

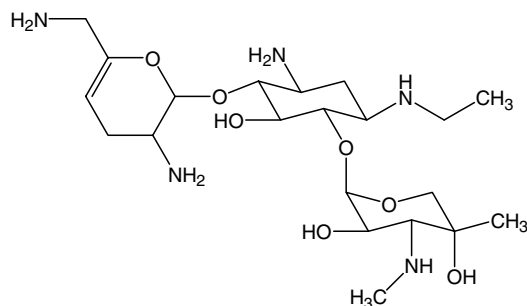
Contents

ARTICLES

Effect of melanin on netilmicin-induced inhibition of collagen biosynthesis in human skin fibroblasts pp 8155–8161

Ewa Buszman,* Dorota Wrześniok, Arkadiusz Surażyński, Jerzy Pałka and Katarzyna Mołęda

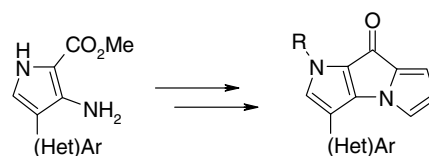
Effect of netilmicin and melanin on collagen and DNA biosynthesis was examined. The role of netilmicin–melanin complex was discussed in relation to aminoglycoside-induced ototoxicity.



Synthesis and biological evaluation of novel pyrrolopyrrolizinones as anticancer agents pp 8162–8175

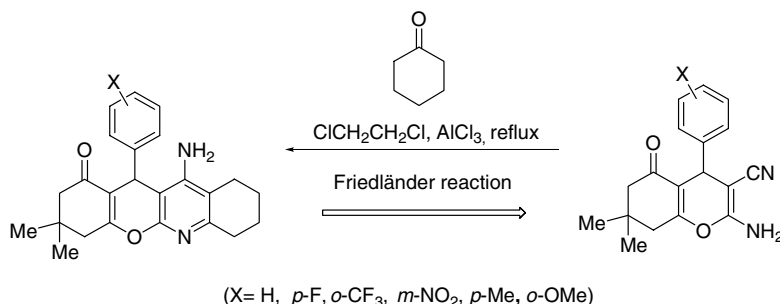
C. Rochais, V. Lisowski, P. Dallemagne and S. Rault*

We herein describe the synthesis of novel 3-(het)aryl-pyrrolo[2,3-*b*]pyrrolizin-8(1*H*)-ones starting from commercial (het)aryl-acetonitriles. A more convergent route was also described through the first synthesis of ethyl 3-amino-4-bromo-1*H*-pyrrole-2-carboxylate **17**. The antiproliferative activities of these compounds were tested toward various cell lines and one of them **10k** shows interesting cytotoxic properties, although it was less potent than our lead compound in thiophene series **1k**.



New multipotent tetracyclic tacrines with neuroprotective activity pp 8176–8185

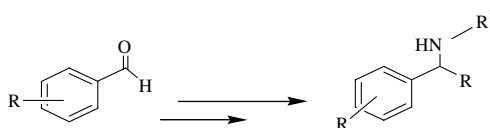
José Marco-Contelles,* Rafael León,* Cristóbal de los Ríos, Antonio G. García, Manuela G. López and Mercedes Villarroya*



Synthesis and antitubercular activity of substituted phenylmethyl- and pyridylmethyl amines

pp 8186–8196

R. P. Tripathi,* Nisha Saxena, V. K. Tiwari, S. S. Verma, Vinita Chaturvedi, Y. K. Manju, A. K. Srivastva, A. Gaikwad and S. Sinha



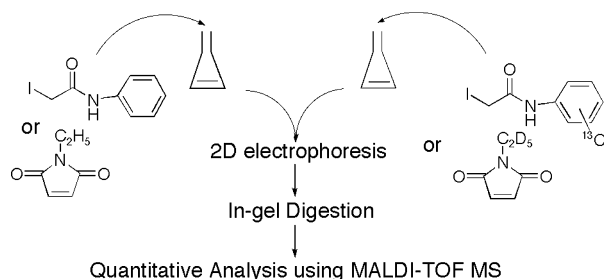
A number of benzyl- and pyridylmethyl amines were synthesized and evaluated against *Mycobacterium tuberculosis* H37Rv strains. The potent compounds were evaluated against clinical isolates of MDR TB and found to be active at one or other concentrations. The MIC was found to be as low as 1.56 µg/mL.

Quantitative proteome analysis using D-labeled N-ethylmaleimide and ¹³C-labeled iodoacetanilide by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry

pp 8197–8209

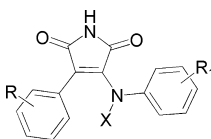
Sadamu Kurono, Tamie Kurono, Naoka Komori, Satomi Niwayama* and Hiroyuki Matsumoto*

A practical method for quantitative analysis of proteins has been developed applying small organic molecule isotope-labeling reagents and 2D electrophoresis as well as MALDI-TOF-MS.

**Probing the physicochemical and structural requirements for glycogen synthase kinase-3α inhibition: 2D-QSAR for 3-anilino-4-phenylmaleimides**

pp 8210–8218

Prasanna Sivaprakasam, Aihua Xie and Robert J. Doerksen*

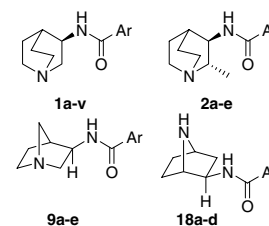


GSK-3 is a potential target for the treatment of Alzheimer's disease, type 2 diabetes, cancer, stroke, bipolar disorder and malaria. A recent study showed that inhibiting the α isoform is most promising in the treatment of Alzheimer's disease. We have prepared a series of robust, systematic, quantitative structure–activity relationship models analyzing important features of GSK-3α inhibition by maleimides.

**Design, synthesis, structure–activity relationship, and in vivo activity of azabicyclic aryl amides as α7 nicotinic acetylcholine receptor agonists**

pp 8219–8248

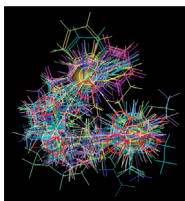
Daniel P. Walker, Donn G. Wishka, David W. Piotrowski, Shaojuan Jia, Steven C. Reitz, Karen M. Yates, Jason K. Myers, Tatiana N. Vetman, Brandon J. Margolis, E. Jon Jacobsen, Brad A. Acker, Vincent E. Groppi, Mark L. Wolfe, Bruce A. Thornburgh, Paula M. Tinholt, Luz A. Cortes-Burgos, Rodney R. Walters, Matthew R. Hester, Eric P. Seest, Lester A. Dolak, Fusen Han, Barbara A. Olson, Laura Fitzgerald, Brian A. Staton, Thomas J. Raub, Mihaly Hajos, William E. Hoffmann, Kai S. Li, Nicole R. Higdon, Theron M. Wall, Raymond S. Hurst, Erik H. F. Wong and Bruce N. Rogers*



Synthesis of some substituted pyrazinopyridoindoles and 3D QSAR studies along with related compounds: Piperazines, piperidines, pyrazinoisoquinolines, and diphenhydramine, and its semi-rigid analogs as antihistamines (H₁)

pp 8249–8258

Mridula Saxena, Stuti Gaur, Philip Prathipati and Anil K. Saxena*

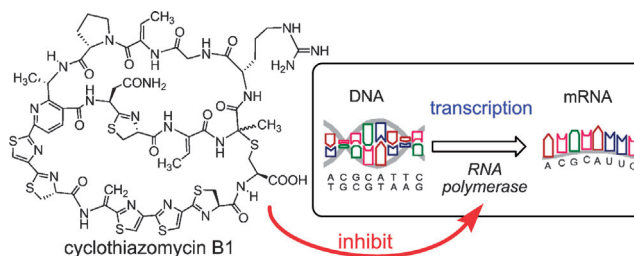


A pharmacophoric model with three biophoric and six secondary sites explaining well the variation in activity and three new antihistamines H₁ with low toxicity and sedation potential are described.

An RNA polymerase inhibitor, cyclothiazomycin B1, and its isomer

pp 8259–8270

Masaru Hashimoto,* Takanori Murakami, Katsuyuki Funahashi, Takashi Tokunaga, Ken-ichi Nihei, Toshikatsu Okuno, Takatsugu Kimura, Hideo Naoki and Hyouta Himeno



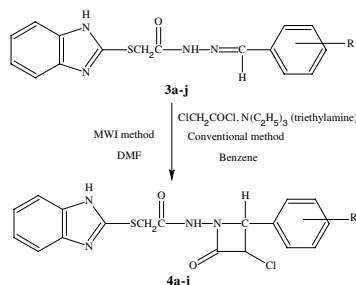
The title compounds were revealed. These potentially exhibited DNA-dependent RNA synthesis.



Green route for the heterocyclization of 2-mercaptobenzimidazole into β -lactum segment derivatives containing –CONH– bridge with benzimidazole: Screening in vitro antimicrobial activity with various microorganisms

pp 8271–8279

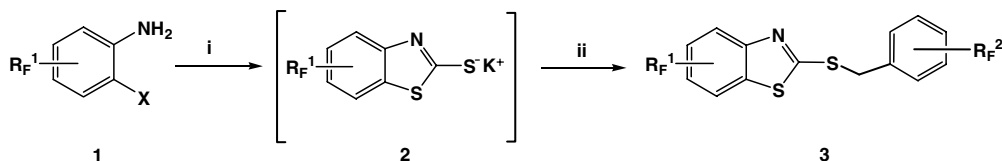
Krunal G. Desai* and Kishor R. Desai



Microwave-assisted, one-pot syntheses and fungicidal activity of polyfluorinated 2-benzylthiobenzothiazoles

pp 8280–8285

Wei Huang and Guang-Fu Yang*



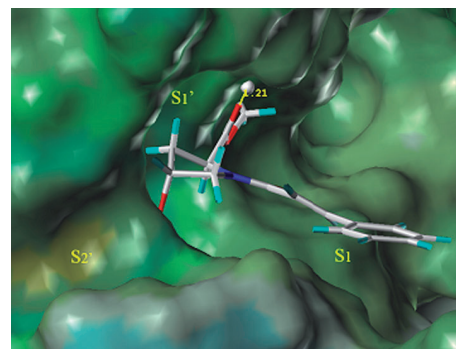
Reagents and conditions: (i) potassium *O*-ethyl dithiocarbonate, DMF, MW, 120 °C; (ii) benzyl bromide, MW, 90 °C.

Design, synthesis and preliminary evaluation of new cinnamoyl pyrrolidine derivatives as potent gelatinase inhibitors

pp 8286–8294

Li Zhang, Jie Zhang, Hao Fang, Qiang Wang and Wenfang Xu*

The FlexX docking of compound **A8** with MMP. The synthesis and preliminary biological evaluation of cinnamoyl pyrrolidine derivatives as MMPs inhibitors are reported in this paper. Compound **A8** showed the lowest IC_{50} at 5.2 nM, indicating that it might be a promising lead compound.

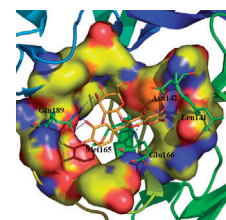


Binding interaction of quercetin-3- β -galactoside and its synthetic derivatives with SARS-CoV 3CL^{pro}: Structure–activity relationship studies reveal salient pharmacophore features

pp 8295–8306

Lili Chen, Jian Li, Cheng Luo, Hong Liu, Weijun Xu, Gang Chen, Oi Wah Liew, Weiliang Zhu,* Chum Mok Puah,* Xu Shen* and Hualiang Jiang

A new class of compounds that have been designed and synthesized based on a natural product, quercetin-3- β -galactoside, has been discovered to be effective inhibitors of SARS coronavirus 3CL protease (SARS-CoV 3CL^{pro}), which could be developed as drug leads for SARS.

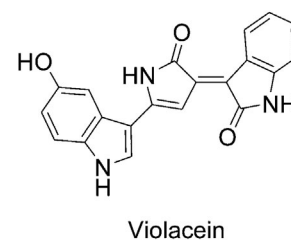


Antioxidant properties of violacein: Possible relation on its biological function

pp 8307–8313

Marlon Konzen, Daniela De Marco, Clarissa A. S. Cordova, Tiago O. Vieira, Regina V. Antônio and Tânia B. Creczynski-Pasa*

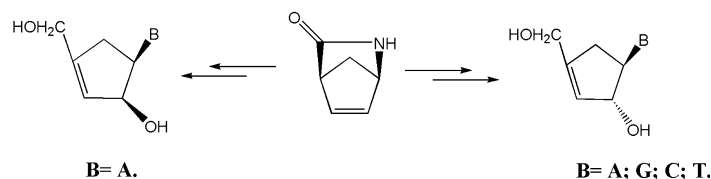
Chromobacterium violaceum has attracted much attention in recent literature due to its genome elucidation. In this work we report violacein (a pigment produced by the bacterium) antioxidant efficiency against oxygen and nitrogen reactive species and to inhibit the myeloperoxidase (MPO) activity. Additionally we show that violacein reconstituted into liposomes has its antioxidant potential increased. We suggest a possible role of the pigment for the microorganism.



Synthesis of neplanocin F analogues as potential antiviral agents

pp 8314–8322

Hongwang Zhang, Raymond F. Schinazi and Chung K. Chu*

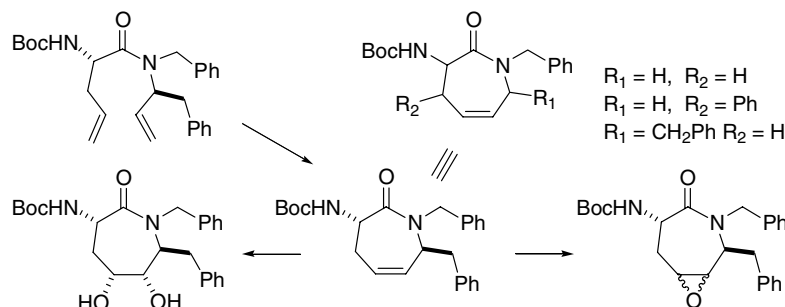


Neplanocin F is a natural carbocyclic nucleoside. Herein, we describe the synthesis and antiviral activity of (\pm)-5'-deoxy-neplanocin F analogues. The key intermediate **4**, synthesized from the commercially available (\pm)-2-azabicyclo[2.2.1]-hept-5-en-3-one (ABH), was utilized to prepare the target nucleosides. Among the target compounds, 5'-deoxyneplanocin F adenine exhibited moderate anti-HIV activity in human lymphocytes without any marked cytotoxicity.

Synthesis of amino acid derived seven-membered lactams by RCM and their evaluation against HIV protease

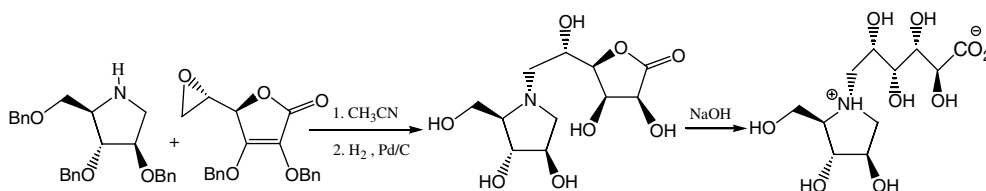
pp 8323–8331

Shazia Zaman, Pietro Campaner and Andrew D. Abell*

**Synthesis, enzymatic activity, and X-ray crystallography of an unusual class of amino acids**

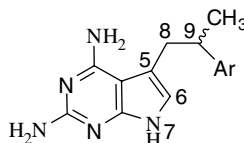
pp 8332–8340

Wang Chen, Douglas A. Kuntz, Tamika Hamlet, Lyann Sim, David R. Rose and B. Mario Pinto*

**Novel non-classical C9-methyl-5-substituted-2,4-diaminopyrrolo[2,3-d]pyrimidines as potential inhibitors of dihydrofolate reductase and as anti-opportunistic agents**

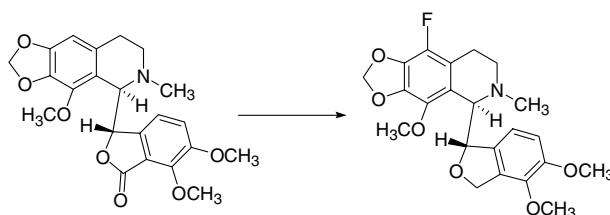
pp 8341–8351

Aleem Gangjee,* Jie Yang and Sherry F. Queener

**Synthesis and biological evaluation of a cyclic ether fluorinated noscapine analog**

pp 8352–8358

Ritu Aneja,* Surya N. Vangapandu and Harish C. Joshi

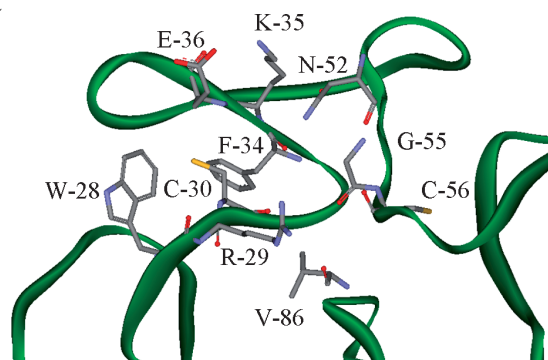


Structure of C-terminal fragment of merozoite surface protein-1 from *Plasmodium vivax* determined by homology modeling and molecular dynamics refinement

pp 8359–8365

María Luisa Serrano,* Hilda A. Pérez and J. D. Medina

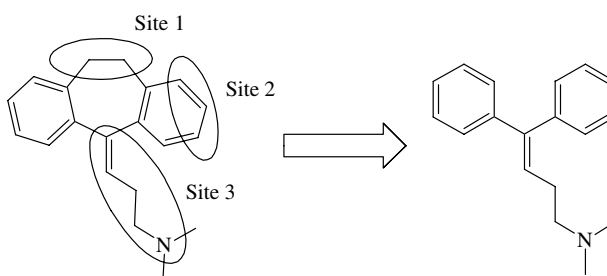
The C-terminal merozoite surface protein-1 from *Plasmodium vivax* was determined by a combined use of various molecular modeling techniques. The main binding pocket was determined by CASTp. Corrections reported to the sequence of PvMSP-1₁₉ Belem strain were also inspected.



Discovery of diphenyl amine based sodium channel blockers, effective against hNa_v1.2

pp 8366–8378

Debjani P. Hudgens, Catherine Taylor, Timothy W. Batts, Manoj K. Patel and Milton L. Brown*

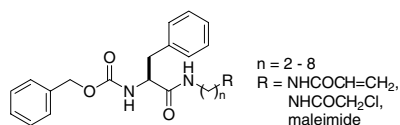


Modification of an amitriptyline scaffold has provided a potent class of diphenyl amine sodium channel blockers.

Synthesis and evaluation of peptidic irreversible inhibitors of tissue transglutaminase

pp 8379–8385

Christophe Pardin, Steve M. F. G. Gillet and Jeffrey W. Keillor*

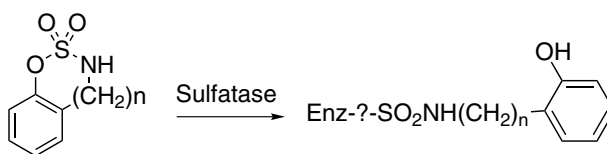


Eight novel irreversible inhibitors of tissue transglutaminase were prepared and evaluated, bearing alkyl chains of varied length and different pharmacophores.

Synthesis and evaluation of general mechanism-based inhibitors of sulfatases based on (difluoro)methyl phenyl sulfate and cyclic phenyl sulfamate motifs

pp 8386–8395

Sarah R. Hanson, Lisa J. Whalen and Chi-Huey Wong*

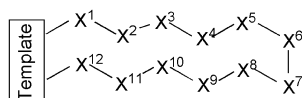


Sulfatases are emerging as an important class of enzymes that modulate the activity of a variety of small molecules and complex glycans by cleaving sulfate esters. Herein, general mechanism-based inhibitors modeled from commonly accepted phenyl sulfate substrates of this enzyme class were designed and evaluated. Phenyl cyclic sulfamate motifs were found to be novel specific-irreversible inhibitors that will be useful for probing the catalytic mechanism of sulfatases.

Discovery of novel, highly potent and selective β -hairpin mimetic CXCR4 inhibitors with excellent anti-HIV activity and pharmacokinetic profiles

pp 8396–8404

Steven J. DeMarco, Heiko Henze, Alexander Lederer, Kerstin Moehle, Reshmi Mukherjee, Barbara Romagnoli, John A. Robinson, Federico Brianza, Frank O. Gombert, Sergio Lociuoro, Christian Ludin, Jan Willem Vrijbloed, Jürg Zumbunn, Jean-Pierre Obrecht, Daniel Obrecht,* Vincent Brondani, François Hamy and Thomas Klimkait

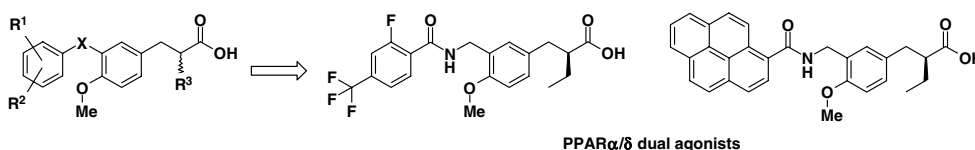


Protein epitope mimetics (PEM) of Polyphemus II act as highly potent CXCR4 inhibitors with good in vivo pharmacokinetic properties.

Design, synthesis, and evaluation of a novel series of α -substituted phenylpropanoic acid derivatives as human peroxisome proliferator-activated receptor (PPAR) α/δ dual agonists for the treatment of metabolic syndrome

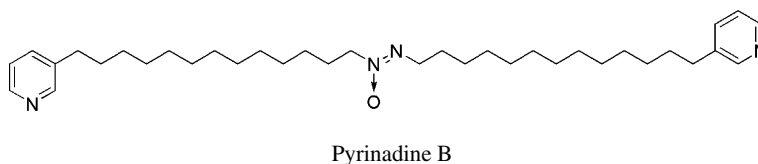
pp 8405–8414

Jun-ichi Kasuga, Daisuke Yamasaki, Yoko Araya, Aya Nakagawa, Makoto Makishima, Takefumi Doi, Yuichi Hashimoto and Hiroyuki Miyachi*


Pyrinadines B–G, new bis-pyridine alkaloids with an azoxy moiety from sponge *Cribrochalina* sp.

pp 8415–8419

Yuuko Kariya, Takaaki Kubota, Jane Fromont and Jun'ichi Kobayashi*



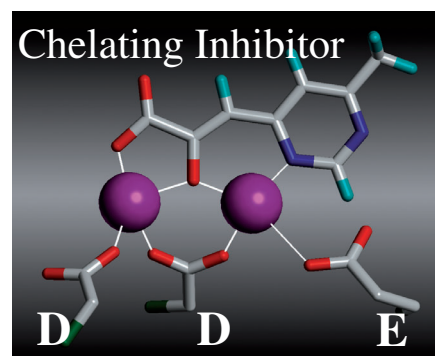
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A platform for designing HIV integrase inhibitors. Part 2: A two-metal binding model as a potential mechanism of HIV integrase inhibitors

pp 8420–8429

Takashi Kawasuji,* Masahiro Fuji, Tomokazu Yoshinaga, Akihiko Sato, Tamio Fujiwara and Ryuichi Kiyama

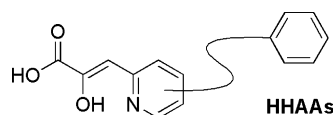
For advanced understanding of mechanism of chelating inhibitors.



A platform for designing HIV integrase inhibitors. Part 1: 2-Hydroxy-3-heteroaryl acrylic acid derivatives as novel HIV integrase inhibitor and modeling of hydrophilic and hydrophobic pharmacophores

pp 8430–8445

Takashi Kawasuji,* Tomokazu Yoshinaga, Akihiko Sato, Mitsuaki Yodo, Tamio Fujiwara and Ryuichi Kiyama

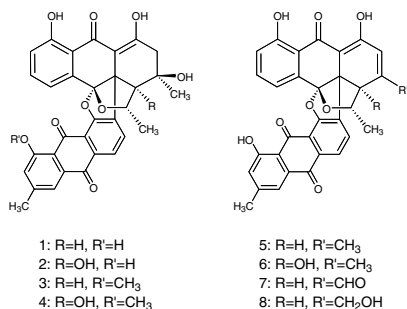


A novel class of HIV integrase inhibitors and a critical pharmacophore model useful for designing other classes of inhibitors.

New bisanthraquinone antibiotics and semi-synthetic derivatives with potent activity against clinical *Staphylococcus aureus* and *Enterococcus faecium* isolates

pp 8446–8454

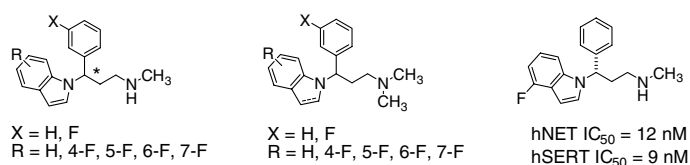
Aaron M. Socha, Kerry L. LaPlante and David C. Rowley*



Synthesis and activity of a new class of dual acting norepinephrine and serotonin reuptake inhibitors: 3-(1*H*-indol-1-yl)-3-arylpropan-1-amines

pp 8455–8466

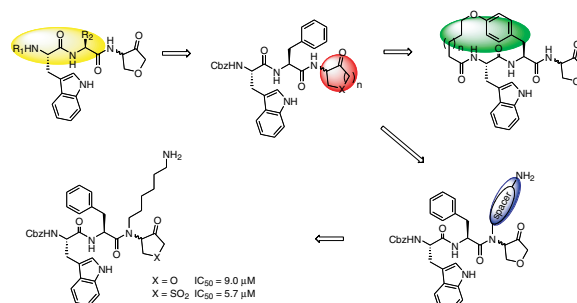
Paige E. Mahaney,* An T. Vu, Casey C. McComas, Puwen Zhang, Lisa M. Nogle, William L. Watts, Ani Sarkahian, Liza Leventhal, Nicole R. Sullivan, Albert J. Uveges and Eugene J. Trybulski



Structure–activity studies of cyclic ketone inhibitors of the serine protease plasmin: Design, synthesis, and biological activity

pp 8467–8487

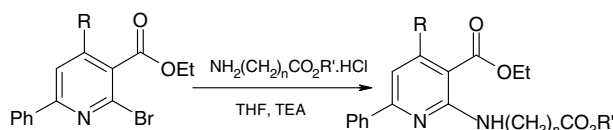
Fengtian Xue and Christopher T. Seto*



Synthesis of novel vasodilatory active nicotinate esters with amino acid function

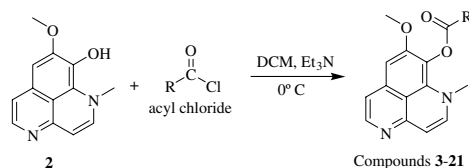
pp 8488–8494

Adel S. Girgis,* Atef Kalmouch and Mohey Ellithey

**Modification at the C9 position of the marine natural product isoaptamine and the impact on HIV-1, mycobacterial, and tumor cell activity**

pp 8495–8505

Waseem Gul, Nicholas L. Hammond, Muhammad Yousaf, John J. Bowling, Raymond F. Schinazi, Susan S. Wirtz, Garcia de Castro Andrews, Carmen Cuevas and Mark T. Hamann*



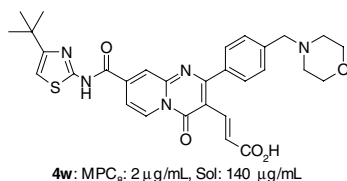
A series of isoaptamine analogs were prepared at the C9 position of isoaptamine (**2**) and were evaluated for their biological activity against HIV-1, Mtb, AIDS-OI, tropical parasitic diseases, and cancer.

**MexAB-OprM specific efflux pump inhibitors in *Pseudomonas aeruginosa*.**

pp 8506–8518

Part 6: Exploration of aromatic substituents

Ken-ichi Yoshida,* Kiyoshi Nakayama, Yoshihiro Yokomizo, Masami Ohtsuka, Makoto Takemura, Kazuki Hoshino, Hiroko Kanda, Kenji Namba, Hironobu Nitani, Jason Z. Zhang, Ving J. Lee and William J. Watkins

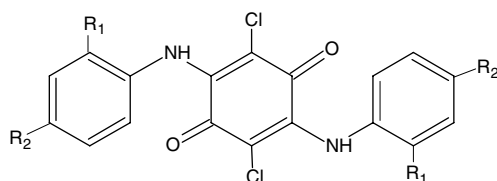


A series of 2-aryl-substituted pyridopyrimidine derivatives were synthesized by palladium catalyzed cross-coupling reaction and evaluated for their ability to potentiate the activity of Levofloxacin and Aztreonam in *Pseudomonas aeruginosa*.

An efficient synthesis and biological activity of substituted *p*-benzoquinones

pp 8519–8526

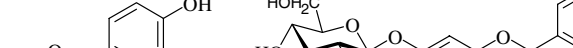
Manoj Batra,* Prashant Kriplani, Chhavi Batra and K. G. Ojha



Comparative profile of synthesis of substituted-*p*-benzoquinones is described. The synthesized compounds were screened for antibacterial and 'in vitro' antitumour activity.

pp 8527–8532

pp 8533–8538



Luteolin
 R = OH, Luteolin 7-O-glucoside
 R = H, Apigenin 7-O-glucoside

The phenolic compounds in '*alcaparra*' table olives were determined by reversed-phase HPLC/DAD and a study on its extracts antimicrobial activity is presented.

pp 8539–8549

pp 8550–8563

[0,0]-rhodacyanine

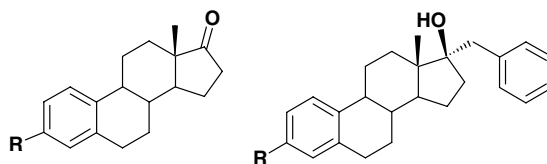
[1,0]-rhodacyanine

[0,0,0]-rhodacyanine

Boronic acids as inhibitors of steroid sulfatase

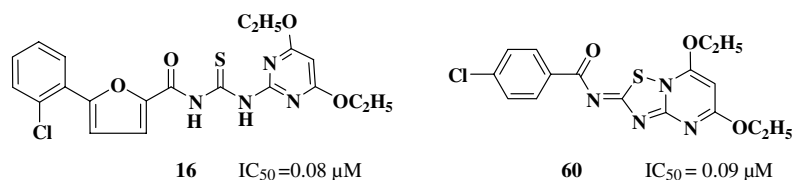
pp 8564–8573

Vanessa Ahmed, Yong Liu, Cassandra Silvestro and Scott D. Taylor*

R = B(OH)₂, competitive inhibitor
of steroid sulfatase K_i = 2.8 μMR = OH, noncompetitive inhibitor
of steroid sulfatase K_i = 63 μM,R = B(OH)₂, noncompetitive inhibitor
of steroid sulfatase, K_i = 0.25 μM, pH 7.0R = OH, noncompetitive inhibitor
of steroid sulfatase, K_i = 0.25 μM, pH 7.0**Synthesis and evaluation of a new series of substituted acyl(thio)urea and thiadiazolo [2,3-*a*] pyrimidine derivatives as potent inhibitors of influenza virus neuraminidase**

pp 8574–8581

Chuanwen Sun, Xiaodong Zhang, Hai Huang and Pei Zhou*

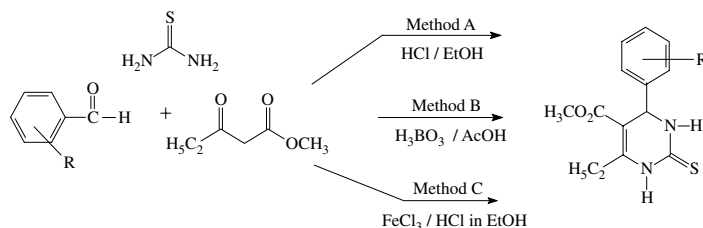


A series of substituted acyl(thio)urea and substituted acylimine derivatives were designed and prepared. Both of their cell culture and enzymatic activity against influenza virus were investigated and they were evaluated as potent neuraminidase inhibitors. Derivatives **16** and **60** were further investigated as potential candidates for future development.

Synthesis of 4-aryl-3,4-dihydropyrimidin-2(1*H*)-thione derivatives as potential calcium channel blockers

pp 8582–8589

İnci Selin Zorkun, Selma Saraç,* Semra Çelebi and Kevser Erol

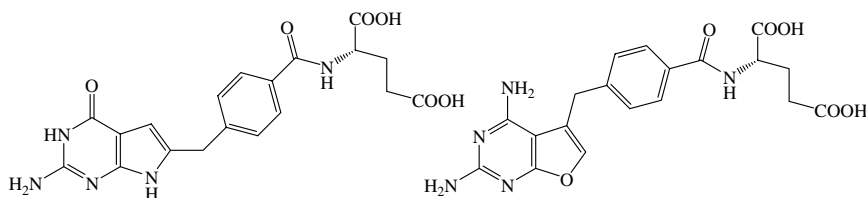


4-Aryl-3,4-dihydropyrimidin-2(1*H*)-thiones were synthesized by Lewis acid-catalyzed Biginelli condensation (Methods B and C). Dihydropyrimidin-2-thiones were obtained in significantly better reaction yields and shorter reaction times than those utilizing the conventional HCl/ethanol method (Method A). The calcium channel blocker activity of the compounds was evaluated.

Synthesis and evaluation of a classical 2,4-diamino-5-substituted-furo[2,3-*d*]pyrimidine and a 2-amino-4-oxo-6-substituted-pyrrolo[2,3-*d*]pyrimidine as antifolates

pp 8590–8598

Aleem Gangjee,* Jie Yang, John J. McGuire and Roy L. Kisliuk

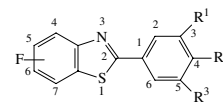


Synthesis of carbon-11 labeled fluorinated 2-arylbenzothiazoles as novel potential PET cancer imaging agents

pp 8599–8607

Min Wang, Mingzhang Gao, Bruce H. Mock, Kathy D. Miller, George W. Sledge, Gary D. Hutchins and Qi-Huang Zheng*

Synthesis of carbon-11 labeled fluorinated 2-arylbenzothiazoles as novel potential PET cancer imaging agents is reported.

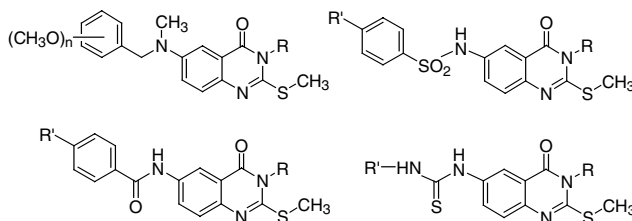


3-[¹¹C]6b: 4-F, R¹=O¹¹CH₃, R²=OCH₃, R³=H
 4-[¹¹C]11c: 5-F, R¹=OCH₃, R²=O¹¹CH₃, R³=H
 3-[¹¹C]11e: 5-F, R¹=O¹¹CH₃, R²=OCH₃, R³=H
 5-[¹¹C]11f: 5-F, R¹=OCH₃, R²=OCH₃, R³=O¹¹CH₃
 4-[¹¹C]11f: 5-F, R¹=OCH₃, R²=O¹¹CH₃, R³=OCH₃
 4-[¹¹C]11i: 6-F, R¹=OCH₃, R²=O¹¹CH₃, R³=H
 3-[¹¹C]11i: 6-F, R¹=O¹¹CH₃, R²=OCH₃, R³=H
 5-[¹¹C]11i: 6-F, R¹=OCH₃, R²=OCH₃, R³=O¹¹CH₃
 4-[¹¹C]11i: 6-F, R¹=OCH₃, R²=O¹¹CH₃, R³=OCH₃

Synthesis, dihydrofolate reductase inhibition, antitumor testing, and molecular modeling study of some new (3H)-quinazolinone analogs

pp 8608–8621

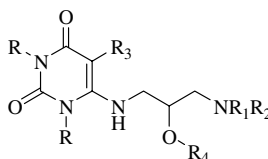
Sarah T. Al-Rashood, Ihsan A. Aboldahab, Mahmoud N. Nagi, Laila A. Abouzeid, Alaa A. M. Abdel-Aziz, Sami G. Abdel-hamide, Khairia M. Youssef, Abdulrahman M. Al-Obaid and Hussein I. El-Subbagh*



Anti-cancer activities of 5-acyl-6-[2-hydroxy/benzyloxy-3-(amino)-propylamino]-1,3-dialkyl-1H-pyrimidin-2,4-diones

pp 8622–8625

Palwinder Singh* and Kamaldeep Paul



R = CH₃, CH₂Ph; R₁R₂ = 1-pyrrolidinyl, 1-piperidinyl, 4-morpholinyl;
 R₃ = H, C(=O)Ph; R₄ = H, C(=O)Ph

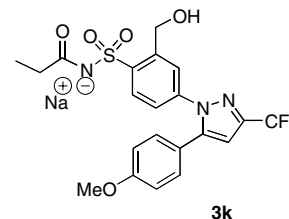
Two of the nine pyrimidine derivatives investigated here show promising anti-cancer activities.

Identification of 2-hydroxymethyl-4-[5-(4-methoxyphenyl)-3-trifluoromethyl-pyrazol-1-yl]-N-propionylbenzenesulfonamide sodium as a potential COX-2 inhibitor for oral and parenteral administration

pp 8626–8634

Sunil Kumar Singh,* Saibaba Vobbalareddy, Srinivasa Rao Kalleda, Seshagiri Rao Casturi, Srinivasa Raju Datla, Rao N. V. S. Mamidi, Ramesh Mullangi, Rajagopalan Ramanujam, Koteswar Rao Yeleswarapu and Javed Iqbal*

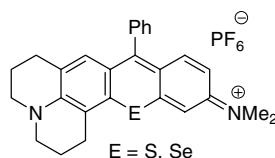
Synthesis and biological evaluation of the prodrugs of a potent COX-2 inhibitor of 1,5-diarylpyrazole class are described. Through this exercise, N-propionyl sulfonamide sodium **3k** has been identified as a potential candidate for oral as well as parenteral administration.



A cationic chalcogenoxanthylum photosensitizer effective in vitro in chemosensitive and multidrug-resistant cells

pp 8635–8643

Jason J. Holt, M. K. Gannon, II, Gregory Tomblin, Taylor A. McCarty, Phillip M. Page, Frank V. Bright and Michael R. Detty*



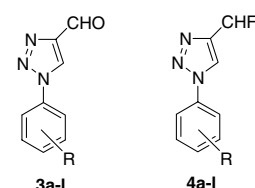
Thio- and seleno-analogues of tetramethylrosamine with a julolidyl fragment replacing one NMe₂ group were evaluated as photosensitizers toward chemosensitive AUXB1 and multidrug-resistant CR1R12 cells.

Synthesis, tuberculosis inhibitory activity, and SAR study of N-substituted-phenyl-1,2,3-triazole derivatives

pp 8644–8653

Marilia S. Costa, Núbia Boechat, Érica A. Rangel, Fernando de C. da Silva, Alessandra M. T. de Souza, Carlos R. Rodrigues, Helena C. Castro, Ivan N. Junior, Maria Cristina S. Lourenço, Solange M. S. V. Wardell and Vitor F. Ferreira*

Tuberculosis (TB) is caused by *Mycobacterium tuberculosis* and remains as a leading cause of mortality worldwide. The in vitro anti-tuberculosis screening of two series of 1,2,3-triazole compounds showed that all compounds were active, although in general **3a–l** were more effective than **4a–l**. SAR study indicated the importance of the hydrogen bond acceptor subunit **3a–l**, the position in the aromatic ring, the planarity of triazole and phenyl rings, and the uniform HOMO coefficient distribution for the anti-tubercular activity.



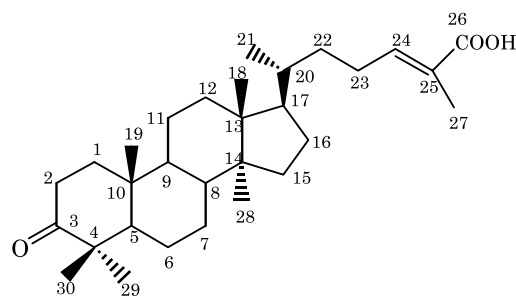
a. R = 3,5-diCl; b. R = 3-CN; c. R = 4-CN; d. R = 2-OCH₃; e. R = 4-OCH₃; f. R = 2,5-(OCH₃)₂; g. R = 3,4-(OCH₃)₂; h. R = 3-Cl; i. R = 4-Cl; j. R = 4-Br; k. R = 4-CH₃; l. R = 4-NO₂

Structure–activity relationship for inhibition of 5 α -reductase by triterpenoids isolated from *Ganoderma lucidum*

pp 8654–8660

Jie Liu, Kenji Kurashiki, Kuniyoshi Shimizu and Ryuichiro Kondo*

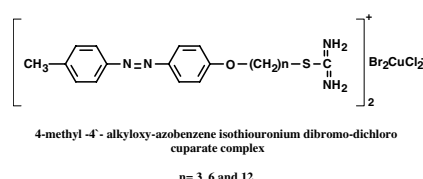
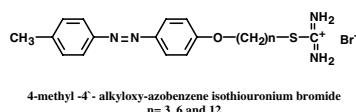
The structure–activity relationship of triterpenoids, which isolated from the ethanol extract of *Ganoderma lucidum*, is reported. Triterpenoids isolated from ethanol extracts of *Ganoderma lucidum* (Fr.) Krast (Ganodermataceae) inhibited 5 α -reductase activity. The presence of the C-3 carbonyl group and of the C-26- α,β -unsaturated carbonyl group was characteristic of almost all inhibitors isolated from *G. lucidum*.



Surface and biocidal activity of some synthesized metallo azobenzene isothiuronium salts

pp 8661–8665

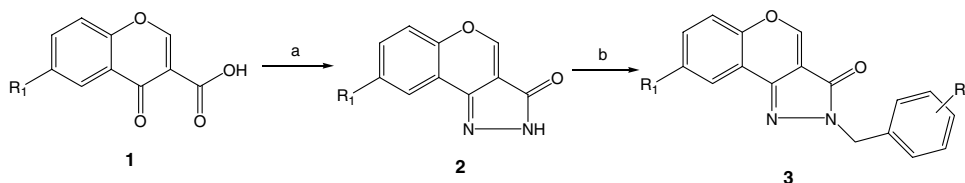
A. M. Badawi, E. M. S. Azzam* and S. M. I. Morsy



Insecticidal lead identification by screening benzopyrano[4,3-*c*]-pyrazol-3(2*H*)-ones library constructed from multiple-parallel synthesis under microwave irradiation

pp 8666–8674

Zhong-Zheng Zhou and Guang-Fu Yang*



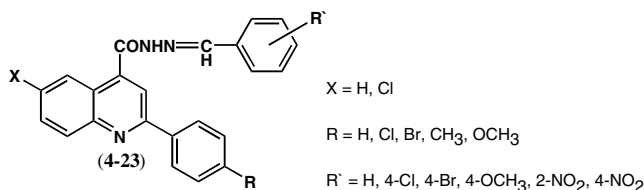
Reagent and condition: (a) $\text{NH}_2\text{NH}_2 \cdot \text{H}_2\text{O}$, HOAc, MW; (b) substituted benzyl chloride, base, MW.

Hydrazones of 2-aryl-quinoline-4-carboxylic acid hydrazides:

pp 8675–8682

Synthesis and preliminary evaluation as antimicrobial agents

Kamel A. Metwally,* Lobna M. Abdel-Aziz, El-Sayed M. Lashine, Mohamed I. Hussein and Rania H. Badawy

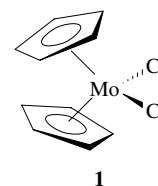


Molybdenocene–oligonucleotide binding study at physiological pH using NMR spectroscopy and cyclic voltammetry

pp 8683–8691

José L. Vera, Félix R. Román and Enrique Meléndez*

Binding interaction studies of antitumor molybdenocene dichloride (**1**) and self-complementary oligonucleotide CGCATATATGCG were accomplished using NMR spectroscopy and cyclic voltammetry in order to elucidate possible interactions between DNA and the organometallic species at physiological pH in buffer solutions. NMR spectroscopic studies showed molybdenocene binds the oligonucleotide weakly and has no preference for guanine over adenine bases. Cyclic voltammetry corroborates in a quantitative manner that the interaction in fact is weak, showing only 4.9% of molybdenocene–oligonucleotide binding. This implicates that DNA cannot be completely ruled out as a target place but the mechanism is more complex than *cis*-platin.



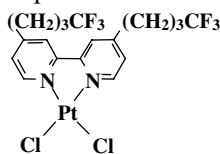
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i⁺

A fluorine containing bipyridine cisplatin analog is more effective than cisplatin at inducing apoptosis in cancer cell lines

pp 8692–8700

Kyler E. Elwell, Casey Hall, Shweta Tharkar, Yvonne Giraud, Byron Bennett, Chulsung Bae and Stephen W. Carper*



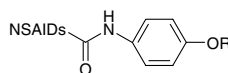
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The synthesis of dichloro[4,4'-bis(4,4,4-trifluorobutyl)-2,2'-bipyridine]platinum (**1**), a cisplatin analog, and a preliminary study of its cytotoxicity are reported. Compound **1** is 14 to 125 times more effective than cisplatin in inducing apoptosis in breast, lung, and prostate cancer cell lines.

Synthesis of new chemical entities from paracetamol and NSAIDs with improved pharmacodynamic profile

pp 8701–8706

Mange Ram Yadav,* Datta M. Nimekar, A. Ananthakrishnan, Pathik S. Brahmakshatriya, Shrikant T. Shirude, Rajani Giridhar, Arvind Parmar and R. Balaraman



Where: R = H, COCH₃

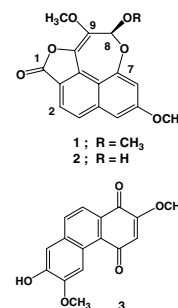
New chemical entities from paracetamol and NSAIDs were synthesized and evaluated for bioactivity. All the synthesized *p*-amidophenol derivatives showed improved antipyretic activity than paracetamol with retention of anti-inflammatory activity and no ulcerogenicity.

Anti-allergic substances from the rhizomes of *Dioscorea membranacea*

pp 8707–8711

Supinya Tewtrakul* and Arunporn Itharat

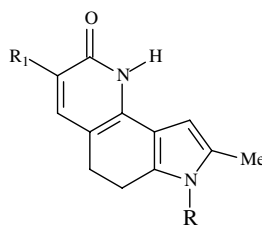
Eight compounds [two naphthofuranoxepins (**1**, **2**), one phenanthraquinone (**3**), three steroids (**4**–**6**), and two steroidal saponins (**7**, **8**)] were isolated from the ethanolic extract of *Dioscorea membranacea* rhizomes and tested for anti-allergic activities. The results showed that dioscorealide B (**2**) possessed the highest activity with an IC₅₀ value of 5.7 μM, followed by dioscoreanone (**3**, IC₅₀ = 7.7 μM), dioscorealide A (**1**, IC₅₀ = 27.9 μM), and diosgenin (**9**, IC₅₀ = 29.9 μM). Structure–activity relationship studies of naphthofuranoxepins on anti-allergic activity revealed that the hydroxylation at position 8 conferred higher activity than methoxylation. For diosgenin derivatives, the aglycone was found to possess higher activity than the diglucosylated molecule; whereas substitution with rhamnoglucosides apparently results in loss of activity. Furthermore, effects of dioscorealide A (**1**), dioscorealide B (**2**), and dioscoreanone (**3**) on antigen-induced release of TNF-α and IL-4 were also examined.



Pyrrolo[2,3-*h*]quinolinones: A new ring system with potent photoantiproliferative activity

pp 8712–8728

Paola Barraja, Patrizia Diana, Alessandra Montalbano, Gaetano Dattolo, Girolamo Cirrincione,* Giampietro Viola,* Daniela Vedaldi and Francesco Dall'Acqua



OTHER CONTENTS

Summary of instructions to authors

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*Corresponding author

①⁺ Supplementary data available via ScienceDirect

COVER

2006: The cover figure shows a synthetic multifunctional pore that is composed of rigid-rod staves (para-octiphenyls, tan) and beta-sheet hoops (arrows) and can be activated with external ligands (fullerenes, golden spheres) and closed with internal blockers (alpha-helix, red ribbon) [Gorteau, V.; Bollot, G.; Mareda, J.; Pasini, D.; Tran, D.-H.; Lazar, A. N.; Coleman, A. W.; Sakai, N.; Matile, S. *Bioorg. Med. Chem.* **2005**, *13*, 5171–5180].

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