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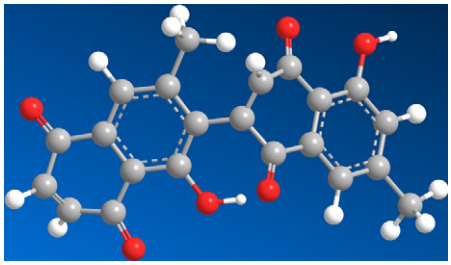
Contents

INVITED REVIEW

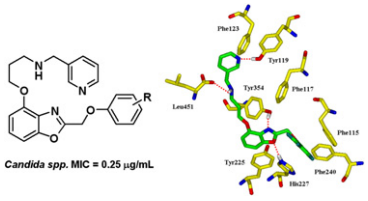
Anti-cancer activities of diospyrin, its derivatives and analogues pp. 3519–3530
Sunil Sagar*, Mandeep Kaur, Kenneth P. Minneman and Vladimir B. Bajic



ORIGINAL ARTICLES

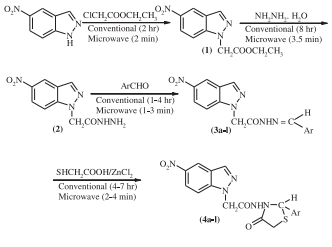
Design, synthesis and antifungal activity of isosteric analogues of benzoheterocyclic *N*-myristoyltransferase inhibitors pp. 3531–3540
Chunquan Sheng, Hui Xu, Wenya Wang, Yongbing Cao, Guoqiang Dong, Shengzheng Wang, Xiaoying Che, Haitao Ji, Zhenyuan Miao, Jianzhong Yao and Wannian Zhang*

A series of benzoxazole and indole derivatives were designed and synthesized as isosteric analogues of benzoheterocyclic NMT Inhibitors. The binding mode was investigated by molecular docking.



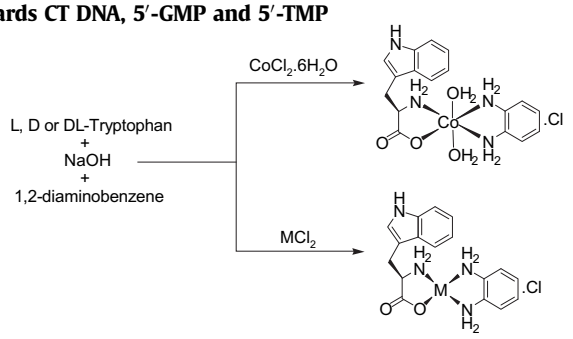
Conventional and microwave assisted synthesis of Some new N-[(4-oxo-2-substituted aryl −1, 3-thiazolidine)-acetamidyl]-5-nitroindazoles and its antimicrobial activity pp. 3541–3548
Apoorva Upadhyay*, S.K. Srivastava and S.D. Srivastava

Several new N-[(4-oxo-2-substituted aryl-1,3-thiazolidine)-acetamidyl] -5-nitroindazole (**4a–l**) were synthesized from N-(arylidene amino acetamidyl) – 5-nitroindazoles (**3a–l**). The reactions were carried out by both conventional as well as microwave method. some of these compounds have shown significant antibacterial and antifungal activities



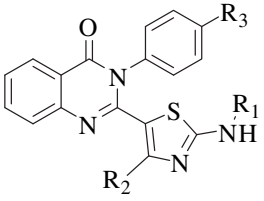
Chiral preference of L-tryptophan derived metal-based antitumor agent of late 3d-metal ions (Co(II), Cu(II) and Zn(II)) in comparison to D- and DL-tryptophan analogues: Their *in vitro* reactivity towards CT DNA, 5′-GMP and 5′-TMP pp. 3549–3557
Farukh Arjmand*, Mohd. Muddassir and Rizwan Hasan Khan

To evaluate chiral preference of two enantiomeric forms L, D and their racemic counterpart DL-tryptophan, new mononuclear complexes **1**–**3** were synthesized. They can bind to DNA via electrostatic interaction.

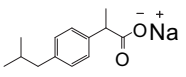


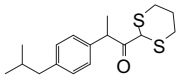
Synthesis and evaluation of quinazolinone derivatives as inhibitors of NF-κB, AP-1 mediated transcription and eIF-4E mediated translational activation: Inhibitors of multi-pathways involve in cancer pp. 3558–3563
Rajan S. Giri, Hardik M. Thaker, Tony Giordano, Bing Chen, Sam Nuthalapaty, Kamala K. Vasu* and Vasudevan Sudarsanam

This study describes the synthesis and evaluation of 2-thiazole-5-yl-3*H*-quinazolin-4-one derivatives as inhibitors of multiple pathways involved in cancerous conditions.



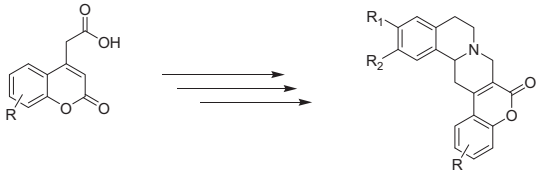
Chemistry around imidazopyrazine and ibuprofen: Discovery of novel fatty acid amide hydrolase (FAAH) inhibitors pp. 3564–3574
Frédéric De Wael, Giulio G. Muccioli, Didier M. Lambert, Thérèse Sergent, Yves-Jacques Schneider, Jean-François Rees and Jacqueline Marchand-Brynaert*


ibuprofen
pI_{50} (FAAH) = 3.42 +/- 0.03

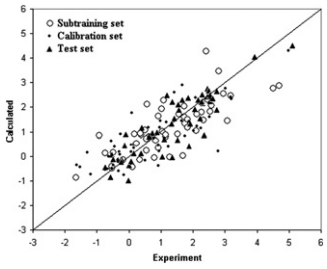

4a
pI_{50} (FAAH) = 5.86 +/- 0.03

Synthesis, structure and DNA cleavage studies of coumarin analogues of tetrahydroisoquinoline and protoberberine alkaloids pp. 3575–3580
Vithal B. Jadhav, Susanta K. Nayak, T.N. Guru Row and M.V. Kulkarni*

A series of novel coumarin analogues of 1,2,3,4-tetrahydroisoquinoline and protoberberine alkaloids have been synthesized from coumarin-4-acetic acids. The DNA cleavage study has been performed on Gram positive, Gram negative bacteria and fungi strains.

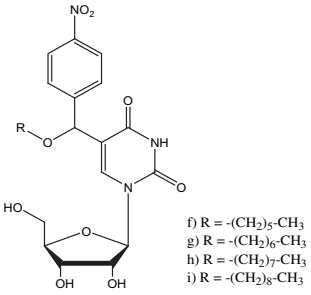


SMILES-based optimal descriptors:QSAR modeling of carcinogenicity by balance of correlations with ideal slopes **pp. 3581–3587**
A.A. Toropov*, A.P. Toropova and E. Benfenati



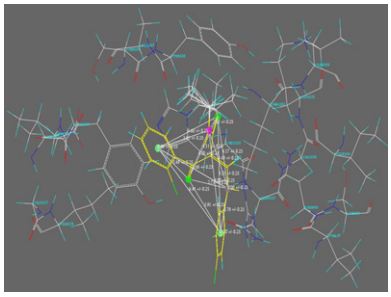
Synthesis of 5-[alkoxy-(4-nitro-phenyl)-methyl]-uridines and study of their cytotoxic activity **pp. 3588–3594**
Lucie Brulíková, Petr Džubák, Marián Hajdúch, Lenka Lachnitová, Madhusudhan Kollareddy, Milan Kolář, Kateřina Bogdanová and Jan Hlaváč*

The synthesis, cytotoxic activity, DNA/RNA synthesis inhibition and apoptosis induction of target compounds in their both diastereoisomeric forms were studied.



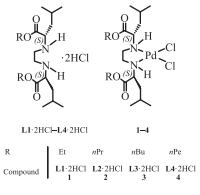
Homology modeling and atomic level binding study of $GABA_A$ receptor with novel enaminone amides **pp. 3595–3600**
Jin Cheng and Xiu-Lian Ju*

The binding modes of novel enaminone amides with rat α1β2γ2 GABAR were studies by molecular docking and pharmacophore analyses. The results indicate His128, Tyr186 and Tyr236 of α subunit of GABAR are essential to form protein–ligand interactions.



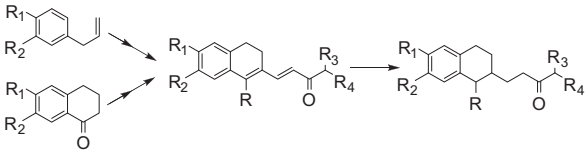
Palladium(II) complexes with R_2edda derived ligands. Part IV. *O,O′*-dialkyl esters of (*S,S*)-ethylenediamine-*N,N′*-di-2-(4-methyl)-pentanoic acid dihydrochloride and their palladium(II) complexes: Synthesis, characterization and *in vitro* antitumoral activity against chronic lymphocytic leukemia (CLL) cells **pp. 3601–3606**
Jelena M. Vujić, Milica Cvijović, Goran N. Kaluđerović*, Marija Milovanović, Bojana B. Zmejkovski, Vladislav Volarević, Nebojša Arsenijević, Tibor J. Sabo and Srećko R. Trifunović

Compounds R_2edda·2HCl-type esters (**L1**·2HCl–**L4**·2HCl) and corresponding palladium(II) complexes (**1–4**) were synthesized, characterized and tested *in vitro* against chronic lymphocytic leukemia cells. Cytotoxicity depends on ester R substituents in both esters (IC_{50}: *n*Pe < *n*Bu ≈ *n*Pr < Et) and palladium(II) complexes (IC_{50}: *n*Pr < *n*Pe < *n*Bu ≈ Et). The most active compound **2**, [$PdCl_2${(*S,S*)-*n*Pr_2eddl}], was found to be 13.6 times more active than cisplatin on CLL cells.



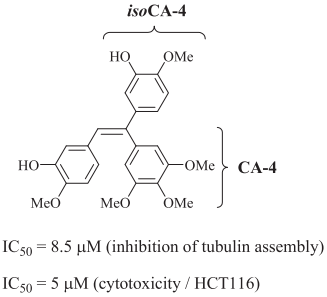
Substituted dihydronaphthalenes as efflux pump inhibitors of *Staphylococcus aureus* **pp. 3607–3616**
Niranjan Thota, Mallepally V. Reddy, Ashwani Kumar, Inshad A. Khan, Payare L. Sangwan, Nitin P. Kalia, Jawahir L. Koul and Surrinder Koul*

Design and synthesis of new series of 3-(substituted 3,4-dihydronaphthyl)-propenoic acid amides as efflux pump inhibitors has resulted in the MIC reduction of ciprofloxacin.



Regioselective hydrostannation of diarylalkynes directed by a labile *ortho* bromine atom: An easy access to stereodefined triarylolefins, hybrids of combretastatin A-4 and *iso*combretastatin A-4 **pp. 3617–3626**
Evelia Rasolofonjatovo, Olivier Provot, Abdallah Hamze, Jérome Bignon, Sylviane Thoret, Jean-Daniel Brion and Mouâd Alami*

A novel series of CA-4-*iso*CA-4 hybrids have been synthesized. All of the compounds were evaluated for their cytotoxic and antimitotic properties.

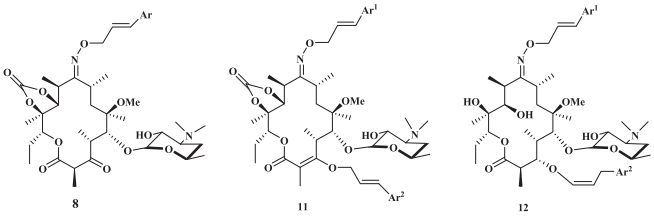


IC_{50} = 8.5 μM (inhibition of tubulin assembly)

IC_{50} = 5 μM (cytotoxicity / HCT116)

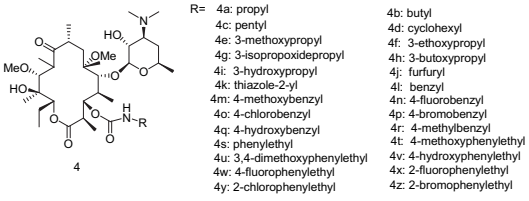
Synthesis and antibacterial activities of 6-*O*-methylerythromycin A 9-*O*-(3-aryl-2-propenyl) oxime ketolide, 2,3-enol ether, and alkylide analogues **pp. 3627–3635**
Jian-Hua Liang*, Li-Jing Dong, He Wang, Kun An, Xiao-Li Li, Li Yang, Guo-Wei Yao and Ying-Chun Xu

Among the candidates, **8b** (3-quinolyl), **8d** (6-quinolyl) and **8e** [4-(1-imidazolyl)phenyl] displayed a good antibacterial profile against both susceptible and resistant respiratory pathogens.

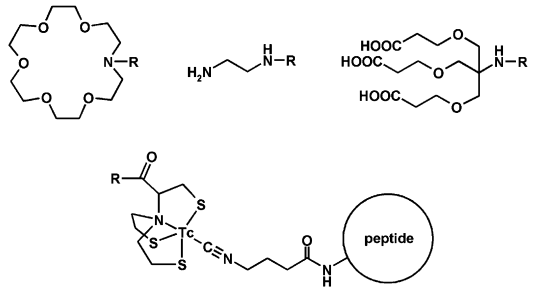


Synthesis and antibacterial activity of 3-*O*-carbamoyl derivatives of 6,11-di-*O*-methylerythromycin A: A novel class of acylides **pp. 3636–3644**
Zhongyuan Wu, Yong Lu, Ming Luo, Xianran He, Yuling Xiao, Jin Yang, Yuanhu Pan, Guofu Qiu, Hao Guo, Hao Hu, Dingshan Zhou and Xianming Hu*

Novel 3-*O*-carbamate derivatives of 6,11-di-*O*-methylerythromycin A were synthesized by substituting L-cladinose with various carbamate groups. This new class of antibiotics exhibited potent activity against some key erythromycin-resistant pathogens.

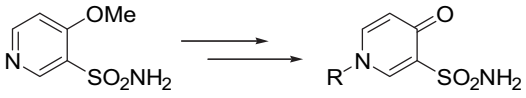


Novel ^{99m}Tc '4 + 1' peptide conjugates: Tuning the biodistribution by variation of coligands pp. 3645–3655
Jens-Uwe Kunstler, Gesine Seidel, Ralf Bergmann, Ewa Gniazdowska, Martin Walther, Eik Schiller, Clemens Decristoforo, Holger Stephan, Roland Haubner, Jorg Steinbach and Hans-Jurgen Pietzsch*



Carbonic anhydrase inhibitors. Regioselective synthesis of novel 1-substituted 1,4-dihydro-4-oxo-3-pyridinesulfonamides and their inhibition of the human cytosolic isozymes I and II and transmembrane cancer-associated isozymes IX and XII pp. 3656–3661
Zdzisław Brzozowski, Jarosław Sławiński*, Alessio Innocenti and Claudiu T. Supuran

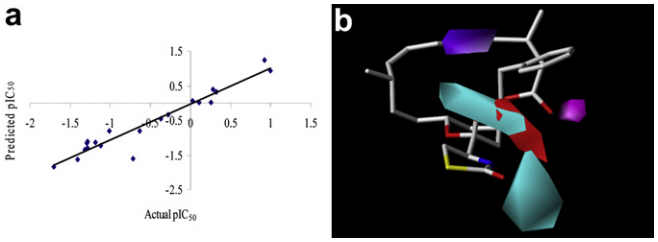
A novel 1-substituted 1,4-dihydro-4-oxo-3-pyridinesulfonamides have been synthesized and investigated as inhibitors of carbonic anhydrase isozymes hCA I, II, IX and XII. Some of them showed excellent hCA IX and XII inhibitory efficacy.



1 2-16

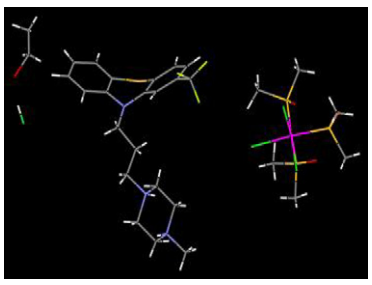
R = alkyl or substituted alkyl, heteroaryl, aryl or aroyl

3D-QSAR studies of latrunculin-based actin polymerization inhibitors using CoMFA and CoMSIA approaches pp. 3662–3668
Mohammad A. Khanfar, Diaa T.A. Youssef and Khalid A. El Sayed*



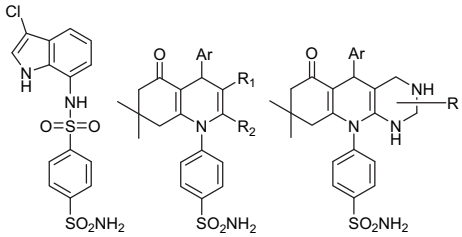
New ruthenium(II) complexes with N-alkylphenothiazines: Synthesis, structure, *in vivo* activity as free radical scavengers and *in vitro* cytotoxicity pp. 3669–3676
Milena Krstić, Sofija P. Sovilj*, Sanja Grgurić-Šipka, Ivana Radosavljević Evans, Sunčica Borozan, Juan Francisco Santibanez and Jelena Kocić

New Ru(II) complexes with N-alkylphenothiazines were prepared, characterized and evaluated for their cytotoxicity against four human cancer cell lines. The trifluoroperazine complex was investigated on the antioxidant enzyme activities, too.



In vitro anticancer screening and radiosensitizing evaluation of some new quinolines and pyrimido[4,5-_b_]quinolines bearing a sulfonamide moiety **pp. 3677–3684**
Mostafa M. Ghorab*, Fatma A. Ragab, Helmy I. Heiba, Reem K. Arafa and Ebaa M. El-Hossary

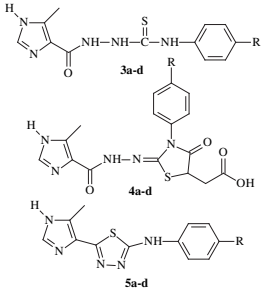
The present work reports the synthesis of twenty novel quinoline and pyrimido[4,5-*b*]quinoline derivatives bearing a sulfonamide moiety (**6–25**), and the evaluation of their *in vitro* anticancer activity alone or in combination with γ-irradiation.



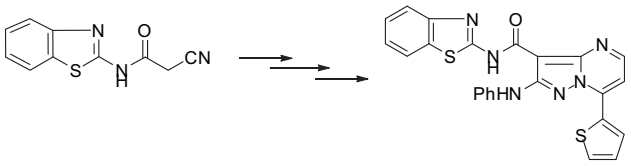
(E7070)

Synthesis and evaluation of anti-_Toxoplasma gondii_ and antimicrobial activities of thiosemicarbazides, 4-thiazolidinones and 1,3,4-thiadiazoles **pp. 3685–3691**
André P. Liesen, Thiago M. de Aquino, Cristiane S. Carvalho, Vânia T. Lima, Janete M. de Araújo, José G. de Lima, Antônio R. de Faria, Edésio J.T. de Melo, Antonio J. Alves, Elias W. Alves, Anselmo Q. Alves and Alexandre J.S. Góes*

Three new series of compounds were synthesized from ethyl(5-methyl-1-*H*-imidazole-4-carboxylate): acylthiosemicarbazide analogues (**3a-d**), 4-thiazolidinone analogues (**4a-d**) and 1,3,4-thiadiazole analogues (**5a-d**). All compounds were screened for their anti-*Toxoplasma gondii* and antimicrobial activity.

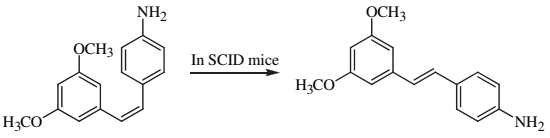


Synthesis and antimicrobial activity of some new thiazole, thiophene and pyrazole derivatives containing benzothiazole moiety **pp. 3692–3701**
Samir Bondock*, Walid Fadaly and Mohamed A. Metwally



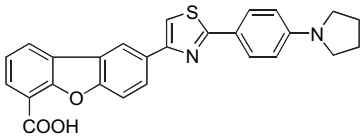
In vitro and _in vivo_ studies on stilbene analogs as potential treatment agents for colon cancer **pp. 3702–3708**
Shiby Paul, Cassia S. Mizuno, Hong Jin Lee, Xi Zheng, Sarah Chajkowisk, John M. Rimoldi, Allan Conney, Nanjoo Suh and Agnes M. Rimando*

Twenty-seven stilbene analogs were tested, and the *cis* isomers were more inhibitory than the *trans* isomers against colon cancer cells *in vitro*. The *cis*-amino analog isomerized to the *trans*-amino isomer *in vivo* and suppressed tumor growth in SCID mice the most.



Synthesis and evaluation of some novel dibenzo[*b*,*d*]furan carboxylic acids as potential anti-diabetic agents **pp. 3709–3718**
N. Lakshminarayana, Y. Rajendra Prasad*, Laxmikant Gharat, Abraham Thomas, Shridhar Narayanan, A. Raghuram, C.V. Srinivasan and Balasubramanian Gopalan

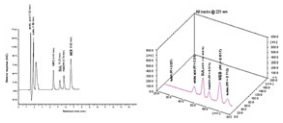
A series of dibenzo[*b*,*d*]furan carboxylic acids were synthesized and evaluated for anti-diabetic activity. Compound **5E** inhibited PTP1B with IC_{50} of 82 nM and reduced WBG and plasma glucose in *obob* mice.



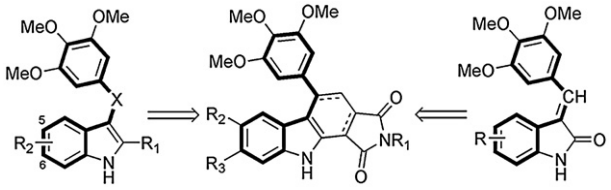
5E IC_{50}: 82 ± 0.43 nM

Development and validation of stability indicating HPLC and HPTLC methods for determination of sulpiride and mebeverine hydrochloride in combination **pp. 3719–3725**
Ibrahim A. Naguib* and Mohammed Abdelkawy

HPLC and HPTLC methods are used for the analysis of sulpiride and mebeverine hydrochloride together and in presence of their reported impurities and degradation products.

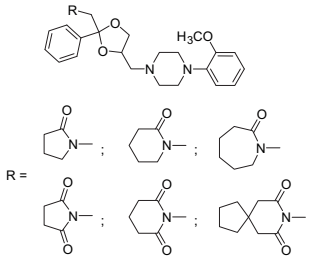


Structure–activity relationships of indole compounds derived from combretastatin A4: Synthesis and biological screening of 5-phenylpyrrolo[3,4-*a*]carbazole-1,3-diones as potential antivascular agents **pp. 3726–3739**
Nancy Ty, Grégory Dupeyre, Guy G. Chabot*, Johanne Seguin, Lionel Quentin, Angèle Chiaroni, François Tillequin, Daniel Scherman, Sylvie Michel and Xavier Cachet*



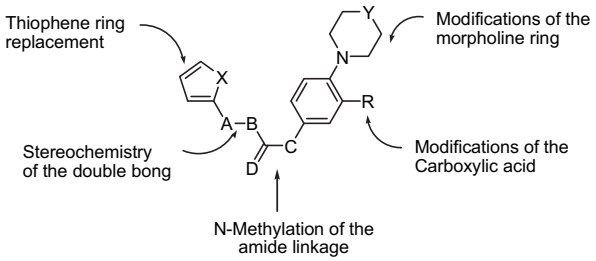
1,3-Dioxolane-based ligands incorporating a lactam or imide moiety: Structure–affinity/activity relationship at α_1-adrenoceptor subtypes and at 5-HT_{1A} receptors **pp. 3740–3751**
Silvia Franchini, Adolfo Prandi, Annamaria Baraldi, Claudia Sorbi, Annalisa Tait, Michela Buccioni, Gabriella Marucci, Antonio Cilia, Lorenza Pirona, Paola Fossa, Elena Cichero and Livio Brasili*

The lactam derivatives seems to favour 5-HT_{1A} receptor antagonism and α_{1B}-adrenoceptor antagonist selectivity. The imide derivative **7*t*** is a selective α_{1D}-adrenoceptor antagonist whereas at 5-HT_{1A} receptor it is a potent partial agonist.



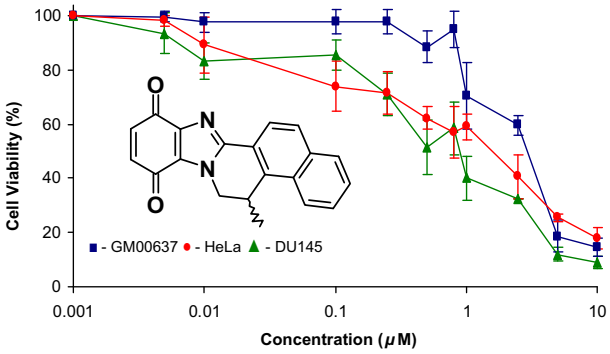
Synthesis and structure activity relationship studies of novel *Staphylococcus aureus* Sortase A inhibitors pp. 3752–3761
Bala Chandra Chenna, Jason R. King, Bidhan A. Shinkre, Amanda L. Glover, Aaron L. Lucius and Sadanandan E. Velu*

Synthesis and structure activity relationship studies of a lead structural template of *Staphylococcus aureus* Sortase A inhibitor are described.



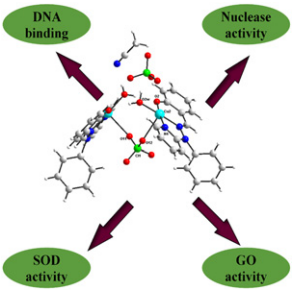
Synthesis and toxicity towards normal and cancer cell lines of benzimidazolequinones containing fused aromatic rings and 2-aromatic ring substituents pp. 3762–3769
Eoin Moriarty, Miriam Carr, Sarah Bonham, Michael P. Carty and Fawaz Aldabbagh*

The naphthyl fused benzimidazolequinone showed the highest specificity towards human cervical (HeLa) and prostate (DU145) cancer cell lines, with little toxicity towards a human normal (GM00637) cell line at doses of <1 μM.



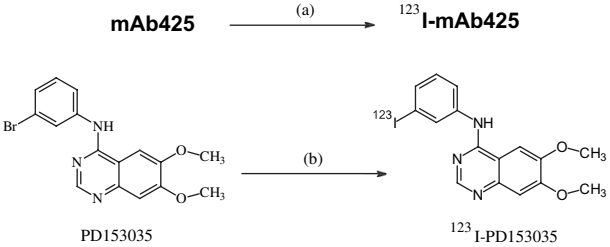
Synthesis and reactivity studies on new copper(II) complexes: DNA binding, generation of phenoxyl radical, SOD and nuclease activities pp. 3770–3779
Kaushik Ghosh*, Pramod Kumar, Nidhi Tyagi, Udai P. Singh, Vaibhave Aggarwal and Maria Camilla Baratto

Novel copper complexes were synthesized by a tridentate ligand having phenolato, pyridine and azomethine nitrogen donors. Phenoxyl radical complexes were generated; DNA interaction, SOD and nuclease activities were investigated.



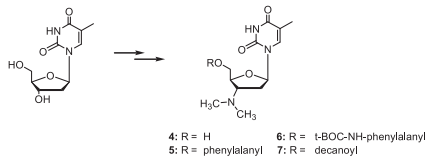
Synthesis and initial tumor affinity testing of iodine-123 labelled EGFR-affine agents as potential imaging probes for hormone-refractory prostate cancer pp. 3780–3786
Thierry Fozing, Claudia Scheuer and Samuel Samnick*

The epidermal growth factor receptor (EGFR) is over-expressed in a variety of human cancers, including in hormone-refractory prostate carcinomas, in which the EGFR has been associated with advanced disease stage, resistance to standard treatment and poor prognosis. Therefore, the EGFR is considered to be a promising molecular target for molecular imaging and therapy for hormone-refractory prostate cancer. This work describes the synthesis and initial tumor affinity testing of the EGFR antagonist ^{123}I-mAb425 and the EGF receptor tyrosine kinase (EGFR-TK) inhibitor ^{123}I-PD153035 as potential imaging probes for studying EGFR-expressing prostate cancer using single photon emission tomography.



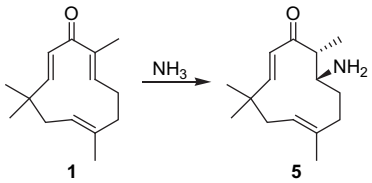
Synthesis, structure–activity relationship and antiviral activity of 3′-*N*,*N*-dimethylamino-2′,3′-dideoxythymidine and its prodrugs **pp. 3787–3793**
Ramendra K. Singh*, Dipti Yadav, Diwakar Rai, Garima Kumari, C. Pannecouque and Erik De Clercq

Synthesis, molecular modeling and antiviral/anti-HIV activity of 3′-*N*,*N*-dimethylamino-2′,3′-dideoxythymidine and its prodrugs have been described.



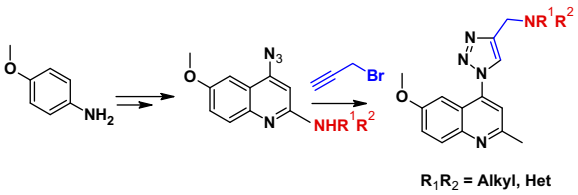
Cytotoxicity against cholangiocarcinoma cell lines of zerumbone derivatives **pp. 3794–3802**
Uraiwan Songsiang, Siripit Pitchuanchom, Chantana Boonyarat, Chariya Hahnvajanawong and Chavi Yenjai*

Amine **5** modified from zerumbone (**1**) exhibited very strong cytotoxicity against cholangiocarcinoma cells (KKU-100; the least sensitive cells) with an IC_{50} value of 16.44 μM. The docking experiment showed that **5** exhibited better binding interaction to EGFR than CDK-2, CDK-5 and GSK-3.



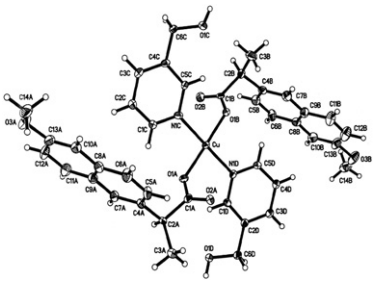
Design, synthesis and antimicrobial activities of some new quinoline derivatives carrying 1,2,3-triazole moiety **pp. 3803–3810**
K.D. Thomas, Airody Vasudeva Adhikari* and N. Suchetha Shetty

Twenty five new derivatives of [1-(6-methoxy-2-methylquinolin-4-yl)-1*H*-1,2,3-triazol-4-yl] methanamine have been synthesized and the most effective compounds have MIC of 6.25 μg/mL, which are in comparable with present antibiotics.



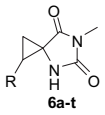
Copper (II) complexes of the anti-inflammatory drug naproxen and 3-pyridylmethanol as auxiliary ligand. Characterization, superoxide dismutase and catecholase – mimetic activities **pp. 3811–3817**
A. Latif Abuhijleh* and Juhienah Khalaf

Binary copper (II) naproxenate complex and its ternary complex with 3-pyridylmethanol were found to be potent SOD mimics and have moderate catecholase mimetic activities.



Synthesis and anticonvulsant activity of new 6-methyl-1-substituted- 4,6- diazaspiro[2.4]heptane-5,7-diones **pp. 3818–3830**
Xianran He, Guanpeng Qiu, Jin Yang, Yuling Xiao, Zhongyuan Wu, Guofu Qiu and Xianming Hu*

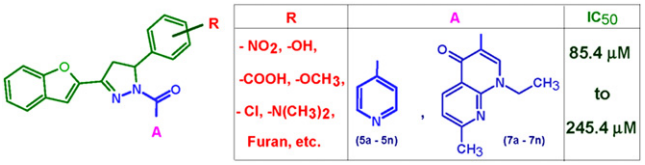
A series of 6-methyl-1-substituted-4,6-diazaspiro[2.4]heptane-5,7-diones(**6a**–**t**) were synthesized. Their anticonvulsant activity was evaluated by the maximal electroshock (MES) and *sc*PTZ test, and their neurotoxicity was evaluated by the rotarod neurotoxicity test.



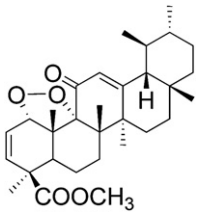
R	R
a: R=$(CH_3)_2CH$	k: R=3,4-di$CH_3OC_6H_3$
b: R=CH_3CH_2	l: R=2,3-di$CH_3OC_6H_3$
c: R=$CH_3CH_2CH_2$	m: R=2,3,4-tri$CH_3OC_6H_2$
d: R=$CH_3CH_2CH_2CH_2$	n: R=3,4,5-tri$CH_3OC_6H_2$
e: R=$(CH_3)_2CHCH_2$	o: R=4-FC_6H_4
f: R=$(CH_3CH_2)_2CH$	p: R=4-ClC_6H_4
g: R=C_6H_5	q: R=2-ClC_6H_4
h: R=4-$CH_3C_6H_4$	r: R=4-BrC_6H_4
i: R=4-$CH_3OC_6H_4$	s: R=C_4H_3O
j: R=2,5-di$CH_3OC_6H_3$	t: R=4-$CH_3SO_2C_6H_4$

Design, synthesis, and antitubercular evaluation of novel series of 3-benzofuran-5-aryl-1-pyrazolyl-pyridylmethanone and 3-benzofuran-5-aryl-1-pyrazolylcarbonyl-4-oxo-naphthyridin analogs **pp. 3831–3839**
Kuntal Manna* and Yadvendra K. Agrawal

In-vivo & *in-vitro* antitubercular results of synthesized drugs (**7j**, **7f**, **7a**, **5d** & **5f**) has drastically been reduced bacterial counts in mice lungs and spleen tissues, which comparable with standard drugs INH and Rifampin.

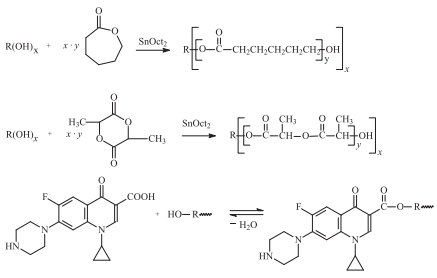


Synthesis of an antitumor active endoperoxide from 11-keto-β-boswellic acid **pp. 3840–3843**
René Csuk*, Anja Niesen-Barthel, Alexander Barthel, Ralph Kluge and Dieter Ströhl



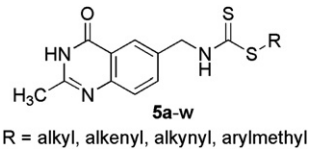
Synthesis and characterization of polyester conjugates of ciprofloxacin **pp. 3844–3849**
Marcin Sobczak*

The ciprofloxacin was covalently connected to the chain end of the two-, three-, four- and six-arm, star-shaped PCL and PLA via an ester linkage. The CIP release could be effectively controlled by altering the pH values of the environment.



Synthesis and cytotoxic activity of *N*-((2-methyl-4(3*H*)-quinazolinon-6-yl)methyl)dithiocarbamates **pp. 3850–3857**
Sheng-Li Cao*, Yao Wang, Lin Zhu, Ji Liao, Yan-Wen Guo, Lin-Lin Chen, Hong-Qin Liu and Xingzhi Xu**

Compounds **5a**–**w** were synthesized and their cytotoxic activity against five human cancer cell lines together with the effects of three representative compounds on A549 cell cycle progression were examined.

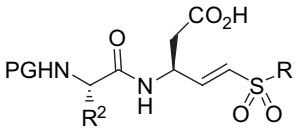


5a-w

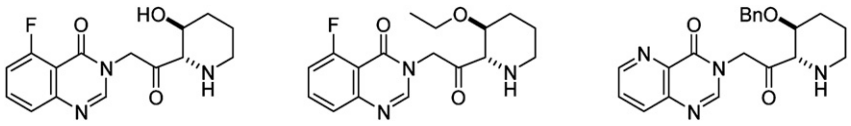
R = alkyl, alkenyl, alkynyl, arylmethyl

Synthesis and evaluation of vinyl sulfones as caspase-3 inhibitors. A structure–activity study **pp. 3858–3863**
Ana S. Newton, Paulo M.C. Glória, Lídia M. Gonçalves, Daniel J.V.A. dos Santos, Rui Moreira, Rita C. Guedes and Maria M.M. Santos*

The first structure–activity relationship study of vinyl sulfones as caspase-3 inhibitors is reported. A series of 12 vinyl sulfones was synthesized and evaluated for caspase-3 inhibition.

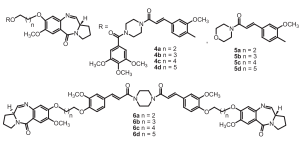


Synthesis and evaluation of 4-quinazolinone compounds as potential antimalarial agents **pp. 3864–3869**
Shuren Zhu*, Joe Wang, Gudise Chandrashekar, Erika Smith, Xianjun Liu and Yongshen Zhang



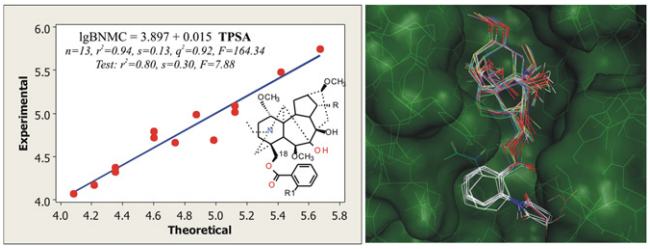
Synthesis and biological evaluation of cinnamido linked pyrrolo[2,1-*c*][1,4]benzodiazepines as antimitotic agents **pp. 3870–3884**
Ahmed Kamal*, G. Balakishan, G. Ramakrishna, T. Basha Shaik, K. Sreekanth, M. Balakrishna, Rajender, D. Dastagiri and Shasi V. Kalivendi

A series of new cinnamido-pyrrolo[2,1-*c*][1,4]benzodiazepine conjugates and their dimers have been designed, synthesized and evaluated for antiproliferative activity, inhibition of tubulin polymerization, and cell cycle effects.

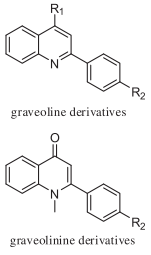


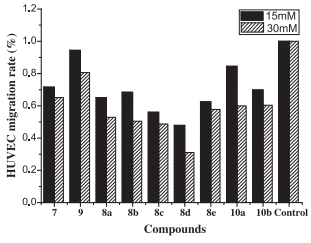
Aconitum and _Delphinium_ alkaloids of curare-like activity. QSAR analysis and molecular docking of alkaloids into AChBP pp. 3885–3894
M.A. Turabekova, B.F. Rasulev, F.N. Dzhakhangirov, D. Leszczynska* and J. Leszczynski

Classical QSAR and molecular docking approaches have been applied to reveal factors determining N-cholinolytic activity and AChBP-binding affinity of 19 curare-like *Aconitum* and *Delphinium* sp. alkaloids.



Synthesis and evaluation of graveoline and graveolinine derivatives with potent anti-angiogenesis activities pp. 3895–3903
Zeng-Yun An, Yi-Yong Yan, Dan Peng, Tian-Miao Ou, Jia-Heng Tan**, Shi-Liang Huang, Lin-Kun An, Lian-Quan Gu and Zhi-Shu Huang*

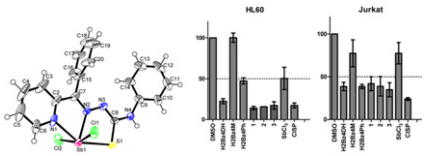




Inhibition of HUVEC migration by graveoline derivatives

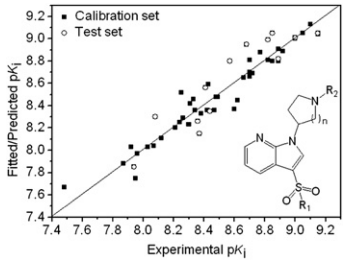
Antimony(III) complexes with 2-benzoylpyridine-derived thiosemicarbazones: Cytotoxicity against human leukemia cell lines pp. 3904–3910
Débora C. Reis, Mauro C.X. Pinto, Elaine M. Souza-Fagundes, Solange M.S.V. Wardell, James L. Wardell and Heloisa Beraldo*

[Sb(2Bz4DH)Cl_2] (**1**), [Sb(H2Bz4M)Cl_3] (**2**) and [Sb(2Bz4Ph)Cl_2] (**3**) were obtained with 2-benzoylpyridine thiosemicarbazone (H2Bz4DH) and its *N*(4)-methyl (H2Bz4M) and *N*(4)-phenyl (H2Bz4Ph) derivatives. H2Bz4DH, H2Bz4Ph and **1**–**3** were highly cytotoxic to leukemia cells.



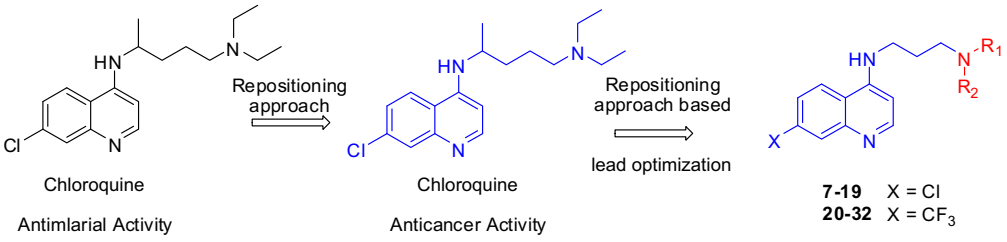
QSAR studies of bioactivities of 1-(azacyclyl)-3-arylsulfonyl-1*H*-pyrrolo[2,3-*b*]pyridines as 5-HT$_6$ receptor ligands using physicochemical descriptors and MLR and ANN-modeling pp. 3911–3915
Mohammad Goodarzi, Matheus P. Freitas* and Nahid Ghasemi

Few physicochemical descriptors were used to model the bioactivities of a series of 1-(azacyclyl)-3-arylsulfonyl-1*H*-pyrrolo[2,3-*b*]pyridines as 5-HT$_6$ receptor inhibitors, giving predictive QSAR models, especially when using ANN as a nonlinear regression.



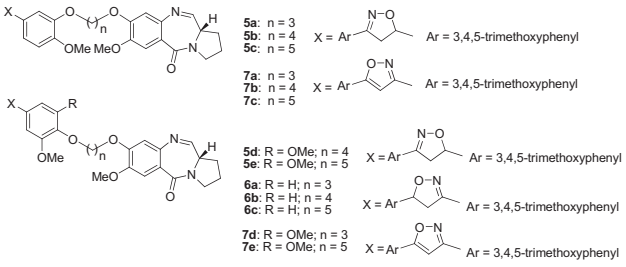
Design and synthesis of chloroquine analogs with anti-breast cancer property pp. 3916–3923
V.R. Solomon, Changkun Hu and Hoyun Lee*

A series of chloroquine (CQ) analogs were designed and synthesized by a *repositioning* approach-based lead optimization concept to improve their anti-breast cancer property.



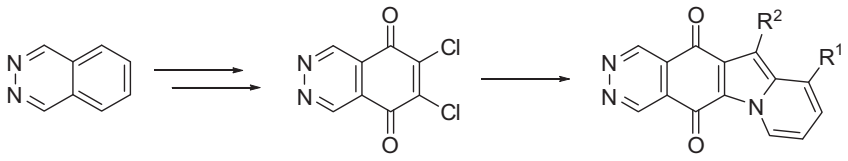
Design, synthesis and biological evaluation of 3,5-diaryl-isoxazoline/isoxazole-pyrrolobenzodiazepine conjugates as potential anticancer agents pp. 3924–3937
Ahmed Kamal*, J. Surendranadha Reddy, M. Janaki Ramaiah, D. Dastagiri, E. Vijaya Bharathi, M. Ameruddin Azhar, Farheen Sultana, S.N.C.V.L. Pushpavalli, Manika Pal-Bhadra*, Aarti Juvekar, Subrata Sen and Surekha Zingde

New class of 3,5-diaryl-isoxazoline/isoxazole-pyrrolobenzodiazepine conjugates were prepared and evaluated for their anticancer activity. Further, some of the biological assays related to mechanism aspects were also carried out.



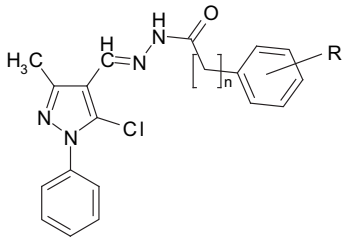
Synthesis and antiproliferative activity of indolizinophthalazine-5,12-dione derivatives, DNA topoisomerase IB inhibitors pp. 3938–3942
De-Qing Shen, Zu-Ping Wu, Xi-Wei Wu, Zeng-Yun An, Xiang-Zhang Bu, Lian-Quan Gu*, Zhi-Shu Huang and Lin-Kun An*

A series of novel indolizinophthalazine-5,12-dione derivatives were synthesized. Their in vitro anti-proliferative activity toward four human tumor cell lines and DNA topoisomerase IB inhibitory activity was investigated.

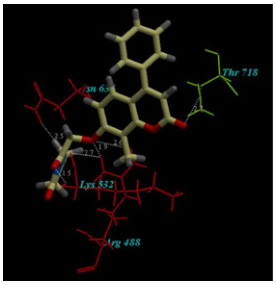


***N'*-[(5-chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylene] 2/4-substituted hydrazides: Synthesis and anticonvulsant activity** pp. 3943–3949
Darpan Kaushik*, Suroor Ahmad Khan, Gita Chawla and Suresh Kumar

A series of substituted hydrazide derivatives were synthesized, evaluated for their anticonvulsant potency in two animal models along with behavioural and neurotoxicity screen and also subjected to computational parameters.

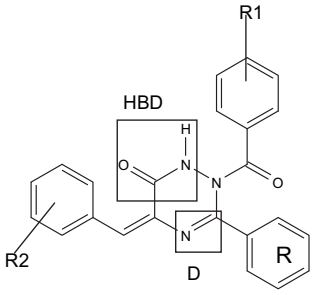


Synthesis and docking studies of novel benzopyran-2-ones with anticancer activity pp. 3950–3959
Magda M.F. Ismail*, Heba S. Rateb and Mohammad M.M. Hussein



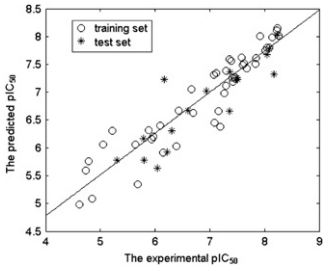
Design & synthesis of 2-(substituted aryloxy)-5-(substituted benzylidene)-3-phenyl-2,5-dihydro-1*H*-[1,2,4] triazin-6-one as potential anticonvulsant agents pp. 3960–3969
Darpan Kaushik*, Suroor Ahmad Khan and Gita Chawla

A series of substituted [1,2,4] triazin-6-one derivatives were synthesized, evaluated for their anticonvulsant potency on two animal models along with CNS activity and neurotoxicity and also subjected to computational parameter.



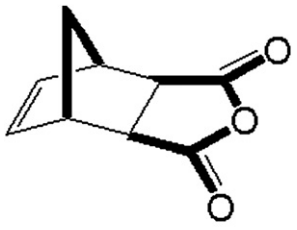
QSAR study of carboxylic acid derivatives as HIV-1 Integrase inhibitors pp. 3970–3980
Zhengjun Cheng, Yuntao Zhang* and Weizhong Fu

QSAR studies of a series of HIV-1 Integrase inhibitors are performed based on six different methods: stepwise-MLR, stepwise-BPNN, stepwise-SVM, RM-MLR, RM-BPNN, RM-SVM. Moreover, RM-SVM is the best models for predicting new HIV-1 Integrase inhibitors.



Therapeutic effects of cantharidin analogues without bridging ether oxygen on human hepatocellular carcinoma cells pp. 3981–3985
Chao-Bin Yeh, Chi-Jung Su, Jin-Ming Hwang and Ming-Chih Chou*

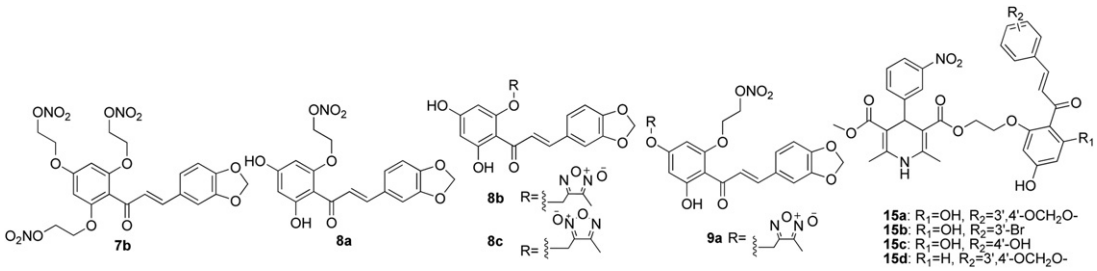
Elimination of bridging ether oxygen on the ring, such as in compound **10**, can` decrease their cytotoxicity. Anhydride ether oxygen is crucial for inducing HCC cytotoxicity.



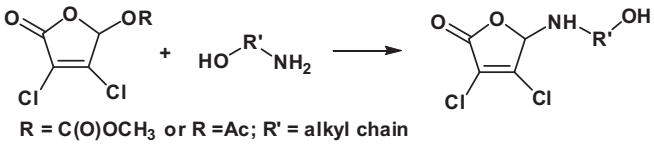
Compound **10**

Synthesis and biological evaluation of novel hybrid chalcone derivatives as vasorelaxant agents pp. 3986–3992
Xiaowu Dong, Lilin Du, Zhichao Pan, Tao Liu, Bo Yang and Yongzhou Hu*

Nine hybrid chalcone derivatives conjugated with nitric oxide (NO) donors or 1,4-dihydropyridyl moiety were designed, synthesized and biological evaluated for their vasorelaxant activities.

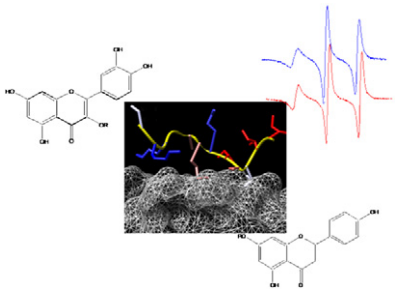


Synthesis and preliminary bioactivity assays of 3,4-dichloro-5-(ω-hydroxyalkylamino)-2(5*H*)-furanones pp. 3993–3997
Edyta Gondela and Krzysztof Z. Walczak*



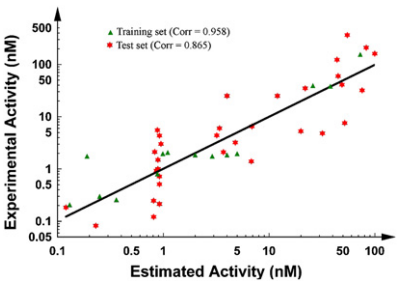
Effect of flavonoids on the Aβ(25-35)-phospholipid bilayers interaction pp. 3998–4003
Annamaria Tedeschi, Gerardino D'Errico, Maria Rosaria Lauro, Francesca Sansone, Sara Di Marino, Anna Maria D'Ursi* and Rita Patrizia Aquino

The effect of several flavonoids on the interaction Aβ(25-35)-phospholipid bilayer is studied by means of Electron Paramagnetic Resonance spectroscopy. The results provide a molecular explanation of the known neuroprotective effect of flavonoids.



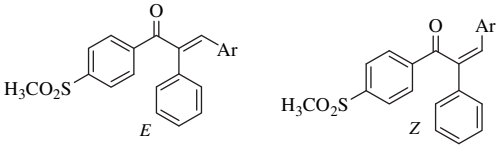
Identification of potent virtual leads to design novel indoleamine 2,3-dioxygenase inhibitors: Pharmacophore modeling and molecular docking studies pp. 4004–4012
Shalini John, Sundarapandian Thangapandian, Sugunadevi Sakkiah and Keun Woo Lee*

A high-correlation four-feature pharmacophore hypothesis was developed based on experimentally known IDO inhibitors. Three potent virtual leads are reported for novel IDO inhibitor designing.

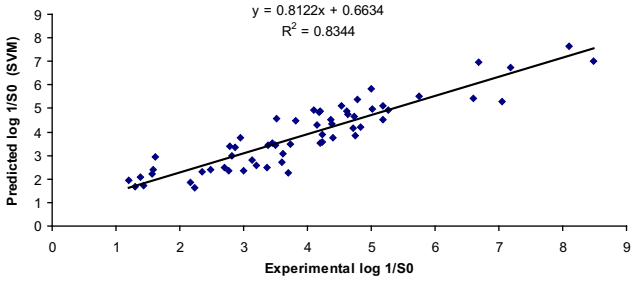


Design, synthesis and biological evaluation of new (*E*)- and (*Z*)-1,2,3-triaryl-2-propen-1-ones as selective COX-2 inhibitors **pp. 4013–4017**
Sara Arfaie and Afshin Zarghi*

A group of (*E*)- and (*Z*)-1,2,3-triaryl-2-propen-1-one derivatives were synthesized and evaluated as selective COX-2 inhibitors. In vitro COX-1/COX-2 structure–activity relationships were determined by varying the substituents on the C-3 propenone moiety.

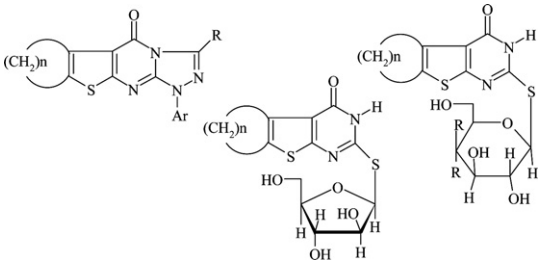


Prediction of intrinsic solubility of generic drugs using MLR, ANN and SVM analyses **pp. 4018–4025**
Bruno Louis, Vijay K. Agrawal* and Padmakar V. Khadikar



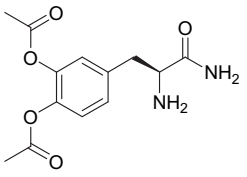
Synthesis of substituted thieno[2,3-*d*]pyrimidine-2,4-dithiones and their *S*-glycoside analogues as potential antiviral and antibacterial agents **pp. 4026–4034**
Hend N. Hafez, Hoda A.R. Hussein and Abdel-Rahman B.A. El-Gazzar*

Thienopyrimidine derivatives containing heterocyclic ring substituent linked to the pyrimidine-2-thione nucleus at C-2 by a two- to four-atom spacer as potential anti-HIV-1 and antimicrobial agents. The compounds were designed to comprise the heterocyclic substituent directly linked to the thienopyrimidines nucleus at C-2. Also, related triazolo[4,3-a]benzothieno[2,3-*d*]pyrimidines were also prepared as isosteres. Among the synthesized derivatives some of these were showing complete inhibition at 128 mg/mL or less.



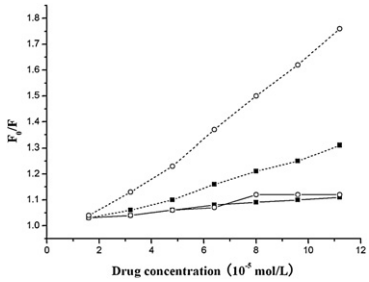
Design, synthesis and biological evaluation of L-dopa amide derivatives as potential prodrugs for the treatment of Parkinson's disease **pp. 4035–4042**
Tao Zhou, Robert C. Hider*, Peter Jenner, Bruce Campbell, Christopher J. Hobbs**, Sarah Rose, Mark Jairaj, Kayhan A. Tayarani-Binazir and Alexander Syme

A range of amide derivatives of L-dopa were synthesized and investigated for their pharmacological activity and their ability to be converted to L-dopa in the unilaterally 6-hydroxydopamine (6-OHDA)-lesioned rat, as an experimental model of Parkinson's disease.

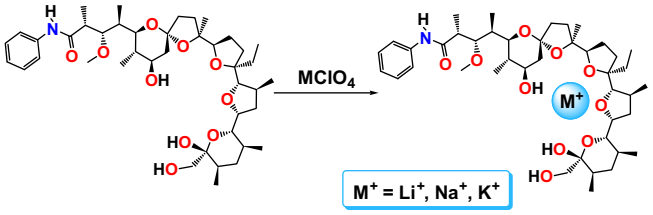


Study on the binding of chiral drug duloxetine hydrochloride to human serum albumin pp. 4043–4049
Xiangping Liu and Yingxiang Du*

Duloxetine can quench DLP–HSA complex fluorescence (pH = 7.4 (solid); pH = 8.5 (dashed line); duloxetine (○); R-isomer (■)), and this meant the specific binding site of duloxetine was located in site II of HSA.

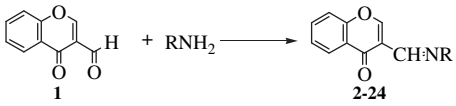


Structural characterization and antibacterial activity against clinical isolates of *Staphylococcus* of *N*-phenylamide of monensin A and its 1:1 complexes with monovalent cations pp. 4050–4057
Daniel Łowicki, Adam Huczyński, Joanna Stefańska and Bogumil Brzezinski*



3-Formylchromones: Potential antiinflammatory agents pp. 4058–4064
Khalid M. Khan*, Nida Ambreen, Uzma Rasool Mughal, Saima Jalil, Shahnaz Perveen and M. Iqbal Choudhary

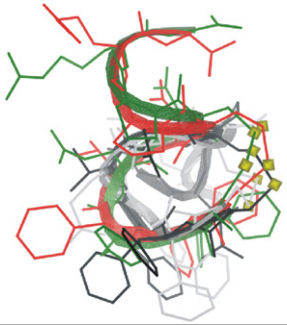
The synthesis and potential antiinflammatory activities of 3-formylchromone (**1**) and its derivatives **2**–**24** is reported here. The synthesized compounds were evaluated by using various *in vitro* and *in vivo* assay models for antiinflammatory activity.



1 **2-24**

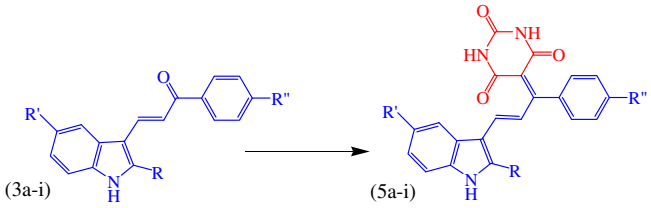
R may be any alkyl or aryl group

Influence of bulky 3,3′-diphenylalanine enantiomers replacing position 2 of AVP analogues on their conformations: NMR and molecular modeling studies pp. 4065–4073
Emilia Sikorska*, Anna Kwiatkowska, Dariusz Sobolewski, Rafał Ślusarz and Magdalena J. Ślusarz



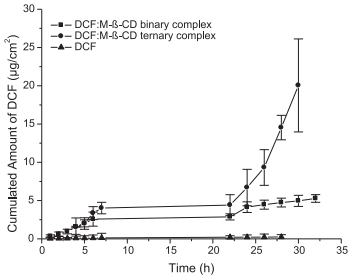
Synthesis, antioxidant and DNA cleavage activities of novel indole derivatives **pp. 4074–4078**
J.S. Biradar*, B.S. Sasidhar and R. Parveen

A new series of novel indole analogues are evaluated for their antioxidant and DNA cleavage activities.



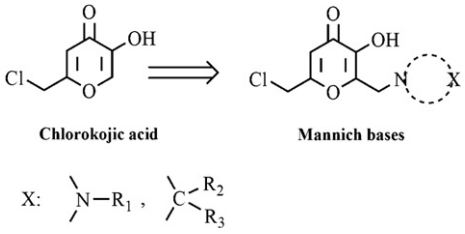
Synthesis and characterization of binary and ternary complexes of diclofenac with a methyl-β-CD and monoethanolamine and *in vitro* transdermal evaluation **pp. 4079–4088**
María Julia Mora, Marcela R. Longhi and Gladys E. Granero*

The aim of our work was to develop a ternary inclusion complex of diclofenac with methyl-β-cyclodextrin and monoethanolamine. This complex may be a promising formulation for percutaneous administration of diclofenac.



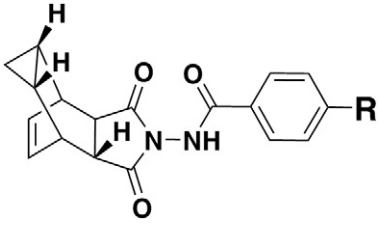
A study of cytotoxicity of novel chlorokojic acid derivatives with their antimicrobial and antiviral activities **pp. 4089–4095**
Mutlu Dilsiz Aytemir* and Berrin Özçelik

Seven novel 6-chloromethyl-3-hydroxy-2-substituted 4*H*-pyran-4-one derivatives (compounds **1**–**7**) were synthesized and tested for their antimicrobial and antiviral activities.



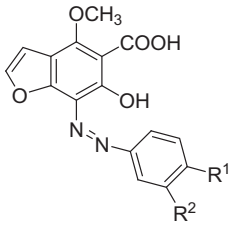
Tricyclononene carboxamide derivatives as novel anti-HIV-1 agents **pp. 4096–4103**
Ming-xin Dong, Jian Zhang, Xu-qing Peng, Hong Lu, Liu-hong Yun, Shibo Jiang** and Qiu-yun Dai*

A series of tricyclononene carboxamide derivatives based on anti-orthopoxvirus compound ST-246 were synthesized and characterized as novel anti-HIV-1 agents.



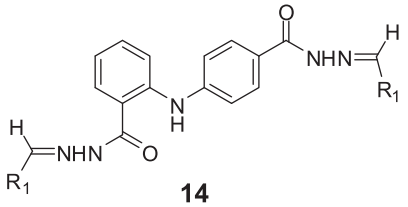
Design, synthesis and anti-ulcerogenic effect of some of furo-salicylic acid derivatives on acetic acid-induced ulcerative colitis **pp. 4104–4112**
Ghaneya S. Hassan* and Gamal A. Soliman

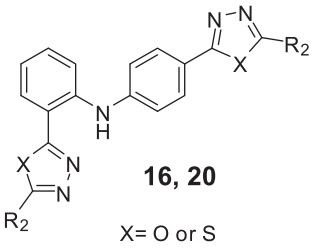
The present work describes design and synthesis of 3-aminofurosalicylic acid **4**, azo-conjugates **2a–c**, N-arylsulphonamido **5**, chlorosulphonyl **6**, aminosulphonyl **7** and N-arylaminosulphonyl derivatives **8**. All the synthesized compounds and sulphasalazine (a reference) were evaluated for their anti-ulcerogenic effect on acetic acid-induced ulcerative colitis in rats.

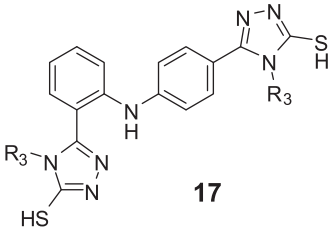


Synthesis and biological evaluation of novel 2,4′-bis substituted diphenylamines as anticancer agents and potential epidermal growth factor receptor tyrosine kinase inhibitors **pp. 4113–4121**
Sahar Mahmoud Abou-Seri*

Several analogues of 2,4′-bis substituted diphenylamines were synthesized and evaluated as EGFR tyrosine kinase inhibitors as well as for their antiprolifertive properties on human breast cancer cell lines (MCF-7).

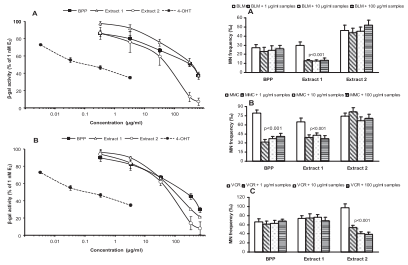






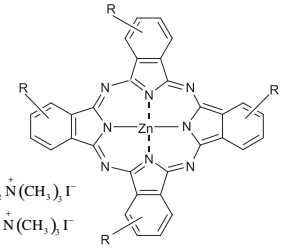
Antiestrogenic and antigenotoxic activity of bee pollen from *Cystus incanus* and *Salix alba* as evaluated by the yeast estrogen screen and the micronucleus assay in human lymphocytes **pp. 4122–4128**
Barbara Pinto*, Francesca Caciagli, Elisabetta Riccio, Daniela Reali, Ana Šarić, Tihomir Balog, Saša Likić and Roberto Scarpato

The estrogenic/antiestrogenic activity and the genotoxicity/antigenotoxicity of bee pollen of *Cystus incanus* and *Salix alba* and its derivative extracts in yeast and human cells was investigated.

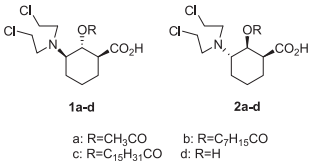


Photodynamic effects of isosteric water-soluble phthalocyanines on human nasopharynx KB carcinoma cells **pp. 4129–4139**
Julieta Marino, María C. García Vior, Lelia E. Dicelio, Leonor P. Roguin and Josefina Awruch*

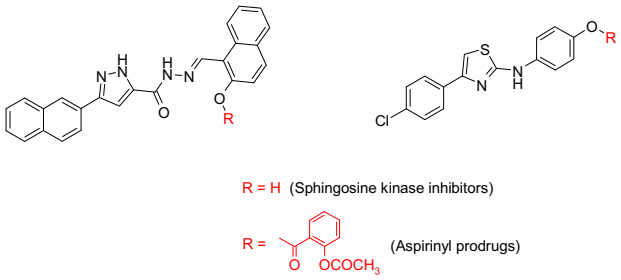
β-Sulfur-linked cationic aliphatic phthalocyanine **13** shows a $\Phi_{\Delta} = 0.58$ and $\lambda_{max} = 686$ nm, no dark cytotoxicity and triggers lysosomal-induced apoptosis after irradiation leading to 90% cell death.



Synthesis and biological evaluation of cyclic nitrogen mustards based on carnitine framework pp. 4140–4148
Simon Leiris, Marc Lucas, Arnaud Dupuy d'Angeac and Alain Morère*

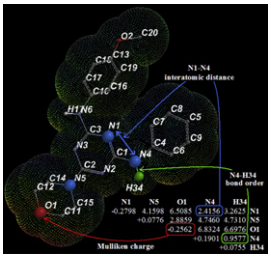


Synthesis and bioactivity of sphingosine kinase inhibitors and their novel aspirinyl conjugated analogs pp. 4149–4156
Arun K. Sharma*, Ugir Hossain Sk, Melissa A. Gimbor, Jeremy A. Hengst, Xujun Wang, Jong Yun and Shantu Amin

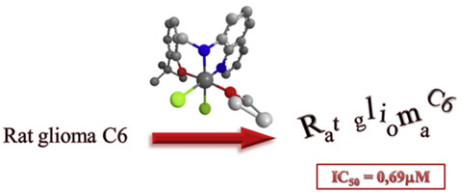


Pharmacophore identification and bioactivity prediction for triaminotriazine derivatives by electron conformational-genetic algorithm QSAR method pp. 4157–4168
Emin Sarıpınar*, Nazmiye Geçen, Kader Sahin and Ersin Yanmaz

The electron conformational–genetic algorithm (EC–GA) method has been employed to reveal the pharmacophore (Pha) and to predict anticancer activity, studying in the class of triaminotriazine derivatives.

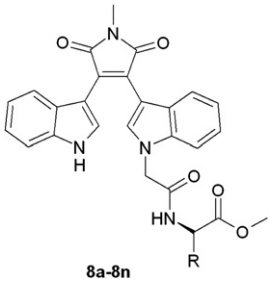


Synthesis and cytotoxic activities of group 3 metal complexes having monoanionic tridentate ligands pp. 4169–4174
Carmela Saturnino*, Mariagrazia Napoli, Gino Paolucci, Marco Bortoluzzi, Ada Popolo, Aldo Pinto and Pasquale Longo



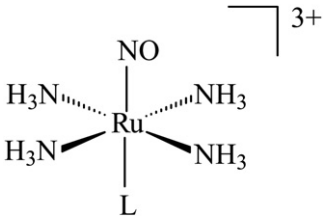
Synthesis of *N*-methyl-bisindolylmaleimide amino acid methyl ester conjugates and cytotoxicity study **pp. 4175–4179**
Ke Wang and Zhan-Zhu Liu*

A novel series of *N*-methylbisindolylmaleimides derivatives bearing 2-acetamino acid moieties were synthesized. The most potent compound **8d** displayed cytotoxicity against six human tumor cell lines in the micromolar range.

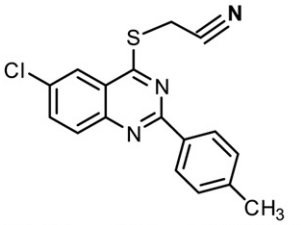


Antileishmanial activity of ruthenium(II)tetraammine nitrosyl complexes **pp. 4180–4187**
José Clayston Melo Pereira, Vanessa Carregaro, Diego Luís Costa, João Santana da Silva, Fernando Q. Cunha and Douglas Wagner Franco*

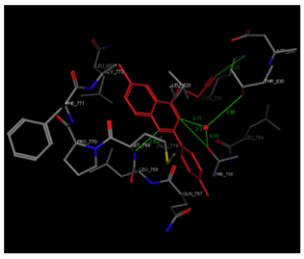
Complexes *trans*-[Ru(NO)(NH_3)$_4$L](X)$_3$ where X = BF_4^-, PF_6^- or Cl^- and L = imN ($C_3H_4N_2$), 4-pic (C_6H_7N), pz ($C_4H_4N_2$), py (C_5H_5N), P(OEt)$_3$ ($C_6H_{15}O_3P$), L-hist ($C_6H_9N_3O_2$), isn ($C_6H_5N_2O$), SO_3^{-2}, nic ($C_6H_6N_2O$), imC ($C_3H_4N_2$) and [Ru(NO) Hedta)] proved to exhibit *in vitro* antileishmanial effect. The *trans*-[Ru(NO)(NH_3)$_4$imN](BF$_4$)$_3$ compound was found to exhibit a significant *in vivo* effect against *Leishmania major*.



Design, synthesis and biological evaluation of novel quinazoline derivatives as potential antitumor agents: Molecular docking study **pp. 4188–4198**
Adel S. El-Azab*, Mohamed A. Al-Omar, Alaa A.-M. Abdel-Aziz, Naglaa I. Abdel-Aziz, Magda A.-A. El-Sayed, Abdulaziz M. Aleisa, Mohamed M. Sayed-Ahmed and Sami G. Abdel-Hamide**

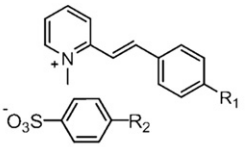


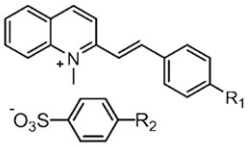
18; IC_{50} = 3.35 μg/ml (MCF-7)



Synthesis, structure and *in vitro* antibacterial activities of new hybrid disinfectants quaternary ammonium compounds: Pyridinium and quinolinium stilbene benzenesulfonates **pp. 4199–4208**
Kullapa Chanawanno, Suchada Chantrapromma*, Theerasak Anantapong, Akkharawit Kanjana-Opas and Hoong-Kun Fun

The new pyridinium and quinolinium stilbene benzenesulfonates have been synthesized and characterized. All compounds were evaluated for their antibacterial activities against the tested Gram-positive and Gram-negative bacteria using colorimetric assay.

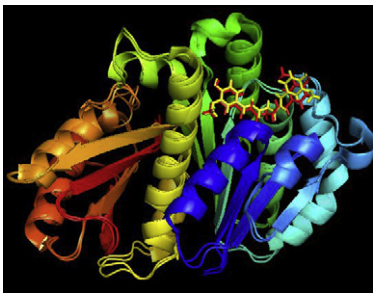




1; R_1=N(CH_3)$_2$, R_2 = CH_3
2; R_1=N(CH_3)$_2$, R_2 = OCH_3
3; R_1=N(CH_3)$_2$, R_2 = Br
4; R_1=N(CH_3)$_2$, R_2 = Cl
5; R_1=N(CH_3)$_2$, R_2 = NH_2
6; R_1=OEt, R_2 = CH_3
7; R_1=OEt, R_2 = OCH_3
8; R_1=OEt, R_2 = Br
9; R_1=OEt, R_2 = Cl
10; R_1=OEt, R_2 = NH_2
11; R_1=N(CH_3)$_2$, R_2 = CH_3
12; R_1=N(CH_3)$_2$, R_2 = OCH_3
13; R_1=N(CH_3)$_2$, R_2 = Br
14; R_1=N(CH_3)$_2$, R_2 = Cl
15; R_1=N(CH_3)$_2$, R_2 = NH_2
16; R_1=OEt, R_2 = CH_3
17; R_1=OEt, R_2 = OCH_3
18; R_1=OEt, R_2 = Br
19; R_1=OEt, R_2 = Cl
20; R_1=OEt, R_2 = NH_2

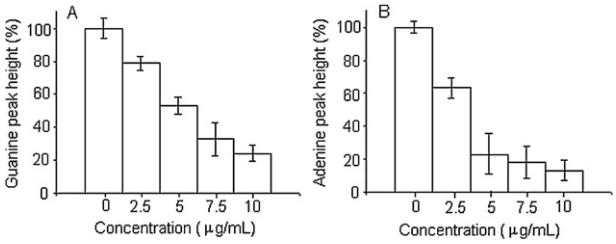
Probing the binding site of curcumin in *Escherichia coli* and *Bacillus subtilis* FtsZ – A structural insight to unveil antibacterial activity of curcumin **pp. 4209–4214**
Simranjeet Kaur, Niraj H. Modi, Dulal Panda and Nilanjan Roy*

We propose the binding conformation of curcumin in *E. coli* and *B. subtilis* FtsZ and suggest plausible critical interactions with the active site residues.



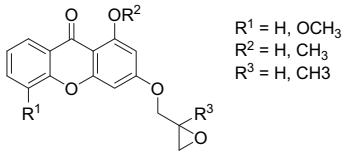
Palladium(II) and platinum(II) complexes of a symmetric Schiff base derived from 2,6,diformyl-4-methylphenol with N-aminopyrimidine: Synthesis, characterization and detection of DNA interaction by voltammetry **pp. 4215–4220**
Mehmet Sönmez*, Metin Çelebi, Yavuz Yardım and Zühre Sentürk

New Pd(II) and Pt(II) complexes of a symmetric Schiff base containing pyrimidine rings have been synthesized and characterized. All the compounds were tested for their DNA interaction ability with the fish sperm DNA.
The effect of Pd(II) complex upon the DP voltammetric response of guanine (A) and adenine (B) after interaction of solution-phase DNA.

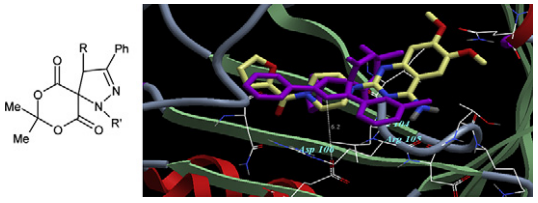


Synthesis and pharmacological evaluation of new methyloxiranylmethoxyxanthone analogues **pp. 4221–4228**
Sangwook Woo, Da-hye Kang, Jung Min Nam, Chong Soon Lee, Eun-Mi Ha, Eung-Seok Lee, Youngjoo Kwon** and Younghwa Na*

In order to develop potential anti-cancer agents that act on topoisomerase II and DNA, we have synthesized 12 new xanthone derivatives.

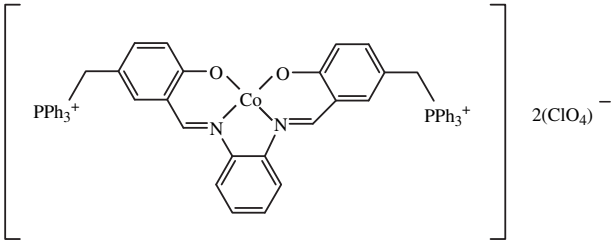


Regioselective synthesis and molecular modeling study of vasorelaxant active 7,9-dioxa-1,2-diaza-spiro[4.5]dec-2-ene-6,10-diones **pp. 4229–4238**
Adel S. Girgis*, Nasser S.M. Ismail, Hanaa Farag, Wafaa I. El-Eraky, Dalia O. Saleh, Srinivasa R. Tala and Alan R. Katritzky



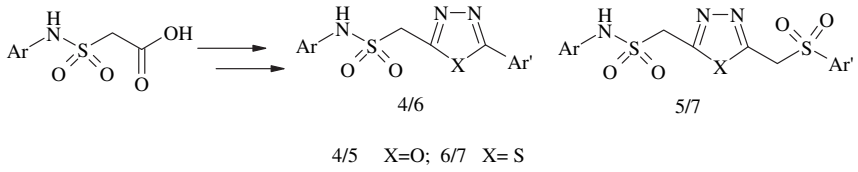
DNA binding and DNA cleavage studies of a water soluble cobalt(II) complex containing dinitrogen Schiff base ligand: The effect of metal on the mode of binding **pp. 4239–4245**
Nahid Shahabadi*, Soheila Kashanian and Farivash Darabi

Binding interaction of water soluble cobalt(II) complex containing Schiff base ligand, SF, with calf thymus DNA (CT-DNA) has been investigated and the result were compared with the SF.



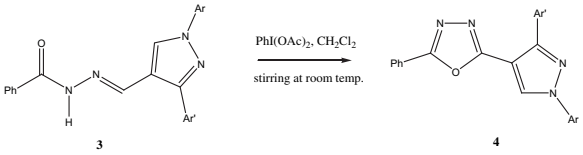
Synthesis and bioassay of aminosulfonyl-1,3,4-oxadiazoles and their interconversion to 1,3,4-thiadiazoles **pp. 4246–4251**
V. Padmavathi*, S. Nagi Reddy, G. Dinneswara Reddy and A. Padmaja

A new class of 1,3,4- oxadiazoles are prepared by treating aminosulfonylacetic acids with different carboxylic acid hydrazides in the presence of phosphorus oxychloride. Interconversion of oxadiazoles to thiadiazoles is carried out with thiourea intetrahydrofuran. Preliminary antimicrobial activity is tested for the synthesized 1,3,4- oxadiazoles and 1,3,4- thiadiazoles.

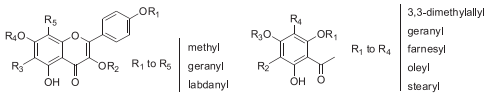


Hypervalent iodine(III) mediated synthesis of novel unsymmetrical 2,5-disubstituted 1,3,4-oxadiazoles as antibacterial and antifungal agents **pp. 4252–4257**
Om Prakash*, Manoj Kumar, Rajesh Kumar, Chetan Sharma and K.R. Aneja

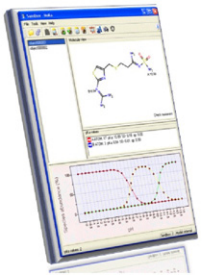
A series of novel 2,5-disubstituted 1,3,4-oxadiazoles **4** have been conveniently synthesized by oxidative cyclization of pyrazolylaldehyde N-acylhydrazones **3** promoted by iodobenzene diacetate under mild conditions (11 examples, up to 92% isolated yields).



Prenylflavonoids and prenyl/alkyl-phloroacetophenones: Synthesis and antitumour biological evaluation **pp. 4258–4269**
P. Basabe*, M. de Román, I.S. Marcos, D. Diez, A. Blanco, O. Bodero, F. Mollinedo, B.G. Sierra and J.G. Urones

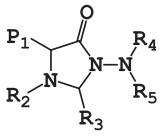


Extending pK_a prediction accuracy: High-throughput pK_a measurements to understand pK_a modulation of new chemical series pp. 4270–4279
Francesca Milletti*, Loriano Storchi, Laura Goracci, Stefanie Bendels, Bjoern Wagner, Manfred Kansy and Gabriele Cruciani



Inhibitors of human neutrophil elastase based on a highly functionalized *N*-amino-4-imidazolidinone scaffold pp. 4280–4287
Guijia He, Dengfeng Dou, Liuqing Wei, Kevin R. Alliston and William C. Groutas*

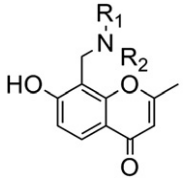
A series of derivatives based on the *N*-amino-4-imidazolidinone scaffold (I) was synthesized and shown to inhibit human neutrophil elastase.



(I)

Synthesis and anticancer activity of chromone-based analogs of lavendustin A pp. 4288–4292
Dong Hyuk Nam, Ki Yong Lee, Chang Sang Moon and Yong Sup Lee*

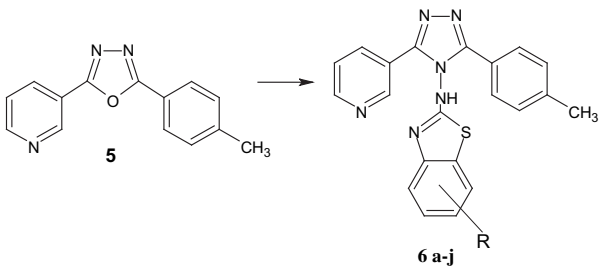
Chromone-based lavendustin A analogs were synthesized as a simplified hybrid of hormothamnione and lavendustin



4a-4k

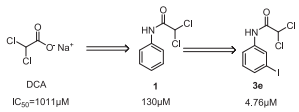
Pharmacological evaluation and characterizations of newly synthesized 1,2,4-triazoles pp. 4293–4299
Navin B. Patel*, Imran H. Khan and Smita D. Rajani

3-(3-Pyridyl)-5-(4-methylphenyl)-4-(*N*-substituted-1,3-benzothiazol-2-amino)-4*H*-1,2,4-triazole **6a–j** were synthesized and their antitubercular activity against $H_{37}Rv$ and antimicrobial activities have been tested.



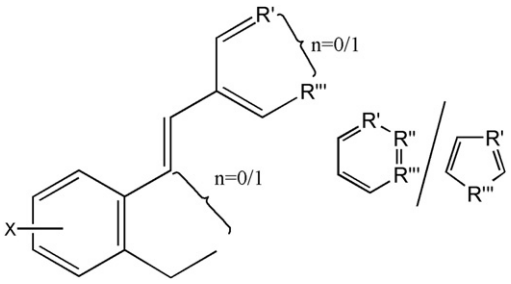
Novel N-phenyl dichloroacetamide derivatives as anticancer reagents: Design, synthesis and biological evaluation **pp. 4300–4306**
Yongchong Yang, Peihua Shang, Changmei Cheng*, Dongchun Wang, Ping Yang, Feng Zhang, Tianwen Li, Aijun Lu and Yufen Zhao

N-phenyl-2,2-dichloroacetamide analogues has higher cytotoxic activity and N-(3-iodophenyl)-2,2-dichloroacetamide (**3e**) is an optimized lead compound.

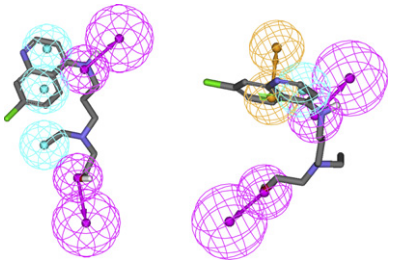


Exploring benzcyclo derivatives as potent aromatase inhibitors using ligand-based modeling studies **pp. 4307–4315**
Shuchi Nagar and Achintya Saha*

QSAR modeling and pharmacophore mapping have been explored to investigate the structural pattern of benzcyclo hexane/pentane derivative for inhibition of aromatase (CYP19) enzyme.

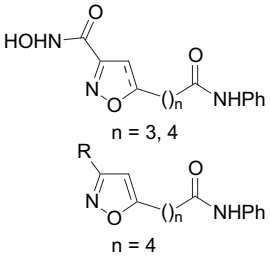


Discovery of novel CDK1 inhibitors by combining pharmacophore modeling, QSAR analysis and *in silico* screening followed by *in vitro* bioassay **pp. 4316–4330**
Mahmoud A. Al-Sha'er and Mutasem O. Taha*



Design and synthesis of novel isoxazole-based HDAC inhibitors **pp. 4331–4338**
Paola Conti*, Lucia Tamborini, Andrea Pinto, Laura Sola, Roberta Ettari, Ciro Mercurio and Carlo De Micheli

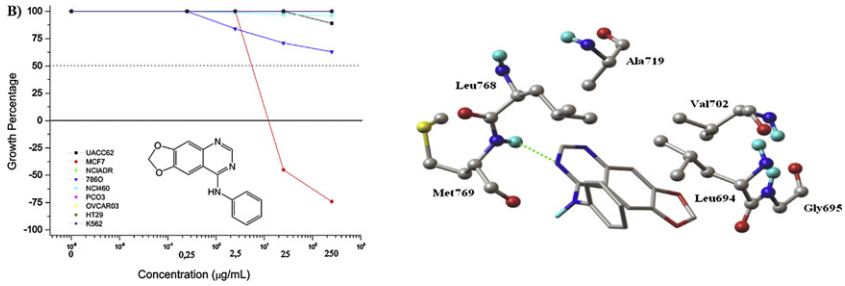
New isoxazole-based histone deacetylase inhibitors structurally related to SAHA were designed and synthesized to check the participation of the isoxazole moiety in the Zn^{2+}coordination.



SHORT COMMUNICATIONS

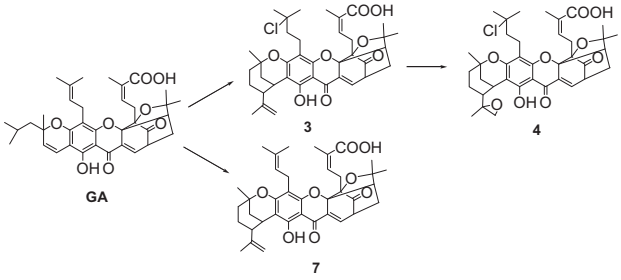
New substituted 4-arylaminoquinazolines as potent inhibitors of breast tumor cell lines: *In vitro* and docking experiments pp. 4339–4342
André N. de Oliveira, Cleverson C. Bocca, João E. Carvalho, Ana Lúcia G. Ruiz, Thiago P. Silva, Roberto Rittner and Nelci F. Hoehr*

The 4-arylaminoqinazolines prepared and tested in this work provide the confirmation of the many theoretical studies and may serve as basis for the design of the novel inhibitors against breast cancer.



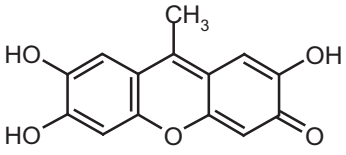
Studies on chemical modification and biology of a natural product, gambogic acid (II): Synthesis and bioevaluation of gambogellic acid and its derivatives from gambogic acid as antitumor agents pp. 4343–4353
Jinxin Wang, Junhai Ma, Qidong You*, Li Zhao, Fan Wang, Chong Li and Qinglong Guo*

Thirteen gambogellic acid analogues from gambogic acid were synthesized. We also performed their SAR studies. A promising derivative **4** as a potent apoptosis inducer in BGC-823 cells was characterized.



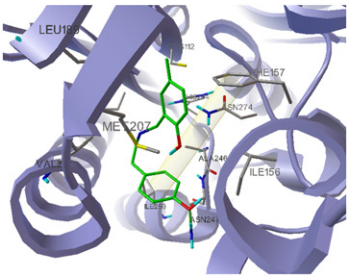
Selectivity determinants of inhibitor binding to the tumour marker human aldose reductase-like protein (AKR1B10) discovered from molecular docking and database screening pp. 4354–4357
Hai-Tao Zhao, Midori Soda, Satoshi Endo, Akira Hara and Ossama El-Kabbani*

A novel AKR1B10 inhibitor, 9-methyl-2,3,7-trihydroxy-6-fluorone (MTF), discovered from molecular docking and database screening, revealed non-conserved residues involved in the binding of inhibitor to AKR1B10 and AKR1B1.



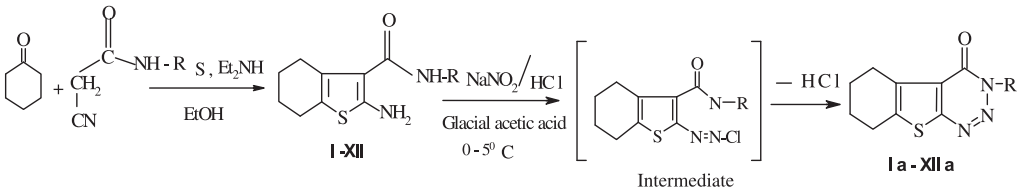
Design and synthesis of potent inhibitors of β-ketoacyl-acyl carrier protein synthase III (FabH) as potential antibacterial agents pp. 4358–4364
Lei Shi, Rui-Qin Fang, Zhen-Wei Zhu, Ying Yang, Kui Cheng, Wei-Qing Zhong* and Hai-Liang Zhu*

Twenty new Schiff bases were synthesized as potent inhibitors of FabH. (*E*)-4-fluoro-2-((4-hydroxyphenethylimino)methyl)phenol (**10**) showed the most potent antibacterial activity and exhibited the most potent *E. coli* FabH inhibitory activity.

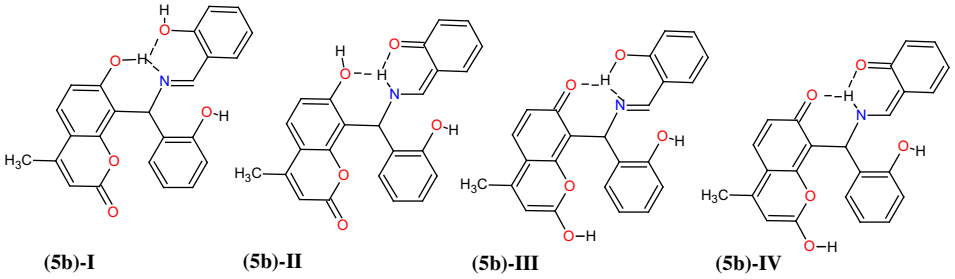


Synthesis of some 3-substituted amino-4,5-tetramethylene thieno[2,3-*d*][1,2,3]-triazin-4(3*H*)-ones as potential antimicrobial agents pp. 4365–4369
Janardhanan Saravanan*, Shamanna Mohan and Jay Jyoti Roy

The required title compounds were synthesized by adapting Gewald & diazotization reaction and the compounds were screened for antimicrobial activity. Some of the compounds exhibited considerable activity.

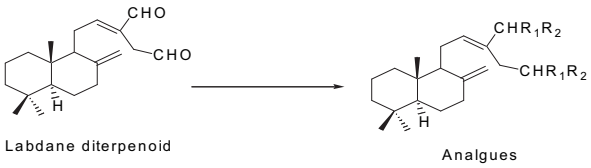


Pharmacophores modeling in terms of prediction of theoretical physico-chemical properties and verification by experimental correlations of novel coumarin derivatives produced via Betti's protocol pp. 4370–4378
Ali Parvez*, Jyotsna Meshram, Vandana Tiwari, Javed Sheik, Rajendra Dongre, Moulay H. Youssoufi and Taibi Ben Hadda



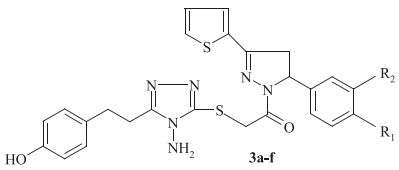
A bioactive labdane diterpenoid from *Curcuma amada* and its semisynthetic analogues as antitubercular agents pp. 4379–4382
Sailendra Singh, Jonnala Kotesh Kumar, Dharmendra Saikia, Karuna Shanker, Jay Prakash Thakur, Arvind Singh Negi* and Suchitra Banerjee**

An antitubercular labdane diterpene dialdehyde (**1**) was isolated from *C. amada*. Two of the semisynthetic analogues possessed good antitubercular activity



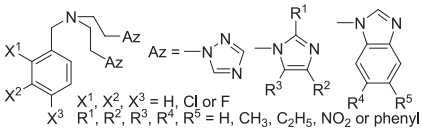
New pyrazoline derivatives and their antidepressant activity pp. 4383–4387
Zafer Asım Kaplancıklı*, Ahmet Özdemir, Gülhan Turan-Zitouni, Mehlika Dilek Altıntop and Özgür Devrim Can

The study supports the antidepressant-like activities of various pyrazoline and/or triazole derivatives and suggests a possible serotonin related mechanism of action for the tested compounds.

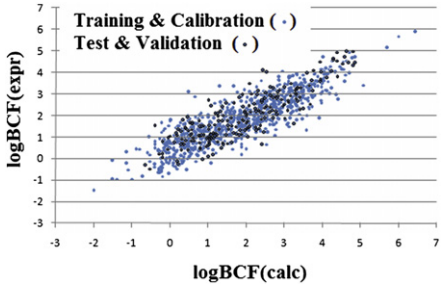


Synthesis and biological activities of novel amine-derived bis-azoles as potential antibacterial and antifungal agents pp. 4388–4398
Bo Fang, Cheng-He Zhou* and Xian-Cai Rao

A series of novel amine-derived bis-azoles were synthesized and evaluated for antibacterial and antifungal activities. Some synthesized compounds exhibited better antibacterial and antifungal efficacy than clinical drugs Fluconazole, Norfloxacin and Chloramphenicol.

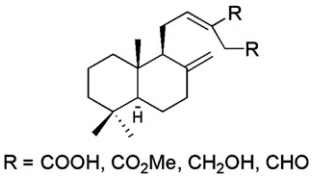


A new bioconcentration factor model based on SMILES and indices of presence of atoms pp. 4399–4402
A.P. Toropova, A.A. Toropov*, A. Lombardo, A. Roncaglioni, E. Benfenati and G. Gini



Synthesis and biological evaluation of (+)-labdadienedial, derivatives and precursors from (+)-sclareolide pp. 4403–4408
Miguel A. González*, Juan Mancebo-Aracil, Veronica Tangarife-Castaño, Lee Agudelo-Goméz, Bibiana Zapata, Ana Mesa-Arango and Liliana Betancur-Galvis**

Labdadienedial and a series of C15,C16-functionalized derivatives were synthesized from commercial (+)-sclareolide and evaluated for their cytotoxic, antimycotic and antiviral activities. Their precursors were similarly evaluated.



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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