



European Journal of Medicinal Chemistry Vol 47, 2012

Contents

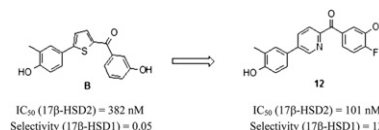
ORIGINAL ARTICLES

Discovery of a new class of bicyclic substituted hydroxyphenylmethanones as 17 β -hydroxysteroid dehydrogenase type 2 (17 β -HSD2) inhibitors for the treatment of osteoporosis

pp. 1–17

Marie Wetzel, Emanuele M. Gargano, Stefan Hinsberger, Sandrine Marchais-Oberwinkler and Rolf W. Hartmann*

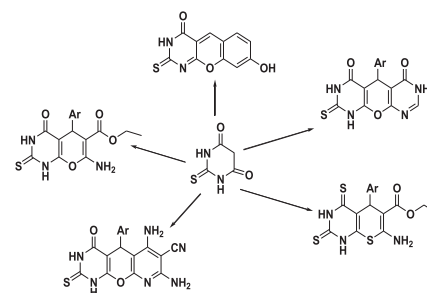
Starting from nonselective compound **B**, potent and selective 17 β -HSD2 inhibitors were obtained by structural modification.


Efficient one-pot preparation of novel fused chromeno[2,3-*d*]pyrimidine and pyrano[2,3-*d*]pyrimidine derivatives

pp. 18–23

Hala M. Aly* and Mona M. Kamal

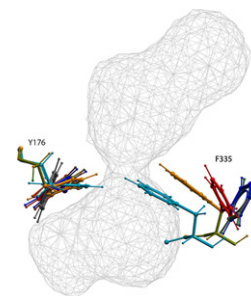
Synthesis and Preliminary Antimicrobial Activity of Some New Pyrano[2,3-*d*]pyrimidine Derivatives.


Molecular mechanism of serotonin transporter inhibition elucidated by a new flexible docking protocol

pp. 24–37

Mari Gabrielsen, Rafał Kurczab, Aina W. Ravna, Irina Kufareva, Ruben Abagyan, Zdzisław Chiltonczyk, Andrzej J. Bojarski and Ingebrigt Sylte*

Figure showing the orientation of Y176 and F335, the aromatic amino acids of extracellular gate (xstick representation), in the occluded (cyan) and outward-facing (orange) SERT homology models and in four binding pocket conformations (red, blue, grey and green) generated through BPMC side chain sampling. The binding pocket detected by ICM PocketFinder in the outward-facing model is shown in grey wire representation.

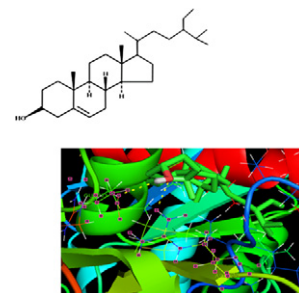


Molecular docking of γ -sitosterol with some targets related to diabetes

pp. 38–43

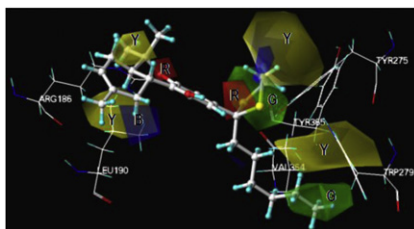
Rangachari Balamurugan, Antony Stalin and Savarimuthu Ignacimuthu*

γ -sitosterol isolated from *Lippia nodiflora* was taken as ligand for molecular docking. The molecular targets from PDB database 1V4S, 2JJJ, 3LC4, 2CBZ were used for the docking analysis using Autodocktool.

**An effort to discover the preferred conformation of the potent AMG3 cannabinoid analog when reaching the active sites of the cannabinoid receptors**

pp. 44–51

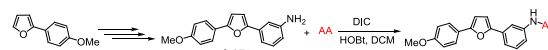
Serdar Durdagi*, Manthos G. Papadopoulos and Thomas Mavromoustakos**

**Synthesis, anti-inflammatory activity and molecular docking studies of 2,5-diarylfuran amino acid derivatives**

pp. 52–58

Hélio A. Stefani*, Giancarlo V. Botteselle, Julio Zukerman-Schpector, Ignez Caracelli, Denis da Silva Corrêa, Sandra H.P. Farsky, Isabel D. Machado, José R. Santin and Cristina B. Hebeda

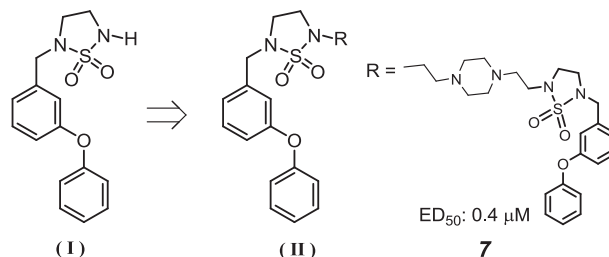
Describe herein the synthesis of a novel 2,5-diarylfuran scaffold suitable for conjugation with amino acids. We also show that the proline-substituted compound inhibited PGE2 secretion by LPS-stimulated neutrophils, suggesting selectivity for COX-2 activity. Molecular docking studies, in COX-2, were performed in order to shed light on the nature of their different activities. The biological and docking results showed that the activity of this kind of molecule can be modulated by the hydrophilicity of the conjugated amino acid.

**Cyclosulfamide-based derivatives as inhibitors of noroviruses**

pp. 59–64

Dengfeng Dou, Sivakoteswara R. Mandadapu, Kevin R. Alliston, Yunjeong Kim, Kyeong-Ok Chang* and William C. Groutas

An optimization campaign focused on improving pharmacological activity and physicochemical properties of a new class of norovirus inhibitors has been conducted. The dimeric compound **7** was found to be ~10-fold more potent norovirus inhibitor compared to the original hit.

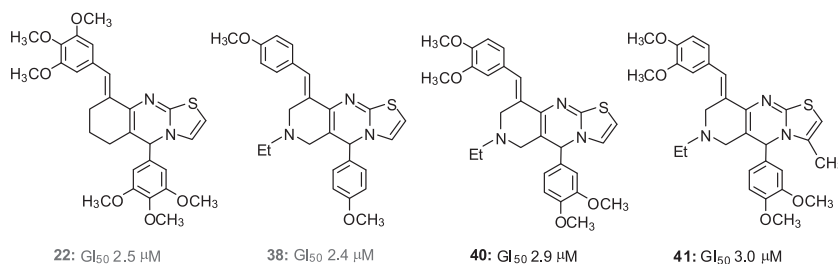


Substituted thiazoles V. Synthesis and antitumor activity of novel thiazolo[2,3-*b*]quinazoline and pyrido[4,3-*d*]thiazolo [3,2-*a*]pyrimidine analogues

pp. 65–72

Fatmah A.M. Al-Omary, Ghada S. Hassan, Shahenda M. El-Messery and Hussein I. El-Subbagh*

Compounds **22** and **38** are almost nine fold, while **40** and **41** are almost seven fold, more active than the known antitumor 5-FU.

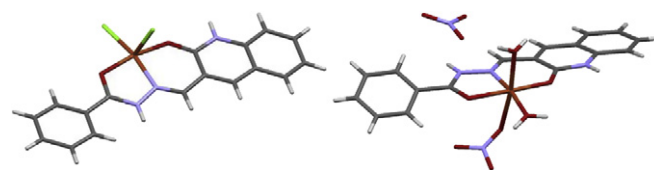


Synthesis, crystal structure and pharmacological evaluation of two new Cu(II) complexes of 2-oxo-1,2-dihydroquinoline-3-carbaldehyde (benzoyl) hydrazone: A comparative investigation

pp. 73–85

Duraismy Senthil Raja, Nattamai S.P. Bhuvanesh and Karuppannan Natarajan*

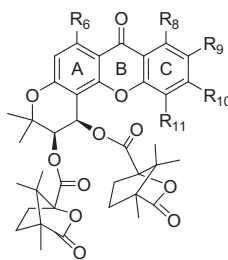
2-oxo-1,2-dihydroquinoline-3-carbaldehyde(benzoyl)hydrazone and its copper(II) complexes have been synthesized. Their structure activity relationships on DNA and protein binding, antioxidative and cytotoxic activity have been investigated.



Anti-AIDS agents 85. Design, synthesis, and evaluation of 1*R*,2*R*-dicamphanoyl-3,3-dimethyldihydropyrano-[2,3-*c*] xanthen-7(1*H*)-one (DCX) derivatives as novel anti-HIV agents

pp. 86–96

Ting Zhou, Qian Shi*, Chin-Ho Chen, Li Huang, Phong Ho, Susan L. Morris-Natschke and Kuo-Hsiung Lee**

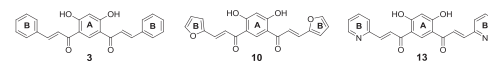


Bis-chalcone analogues as potent NO production inhibitors and as cytotoxic agents

pp. 97–103

M. Vijaya Bhaskar Reddy, Yuh-Chiang Shen, Emika Ohkoshi, Kenneth F. Bastow, Keduo Qian, Kuo-Hsiung Lee and Tian-Shung Wu*

Several synthetic bis-chalcones showed significant cytotoxic activity and potent inhibition of NO production. The compounds down-regulated iNOS expression by inhibiting p65 NF- κ B activation/ nuclear translocation due to prevention of I κ B α degradation.

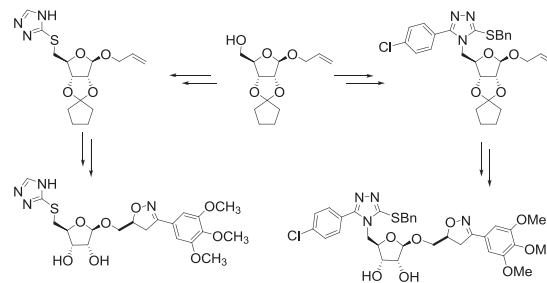


1,2,4-Triazole D-ribose derivatives: Design, synthesis and antitumoral evaluation

pp. 104–110

Romina E. Avanzo, Claudia Anesini, Mirta L. Fascio, María I. Errea and Norma B. D'Accorso*

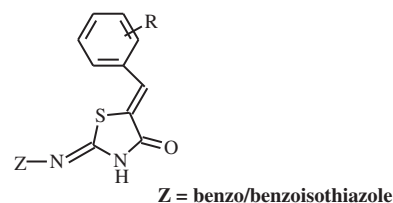
Novel 1,2,4-triazole D-ribose derivatives were synthesized and their antitumoral activity on a T cell lymphoma cell line was evaluated.

**Fragment-based design, docking, synthesis, biological evaluation and structure–activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as cyclooxygenase/lipoxygenase inhibitors**

pp. 111–124

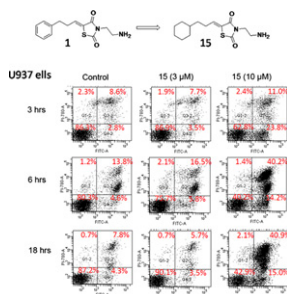
Phaedra Eleftheriou, Athina Geronikaki*, Dimitra Hadjipavlou-Litina, Paola Vicini, Olga Filz**, Dmitry Filimonov, Vladimir Poroikov, Shailendra S. Chaudhaery, Kuldeep K. Roy and Anil K. Saxena

A new statistical method was proposed and applied to identify the fragments involved in the inhibition of COX-1, COX-2 and LOX enzymes. The further chemicals synthesis of designed compounds and both *in vitro* and *in vivo* biological testing confirmed the results of computational modelling.

**3,5-Disubstituted-thiazolidine-2,4-dione analogs as anticancer agents: Design, synthesis and biological characterization**

pp. 125–137

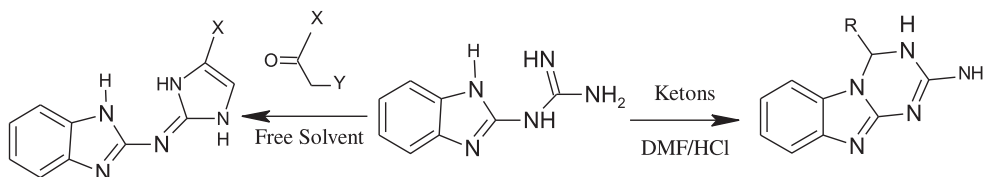
Kai Liu, Wei Rao, Hardik Parikh, Qianbin Li, Tai L. Guo, Steven Grant, Glen E. Kellogg and Shijun Zhang*

**Synthesis and biological activity of dihydroimidazole and 3,4-dihydrobenzo[4,5]imidazo[1,2-a][1,3,5]triazins**

pp. 138–142

Ahmed M. Soliman*, Shaaban K. Mohamed, Mahmoud A.A. El Remaily and H. Abdel-Ghany

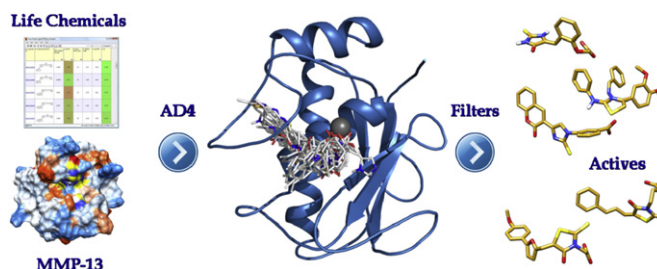
Reaction of 2-guanidinobenzimidazole with halogenated active methylenes and ketones gave dihydroimidazole and 3,4-dihydrobenzo [4,5]imidazo [1,2-a] [1,3,5]triazin derivatives. The anti-bacterial evaluation of the synthesized products showed excellent zone of inhibition against tested bacteria.



Identification of novel molecular scaffolds for the design of MMP-13 inhibitors: A first round of lead optimization

pp. 143–152

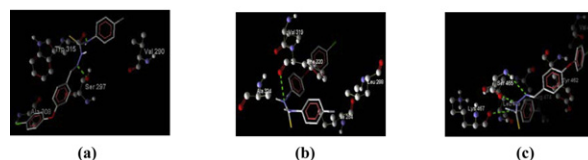
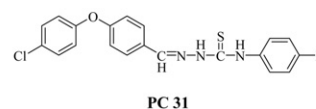
Valeria La Pietra, Luciana Marinelli*, Sandro Cosconati, Francesco Saverio Di Leva, Elisa Nuti, Salvatore Santamaria, Isabella Pugliesi, Matteo Morelli, Francesca Casalini, Armando Rossello, Concettina La Motta, Sabrina Taliani, Robert Visse, Hideaki Nagase, Federico da Settimo and Ettore Novellino

**Design, synthesis and anticonvulsant evaluation of novel *N*-(4-substituted phenyl)-2-[4-(substituted) benzylidene]-hydrazinecarbothio amides**

pp. 153–166

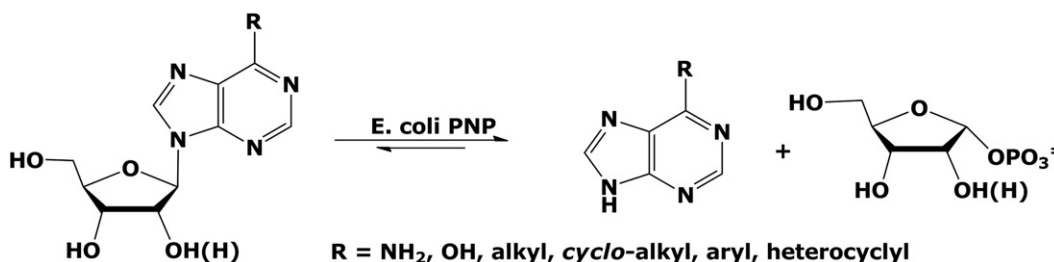
Laxmi Tripathi*, Praveen Kumar, Ranjit Singh and James P. Stables

Thirty six novel *N*-(4-substituted phenyl)-2-[4-(substituted)benzylidene] hydrazinecarbothioamides were synthesized and evaluated for anticonvulsant activity. Their computational studies were also reported. 2-[4-(4-Chlorophenoxy)benzylidene]-*N*-(4-fluorophenyl)hydrazinecarbothioamide **PC 31** emerged as most active compound of the series.

**Synthesis and evaluation of the substrate activity of C-6 substituted purine ribosides with *E. coli* purine nucleoside phosphorylase: Palladium mediated cross-coupling of organozinc halides with 6-chloropurine nucleosides**

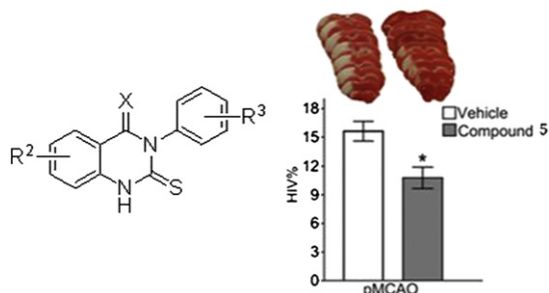
pp. 167–174

Abdalla E.A. Hassan, Reham A.I. Abou-Elkhair, James M. Riordan, Paula W. Allan, William B. Parker, Rashmi Khare, William R. Waud, John A. Montgomery and John A. Secrist III*

**Neuroprotective efficacy of quinazoline type phosphodiesterase 7 inhibitors in cellular cultures and experimental stroke model**

pp. 175–185

Miriam Redondo, Juan G. Zaruk, Plácido Ceballos, Daniel I. Pérez, Concepción Pérez, Ana Perez-Castillo, María A. Moro, José Brea, Cristina Val, María I. Cadavid, María I. Loza, Nuria E. Campillo, Ana Martínez and Carmen Gil*

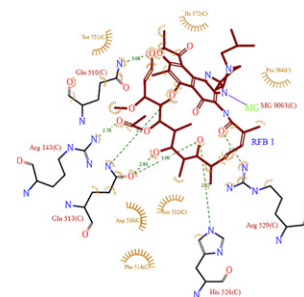


Pharmacophore insights into rpoB gene mutations in *Mycobacterium tuberculosis* rifampicin resistant isolates

pp. 186–193

Ricardo Figueiredo, Daniela F. Ramos, Cristina Moiteiro, Maria Augusta Medeiros, Maria João Marcelo Curto, José Cardoso de Menezes, Rogelio Hernandez Pando, Pedro E.A. Silva and Maria do Céu Costa*

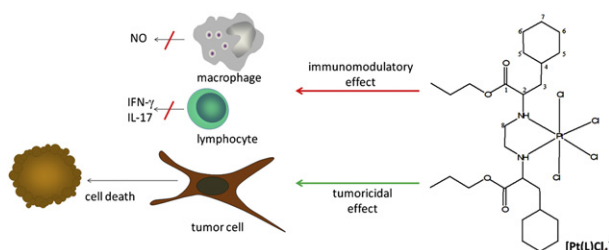
Interactions of RFB 1 backbone with distance interacting residues of *T. thermophilus* RNAP chain (Chain C) containing positions corresponding to codons 514, 516, 529 and 531 of investigated mutations, where hydrogen bonds are represented by dashed green lines while non specific van der Waals interactions with RNAP rpoB aa are in orange.



Novel octahedral Pt(IV) complex with di-*n*-propyl-(*S,S*)-ethylenediamine-*N,N'*-di-2-(3-cyclohexyl)propanoato ligand exerts potent immunomodulatory effects

pp. 194–201

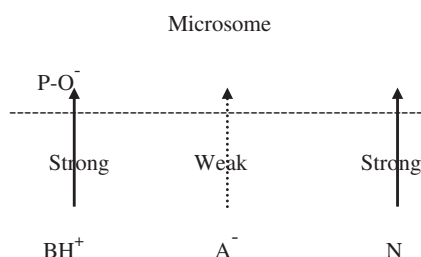
Djordje Miljković*, Jelena M. Poljarević, Filip Petković, Jana Blaževski, Miljana Momčilović, Ivana Nikolić, Tamara Saksida, Stanislava Stošić-Grujičić, Sanja Grgurić-Šipka and Tibor J. Sabo



The effect of ionized species on microsomal binding

pp. 202–205

Michael H. Abraham* and Rupert P. Austin

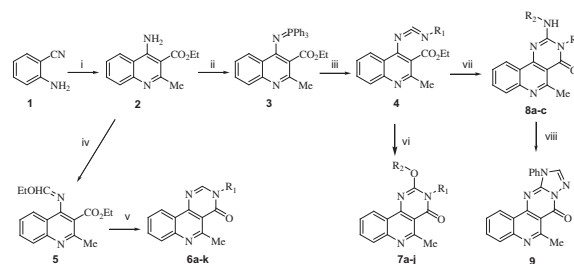


Synthesis and in vitro antiproliferative evaluation of pyrimido[5,4-*c*]quinoline-4-(3*H*)-one derivatives

pp. 206–213

Yong Ai, Yong-Ju Liang, Jian-Chao Liu, Hong-Wu He, Yu Chen, Chu Tang, Guang-Zhong Yang* and Li-Wu Fu*

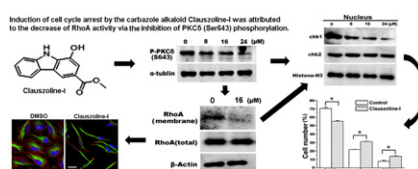
A series of pyrimido[5,4-*c*]quinoline-4-(3*H*)-one derivatives variously substituted at positions 2 and 3 were synthesized and evaluated for their in vitro antiproliferative activities.



Induction of cell cycle arrest by the carbazole alkaloid *Clauszoline-I* from *Clausena vestita* D. D. Tao via inhibition of the PKC δ phosphorylation

pp. 214–220

Wei Lin, Ying Wang, Sisi Lin, Cuixian Li, Chun Zhou, Shaogui Wang, Heqing Huang, Peiqing Liu, Guan Ye* and Xiaoyan Shen**

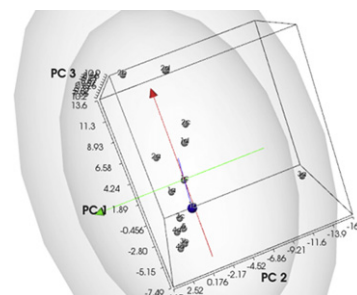


Design, synthesis and in vitro antitumour activity of new heteroaryl ethylenes

pp. 221–227

Cosimo G. Fortuna*, Vincenza Barresi, Carmela Bonaccorso, Giuseppe Consiglio, Salvatore Failla, Angela Trovato-Salinaro and Giuseppe Musumarra

Almond and VolSurf + approaches allowed the design of new derivatives, which after synthesis and biological evaluation, exhibited in vitro antiproliferative activity significantly higher than that of the most active compound previously synthesized in our laboratory.

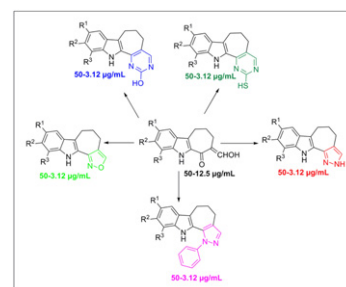


Synthesis, antimicrobial, antimycobacterial and structure–activity relationship of substituted pyrazolo-, isoxazolo-, pyrimido- and mercaptopyrimidocyclohepta[b]indoles

pp. 228–238

Ezhumalai Yamuna, R. Ajay Kumar, Matthias Zeller and Karnam Jayarampillai Rajendra Prasad*

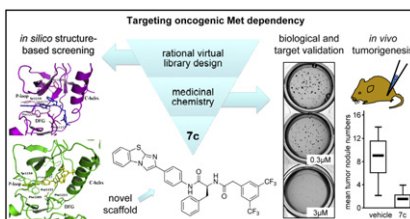
The hererofused cyclohepta[b]indoles were synthesized and subjected to in vitro antimicrobial and anti-mycobacterial activities.



Identification of new aminoacid amides containing the imidazo[2,1-b]benzothiazol-2-ylphenyl moiety as inhibitors of tumorigenesis by oncogenic Met signaling

pp. 239–254

Alessandro Furlan, Francesco Colombo, Andrea Kover, Nathalie Issaly, Cristina Tintori, Lucilla Angeli, Vincent Leroux, Sébastien Letard, Mercedes Amat, Yasmine Asses, Bernard Maigret, Patrice Dubreuil, Maurizio Botta, Rosanna Dono****, Joan Bosch****, Oreste Piccolo***, Daniele Passarella** and Flavio Maina*

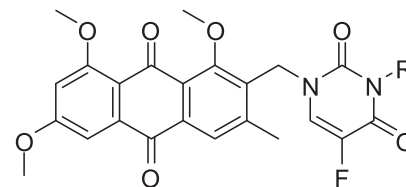


Synthesis and antitumor activity of conjugates of 5-Fluorouracil and emodin

pp. 255–260

Li-Ming Zhao*, Li-Ming Zhang, Jin-Juan Liu, Li-Jing Wan, Yong-Qiang Chen, Shu-Qing Zhang, Zhi-Wei Yan and Ji-Hong Jiang*

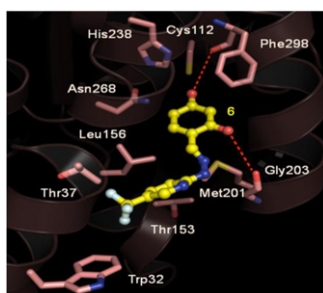
A series of conjugates of 5-FU and emodin were synthesized and evaluated for their antitumor activity. The structure–activity relationship showed N³-aromatic substituent is important for their cytotoxic activity.



Discovery of novel selective inhibitors of *Staphylococcus aureus* β -ketoacyl acyl carrier protein synthase III

pp. 261–269

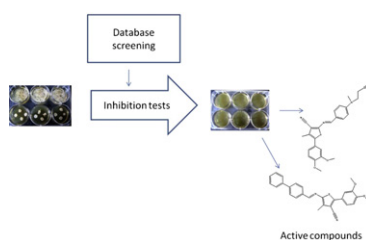
Jee-Young Lee, Ki-Woong Jeong, Soyoung Shin, Ju-Un Lee and Yangmee Kim*



Antifungal activities of novel non-azole molecules against *S. cerevisiae* and *C. albicans*

pp. 270–277

Niina Tani*, Minna Rahnasto-Rilla, Carsten Wittekindt, Kaisa A. Salminen, Anniina Ritvanen, Riina Ollakka, Jenna Koskiranta, Hannu Raunio and Risto O. Juvonen

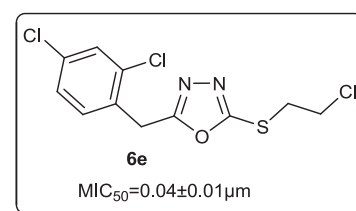


Identification and development of 2,5-disubstituted oxadiazole as potential candidate for treatment of XDR and MDR tuberculosis

pp. 278–282

Ravi L. Bakal* and Surendra G. Gattani

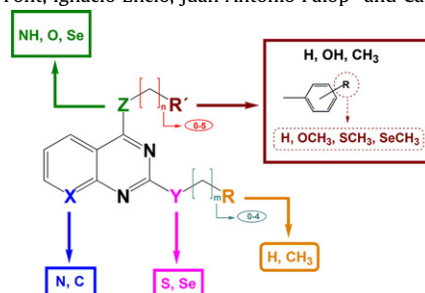
A substituted oxadiazole has been identified and then modified to yield **6e**, a potent anti-tubercular agent. The anti-XDR & MDR-TB activity is discussed using 25 different isolates.



Sulfur and selenium derivatives of quinazoline and pyrido[2,3-*d*]pyrimidine: Synthesis and study of their potential cytotoxic activity *in vitro*

pp. 283–298

Esther Moreno, Daniel Plano, Iranzu Lamberto, María Font, Ignacio Encío, Juan Antonio Palop* and Carmen Sanmartín

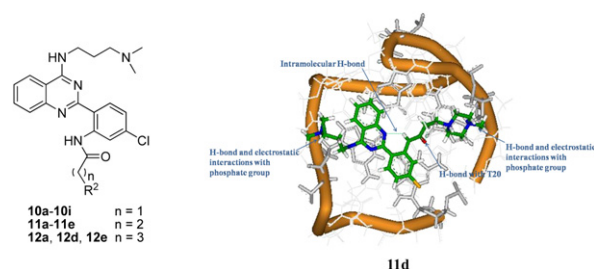


Disubstituted quinazoline derivatives as a new type of highly selective ligands for telomeric G-quadruplex DNA

pp. 299–311

Zeng Li, Jia-Heng Tan, Jin-Hui He, Yi Long, Tian-Miao Ou, Ding Li*, Lian-Quan Gu and Zhi-Shu Huang*

A series of quinazoline derivatives as novel telomeric G-quadruplex ligands were synthesized and evaluated. These derivatives could well recognize G-quadruplex DNA and have significant cellular biological activity.

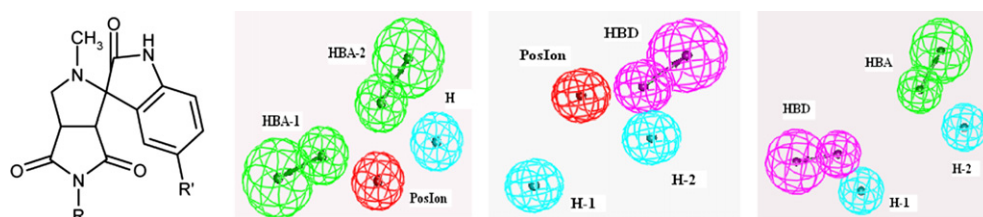


Synthesis and QSAR study of novel cytotoxic spiro[3H-indole-3,2'-(1'H)-pyrrolo[3,4-c]pyrrole]-2,3',5'-(1H,2'aH,4'H)-triones

pp. 312–322

Adel S. Girgis*, Jacek Stawinski**, Nasser S.M. Ismail and Hanaa Farag

Anti-tumor active 4'-aryl-5'a,6'-dihydro-1'-methyl-spiro[3H-indole-3,2'-(1'H)-pyrrolo[3,4-c]pyrrole]-2,3',5'-(1H,2'aH,4'H)-triones were synthesized via dipolar cycloaddition reaction of azomethine ylides with 1-aryl-1H-pyrrole-2,5-diones.

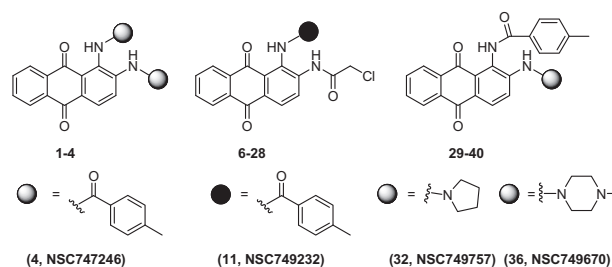


Synthesis, antiproliferative activities and telomerase inhibition evaluation of novel asymmetrical 1,2-disubstituted amidoanthraquinone derivatives

pp. 323–336

Chia-Chung Lee, Kuo-Feng Huang, Pen-Yuan Lin, Fong-Chun Huang, Chun-Liang Chen, Tsung-Chih Chen, Jih-Hwa Guh, Jing-Jer Lin** and Hsu-Shan Huang*

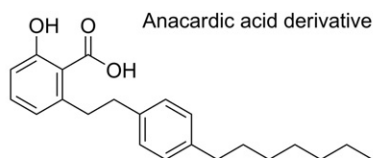
A series of diversely asymmetrical mono- or disubstituted 1,2-diamidoanthraquinone derivatives were synthesized and evaluated for drug-induced cytotoxicity by SRB assay, telomerase inhibitory activity by TRAP assay, and *hTERT* expression by SEAP assay.



6-alkylsalicylates are selective Tip60 inhibitors and target the acetyl-CoA binding site

pp. 337–344

Massimo Ghizzoni, Jiang Wu, Tielong Gao, Hidde J. Haisma, Frank J. Dekker* and Y. George Zheng**



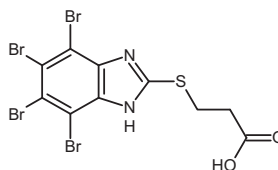
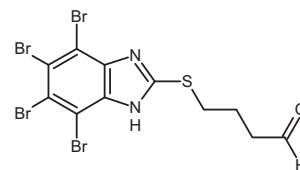
Tip60 IC₅₀ 74 μM p300 IC₅₀ > 200 μM
 MOF IC₅₀ 47 μM PCAF IC₅₀ >> 200 μM

CK2α and CK2α' subunits differ in their sensitivity to 4,5,6,7-tetrabromo- and 4,5,6,7-tetraiodo-1H-benzimidazole derivatives

pp. 345–350

Monika Janeczko, Andrzej Orzeszko, Zygmunt Kazimierczuk, Ryszard Szyszka and Andrea Baier*

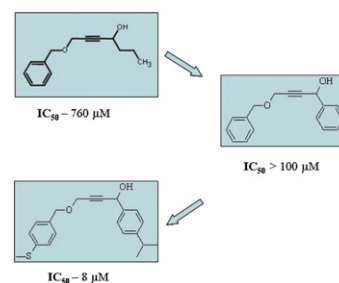
4,5,6,7-tetrabromo- and 4,5,6,7-tetraiodo-1H-benzimidazoles and their newly obtained N¹- and 2-S-carboxyalkyl derivatives showed potent inhibitory activity against human protein kinase CK2 catalytic subunits. Among newly synthesized compounds **5c** and **5e** exert the highest anti-CK2 activity. CK2α' was up to 6 times more sensitive to the studied compounds than CK2α.

**5c****5e****Structure based drug design, synthesis and evaluation of 4-(benzyloxy)-1-phenylbut-2-yn-1-ol derivatives as 5-lipoxygenase inhibitors**

pp. 351–359

Nimmanapalli P. Reddy, T. Chandramohan Reddy, Polamarasetty Aparoy, Chandrani Achari, P. Ramu Sridhar and Pallu Reddanna*

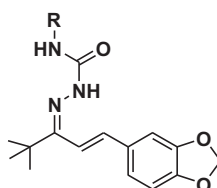
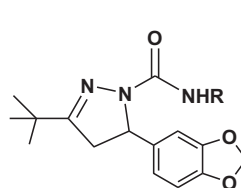
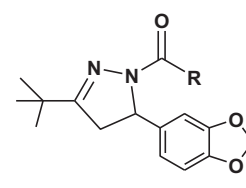
In this study, a group of 4-(benzyloxy)-1-phenylbut-2-yn-1-ol derivatives were designed using Site point connection method, synthesized and evaluated for their 5-Lipoxygenase (5-LOX) inhibitory activity.

**Design and synthesis of novel stiripentol analogues as potential anticonvulsants**

pp. 360–369

Mohamed N. Aboul-Enein*, Aida A. El-Azzouny, Mohamed I. Attia, Yousreya A. Maklad, Kamilia M. Amin, Mohamed Abdel-Rehim and Mohammed F. El-Beahry

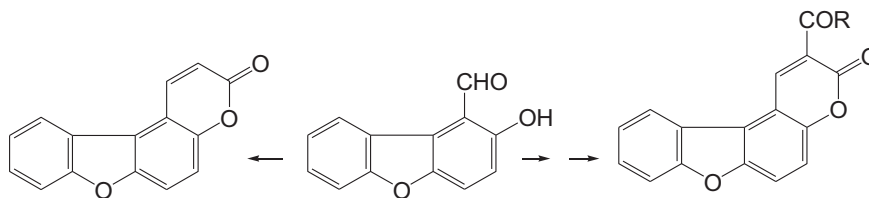
The synthesis and anticonvulsant activity of certain novel stiripentol analogues **7a–h**, (±) **8a–h**, and (±) **13a–f** are reported. The anticonvulsant potential of the prepared compounds was evaluated using subcutaneous pentylenetetrazole (scPTZ) and maximal electroshock seizures (MES) screens.

**7a-h**(±)-**8a-h**(±)-**13a-f**

Synthesis of novel benzofurocoumarin analogues and their anti-proliferative effect on human cancer cell lines

pp. 370–376

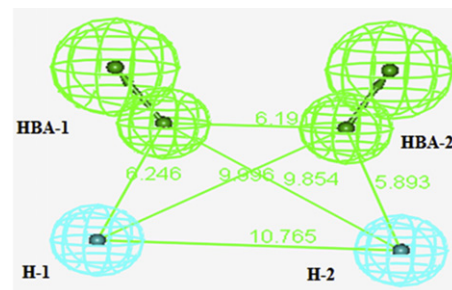
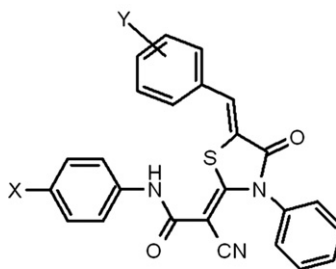
Carla S. Francisco, Lúcia R. Rodrigues, Nuno M.F.S.A. Cerqueira, Ana M.F. Oliveira-Campos and Lúcia M. Rodrigues*

**Stereoselective synthesis and QSAR study of cytotoxic 2-(4-oxo-thiazolidin-2-ylidene)-2-cyano-N-arylacetamides**

pp. 377–386

Riham F. George*

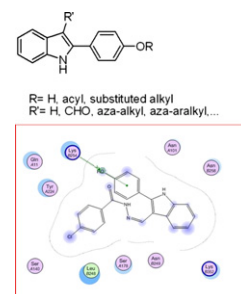
4-Thiazolidinones were prepared in a high stereo-selective manner and tested for their antitumor activity. Compound **4b** was the most effective agent against colon HCT116 and breast MCF7 cancer cell lines.

**Synthesis, molecular docking study and antitumor activity of novel 2-phenylindole derivatives**

pp. 387–398

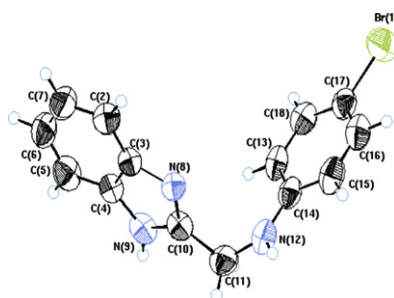
Sally S. El-Nakkady, Mona M. Hanna*, Hanaa M. Roaiah and Iman A.Y. Ghannam

Several 3-(un)substituted-2-phenylindoles were synthesized according to Schemes 1–3. Their antitumor activity was evaluated against MCF-7 cell line. Compound **3e** was more potent than vincristine. Docking study suggested their antitubulin activity.

**Novel palladium(II) and platinum(II) complexes with 1H-benzimidazol-2-ylmethyl-N-(4-bromo-phenyl)-amine: Structural studies and anticancer activity**

pp. 399–411

Nour T. Abdel Ghani and Ahmed M. Mansour*

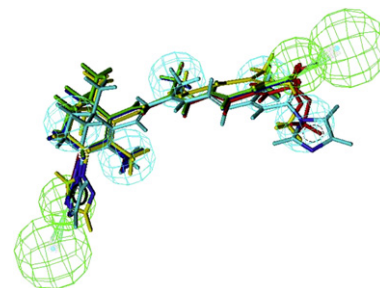


First chemical feature-based pharmacophore modeling of potent retinoidal retinoic acid metabolism blocking agents (RAMBAs): Identification of novel RAMBA scaffolds

pp. 412–423

Puranik Purushottamachar, Jyoti B. Patel, Lalji K. Gediya, Omoshile O. Clement and Vincent C.O. Njar*

Using the first chemical feature-based pharmacophore modeling of our retinoidal RAMBAs, we have identified novel RAMBAs with new scaffolds.

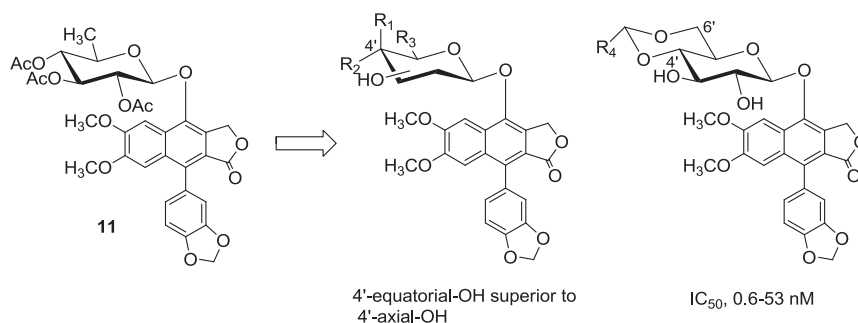


Design, synthesis and biological evaluation of novel glycosylated diphyllin derivatives as topoisomerase II inhibitors

pp. 424–431

Da-Kuo Shi, Wei Zhang, Ning Ding, Ming Li** and Ying-Xia Li*

A series of glycosylated diphyllin derivatives were designed for anti-tumor activity and SAR studies were revealed.

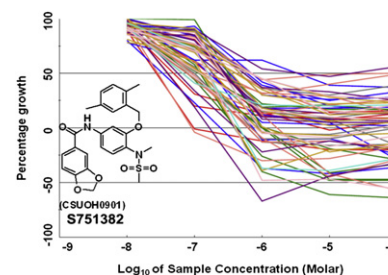


From COX-2 inhibitor nimesulide to potent anti-cancer agent: Synthesis, *in vitro*, *in vivo* and pharmacokinetic evaluation

pp. 432–444

Bo Zhong, Xiaohan Cai, Snigdha Chennamaneni, Xin Yi, Lili Liu, John J. Pink, Afshin Dowlati, Yan Xu, Aimin Zhou and Bin Su*

CSUOH0901, a non-COX-2 inhibitory derivative of COX-2 inhibitor nimesulide, significantly suppresses the growth of multiple cancer cell lines with IC₅₀s around 100–500 nM.

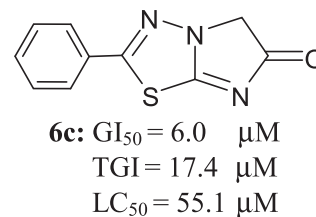


Novel 1,3,4-heterodiazole analogues: Synthesis and *in-vitro* antitumor activity

pp. 445–451

Azza T. Taher, Hanan H. Georgey* and Hussein I. El-Subbagh

The manuscript deals with the synthesis of 1,3,4-oxa/thiadiazole and their annelated imidazo[2,1-*b*]1,3,4-oxa/thiadiazolone derivatives. The obtained compounds were evaluated for their *in-vitro* antitumor activity.

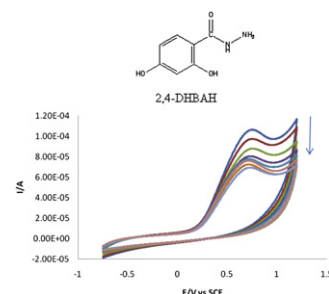


Electrochemical and spectroscopic investigations of isoniazide and its analogs with ds.DNA at physiological pH: Evaluation of biological activities

pp. 452–461

Nasima Arshad*, Uzma Yunus, Shumaila Razzque, Maliha Khan, Samreen Saleem, Bushra Mirza and Naghmana Rashid

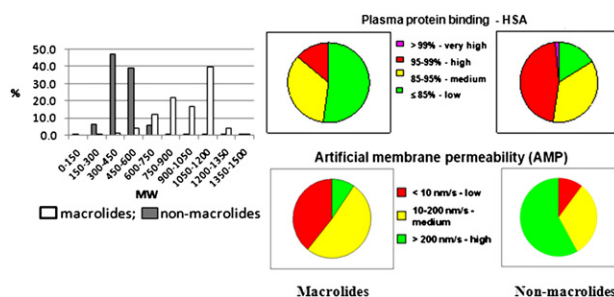
Isonicotinic acid hydrazide, pyrazine carboxylic acid hydrazide and 2,4-dihydroxy benzoic acid hydrazide showed good DNA binding ability *via* intercalation. All hydrazides have anti-oxidant potential, while 2,4-DHBAH showed promising anti-bacterial activities.



Physicochemical profile of macrolides and their comparison with small molecules

pp. 462–472

Višnja Stepanić*, Dinko Žiher, Vesna Gabelica-Marković, Dubravko Jelić, Shenaz Nunhuck, Klara Valko and Sanja Koštrun

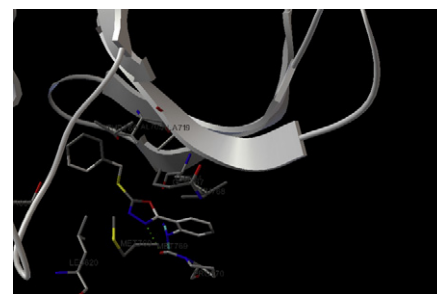


Synthesis, molecular modeling and biological evaluation of 2-(benzylthio)-5-aryloxadiazole derivatives as anti-tumor agents

pp. 473–478

Kai Liu, Xiang Lu, Hong-Jia Zhang, Juan Sun and Hai-Liang Zhu*

A series of 2-benzylthio-5-aryloxadiazole derivatives have been designed and synthesized, and their biological activities were also evaluated for EGFR inhibitory activity. Compound **3e** possessed the most potent biological activity ($IC_{50} = 1.09 \mu M$ for MCF-7 and $IC_{50} = 1.51 \mu M$ for EGFR). Docking simulation was performed to explore the binding model of compound **3e** with EGFR kinase.

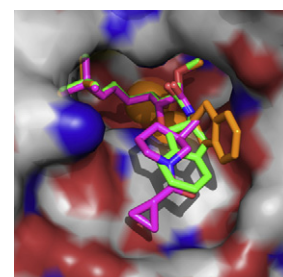


Structural analysis of inhibition of *Mycobacterium tuberculosis* methionine aminopeptidase by bengamide derivatives

pp. 479–484

Jing-Ping Lu, Xiu-Hua Yuan and Qi-Zhuang Ye*

The X-ray structures of tubercular methionine aminopeptidase in complex with different bengamide-derived inhibitors.

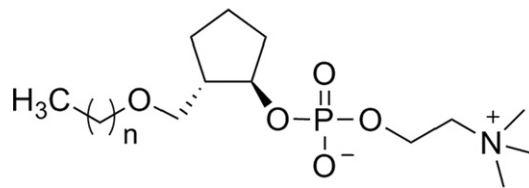


Synthesis and biological evaluation of cyclopentane-linked alkyl phosphocholines as potential anticancer agents that act by inhibiting Akt phosphorylation

pp. 485–492

Md. Maqsood Alam, Eun-Ha Joh, Yuri Kim, Yeon Il Oh, Jongki Hong,
Baek Kim, Dong-Hyun Kim and Yong Sup Lee*

The cyclopentane-linked alkylphosphocholines were synthesized. Compound **6d** was found to more potently inhibit Akt phosphorylation ($IC_{50} = 3.6 \mu M$) than miltefosine. This compound also exhibited potent cytotoxicity against A549 ($IC_{50} = 6.4 \mu M$).

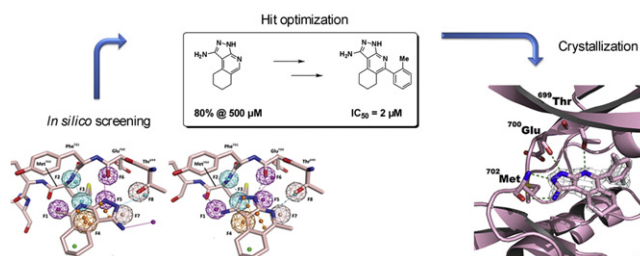


6a-e, $n = 11, 12, 17, 19, 21$

Fragment based lead discovery of small molecule inhibitors for the EPHA4 receptor tyrosine kinase

pp. 493–500

Oscar P.J. van Linden, Carine Farenc, Willem H. Zoutman, Liesbeth Hameetman, Maikel Wijtmans, Rob Leurs, Cornelis P. Tensen, Gregg Siegal and Iwan J.P. de Esch*

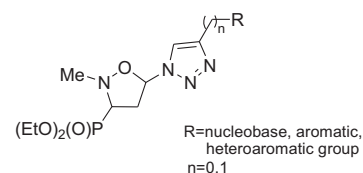


Design, synthesis, antiviral and cytostatic evaluation of novel isoxazolidine nucleotide analogues with a 1,2,3-triazole linker

pp. 501–509

Dorota G. Piotrowska*, Jan Balzarini and Iwona E. Głowacka

Inhibitory activity of cell proliferation for HEL cells as well as L1210, CEM and HeLa cells of several (1,2,3-triazolyl)isoxazolidine phosphonates was evaluated. The unsubstituted and fluoro-substituted phenyl derivatives appeared cytostatic (CC_{50} 40–250 μM).

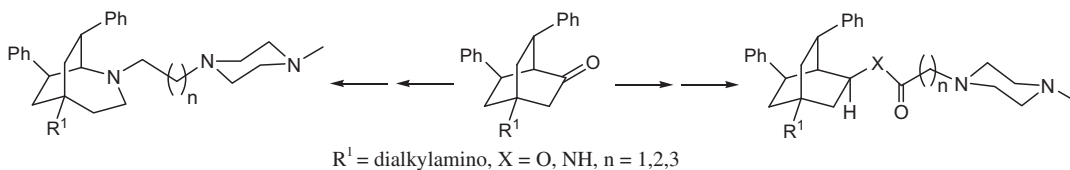


New N-methylpiperazinyl derivatives of bicyclic antiprotozoal compounds

pp. 510–519

Johanna Faist, Werner Seebacher, Robert Saf, Reto Brun, Marcel Kaiser and Robert Weis*

New compounds with increased antitrypanosomal and antiplasmodial activity

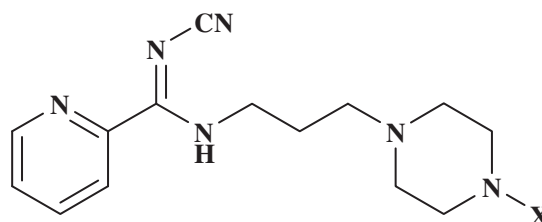


New potent 5-HT_{2A} receptor ligands containing an N'-cyanopicolinamidine nucleus: Synthesis and in vitro pharmacological evaluation

pp. 520–529

Ferdinando Fiorino, Beatrice Severino, Elisa Magli, Elisa Perissutti, Francesco Frecentese, Antonella Esposito, Giuseppina Maria Incisivo, Antonio Ciano, Paola Massarelli, Cristina Nencini, Vincenzo Santagada and Giuseppe Caliendo*

N'-cyanopicolinamidine derivatives were prepared to obtain a structure-affinity/selectivity relationship study between N'-cyanoisocotinamidine and the precedently synthesized N'-cyanopicolinamidine derivatives. N-(3-(4-(3-chlorophenyl)piperazin-1-yl)propyl)-N'-cyanopicolinamidine (**4I** K_i = 0.000185 nM) was the most active 5-HT_{2A} ligand.

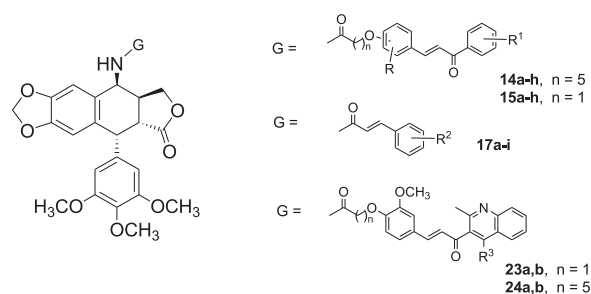


Synthesis and anticancer activity of 4β-alkylamidochalcone and 4β-cinnamido linked podophyllotoxins as apoptotic inducing agents

pp. 530–545

Ahmed Kamal*, Adla Mallareddy, Paidakula Suresh, V. Lakshma Nayak, Rajesh V.C.R.N.C. Shetti, N. Sankara Rao, Jaki R. Tamboli, Thokhir B. Shaik, M.V.P.S. Vishnuvardhan and S. Ramakrishna

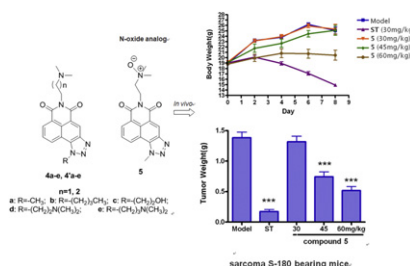
A series of 4β-alkylamidochalcone and 4β-cinnamido linked podophyllotoxins have been synthesized and evaluated for their anticancer activity and apoptotic inducing ability.



Unprecedented synthesis, in vitro and in vivo anti-cancer evaluation of novel triazolonaphthalimide derivatives

pp. 546–552

Shasha Li, Wenhe Zhong, Zhongjun Li* and Xiangbao Meng*

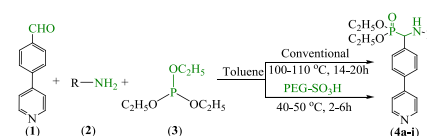


PEG-SO₃H catalyzed synthesis and cytotoxicity of α-aminophosphonates

pp. 553–559

C. Bhupendra Reddy, K. Suresh Kumar, M. Anil Kumar, M. Veera Narayana Reddy, B. Satheesh Krishna, M. Naveen, M.K. Arunasree, C. Suresh Reddy, C. Naga Raju and C. Devendranath Reddy*

PEG-SO₃H was found to be an efficient catalyst for the one pot synthesis of α-aminophosphonates with excellent yields. The cytotoxicity of the synthesized compounds was studied on K562, Colo205 and HEK 293.

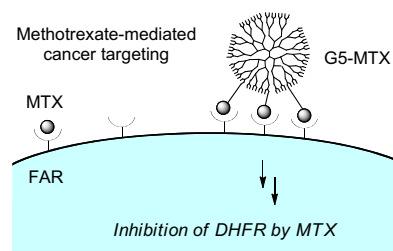


Dendrimer-based multivalent methotrexates as dual acting nanoconjugates for cancer cell targeting

pp. 560–572

Ming-Hsin Li, Seok Ki Choi*, Thommey P. Thomas, Ankur Desai, Kyung-Hoon Lee, Alina Kotlyar, Mark M. Banaszak Holl and James R. Baker, Jr.**

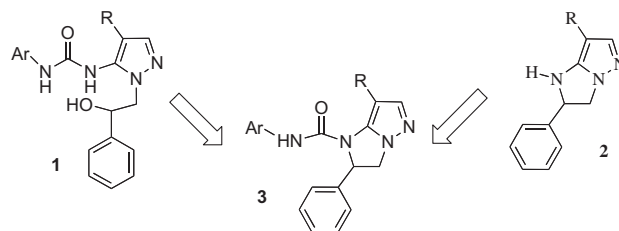
Nanotechnology platform for cancer-targeting drug delivery is designed by employing methotrexate (MTX) as a dual-acting cytotoxic molecule that targets folic acid receptor (FAR), a cancer surface biomarker.

**N-Aryl-2-phenyl-2,3-dihydro-imidazo[1,2-b]pyrazole-1-carboxamides 7-substituted strongly inhibiting both fMLP-OMe- and IL-8-induced human neutrophil chemotaxis**

pp. 573–579

Chiara Brullo, Susanna Spisani, Rita Selvatici and Olga Bruno*

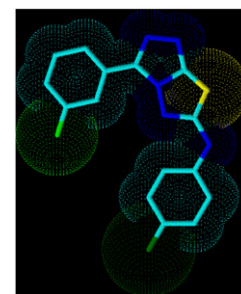
New N-aryl-2-phenyl-2,3-dihydro-imidazo[1,2-b]pyrazole-1-carboxamides 7-substituted able to inhibit at nanomolar concentration both fMLP-OMe- and IL8-induced neutrophil chemotaxis.

**PRELIMINARY COMMUNICATIONS****Studies on the synthesis and antibacterial activity of 3,6-disubstituted 1,2,4-triazolo[3,4-b][1,3,4-thiadiazoles**

pp. 580–584

Tomasz Plech*, Monika Wujec, Urszula Kosikowska, Anna Malm and Barbara Kaproń

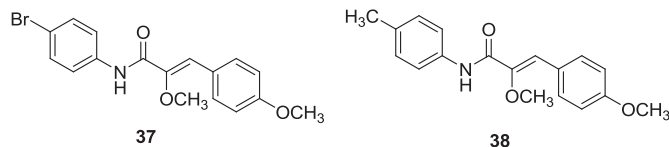
Two new derivatives (**5** and **6**) are as effective towards the MRSA strain as vancomycin.

**SHORT COMMUNICATIONS****Synthesis of novel cinnamanilides as potential immunosuppressive agents**

pp. 585–593

Lei Shi*, Lu Wang, Zhi Wang, Hai-Liang Zhu** and Qiao Song

A series of new cinnamanilides were synthesized and their immunosuppressive activities were evaluated. Compounds **37** and **38** exhibited most potent immunosuppressive activity ($IC_{50} = 1.77 \pm 0.33$ and $0.94 \pm 0.13 \mu M$).

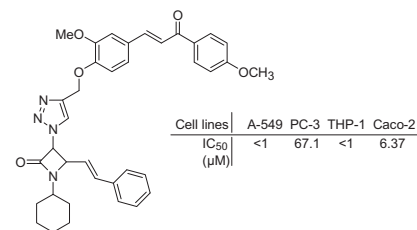


1,2,3-Triazole tethered β -lactam-Chalcone bifunctional hybrids: Synthesis and anticancer evaluation

pp. 594–600

Pardeep Singh, Raghu Raj, Vipin Kumar*, Mohinder P. Mahajan, P.M.S. Bedi, Tandeep Kaur and A.K. Saxena

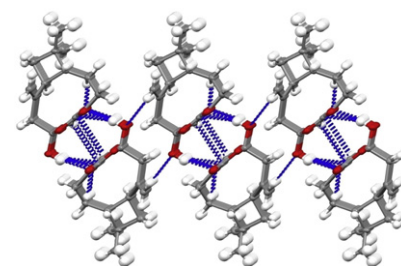
A series of β -lactam-chalcone bifunctional hybrids were synthesized and screened for their anti-cancer evaluation.

**A novel caryophyllene type sesquiterpene lactone from *Asparagus falcatus* (Linn.); Structure elucidation and anti-angiogenic activity on HUVECs**

pp. 601–607

Raza Murad Ghalib*, Rokiah Hashim, Othman Sulaiman, Sayed Hasan Mehdi, Arto Valkonen, Kari Rissanen, Srećko R. Trifunović, Mohamed. B. Khadeer Ahamed, Amin Malik Shah Abdul Majid and Fumio Kawamura

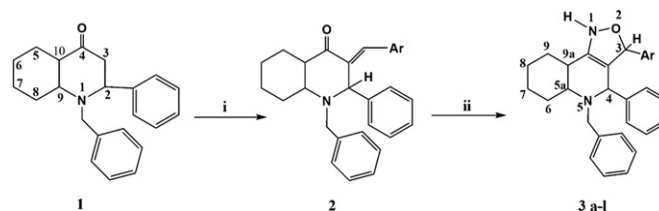
Here is a report of novel caryophyllene type sesquiterpene lactone from *Asparagus falcatus* (Linn.) with its anti-angiogenic activity on HUVECs.

**Isoxazoles incorporated N-substituted decahydroquinolines: A precursor to the next generation antimicrobial drug**

pp. 608–614

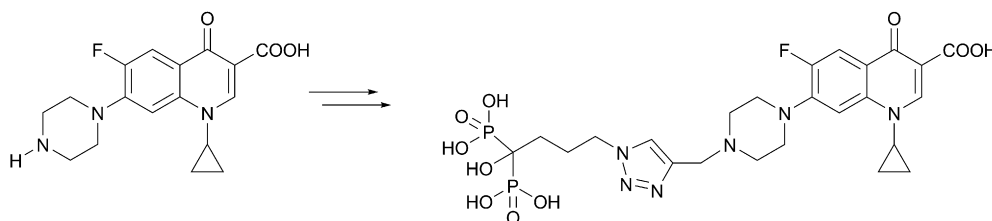
Mariappan Babu, Kasi Pitchumani and Penugonda Ramesh*

We report here a simple entry into N-substituted decahydroisoxazoloquinoline system containing a substituent at position 3, 4 and 5 using the readily available substrates and they were evaluated for antimicrobial activities against six bacterial and four fungal strains. Compounds **3b**, **3c**, **3e** (100 μ g/mL) exhibits excellent antifungal activity compared with the standard ketoconazole.

**Synthesis of osteotropic hydroxybisphosphonate derivatives of fluoroquinolone antibacterials**

pp. 615–618

James C. McPherson, III, Royce Runner, Thomas B. Buxton, John F. Hartmann, Dan Farcasiu, Ilona Bereczki, Erzsébet Róth, Szilvia Tollas, Eszter Ostorházi, Ferenc Rozgonyi and Pál Herczegh*

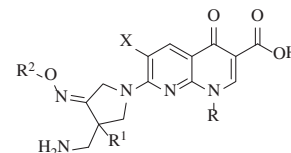


Synthesis and antibacterial activity of naphthyridone derivatives containing mono/difluoro-methyloxime pyrrolidine scaffolds

pp. 619–625

Kai Lv, Ming-Liang Liu*, Lian-Shun Feng, Lan-Ying Sun, Ye-Xin Sun, Zeng-Quan Wei and Hui-Quan Guo

A series of novel naphthyridone derivatives containing mono/difluoro-methyloxime pyrrolidine scaffolds were designed, synthesized. All of the target compounds have considerable antibacterial activity.

**RETRACTION NOTICE**

'Retraction notice to "Synthesis and biological screening of some novel amidocarbamate derivatives of ketoprofen" [Eur. J. Med. Chem. (2010) 3162–3168]'

p. 626

Prasanta Kumar Sahoo* and Pritishova Behera

COVER

This picture is taken from the review published in: European Journal of Medicinal Chemistry, 2010, Volume 45, Pages 2095–2116. The review is focused on the binding of inhibitors to the catalytic site of histone deacetylase © 2010 Published by Elsevier Masson SAS

* Corresponding authors.

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