydrazides

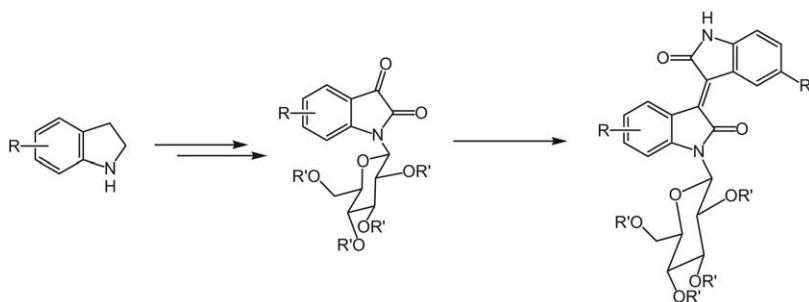
Alice M.R. Bernardino, Adriana O. Gomes, Karen S. Charret, Antônio C.C. Freitas, Gêrzia M.C. Machado, Marilene M. Canto-Cavalheiro, Leonor L. Leon and Veronica F. Amaral*

1H-pyrazole-4-carbohydrazides were synthesized and their leishmanicidal in vitro activities and cytotoxic effects were investigated.

**Synthesis and antiproliferative activities of diversely substituted glycosyl-isoidindigo derivatives**

pp 88–100

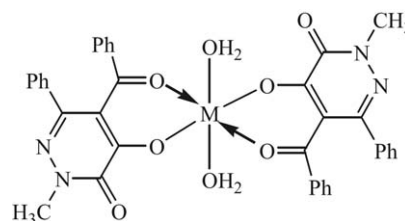
Mathieu Sassatelli, Fadoua Bouchikhi, Samir Messaoudi, Fabrice Anizon, Eric Debiton, Chantal Barthomeuf, Michelle Prudhomme and Pascale Moreau*

**Synthesis, antibacterial and antifungal activity of some new pyridazinone metal complexes**

pp 101–105

Mehmet Sönmez*, İsmet Berber and Esvet Akbaş

The new various metal complexes of 5-benzoyl-4-hydroxy-2-methyl-6-phenyl-2H-pyridazin-3-one have been synthesized and characterized. All the complexes were evaluated for their antimicrobial activities against Gram-positive, Gram-negative bacteria and fungi using micro-dilution procedure.



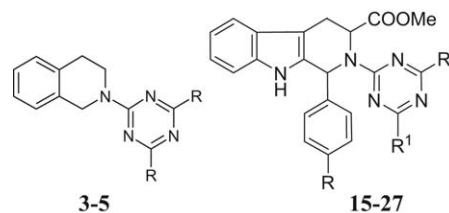
M: Co(II), Ni(II), Zn(II), Cd(II)

Syntheses of new substituted triazino tetrahydroisoquinolines and β -carbolines as novel antileishmanial agents

pp 106–113

Arun Kumar, Sanjay Babu Katiyar, Suman Gupta and Prem M.S. Chauhan*

A series of triazino tetrahydroisoquinolines (**3–5**) and β -carboline derivatives (**15–27**) have been synthesized as novel antileishmanial agents. Among them, compounds **15**, **16** and **25** have shown 78.0%, 78.6% and 68.0% in vivo inhibition against *Leishmania donovani* at a dose of 50 mg kg⁻¹ x 5 days respectively, while compounds **3** and **18** exhibited 55.6% and 53.3% in vivo inhibitions, respectively, against *L. donovani* at a dose of 50 mg kg⁻¹ x 5 days.

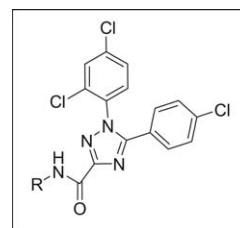


Structural–activity relationship study on C-4 carbon atom of the CB₁ antagonist SR141716: synthesis and pharmacological evaluation of 1,2,4-triazole-3-carboxamides

pp 114–120

Nadine Jagerovic*, Laura Hernandez-Folgado, Ibon Alkorta, Pilar Goya, María Isabel Martín, María Teresa Dannert, Ángela Alsasua, Jordi Frigola, María Rosa Cuberes, Alberto Dordal and Jörg Holenz

1,2,4-Triazole-3-carboxamides have been prepared under mild conditions. Their ability to displace [³H]-CP55940 from CB₁ cannabinoid receptor and their antagonistic properties in the mouse vas deferens functional assay were evaluated.

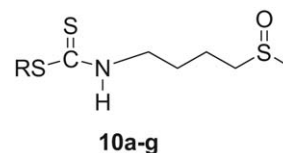


Cancer chemopreventive activity of sulforamate derivatives

pp 121–124

Robert M. Moriarty, Rajesh Naithani*, Jerome Kosmeder and Om Prakash

Synthesis of several derivatives of (+)(-) 4-methylsulfinyl-1-(S-methyl-dithio-carbamyl)butane (sulforamate) and their evaluation as mono-functional inducer of NAD(P)H quinone oxidoreductase [quinone reductase (QR)] was carried out.

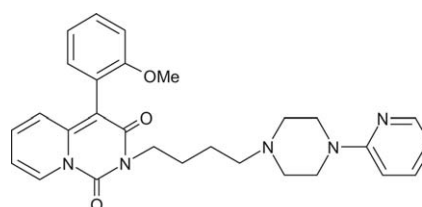


Synthesis of new hexahydro- and octahydropyrido[1,2-c]pyrimidine derivatives with an arylpiperazine moiety as ligands for 5-HT_{1A} and 5-HT_{2A} receptors. Part 4

pp 125–134

Franciszek Herold*, Marek Król, Jerzy Kleps and Gabriel Nowak

The synthesis and biological activity of a novel series of 4-aryl-2H-pyrido[1,2-c]pyrimidine-1,3-dione derivatives **6–18** with potent binding affinity for 5-HT_{1A} receptor are reported.

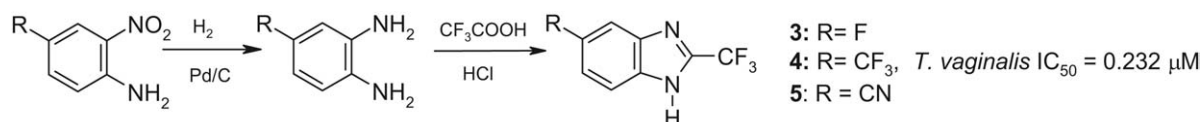


10
5-HT_{1A} K_i = 2.2 nM

Synthesis and antiprotozoal activity of some 2-(trifluoromethyl)-1H-benzimidazole bioisosteres

pp 135–141

Gabriel Navarrete-Vázquez*, María de Monserrat Rojano-Vilchis, Lilián Yépez-Mulia, Víctor Meléndez, Lucia Gerena, Alicia Hernández-Campos, Rafael Castillo and Francisco Hernández-Luis

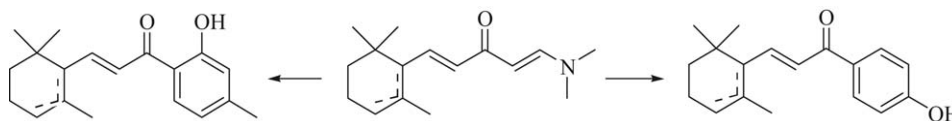


A series of 2-(Trifluoromethyl)-1H-benzimidazole derivatives with various 5- and 6-position bioisosteric substituents were prepared using a short synthetic route. Each analogue was tested *in vitro* against the protozoa *G. intestinalis*, *T. vaginalis* and *P. falciparum*. Compound 4, was 14 times more active than albendazole against *T. vaginalis* and also showed moderate antimalarial activity.

New syntheses and potential antimalarial activities of new ‘retinoid-like chalcones’

pp 142–146

Alain Valla*, Benoist Valla, Dominique Cartier, Régis Le Guillou, Roger Labia, Loïc Florent, Sébastien Charneau, Joseph Schrevel and Pierre Potier



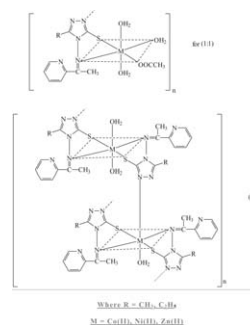
A series of ‘retinoid-like chalcones’ were synthesized from a new enaminone synthon, via a new aromatic annelation. These new derivatives have been tested *in vitro* as potential antimalarial agents

Synthesis, characterization and biological studies of Co(II), Ni(II), Cu(II) and Zn(II) complexes with bidentate Schiff bases derived by heterocyclic ketone

pp 147–153

Kiran Singh*, Manjeet Singh Barwa and Parikshit Tyagi

A series of metal complexes of Co(II), Ni(II), Cu(II) and Zn(II) have been synthesized by 1,2,4-triazole and 2-acetylpyridine. The structures of the complexes have been proposed on the bases of various physico-chemical techniques. Antibacterial activities of few complexes have been studied.



OTHER CONTENTS**Instructions to authors****pp I–III**

* Corresponding Author

COVER

Crystallographic structure of a histone deacetylase-like amidohydrolase from *Bordetella/Alcaligenes* strain FB188 (FB188 HDAH), a bacterial homologue of class 2 histone deacetylase, with a docked inhibitor. Image provided by L. Giurato, Professor A. Schwienhorst and Professor R. Ficner's group, S. Forte. © 2006. Published by Elsevier SAS



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