



## European Journal of Medicinal Chemistry Vol 46, No 1, 2011

## Contents

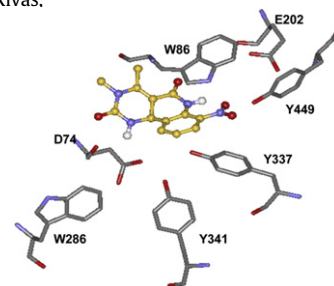
## ORIGINAL ARTICLES

**Synthesis, biological assessment and molecular modeling of new dihydroquinoline-3-carboxamides and dihydroquinoline-3-carbohydrazide derivatives as cholinesterase inhibitors, and Ca channel antagonists**

pp. 1–10

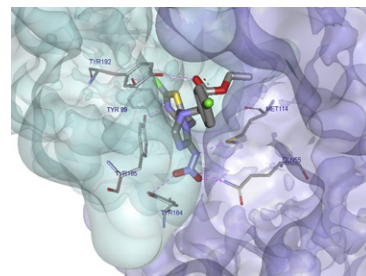
Isabelle Tomassoli, Lhassane Ismaili, Marc Pudlo, Cristóbal de los Ríos, Elena Soriano, Inés Colmena, Luis Gandía, Luis Rivas, Abdelouahid Samadi, José Marco-Contelles and Bernard Refouvet\*

A series of quinoline derivatives have been designed, synthesized and evaluated in vitro for their cholinesterase inhibitory activity and selectivity and Ca channel antagonist. Docking analysis allowed to identify the binding mode in the active site and to explain the observed selectivities.


**Chiral 1,5-disubstituted 1,3,5-hexahydrotriazine-2-*N*-nitroimine analogues as novel potent neonicotinoids: Synthesis, insecticidal evaluation and molecular docking studies**

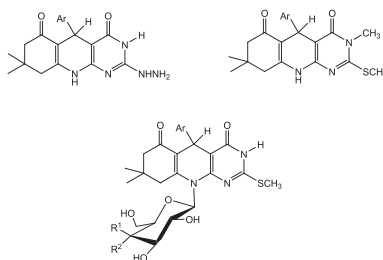
pp. 11–20

Chuanwen Sun\*, Jun Zhu, Haifeng Wang, Jia Jin, Jiahua Xing and Dingrong Yang

 A series of new chiral neonicotinoid analogues (**4a–4x**) were prepared and evaluated for the insecticidal activity, and their binding interactions with the receptor were investigated by molecular docking studies

**Synthesis, *in vitro* antimicrobial and *in vivo* antitumor evaluation of novel pyrimidoquinolines and its nucleoside derivatives**

pp. 21–30

Hebat-Allah S. Abbas\*, Hend N. Hafez and Abdel-Rahman B.A. El-Gazzar

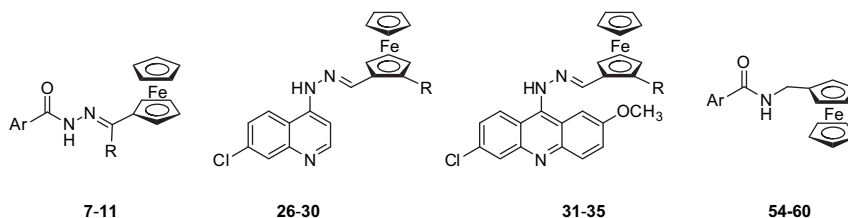


**Synthesis and antimycobacterial activity of a series of ferrocenyl derivatives**

pp. 31–38

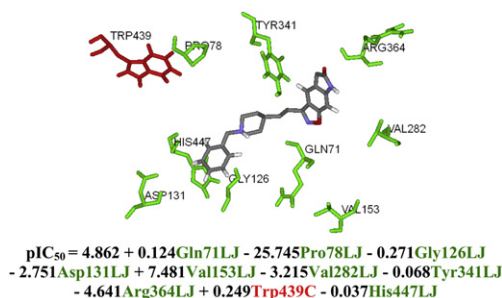
Gabin Mwande Maguene, Jouda Jakhlal, Melissa Ladyman, Aurélie Vallin, Dimby Andrianina Ralambomanana, Till Bousquet, Jeanne Maugein, Jacques Lebibi\*\* and Lydie Pélinski\*

The synthesis of twenty five ferrocenyl derivatives was presented. All compounds were screened for their antimycobacterial activities.

**Receptor-dependent (RD) 3D-QSAR approach of a series of benzylpiperidine inhibitors of human acetylcholinesterase (HuAChE)**

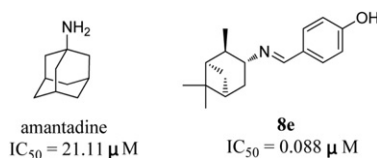
pp. 39–51

Jocley Queiroz Araújo\*, Monique Araújo de Brito, Lucas Villas Bôas Hoelz, Ricardo Bicca de Alencastro, Helena Carla Castro, Carlos Rangel Rodrigues and Magaly Girão Albuquerque\*

**Discovery of highly potent agents against influenza A virus**

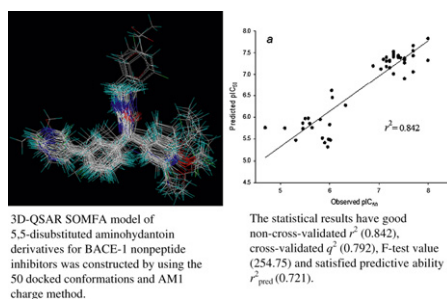
pp. 52–57

Xin Zhao, Chufang Li, Shaogao Zeng and Wenhui Hu\*

**Self-organizing molecular field analysis on human  $\beta$ -secretase nonpeptide inhibitors: 5, 5-disubstituted aminohydantoins**

pp. 58–64

Zhi Li, Meng Zhou, Feng Wu, Rui Li\* and Zhenyu Ding

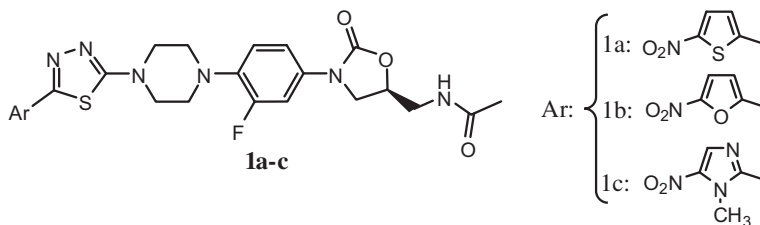


### Discovery of a novel nitroimidazolyl–oxazolidinone hybrid with potent anti Gram-positive activity: Synthesis and antibacterial evaluation

pp. 65–70

Ali Khalaj, Maryam Nakhjiri, Amir Soheil Negahbani, Marjaneh Samadizadeh, Loghman Firoozpour, Saeed Rajabalian, Nasrin Samadi, Mohammad Ali Faramarzi, Neda Adibpour, Abbas Shafiee and Alireza Foroumadi\*

Novel linezolid analogues containing a nitroaryl-1,3,4-thiadiazole moiety, were synthesized and evaluated against a panel of Gram-positive and Gram-negative bacteria.

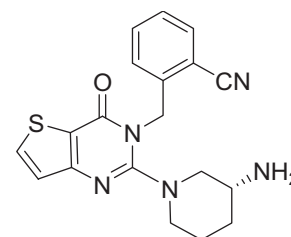


### The highly potent and selective dipeptidyl peptidase IV inhibitors bearing a thienopyrimidine scaffold effectively treat type 2 diabetes

pp. 71–76

Jifeng Deng, Li Peng, Guicheng Zhang, Xiaobing Lan, Chufang Li, Fuxin Chen, Yayao Zhou, Zuoxian Lin, Ling Chen, Renke Dai, Hongjiang Xu, Ling Yang, Xiquan Zhang and Wenhui Hu\*

Compound **10d** was found to be a highly potent DPP-IV inhibitor ( $IC_{50} = 0.33$  nM) and exhibited good *in vivo* efficacy and an acceptable pharmacokinetic profile.

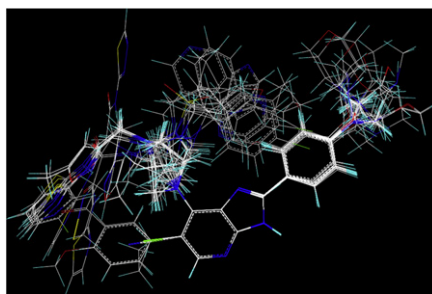


**10d**,  $IC_{50} = 0.33$  nM

### Molecular modeling studies on imidazo[4,5-b]pyridine derivatives as Aurora A kinase inhibitors using 3D-QSAR and docking approaches

pp. 77–94

Ping Lan, Wan-Na Chen and Wei-Min Chen\*

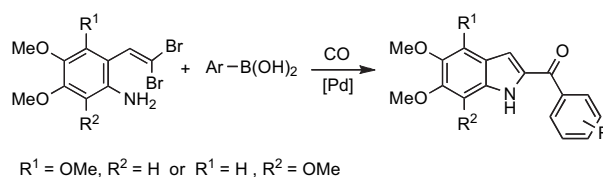


### Domino approach to 2-aryltrimethoxyindoles as novel heterocyclic combretastatin A4 analogues

pp. 95–100

Martin Arthuis, Renée Pontikis\*, Guy G. Chabot, Lionel Quentin, Daniel Scherman and Jean-Claude Florent\*

An efficient synthesis of 2-aryltrimethoxyindoles is reported via a domino palladium-catalyzed sequence. The antiproliferative activity and tubulin polymerization inhibition were evaluated.

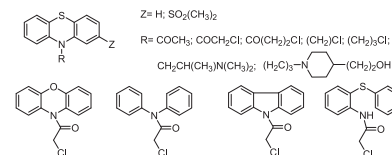


**Synthesis and antifungal activity of some substituted phenothiazines and related compounds**

pp. 101–105

Gabriela P. Sarmiento, Roxana G. Vitale, Javier Afeltra, Graciela Y. Moltrasio and Albertina G. Moglioni\*

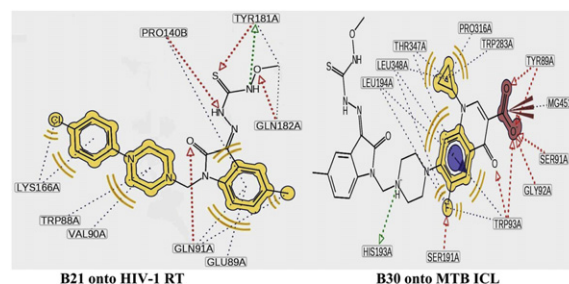
Some phenothiazine derivatives and related compounds have been prepared and evaluated as potential antifungal agents against 14 nosocomial strains of fungi. Pipothiazine and promethazine showed activity at high concentrations, but one of the simplest derivatives, compound **6** ( $Z = H$ ;  $R = COCH_2Cl$ ), showed an important activity at low concentrations.

**Novel isatinyl thiosemicarbazones derivatives as potential molecule to combat HIV-TB co-infection**

pp. 106–121

Debjani Banerjee, Perumal Yogeeswari, Pritesh Bhat, Anisha Thomas, Madala Srividya and Dharmarajan Sriram\*

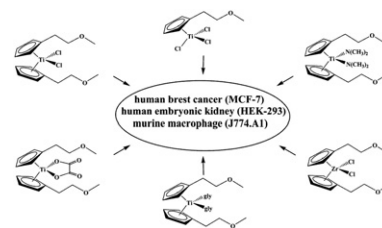
A series of novel 5-substituted-1-(arylmethyl/alkylmethyl)-1H-indole-2,3-dione-3-(N-hydroxy/methoxy thiosemicarbazone) analogues were synthesized and evaluated for their anti-HIV activity and anti-tubercular activity.

**Synthesis, characterization and cytotoxicity studies of methoxy alkyl substituted metallocenes**

pp. 122–128

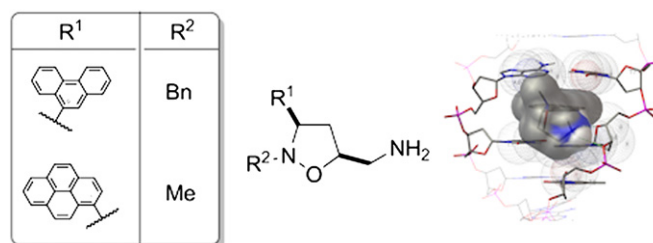
Mariagrazia Napoli\*, Carmela Saturnino, Esther Sirignano, Ada Popolo, Aldo Pinto and Pasquale Longo

Five titanocene derivatives and one zirconium analogous, having cyclopentadienylethenylmethoxy ligand, were synthesized and fully characterized. The rate of hydrolysis of these compounds was studied and the cytotoxic activities have been evaluated on human breast cancer (MCF-7) human embryonic kidney (HEK-293) and murine macrophage (J774.A1) cell lines.

**Isoxazolidinyl polycyclic aromatic hydrocarbons as DNA-intercalating antitumor agents**

pp. 129–136

Antonio Rescifina\*, Ugo Chiacchio, Antonino Corsaro, Anna Piperno and Roberto Romeo

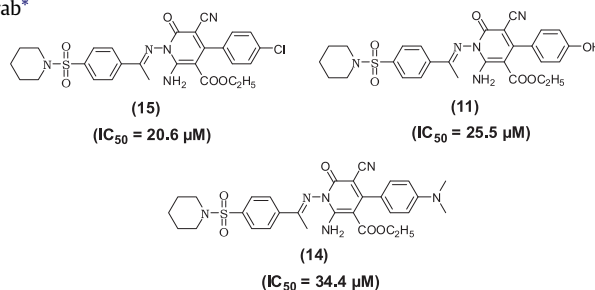


**Anti-breast cancer activity of some novel 1,2-dihydropyridine, thiophene and thiazole derivatives**

pp. 137–141

Mansour S. Al-Said, Mahmoud S. Bashandy, Saleh I. Al-qasoumi and Mostafa M. Ghorab\*

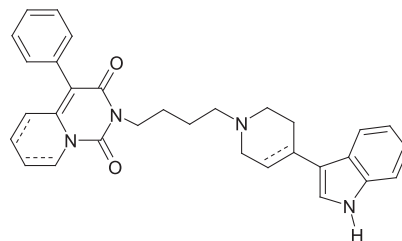
A variety of novel 1,2-dihydropyridines **10–17**, thiophenes **18–21** and thiazole **22** having a biologically active sulfone moiety were synthesized to evaluate their anti-breast cancer activity. Compounds **15** and **11** with  $IC_{50}$  values (20.6, 25.5  $\mu M$ ) exhibited better activity than Doxorubicin as a reference drug with  $IC_{50}$  value (32.02  $\mu M$ ), while compound **14** is nearly as active as Doxorubicin as positive control.

**Novel 4-aryl-pyrido[1,2-c]pyrimidines with dual SSRI and 5-HT<sub>1A</sub> activity. part 3**

pp. 142–149

Franciszek Herold\*, Andrzej Chodkowski, Łukasz Izbiński, Jadwiga Turło, Maciej Dawidowski, Jerzy Kleps, Gabriel Nowak, Katarzyna Stachowicz, Małgorzata Dytała, Agata Siwek, Aleksander P. Mazurek, Andrzej Mazurek and Franciszek Pluciński

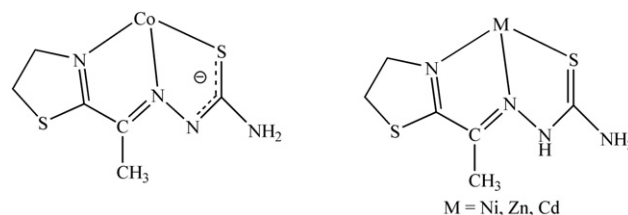
Structure of pyrido[1,2-c]pyrimidines with dual 5-HT<sub>1A</sub>/SERT activity

**Co(III), Ni(II), Zn(II) and Cd(II) complexes with 2-acetyl-2-thiazoline thiosemicarbazone: Synthesis, characterization, X-ray structures and antibacterial activity**

pp. 150–159

E. Viñuelas-Zahinos, F. Luna-Giles\*, P. Torres-García and M.C. Fernández-Calderón

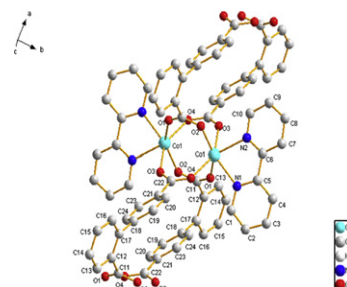
Six metal complexes of a novel thiosemicarbazone-thiazoline derivative ligand were characterized and their antimicrobial activity studied. Cadmium(II) complexes were more active than the ligand against most of tested microorganisms.

**Synthesis and crystal structure of two new dinuclear cobalt(II) complexes interaction with HeLa cells**

pp. 160–167

En-jun Gao\*, Xia-nan Gao, Feng Guan, Ming-chang Zhu, Lei Liu, Min Zhang, Ying-xing Zhang, Ying Wang, Zheng Wen, Yan Zhang, Ying Zhang and Qi Liang

Two Co(II) atoms' coordinate pattern is the same, both Co(II) atoms are six coordinated by two nitrogen atoms from the bipy, four oxygen atoms from four different biphenyl-2,4'-dicarboxylic acid ligands.

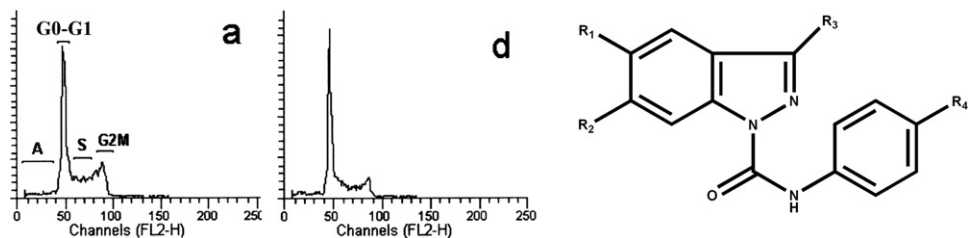


### Synthesis of substituted 3-amino-N-phenyl-1H-indazole-1-carboxamides endowed with antiproliferative activity

pp. 168–174

Benedetta Maggio, Maria Valeria Raimondi, Demetrio Raffa, Fabiana Plescia, Stella Cascioferro, Salvatore Plescia, Manlio Tolomeo, Antonietta Di Cristina, Rosaria Maria Pipitone, Stefania Grimaudo and Giuseppe Daidone\*\*

A series of N-phenyl-1H-indazole-1-carboxamide derivatives have been synthesized and tested against the full panel NCL cell lines. The most active compound **1c** showed a mean GI<sub>50</sub> value of 1.90 μM. It was able to induce G0–G1 arrest.

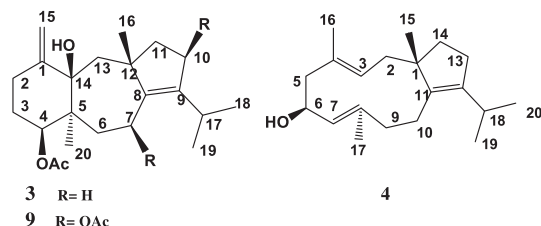


### Cytotoxic and protective DNA damage of three new diterpenoids from the brown alga *Dictyota dichotoma*

pp. 175–182

Seif-Eldin N. Ayyad\*, Mohamed S. Makki, Nazeeha S. Al-kayal, Salim A. Basaif, Kalid O. El-Foty, Abdullah M. Asiri, Walied M. Alarif and Farid A. Badria

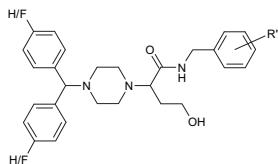
New diterpenes **3**, **4** and **9** isolated from the brown alga *D. dichotoma* showed highest protection activity against DNA damage, strong cytotoxic activity, antitumor and antioxidant activity.



### Synthesis and biological evaluation of new derivatives of 2-substituted 4-hydroxybutanamides as GABA uptake inhibitors

pp. 183–190

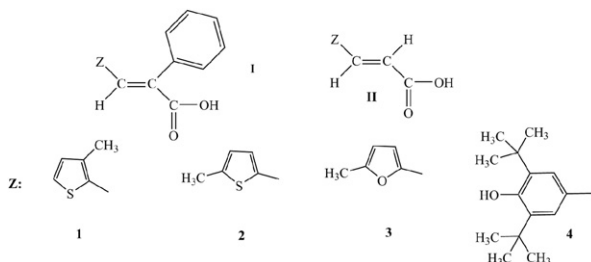
Katarzyna Kulig, Krzysztof Więckowski, Anna Więckowska, Justyna Gajda, Bartłomiej Pochwat, Georg C. Höfner, Klaus T. Wanner and Barbara Malawska\*



### Design, synthesis and pharmacobiological evaluation of novel acrylic acid derivatives acting as lipoxygenase and cyclooxygenase-1 inhibitors with antioxidant and anti-inflammatory activities

pp. 191–200

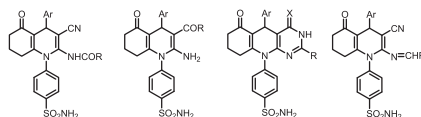
Eleni Pontiki\*, Dimitra Hadjipavlou-Litina\*, Konstantinos Litinas, Orazio Nicolotti and Angelo Carotti



## Synthesis and *in vitro* anticancer evaluation of some novel hexahydroquinoline derivatives having a benzenesulfonamide moiety

pp. 201–207

Mansour S. Al-Said, Mostafa M. Ghorab\*, Mohammed S. Al-Dosari and Mostafa M. Hamed

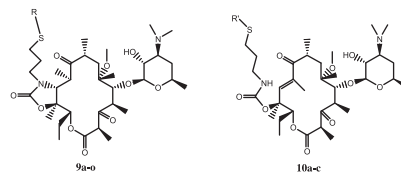
Ar = C<sub>6</sub>H<sub>3</sub>Cl<sub>2</sub>-2,4

## Synthesis and antibacterial activity of novel ketolides with 11,12-sulfur contained aryl alkyl side chains

pp. 208–217

Xiao-zhuo Chen, Peng Xu, Lu Liu, Dan Zheng and Ping-sheng Lei\*

A novel series of ketolides with 11,12-sulfur contained aryl alkyl side chains were synthesized and evaluated for their antibacterial activity.

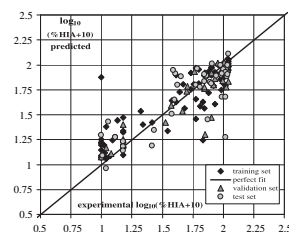


## Prediction of drug intestinal absorption by new linear and non-linear QSPR

pp. 218–228

Alan Talevi, Mohammad Goodarzi, Erlinda V. Ortiz, Pablo R. Duchowicz\*, Carolina L. Bellera, Guido Pesce, Eduardo A. Castro and Luis E. Bruno-Blanch

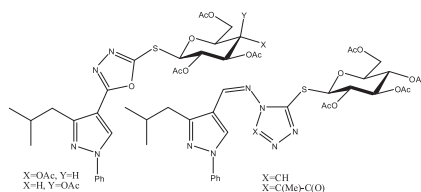
Dragon molecular descriptors based linear and non-linear QSPR Analysis for the intestinal absorption of drug like compounds.



## Synthesis and *in vitro* anti-tumor activity of new oxadiazole thioglycosides

pp. 229–235

M.A. Abu-Zaied, E.M. El-Telbani, G.H. Elgemeie and G.A.M. Nawwar\*

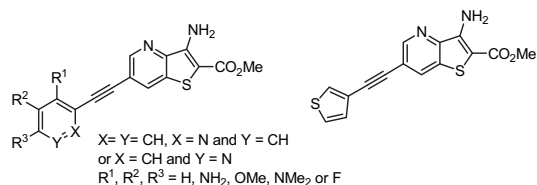


### Synthesis and evaluation of tumor cell growth inhibition of methyl 3-amino-6-[(hetero)arylethynyl]thieno[3,2-*b*]pyridine-2-carboxylates. Structure–activity relationships, effects on the cell cycle and apoptosis

pp. 236–240

Maria-João R.P. Queiroz\*, Ricardo C. Calhella, Luís A. Vale-Silva, Eugénia Pinto, Gabriela M. Almeida and M. Helena Vasconcelos

Several methyl 3-amino-6-[(hetero)arylethynyl]thieno[3,2-*b*]pyridines were prepared by Sonogashira coupling and their growth inhibitory effects were evaluated in three human tumor cell lines. The most promising compounds were submitted to cell cycle analysis and apoptosis detection.

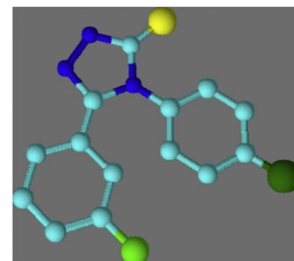


### Synthesis and antimicrobial activity of thiosemicarbazides, *s*-triazoles and their Mannich bases bearing 3-chlorophenyl moiety

pp. 241–248

Tomasz Plech\*, Monika Wujec, Agata Siwek, Urszula Kosikowska and Anna Malm

Synthesis and antimicrobial evaluation of some 1,4-disubstituted thiosemicarbazides, *s*-triazoles and Mannich bases were described. Compounds **4**, **6**, **15** appeared to be four-fold more effective against *Bacillus cereus* ATCC 10876 than ampicillin.

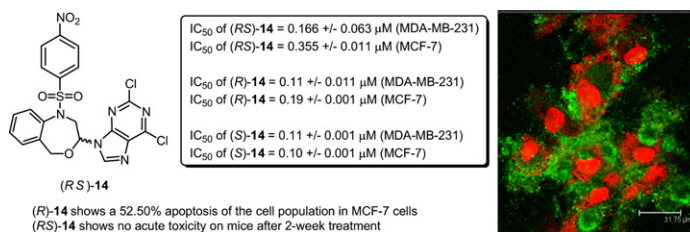


Compound 15, MIC=15.63–31.25 µg/mL

### New (*RS*)-benzoxazepin-purines with antitumour activity: The chiral switch from (*RS*)-2,6-dichloro-9-[1-(*p*-nitrobenzenesulfonyl)-1,2,3,5-tetrahydro-4,1-benzoxazepin-3-yl]-9*H*-purine

pp. 249–258

Luisa C. López-Cara, Ana Conejo-García, Juan A. Marchal, Giuseppe Macchione, Olga Cruz-López, Houria Boulaiz, María A. García, Fernando Rodríguez-Serrano, Alberto Ramírez, Carlos Cativiela, Ana I. Jiménez, Juan M. García-Ruiz, Duane Choquesillo-Lazarte, Antonia Aránega and Joaquín M. Campos\*

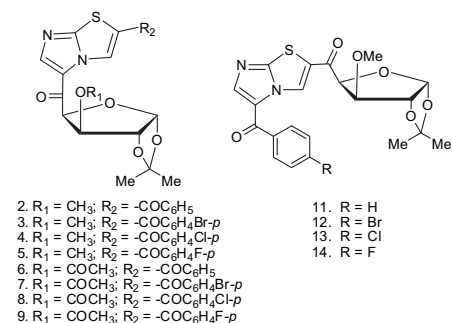


### Imidazo[2,1-*b*]thiazole carbohydrate derivatives: Synthesis and antiviral activity against Junin virus, agent of Argentine hemorrhagic fever

pp. 259–264

José Sebastián Barradas, María Inés Errea, Norma B. D'Accorso\*, Claudia Soledad Sepúlveda and Elsa Beatriz Damonte

A series of 3,5-disubstituted imidazo[2,1-*b*]thiazoles were synthesized and their activity against the etiological agent of Argentine hemorrhagic fever (JUNV), was evaluated.



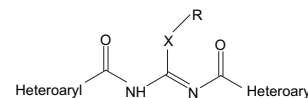


**Synthesis and antiproliferative activity of novel symmetrical alkylthio- and alkylseleno-imidocarbamates**

pp. 265–274

Elena Ibáñez, Daniel Plano, María Font, Alfonso Calvo, Celia Prior, Juan Antonio Palop\* and Carmen Sanmartín

A series of novel symmetrical alkylthio- and alkylseleno-imidocarbamates was prepared and their antitumor activities were evaluated against a panel of five human tumor cell lines and one non-malignant cell line.



X= S, Se

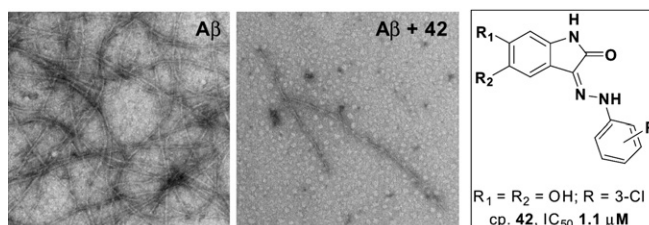
R= methyl, benzyl

Heteroaryl = 2-furyl, 2-thienyl, 3-chloro-2-thienyl, 5-nitro-3-thienyl, 5-isoxazolyl, benzothienyl, 3,4-methylenedioxybenzyl, 3-quinoliny, 2-phenyl-3-quinoliny, 9-acridinyl.

**Synthesis and biophysical evaluation of arylhydrazono-1*H*-2-indolinones as  $\beta$ -amyloid aggregation inhibitors**

pp. 275–284

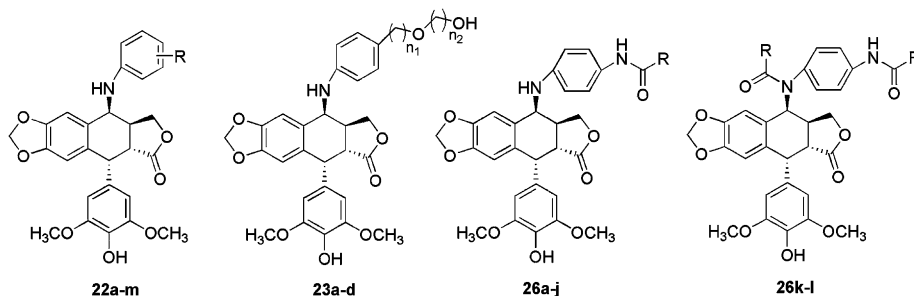
Francesco Campagna\*, Marco Catto, Rosa Purgatorio, Cosimo D. Altomare, Angelo Carotti, Angelo De Stradis and Gerardo Palazzo

**Synthesis and biological evaluation of new 4 $\beta$ -anilino-4'-*O*-demethyl-4-desoxypodophyllotoxin derivatives as potential antitumor agents**

pp. 285–296

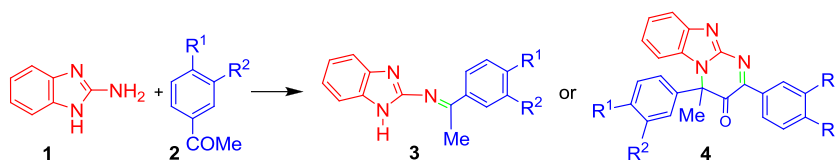
Li Wang, Fenyan Yang, Xiaochun Yang, Xianghong Guan, Chunqi Hu, Tao Liu, Qiaojun He, Bo Yang and Yongzhou Hu\*

A series of new 4 $\beta$ -anilino-4'-*O*-demethyl-4-desoxypodophyllotoxin derivatives were synthesized and evaluated for their cytotoxicities against four human cancer cell lines. Compound **26c** showed good tumor growth inhibition on highly metastatic human lung cancer xenograft in nude mice with administrating by oral route.

**One-pot microwave assisted synthesis under green chemistry conditions, antioxidant screening, and cytotoxicity assessments of benzimidazole Schiff bases and pyrimido[1,2-*a*]benzimidazol-3(4*H*)-ones**

pp. 297–306

Constantinos G. Neochoritis, Tryfon Zarganes-Tzitzikas, Constantinos A. Tsoleridis\*, Julia Stephanidou-Stephanatou\*, Christos A. Kontogiorgis, Dimitra J. Hadjipavlou-Litina and Theodora Choli-Papadopoulou

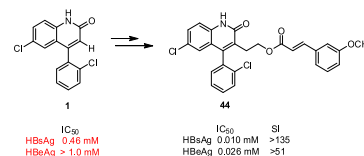


### Structure–activity relationships study of 6-chloro-4-(2-chlorophenyl)-3-(2-hydroxyethyl) quinolin-2(1H)-one derivatives as novel non-nucleoside anti-hepatitis B virus agents

pp. 307–319

Rui-Hua Guo, Quan Zhang, Yun-Bao Ma, Jie Luo, Chang-An Geng, Li-Jun Wang, Xue-Mei Zhang, Jun Zhou, Zhi-Yong Jiang and Ji-Jun Chen\*

6-Chloro-4-(2-chlorophenyl)-3-(2-hydroxyethyl)quinolin-2(1H)-one analogues were synthesized and evaluated for the anti-HBV activities in vitro. Most of compounds possessed potent activities, of which the promising compound **44** exhibited significantly inhibitory activities.

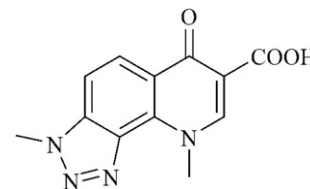


### Synthesis and anti-mycobacterial activities of triazoloquinolones

pp. 320–326

Antonio Carta\*, Michele Palomba, Irene Briguglio, Paola Corona, Sandra Piras, Daniela Jabes, Paola Guglielame, Paola Molicotti and Stefania Zanetti

In this study it is confirmed that triazolo[4,5-*h*]quinolone-carboxylic acid derivatives belong to a novel class of quinolones endowed with a selective anti-mycobacterial activity. The SAR analysis of the new derivatives in comparison with the previous series shows that the methyl group is the most effective substituent in both N-3 and N-9 positions of the ring system.

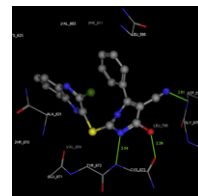


### Part I: Synthesis, cancer chemopreventive activity and molecular docking study of novel quinoxaline derivatives

pp. 327–340

Shadia A. Galal\*, Ahmed S. Abdelsamie, Harukuni Tokuda, Nobutaka Suzuki, Akira Lida, Mahmoud M. ElHefnawi, Raghdha A. Ramadan, Mona H.E. Atta and Hoda I. El Diwani

Ligand interaction and the binding mode of compound **17** with c-kit receptor, it exhibited 3 H-bonds with the amino acids in C-kit two of them with CYS 673 and one with ASP 677, the hydrogen bonds formed colored in green.

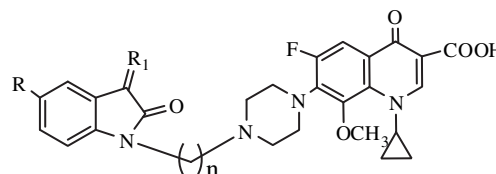


### Synthesis and *in vitro* antimycobacterial activity of 8-OCH<sub>3</sub> ciprofloxacin methylene and ethylene isatin derivatives

pp. 341–348

Lian-Shun Feng, Ming-Liang Liu\*, Shu Zhang, Yun Chai, Bo Wang, Yi-Bin Zhang, Kai Lv, Yan Guan, Hui-Yuan Guo and Chun-Ling Xiao\*\*

A series of novel 8-OCH<sub>3</sub> ciprofloxacin methylene and ethylene isatin derivatives were synthesized. These compounds have considerable activity against *M. smegmatis* CMCC 93202, MTB H37Rv ATCC 27294 and MDR-MTB 09710.

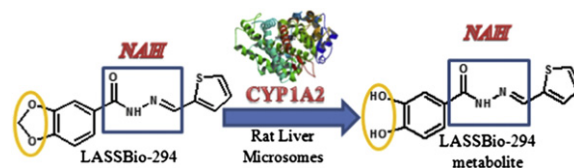
**3a-k and 5a-l**

### CYP1A2-mediated biotransformation of cardioactive 2-thienylidene-3,4-methylenedioxybenzoylhydrazine (LASSBio-294) by rat liver microsomes and human recombinant CYP enzymes

pp. 349–355

Aline Guerra M. Fraga, Leandro Louback da Silva, Carlos Alberto Manssour Fraga and Eliezer J. Barreiro\*

We describe herein the metabolic fate of cardioactive 1,3-benzodioxolyl *N*-acylhydrazine, LASSBio-294 (**4**), and the structural identification of its principal metabolite formed by CYP1A2 from rat liver microsomal assays.

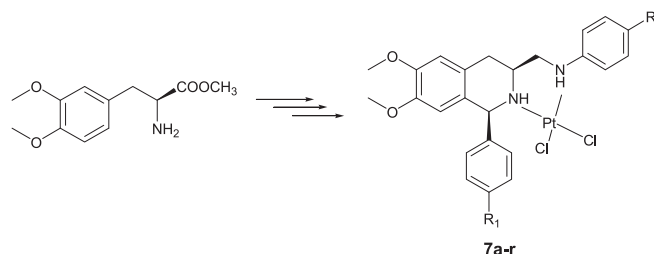


### Synthesis and cytotoxicity of *cis*-dichloroplatinum (II) complexes of (1*S*,3*S*)-1,2,3,4-tetrahydroisoquinolines

pp. 356–363

Geng Xu, Zheng Yan, Nan Wang and Zhanzhu Liu\*

A series of novel cisplatin analogues were designed and synthesized. Some compounds exhibited better cytotoxic activity than cisplatin. The structure–activity relationship was revealed.



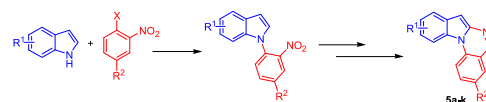
## SHORT COMMUNICATIONS

### Antifungal agents. Part 4: Synthesis and antifungal activities of novel indole[1,2-*c*]-1,2,4-benzotriazine derivatives against phytopathogenic fungi *in vitro*

pp. 364–369

Hui Xu\* and Ling-ling Fan

Two indole[1,2-*c*]-1,2,4-benzotriazine derivatives have been identified as potent antifungal agents and might be considered as novel promising lead candidates for further design and synthesis of agricultural fungicides.

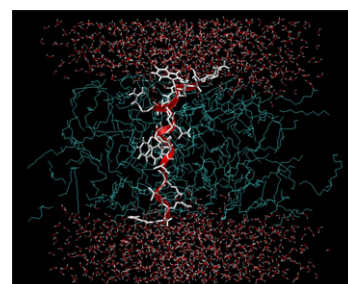


### Penetratin analogues acting as antifungal agents

pp. 370–377

Francisco M. Garibotto, Adriana D. Garro, Ana M. Rodríguez, Marcela Raimondi, Susana A. Zacchino, Andras Perczel, Csaba Somlai, Botond Penke and Ricardo D. Enriz\*

We designed, synthesized and tested penetratin analogues possessing antifungal activity against *C. neoformans* and *C. albicans*. A pharmacophoric patron for these peptides is also discussed.

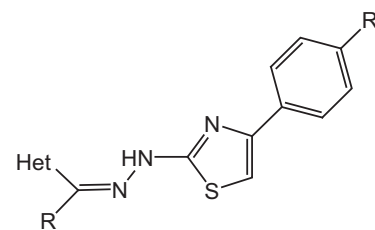


### Synthesis and biological evaluation of novel 2,4-disubstituted-1,3-thiazoles as anti-*Candida* spp. agents

pp. 378–382

Franco Chimenti, Bruna Bizzarri\*, Adriana Bolasco, Daniela Secci, Paola Chimenti, Arianna Granese, Simone Carradori, Melissa D'Ascenzio, Daniela Lilli and Daniela Rivanera

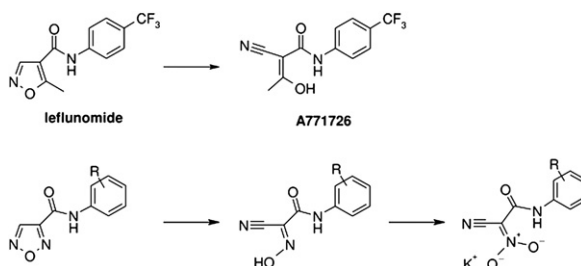
A new series of [4-(4'-substituted-phenyl)thiazol-2-yl]hydrazine derivatives were synthesized and assayed for their *in vitro* antifungal activity against 20 clinical isolates of pathogenic *Candida* spp.



### 1,2,5-Oxadiazole analogues of leflunomide and related compounds

pp. 383–392

Marta Giorgis, Marco Lucio Lolli, Barbara Rolando, Angela Rao, Paolo Tosco, Shilpi Chaurasia, Domenica Marabello, Roberta Fruttero and Alberto Gasco\*

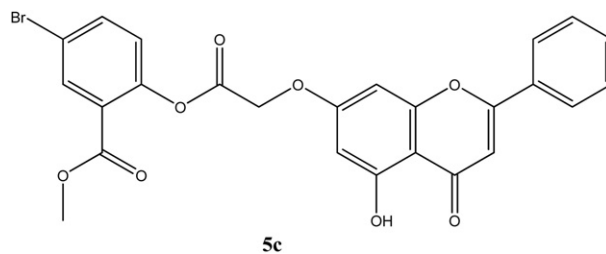


### Synthesis, biological evaluation of chrysin derivatives as potential immunosuppressive agents

pp. 393–398

Peng-Cheng Lv, Tian-Tian Cai, Yong Qian, Juan Sun and Hai-Liang Zhu\*

Compound **5c** exhibited lower cytotoxicity and higher inhibition activity on CD3/CD28 co-stimulated T cell proliferation than other compounds.

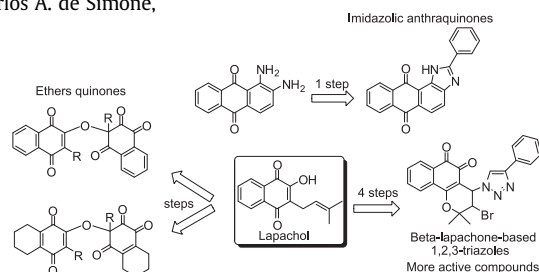


### Synthesis and evaluation of quinonoid compounds against tumor cell lines

pp. 399–410

Eufrânio N. da Silva, Jr.\* , Bruno C. Cavalcanti, Tiago T. Guimarães, Maria do Carmo F.R. Pinto, Igor O. Cabral, Cláudia Pessoa, Letícia V. Costa-Lotufo, Manoel O. de Moraes, Carlos K.Z. de Andrade, Marcelo R. dos Santos, Carlos A. de Simone, Marília O.F. Goulart and Antonio V. Pinto

Thirty two compounds were synthesized in moderate to high yields and showed activity against cancer cells HL-60, MDA-MB435, HCT-8 and SF295, with IC<sub>50</sub> below 2 μM for some compounds.

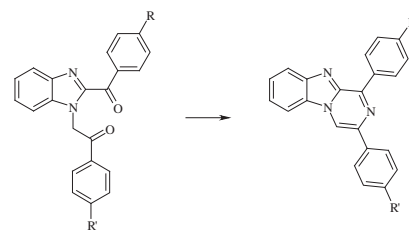


**Microwave supported synthesis of some novel 1,3-Diarylpyrazino[1,2-a]benzimidazole derivatives and investigation of their anticancer activities**

pp. 411–416

Seref Demirayak, Ismail Kayagil\* and Leyla Yurttas

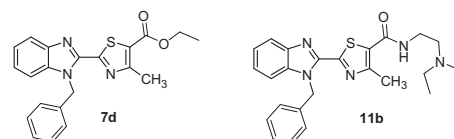
The syntheses of 1,3-diarylpyrazino[1,2-a]benzimidazole derivatives and the investigation of their anti-cancer activities were studied. For this, 2-arylpyrazino[1,2-a]benzimidazole derivatives were reacted with 2-bromoacetophenones in acetone to give 1-(2-aryl-2-oxoethyl)-2-arylpyrazino[1,2-a]benzimidazoles.

**Synthesis and *in vitro* cytotoxic evaluation of some thiazolylbenzimidazole derivatives**

pp. 417–422

Yu Luo, Feng Xiao, Shijing Qian, Wei Lu\* and Bo Yang

Synthesis of a series of 2-thiazol-2-yl derivatives and some of them exhibit significant inhibitory activities against SMMC-7721 and A549 cell lines *in vitro*.

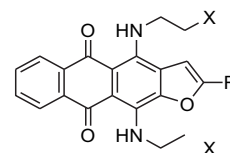
**The first series of 4,11-bis[(2-aminoethyl)amino]anthra[2,3-b]furan-5,10-diones:**

pp. 423–428

**Synthesis and anti-proliferative characteristics**

Andrey E. Shchekotikhin\*, Valeria A. Glazunova, Lyubov G. Dezhenskova, Elena K. Shevtsova, Valery F. Traven', Jan Balzarini, Hsu-Shan Huang, Alexander A. Shtil and Maria N. Preobrazhenskaya

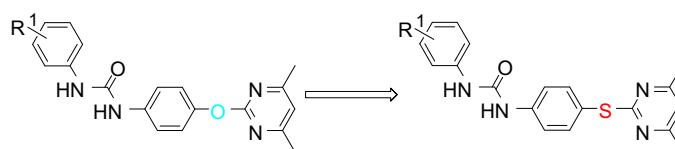
The synthesis and cytotoxic properties of novel 4,11-bis[(2-aminoethyl)amino]anthra[2,3-b]furan-5,10-diones are described. The selected compounds potently killed mammalian tumor cell lines, including drug-resistant variants. Critical role of the structure of distal amino groups for cytotoxicity of anthrafurandiones is demonstrated.

**Synthesis and antitumor activity of ureas containing pyrimidinyl group**

pp. 429–432

Chuanfei Jin, Yong-Ju Liang, Hongwu He\* and Liwu Fu\*\*

From the structure-activity relationships we may conclude that introduction of a sulfide bridge between phenyl and pyrimidinyl rings would be critical for their biological activities.



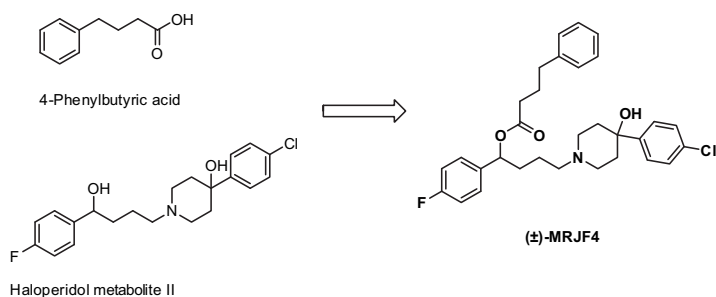
## PRELIMINARY COMMUNICATIONS

**Antiproliferative activity of phenylbutyrate ester of haloperidol metabolite II [(±)-MRJF4] in prostate cancer cells**

pp. 433–438

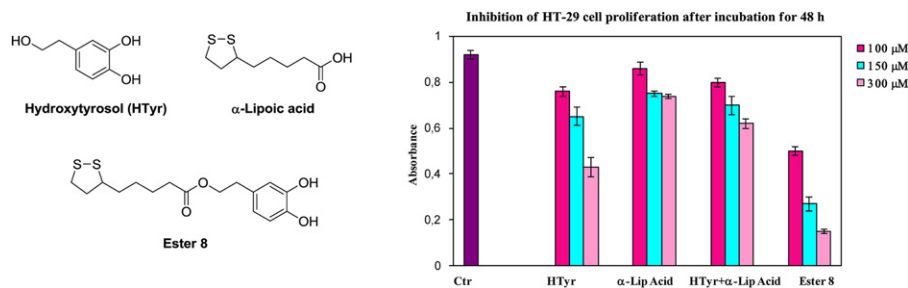
Agostino Marrazzo\*, Jole Fiorito, Laura Zappalà, Orazio Prezzavento, Simone Ronsisvalle, Lorella Pasquinucci, Giovanna M. Scoto, Renato Bernardini and Giuseppe Ronsisvalle

(±)-MRJF4 showed a better antiproliferative activity on LNCaP and PC3 prostate cancer cells ( $IC_{50} = 11$  and  $13 \mu M$  for LNCaP and PC3, respectively) compared to 4-phenylbutyric acid, haloperidol metabolite II and equimolar mixture of both compounds.

**Synthesis of a novel ester of hydroxytyrosol and  $\alpha$ -lipoic acid exhibiting an antiproliferative effect on human colon cancer HT-29 cells**

pp. 439–446

Roberta Bernini\*, Fernanda Crisante, Nicolò Merendino, Romina Molinari, Maria Chiara Soldatelli and Francesca Velotti



**COVER**

An evaluation of hsp90 inhibitors chemical diversity has been performed. 2D-molecular descriptors, principal component analysis and fragment-based approach have been used to explore their chemical space. 45/5, P2000-2009 by Davide Audisio, Samir Messaoudi, Ismail Ijjaali, Elodie Dubus, François Petitot, Jean-François Peyrat, Jean-Daniel Brion, Mouâd Alami © 2010 Published by Elsevier Masson SAS

\* Corresponding authors.



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ISSN 0223-5234