

Contents lists available at ScienceDirect

Bioorganic & Medicinal Chemistry

journal homepage: www.elsevier.com/locate/bmc



Bioorganic & Medicinal Chemistry Volume 18, Issue 22, 2010

Symposium-in-Print

Chemical Neurobiology

Edited by: Prof. Dirk Trauner

University of Munich, Department of Chemistry, Butenandtstr. 5-13, 81377 Munich, Germany

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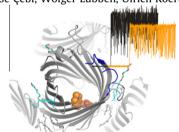
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SPECIAL ISSUE ARTICLES

Structural and functional characterization of a synthetically modified OmpG

pp 7716-7723

Wolfgang Grosse, Philipp Reiß, Simon Reitz, Menekse Çebi, Wolger Lübben, Ulrich Koert*, Lars-Oliver Essen*

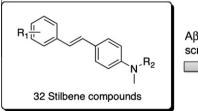


The first structure of the OmpG porin covalently modified by a synthetic compound is reported. Intimate lining of the modulator to the pore interior leads to partial current blockage.

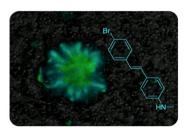
Synthesis and evaluation of stilbene derivatives as a potential imaging agent of amyloid plaques

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Aβ40 fibril screening

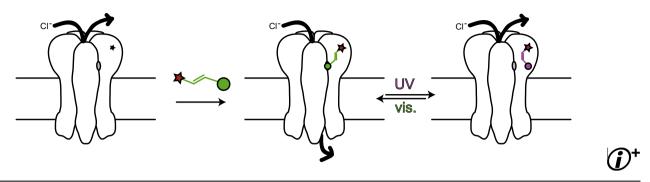




The GABA_A receptor as a target for photochromic molecules

pp 7731-7738

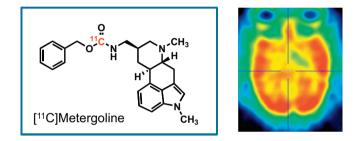
Mariel Feliciano, Devaiah Vytla, Kathryne A. Medeiros, James J. Chambers*



Evaluation of [11C]metergoline as a PET radiotracer for 5HTR in nonhuman primates

pp 7739-7745

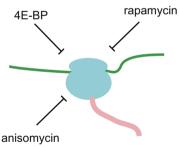
Jacob M. Hooker*, Sung Won Kim, Achim T. Reibel, David Alexoff, Youwen Xu, Colleen Shea



A collection of caged compounds for probing roles of local translation in neurobiology

pp 7746-7752

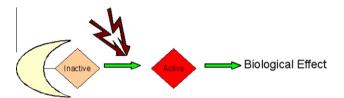
Oleg Sadovski, Anna S. I. Jaikaran, Subhas Samanta, Marc R. Fabian, Ryan J. O. Dowling, Nahum Sonenberg, G. Andrew Woolley*



Two-photon uncaging: New prospects in neuroscience and cellular biology

pp 7753-7758

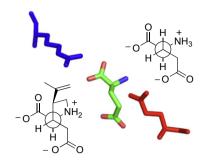
D. Warther, S. Gug, A. Specht, F. Bolze, J.-F. Nicoud, A. Mourot, M. Goeldner*



Pharmacology of ionotropic glutamate receptors: A structural perspective

pp 7759-7772

Philipp Stawski, Harald Janovjak, Dirk Trauner*

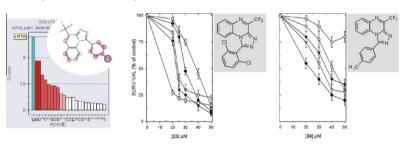


REGULAR ARTICLES

Ligand-based virtual screening and ADME-tox guided approach to identify triazolo-quinoxalines as folate cycle inhibitors

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Emanuele Carosati, Gianluca Sforna, Massimiliano Pippi, Gaetano Marverti, Alessio Ligabue, Davide Guerrieri, Sandra Piras, Giambattista Guaitoli, Rosaria Luciani, Maria Paola Costi, Gabriele Cruciani*





Parallel synthesis and nucleic acid binding properties of C(6')- α -functionalized bicyclo-DNA

pp 7786-7793

Peter Šilhár, Christian J. Leumann*

Probing the active-site requirements of human intestinal N-terminal maltase-glucoamylase: Synthesis and enzyme inhibitory activities of a six-membered ring nitrogen analogue of kotalanol and its de-O-sulfonated derivative

pp 7794-7798

Sankar Mohan, Lyann Sim, David R. Rose, B. Mario Pinto*



Intramolecular reductive cyclization strategy to the synthesis of (–)-6-methyl-3-hydroxy-piperidine-2-carboxylic acid, pp 7799–7803 (+)-6-methyl-(2-hydroxymethyl)-piperidine-3-ol and their glycosidase inhibitory activity

Vishwas U. Pawar, Sanjay T. Chavan, Sushma G. Sabharwal, Vaishali S. Shinde*



Selective accumulation of a novel antimalarial rhodacyanine derivative, SSJ-127, in an organelle of *Plasmodium berghei* pp 7804–7808 Mayumi Ikegami-Kawai*, Chika Arai, Yuko Ogawa, Ryohei Yanoshita, Masataka Ihara

A novel antimalarial rhodacyanine derivative, SSJ-127, is detected in mouse malaria parasites using fluorescence imaging. The SSJ-127-accumulating organelle is clearly different from the mitochondrion and the nucleus in terms of morphology.

1-Bromo-3-(1',1'-dimethylalkyl)-1-deoxy- Δ^8 -tetrahydrocannabinols: New selective ligands for the cannabinoid CB₂ pp 7809–7815 receptor

John W. Huffman*, Seon A. Hepburn, Nataliya Lyutenko, Alicia L. S. Thompson, Jenny L. Wiley, Dana E. Selley, Billy R. Martin

The synthesis and pharmacology of a series of 1-bromo-1-deoxy-3-(1',1'-dimethylalkyl)- Δ^8 -THCs is described. One of these compounds (R = dimethylhexyl) is 52-fold selective for the CB₂ receptor with good (28 nM) affinity for this receptor.

Discovery and biological evaluation of potent, selective, orally bioavailable, pyrazine-based blockers of the $Na_v 1.8$ pp 7816–7825 sodium channel with efficacy in a model of neuropathic pain

Marc J. C. Scanio*, Lei Shi, Irene Drizin, Robert J. Gregg, Robert N. Atkinson, James B. Thomas, Matthew S. Johnson, Mark L. Chapman, Dong Liu, Michael J. Krambis, Yi Liu, Char-Chang Shieh, XuFeng Zhang, Gricelda H. Simler, Shailen Joshi, Prisca Honore, Kennan C. Marsh, Alison Knox, Stephen Werness, Brett Antonio, Douglas S. Krafte, Michael F. Jarvis, Connie R. Faltynek, Brian E. Marron, Michael E. Kort

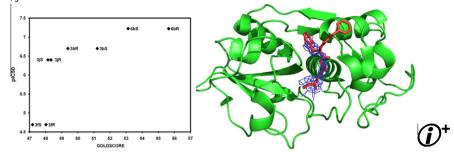
$$R^1$$
 N N R^2

Studies toward the structural optimization of novel thiazolylhydrazone-based potent antitrypanosomal agents

pp 7826-7835

Marcelo Zaldini Hernandes, Marcelo Montenegro Rabello, Ana Cristina Lima Leite*, Marcos Veríssimo Oliveira Cardoso, Diogo Rodrigo Magalhaes Moreira, Dalci José Brondani, Carlos Alberto Simone, Luiza Campos Reis, Marina Assis Souza, Valéria Rego Alves Pereira, Rafaela Salgado Ferreira, James Hobson McKerrow

Optimization of antichagasic structures: thiazolylhydrazones represent a class of compounds that exhibit powerful trypanocidal properties, as confirmed by in vitro and in silico (docking) evaluation using the *Trypanosoma cruzi* cruzain as drug target. Strategies for molecular optimization are presented here and structure–activity relationships (SAR) data are subsequently gathered. This represents an important progress on previously reported SAR studies for this scaffold.

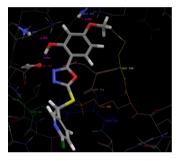


Synthesis, biological evaluation, and molecular docking studies of 2-chloropyridine derivatives possessing 1,3,4-oxadiazole moiety as potential antitumor agents

pp 7836-7841

Qing-Zhong Zheng, Xiao-Min Zhang, Ying Xu, Kui Cheng, Qing-Cai Jiao*, Hai-Liang Zhu*

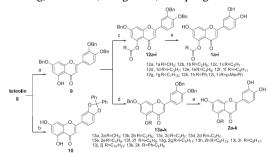
Antiproliferative assay results indicated that compounds **60** and **6u** exhibited the most potent activity against gastric cancer cell SGC-7901, which was more potent than the positive control. Especially, compound **60** exhibited significant telomerase inhibitory activity (IC $_{50}$ = 2.3 ± 0.07 μ M), which was comparable to the positive control ethidium bromide. Docking simulation was performed to position compound **60** into the active site of telomerase (3DU6) to determine the probable binding model.



Discovery and synthesis of novel luteolin derivatives as DAT agonists

pp 7842-7848

Jiange Zhang*, Xianbo Liu, Xinsheng Lei*, Lei Wang, Lihe Guo*, Gang Zhao, Guoqiang Lin



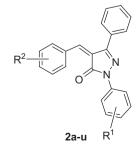
The synthesis of the novel dopamine transporter (DAT) agonist luteolin derivative $\mathbf{1d}$ (EC50 = 0.046 μm) is reported.



Synthesis and evaluation of pyrazolone compounds as SARS-coronavirus 3C-like protease inhibitors

R. Ramajayam, Kian-Pin Tan, Hun-Ge Liu, Po-Huang Liang*

A series of pyrazolone compounds as possible SARS-CoV 3CL protease inhibitors were designed, synthesized, and evaluated by in vitro protease assay using fluorogenic substrate peptide in which several showed potent inhibition against the 3CL protease. Interestingly, one of the inhibitors was also active against 3C protease from coxsackievirus B3. These inhibitors could be potentially developed into anti-coronaviral and anti-picornaviral agents.



pp 7849-7854

Synthesis and SAR studies of chiral non-racemic dexoxadrol analogues as uncompetitive NMDA receptor antagonists pp 7855–7867
Ashutosh Banerjee, Dirk Schepmann, Jens Köhler, Ernst-Ulrich Würthwein, Bernhard Wünsch*

Inhibition of Helicobacter pylori aminoacyl-tRNA amidotransferase by chloramphenicol analogs

pp 7868-7872

Christian Balg, Maria De Mieri, Jonathan L. Huot, Sébastien P. Blais, Jacques Lapointe, Robert Chênevert*

4-Phenylcoumarins from Mesua elegans with acetylcholinesterase inhibitory activity

pp 7873-7877

Khalijah Awang*, Gomathi Chan, Marc Litaudon, Nor Hadiani Ismail, Marie-Thérèse Martin, Françoise Gueritte

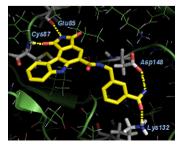
Nine 4-phenylcoumarins have been isolated from *Mesua elegans*, in which three are new; mesuagenin A, mesuagenin C, mesuagenin D, and one is a newly reported natural product; mesuagenin B. Chemical structures were elucidated using spectroscopic techniques, notably 1D and 2D NMR spectroscopy. Four compounds showed significant inhibitory activity against acetylcholinesterase, with mesuagenin B being the most potent ($IC_{50} = 0.7 \mu M$).

(i)+

Synthesis and evaluation of 5-substituted 9-hydroxypyrrolo[3,4-c]carbazole-1,3(2H,6H)-diones as check point 1 kinase inhibitors

pp 7878-7889

Yuki Sako, Satoshi Ichikawa*, Akiko Osada, Akira Matsuda*





Potent inhibitors of Check point kinase 1 have been developed by a structure-based drug design.

Pyrazolo[1',5':1,6]pyrimido[4,5-d]pyridazin-4(3H)-ones as selective human A₁ adenosine receptor ligands

pp 7890-7999

Maria Paola Giovannoni*, Claudia Vergelli, Agostino Cilibrizzi, Letizia Crocetti, Claudio Biancalani, Alessia Graziano, Vittorio Dal Piaz, Maria Isabel Loza, Maria Isabel Cadavid, José Luis Díaz, Amadeu Gavaldà

R₁ = CH₃, Ph, Cl, 3-Pyridine, 4-Pyridine3-F-Ph, 4-F-Ph

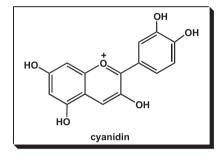
R₃ = PhCH₂, C₄H₉, Ph(CH)CH₃ R₆ = Ph, 3-thienyl, 4-OCH₃-Ph R₉ = CH₃, C₂H₅, iC₃H₇, nC₃H₇, CF₃

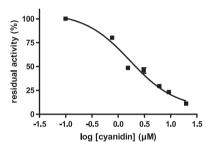


Identification by high-throughput screening of inhibitors of Schistosoma mansoni NAD* catabolizing enzyme

pp 7900-7910

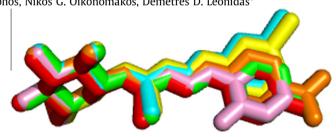
Isabelle Kuhn, Esther Kellenberger, Fatouma Said-Hassane, Pascal Villa, Didier Rognan, Annelise Lobstein, Jacques Haiech, Marcel Hibert, Francis Schuber, Hélène Muller-Steffner*







The binding of β-p-glucopyranosyl-thiosemicarbazone derivatives to glycogen phosphorylase: A new class of inhibitors pp 7911–7922 Kyra-Melinda Alexacou, Alia-Cristina Tenchiu (Deleanu), Evangelia D. Chrysina, Maria-Despoina Charavgi, Ioannis D. Kostas*, Spyros E. Zographos, Nikos G. Oikonomakos, Demetres D. Leonidas*



The catalytic site of muscle glycogen phosphorylase b (GPb) has been probed with a group of fifteen aromatic aldehyde 4-(β-p-glucopyranosyl)thiosemicarbazones. The best of these inhibitors displays a IC_{50} value of 5.7 μM .

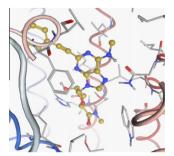


Molecular modeling study on potent and selective adenosine A₃ receptor agonists

pp 7923-7930

Diego Dal Ben, Michela Buccioni, Catia Lambertucci, Gabriella Marucci, Ajiroghene Thomas, Rosaria Volpini, Gloria Cristalli*

Adenosine A₃ receptor is involved in a variety of key physio-pathological processes and its agonists represent interesting tools for the development of new drugs. In this molecular modeling study, high adenosine A₃ receptor affinities and selectivities of recently reported MECA derivatives were analyzed by using adenosine receptor structural models based on the adenosine A_{2A} receptor crystal structure and molecular docking analysis.



Synthesis and antioxidant properties of pulvinic acids analogues

pp 7931-7939

Brice Nadal, Sophie A.-L. Thetiot-Laurent, Serge Pin, Jean-Philippe Renault, Damien Cressier, Ghassoub Rima, Antoine Le Roux, Stéphane Meunier, Alain Wagner, Claude Lion, Thierry Le Gall*

The synthesis of 28 pulvinic acids analogues from dimethyl L-tartrate and the evaluation of their antioxidant properties, using antioxidant capacity assays and free radical scavenging assays, are described.



Biflavonoids from Torreya nucifera displaying SARS-CoV 3CL^{pro} inhibition

pp 7940-7947

Young Bae Ryu, Hyung Jae Jeong, Jang Hoon Kim, Young Min Kim, Ji-Young Park, Doman Kim, Thi Thanh Hanh Naguyen, Su-Jin Park, Jong Sun Chang, Ki Hun Park, Mun-Chual Rho*, Woo Song Lee*

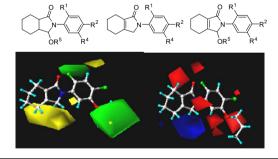
Inhibitory activity appeared to be associated with the presence of an apigenin moiety at position C-3' of flavones, as biflavonoid had an effect on SARS-CoV 3CL^{pro} inhibitory activity.



Design, syntheses and 3D-QSAR studies of novel N-phenyl pyrrolidin-2-ones and N-phenyl-1H-pyrrol-2-ones as protoporphyrinogen oxidase inhibitors

pp 7948-7956

Li Zhang, Yin Tan, Neng-Xue Wang, Qiong-You Wu, Zhen Xi*, Guang-Fu Yang*



Anticonvulsant activity of 2,4(1H)-diarylimidazoles in mice and rats acute seizure models

pp 7957-7965

Valentina Zuliani*, Marco Fantini, Aradhya Nigam, James P. Stables, Manoj K. Patel, Mirko Rivara

$$\begin{array}{c} R = R_1 = H - ED_{50} \ (MES) = 61.7; TD_{50} = 126.8; PI = 2.1 \\ R = \textit{m-OCH}_3, \ R_1 = H - ED_{50} \ (MES) = 46.8; TD_{50} = 200.8; PI = 4.3 \\ R = \textit{p-CF}_3, \ R_1 = H - ED_{50} \ (MES) = 129.5; TD_{50} > 500; PI > 3.8 \\ R = H, \ R_1 = \textit{m-CI} - ED_{50} \ (MES) = 136.7; TD_{50} > 500; PI > 3.6 \\ \end{array}$$



Synthesis and anticancer activity of new 1-[(5 or 6-substituted 2-alkoxyquinoxalin-3-yl)aminocarbonyl]-4-(hetero)arylpiperazine derivatives

pp 7966-7974

Young Bok Lee*, Young-Dae Gong*, Heejeong Yoon, Chang-Ho Ahn, Moon-Kook Jeon, Jae-Yang Kong

Compound 25:
$$R^1 = H$$

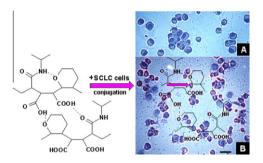
 $R^2 = F$
 $R^2 = 3,5$ -dimethoxyphenyl $R^2 = 11 \sim 21 \text{ nM}$



Bioengineering functional copolymers. XIV. Synthesis and interaction of poly(*N*-isopropylacrylamide-*co*-3,4-dihydro-pp 7975–7984 2*H*-pyran-*alt*-maleic anhydride)s with SCLC cancer cells

Mustafa Türk, Zakir M. O. Rzayev*, Sevda A. Khalilova

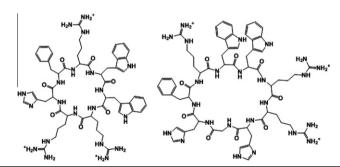
Novel bioengineering functional terpolymers containing a combination of H-bonded ionizable amide-pyran and carboxylic groups as antitumor sites were synthesized and their cytotoxic, apoptotic and necrotic effects on human lung small cell carcinoma (SCLC) are investigated. LM images: (A) non-apoptotic and (B) conjugated cells.



Synthesis of new antifungal peptides selective against Cryptococcus neoformans

pp 7985-7990

Manuela Grimaldi, Margherita De Rosa, Sara Di Marino, Mario Scrima, Brunella Posteraro, Maurizio Sanguinetti, Giovanni Fadda, Annunziata Soriente, Anna Maria D'Ursi*

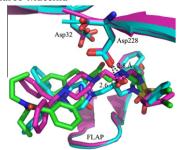




BACE1 inhibitory activities of enantiomerically pure, variously substituted N-(3-(4-benzhydrylpiperazin-1-yl)-2-hydroxypropyl) arylsulfonamides

pp 7991-7996

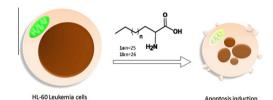
Simone Bertini, Elisa Ghilardi, Valentina Asso, Carlotta Granchi, Filippo Minutolo, Mauro Pineschi, Valeria Di Bussolo, Andrea Bortolato, Stefano Moro, Alessandro Saba, Marco Macchia*



Pro-apoptotic activity of lipidic α -amino acids isolated from *Protopalythoa variabilis*

pp 7997-8004

Diego Veras Wilke, Paula Christine Jimenez, Renata Mendonça Araújo, Wildson Max Barbosa da Silva, Otília Deusdênia Loiola Pessoa, Edilberto Rocha Silveira, Claudia Pessoa, Manoel Odorico de Moraes, Mariusz Skwarczynski, Pavla Simerska, Istvan Toth, Letícia Veras Costa-Lotufo*



The anti-proliferative potential of 14 synthetic LAAs were evaluated on several tumor cell lines, as well as the anti-proliferative and pro-apoptotic effects of cytotoxic LAAs (1a/1b) isolated from the marine zoanthid *Protopalythoa variabilis*.

Conformationally constrained NR2B selective NMDA receptor antagonists derived from ifenprodil: Synthesis and biological evaluation of tetrahydro-3-benzazepine-1,7-diols

pp 8005-8015

Bastian Tewes, Bastian Frehland, Dirk Schepmann, Kai-Uwe Schmidtke, Thomas Winckler, Bernhard Wünsch*

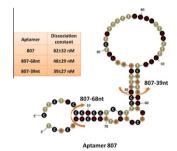


In vitro lectin-mediated selection and characterization of rHuEPO-α-binding ssDNA aptamers

pp 8016-8025

Zhaoyang Zhang, Lei Guo, Aitao Guo, Hua Xu, Jijun Tang, Xingjie Guo, Jianwei Xie*

After eight rounds of lectin-mediated affinity chromatographic SELEX, aptamer 807 of recombinant human erythropoietin- α was successfully evolved as a prevalent one for the first time. Characterization of aptamer 807 was fully investigated from the point of its secondary structural information and specific recognition towards malignant tumor cells and human urothelium tumors.





Naphthylchalcones induce apoptosis and caspase activation in a leukemia cell line: The relationship between mitochondrial damage, oxidative stress, and cell death

pp 8026-8034

Evelyn Winter, Louise Domeneghini Chiaradia, Clarissa A. S. de Cordova, Ricardo José Nunes, Rosendo Augusto Yunes, Tânia Beatriz Creczynski-Pasa*

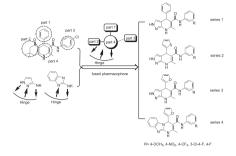


Design, synthesis and bioevaluation of dihydropyrazolo[3,4-b]pyridine and benzo[4,5]imidazo[1,2-a]pyrimidine compounds as dual KSP and Aurora-A kinase inhibitors for anti-cancer agents

pp 8035-8043

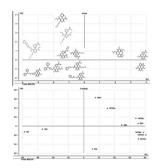
Rong-geng Fu, Qi-dong You*, Lei Yang, Wu-tong Wu, Cheng Jiang, Xiao-li Xu

Four series of dihydropyrazolo[3,4-b]pyridines and benzo[4,5]imidazo[1,2-a]pyrimidines were designed and synthesized as dual KSP and Aurora-A kinase inhibitors for anti-cancer agents by introducing some fragments of Aurora-A kinase inhibitors into KSP inhibitor CPUYL064.



Anti-leishmanial and anti-trypanosomal activities of 1,4-dihydropyridines: In vitro evaluation and structure-activity pp 8044–8053 relationship study

Juliana Q. Reimão, Marcus T. Scotti, André G. Tempone*



Structure-activity relationships of benzimidazole-based selective inhibitors of the mitogen activated kinase-5 signaling pathway

pp 8054-8060

Patrick T. Flaherty*, Ishveen Chopra, Prashi Jain, Darlene Monlish, Jane Cavanaugh

Inhibition of EGF-mediated ERK5 phosphorylation is examined for several 1-isopropyl-4-amino-6-ether linked benzimidazole-based compounds.



Synthesis and evaluation of 2'-O-allyl substituted dinucleotide cap analog for mRNA translation

pp 8061-8065

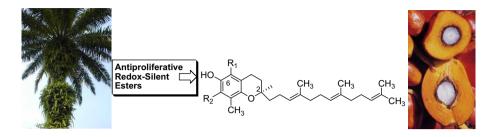
Anilkumar R. Kore*, Irudaya Charles

 $Design, synthesis \ and \ substrate \ properties \ of \ 2'-0-allyl \ substituted \ dinucleotide \ cap \ analog, \ that \ is, \ m^{7,2'-0-Allyl} GpppG \ is \ reported.$

Redox-silent tocotrienol esters as breast cancer proliferation and migration inhibitors

pp 8066-8075

Fathy A. Behery, Ahmed Y. Elnagar, Mohamed R. Akl, Vikram B. Wali, Bilal Abuasal, Amal Kaddoumi, Paul W. Sylvester, Khalid A. El Sayed*



Identification of a novel pyrrole derivative endowed with antimycobacterial activity and protection index comparable to pp 8076–8084 that of the current antitubercular drugs streptomycin and rifampin

Mariangela Biava*, Giulio Cesare Porretta, Giovanna Poce, Claudio Battilocchio, Salvatore Alfonso, Alessandro De Logu, Nadia Serra, Fabrizio Manetti, Maurizio Botta

Synthesis and antimalarial activities of rhenium bioorganometallics based on the 4-aminoquinoline structure

pp 8085-8091

Rodrigo Arancibia, Faustine Dubar, Bruno Pradines, Isabelle Forfar, Daniel Dive, A. Hugo Klahn, Christophe Biot*

A series of new 4-aminoquinoline-cyrhetrene derivatives have been synthesized and tested for efficacy against both chloroquine-susceptible and chloroquine-resistant strains of *Plasmodium falciparum*. To establish the role of the cyrhethrenyl moiety in the antimalarial activity of this series, purely organic parent compounds were also synthesized and tested.

Halogenation of 4-hydroxy/amino-3-methoxyphenyl acetamide TRPV1 agonists showed enhanced antagonism to capsaicin

pp 8092-8105

Dong Wook Kang, Yong Soo Kim, Kwang Su Lim, Myeong Seop Kim, Larry V. Pearce, Vladimir A. Pavlyukovets, Andy K. Tao, Krystle A. Lang-Kuhs, Peter M. Blumberg, Jeewoo Lee*

$$R_{5}$$
 R_{6} R_{5} R_{6} = H, halogens R_{4} R_{4} = OH, OAc, NH₂, NHSO₂CH₃

Structure-activity relationships for inhibition of inosine monophosphate dehydrogenase and differentiation induction pp 8106-8111 of K562 cells among the mycophenolic acid derivatives

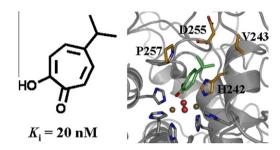
Shinya Mitsuhashi, Junichi Takenaka, Katsushige Iwamori, Noriyuki Nakajima, Makoto Ubukata*



Structural insights into the hot spot amino acid residues of mushroom tyrosinase for the bindings of thujaplicins

pp 8112-8118

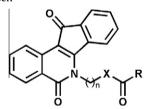
Satoshi Takahashi, Takanori Kamiya, Kazunori Saeki, Tomoka Nezu, Shin-ichiro Takeuchi, Ryoko Takasawa, Satoshi Sunaga, Atsushi Yoshimori, Shigeo Ebizuka, Takehiko Abe, Sei-ichi Tanuma*



Indeno[1,2-c]isoquinolin-5,11-diones conjugated to amino acids: Synthesis, cytotoxicity, DNA interaction, and topoisomerase II inhibition properties

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Gang Ahn, Amélie Lansiaux, Jean-François Goossens, Christian Bailly, Brigitte Baldeyrou, Nadège Schifano-Faux, Pierre Grandclaudon, Axel Couture, Adina Ryckebusch*



32: n = 2, X = NH, COR = Arg

topoisomerase II inhibitor

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*Corresponding author

(1) Supplementary data available via ScienceDirect

COVER

The cover shows the crystal structure of an AMPA receptor, as elucidated by Eric Gouaux and colleagues, surrounded by various agonists and antagonists of ionotropic glumatate receptors. It was designed by Dirk Trauner.

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