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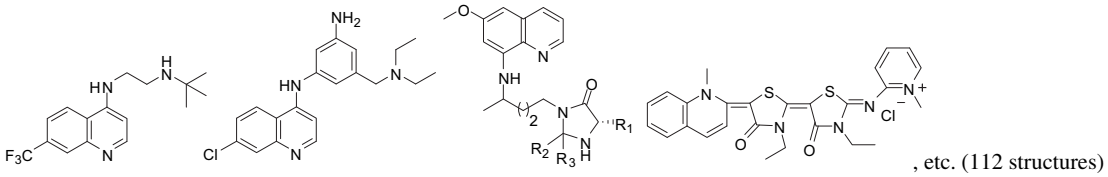
Contents

INVITED REVIEW

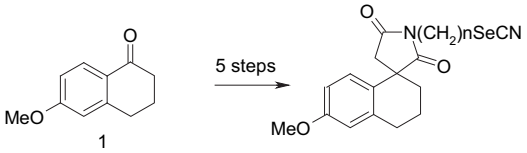
Quinolines and structurally related heterocycles as antimalarials **pp. 3245–3264**
Kirandeep Kaur, Meenakshi Jain, Ravi P. Reddy and Rahul Jain*



ORIGINAL ARTICLES

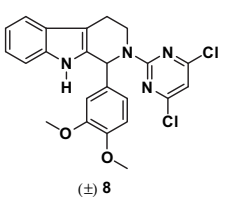
Synthesis and biological evaluation of novel spiro 6-methoxytetralin-1,3′-pyrrolidine based organoselenocyanates against cadmium-induced oxidative and hepatic damage in mice **pp. 3265–3273**
Ugir Hossain Sk, Arun K. Sharma, Sulekha Ghosh and Sudin Bhattacharya*

A series of spiro[6-methoxytetralin-1,3′-pyrrolidine] based organoselenocyanates were synthesized and evaluated against cadmium induced lipid peroxidation and hepatotoxicity in mice.



Synthesis of 2-(pyrimidin-2-yl)-1-phenyl-2,3,4,9-tetrahydro-1*H*-β-carbolines as antileishmanial agents **pp. 3274–3280**
Ravi Kumar, Shahnawaz Khan, Aditya Verma, Saumya Srivastava, Preeti Viswakarma, Suman Gupta, Sanjeev Meena, Neetu Singh, Jayanta Sarkar and Prem M.S. Chauhan*

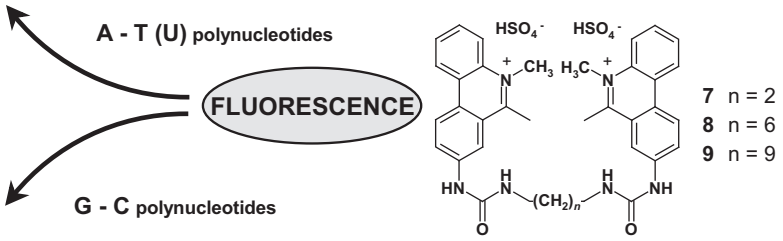
A novel series of 2-(pyrimidin-2-yl)-1-phenyl-2,3,4,9-tetrahydro-1*H*-β-carbolines has been synthesized and evaluated for their antileishmanial activity against *Leishmania donovani*.



Antipromastigote activity: 93% inhibition at 10μg/ml
Antiamastigote activity: IC_{50} = 1.93 μg/ml
Slectivity index = 15.43.

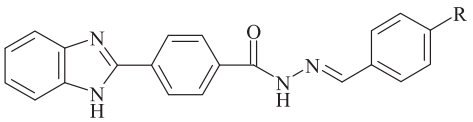
Permanent positive charge strongly influences DNA/RNA binding and antiproliferative activity of urea–phenanthridinium conjugates **pp. 3281–3292**
Marijana Radić Stojković, Saška Marczi, Ljubica Glavaš-Obrovac* and Ivo Piantanida**

A methylation of heterocyclic nitrogen on a previously studied bis-urea phenanthridines substantially changed their interactions with DNA, RNA and biological activity. Novel compounds act as basepair selective fluorescence probes.



Antimicrobial activity and a SAR study of some novel benzimidazole derivatives bearing hydrazone moiety **pp. 3293–3298**
Yusuf Özkay*, Yağmur Tunalı, Hülya Karaca and İlhan Isıkdağ

Twelve novel benzimidazole compounds bearing hydrazone moiety were synthesized in order to investigate their possible antibacterial and antifungal activity. Characterized compounds were subjected to a structure–activity relationship (SAR) study.

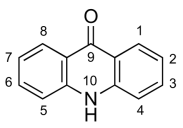


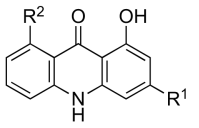
4a-4l

R: **4a**; -H, **4b**; -OH, **4c**; -$N(CH_3)_2$, **4d**; -Cl, **4e**; -Br, **4f**; -F, **4g**; -CH_3, **4h**; -OCH_3, **4i**; -NO_2, **4j**; -CF_3, **4k**; COOH, **4l**: CN

Structure–activity relationship studies of acridones as potential antipsoriatic agents. 1. Synthesis and antiproliferative activity of simple N-unsubstituted 10*H*-acridin-9-ones against human keratinocyte growth **pp. 3299–3310**
Aleksandar Putic, Lambert Stecher, Helge Prinz and Klaus Müller*

A series of N-unsubstituted hydroxy-10*H*-acridin-9-ones were synthesized and evaluated for their inhibitory action against the growth of HaCaT keratinocytes, capability to interact with the free radical 2,2-diphenyl-1-picrylhydrazyl, and release of lactate dehydrogenase into the culture medium.

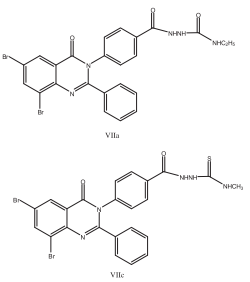




4 R^1 = H, R^2 = OH
5ee R^1 = OH, R^2 = Me

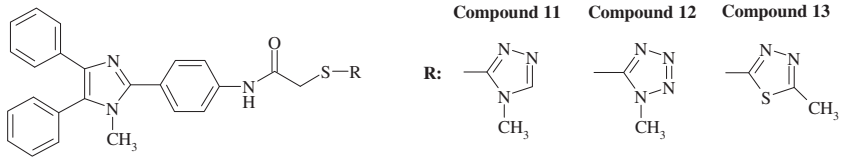
Novel 6,8-dibromo-4(3*H*)quinazolinone derivatives of anti-bacterial and anti-fungal activities **pp. 3311–3319**
Mosaad S. Mohamed, Mohsen M. Kamel, Emad M.M. Kassem, Nageh Abotaleb, Sherein I. Abd El-moez and Marwa F. Ahmed*

Compound **VIIa** was found to exhibit the most potent in vitro anti-microbial activity with the MICs of 1.56, 3.125, 1.56, 25, 25 and 25 μg/ml against *E. coli, S. typhimurium, L. monocytogenes, S. aureus, P. aeruginosa*, and *B. cereus* respectively. Compound **VIIc** showed pronounced in vitro anti-fungal activity with MICs of 0.78 and 0.097 μg/ml against *C. albicans* and *A. flavus*.



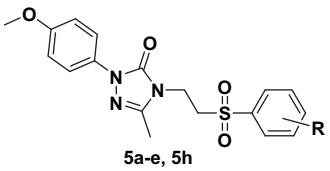
Synthesis of 2-substituted-*N*-[4-(1-methyl-4,5-diphenyl-1*H*-imidazole-2-yl)phenyl]acetamide derivatives and evaluation of their anticancer activity pp. 3320–3328
Yusuf Özkay*, İlhan Isıkdağ, Zerrin İncesu and Gülsen Akalın

Some imidazole-(benz)azole and imidazole-piperazine derivatives were synthesized to investigate their probable anticancer activity. The compounds **11**, **12** and **13** were determined as the most active derivatives in the series.



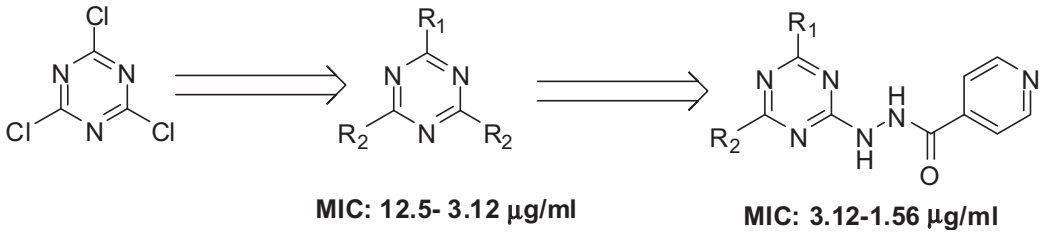
Synthesis, characterization and antimicrobial studies of 2-(4-methoxy-phenyl)-5-methyl-4-(2-arylsulfanyl-ethyl)-2,4-dihydro-[1,2,4] triazolo-3-ones and their corresponding sulfones pp. 3329–3334
Bhimagouda S. Patil*, G. Krishnamurthy, H.S. Bhojya Naik, Prashant R. Latthe and Manjunath Ghate

Synthesis, characterization, antibacterial and antifungal properties of some novel 1,2,4-triazol-3-ones have been described.



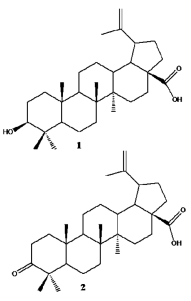
Discovery of new 1,3,5-triazine scaffolds with potent activity against *Mycobacterium tuberculosis* H37Rv pp. 3335–3345
Naresh Sunduru, Leena Gupta, Vinita Chaturvedi, Richa Dwivedi, Sudhir Sinha and Prem M.S. Chauhan*

A series of 2,4,6-trisubstitutesd-1,3,5-triazines were synthesized and identified as a promising inhibitors of *Mycobacterium tuberculosis* H37Rv.



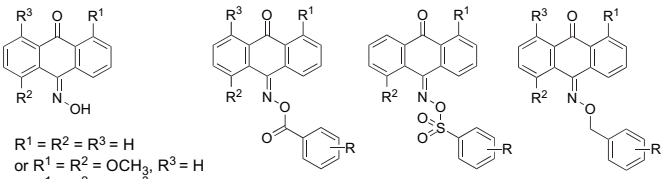
Small structural changes of pentacyclic lupane type triterpenoid derivatives lead to significant differences in their anticancer properties pp. 3346–3353
Harish Kommera, Goran N. Kaluđerović, Jutta Kalbitz, Birgit Dräger and Reinhard Paschke*

Synthesis, characterization and *in vitro* antitumoral activity of novel betulinic (**1**) and betulonic acid (**2**) derivatives against eight tumor cell lines of different histogenic origin has been carried out. Furthermore, structure activity relationships and mode of cell death are described. The drastic influence of minor structural changes on the anticancer properties is shown.

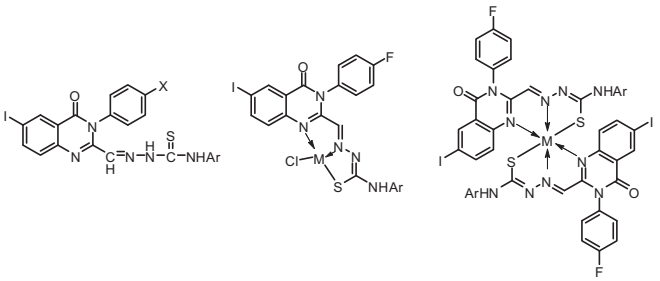


Synthesis, antiproliferative activity and inhibition of tubulin polymerization by anthracenone-based oxime derivatives pp. 3354–3364
Georg Surkau, Konrad J. Böhm, Klaus Müller and Helge Prinz*

A novel series of anthracenone-derived oxime ethers and -esters were synthesized and evaluated for antiproliferative activity and inhibition of tubulin polymerization.

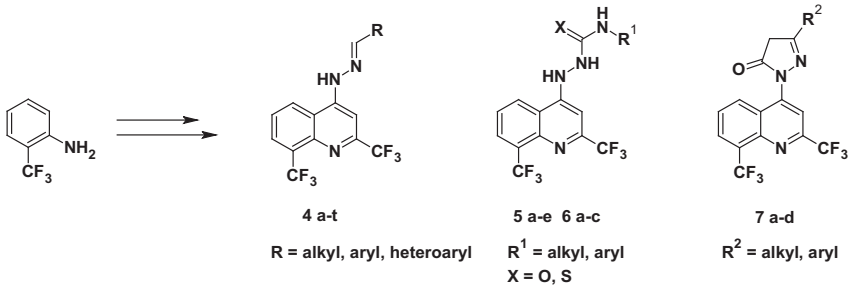


Synthesis of some new 4(3*H*)-quinazolinone-2-carboxaldehyde thiosemicarbazones and their metal complexes and a study on their anticonvulsant, analgesic, cytotoxic and antimicrobial activities – Part-1 pp. 3365–3373
Mohsen M. Aly*, Yahia A. Mohamed, Khairy A.M. El-Bayouki, Wahid M. Basyouni and Samir Y. Abbas*

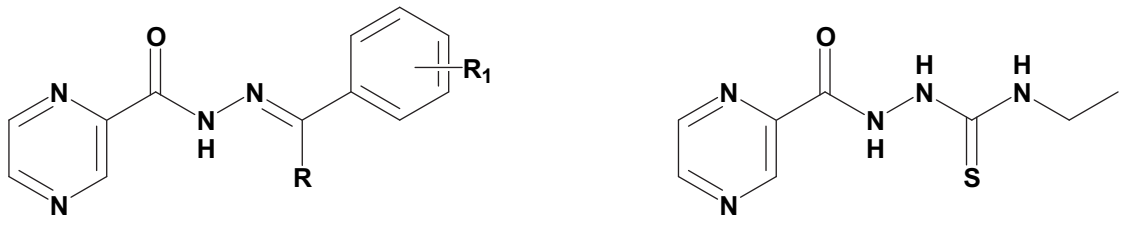


New quinoline derivatives: Synthesis and investigation of antibacterial and antituberculosis properties pp. 3374–3383
Sumesh Eswaran, Airody Vasudeva Adhikari*, Imran H. Chowdhury, Nishith K. Pal and K.D. Thomas

Four new series of quinoline derivatives have been synthesized from 2-trifluoromethyl aniline and evaluated for antibacterial and antituberculosis studies. Majority of them showed moderate to good antimicrobial activity.

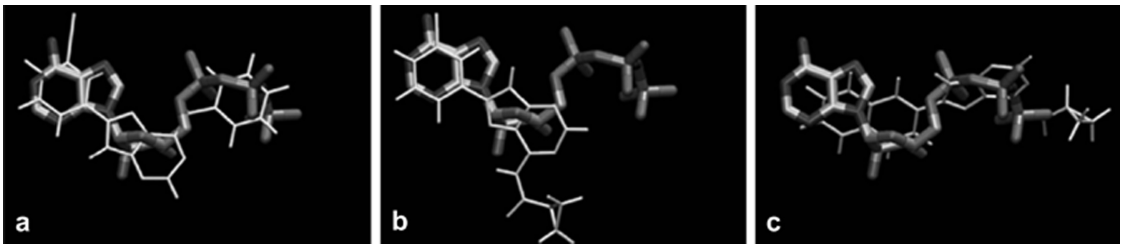


Synthesis and anti-mycobacterial evaluation of some pyrazine-2-carboxylic acid hydrazide derivatives pp. 3384–3388
Mohamed Abdel-Aziz* and Hamdy M. Abdel-Rahman

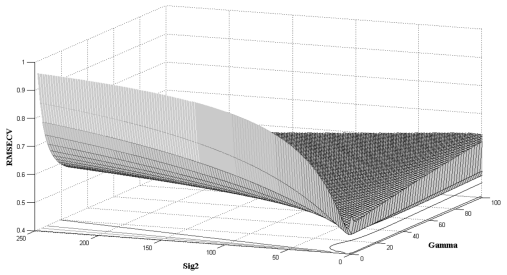


Novel 8-arylated purines as inhibitors of glycogen synthase kinase pp. 3389–3393
Nada Ibrahim, Liliane Mouawad and Michel Legraverend*

The synthesis of a library of 8-arylated-6-substituted purines allowed the identification of inhibitors of Glycogen Synthase Kinase (GSK-3) which were docked in the ATP binding site of the kinase.

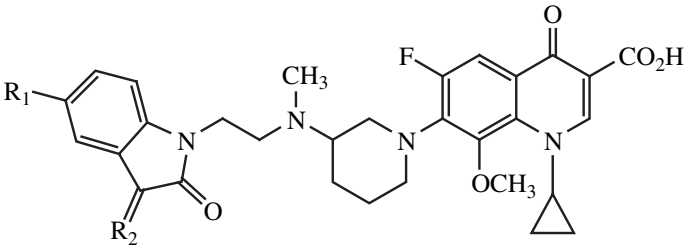


Validated QSAR analysis of some diaryl substituted pyrazoles as CCR2 inhibitors by various linear and nonlinear multivariate chemometrics methods pp. 3394–3406
Elham Arkan, Mohsen Shahlaei*, Alireza Pourhossein, Kambiz Fakhri and Afshin Fassihi**



Synthesis and *in vitro* antimycobacterial activity of balofloxacin ethylene isatin derivatives pp. 3407–3412
Lian-Shun Feng, Ming-Liang Liu*, Bo Wang, Yun Chai, Xue-Qin Hao, Shuai Meng and Hui-Yuan Guo

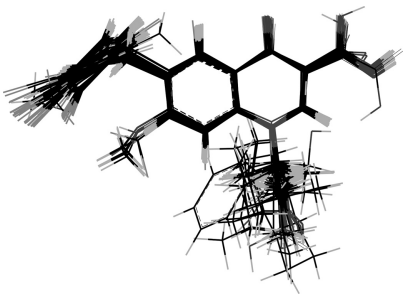
A series of novel balofloxacin ethylene isatin derivatives were synthesized. These compounds have considerable activity against *M. phlei* CMCC 93201, *M. smegmatis* CMCC 93202, MTB 09710 and MTB H37Rv ATCC 27294



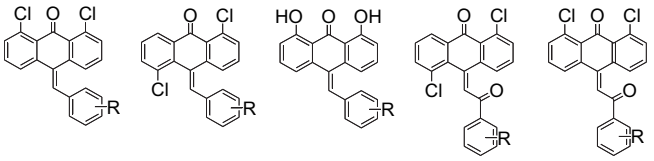
3a-n

CoMFA and CoMSIA 3D-QSAR studies on quionolone caroxylic acid derivatives inhibitors of HIV-1 integrase pp. 3413–3419
Peng Lu, Xia Wei and Ruisheng Zhang*

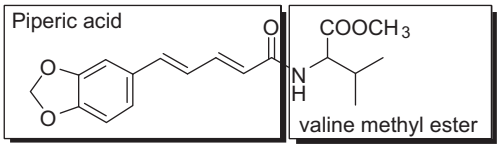
3D-QSAR studies were performed on 48 HIV-1 integrase inhibitors by CoMFA and CoMSIA methods.



Synthesis, antiproliferative activity and inhibition of tubulin polymerization by 1,5- and 1,8-disubstituted 10*H*-anthracen-9-ones bearing a 10-benzylidene or 10-(2-*oxo*-2-phenylethylidene) moiety **pp. 3420–3438**
Holger C. Nickel, Peter Schmidt, Konrad J. Böhm, Silke Baasner, Klaus Müller, Matthias Gerlach, Eberhard Unger, Eckhard G. Günther and Helge Prinz*



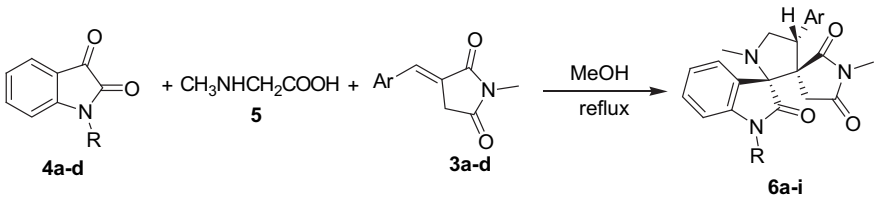
Synthesis and Antileishmanial activity of Piperoyl-Amino Acid Conjugates **pp. 3439–3445**
Inder Pal Singh*, Shreyans Kumar Jain, Amandeep Kaur, Sukhvinder Singh, Rajender Kumar, Prabha Garg, Shyam Sundar Sharma and Sunil Kumar Arora



5: IC_{50} = 0.075 mM

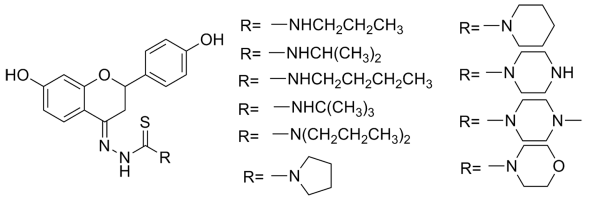
Synthesis, antibacterial activity evaluation and QSAR studies of novel dispiropyrrolidines **pp. 3446–3452**
K. Karthikeyan, P.M. Sivakumar, M. Doble and P.T. Perumal*

A series of novel dispiropyrrolidines have been synthesized through 1,3-dipolar cycloaddition of azomethine ylide. The products exhibits good antibacterial activity and QSAR were developed for the antibacterial activities.



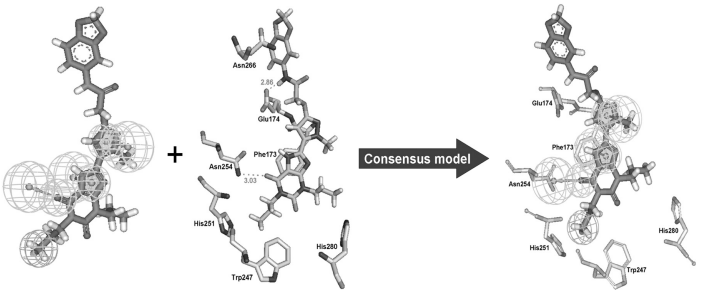
Synthesis and antitumor activity of liquiritigenin thiosemicarbazone derivatives **pp. 3453–3458**
Kun Hu, Ze-hua Yang, Sha-Sha Pan, Hua-jin Xu and Jie Ren*

The synthesis and antitumor activities of a series liquiritigenin thiosemicarbazone derivatives were described.



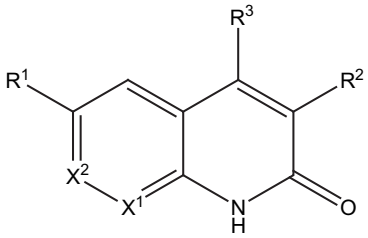
Insights into binding modes of adenosine A_{2B} antagonists with ligand-based and receptor-based methods pp. 3459–3471
Feixiong Cheng, Zhejun Xu, Guixia Liu and Yun Tang*

A consensus model of human A_{2B} antagonists was developed. These results provided helpful information for the discovery of novel and potent A_{2B} antagonists.



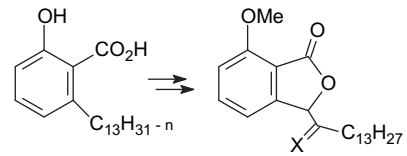
Insights through AM1 calculations into the structural requirement of 3,4,6-substituted-2-quinolone analogs towards FMS kinase inhibitory activity pp. 3472–3479
Arun Kumar Gupta*, Neetu Sabarwal, Yogesh P. Agrawal, Sumeet Prachand and Sanjay Jain

Amalgamated QSAR model of FMS kinase inhibitory activity against 3,4,6-substituted-2-quinolones showed coefficient of determination (0.891), cross validated correlation coefficient (0.776) and external predictivity (0.668).



Synthesis and cytotoxicity screening of substituted isobenzofuranones designed from anacardic acids pp. 3480–3489
Lúcio P.L. Logrado, Camila O. Santos, Luiz A.S. Romeiro, Arinice M. Costa, José R.O. Ferreira, Bruno C. Cavalcanti, O. Manoel de Moraes, Letícia V. Costa-Lotufo, Cláudia Pessoa and Maria L. dos Santos*

A simple approach to isobenzofuranones from anacardic acids is described. Compound (**1b**) showed a discriminatory antiproliferative effects against HL-60 cells.



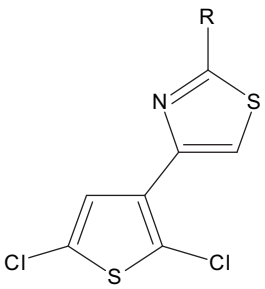
n = 0, 2, 4 or 6
Anacardic acids

1a: X = OH, H
1b: X = O

SHORT COMMUNICATIONS

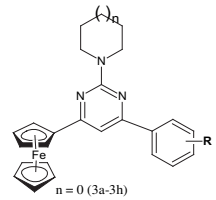
Synthesis, characterization, *in vitro* and molecular docking studies of new 2,5-dichloro thienyl substituted thiazole derivatives for antimicrobial properties pp. 3490–3496
Balladka Kunhanna Sarojini*, Bettadapura Gundappa Krishna, Chenna Govindaraju Darshanraj, Basavapattana Rudresh Bharath and Hanumanthappa Manjunatha

A new series of 2-substituted 4-(2,5-dichloro thienyl)-1,3-thiazoles are synthesized and screened for their antifungal and antibacterial activities *in vitro* and *in silico*. Some of them have showed promising activities.



Synthesis, characterization and biological evaluation of novel 6-ferrocenyl-4-aryl-2-substituted pyrimidine derivatives **pp. 3497–3503**
Humaira Parveen*, Faisal Hayat, Attar Salahuddin and Amir Azam

A series of novel 6-ferrocenyl-4-aryl-2-substituted pyrimidine derivatives were synthesized and screened for antiamoebic activity and toxicity. Out of 16 compounds **4f** was found most active and least toxic.



n = 0 (3a-3h)

n = 1 (4a-4h)

a = H, b = 4-Me, c = 2,5- DiOMe

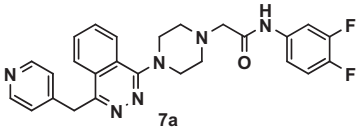
d = 4-OMe, e = 3,4,5- triOMe, f = 4-Cl

g = 3,4-DiMe, h = 4-SMe

PRELIMINARY COMMUNICATION

Synthesis and antitumor activities of novel 1,4-disubstituted phthalazine derivatives **pp. 3504–3510**
Shulan Zhang, Yanfang Zhao, Yajing Liu, Dong Chen, Weihuan Lan, Qiaoling Zhao, Chengcheng Dong, Lin Xia and Ping Gong*

The most promising compound, 7a (IC_{50} = 3.79 μM, 2.32 μM, 0.84 nM), showed excellent cytotoxic activities against A549, HT-29 and MDA-MB-231 cell lines *in vitro* by the MTT method.

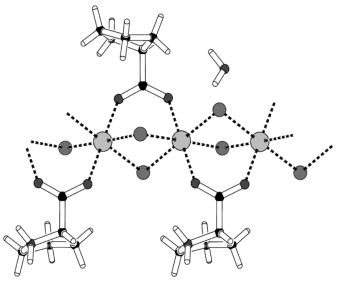


7a

LABORATORY NOTE

Advantages of cocrystallization in the field of solid-state pharmaceutical chemistry: L-Proline and $MnCl_2$ **pp. 3511–3517**
Anaëlle Tilborg, Catherine Michaux, Bernadette Norberg and Johan Wouters*

Dry grinding has been used here to obtain cocrystals of L-Proline and $MnCl_2$. The complex was characterized by powder and single-crystal X-ray diffraction and differential scanning calorimetry. This contribution provides structural basis for the role that L-Proline could play within multicomponent solid-state molecular complexes, in particular as a potential cocrystal former acting by both ionic and H-bond interactions when combined to molecules of pharmaceutical interest.



CORRIGENDUM

Corrigendum to "Synthesis and in vivo antidiabetic activity of novel dispiropyrrolidines through [3 + 2] cycloaddition reactions with thiazolidinedione and rhodanine derivatives " [European Journal of Medicinal Chemistry 44 3272–3279] **pp. 3518–3518**
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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

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