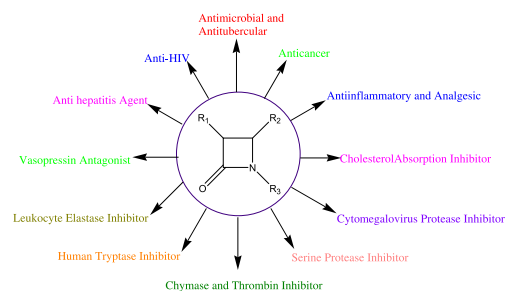


Contents

pp. 5541–5560

2-Azetidinone and their derivatives occupy a central place in medicinal chemistry due to their diverse and broad pharmacological profile. This article focuses on the various pharmacological profile of 2-azetidinone scaffold and development of novel derivatives with their potential activity.



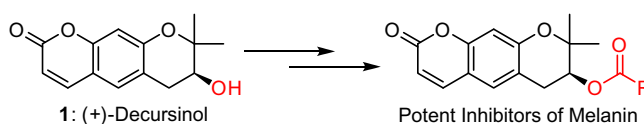
Identification of efficient fluorophores for the direct labeling of DNA via rolling circle amplification (RCA) polymerase

pp. 5561–5566

Synthesis of (S)-(+)-decursin and its analogues as potent inhibitors of melanin formation in B16 murine melanoma cells

pp. 5567–5575

Kyeong Lee, Jee-Hyun Lee, Shanthaveerappa K. Boovanahalli, Yongseok Choi, Soo-Jin Choo, Ick-dong Yoo, Dong Hee Kim, Mi Young Yun, Gye Won Lee and Gyu-Yong Song*

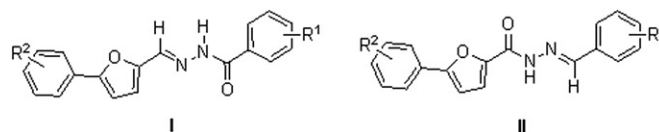


New class of potent antitumor acylhydrazone derivatives containing furan

pp. 5576–5584

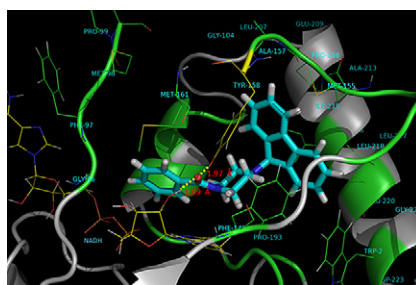
Zining Cui, Ying Li, Yun Ling, Juan Huang, Jingrong Cui, Ruiqing Wang and Xinling Yang*

A pair of *N*-acylhydrazones **I** and **II** were synthesized in excellent yields. The antitumor bioassay revealed some compounds exhibited excellent activity. Their toxicities were predicted by *in silico* methods.

**Investigating the structural basis of arylamides to improve potency against *M. tuberculosis* strain through molecular dynamics simulations**

pp. 5585–5593

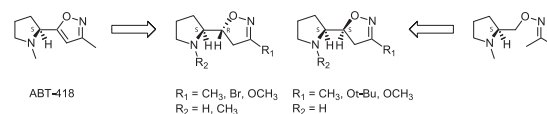
Auradee Punkvang, Patchreenart Saparpakorn, Supa Hannongbua, Peter Wolschann, Anton Beyer and Pornpan Pungpo*

**Synthesis of novel chiral Δ^2 -isoxazoline derivatives related to ABT-418 and estimation of their affinity at neuronal nicotinic acetylcholine receptor subtypes**

pp. 5594–5601

Clelia Dallanocce*, Pietro Magrone, Carlo Matera, Leonardo Lo Presti, Marco De Amici, Loredana Riganti, Francesco Clementi, Cecilia Gotti and Carlo De Micheli

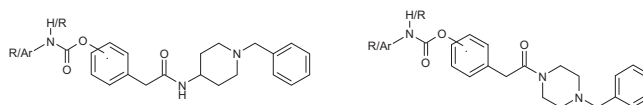
A group of novel Δ^2 -isoxazolines structurally related to oxyimino ethers and to the isoxazole nicotinic agonist ABT-418 were prepared and assayed for their binding affinity at $\alpha 4\beta 2$ and $\alpha 7$ nicotinic acetylcholine receptor subtypes.

**Novel alkyl- and arylcarbamate derivatives with *N*-benzylpiperidine and *N*-benzylpiperazine moieties as cholinesterases inhibitors**

pp. 5602–5611

Anna Wieckowska, Marek Bajda, Natalia Guzik and Barbara Malawska*

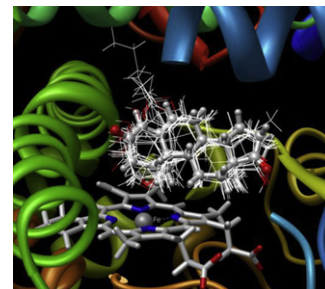
This study presents a synthesis of novel carbamates and their inhibitory activity against cholinesterases.



Molecular docking and QSAR study on steroidal compounds as aromatase inhibitors

pp. 5612–5620

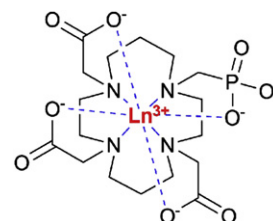
Yujie Dai*, Qiang Wang, Xiuli Zhang, Shiru Jia, Heng Zheng, Dacheng Feng and Peng Yu

Docked positions with the minimized CDOCKER interaction energies (E_{CD}) of the 32 steroidal compounds.**TETA analogue containing one methylenephosphonate pendant arm: Lanthanide complexes and biological evaluation of its ^{153}Sm and ^{166}Ho complexes**

pp. 5621–5627

Luís M.P. Lima, Rita Delgado*, Fernanda Marques, Lurdes Gano and Isabel Santos*

The thermodynamic stability of lanthanide complexes of $\text{H}_5\text{te3a1p}$, and the *in vitro* and *in vivo* behaviours of $^{153}\text{Sm}/^{166}\text{Ho}$ -te3a1p complexes were evaluated. The results indicate that the replacement of one acetate pendant arm of H_4teta by a methylphosphonate one does not provide promising chelators for *in vivo* application.

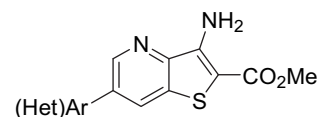
**Efficient synthesis of 6-(hetero)arylthieno[3,2-*b*]pyridines by Suzuki–Miyaura coupling.**

pp. 5628–5634

Evaluation of growth inhibition on human tumor cell lines, SARs and effects on the cell cycle

Maria-João R.P. Queiroz*, Ricardo C. Calhelha, Luís A. Vale-Silva, Eugénia Pinto, Raquel T. Lima and M. Helena Vasconcelos

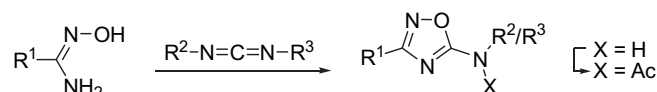
Bi(hetero)aryl derivatives of the thieno[3,2-*b*]pyridine were obtained by Suzuki–Miyaura cross-coupling of the methyl 3-amino-6-bromothieno[3,2-*b*]pyridine-2-carboxylate with aryl or heteroaryl pinacolborane esters or potassium trifluoroborates, in good to excellent yields. The coupling products were evaluated for their growth inhibitory effect on three human tumor cell lines, representing different tumor models. For the two most promising compounds, cell cycle analysis was performed in one of the cell lines in study.

**Convenient synthesis and biological profile of 5-amino-substituted 1,2,4-oxadiazole derivatives**

pp. 5635–5645

Maria Ispikoudi, Michalis Amvrazis, Christos Kontogiorgis, Alexandros E. Koumbis, Konstantinos E. Litinas, Dimitra Hadjipavlou-Litina* and Konstantina C. Fylaktakidou**

5-Amino substituted 1,2,4-oxadiazole derivatives were easily prepared, in one step and in high yields, upon the reactions of a variety of amidoximes with carbodiimides. Subsequent acetylation provided the corresponding acetamides. A number of compounds exhibited significant *in vivo* anti-inflammatory activity (up to 51%).

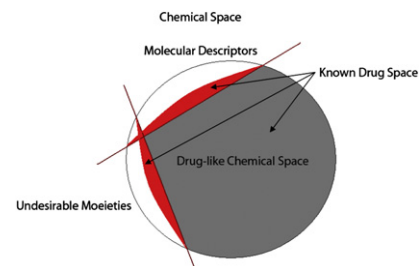


Characteristics of known drug space. Natural products, their derivatives and synthetic drugs

pp. 5646–5652

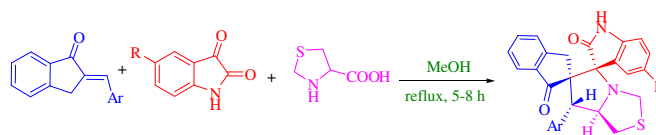
Richard Bade, Ho-Fung Chan and Jóhannes Reynisson*

Chemical space portrayed as a sphere with molecular descriptors and “undesirable” moieties defining an area of drug-like chemical space within it. Known drug space (KDS) fully encompasses drug-like chemical space with the parameters of molecular weight $\leq 800 \text{ g mol}^{-1}$, $\log P \leq 6.5$, hydrogen bond acceptors ≤ 15 , hydrogen bond donors ≤ 7 , polar surface area $\leq 180 \text{ \AA}^2$, and rotatable bonds ≤ 17 . It was found that 10% of the drugs on the market are unaltered natural products, 29% are their derivatives (semi-synthetics) and the rest (61%) have a synthetic origin.

**A regio- and stereoselective 1,3-dipolar cycloaddition for the synthesis of novel spiro-pyrrolothiazolyloxindoles and their antitubercular evaluation**

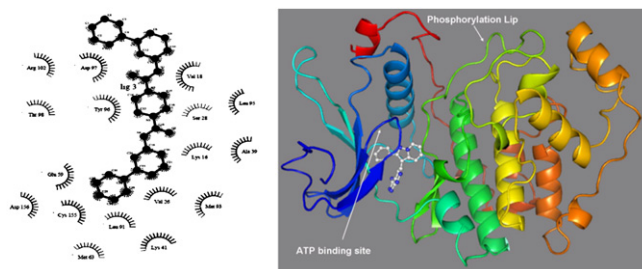
pp. 5653–5661

Pitchaimani Prasanna, Kamaraj Balamurugan, Subbu Perumal*, Perumal Yogeeswari and Dharmarajan Sriram

**Mitogen-activated protein kinase 4 of *Leishmania* parasite as a therapeutic target**

pp. 5662–5670

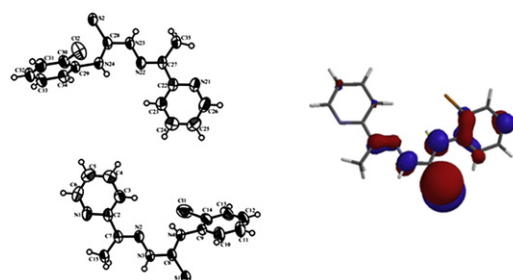
Parameswaran Saravanan, Santhosh K. Venkatesan, C. Gopi Mohan, Sanjukta Patra* and Vikash Kumar Dubey*

**2-Acetylpyridine thiosemicarbazones: Cytotoxic activity in nanomolar doses against malignant gliomas**

pp. 5671–5677

Josane A. Lessa, Isolda C. Mendes, Paulo R.O. da Silva, Marcella A. Soares, Raquel G. dos Santos, Nivaldo L. Speziali, Nelilma C. Romeiro, Eliezer J. Barreiro and Heloisa Beraldo*

2-Acetylpyridine *N*(4)-phenyl thiosemicarbazone, and its *N*(4)-*ortho*-, *meta*-, and *para*-tolyl, and *N*(4)-*ortho*-, *meta*- and *para*-chlorophenyl derivatives are cytotoxic at nanomolar doses against glioma cells. SAR studies were carried out.

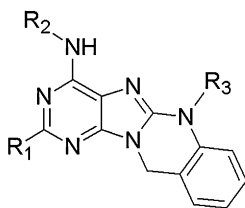


Synthesis, biological evaluation and docking studies of 4-amino-tetrahydroquinazolino[3,2-e]purine derivatives

pp. 5678–5684

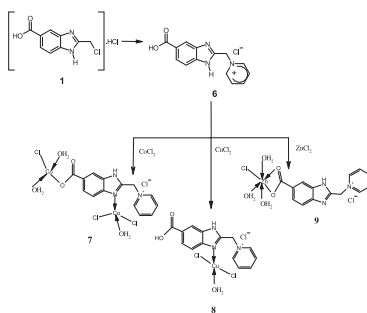
Valerie Verones, Nathalie Flouquet, Amaury Farce, Pascal Carato, Stephane Leonce, Bruno Pfeiffer, Pascal Berthelot and Nicolas Lebegue*

A series of 4-amino-tetrahydroquinazolino[3,2-e]purine derivatives was synthesized and evaluated for its Src cell-free enzymatic inhibitory and anti-proliferative activity on the murine leukemia L1210 cell line.

**9a** R₁, R₂, R₃ = H**9b** R₁ = Cl; R₂, R₃ = H**11a** R₁, R₃ = H; R₂ = phenyl**11b** R₁ = H; R₂ = phenyl; R₃ = *N,N*-diethylaminoethyl**11c** R₁ = H; R₂ = phenyl; R₃ = *N*-ethylmorpholine**11d** R₁ = H; R₂ = 2-chlorophenyl; R₃ = *N*-ethylmorpholine**11e** R₁ = H; R₂ = 2-bromophenyl; R₃ = *N*-ethylmorpholine**11f** R₁ = H; R₂ = benzyl; R₃ = *N*-ethylmorpholine**Synthesis and antitumor activity of novel benzimidazole-5-carboxylic acid derivatives and their transition metal complexes as topoisomerase II inhibitors**

pp. 5685–5691

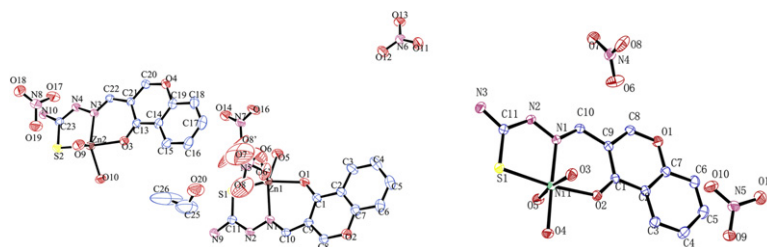
Shadia A. Galal*, Khaled H. Hegab, Ahmed M. Hashem and Nabil S. Youssef

**Synthesis, crystal structures, biological activities and fluorescence studies of transition metal complexes with 3-carbaldehyde chromone thiosemicarbazone**

pp. 5692–5701

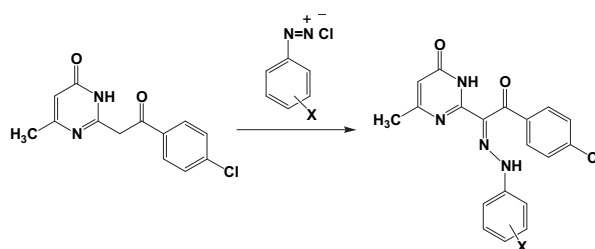
Yong Li, Zheng-Yin Yang* and Jin-Cai Wu

3-Carbaldehyde chromone thiosemicarbazone and its Copper (II), Zinc (II) and Nickel (II) complexes were synthesized and characterized. Their DNA binding properties and antioxidant activity were investigated systematically.

**Antimicrobial, antitumor and 5α-reductase inhibitor activities of some hydrazoneyl substituted pyrimidinones**

pp. 5702–5707

Mastoura M. Edrees*, Thoraya A. Farghaly, Fatma A.A. El-Hag and Mohamed M. Abdalla

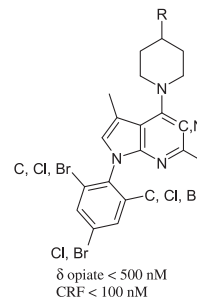


Knowledge-based analysis of multi-potent G-protein coupled receptors ligands

pp. 5708–5717

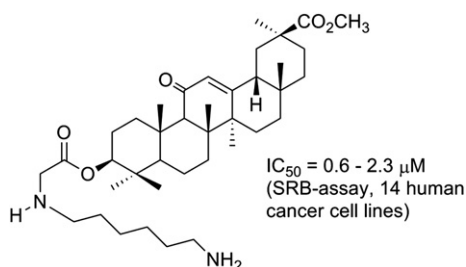
Patricia Faure*, Elodie Dubus, Ismail Ijjaali*, Christelle Morlière, Olivier Barberan and François Petitet

General structure of compound recognizing both class A and B GPCRs.

**Synthesis and biological activity of some antitumor active derivatives from glycyrrhethinic acid**

pp. 5718–5723

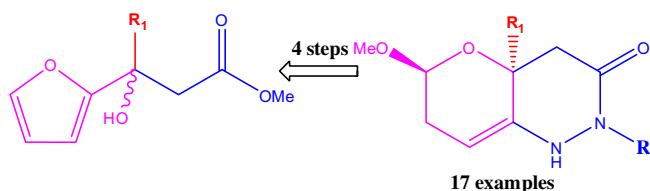
René Csuk*, Stefan Schwarz, Ralph Kluge and Dieter Ströhl

**Design and synthesis of novel tetrahydro-2H-Pyrano[3,2-c]Pyridazin-3(6H)-one derivatives as potential anticancer agents**

pp. 5724–5731

Taleb H. Al-Tel*

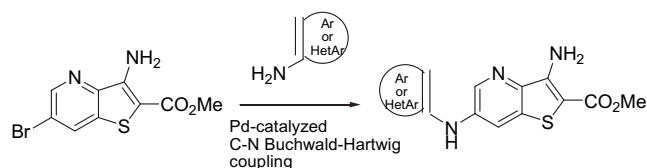
Polyfunctional tetrahydro-2H-pyrano[3,2-c]pyridazin-3(6H)-one derivatives were synthesized and biologically evaluated as novel anticancer agents. Compounds **16c** and **16d** were found to be 30-fold more potent against SK-BR-3 (IC₅₀ 0.21 and 0.15 μM, respectively) compared to other cancer cell lines tested.

**Novel 6-[(hetero)arylamino]thieno[3,2-b]pyridines: Synthesis and antitumoral activities**

pp. 5732–5738

Maria-João R.P. Queiroz*, Ricardo C. Calhelha, Luís A. Vale-Silva, Eugénia Pinto and M. São-José Nascimento

The novel di(hetero)arylamines derivatives of the thieno[3,2-b]pyridine moiety were submitted to *in vitro* antitumoral evaluation and some structure–activity relationships (SARs) were established.

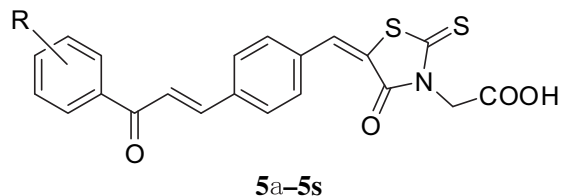


Synthesis of new chalcone derivatives containing a rhodanine-3-acetic acid moiety with potential anti-bacterial activity

pp. 5739–5743

Zhen-Hua Chen, Chang-Ji Zheng, Liang-Peng Sun and Hu-Ri Piao*

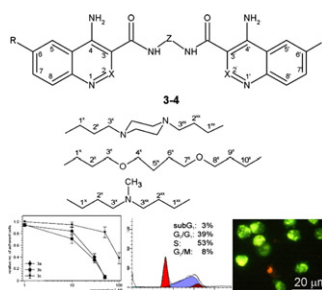
With an intention to synergize the anti-bacterial activity of chalcones and rhodanine-3-acetic acid, several hybrid compounds possessing chalcone and rhodanine-3-acetic acid moieties were synthesized and tested for their anti-bacterial activity.



Synthesis and *in vitro* biological evaluation of new polyamine conjugates as potential anticancer drugs

pp. 5744–5751

Marta Szumilak, Agata Szulawska-Mroczek, Kamila Koprowska, Marta Stasiak, Wiesława Lewgowd, Andrzej Stanczak and Małgorzata Czyż*

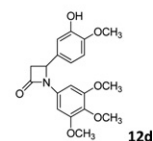
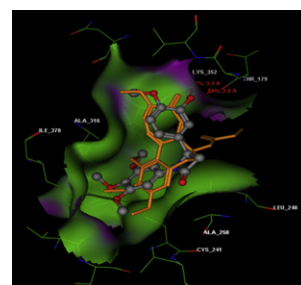


Lead identification of conformationally restricted β-lactam type combretastatin analogues: Synthesis, antiproliferative activity and tubulin targeting effects

pp. 5752–5766

Miriam Carr, Lisa M. Greene, Andrew J.S. Knox, David G. Lloyd, Daniela M. Zisterer and Mary J. Meegan*

Docked pose of β-lactam **12d** overlayed with N-deacetyl-N-(2-mercaptoacetyl)colchicine (DAMA-colchicine) in the tubulin binding site.



Massive screening yields novel and selective *Trypanosoma cruzi* triosephosphate isomerase dimer-interface-irreversible inhibitors with anti-trypanosomal activity

pp. 5767–5772

Guzmán Álvarez, Beatriz Aguirre-López, Javier Varela, Mauricio Cabrera, Alicia Merlino, Gloria V. López, María Laura Lavaggi, Williams Porcal, Rossanna Di Maio, Mercedes González*, Hugo Cerecetto*, Nallely Cabrera, Ruy Pérez-Montfort**, Marieta Tuena de Gómez-Puyou and Armando Gómez-Puyou**

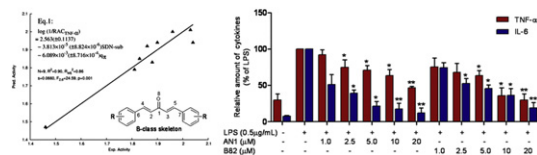
TcTIM IC ₅₀	20.0 μM	13.0 μM	26.0 μM	3.5 μM	10.0 μM
HTIM IC ₅₀	-	> 100.0 μM	> 100.0 μM	~ 100.0 μM	> 100.0 μM
<i>T. cruzi</i> IC ₅₀	50.0 μM	50.0 μM	2.9 μM	> 25.0 μM	22.0 μM

Synthesis and anti-inflammatory evaluation of novel mono-carbonyl analogues of curcumin in LPS-stimulated RAW 264.7 macrophages

pp. 5773–5780

Chengguang Zhao, Yuepiao Cai, Xuzhi He, Jianling Li, Li Zhang, Jianzhang Wu, Yunjie Zhao, Shulin Yang, Xiaokun Li, Wulan Li** and Guang Liang*

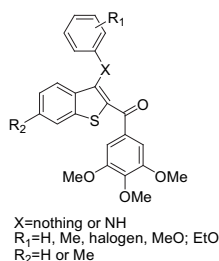
Curcumin analogues were synthesized and evaluated for inhibition of LPS-induced TNF- α and IL-6 production in macrophages. The quantitative SAR indicates that electron-withdrawing groups benefit anti-inflammatory activities of B-class compounds.



Synthesis and biological evaluation of 2-(3',4',5'-trimethoxybenzoyl)-3-aryl/arylaminothiophene derivatives as a novel class of antiproliferative agents

pp. 5781–5791

Romeo Romagnoli*, Pier Giovanni Baraldi, Carlota Lopez Cara, Ernest Hamel, Giuseppe Basso, Roberta Bortolozzi and Giampietro Viola**

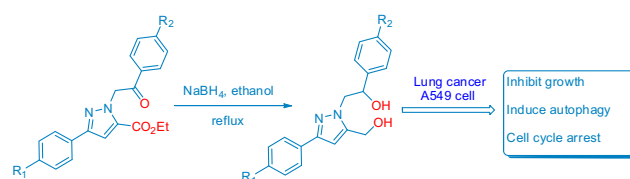


Synthesis, crystal structure and biological evaluation of novel 2-(5-(hydroxymethyl)-3-phenyl-1H-pyrazol-1-yl)-1-phenylethanol derivatives

pp. 5792–5799

Liang-Wen Zheng, Jian Zhu, Bao-Xiang Zhao*, Yao-Hui Huang, Jun Ding and Jun-Ying Miao*

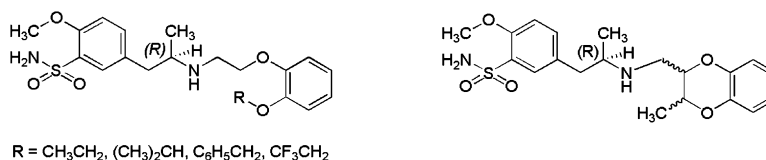
Biological evaluation showed that compounds **4d** and **4e** could suppress A549 lung cancer cell growth through cell cycle arrest and autophagy.



Synthesis and α_1 -adrenoceptor antagonist activity of tamsulosin analogues

pp. 5800–5807

Gianni Sagratini, Piero Angeli, Michela Buccioni, Ugo Gulini, Gabriella Marucci, Carlo Melchiorre, Elena Poggesi and Dario Giardinà*

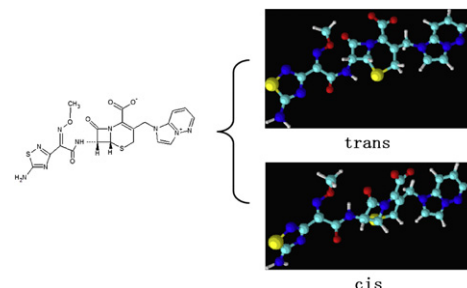


On the isomerisation of cefozopran in solution

pp. 5808–5816

Shu-Yu Liu, Dou-Sheng Zhang and Chang-Qin Hu*

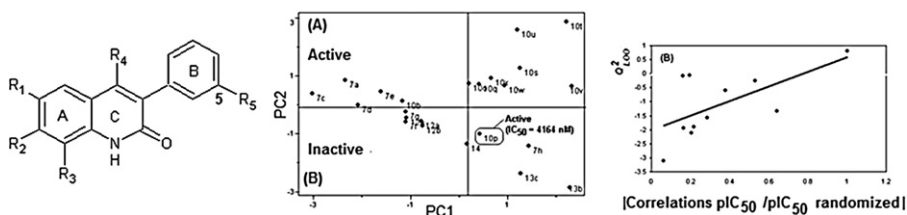
We reported two kinds of configurations of cefozopran in solution, determined their molecular structures and evaluated their biological activity.

**Multivariate SAR/QSAR of 3-aryl-4-hydroxyquinolin-2(1H)-one derivatives as type I fatty acid synthase (FAS) inhibitors**

pp. 5817–5826

Eduardo Borges de Melo*

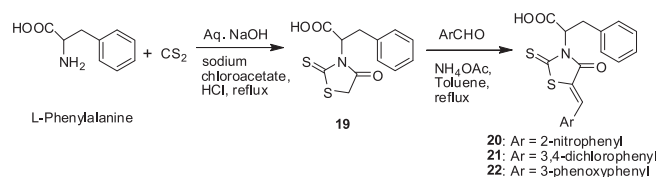
Two multivariate structure–activity relationships studies (PCA and PLS) were performed with a set of 3-aryl-4-hydroxyquinolin-2(1H)-one derivatives described as type I fatty acid synthase (FAS) inhibitors.

**The synthesis of phenylalanine-derived C5-substituted rhodanines and their activity against selected methicillin-resistant *Staphylococcus aureus* (MRSA) strains**

pp. 5827–5832

Diane Hardej, Charles R. Ashby, Jr., Nikhil S. Khadtare, Shridhar S. Kulkarni, Satyakam Singh and Tanaji T. Talele*

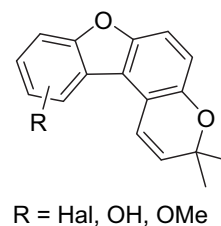
The anti-MRSA activity of the phenylalanine-derived rhodanine analogs **21** (MIC = 3.9 µg/mL, MBC = 7.8 µg/mL) and **22** (MIC = 1.95 µg/mL, MBC = 7.8 µg/mL) was found to be comparable to the reference antibiotic vancomycin (MIC = 0.97 µg/mL).

**Synthesis, biological activity, and evaluation of the mode of action of novel antitubercular benzofurobenzopyrans substituted on A ring**

pp. 5833–5847

Aikaterini Termentzi, Inana Khouri, Thomas Gaslonde, Soizic Prado, Brigitte Saint-Joanis, Fabienne Bardou, Elsa P. Amanatiadou, Ioannis S. Vizirianakis, Jana Kordulakova, Mary Jackson, Roland Brosch, Yves L. Janin, Mamadou Daffé, François Tillequin and Sylvie Michel*

Halo, hydroxy, and methoxy derivatives of 3,3-dimethyl-3H-benzofuro[3,2-f][1]benzopyran were synthesized and tested against *Mycobacterium bovis* and *Mycobacterium tuberculosis*. Effect of the most active derivatives on mycolate synthesis was explored.

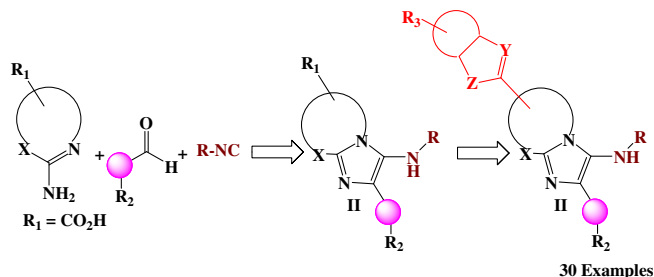


Post Groebke–Blackburn multicomponent protocol: Synthesis of new polyfunctional imidazo[1,2-a]pyridine and imidazo[1,2-a]pyrimidine derivatives as potential antimicrobial agents

pp. 5848–5855

Taleb H. Al-Tel* and Raed A. Al-Qawasmeh

New antimicrobial agents [imidazo[1,2-a]pyridine and imidazo[1,2-a]pyrimidine] have been synthesized and biologically evaluated as antimicrobial agents against various Gram-positive and Gram-negative bacteria.

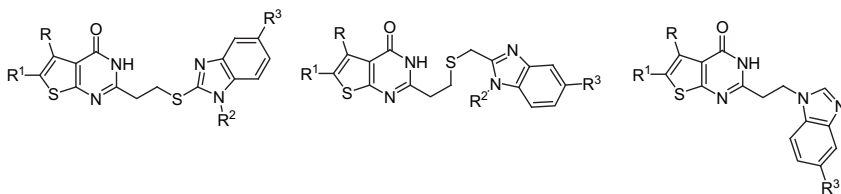


Synthesis, antitrichinellosis and antiprotozoal activity of some novel thieno[2,3-d]pyrimidin-4(3H)-ones containing benzimidazole ring

pp. 5856–5861

Anelia Ts. Mavrova*, Dimitar Vuchev, Kameliya Anichina and Nikolay Vassilev

Novel benzimidazole derivatives of thieno[2,3-d]pyrimidin-4(3H)-ones were synthesized. Significant activity of the compounds against *Trichinella spiralis* in vitro and 100% efficacy against *Lambliam muris* were ascertained in the parasitological screening in vivo.

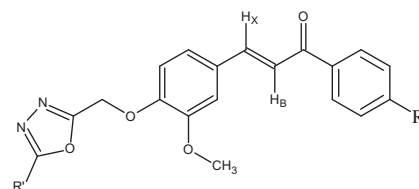


Molecular properties prediction, synthesis and antimicrobial activity of some newer oxadiazole derivatives

pp. 5862–5869

Mohammed Afroz Bakht*, M. Shahar Yar, Sami Gaber Abdel-Hamid, Saleh I. Al Qasoumi and Abdul Samad

Twenty eight oxadiazole analogues (**AB1–AB28**) were subjected to molecular properties prediction. Out of which sixteen (**AB1–AB2**), (**AB5–AB9**), (**AB12–AB16**), (**AB18–AB21**) were chosen on the basis of Lipinski “Rule of Five” (Ro5) for the synthesis and antimicrobial screening as oral bioavailable drugs/leads. Compounds (**AB13**, **AB20**) having maximum drug-likeness model score were found to have good results against bacterial and fungal strains.



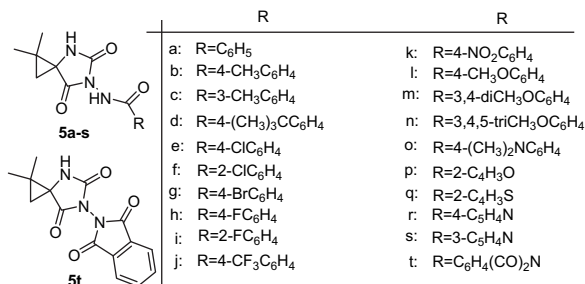
(AB1-AB2), (AB5-AB9), (AB12-AB16), (AB18-AB21)

Synthesis and anticonvulsant activity of N-3-arylamide substituted 5,5-cyclopropanespirohydantoin derivatives

pp. 5870–5877

Xianran He, Min Zhong, Tao Zhang, Wen Wu, Zhongyuan Wu, Jin Yang, Yuling Xiao, Yuanhu Pan, Guofu Qiu and Xianming Hu*

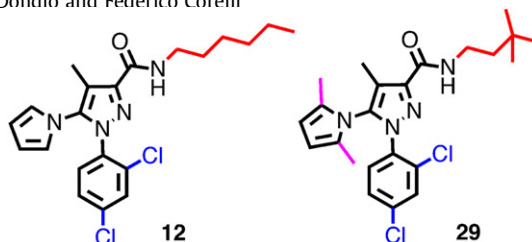
A series of 6-methyl-1-substituted-4,6-diazaspiro[2.4]heptane-5,7-diones (**5a–t**) were synthesized. Their anticonvulsant activities were evaluated by the maximal electroshock (MES) and scPTZ test, and their neurotoxicity was evaluated by the rotarod neurotoxicity test.



Synthesis and biological evaluation of new *N*-alkyl 1-aryl-5-(1*H*-pyrrol-1-yl)-1*H*-pyrazole-3-carboxamides as cannabinoid receptor ligands

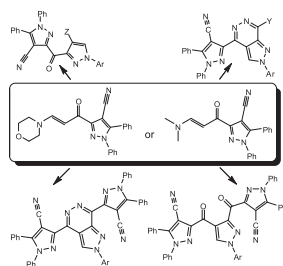
pp. 5878–5886

Romano Silvestri*, Alessia Ligresti, Giuseppe La Regina, Francesco Piscitelli, Valerio Gatti, Antonio Lavecchia**, Antonella Brizzi, Serena Pasquini, Marco Allarà, Noemi Fantini, Mauro Antonio Maria Carai, Chiara Bigogno, Marco Giulio Rozio, Roberta Sinisi, Ettore Novellino, Giancarlo Colombo, Vincenzo Di Marzo, Giulio Dondio and Federico Corelli***

**Design, synthesis and structure–activity relationship study of novel pyrazole-based heterocycles as potential antitumor agents**

pp. 5887–5898

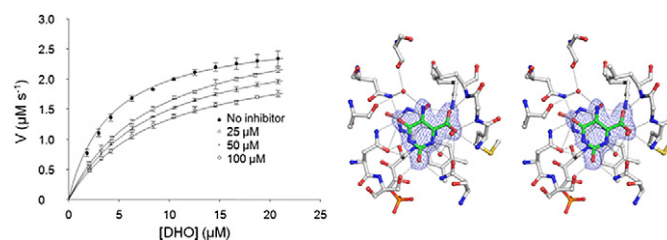
Ahmad M. Farag*, Korany A.K. Ali, Taha M.A. El-Debss, Abdelrahman S. Mayhoub, Abdel-Galil E. Amr, Naglaa A. Abdel-Hafez and Mohamed M. Abdulla

**Novel insights for dihydroorotate dehydrogenase class 1A inhibitors discovery**

pp. 5899–5909

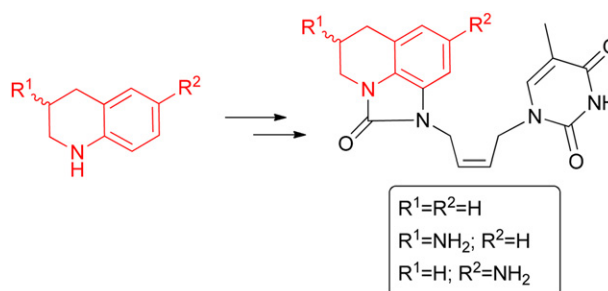
Juliana Cheleski, Josmar R. Rocha, Matheus P. Pinheiro, Helton José Wiggers, Albérico B.F. da Silva, Maria C. Nonato* and Carlos A. Montanari*

Orthogonal validation of ITC nonlinear least squares fit of Michaelis–Menten curves and X-Ray data for 5-aminoorotic acid competitive inhibition.

**Design, synthesis and inhibitory activity against *Mycobacterium tuberculosis* thymidine monophosphate kinase of acyclic nucleoside analogues with a distal imidazoquinolinone**

pp. 5910–5918

Olga Familiar, Hélène Munier-Lehmann, José Antonio Ainsa, María-José Camarasa and María-Jesús Pérez-Pérez*

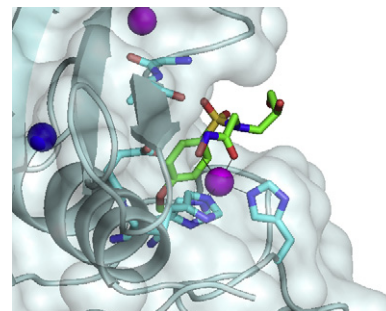


Structure-based approach to nanomolar, water soluble matrix metalloproteinases inhibitors (MMPIs)

pp. 5919–5925

Emanuele Attolino, Vito Calderone, Elisa Dragoni, Marco Fragai, Barbara Richichi, Claudio Luchinat and Cristina Nativi*

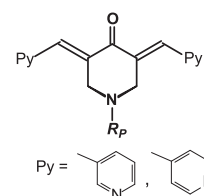
Sulfonamidic MMPs inhibitors soluble in water were obtained relying on structural-based approach. This new family of large spectrum, nanomolar inhibitors can be seen as water soluble NNHG analogues.

**Structure–cytotoxicity relationship in a series of N-phosphorus substituted *E,E*-3,5-bis(3-pyridinylmethylene)- and *E,E*-3,5-bis(4-pyridinylmethylene)piperid-4-ones**

pp. 5926–5934

Evgeniya S. Leonova, Michael V. Makarov, Ekaterina Yu. Rybalkina, Shravana L. Nayani, Paul Tongwa, Alexander Fonari, Tatiana V. Timofeeva and Irina L. Odinets*

Phosphorus substituted 3,5-bis(pyridinylmethylene)-piperid-4-ones possess high cytotoxicity towards human carcinoma cell lines Caov3, A549, KB 3-1, including multi-drug resistant subline KB 8-5, where the derivatives with more electron-withdrawing 4-pyridine rings are more potent.



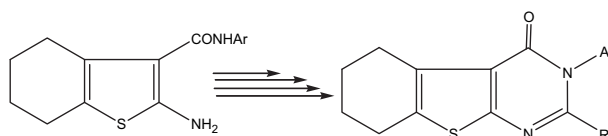
$R_P = \text{P}(\text{O})(\text{OEt})_2, \text{P}(\text{O})(\text{OPh})_2, \text{P}(\text{O})\text{Me}(\text{OPh});$
 $(\text{CH}_2)_n\text{P}(\text{O})(\text{OEt})_2; n=1, 2, 4$

IC_{50} 2–45 μM (Caov3, A549, KB 3-1, KB 8-5)

Antiarrhythmic, serotonin antagonist and antianxiety activities of novel substituted thiophene derivatives synthesized from 2-amino-4,5,6,7-tetrahydro-N-phenylbenzo[b]thiophene-3-carboxamide

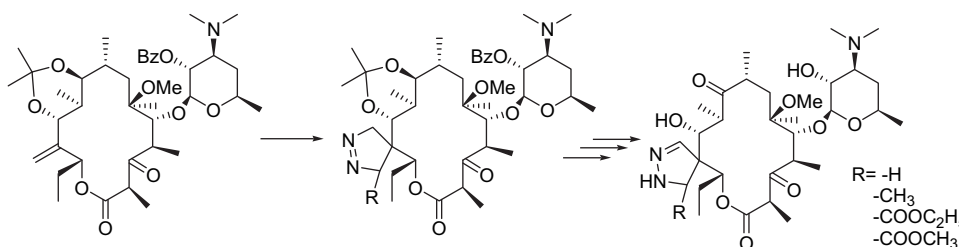
pp. 5935–5942

Abd El-Galil E. Amr*, Mohamed H. Sherif, Mohamed G. Assy, Mohamed A. Al-Omar and Islam Ragab

**Synthesis and antibacterial activity of C-12 pyrazolanyl spiro ketolides**

pp. 5943–5949

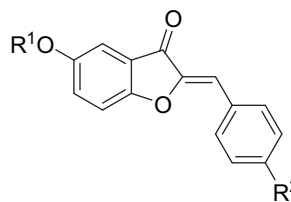
Lei Hu, Ping Lan, Qiu-Ling Song, Zhi-Jian Huang, Ping-Hua Sun, Chao Zhuo, Ying Wang, Shunian Xiao and Wei-Min Chen*



Design, synthesis and discovery of 5-hydroxyaurone derivatives as growth inhibitors against HUVEC and some cancer cell lines pp. 5950–5957

Huimin Cheng, Lianwen Zhang, Yingxue Liu, Shaopeng Chen, Hao Cheng, Xin Lu, Zhuxia Zheng and Guo-Chun Zhou*

5-Hydroxyaurone compounds **16** and **27** exhibited potent inhibitory activity against the proliferation of endothelial cells and cancer cells. They effectively inhibited *in vitro* endothelial cell motility and tube formation and also *in vitro* cancer cell invasion.



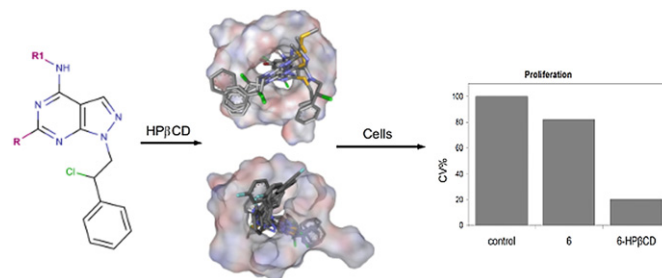
$R^1 = \text{H}$, $R^2 = \text{NEt}_2$, **16**
 $\text{IC}_{50}(\text{HUVEC}) = 0.25 \mu\text{M}$
 $\text{IC}_{50}(\text{MCF-7}) = 1.81 \mu\text{M}$
 $\text{IC}_{50}(\text{A549}) = 1.25 \mu\text{M}$

$R^1 = \text{Ac}$, $R^2 = \text{NEt}_2$, **27**
 $\text{IC}_{50}(\text{HUVEC}) = 0.23 \mu\text{M}$
 $\text{IC}_{50}(\text{MCF-7}) = 2.95 \mu\text{M}$
 $\text{IC}_{50}(\text{A549}) = 1.29 \mu\text{M}$

2-Hydroxypropyl- β -cyclodextrin strongly improves water solubility and anti-proliferative activity of pyrazolo[3,4-d]pyrimidines Src-Abl dual inhibitors pp. 5958–5964

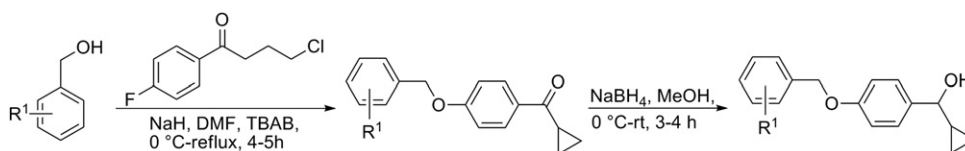
Elena Dreassi, Alessandra Tania Zizzari, Mattia Mori, Irene Filippi, Amalia Belfiore, Antonella Naldini, Fabio Carraro, Annalisa Santucci, Silvia Schenone** and Maurizio Botta*

Phase solubility studies were conducted for a class of very insoluble pyrazolo-pyrimidines and for their complexes with HP β CD. Increased solubility observed for all compounds, together with the very significant improvement of their biological activity, set the bases for enhancing the bioavailability of these promising candidate-drugs.



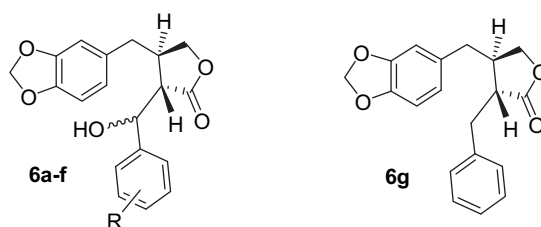
Synthesis and optimization of antitubercular activities in a series of 4-(aryloxy)phenyl cyclopropyl methanols pp. 5965–5978

Surendra S. Bisht, Namrata Dwivedi, Vinita Chaturvedi, Namrata Anand, Mridul Misra, Rahul Sharma, Brijesh Kumar, Richa Dwivedi, Shyam Singh, Sudhir Kumar Sinha, Versha Gupta, P.R. Mishra, Anil K. Dwivedi and Rama P. Tripathi



Isochaihulactone analogues: Synthesis and anti-proliferative activity of novel dibenzylbutyrolactones pp. 5979–5984

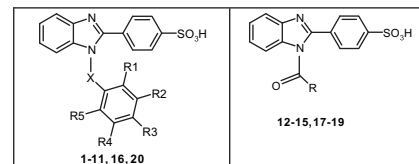
Babak Heidary Alizadeh, Alireza Foroumadi, Saeed Emami, Mehdi Khoobi, Fatemeh Panah, Sussan K. Ardestani and Abbas Shafiee*



4-[1-(Substituted aryl/alkyl carbonyl)-benzimidazol-2-yl]-benzenesulfonic acids: Synthesis, antimicrobial activity, QSAR studies, and antiviral evaluation pp. 5985–5997

Snehlata Yadav, Pradeep Kumar, Erik De Clercq, Jan Balzarini, Christophe Pannecouque, Sharwan Kumar Dewan and Balasubramanian Narasimhan*

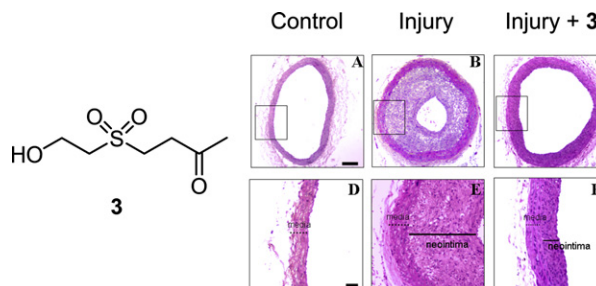
The *in vitro* antimicrobial activity of a series of substituted benzimidazoles (**1–20**) indicated that compounds 4-[1-(4-Nitrobenzoyl)-1H-benzimidazol-2-yl]-benzene sulfonic acid (**9**) and 4-(1-octadec-9-enoyl-1H-benzimidazol-2-yl)-benzenesulfonic acid (**18**) were found to be the most active ones.



A neuroprotective sulfone of marine origin and the *in vivo* anti-inflammatory activity of an analogue pp. 5998–6004

Zhi-Hong Wen, Chih-Hua Chao, Ming-Hsuan Wu and Jyh-Horng Sheu*

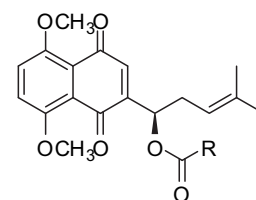
Isolation, activity, and synthesis of a new soft coral metabolite, austrasulfone (**1**), were described. Its synthetic intermediate, dihydroaustrasulfone alcohol (**3**), also exhibited promising *in vitro* and *in vivo* anti-inflammatory activity.



Semi-synthesis and anti-tumor activity of 5,8-O-dimethyl acylshikonin derivatives pp. 6005–6011

Wen Zhou, Ying Peng and Shao-Shun Li*

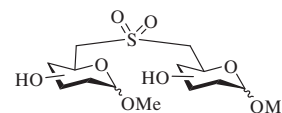
Twenty-two 5,8-O-dimethyl acylshikonin derivatives were synthesized and evaluated for their cytotoxicity to three cancer cells. The *in vivo* anti-tumor activities of three derivatives were also reported.



Efficient synthesis of (6-deoxyglycopyranosid-6-yl) sulfone derivatives and their effect on Ca²⁺-ATPase pp. 6012–6019

Chinmoy Mukherjee, Swatilekha Ghosh, Pinki Nandi, Parimal C. Sen and Anup Kumar Misra*

Convenient synthesis of a series of novel (6-deoxyglycopyranosid-6-yl) sulfone derivatives and their bioevaluation against Ca²⁺-ATPase is reported. Yields were excellent in every case.



pp. 6020–6026

pp. 6027–6038

Chemical structures of compounds 4a,b, 6a,b, and 10a,b are shown. The structures are based on a 1-phenyl-2-(4-R-phenyl)-1H-imidazole-5-ylidene-1,3-dithiane core. The substituent R is defined as R = H, CH₃.

4a,b

6a,b

10a,b

R = H, CH₃

pp. 6039–6044

$$\text{CH}_3\text{O}-\text{P}\left(\begin{array}{c} \text{O} \\ \parallel \\ \text{RCHNH} \\ | \\ \text{C}_6\text{H}_4 \\ | \\ \text{CH}_2 \end{array}\right)\left[\text{O}(\text{CH}_2\text{CH}_2\text{O})_k\right]_n-\text{P}\left(\begin{array}{c} \text{O} \\ \parallel \\ \text{RCHNH} \\ | \\ \text{C}_6\text{H}_4 \\ | \\ \text{CH}_3 \end{array}\right)_n-\text{P}\left(\begin{array}{c} \text{O} \\ \parallel \\ \text{RCHNH} \\ | \\ \text{C}_6\text{H}_4 \\ | \\ \text{CH}_3 \end{array}\right)\text{OH}$$

pp. 6045–6051

Chemical structures of [alpha]-santonin, [3], and [13] derivatives are shown. The structures are tricyclic compounds with a central seven-membered ring fused to two six-membered rings. The central ring has a ketone group at C1 and a double bond between C2 and C3. The left six-membered ring has a ketone group at C4 and a double bond between C5 and C6. The right six-membered ring has a ketone group at C7 and a double bond between C8 and C9. The central ring has a hydroxyl group at C10 and a double bond between C11 and C12. The left six-membered ring has a double bond between C13 and C14. The right six-membered ring has a double bond between C15 and C16. The structures are labeled [alpha]-santonin, [3], and [13].

[α -santonin] R = H, CH₃
 [1] R = CH₂
 [11] R = H, CH₂COCH₂

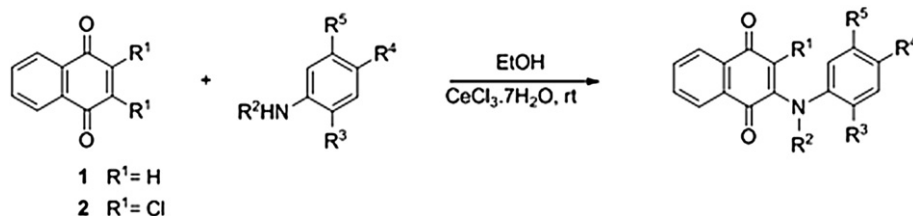
[3] R = CH₂
 [13] R = H, CH₂COCH₂

isomeric mixture [5] and [6]

Biological evaluation of donor-acceptor aminonaphthoquinones as antitumor agents

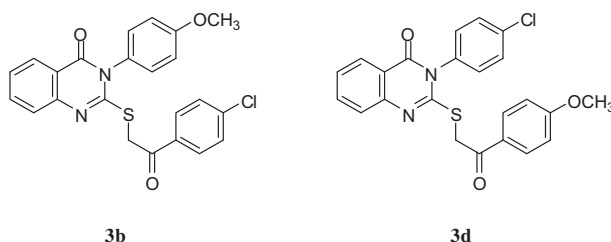
pp. 6052–6057

Julio Benites, Jaime A. Valderrama, Karina Bettega, Rozangela Curi Pedrosa, Pedro Buc Calderon and Julien Verrax*

**Synthesis and antitumor activity of some 2, 3-disubstituted quinazolin-4(3H)-ones and 4, 6-disubstituted- 1, 2, 3, 4-tetrahydroquinazolin-2H-ones**

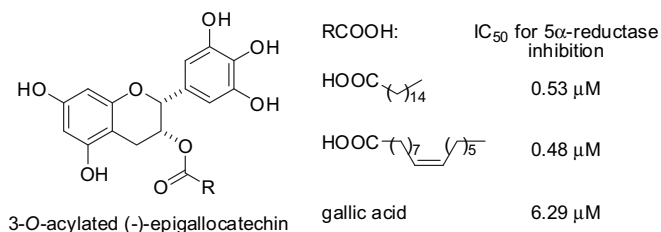
pp. 6058–6067

Nagwa M. Abdel Gawad, Hanan H. Georgey*, Riham M. Youssef and Nehad A. El-Sayed

**Synthesis and structure–activity relationship of 3-O-acylated (–)-epigallocatechins as 5 α -reductase inhibitors**

pp. 6068–6076

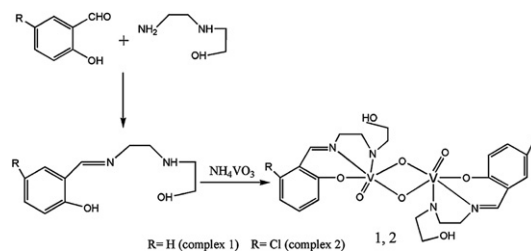
Shu Fu Lin, Yu-Hsiang Lin, Mengju Lin, Yi-Feng Kao, Ru-Wen Wang, Li-Wei Teng, Shih-Hsien Chuang, Jia-Ming Chang, Ta-Tung Yuan, Kuo Chu Fu, Kuan Pin Huang, Ying-Shuen Lee, Chao-Cheng Chiang, Sheng-Chuan Yang, Chun-Liang Lai, Chu-Bin Liao, Paonien Chen, Young-Sun Lin, Kuei-Tai Lai, Hung-Jyun Huang, Ju-Ying Yang, Chia-Wei Liu, Win-Yin Wei, Chi-Kuan Chen, Richard A. Hiipakka, Shutsung Liao and Jiann-Jyh Huang*

Introduction of fatty acid to the C3-O position of (–)-epigallocatechin increases the potency for the inhibition of steroid 5 α -reductase.**Effect of the chloro-substitution on lowering diabetic hyperglycemia of vanadium complexes with their permeability and cytotoxicity**

pp. 6077–6084

Ming-Jin Xie*, Yan-Fen Niu, Xiao-Da Yang, Wei-Ping Liu, Ling Li, Li-Hui Gao, Shi-Ping Yan and Zhao-Hui Meng

The effect of the chloro-substitution of dinuclear vanadium (V) complexes on lowering diabetic hyperglycemia was the chloro substituent may be increased the insulin-enhancing properties of the complex 2.



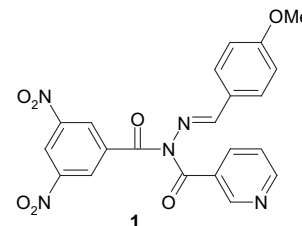
SHORT COMMUNICATIONS

Synthesis and antitubercular activities of substituted benzoic acid *N'*-(substituted benzylidene/furan-2-ylmethylene)-*N*-(pyridine-3-carbonyl)-hydrazides

pp. 6085–6089

Pradeep Kumar, Balasubramanian Narasimhan*, Perumal Yogeeswari and Dharmarajan Sriram

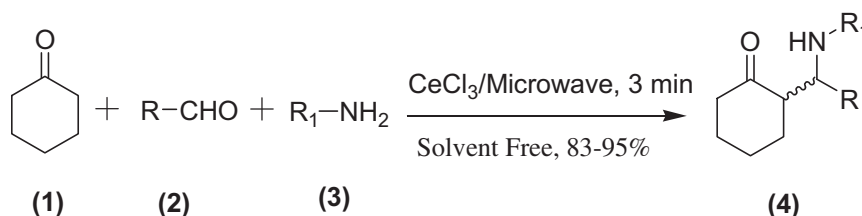
A series of benzoic acid hydrazones (**1–10**) evaluated for their antitubercular activity indicated that nicotinic acid *N*-(3,5-dinitro-benzoyl)-*N'*-(4-methoxy-benzylidene)-hydrazide (**1**) is the most potent one.

**Synthesis and biological evaluation of aminoketones**

pp. 6090–6094

U. Sankappa Rai, Arun M. Isloor*, Prakash Shetty, Nishitha Isloor, Shridhar Malladi and Hoong-Kun Fun

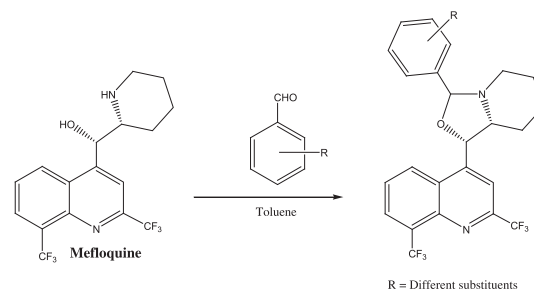
Three-component Mannich reaction of ketones with aromatic aldehydes and different amines in microwave irradiation afforded corresponding β -amino carbonyl compounds in good yields. Structure of the synthesized compounds were confirmed by spectral studies. Few compounds showed excellent antibacterial activity.

**Synthesis and antitubercular activity of new mefloquine-oxazolidine derivatives**

pp. 6095–6100

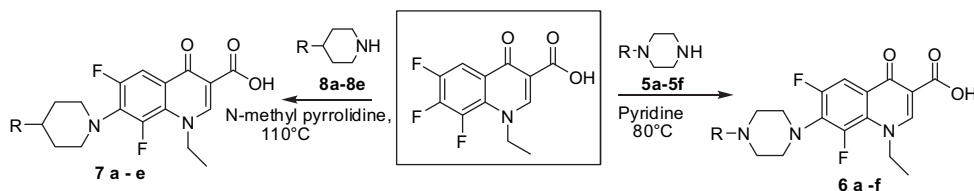
Raoni S.B. Gonçalves, Carlos R. Kaiser, Maria C.S. Lourenço, Marcus V.N. de Souza*, James L. Wardell, Solange M.S.V. Wardell and Adilson D. da Silva

Several new mefloquine-oxazolidine derivatives have been synthesized and evaluated as antituberculosis agents. The compounds displayed substantial activities and high cell viability.

**Synthesis and *in vitro* antimicrobial evaluation of novel fluoroquinolone derivatives**

pp. 6101–6105

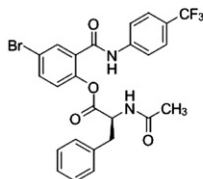
Shanmugam Srinivasan, Raja Mohmed Beema Shaheen, Paramasivam Nithyanand, Paramasivam Manisankar and Shunmugiah Karutha Pandian*



New amino acid esters of salicylanilides active against MDR-TB and other microbes

pp. 6106–6113

Martin Krátký, Jarmila Vinšová*, Vladimír Buchta, Kata Horvati, Szilvia Bösze and Jirina Stolaříková



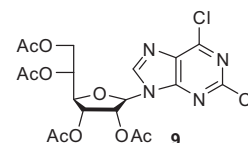
MIC = 0.25 - 2 $\mu\text{mol/L}$ against *M. tuberculosis* including MDR-TB
 MIC = 3.9 - 7.81 $\mu\text{mol/L}$ against *Trichophyton mentagrophytes*
 SI = 24.1 - 194.8

Synthesis and cytostatic activity of purine nucleosides derivatives of allofuranose

pp. 6114–6119

Pedro Besada**, Tamara Costas, Marta Teijeira and Carmen Terán*

Several new purine nucleosides derivatives of allofuranose were synthesized and evaluated for their cytotoxicity *in vitro* in three human cancer cell lines. Among the studied compounds, the acetyl derivative **9** was the most potent one on the three cell lines evaluated.

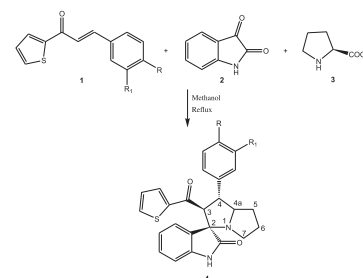


Regiospecific synthesis and biological evaluation of spirooxindolopyrrolizidines via [3 + 2] cycloaddition of azomethine ylides

pp. 6120–6126

Arumugam Thangamani*

A series of spirooxindolopyrrolizidines prepared in good yields from the reaction of thiophenyl-substituted dipolarophiles, isatin and *L*-proline under reflux conditions show good *in vitro* antibacterial and antifungal activity.

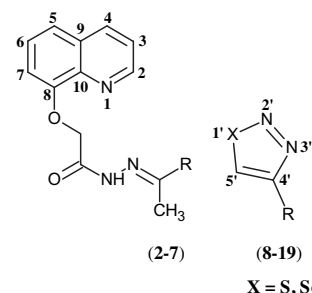


Synthesis, characterization, antiamebic activity and cytotoxicity of novel 2-(quinolin-8-yloxy) acetohydrazone and their cyclized products (1,2,3-thiadiazole and 1,2,3-selenadiazole derivatives)

pp. 6127–6134

Faisal Hayat, Attar Salahuddin, Jamil Zargan and Amir Azam

Novel 1,2,3-thiadiazole, 1,2,3-selenadiazole and 2-(quinolin-8-yloxy) acetohydrazone derivatives (**2–19**) were synthesized. Compounds (**2–7**), **9**, **10**, **12**, **16** and **17** exhibited better antiamebic activity and screened for cytotoxicity.

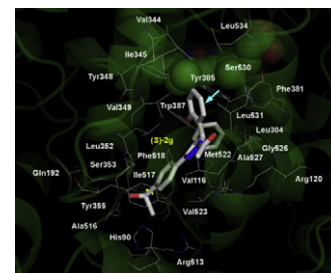


Synthesis and biological evaluation of N-substituted-3,5-diphenyl-2-pyrazoline derivatives as cyclooxygenase (COX-2) inhibitors

pp. 6135–6138

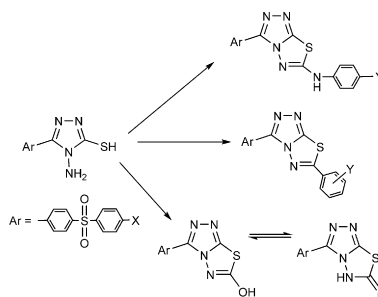
Rossella Fioravanti*, Adriana Bolasco, Fedele Manna, Francesca Rossi, Francisco Orallo, Francesco Ortuso, Stefano Alcaro and Roberto Cirilli

In this paper, eighteen new 1-N-substituted-3,5-diphenyl-2-pyrazoline derivatives have been synthesized and tested *in vitro*, as anti-inflammatory agents. The results of these biological assays showed that all of new derivatives are not endowed with improved anti-inflammatory activity against COX-1, but some of them showed a good activity against COX-2.

**Synthesis and antimicrobial evaluation of some fused heterocyclic [1,2,4]triazolo[3,4-b][1,3,4]thiadiazole derivatives**

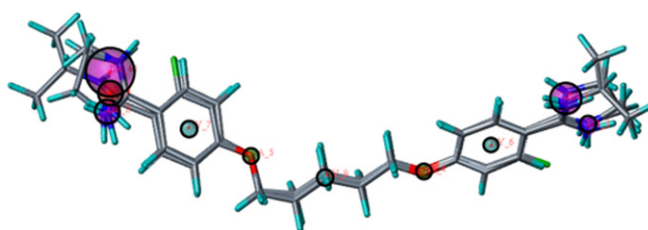
pp. 6139–6146

Gabriela Laura Almajan*, Stefania-Felicia Barbuceanu, Gabriela Bancescu, Ioana Saramet, Gabriel Saramet and Constantin Draghici

**PRELIMINARY COMMUNICATIONS****Pharmacophore model for pentamidine analogs active against *Plasmodium falciparum***

pp. 6147–6151

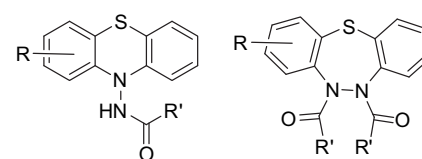
Prashanth Athri*, Tanja Wenzler, Richard Tidwell, Svetlana M. Bakunova and W. David Wilson

**Old phenothiazine and dibenzothiadiazepine derivatives for tomorrow's neuroprotective therapies against neurodegenerative diseases**

pp. 6152–6158

Gema C. González-Muñoz, Mariana P. Arce, Beatriz López, Concepción Pérez, Mercedes Villarroya, Manuela G. López, Antonio G. García, Santiago Conde* and María Isabel Rodríguez-Franco*

From an in-house library of compounds, one *N*-acylaminophenothiazine and one 1,4,5-dibenzo[*b,f*]thiadiazepine have been selected as lead compounds to develop two new lines, currently in progress.



COVER

Image of Antibacterial activities of urea and thiourea derivatives of 15-membered azalides in comparison to sulfonylurea analogs. 44/9, P3459–3470 by Mirjana Bukvić Krajačić, Predrag Novak, Miljenko Dumić, Mario Cindrić, Hana Čipčić Paljetak and Nedjeljko Kujundžić © 2009 Published by Elsevier Masson SAS

* Corresponding authors.



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