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# European Journal of Medicinal Chemistry

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# European Journal of Medicinal Chemistry Vol 45, No 3, 2010

#### **Contents**

#### **ORIGINAL ARTICLES**

## Design, synthesis and pharmacological screening of potential anticonvulsant agents using hybrid approach

J.G. Ghogare, S.V. Bhandari\*, K.G. Bothara, A.R. Madgulkar, G.A. Parashar, B.G. Sonawane and P.R. Inamdar

pp. 857-863

#### Synthesis and antiprotozoal activity of 4-arylcoumarins

Jean-Thomas Pierson, Aurélien Dumètre, Sébastien Hutter, Florence Delmas, Michèle Laget, Jean-Pierre Finet, Nadine Azas\* and Sébastien Combes\*\*

pp. 864–869

Synthesis and biological evaluation of 4-arylcoumarins as antiprotozoal agents were investigated. The 4-(3,4-dimethoxyphenyl)-6,7-dimethoxycoumarin was found to exhibit a potent activity on*Leishmania donovani*amastigotes with a selectivity index (<math>SI=265) twice than amphotericin B (SI=140).

### Synthesis of potent BACE-1 inhibitors incorporating a hydroxyethylene isostere as central core

pp. 870-882

Fredrik Wångsell, Karin Gustafsson, Ingemar Kvarnström, Neera Borkakoti, Michael Edlund, Katarina Jansson, Jimmy Lindberg, Anders Hallberg, Åsa Rosenquist\* and Bertil Samuelsson\*

$$\begin{array}{c} \mathsf{BnO} \\ \mathsf{BnO} \\ \\ \mathsf{O} \\ \\ \mathsf{O} \\ \\ \mathsf{O} \\ \\ \mathsf{O} \\ \mathsf{O} \\ \\ \mathsf{O} \\ \mathsf{N}_{3} \\ \mathsf{O} \\ \mathsf{O} \\ \mathsf{O} \\ \mathsf{N}_{3} \\ \mathsf{O} \\ \mathsf{O} \\ \mathsf{N}_{1} \\ \mathsf{O} \\ \mathsf{N}_{1} \\ \mathsf{N}_{2} \\ \mathsf{O} \\ \mathsf{N}_{1} \\ \mathsf{O} \\ \mathsf{N}_{1} \\ \mathsf{O} \\ \mathsf{N}_{2} \\ \mathsf{O} \\ \mathsf{N}_{3} \\ \mathsf{O} \\ \mathsf{N}_{4} \\ \mathsf{O} \\ \mathsf{N}_{1} \\ \mathsf{O} \\ \mathsf{N}_{2} \\ \mathsf{O} \\ \mathsf{N}_{3} \\ \mathsf{O} \\ \mathsf{N}_{4} \\ \mathsf{O} \\ \mathsf{N}_{1} \\ \mathsf{O} \\ \mathsf{N}_{2} \\ \mathsf{O} \\ \mathsf{N}_{3} \\ \mathsf{O} \\ \mathsf{N}_{4} \\ \mathsf{O} \\ \mathsf{N}_{5} \\$$

#### Synthesis, characterization and biocidal activity of new organotin complexes of 2-(3-oxocyclohex-1-enyl)benzoic acid

pp. 883-889

Flaviana T. Vieira, Geraldo M. de Lima\*, José R. da S. Maia, Nivaldo L. Speziali, José D. Ardisson, Leonardo Rodrigues, Ary Correa Junior and Oscar B. Romero

Following our interest in the biological aspects of organotin chemistry we have obtained new organotin complexes with 2-(3-oxocyclohex-1-enyl)benzoic. The biological activities of the resultant products were assayed.

# Novel phosphoramidates with porphine and nitrogenous drug: One-pot synthesis and orientation to cancer cells Zhi-Wei Wang, Can-Cheng Guo\*, Wen-Zhong Xie, Chao-Zhou Liu, Chun-Guang Xiao and Ze Tan

pp. 890-895

Five novel porphine phosphoramidates were synthesized by one-spot. Their selectively accumulation and derogation for cancer cells were investigated by MTT test, cell viability test and uptake test.

$$\begin{array}{c} R \\ NH \\ N \end{array}$$

$$\begin{array}{c} HN \\ O-P=0 \\ HN \end{array}$$

$$\begin{array}{c} HN \\ O-P=0 \\ HN \end{array}$$

#### 5-Substituted [1]pyrindine derivatives with antiproliferative activity

pp. 896-901

 $St\'{e}phanie\ Kolb,\ Mary-Lor\`{e}ne\ Goddard,\ Ali\ Loukaci,\ Odile\ Mond\'{e}sert,\ Bernard\ Ducommun,\ Emmanuelle\ Braud\ and\ Christiane\ Garbay^*$ 

Synthesis and biological evaluation of 5-substituted [1]pyrindine derivatives.

$$R$$
 $R$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 

# Conventional and microwave assisted synthesis of small molecule based biologically active heterocyclic amidine derivatives

pp. 902-908

Sham M. Sondhi\*, Reshma Rani, Partha Roy, S.K. Agrawal and A.K. Saxena

Heterocyclic amidine derivatives **3a**–**f**, **4a**–**f**, **5a**–**d** and **5f** have been synthesized by conventional heating as well as *via* microwave irradiation in good yields. Compounds **3a**, **3d**, **4d** and **4e** exhibited good anti-inflammatory activity.

Where **R** is various substituents.

# Synthesis and biological evaluation of [1,2,4]triazino[4,3-a] benzimidazole acetic acid derivatives as selective aldose reductase inhibitors

pp. 909-914

Prasanta Kumar Sahoo\* and Pritishova Behera

The acetic acid derivatives of [1,2,4]triazino[4,3- $\alpha$ ]benzimidazole (TBI) were synthesized and tested in vitro and in vivo as selective aldose reductase (ALR2) inhibitors. Compound **PS11** showed highest inhibitory activity (IC $_{50}$ ) 0.32  $\mu$ M) and was found to be effective in preventing cataract development in severely galactosemic rats when administered as an eyedrop solution. All the compounds investigated were selective for ALR2, since none of them inhibited appreciably aldehyde reductase, sorbitol dehydrogenase, or glutathione reductase.

# Synthesis and antibacterial activity of novel 3-O-carbamoyl derivatives of clarithromycin and 11,12-cyclic carbonate azithromycin

pp. 915-922

Ling Zhang, Linchen Song, Zhaopeng Liu, Hui Li, Yingdong Lu, Zerong Li and Shutao Ma\*

Novel 3-O-carbamoyl derivatives of clarithromycin and 11,12-cyclic carbonate azithromycin were synthesized and evaluated. Some derivatives showed excellent activity against erythromycin-susceptible bacteria and greatly improved activity against erythromycin-resistant *Streptococcus pneumoniae*.

**4j** R<sup>1</sup> = butyl, MIC = 0.03 g/mL **4k** R<sup>1</sup> = pentyl, MIC = 0.03 g/mL

#### Synthesis and biological activity of derivatives of the marine quinone avarone

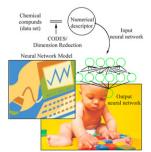
pp. 923-929

Tatjana Božić, Irena Novaković, Miroslav J. Gašić, Zorica Juranić, Tatjana Stanojković, Srđan Tufegdžić, Zoran Kljajić and Dušan Sladić\*

## Neural computational prediction of oral drug absorption based on CODES 2D descriptors

pp. 930-940

A. Guerra, N.E. Campillo\* and J.A. Páez\*



#### Curcuminoid analogs with potent activity against Trypanosoma and Leishmania species

pp. 941-956

Chatchawan Changtam, Harry P. de Koning, Hasan Ibrahim, M. Sohail Sajid, Matthew K. Gould and Apichart Suksamrarn\*

Compound **40** was the most active analog against *Trypanosoma brucei brucei*, with an EC $_{50}$  value of  $0.053\pm0.007~\mu M$ . It was about 2-fold more active than the standard drug diminazene aceturate and exhibited low toxicity to HEK cell with high selectivity index of 453-fold.

# New 1,3-oxazolo[4,5-c]quinoline derivatives: Synthesis and evaluation of antibacterial and antituberculosis properties Sumesh Eswaran, Airody Vasudeva Adhikari\* and R. Ajay Kumar

pp. 957-966

A new series of fused 1,3-oxazolo[4,5-c]quinoline derivatives have been synthesized and evaluated for antimicrobial studies. Majority of them showed good antibacterial and antituberculosis activity.

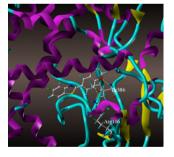
$$R^2$$
 $R^1$ 
 $R^2$ 
 $R^2$ 
 $R^2$ 
 $R^2$ 
 $R^2$ 
 $R^2$ 
 $R^2$ 
 $R^2$ 
 $R^2$ 

R = alkyl/aralkyl/ aryl  $R^1/R^2 = F$ 

# CoMFA and molecular docking studies of benzoxazoles and benzothiazoles as CYP450 1A1 inhibitors Jie Pan, Gen-Yan Liu, Jin Cheng, Xin-Jie Chen and Xiu-Lian Ju\*

pp. 967-972

A three-dimensional model of CYP450 1A1 was generated by homology modeling using CYP450 1A2 as a template, and CYP450 1A1 inhibitors of benzoxazoles and benzothiazoles were docked into the putative binding site of the CYP450 1A1. The results give a deep insight into the hydrogen-bonding interactions between the inhibitors and residues in the active site of CYP450 1A1.



# Synthesis and antitumor activity of new dihydropyridine thioglycosides and their corresponding dehydrogenated forms

pp. 973–982

Hebat-Allah S. Abbas\*, Wael A. El Sayed and Nahed M. Fathy

$$R^3$$
 $R^3$ 
 $R^3$ 
 $R^3$ 
 $R^3$ 

$$R^{2}$$
 $R^{3}$ 
 $R^{2}$ 
 $R^{3}$ 
 $R^{3}$ 
 $R^{3}$ 

## Molecular modeling study of binding site selectivity of TQMP to G-quadruplex DNA

Li Aixiao\*, Maurel François, Barbault Florent, Delamar Michel, Wang Baoshan, Zhou Xiang and Wang Ping

pp. 983-991

Molecular dynamics (MD) simulations of four-stranded G-quadruplex DNA complexes formed by the sequence d(TTAGGG)<sub>4</sub> and the TOMP ligand show that in water medium, TOMP preferentially binds in the diagonal loop position.



### Synthesis, characterization and structure—activity relationship of novel N-phosphorylated E,E-3,5bis(thienylidene)piperid-4-ones

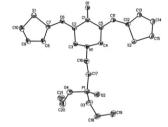
pp. 992-1000

Michael V. Makarov, Evgeniya S. Leonova, Ekaterina Yu. Rybalkina, Paul Tongwa, Victor N. Khrustalev, Tatiana V. Timofeeva and Irina L. Odinets\*

Direct phosphorylation of NH-bis(thienylidene)-4-piperidone and condensation of  $\omega$ -aminophosphonates bearing piperidone or a protected piperidone moiety with thiophen 2-carbaldehyde provide a convenient approach to phosphorus substituted 3,5-bis(thienylidene)piperid-4-ones possessing high cytotoxicity towards human carcinoma cell lines CaOv3, Scov3, and A549. The importance of phosphorylation for cytotoxic properties and influence of olefin configuration on antitumor activity were demonstrated.

 $R_P = P(O)(OEt)_2$ ,  $P(O)(OPh)_2$ , P(O)Me(OPh);  $(CH_2)_n P(O)(OEt)_2$ ; n=1-3

IC<sub>50</sub> 4-44 μM (Scov3, Caov3, A549)



## Synthesis of glycoside derivatives of hydroxyanthraquinone with ability to dissolve and inhibit formation of crystals of calcium oxalate. Potential compounds in kidney stone therapy

pp. 1001-1007

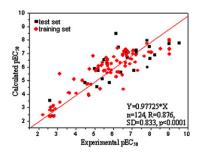
Anna Frackowiak, Przemysław Skibiński, Wiesław Gaweł, Ewa Zaczyńska, Anna Czarny and Roman Gancarz\*

Newly synthesized glycosyl derivatives of hydroxyanthraquinones have shown good properties as substances potentially useful in kidney stone therapy. Tests were performed on calcium oxalate and on real kidney stones in ex vivo test. Tests on L929 and A545 cell lines have shown that the compounds obtained were not cytotoxic.

#### Docking and 3D-QSAR studies of influenza neuraminidase inhibitors using three-dimensional holographic vector of atomic interaction field analysis

Jiaying Sun\*, Shaoxi Cai, Ning Yan and Hu Mei\*

Correlation plot of experimental and calculated pEC<sub>50</sub> elucidates that almost all samples are uniformly distributed in a straight line around 45° origin. 3D-HoVAIF can illustrate structural feature of compounds.



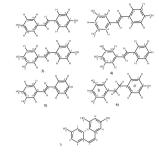
pp. 1008-1014

# A theoretical study of the structure—radical scavenging activity of trans-resveratrol analogues and cis-resveratrol in gas phase and water environment

pp. 1015-1027

Damian Mikulski\*, Rafał Górniak and Marcin Molski

In the present study highly accurate DFT computations have been performed to investigate the relation between the molecular structure and antioxidant activity of trans-resveratrol (TR), cis-resveratrol (CR), trans-4,4'-dihydroxystilbene (trans-4,4'-DHS), trans-3,4-dihydroxystilbene (trans-3,4-DHS), trans-3,4,4'-trihydroxystilbene (trans-3,4,4'-THS), trans-3,4,5-trihydroxystilbene (trans-3,4,5-THS) and  $\alpha$ , $\beta$ -dihydro-3,4',5-trihydroxystilbene ( $\alpha$ , $\beta$ -dihydro-3,4',5-THS) in the gas phase and water environment. The results obtained show that trans-3,4-DHS, trans-3,4,4'-THS, trans-3,4,5-THS and trans-4,4'-DHS exhibit higher antioxidant activity than TR, while  $\alpha$ , $\beta$ -dihydro-3,4',5-THS and CR are a significantly less efficient antioxidants than TR in the mediums considered.



# Synthesis and antimicrobial activities of 3-0-alkyl analogues of (+)-catechin: Improvement of stability and proposed action mechanism

pp. 1028-1033

Ki Duk Park\* and Sung Iin Cho\*

We report here the synthesis and biological properties of 3-O-alkyl analogues of (+)-catechin (5), which itself is one of the major natural polyphenols found in green tea.

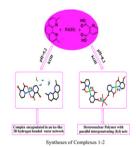
8a-8I

# New pH-dependent complexes, from mononuclear Pd(II) monomer to heteronuclear [Pd(II),K(I)]Polymer: DNA cleavage and cytotoxicity in vitro

pp. 1034-1041

En-Jun Gao\*, Ming-Chang Zhu, Yun Huang, Lei Liu, Hong-Yan Liu, Fu-Chun Liu, Shuang Ma and Chun-Yue Shi

Syntheses of complexes 1 and 2  $\,$ 



New pyrazoles incorporating pyrazolylpyrazole moiety: Synthesis, anti-HCV and antitumor activity Sayed M. Riyadh, Thoraya A. Farghaly, Magda A. Abdallah\*, Mohamed M. Abdalla and Mohamed R. Abd El-Aziz

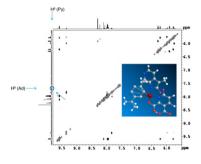
pp. 1042-1050

#### Ruthenium(II)—arene complexes with functionalized pyridines: Synthesis, characterization and cytotoxic activity

pp. 1051-1058

Sanja Grgurić-Šipka\*, Ivanka Ivanović, Gordana Rakić, Nina Todorović, Nevenka Gligorijević, Siniša Radulović, Vladimir B. Arion, Bernhard K. Keppler and Živoslav Lj. Tešić

Ruthenium(II)—arene complexes with functionalized pyridines were synthesized and characterized by elemental analysis, mass spectrometry, IR and NMR spectroscopy and X-ray crystallography. The cytotoxicity and reaction with 9-methyladenine were investigated.



#### Antioxidant and antiviral activities of silybin fatty acid conjugates

pp. 1059-1067

Radek Gažák, Kateřina Purchartová, Petr Marhol, Lucie Živná, Petr Sedmera, Kateřina Valentová, Nobuo Kato, Hiroyo Matsumura, Kunihiro Kaihatsu\*\* and Vladimír Křen\*

Silybin fatty-acyl derivatives were synthesized and their antioxidant and anti-influenza virus activities were tested. The acyl chain size is an important parameter for both biological activities, as they improved with its increasing length.

# Synthesis of new spiroindolinones incorporating a benzothiazole moiety as antioxidant agents Nilgün Karalı, Özlen Güzel\*, Nurten Özsoy, Süheyla Özbey and Aydın Salman

pp. 1068-1077

New series of 3*H*-spiro[1,3-benzothiazole-2,3'-indol]-2'(1'*H*)-ones showed potent scavenging activities against DPPH' and ABTS'<sup>+</sup> radicals, reducing powers, and strong inhibitory capacity on lipid peroxidation. Most compounds displayed very good antioxidant activity.

$$R_1$$
 $R_2$ 
 $R_1$ 
 $R_2$ 
 $R_3$ 
 $R_4$ 
 $R_4$ 
 $R_5$ 
 $R_4$ 
 $R_5$ 
 $R_6$ 

R<sub>1</sub>= CH<sub>3</sub>, CF<sub>3</sub>O, CI, Br, NO<sub>2</sub> R<sub>2</sub>= H, CH<sub>3</sub>

 $Synthesis, antibacterial\ and\ antiviral\ properties\ of\ curcumin\ bioconjugates\ bearing\ dipeptide,\ fatty\ acids\ and\ folic\ acid$ 

pp. 1078-1086

Ramendra K. Singh\*, Diwakar Rai, Dipti Yadav, A. Bhargava, J. Balzarini and E. De Clercq

Curcumin

$$R_1O$$
 $R_3$ 
 $OCH_3$ 
 $OR_2$ 

2:  $R_1 = R_2 = \text{dipeptide}; R_3 = H$ 

4:  $R_1 = R_2 = \text{pamitoyl}, R_3 = H$ 

8:  $R_1 = R_2 = H; R_3 = \text{ethylfolate}$ 

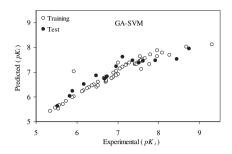
10:  $R_1 = H, R_2 = \text{ethylfolate}, R_3 = H$ 

#### QSAR study on melanocortin-4 receptors by support vector machine

Eslam Pourbasheer, Siavash Riahi\*, Mohammad Reza Ganjali and Parviz Norouzi

pp. 1087-1093

The QSAR of the melanocortin-4 receptor binding affinities of trans-4-(4-chlorophenyl) pyrrolidine-3-carboxamides of piperazinecyclohexanes was studied. The MLR and the SVM were utilized to construct the linear and nonlinear models.



## Synthesis, antibacterial and antifungal activities of 6,5 fused steroidal oxazoles in cholestane series

Shamsuzzaman\*, Mohd. Shaheen Khan, Mahboob Alam, Zishan Tabassum, Anis Ahmad and Asad U. Khan

We have investigated the antibacterial and antifungal activity of 2'-amino-5 $\alpha$ -cholest-6-eno [6,5-d] oxazole derivatives (**4**–**6**) prepared by refluxing cholestan-6-ones (**1**–**3**) with urea and iodine in ethanol. The structures of the compounds were established by means of their IR,  $^1$ H NMR,  $^{13}$ C NMR, FAB mass spectra and micro analytical data. The antibacterial activity of all the synthesized compounds was tested *in vitro* by the disk diffusion assay against three Gram-positive and three Gram-negative strains of bacteria. All the synthesized compounds were also tested for their inhibitory action against five strains of fungus and then the minimum inhibitory concentration (MIC) of all the synthesized compounds were determined. Chloramphenicol (30  $\mu$ g) was used as standard drug in case of bacteria and nystatin was used as a standard drug in case of fungi.

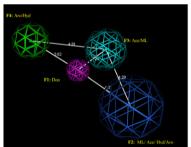
# Pharmacophoric model building for antitubercular activity of the individual Schiff bases of small combinatorial library

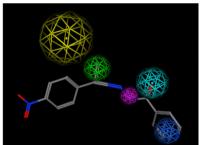
pp. 1098-1106

pp. 1094-1097

Wesam S. Abdel-Aal, Hoda Y. Hassan, Tarek Aboul-Fadl\* and Adel F. Youssef

A 3D pharmacophoric model has been generated by Molecular Operating Environment (MOE) using a training set of 10 reported anti-TB Schiff bases and testing the synthesized ones.





# Synthesis of tropolone derivatives and evaluation of their *in vitro* neuroprotective activity Maria Koufaki\*, Elissavet Theodorou, Xanthippi Alexi, Faidra Nikoloudaki and Michael N. Alexis

pp. 1107-1112

#### OSAR study of isatin analogues as in vitro anti-cancer agents

Razieh Sabet, Mehrdad Mohammadpour, Amir Sadeghi and Afshin Fassihi\*

A series of anti-cancer isatins was subjected to QSAR analysis to find the structural requirements for biological activity. QSAR results were in accordance with previous SAR studies and confirm them.

MIR

pp. 1113-1118

# Experimental activity

#### Predictive comparative QSAR modelling of (phenylpiperazinyl-alkyl) oxindoles as selective 5-HT<sub>1A</sub> antagonists by stepwise regression, PCRA, FA-MLR and PLS techniques

pp. 1119-1127

Nilanjan Adhikari, Milan K. Maiti and Tarun Jha\*

Thirtytwo (phenylpiperazinyl-alkyl) oxindoles are subjected to predictive comparative QSAR modelling by stepwise regression, PCRA, FA-MLR and PLS techniques to find structurally more active and selective 5-HT<sub>1A</sub> receptor antagonist.

#### Synthesis, in vitro antibacterial and antifungal evaluations of new $\alpha$ -hydroxyphosphonate and new $\alpha$ -acetoxyphosphonate derivatives of tetrazolo [1, 5-a] quinoline

pp. 1128-1132

Amol H. Kategaonkar, Rajkumar U. Pokalwar, Swapnil S. Sonar, Vaibhav U. Gawali, Bapurao B. Shingate and Murlidhar S. Shingare\*

A series of new  $\alpha$ -hydroxyphosphonate and  $\alpha$ -acetoxyphosphonate derivatives have been synthesized for the first time of tetrazolo [1, 5-a] quinoline derivatives and screened for antimicrobial activity.

# Discovery of benzhydrylpiperazine derivatives as CB<sub>1</sub> receptor inverse agonists via privileged structure-based approach

pp. 1133-1139

Tao Meng, Jue Wang, Hongli Peng\*, Guanghua Fang, Min Li, Bing Xiong, Xin Xie\*, Yongliang Zhang, Xin Wang and Jingkang Shen\*

A series of benzhydrylpiperazine derivatives was identified as a novel class of CB1 receptor inverse agonists utilizing privileged structure approach.



Privileged Structure Based Library (6 arrays, 230 cpds)

# Structure of aldehyde reductase in ternary complex with a 5-arylidene-2,4-thiazolidinedione aldose reductase inhibitor

pp. 1140-1145

Vincenzo Carbone, Marco Giglio, Roland Chung, Trevor Huyton, Julian Adams, Rosanna Maccari, Rosaria Ottana, Akira Hara and Ossama El-Kabbani\*

A novel inhibitor of aldose reductase-[5-(3-carboxymethoxy-4-methoxybenzylidene)-2,4-dioxothiazolidin-3-yl]acetic acid (CMD) was crystallised in ternary complex with aldehyde reductase. Molecular modelling and inhibitory activity measurements indicated a difference in binding residing predominantly within the non-conserved C-terminal residues of either enzyme.



Structures of 5-arylidene-2,4-thiazolidinediones

CMD bound to ALR1 active site

# Hydrogenative desulphurization of thienopyrrolizinones: An easy and selective access to (Z)-phenethylidenepyrrolizinones with in vitro cytotoxic activity

pp. 1146-1150

Vittoria Perri, Christophe Rochais, Jana Sopkova-de Oliveira Santos, Rémi Legay, Thierry Cresteil, Patrick Dallemagne\* and Sylvain Rault

Attempts in view to dearomatize some previously reported tripentones with potent antineoplastic activities led in thiophene series to an unexpected hydrogenative desulphurization reaction. The resulting (*Z*)-phenethylidenepyrrolizinones were tested in vitro over human epidermoid carcinoma KB cell line. The results of this biological evaluation indicated that the tricyclic core of our model can be cleaved with a partial respect of the activity.

## Synthesis and antimicrobial studies on novel sulfonamides containing 4-azidomethyl coumarin

pp. 1151-1157

Mahantesha Basanagouda, K. Shivashankar, Manohar V. Kulkarni\*, Vijaykumar P. Rasal, Harishchandra Patel, Sumit S. Mutha and Ashwini A. Mohite

A series of new and novel coumarin-6-sulfonamides with a free C4-azidomethyl group have been synthesized and screened for their antimicrobial activity (MICs) against different twelve microbial species.

# Design, synthesis, and biological evaluation of novel pyrimidine derivatives as CDK2 inhibitors Diaa A. Ibrahim\* and Amira M. El-Metwally

pp. 1158-1166

Novel pyrimidine derivatives were designed, synthesized and evaluated for their anti-tumor activities as CDK2 inhibitors, and proved to be both potent and selective as CDK2 inhibitors.

# Prediction of acetylcholinesterase inhibitors and characterization of correlative molecular descriptors by machine learning methods

pp. 1167-1172

pp. 1173-1180

Wei Lv and Ying Xue\*

Several machine learning methods such as support vector machine, k-nearest neighbor, and C4.5 decision tree were used to predict acetylcholinesterase inhibitors (AChEIs) and non- AChEIs.

### Synthesis and antimicrobial activities of novel 1,5-diaryl pyrazoles

R. Venkat Ragavan, V. Vijayakumar\* and N. Suchetha Kumari

# **Synthesis, characterization and antibacterial activities of some new ferrocene-containing penems**Bohua Long, Chunlian He, Yingbin Yang and Jiannan Xiang\*

pp. 1181-1188

A series of new ferrocene-containing penems had been synthesized. The results of bioassay showed that these compounds exhibited potent antibacterial activities and high stability to DHP-I.

#### **SHORT COMMUNICATIONS**

# Identification of antibacterial and antifungal pharmacophore sites for potent bacteria and fungi inhibition: Indolenyl sulfonamide derivatives

pp. 1189—1199

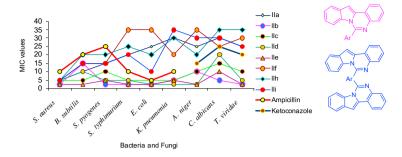
Zahid H. Chohan\*, Moulay H. Youssoufi, Aliasghar Jarrahpour and Taibi Ben Hadda\*

#### Antimicrobial study of newly synthesized 6-substituted indolo[1,2-c]quinazolines

Rondla Rohini, P. Muralidhar Reddy, Kanne Shanker, Anren Hu\* and Vadde Ravinder\*\*

pp. 1200-1205

Synthesis of a new series of mono and bis 6-substituted indolo [1,2-c]quinazoline derivatives and study of their antimicrobial acticities.



# Synthesis, characterization and biological activity of some new 1,3,4-oxadiazole bearing 2-flouro-4-methoxy phenyl moiety

pp. 1206-1210

B. Chandrakantha, Prakash Shetty, Vijesh Nambiyar, Nishitha Isloor and Arun M. Isloor\*

In the present investigation, a new series of 1,3,4-oxadiazoles bearing 2-flouro 4-methoxy phenyl moiety were synthesized, characterized and their antimicrobial studies were performed. Few of the compounds showed significant antimicrobial activity.

$$\frac{\text{POCl}_3 + \text{R-COOH}}{110 \, ^{\circ}\text{C}}$$

# 6-Substituted 2-(N-trifluoroacetylamino)imidazopyridines induce cell cycle arrest and apoptosis in SK-LU-1 human cancer cell line

pp. 1211-1219

Miguel Angel Martínez-Urbina\*, Alejandro Zentella, Miguel Angel Vilchis-Reyes, Ángel Guzmán, Omar Vargas, María Teresa Ramírez Apan, José Luis Ventura Gallegos and Eduardo Díaz\*

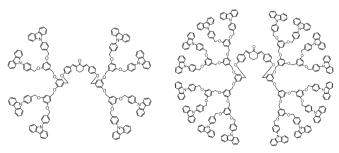
A series of 6-substituted 2-(N-trifluoroacetylamino)imidazopyridine were synthesized an evaluated for in vitro cytotoxicity, apoptosis induction and cyclin B/CDK1, and cyclin A/CDK2 inhibition.

# Synthesis and antioxidant properties of enone core based dendrimers with carbazole as surface group

pp. 1220-1224

Perumal Rajakumar\*, Nagarathinam Venkatesan, Karuppannan Sekar, Subramani Nagaraj and Ramasamy Rengasamy

Synthesis of enone core based dendrimers with carbazole as surface group has been achieved. All the synthesized dendrimers showed excellent antioxidant behavior with commercially available 1,1-diphenyl-2-picryl hydrazyl (DPPH).



#### Synthesis and investigation of inhibition effect of fluorinated sulfonamide derivatives on carbonic anhydrase

pp. 1225-1229

Zohra Benfodda, Franck Guillen, Bernard Romestand, Abdelkader Dahmani and Hubert Blancou\*

Series of perfluoroalkanesulfonamides 1 derivatives were synthesized by reaction of perfluoroalkanesulfonyle fluorides with gaseous ammonia. 1 react with sodium methylate in  $\text{Et}_2\text{O}/\text{methanol}$  media to give the corresponding sodium salt of perfluoroalkanesulfonamides 2.

# New 14-membered octaazamacrocyclic complexes: Synthesis, spectral, antibacterial and antifungal studies D.P. Singh\*, Krishan Kumar and Chetan Sharma

pp. 1230-1236

A novel series of macrocyclic complexes have been synthesized by template method followed by their characterization by various physicochemical techniques. These metal complexes were tested for their *in vitro* antimicrobial activities against some bacterial and fungal strains to assess their inhibiting potential.

Where M = Cr(III), Mn(III), Fe(III) $X = C1^{\circ}$ ,  $NO_3^{\circ}$ ,  $CH_3COO^{\circ}$ 

# Synthesis, cytotoxicity, antiviral activity and interferon inducing ability of 6-(2-aminoethyl)-6H-indolo [2,3-b]quinoxalines

pp. 1237-1243

Marina O. Shibinskaya, Sergey A. Lyakhov\*, Alexander V. Mazepa, Sergey A. Andronati, Alexander V. Turov, Nadezhda M. Zholobak and Nikolay Ya. Spivak

New indolo[2,3-b]quinoxalines (**4–15**) were synthesized with high yields using bromoethylisatin and 6-(2-bromoethyl)-6H-indolo[2,3-b]quinoxaline as intermediates. These compounds are low toxic potent interferon inducers and antivirals as active (or more) than tilorone. Morpholine and 4-methyl-piperidine derivatives appeared as the most active antivirals and the least cytotoxic in the investigated series.

## An expeditious synthesis and anticancer activity of novel 4-(3'-indoly1) oxazoles

pp. 1244–1249

Dalip Kumar\*, N. Maruthi Kumar, Swapna Sundaree, Emmanuel O. Johnson and Kavita Shah\*\*

A novel series of 4-(3'-indolyl)oxazoles have been synthesized and evaluated for their cytotoxicity.

#### Synthesis and evaluation of the $\alpha$ -glucosidase inhibitory activity of 3-[4-(phenylsulfonamido)benzoyl]-2H-1benzopyran-2-one derivatives

pp. 1250-1255

Shaojie Wang\*, Jufang Yan, Xiaoyan Wang, Zhuo Yang, Fengwei Lin and Tingjian Zhang

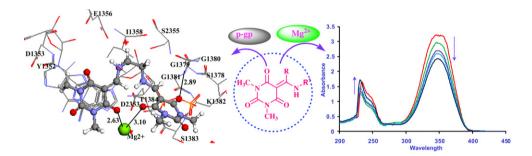
A series of 3-[4-(phenylsulfonamido)benzoyl]-2H-1-benzopyran-2-one derivatives was synthesized and evaluated as  $\alpha$ -glucosidase inhibitors. Compound **7u** showed the strongest inhibitory activity.

7u,  $IC_{50} = 0.0645 \mu M$ .

#### Synthesis of highly functionalized barbituric acids and study of their interactions with p-glycoprotein and ${\rm Mg}^{2+}$ pp. 1256-1262 Potential candidates for multi drug resistance modulation

Palwinder Singh\*, Jatinder Kaur and Atul Bhardwaj

Barbituric acid derivatives exhibit significant interactions with p-gp and Mg<sup>2+</sup> and could be useful for MDR modulation.



### LABORATORY NOTE

## Simultaneous tritium labelling of two potent 5-HT<sub>4</sub> ligands

pp. 1263-1265 Franck Sobrio\*, Stéphane Lemaitre, Antoine Hinsberger, Louisa Barré, Bernard Rousseau and Sylvain Rault\*\* Two selective 5-HT<sub>4</sub> ligands were tritiated simultaneously during a unique tritium labelling reaction.

### 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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