



European Journal of Medicinal Chemistry Vol 45, No 6, 2010

Contents

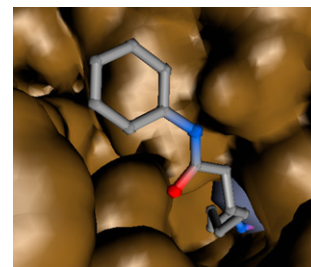
INVITED REVIEW

Inside HDAC with HDAC inhibitors

pp. 2095–2116

Philippe Bertrand

This review focuses on the synthetic and biological results obtained by several research groups with HDAC inhibitors designed from structural analyses of the proteins active sites and mechanistic proposals.



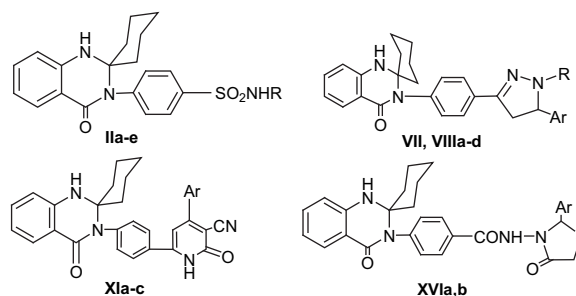
ORIGINAL ARTICLES

Synthesis, biological evaluation and molecular docking of novel series of spiro [(2H,3H) quinazoline-2,1'-cyclohexan]-4(1H)-one derivatives as anti-inflammatory and analgesic agents

pp. 2117–2131

K.M. Amin, M.M. Kamel, M.M. Anwar*, M. Khedr and Y.M. Syam

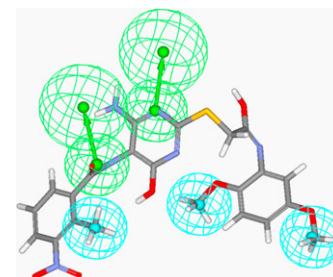
Three series of Spiro [(2H, 3H) quinazoline-2,1'-cyclohexan]-4(1H)-one derivatives have been synthesized. Some of the derivatives were evaluated as anti-inflammatory and analgesic agents using indomethacin and tramadol as reference drugs. The biological data were compared to the molecular docking study.


3D QSAR pharmacophore based virtual screening and molecular docking for identification of potential HSP90 inhibitors

pp. 2132–2140

Sugunadevi Sakthiah, Sundarapandian Thangapandian, Shalini John, Yong Jung Kwon and Keun Woo Lee*

Pharmacophore model was generated using HYPOGEN algorithm in DS v2.1. The well validated Hypo1 was used to screen large databases. Finally, 36 compounds were selected as HSP90 inhibitors.

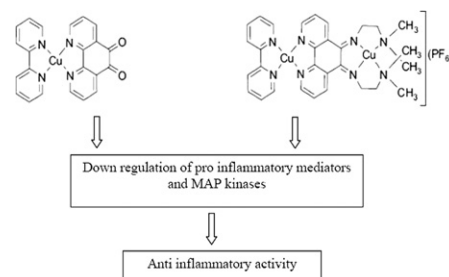


2,2'-Bipyridyl based copper complexes down regulate expression of pro-inflammatory cytokines and suppress MAPKs in mitogen induced Peripheral blood mononuclear cells

pp. 2141–2146

K.R. Rupesh, A. Moushumi Priya, B. Sundarakrishnan, R. Venkatesan, B.S. Lakshmi and S. Jayachandran*

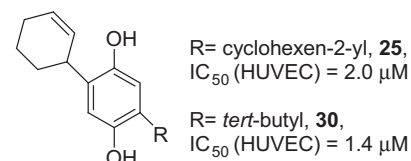
2,2-bipyridyl complexes *I* and *Ia* down regulated pro-inflammatory cytokines and mediating enzymes through inhibition of MAP kinases suggesting that the complexes may be potent anti-inflammatory compounds.

**Synthesis and inhibitory evaluation of cyclohexen-2-yl- and cyclohexyl-substituted phenols and quinones to endothelial cell and cancer cells**

pp. 2147–2153

Xin Liu, Yingyong Ou, Shaopeng Chen, Xin Lu, Hao Cheng, Xian Jia, Decai Wang and Guo-Chun Zhou*

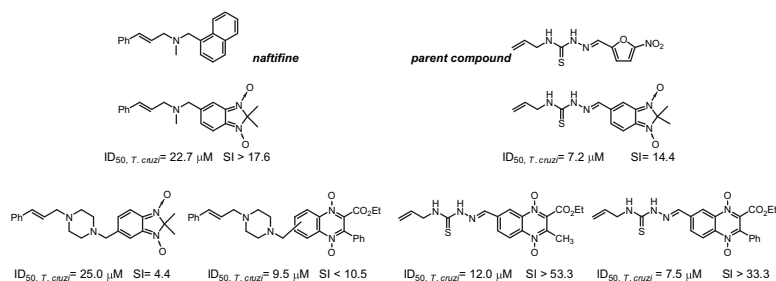
The inhibitory activity and selectivity of cyclohexen-2-yl- and cyclohexyl-substituted phenols and quinones were significantly affected by the sizes and occupied positions of substitutes

**Naftifine-analogues as anti-*Trypanosoma cruzi* agents**

pp. 2154–2164

Alejandra Gerpe, Luc a Boiani, Paola Hern andez, Maximiliano Sortino, Susana Zacchino, Mercedes Gonz alez* and Hugo Cerecetto*

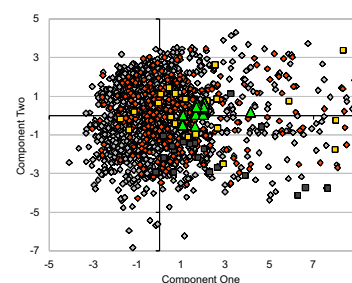
New containing bioactive-heterocycles analogues of naftifine have been synthesized and evaluated for their *in vitro* anti-*Trypanosoma cruzi* activities.

**Assessing the drug-likeness of lamellarins, a marine-derived natural product class with diverse oncological activities**

pp. 2165–2172

Montakarn Chittchang*, M. Paul Gleeson, Poonsakdi Ploypradith and Somsak Ruchirawat

Lamellarins are a class of natural products with diverse biological activities. However, they have not been assessed for their drug-likeness essential for their further development into drug candidates. In this study, experimental logP and other physicochemical properties of lamellarins were studied in conjunction with principal components analysis (PCA)

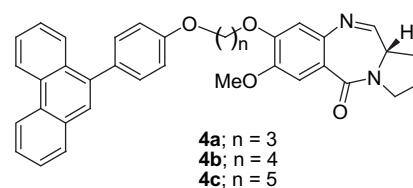


Synthesis and potential cytotoxic activity of new phenanthrylphenol-pyrrolobenzodiazepines

pp. 2173–2181

Ahmed Kamal*, Kokkonda Sreekanth, P. Praveen Kumar, Nagula Shankaraiah, G. Balakishan, M. Janaki Ramaiah, S.N.C.V.L. Pushpavalli, Paramita Ray and Manika Pal Bhadra*

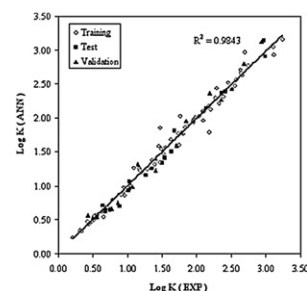
New class of phenanthrylphenol-pyrrolobenzodiazepine (PP-PBD) conjugates has been synthesized and evaluated the cytotoxic effect of these compounds on MCF-7 cell proliferation.

**Prediction of air to liver partition coefficient for volatile organic compounds using QSAR approaches**

pp. 2182–2190

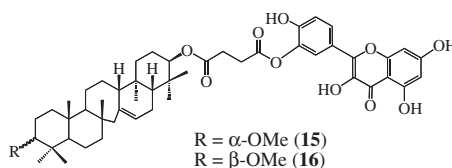
Zahra Dashtbozorgi and Hassan Golmohammadi*

Plot of calculated air to liver partition coefficient against experimental values.

**Hybrids of 3 α -methoxyserrat-14-en-21 β -ol (PJ-1) and 3 β -methoxyserrat-14-en-21 β -ol (PJ-2) and various anti-oxidants as cancer chemopreventive agents**

pp. 2191–2197

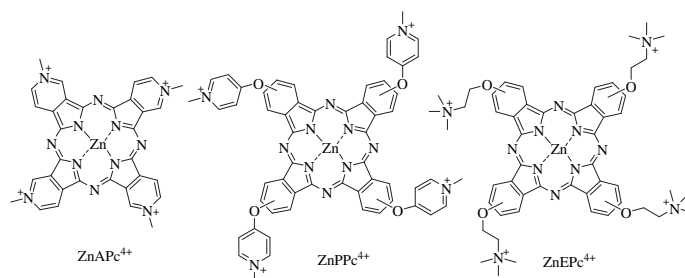
Hiroko Tsujii, Takeshi Yamada, Tetsuya Kajimoto, Reiko Tanaka*, Harukuni Tokuda, Junya Hasegawa, Yoshio Hamashima and Manabu Node

**Photodynamic inactivation of *Escherichia coli* and *Streptococcus mitis* by cationic zinc(II) phthalocyanines in media with blood derivatives**

pp. 2198–2205

Mariana B. Spesia, Marisa Rovera and Edgardo N. Durantini*

The paper reports details about the photodynamic inactivation of bacteria by tetracationic phthalocyanines with different molecular structures in media containing blood derivatives.

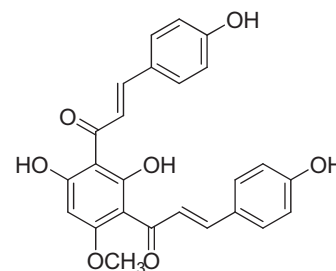


Synthesis, cytotoxicity, anti-oxidative and anti-inflammatory activity of chalcones and influence of A-ring modifications on the pharmacological effect

pp. 2206–2213

Susanne Vogel, Matej Barbic, Guido J rgenliemk and J rg Heilmann*

Several new chalcones based on the natural compounds helichrysetin and xanthohumol were synthesized and characterized concerning their anti-inflammatory, cytotoxic and anti-oxidative activity.

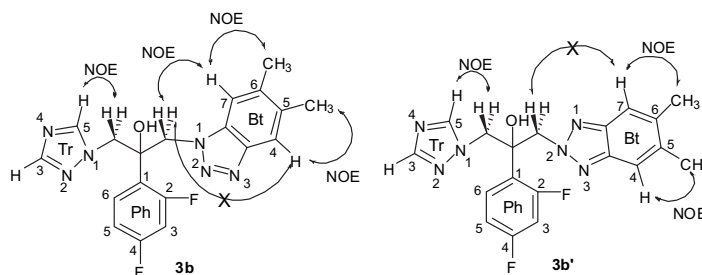


Design, synthesis and determination of antifungal activity of 5(6)-substituted benzotriazoles

pp. 2214–2222

Pallav D. Patel, Maulik R. Patel, Bela Kocsis, Erika Kocsis, Steven M. Graham, Andrew R. Warren, Stacia M. Nicholson, Blase Billack, Frank R. Fronczek and Tanaji T. Talele*

A series of 5(6)-(un)substituted benzotriazole analogs were identified as broad spectrum antifungal agents.

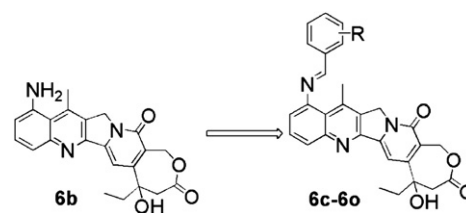


Synthesis and evaluation of 9-benzylideneamino derivatives of homocamptothecin as potent inhibitors of DNA topoisomerase I

pp. 2223–2228

Wei Guo, Zhenyuan Miao**, Chunquan Sheng, Jianzhong Yao, Hao Feng, Wannian Zhang*, Lingjian Zhu, Wenfeng Liu, Pengfei Cheng, Jing Zhang, Xiaoying Che, Wenya Wang, Chuan Luo and Yulan Xu

A series of novel 7-methyl-9-benzylideneamino derivatives of homocamptothecin are synthesized. Compounds **6c–o** showed potent cytotoxic activity against A549, MDA-MB-435 and LOVO cell lines.

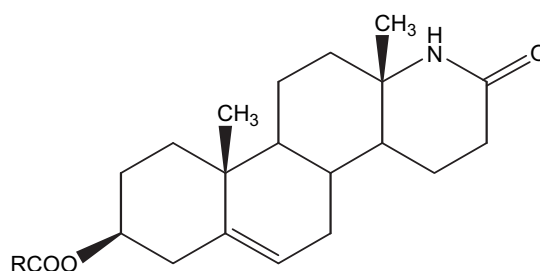


Synthesis, antiproliferative, acute toxicity and assessment of antiandrogenic activities of some newly synthesized steroidal lactams

pp. 2229–2236

Neelima Dhingra, T.R. Bhardwaj, Neeraj Mehta, Tapas Mukhopadhyay, Ashok Kumar and Manoj Kumar*

A series of novel 17-oxo-17a-aza- -homo-5-androsten-3 -yl esters have been synthesized and evaluated for their *in vitro* antiproliferative activity, acute toxicity and effect on serum androgen level.

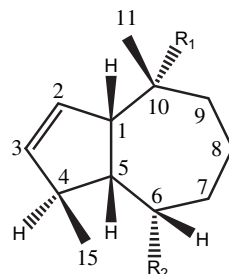


Guaiane sesquiterpenes from seaweed *Ulva fasciata* Delile and their antibacterial properties

pp. 2237–2244

Kajal Chakraborty*, A.P. Lipton, R. Paulraj and Rekha D. Chakraborty

Two novel guaiane sesquiterpenes guai-2-en-10 α -ol (**1**) and guai-2-en-10 α -methanol (**2**) were purified as antibacterial constituents of *Ulva fasciata*. The acetylated derivative of **2** had higher antibacterial activity than the parent compound.



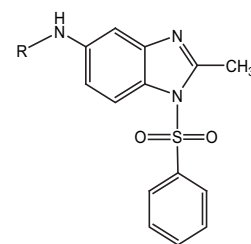
- 1** R₁ = OH, R₂ = CH(CH₃)₂
2 R₁ = CH₂OH, R₂ = CH₂CH₃
3 R₁ = CH₂O(C=O)CH₃, R₂ = CH₂CH₃

Synthesis and pharmacological evaluation of novel 5-substituted-1-(phenylsulfonyl)-2-methylbenzimidazole derivatives as anti-inflammatory and analgesic agents

pp. 2245–2249

Monika Gaba*, Dhandeep Singh, Sarbjot Singh, Vikas Sharma and Punam Gaba

In the present study Novel 5-Substituted -1- (phenylsulphonyl)-2-methylbenzimidazole Derivatives, we have synthesized and screened for their anti-inflammatory as well as analgesic activity.



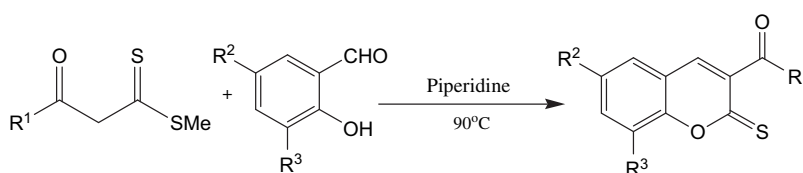
R=Substituted alkyl/aryl

Novel 3-alkanoyl/aroyl/heteroaroyl-2H-chromene-2-thiones: Synthesis and evaluation of their antioxidant activities

pp. 2250–2257

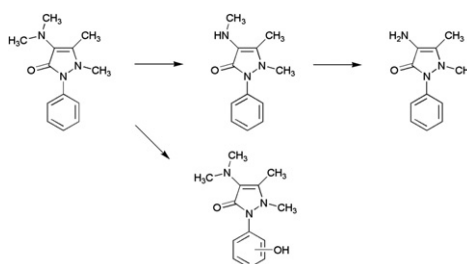
Okram Mukherjee Singh*, Nepram Sushuma Devi, Dhanaraj Singh Thokchom and Gurumayum Jitendra Sharma

A facile synthesis of 3-alkanoyl/aroyl/heteroaroyl- 2H-chromene-2-thiones has been developed by the condensation of easily accessible β -oxodithioesters and salicylaldehyde/substituted 2-hydroxybenzaldehydes under solvent-free conditions. The newly synthesized compounds exhibited profound antioxidant activities.

**Scavenging activity of aminoantipyridines against hydroxyl radical**

pp. 2258–2264

Pedro M.P. Santos, Alexandra M.M. Antunes, João Noronha, Eduarda Fernandes and Abel J.S.C. Vieira*

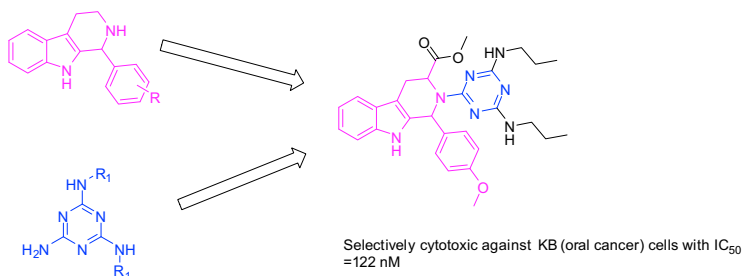


Synthesis and cytotoxicity evaluation of (tetrahydro- β -carboline)-1,3,5-triazine hybrids as anticancer agents

pp. 2265–2276

Ravi Kumar, Leena Gupta, Pooja Pal, Shahnawaz Khan, Neetu Singh, Sanjay Babu Katiyar, Sanjeev Meena, Jayanta Sarkar, Sudhir Sinha, Jitendra Kumar Kanaujiya, Savita Lochab, Arun Kumar Trivedi and Prem M.S. Chauhan*

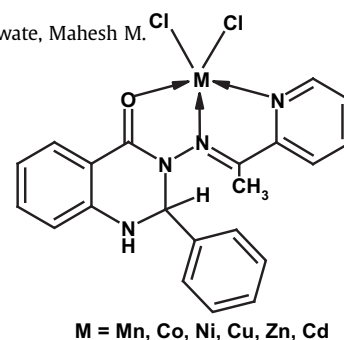
A series of tetrahydro- β -carbolines and 1,3,5-triazine hybrids have been synthesized and evaluated for their cytotoxicity against a panel of eight human cancer cell lines and normal human fibroblasts (NIH3T3).

**Transition metal complexes of 3-aryl-2-substituted 1,2-dihydroquinazolin-4(3H)-one derivatives: New class of analgesic and anti-inflammatory agents**

pp. 2277–2282

Rekha S. Hoonur, Basavaraj R. Patil, Dayananda S. Badiger, Ramesh S. Vadavi, Kalagouda B. Gudasi*, Prasad R. Dandawate, Mahesh M. Ghaisas, Subhash B. Padhye and Munirathinam Nethaji

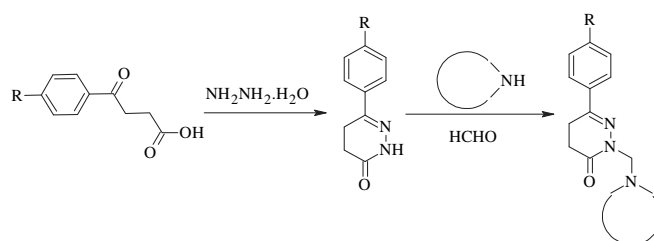
Five-coordinate, neutral transition metal complexes of pyridine-2-ethyl-(3-carboxylideneamino)-3-(2-phenyl)-1,2-dihydroquinazolin-4(3H)-one (**L**) were synthesized, characterized and screened for analgesic and anti-inflammatory activity wherein the copper complex showed most potent activity.

**Synthesis, characterization and antihypertensive activity of pyridazinone derivatives**

pp. 2283–2290

Anees A. Siddiqui*, Ravinesh Mishra and Mohammad Shaharyar

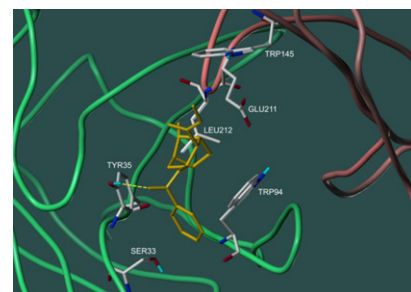
6-(Substituted-phenyl)-2-(substitutedmethyl)-4,5-dihydropyridazin-3(2H)-one derivatives were synthesized by reacting 6-substituted-phenyl-4,5-dihydropyridazine-3(2H)-one with different heterocyclic base under Mannich reaction conditions and evaluated for antihypertensive activity in rats by non-invasive Tail cuff method.

**A molecular model for cocaine binding by the immunotherapeutic human/mouse chimeric monoclonal antibody 2E2**

pp. 2291–2298

Michael Lape, Stefan Paula and William J. Ball Jr*

After determining its amino acid sequence, a homology model of a human/mouse anti-cocaine monoclonal antibody was developed. Subsequent computational docking studies provided a molecular-level characterization of protein/ligand interactions responsible for the antibody's cocaine affinity and specificity and demonstrate its potential as an immunotherapeutic agent.

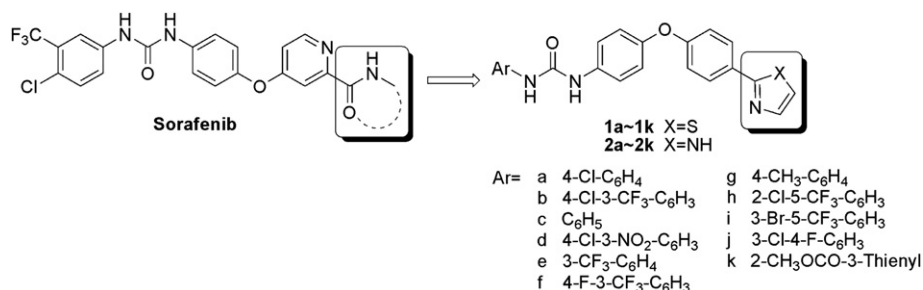


Design, synthesis, and *in vitro* antitumor evaluation of novel diaryl ureas derivatives

pp. 2299–2306

Min Sun, Xiaoqing Wu, Junqing Chen, Jin Cai, Meng Cao and Min Ji*

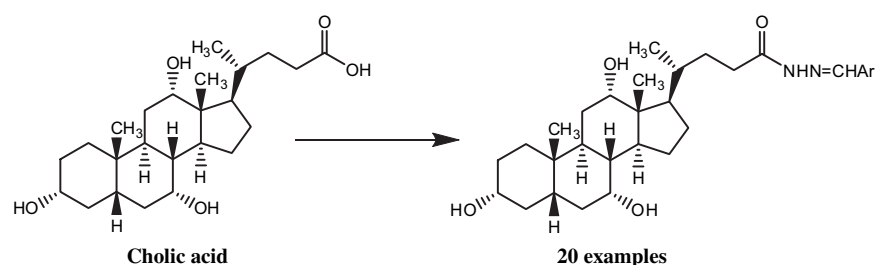
Two series of diaryl ureas derivatives were designed, synthesized, and evaluated for their antitumor activities.

**Synthesis and antimicrobial activity of cholic acid hydrazone analogues**

pp. 2307–2313

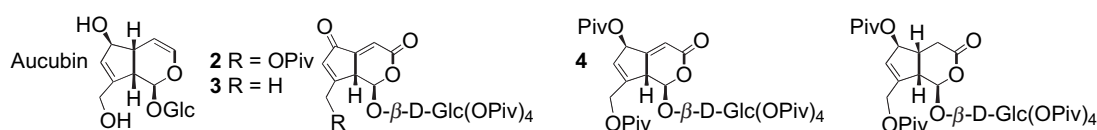
Anas J.M. Rasras, Taleb H. Al-Tel, Amal F. Al-Aboudi and Raed A. Al-Qawasmeh*

Synthesis and antimicrobial activity of cholic acid analogues are reported. Most compounds showed stronger antimicrobial activity against Gram-positive bacteria than Cefaclor and Cefixime. Some of the synthesized compounds indicated twofolds less activity against Gram-negative bacteria than Cefixime.

**A novel series of cytotoxic iridoid glucosides derived from aucubin: Design, synthesis and structure–activity relationships**

pp. 2314–2320

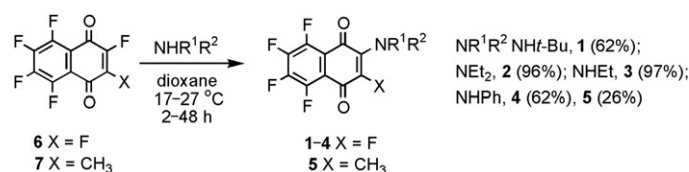
Vokatsoa C. Rakotondramasy, Christine Mouri  s, Xavier Cachet, Abdelhak Neghra, Missam El Mourabet, Fran  ois Tillequin, Michel Koch and Brigitte Deguin*

**Cytotoxicity of new alkylamino- and phenylamino-containing polyfluorinated derivatives of 1,4-naphthoquinone**

pp. 2321–2326

Ol'ga D. Zakharova, Ludmila P. Ovchinnikova, Leonid I. Goryunov, Nadezhda M. Troshkova, Vitalij D. Shteingarts and Georgy A. Nevinsky*

Polyfluorinated derivatives of 1,4-naphthoquinone are highly potent inhibitors of Cdc25A and Cdc25B phosphatases and growth of tumor cells. Five new N-substituted polyfluorinated derivatives of 2-amino-1,4-naphthoquinone were synthesized; all compounds (1)–(5) are effective inhibitors of growing of tumor cells.

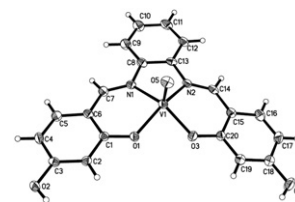


A new insulin-enhancing agent: *[N,N'*-bis(4-hydroxysalicylidene)-*o*-phenylene-diamine]oxovanadium(IV) and its permeability and cytotoxicity

pp. 2327–2335

Ming-jin Xie*, Ling Li, Xiao-Da Yang, Wei-ping Liu, Shi-ping Yan, Yan-fen Niu and Zhao-hui Meng

A new insulin-enhancing agent BPOV could significantly decrease blood glucose level in STZ-diabetic rats and could improve disorder of lipid metabolism in diabetes with insulin, glycogen, serum lipid studies.

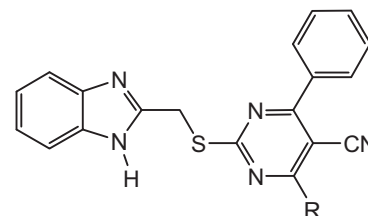


Novel benzimidazole–pyrimidine conjugates as potent antitumor agents

pp. 2336–2344

Heba T. Abdel-Mohsen*, Fatma A.F. Ragab, Mostafa M. Ramla and Hoda I. El Diwani

A series of 2-((1*H*-benzo[*d*]imidazol-2-yl)methylthio)-4-(substituted)-6-phenylpyrimidine-5-carbonitriles was synthesized. The *in vitro* cytotoxic activity against twelve tumor cell lines, revealed their marked potency when compared with known anticancer drugs.

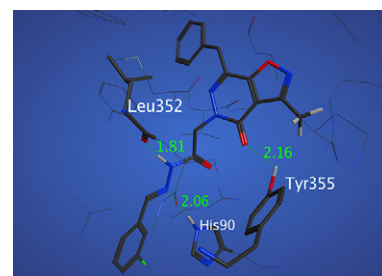


Synthesis and cyclooxygenase inhibitory activities of some *N*-acylhydrazone derivatives of isoxazolo[4,5-*d*]pyridazin-4(5*H*)-ones

pp. 2345–2352

Oya Ünsal-Tan*, Kevser Üzden, Arvi Rauk and Ayla Balkan

New isoxazolo[4,5-*d*]pyridazin-4(5*H*)-one derivatives having an *N*-acylhydrazone moiety were synthesized and tested for their COX inhibitory activities. Docking studies were done to understand the interactions of the compounds with the active site of COX-2.

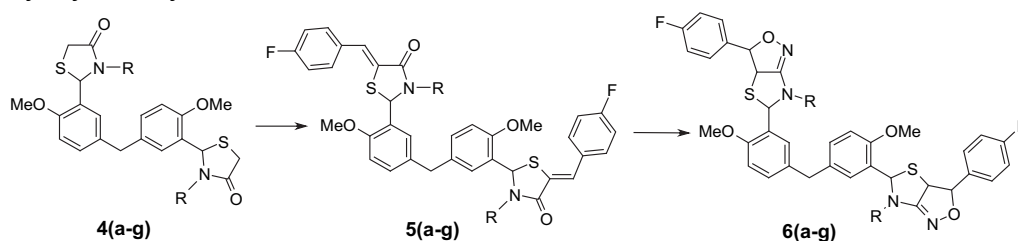


Synthesis and *in vitro* study of methylene-bis-tetrahydro[1,3]thiazolo[4,5-*c*]isoxazoles as potential nematocidal agents

pp. 2353–2358

Avula Srinivas, Adki Nagaraj and Cherkupally Sanjeeva Reddy*

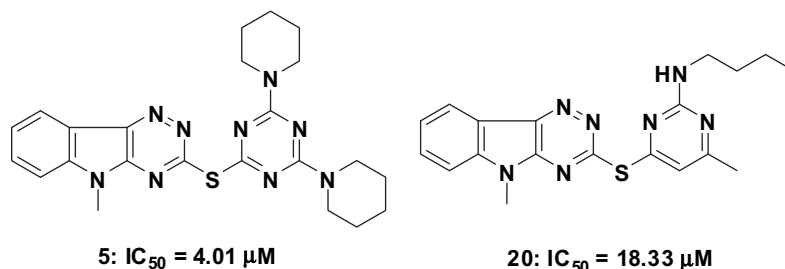
A series of methylene-bis-tetrahydro[1,3]thiazolo[4,5-*c*]isoxazoles have been synthesized and screened for their *in vitro* anti-fungal and nematocidal activities.



Synthesis and biological evaluation of new [1,2,4]triazino[5,6-*b*]indol-3-ylthio-1,3,5-triazines and [1,2,4]triazino[5,6-*b*]indol-3-ylthio-pyrimidines against *Leishmania donovani* pp. 2359–2365

Leena Gupta, Naresh Sunduru, Aditya Verma, Saumya Srivastava, Suman Gupta, Neena Goyal and Prem M.S. Chauhan*

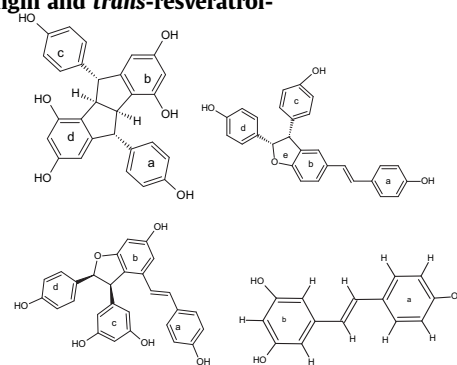
The triazino[5,6-*b*]indol-3-ylthio-1,3,5-triazine derivative (**5**) is the most potent and is 20-fold more selective, while triazino[5,6-*b*]indol-3-ylthio-pyrimidine derivative (**20**) is 2-fold more selective as an antileishmanial agent, in comparison with pentamidine.



Quantitative structure–antioxidant activity relationship of *trans*-resveratrol oligomers, *trans*-4,4'-dihydroxystilbene dimer, *trans*-resveratrol-3-O-glucuronide, glucosides: *Trans*-piceid, *cis*-piceid, *trans*-astringin and *trans*-resveratrol-4'-O-β-D-glucopyranoside pp. 2366–2380

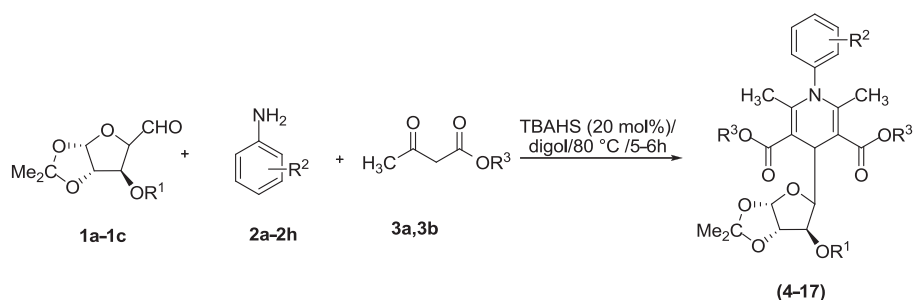
Damian Mikulski* and Marcin Molski

In the present study accurate computations based on DFT method have been performed to investigate the relation between the molecular structure and the antioxidant activity of the oligomers and glucosides of *trans*-resveratrol.



Synthesis and molecular docking studies of 1-phenyl-4-glycosyl-dihydropyridines as potent antileishmanial agents pp. 2381–2388

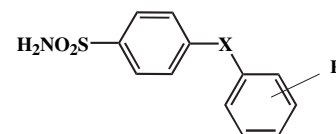
Vivek Parashar Pandey, Surendra Singh Bisht, Mridul Mishra, Ashutosh Kumar, Mohammad Imran Siddiqi, Aditya Verma, Monika Mittal, Shraddha A. Sane, Suman Gupta and Rama P. Tripathi*



A rationale for the activity profile of benzenesulfonamide derivatives as cyclooxygenase (COX) inhibitors pp. 2389–2395

Brij Kishore Sharma*, Prithvi Singh, Manju Shekhawat and Pradeep Pilania

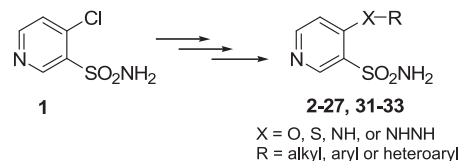
The QSAR analysis of the cyclooxygenase inhibition actions of benzenesulfonamide derivatives suggest that the substituent groups hold scope for further modification in the optimization of the activity.



Carbonic anhydrase inhibitors: Synthesis and inhibition of the human cytosolic isozymes I and II and transmembrane isozymes IX, XII (cancer-associated) and XIV with 4-substituted 3-pyridinesulfonamides pp. 2396–2404

Zdzisław Brzozowski, Jarosław Sławin'ski*, Franciszek Sączewski, Alessio Innocenti and Claudiu T. Supuran

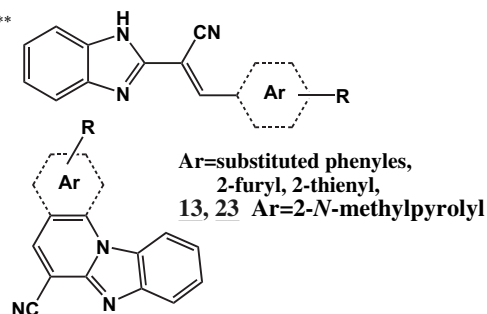
A series of novel 4-substituted-3-pyridinesulfonamides have been synthesized and investigated as inhibitors of five isoforms of zinc enzyme carbonic anhydrase (CA) that is, isozymes hCA I, II, IX, XII and XIV.



Benzimidazole derivatives related to 2,3-acrylonitriles, benzimidazo[1,2-a]quinolines and fluorenes: Synthesis, antitumor evaluation *in vitro* and crystal structure determination pp. 2405–2417

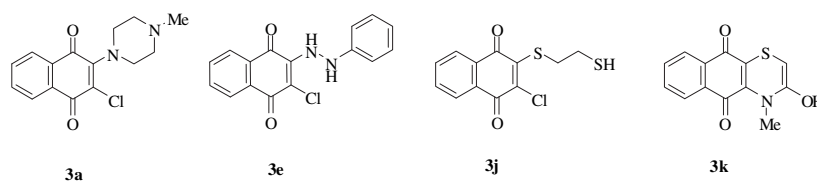
Marijana Hranjec*, Gordana Pavlovic*, Marko Marjanovic*, Marijeta Kralj and Grace Karminski-Zamola**

Newly synthesized benzimidazole derivatives exerted pronounced antiproliferative activity, **13** and **23** showed a special selectivity toward HeLa cells. Some compounds showed significant interaction with ct-DNA.



'On water' assisted synthesis and biological evaluation of nitrogen and sulfur containing hetero-1, 4-naphthoquinones as potent antifungal and antibacterial agents pp. 2418–2426

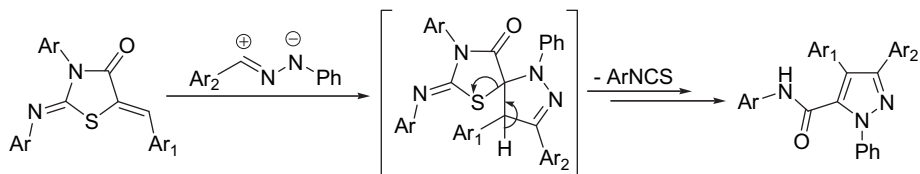
Vishnu K. Tandon*, Hardesh K. Maurya, Manoj K. Verma, Rohitashw Kumar and Praveen K. Shukla



MIC (mmol/mL) against *T.mentagraphytes* = 1.34 (**3a**), 1.31 (**3e**), 1.37 (**3j**), 3.00 (**3k**)

Microwave-assisted synthesis and *in-vitro* anti-tumor activity of 1,3,4-triaryl-5-N-arylpyrazole-carboxamides pp. 2427–2432

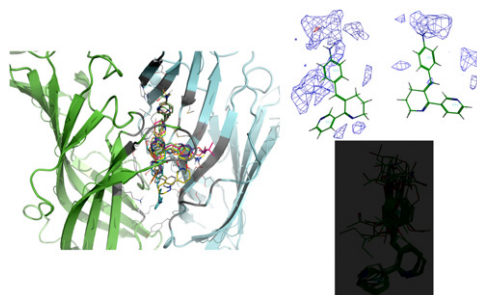
Hatem A. Abdel-Aziz, Heba S.A. El-Zahabi and Kamal M. Dawood*



A computational study of the binding of 3-(arylidene) anabaseines to two major brain nicotinic acetylcholine receptors and to the acetylcholine binding protein

pp. 2433–2446

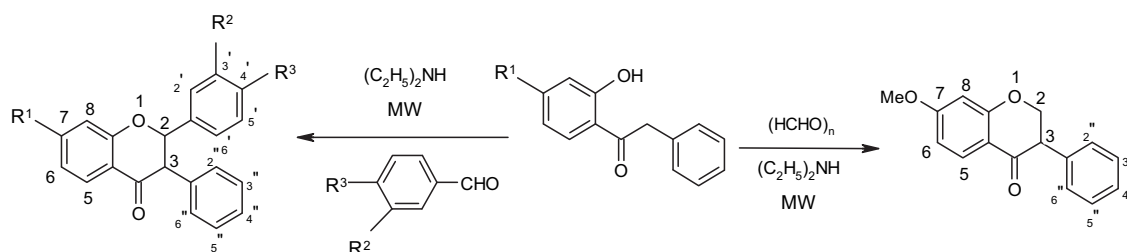
Svetoslav H. Slavov, Maksim Radzvilovits, Susan LeFrancois, Iva B. Stoyanova-Slavova, Ferenc Soti, William R. Kem** and Alan R. Katritzky*

**Synthesis, anticancer and antioxidant activities of 7-methoxyisoflavanone and 2,3-diarylchromanones**

pp. 2447–2452

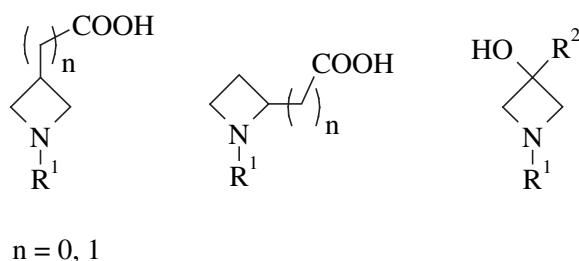
Kanagasabai Kanagalakshmi, Mariappan Premanathan, Ragunathan Priyanka, Balasubramanian Hemalatha and Arumugasamy Vanangamudi*

7-methoxyisoflavanone and 2,3-diarylchromanones have been synthesized and screened for antioxidant and anticancer activities. Diarylchromanone **6c** possess highest anticancer activity and diarylchromanone **6b** have highest antioxidant activity.

**Azetidine derivatives as novel γ -aminobutyric acid uptake inhibitors: Synthesis, biological evaluation, and structure–activity relationship**

pp. 2453–2466

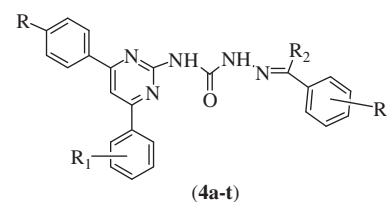
Mark R. Faust, Georg H fner, J rg Pabel and Klaus T. Wanner*

**Synthesis, anticonvulsant and toxicity screening of newer pyrimidine semicarbazone derivatives**

pp. 2467–2472

Ozair Alam*, Pooja Mullick, S.P. Verma, Sadaf J. Gilani, Suroor A. Khan, Nadeem Siddiqui and Waquar Ahsan

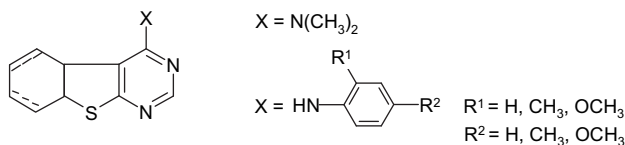
Various pyrimidine incorporated semicarbazones (**4a–t**) have been synthesized keeping in view the structural requirements of the proposed pharmacophore model. Some compounds showed promising anticonvulsant activity with less neurotoxicity and hepatotoxicity.



Synthesis and study of antiproliferative activity of novel thienopyrimidines on glioblastoma cells

pp. 2473–2479

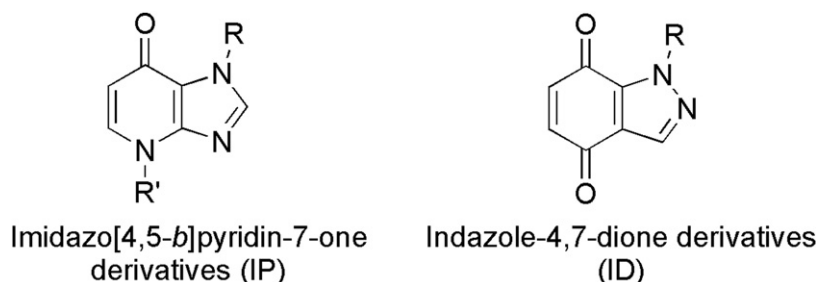
Stéphane Pâdeboscq*, Denis Gravier, Françoise Casadebaig, Geneviève Hou, Arnaud Gissot, Francesca De Giorgi, François Ichas, Jean Cambar and Jean-Paul Pometan

**Synthesis and modulation properties of imidazo[4,5-*b*]pyridin-7-one and indazole-4,7-dione derivatives towards the *Cryptosporidium parvum* CpABC3 transporter**

pp. 2480–2488

Wall Zeinyeh, Hexue Xia, Philippe Lawton, Sylvie Radix*, Christelle Marminon, Pascal Nebois and Nadia Walchshofer*

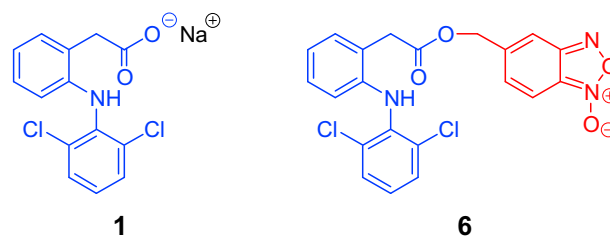
The affinity binding of IP and ID derivatives for the recombinant H6-NBD1 of the *Cryptosporidium parvum* ABC 3 protein was evaluated. These compounds were shown to be suitable scaffolds for designing new ligands of CpABC3.

**Synthesis and pharmacological characterization of a novel nitric oxide-releasing diclofenac derivative containing a benzofuroxan moiety**

pp. 2489–2493

Paulo Sérgio de Carvalho, Marta Marêstica, Alessandra Gambero* and JosÂ Pedrazzoli, Jr.

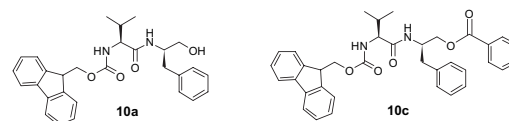
Native diclofenac (1) and benzofuroxan modified diclofenac (6). The structural modification results in anti-inflammatory activity and reduced ulcerogenic effects.

**Cytotoxic *N*-(fluorenyl-9-methoxycarbonyl) (Fmoc)-dipeptides: Structure–activity relationships and synergistic studies**

pp. 2494–2502

Chiao-Ting Yen, Chin-Chung Wu, Jin-Ching Lee, Shu-Li Chen, Susan L. Morris-Natschke, Pei-Wen Hsieh* and Yang-Chang Wu**

Thirty Fmoc-based dipeptides were designed and synthesized. The pharmacological results showed compounds **10a** and **10c** with IC₅₀ values of 1.0 and 0.4 μM against HepG2 and Ca9-22, respectively.



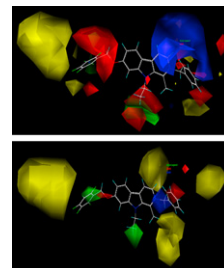
Compound	MDA-MB-231 (IC ₅₀ μg/ml)
10c : Doxo (1:1)	0.03
10c : Doxo (1:5)	0.23
Doxorubicin	0.43

Design, synthesis and 3D-QSAR of β -carboline derivatives as potent antitumor agents

pp. 2503–2515

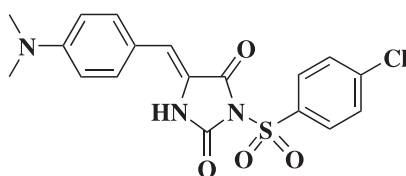
Rihui Cao*, Xiangdong Guan, Buxi Shi, Zhiyong Chen, Zhenhua Ren, Wenlie Peng and Huacan Song

The constructive CoMFA and CoMSIA models with highly predictive capacity provided important structural requirement for further design and synthesis of new β -carboline derivatives as potent antitumor agents.

**Synthesis and antitumor evaluation of novel cyclic arylsulfonylureas: ADME-T and pharmacophore prediction**

pp. 2516–2530

Ibrahim M. El-Deeb, Said M. Bayoumi, Magda A. El-Sherbeny and Alaa A.-M. Abdel-Aziz*



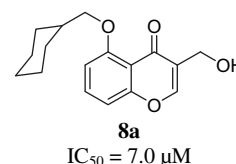
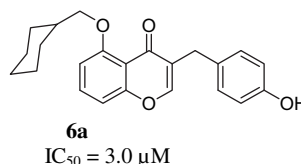
3q
%Inhibition over Melanoma M14
at 10 μ M = 199.6 %

Synthesis and evaluation of novel chromone analogs for their inhibitory activity against interleukin-5

pp. 2531–2536

Pillaiyar Thanigaimalai, Tuan Anh Le Hoang, Ki-Cheul Lee, Vinay K. Sharma, Seong-Cheol Bang, Jun Ho Yun, Eunmiri Roh, Youngsoo Kim and Sang-Hun Jung*

A novel series of chromone analogs **6(a–l)**, **8**, **9**, **10**, **11** and **12(a, b)** were synthesized and evaluated for their inhibitory activity against IL-5.

**Self-organizing molecular field analysis of 2,4-thiazolidinediones: A 3D-QSAR model for the development of human PTP1B inhibitors**

pp. 2537–2546

Suresh Thareja, Saurabh Aggarwal, T.R. Bhardwaj and Manoj Kumar*

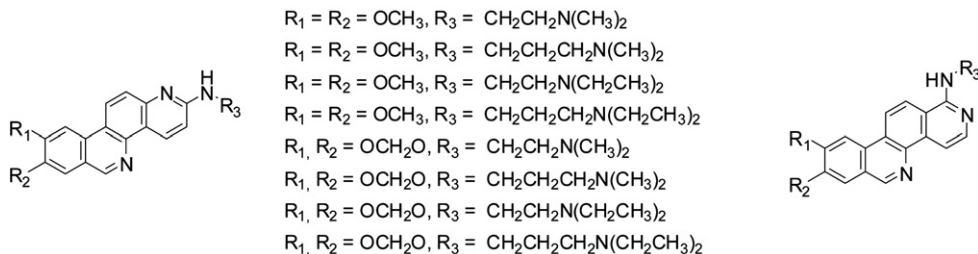
Self-organizing molecular field analysis was performed to generate 3D-QSAR models on a series containing TZD molecular scaffold having *h*-PTP1B inhibitory activities.



Synthesis and biological evaluation of dialkylaminoalkylamino benzo[*c*][1,7] and [1,8]phenanthrolines as antiproliferative agents

pp. 2547–2558

Tuba Şerbetçi, Constance Gen  s, Sabine Depauw, Soizic Prado, Fran  ois-Hugues Por  e, Marie-Paule Hildebrand, Marie-H  l  ne David-Cordonnier, Sylvie Michel and Fran  ois Tillequin*

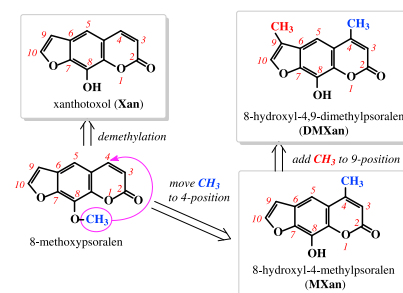


Synthesis of methyl-substituted xanthotoxol to clarify prooxidant effect of methyl on radical-induced oxidation of DNA

pp. 2559–2566

Chuan Xiao, Zhi-Guang Song and Zai-Qun Liu*

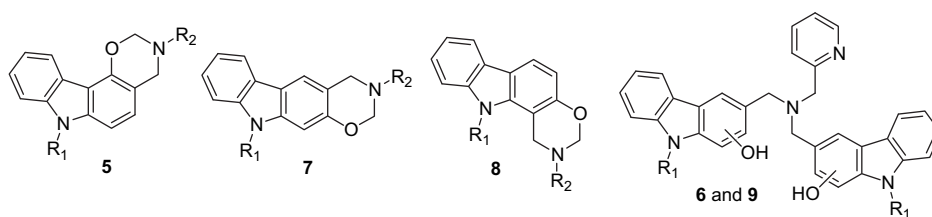
Detect the antioxidant effects of Xan, MXan and DMXan on the oxidation of DNA induced by Cu^{2+} /glutathione and peroxy radical to clarify that methyl attenuated the antioxidant capacity of Xan.



Synthesis and antiproliferative activity of oxazinocarbazole and *N,N*-bis(carbazolylmethyl)amine derivatives

pp. 2567–2577

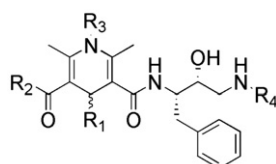
Samar Issa, Nadia Walchshofer, Issam Kassab, Hussein Termoss, Soulaïma Chamat, Aziz Geahchan and Zouhair Bouaziz*



Design and synthesis of 1,4-dihydropyridine derivatives as BACE-1 inhibitors

pp. 2578–2590

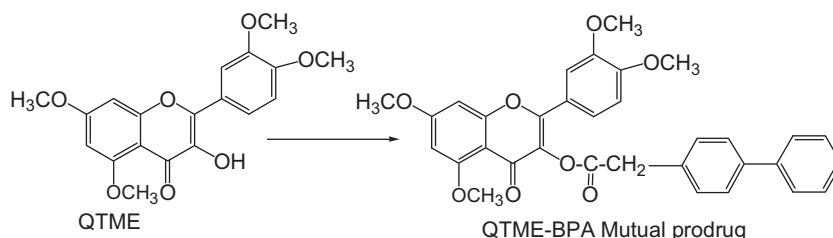
Soo-Jeong Choi, Joong-Heui Cho, Isak Im, So-Deok Lee, Ji-Yeon Jang, Yu-Min Oh, Yong-Keun Jung, Eun-Seok Jeon and Yong-Chul Kim*



Design, synthesis and evaluation of mutual prodrug of 4-biphenylacetic acid and quercetin tetramethyl ether (BPA–QTME) as gastrosparring NSAID

pp. 2591–2596

Mamta Madhukar, Shruti Sawraj and Pritam Dev Sharma*

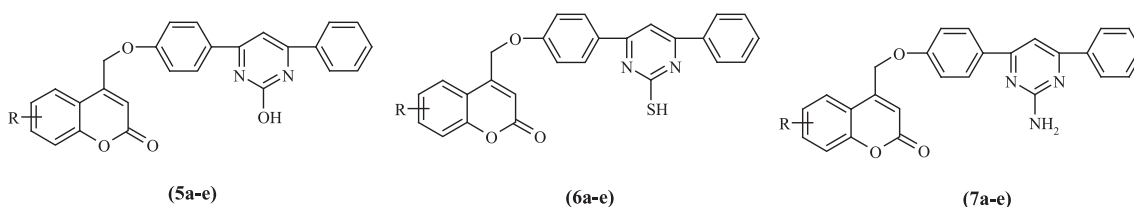


Analgesic, anti-pyretic and DNA cleavage studies of novel pyrimidine derivatives of coumarin moiety

pp. 2597–2605

Rangappa S. Keri, Kallappa M. Hosamani*, Ramya V. Shingalapuri and Mallinath H. Hugar

A series of new pyrimidine derivatives were synthesized and evaluated for their *in-vivo* analgesic, anti-pyretic and DNA cleavage studies. Compounds were characterized by spectroscopic studies and elemental analysis.



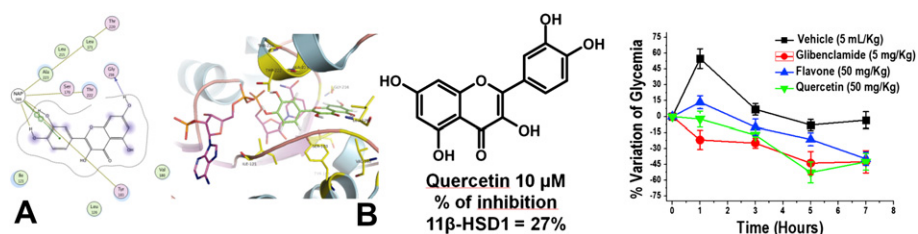
Where, R = a) 6-CH₃, b) 7-CH₃, c) 6-Cl, d) 5,6-Benzo, e) 7,8-Benzo

A comparative study of flavonoid analogues on streptozotocin–nicotinamide induced diabetic rats: Quercetin as a potential antidiabetic agent acting via 11β-Hydroxysteroid dehydrogenase type 1 inhibition

pp. 2606–2612

Mariana Torres-Piedra, Rolffy Ortiz-Andrade, Rafael Villalobos-Molina, Narender Singh, Jose L. Medina-Franco, Scott P. Webster, Margaret Binnie, Gabriel Navarrete-Vázquez and Samuel Estrada-Soto*

Normoglycemic and STZ-nicotinamide induced diabetic rats were treated with flavone (**1**), 3-hydroxyflavone (**2**), 6-hydroxyflavone (**3**), 7-hydroxyflavone (**4**), chrysin (**5**) and quercetin (**6**) (50 mg/kg). Compounds **1**, **5** and **6** were found most active in both experiments in comparison with control group ($p < 0.05$).

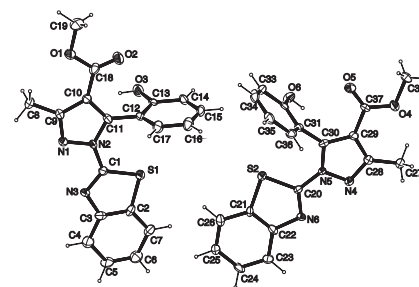


Synthesis, X-ray structures and cytotoxic activity of platinum(II), palladium(II) and copper(II) complexes with chelating ligands

pp. 2613–2621

Elzbieta Budzisz*, Magdalena Miernicka, Ingo-Peter Lorenz, Peter Mayer, Ewa Balcerzak, Urszula Krajewska and Marek Rozalski

Here we present the synthesis of the new pyrazole ligands obtained in the reaction of 2-methyl-4-oxo-4H-chromene-3-carboxylic acid methyl ester with hydrazine derivatives. These ligands create solid complexes with Pt(II), Pd(II) and Cu(II) metal ions or can be cyclized. The crystal and molecular structures of one ligand and its Cu(II) complexes were determined by X-ray diffraction method. Cytotoxic activity of the ligands and their complexes, and modulation of expression of BAX and P53 genes are also shown.



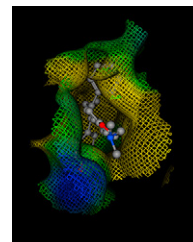
SHORT COMMUNICATIONS

Post-docking virtual screening of diverse binding pockets: Comparative study using DOCK, AMMOS, X-Score and FRED scoring functions

pp. 2622–2628

Tania Pencheva, Oumarou Samna Soumana, Ilza Pajeva and Maria A. Miteva*

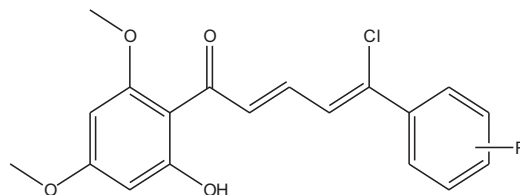
Summary: Thirteen commonly used scoring functions implemented in DOCK, AMMOS, X-Score and FRED are compared at a post-docking stage to examine their performance depending on the binding site properties for five important protein targets.

**Synthesis and biological evaluation of β -chloro vinyl chalcones as inhibitors of TNF- α and IL-6 with antimicrobial activity**

pp. 2629–2633

Babasaheb P. Bandgar*, Sachin A. Patil, Balaji L. Korbadi, Shivraj H. Nile and Chandrasekhar N. Khobragade

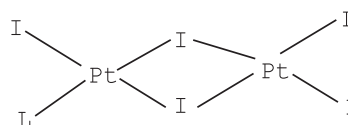
A series of β -chloro vinyl chalcones have been synthesized by Claisen–Schmidt condensation. All the compounds were evaluated for their anti-inflammatory activity (against TNF- α and IL-6) and antimicrobial activity.

**Synthesis, characterization and cytotoxicity of iodo-bridged binuclear platinum(II) complexes**

pp. 2634–2637

Jinchao Zhang*, Luwei Li, Xiaoyu Ji, Jing Sun, Liwei Wang and Ying Zhang

Seven binuclear platinum complexes (**1–7**) have been synthesized and characterized by elemental analysis, conductivity, thermal analysis, IR, ^1H NMR and mass spectra techniques. The cytotoxicity was tested by MTT assay.



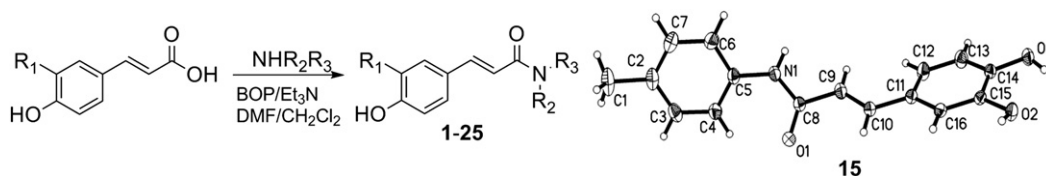
(L = *n*-butylamine, isopropylamine, *m*-toluidine, *p*-toluidine, diethylamine, N-methylaniline and aniline)

Synthesis, structure and structure–activity relationship analysis of caffeic acid amides as potential antimicrobials

pp. 2638–2643

Jie Fu, Kui Cheng, Zhi-ming Zhang, Rui-qin Fang and Hai-liang Zhu*

A series of caffeic acid amides were synthesized and (*E*)-3-(3,4-Dihydroxyphenyl)-*N*-*p*-tolylacrylamide (**15**) showed considerable antibacterial activity against *Bacillus subtilis* with MIC of 1.18 $\mu\text{g/mL}$.

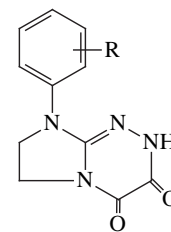


Lipophilicity of novel antitumour and analgesic active 8-aryl-2,6,7,8-tetrahydroimidazo[2,1-c][1,2,4]triazine-3,4-dione derivatives determined by reversed-phase HPLC and computational methods

pp. 2644–2649

Krzysztof Sztanke*, Wojciech Markowski, Ryszard S'wieboda and Beata Polak

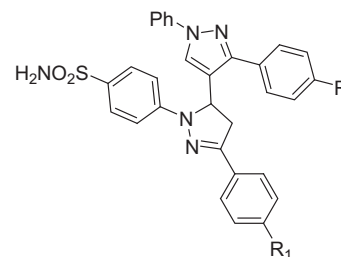
Log P_{HPLC} values of novel biologically active 8-aryl-2,6,7,8-tetrahydroimidazo[2,1-c][1,2,4]triazine-3,4-diones can be regarded as their hydrophobic parameters and these ones were found to be in the range of 0.97–2.63. **1**: R = H; **2**: R = 2-CH₃; **3**: R = 4-CH₃; **4**: R = 2-OCH₃; **5**: R = 4-OCH₃; **6**: R = 3-Cl; **7**: R = 4-Cl; **8**: R = 3,4-Cl₂.

**Synthesis and biological evaluation of some pyrazolypyrazolines as anti-inflammatory–antimicrobial agents**

pp. 2650–2655

Pawan K. Sharma*, Satish Kumar, Pawan Kumar, Pawan Kaushik, Dhirender Kaushik, Yogita Dhingra and Kamal R. Aneja

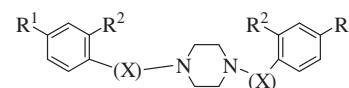
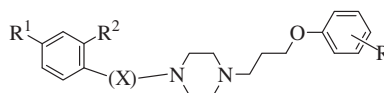
A series of pyrazolypyrazolines with vicinal diaryl substitution pattern on the pyrazole as well as pyrazoline nucleus was synthesized. One of the compounds showed interesting dual anti-inflammatory and antibacterial profile.

**Synthesis, evaluation and computational studies on a series of acetophenone based 1-(aryloxypropyl)-4-(chloroaryl) piperazines as potential atypical antipsychotics**

pp. 2656–2662

Alka Bali*, Komal Sharma, Abhishek Bhalla, Suman Bala, Dinesh Reddy, Anant Singh and Anil Kumar

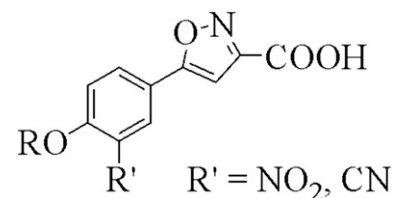
A series of 1-(aryloxypropyl)-4-(chloroaryl) piperazines have been synthesized and the target compounds evaluated for atypical antipsychotic activity in apomorphine induced mesh climbing and stereotypy in mice. 2D similarity studies and log BB calculations have been performed.

**Synthesis of some 5-phenylisoxazole-3-carboxylic acid derivatives as potent xanthine oxidase inhibitors**

pp. 2663–2670

Shaojie Wang*, Jufang Yan, Jian Wang, Jiarun Chen, Tingjian Zhang, Yong Zhao and Mingxing Xue

A number of 5-phenylisoxazole-3-carboxylic acid derivatives were synthesized and tested for their ability to inhibit xanthine oxidase. Most of the compounds exhibited potency levels in the micromolar/submicromolar range.

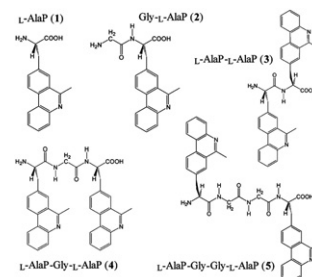


Novel bis-phenanthridine derivatives with easily tunable linkers, study of their interactions with DNA and screening of antiproliferative activity

pp. 2671–2676

Marko Dukii, Domagoj Baretic*, Vesna Čaplar and Ivo Piantanida*

Novel peptide-bridged bis-phenanthridine derivatives, including the first known derivative forming intramolecular excimer, revealed strong interactions with ds-DNA, as well as selective fluorescence response.

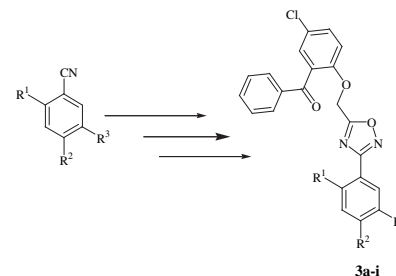


Design, synthesis, characterization, and antibacterial activity of {5-chloro-2-[(3-substitutedphenyl)-1,2,4-oxadiazol-5-yl]-methoxy}-phenyl)-(phenyl)-methanones

pp. 2677–2682

Neithnadka Premsai Rai, Venugopala Katharigatta Narayanaswamy, Thavendran Govender, B.K. Manuprasad, Sheena Shashikanth* and Pirama Nayagam Arunachalam

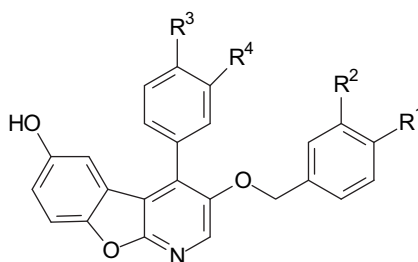
In the present investigation, a series of novel {5-chloro-2-[(3-(substitutedphenyl)-1,2,4-oxadiazol-5-yl)-methoxy]-phenyl)-(phenyl)-methanones (**3a–i**) have been synthesized, characterized and investigated for qualitative (zone of inhibition) and quantitative (MIC) antibacterial activity.



First biological evaluation of developed 3-benzyloxyfluorenes as novel class of MDR modulators

pp. 2683–2688

Martin Krug, Burkhardt Voigt, Christiane Baumert, Ralf Lippken, JosÁf MolnÁr and Andreas Hilgeroth*

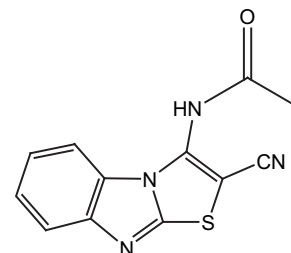


Cell cycle disruption and apoptotic activity of 3-aminothiazolo[3,2-a]benzimidazole-2-carbonitrile and its homologues

pp. 2689–2694

Abdelwareth A.O. Sarhan, Abdullah Al-Dhfyan, Maha A. Al-Mozaini, Chaker N. Adra and Tarek Aboul-Fadl*

Among a synthesized series of aminothiazolo[3,2-a]benzimidazole derivatives *N*-acetylaminothiazolo[3,2-a]benzimidazole-2-carbonitrile revealed significant *in vitro* antiproliferative activity which attributed to its ability to arrest G2/M phase and to induce apoptosis in time dependant manner.

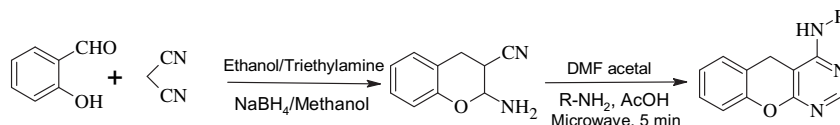


Novel chromeno [2,3-*b*]-pyrimidine derivatives as potential anti-microbial agents

pp. 2695–2699

U. Sankappa Rai, Arun M. Isloor*, Prakash shetty, A.M. Vijesh, Nithin Prabhu, Shrikrishna Isloor, M. Thiageeswaran and Hoong-Kun Fun

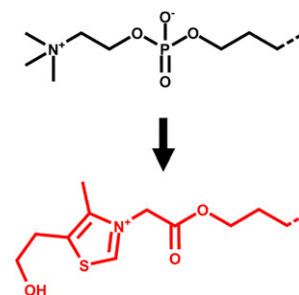
Heterocyclic privileged medicinal scaffolds involving chromeno[2,3-*b*]-pyrimidine frameworks are prepared by microwave irradiation.

**PRELIMINARY COMMUNICATIONS****Computational screening for membrane-directed inhibitors of mast cell activation**

pp. 2700–2704

Jos  Batista, Tim Friedrichson, Georg Schlechtingen, Tobias Braxmeier, Gary Jennings and J rgen Bajorath*

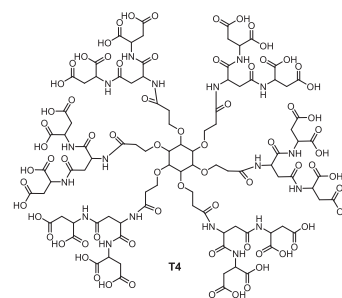
Lipid-like compounds have been explored for their potential to inhibit mast cell activation and degranulation. Shown is the head group of a new inhibitor of mast cell activation (red) identified by computational extrapolation from the alkylphospholipid chemotype represented by miltefosine (black).

**Synthesis of novel dendrimers having aspartate grafts and their ability to enhance the aqueous solubility of model drugs**

pp. 2705–2711

Liang Ouyang, Lifang Ma, Bo Jiang, Yanhua Li, Dongsheng He and Li Guo*

A series of peptide dendrimers bearing aspartate grafts in periphery as macromolecules for solubility enhancer of drug delivery were synthesized.

**BOOK REVIEW****How To Write A Successful Science Thesis- The Concise Guide For Students**

pp. 2712

Alessio Travaglia*

COVER

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

* Corresponding authors.



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