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Bioorganic & Medicinal Chemistry Vol. 16, No. 17, 2008

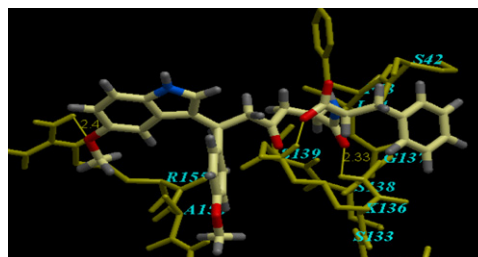
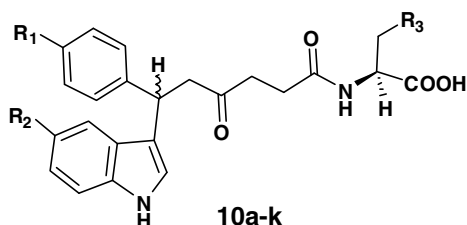
Contents

ARTICLES

Computer based design, synthesis and biological evaluation of novel indole derivatives as HCV NS3-4A serine protease inhibitors

pp 7877–7887

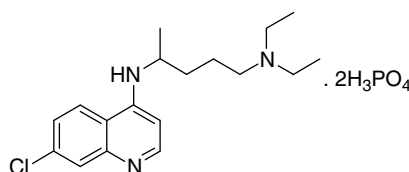
Nasser S. M. Ismail*, Riham Salah El Dine, Masao Hattori, Kazunori Takahashi, Masataka Ihara



The efficacy and selectivity of tumor cell killing by Akt inhibitors are substantially increased by chloroquine

pp 7888–7893

Changkun Hu, V. Raja Solomon, Gerardo Ulibarri, Hoyun Lee*



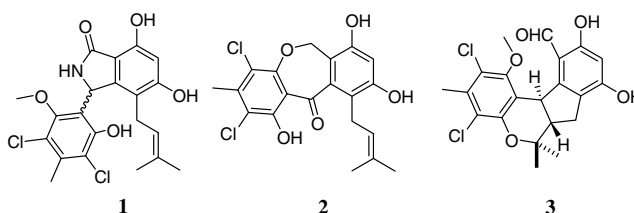
Chloroquine diphosphate (CQ)

In the present study, the combinational effects of CQ and Akt inhibitors were evaluated for their cell killing activity on cancer and non-cancer breast cells.

Pestalachlorides A–C, antifungal metabolites from the plant endophytic fungus *Pestalotiopsis adusta*

pp 7894–7899

Erwei Li, Lihua Jiang, Liangdong Guo, Hua Zhang, Yongsheng Che*



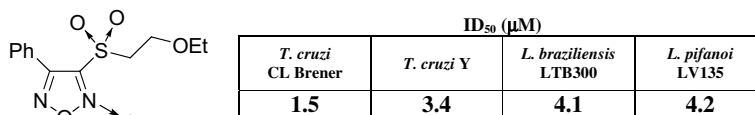
Pestalachlorides A–C (1–3), three new chlorinated benzophenones, have been isolated from the plant endophyte *Pestalotiopsis adusta* and evaluated for their antifungal activities.



Furoxan-, alkyl nitrate-derivatives and related compounds as anti-trypanosomatid agents: Mechanism of action studies

pp 7900–7907

Lucía Boiani, Gabriela Aguirre, Mercedes González, Hugo Cerecetto*, Agustina Chidichimo, Juan J. Cazzulo, Massimo Bertinaria*, Stefano Guglielmo



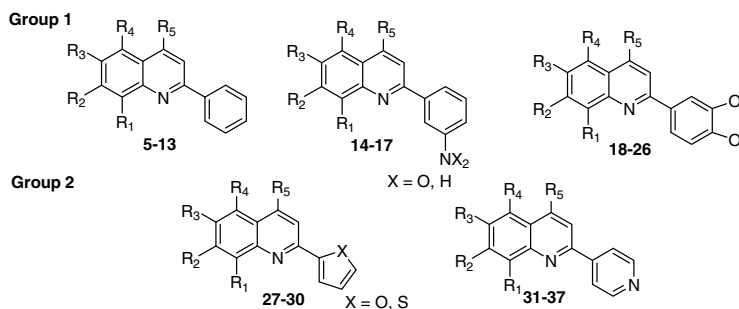
Over a hundred furoxans, alkyl nitrates and related compounds were studied as growth inhibitors of *Trypanosoma cruzi* and *Leishmania* spp.

In vitro antifungal activity of polyfunctionalized 2-(hetero)arylquinolines prepared through imino Diels–Alder reactions

pp 7908–7920

Carlos M. Meléndez Gómez, Vladimir V. Kouznetsov*, Maximiliano A. Sortino, Sandra L. Álvarez, Susana A. Zacchino*

Thirty-three 2-aryl and 2-hetaryl derivatives of polyfunctionalized quinolines (groups 1 and 2) were tested for antifungal properties against standardized and isolates of clinically important fungi. The most active compounds belong to group 2 being playing the positions 4 and 8 of the quinoline ring an important role against dermatophytes.

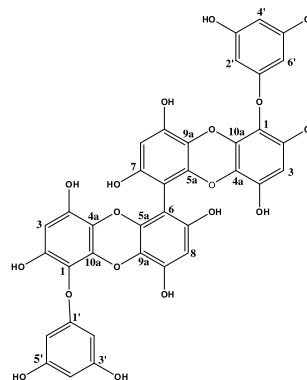


Anti-HIV-1 activity of phloroglucinol derivative, 6,6'-bieckol, from *Ecklonia cava*

pp 7921–7926

Murat Artan, Yong Li, Fatih Karadeniz, Sang-Hoon Lee, Moon-Moo Kim, Se-Kwon Kim*

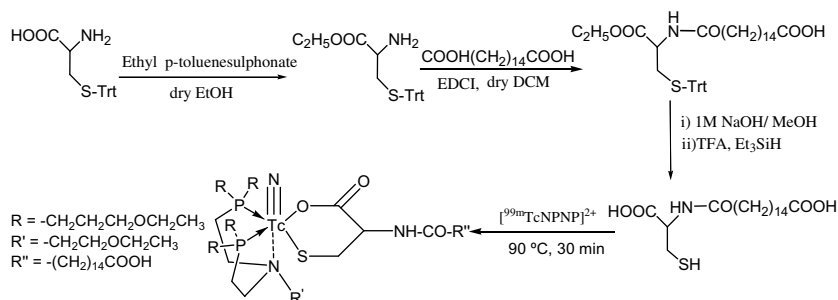
The bioactive 6,6'-bieckol was isolated and characterized by NMR techniques. For the first time, human immunodeficiency virus type-1 (HIV-1) inhibitory activity of 6,6'-bieckol showed wild inhibition against HIV-1 induced syncytia formation (EC₅₀ 1.72 μM), lytic effects (EC₅₀ 1.23 μM), and viral p24 antigen production (EC₅₀ 1.26 μM), respectively. This result was strongly and clearly supported by the further investigation also, which 6,6'-bieckol selectively inhibited the activity of HIV-1 reverse transcriptase (RT) enzyme with EC₅₀ of 1.07 μM, as well as HIV-1 entry. Moreover, unlike most of other tannins, 6,6'-bieckol exhibited no cytotoxicity at concentrations which inhibited HIV-1 replication almost completely. Thus, it can be suggested that the potentially effective 6,6'-bieckol might be employed as a drug candidate for development of new generation therapeutic agents against HIV.



Synthesis and bio-evaluation of a new fatty acid derivative for myocardial imaging

pp 7927–7931

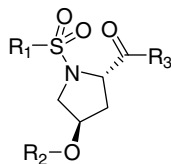
Anupam Mathur, Suresh Subramanian, Madhava B. Mallia, Sharmila Banerjee, Grace Samuel, Haladhar D. Sarma, Meera Venkatesh*



Synthesis of new sulfonyl pyrrolidine derivatives as matrix metalloproteinase inhibitors

pp 7932–7938

Xian-Chao Cheng, Qiang Wang, Hao Fang, Wei Tang, Wen-Fang Xu *



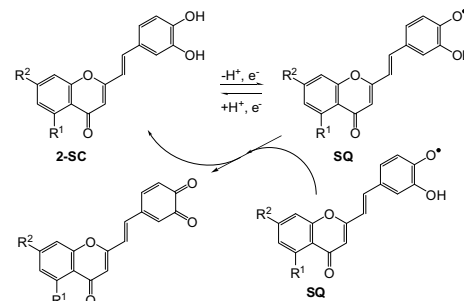
A series of new sulfonyl pyrrolidine derivatives was designed, synthesized, and assayed for their inhibitory activities on matrix metalloproteinase 2 (MMP-2) and aminopeptidase N (AP-N). The results showed that these pyrrolidine derivatives exhibited highly selective inhibition against MMP-2 as compared with AP-N. The compounds **4c**, **4j**, **5a**, and **5b** were equally or more potent MMP-2 inhibitors than the positive control LY52. The FlexX docking was done to explain the reason for the different potency between MMP-2 and AP-N. Structure–activity relationships were also briefly discussed.

Cyclic voltammetric analysis of 2-styrylchromones: Relationship with the antioxidant activity

pp 7939–7943

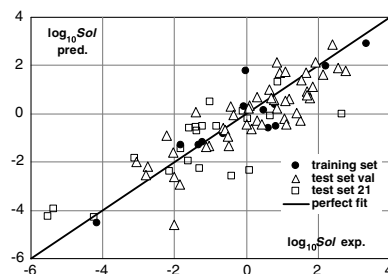
Ana Gomes, Eduarda Fernandes *, M. Beatriz Q. Garcia, Artur M. S. Silva, Diana C. G. A. Pinto, Clementina M. M. Santos, José A. S. Cavaleiro, José L. F. C. Lima

The scavenging effects of the studied 2-styrylchromones are related to their electrochemical behaviour. Our cyclic voltammetry results suggest an oxidation reaction involving only one electron process. This phenomenon can be explained by the formation of a semiquinone (SQ) (or to use the more generic term, an aryloxyl radical), which undergoes disproportionation leading to the *ortho*-quinone formation and to the regeneration of the starting 2-SC.

**New QSPR study for the prediction of aqueous solubility of drug-like compounds**

pp 7944–7955

Pablo R. Duchowicz *, Alan Talevi, Luis E. Bruno-Blanch, Eduardo A. Castro

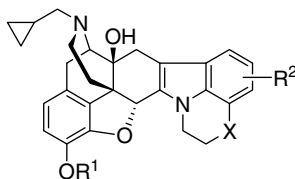


QSPR analysis on 166 drug-like compounds based on linear combinations of novel indices derived from Lipinski's 'rule of five' and Dragon descriptors. Results are compared with previously reported ones.

Design and synthesis of a metabolically stable and potent antitussive agent, a novel δ opioid receptor antagonist, TRK-851

pp 7956–7967

Satoshi Sakami, Koji Kawai, Masayuki Maeda, Takumi Aoki, Hideaki Fujii, Hiroshi Ohno, Tsuyoshi Ito, Akiyoshi Saitoh, Kaoru Nakao, Naoki Izumimoto, Hirotohi Matsuura, Takashi Endo, Shinya Ueno, Kazuto Natsume, Hiroshi Nagase *

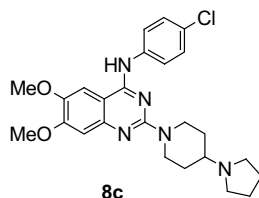


A series of naltrindole derivatives with an extra fused ring structure were synthesized, and their antitussive activities and metabolic stabilities were evaluated.

Potent CCR4 antagonists: Synthesis, evaluation, and docking study of 2,4-diaminoquinazolines

pp 7968–7974

Kazuhiro Yokoyama*, Noriko Ishikawa, Susumu Igarashi, Noriyuki Kawano, Naoyuki Masuda, Kazuyuki Hattori, Takahiro Miyazaki, Shin-ichi Ogino, Masaya Orita, Yuzo Matsumoto, Makoto Takeuchi, Mitsuaki Ohta

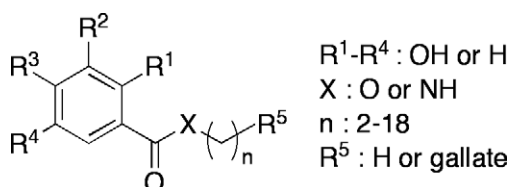


The novel *N*-(4-chlorophenyl)-6,7-dimethoxy-2-(4-pyrrolidin-1-ylpiperidin-1-yl)quinazolin-4-amine **8c** was found to be a potent competitive CCR4 antagonist and showed anti-inflammatory activity in a murine model of acute dermatitis.

Antiproliferative and apoptosis-inducing activities of alkyl gallate and gallamide derivatives related to (–)-epigallocatechin gallate

pp 7975–7982

Kosuke Dodo*, Taro Minato, Tomomi Noguchi-Yachide, Masami Suganuma, Yuichi Hashimoto

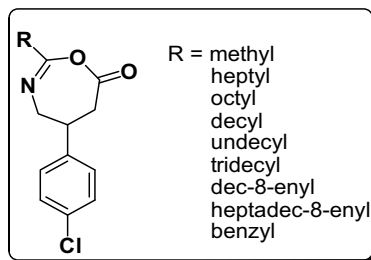


Various alkyl gallate and gallamide derivatives were synthesized and their antiproliferative/apoptosis-inducing activities were evaluated.

5-(4-Chlorophenyl)-5,6-dihydro-1,3-oxazepin-7(4H)-one derivatives as lipophilic cyclic analogues of baclofen: Design, synthesis, and neuropharmacological evaluation

pp 7983–7991

Atef A. Abdel-Hafez*, Basel A. Abdel-Wahab

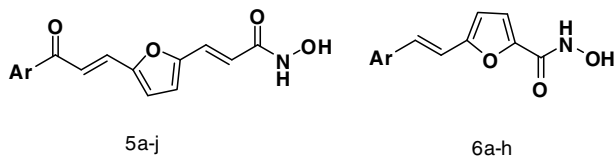


Nine new lipophilic cyclic analogues of baclofen were designed, synthesized and tested for their neuropharmacological activities.

Design, synthesis and biological evaluation of novel compounds with conjugated structure as anti-tumor agents

pp 7992–8002

Hong Su, Angela Nebbioso, Vincenzo Carafa, Yadong Chen, Bo Yang, Lucia Altucci*, Qidong You*

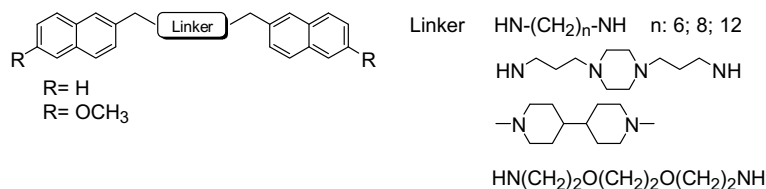


A series of hydroxamic acids with conjugated stereodefined structure were designed as HDAC inhibitors.

Design, synthesis, and antitumor activity of new bis-aminomethylnaphthalenes

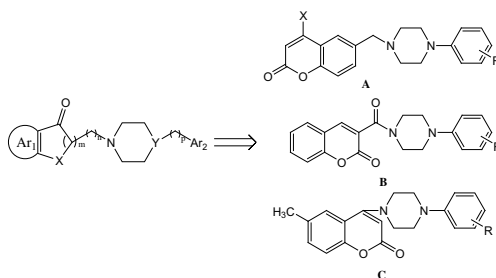
pp 8003–8010

Mariela Bollini, Juan José Casal, Ana María Bruno *

**Design, synthesis, and acetylcholinesterase inhibitory activity of novel coumarin analogues**

pp 8011–8021

Xiang Zhou, Xiao-Bing Wang, Tao Wang, Ling-Yi Kong *

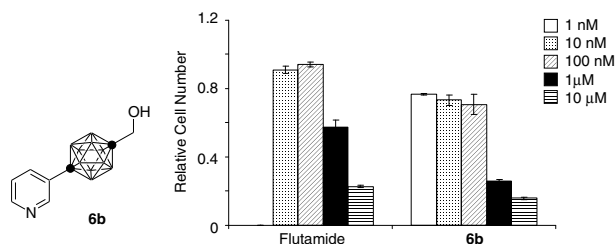


Three series of coumarin compounds were designed and synthesized. Their anti-AChE activities were also determined.

Design and synthesis of carborane-containing androgen receptor (AR) antagonist bearing a pyridine ring

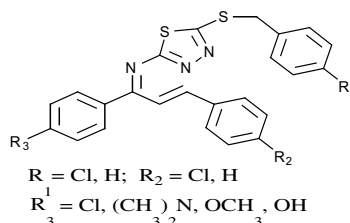
pp 8022–8028

Kiminori Ohta, Tokuhito Goto, Shinya Fijii, Tomoharu Suzuki, Shigeru Ohta, Yasuyuki Endo *

Compound **6b**, which was designed based on the structures of BA321 and BA341, exhibited more potent antiandrogenic activity than that of flutamide in SC-3 cell growth inhibition assay.**Syntheses and anti-depressant activity of 5-amino-1, 3, 4-thiadiazole-2-thiol imines and thiobenzyl derivatives**

pp 8029–8034

Mohammad Yusuf, Riaz A. Khan, Bahar Ahmed *

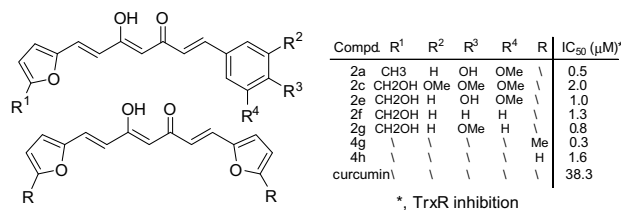


A series of imines of 1, 3, 4-thiadiazol-2-thiol and their thiobenzyl derivatives were synthesized from various chalcones in different reaction conditions and were evaluated for their anti-depressant and neurotoxic activity. Some of the compounds showed potent anti-depressant activity without any serious neurotoxicity as compared to standard drug imipramine.

Synthesis and evaluation of curcumin analogues as potential thioredoxin reductase inhibitors

pp 8035–8041

Xu Qiu, Zhong Liu, Wei-Yan Shao, Xing Liu, Da-Ping Jing, Yan-Jun Yu, Lin-Kun An, Shi-Liang Huang, Xian-Zhang Bu*, Zhi-Shu Huang, Lian-Quan Gu

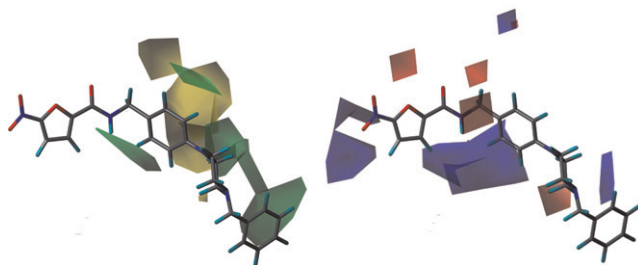


Series of curcumin derivatives were synthesized and evaluated for the inhibitory activities on TrxR by DTNB assay; it is found that most of the analogues can inhibit TrxR in vitro; SAR analysis reveals that analogues with furan moiety have excellent inhibitory effect on TrxR.

Quantitative structure–activity relationship studies on nitrofuranyl anti-tubercular agents

pp 8042–8053

Kirk E. Hevener, David M. Ball, John K. Buolamwini, Richard E. Lee*



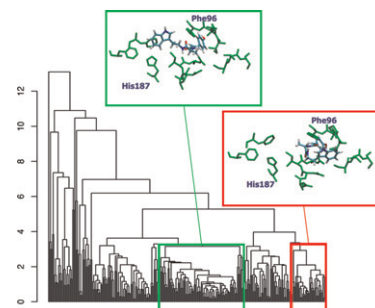
The development of a series of externally validated 3D-QSAR models with high predictive ability against nitrofuranyl agents with antimycobacterial activity is discussed.

Characterization of the binding properties of SIRT2 inhibitors with a *N*-(3-phenylpropenoyl)-glycine tryptamide backbone

pp 8054–8062

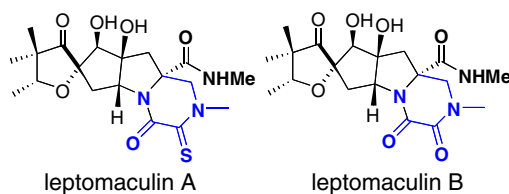
Päivi H. Kiviranta*, Heikki S. Salo*, Jukka Leppänen, Valtteri M. Rinne, Sergiy Kyrylenko, Erkki Kuusisto, Tiina Suuronen, Antero Salminen, Antti Poso, Maija Lahtela-Kakkonen, Erik A. A. Wallén

SIRT2 inhibitors with a *N*-(3-phenylpropenoyl)-glycine tryptamide backbone were studied, and their binding modes were analyzed with molecular modelling methods.

**Stress-driven discovery of metabolites from the phytopathogenic fungus *Leptosphaeria maculans*: Structure and activity of leptomaculins A–E**

pp 8063–8071

M. Soledade C. Pedras*, Yang Yu

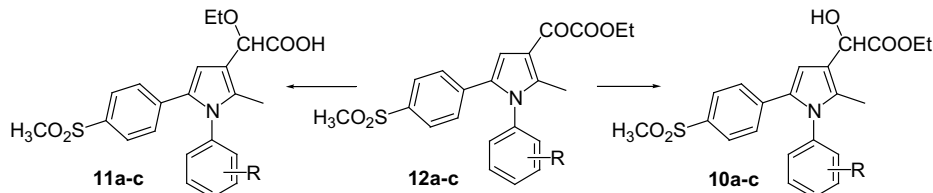


The chemical structures of the first natural 2,3-oxopiperazinethione and 2,3-dioxopiperazine, leptomaculins A and B, together with six new leptomaculins as well as biological activities and proposed biosynthetic pathways are reported.



Synthesis, in vitro, and in vivo biological evaluation and molecular docking simulations of chiral alcohol and ether derivatives of the 1,5-diarylpyrrole scaffold as novel anti-inflammatory and analgesic agents pp 8072–8081

Mariangela Biava*, Giulio C. Porretta, Giovanna Poce, Sibilla Supino, Fabrizio Manetti*, Stefano Forli, Maurizio Botta, Lidia Sautebin, Antonietta Rossi, Carlo Pergola, Carla Ghelardini, Monica Norcini, Francesco Makovec, Antonio Giordani, Paola Anzellotti, Roberto Cirilli, Rosella Ferretti, Bruno Gallinella, Francesco La Torre, Maurizio Anzini, Paola Patrignani

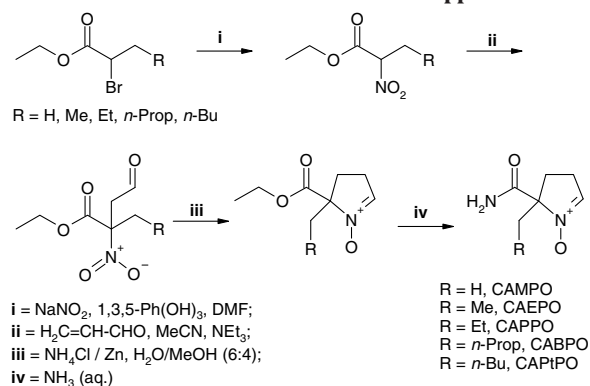


(–)-**10b**: R = 3-F, COX-2 affinity: 0.075 μ M, COX-1/COX-2 selectivity >1300. (+)-**10c**: R = 4-OCH₃, COX-2 affinity: 0.079 μ M, COX-1/COX-2 selectivity >1200. Celecoxib (**1b**): COX-2 affinity: 0.06 μ M, COX-1/COX-2 selectivity: 61.7.

Spin trapping experiments with different carbamoyl-substituted EMPO derivatives pp 8082–8089

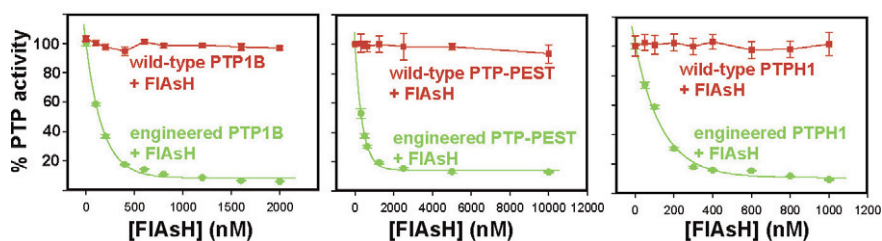
Klaus Stolze*, Natascha Rohr-Udilova, Andreas Hofinger, Thomas Rosenau

Synthesis and spin trapping properties of a series of EMPO-derived nitrones are reported.



Allele-specific inhibition of divergent protein tyrosine phosphatases with a single small molecule pp 8090–8097

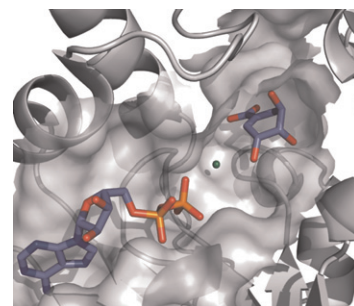
Xin-Yu Zhang, Vincent L. Chen, Mari S. Rosen, Elizabeth R. Blair, Anna Mari Lone, Anthony C. Bishop*



Molecular modeling and dynamics studies of Shikimate Kinase from *Bacillus anthracis* pp 8098–8108

Ivani Pauli, Rafael Andrade Caceres, Walter Filgueira de Azevedo Jr.*

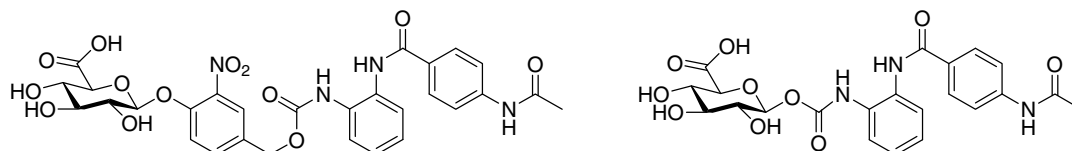
Complexes of BaSK were modeled with natural substrates in different conformational states due ligand-binding. Molecular dynamics simulations have been performed to evaluate structural and dynamical properties of BaSK.



Synthesis and biological evaluation of glucuronide prodrugs of the histone deacetylase inhibitor CI-994 for application in selective cancer chemotherapy

pp 8109–8116

Mickaël Thomas, Jonathan Clarhaut, Isabelle Tranoy-Opalinski, Jean-Pierre Gesson, Joëlle Roche, Sébastien Papot*

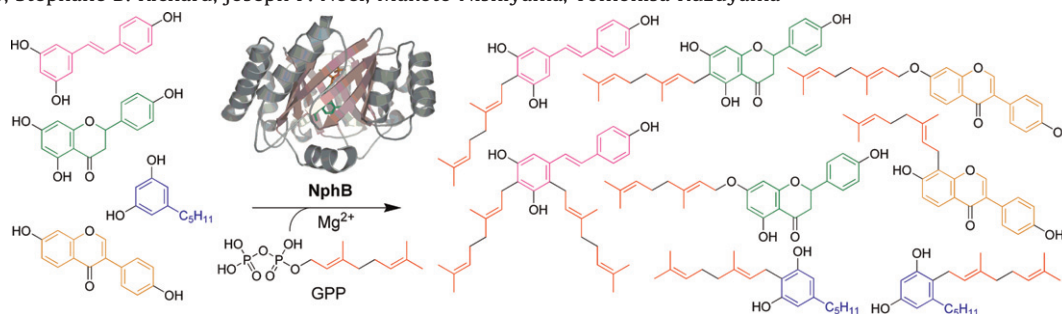


Two glucuronide prodrugs of the histone deacetylase inhibitor CI-994 were synthesized and evaluated as potential selective antitumour agents.

Chemoenzymatic syntheses of prenylated aromatic small molecules using *Streptomyces* prenyltransferases with relaxed substrate specificities

pp 8117–8126

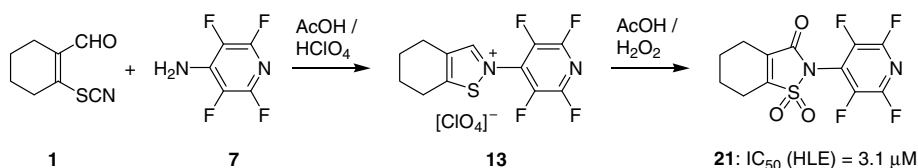
Takuto Kumano, Stéphane B. Richard, Joseph P. Noel, Makoto Nishiyama, Tomohisa Kuzuyama*



Synthesis and elastase-inhibiting activity of 2-pyridinyl-isothiazol-3(2H)-one 1,1-dioxides

pp 8127–8135

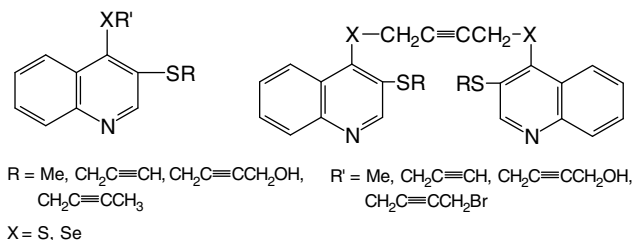
Alexander Eilfeld, Camino M. González Tanarro, Maxim Frizler, Joachim Sieler, Bärbel Schulze, Michael Gütschow*



Synthesis and antiproliferative activity in vitro of novel (2-butynyl)thioquinolines

pp 8136–8141

W. Mól, M. Matyja, B. Filip, J. Wietrzyk, S. Boryczka*

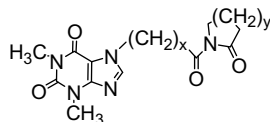


The synthesis of new acetylenic thioquinolines containing propargyl, 2-butynyl, 4-bromo-2-butynyl, and 4-hydroxy-2-butynyl groups exhibiting anti-proliferative activity in vitro against the cells of human and murine cancer cell lines was investigated.

Synthesis and structure–activity relationship studies of theophylline analogs on population responses in the rat hippocampus in vitro

pp 8142–8150

Kethireddy V. V. Ananthalakshmi, Tomáš Bartl, Mohammed H. Aziza, Ladislav Novotný, Radek Marek, Luděk Beneš, Samuel B. Kombian *



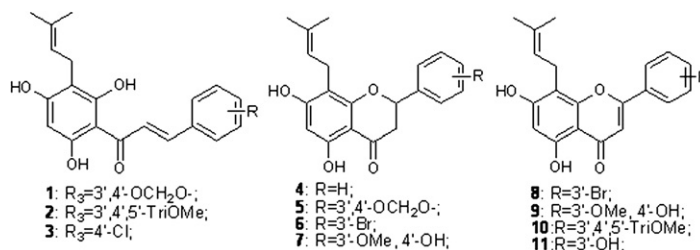
N7-substituted theophylline derivatives bearing various carbon chains ($x = 1-3$) and terminal lactam rings ($y = 1-3$) were synthesized and tested on hippocampal field population responses to see if they enhanced neuronal communication as possible nootropic agents.



Identification of SVM-based classification model, synthesis and evaluation of prenylated flavonoids as vasorelaxant agents

pp 8151–8160

Xiaowu Dong, Yujie Liu, Jingying Yan, Chaoyi Jiang, Jing Chen, Tao Liu, Yongzhou Hu *

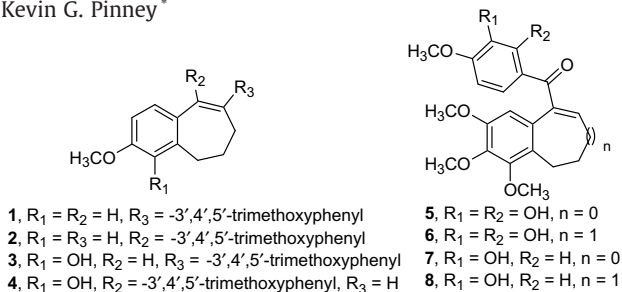


Eleven prenylated flavonoids **1–11** were designed and synthesized according to SVM-based classification model for vasodilators. Their vasorelaxation activities were determined experimentally in rat aorta rings that were pretreated with phenylephrine (PE).

Design, synthesis and biological evaluation of dihydronaphthalene and benzosuberene analogs of the combretastatins as inhibitors of tubulin polymerization in cancer chemotherapy

pp 8161–8171

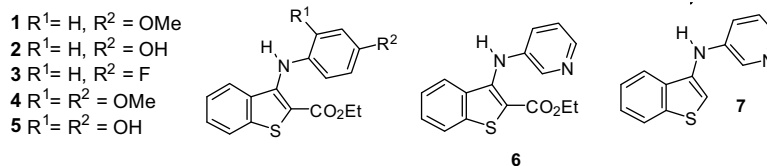
Madhavi Sriram, John J. Hall, Nathan C. Grohmann, Tracy E. Strecker, Taylor Wootton, Andreas Franken, Mary Lynn Trawick, Kevin G. Pinney *



Antifungal activity of synthetic di(hetero)arylamines based on the benzo[b]thiophene moiety

pp 8172–8177

Eugénia Pinto *, Maria-João R. P. Queiroz, Luís A. Vale-Silva, João F. Oliveira, Agathe Begouin, Jeanne-Marie Begouin, Gilbert Kirsch

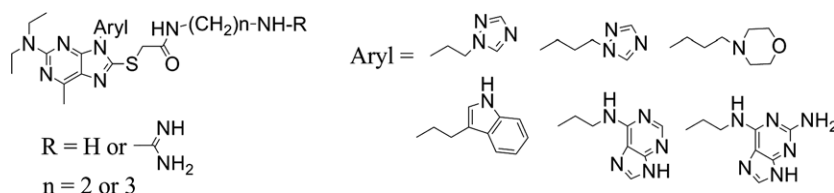


The antifungal activity of new synthesized di(hetero)arylamine derivatives of benzo[b]thiophene, together with some previously reported ones, was evaluated against relevant *Candida*, *Aspergillus*, and dermatophyte species and further confirmed through flow cytometry and germ tube inhibition in *Candida albicans*.

Design and SAR of new substituted purines bearing aryl groups at N9 position as HIV-1 Tat–TAR interaction inhibitors

pp 8178–8186

Ruifang Pang, Chunlei Zhang, Dekai Yuan, Ming Yang*

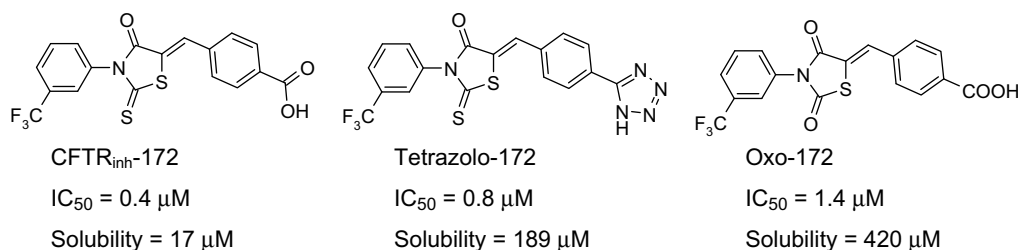


Twenty-four purine derivatives were designed and synthesized as HIV-1 Tat–TAR interaction inhibitors. The aryl groups at N9 position could affect the binding specificity between compounds and TAR.

Thiazolidinone CFTR inhibitors with improved water solubility identified by structure–activity analysis

pp 8187–8195

N. D. Sonawane*, A. S. Verkman

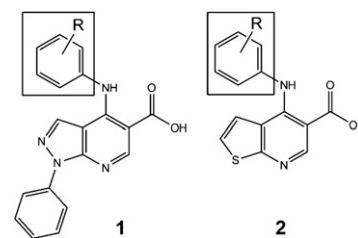


Antibacterial profile against drug-resistant *Staphylococcus epidermidis* clinical strain and structure–activity relationship studies of 1H-pyrazolo[3,4-b]pyridine and thieno[2,3-b]pyridine derivatives

pp 8196–8204

Bruno Leal, Ilídio F. Afonso, Carlos R. Rodrigues*, Paula A. Abreu, Rafael Garrett, Luiz Carlos S. Pinheiro, Alexandre R. Azevedo, Julio C. Borges, Percilene F. Vegi, Cláudio C. C. Santos, Francisco C. A. da Silveira, Lúcio M. Cabral, Izabel C. P. P. Frugulhetti, Alice M. R. Bernardino, Dilvani O. Santos, Helena C. Castro*

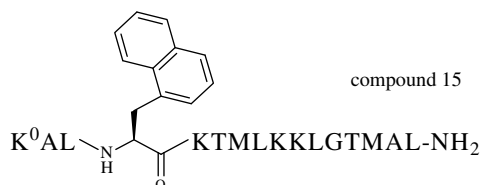
In this work, we report the antibacterial and theoretical evaluations of a pyrazolo[3,4-*b*]pyridine series (**1**, **1a–l**) and the comparison with a new isosteric thieno[2,3-*b*]pyridine derivatives series (**2**, **2a–l**). Several analyses that included molecular modeling studies and in silico ADMET evaluation revealed 1 series with four potential antibacterial lead compounds for treating infections caused by drug-resistant *Staphylococcus epidermidis* clinical strain.



Synthesis and antimicrobial activity of dermaseptin S1 analogues

pp 8205–8209

Dianella Savoia, Remo Guerrini*, Erika Marzola, Severo Salvadori

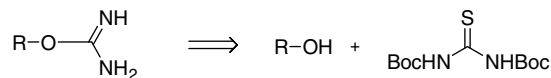


Novel dermaseptin S1 (DS1) analogues were synthesized and evaluated biologically. The replacement of Trp³ with naphthyl-Ala and the insertion of a Lys⁰ in the DS1(1–15) fragment generated a highly potent antimicrobial peptide.

Novel synthesis and pharmacological evaluation as α_2 -adrenoceptor ligands of *O*-phenylisouronium salts

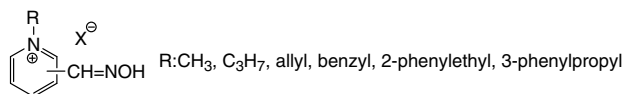
pp 8210–8217

Áine Goonan[†], Amila Kahvedžić, Fernando Rodriguez, Padraic S. Nagle, Thomas McCabe, Isabel Rozas^{*}, Amaia M. Erdozain, J. Javier Meana, Luis F. Callado

**Monoquatary pyridinium salts with modified side chain—synthesis and evaluation on model of tabun- and paraoxon-inhibited acetylcholinesterase**

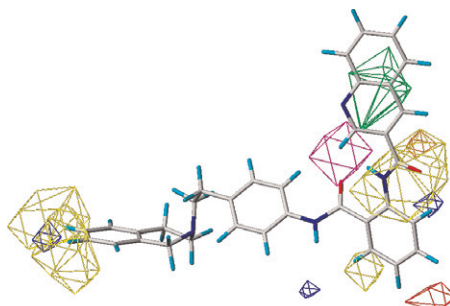
pp 8218–8223

Kamil Musilek^{*}, Jiri Kucera, Daniel Jun, Vlastimil Dohnal, Veronika Opletalova, Kamil Kuca

**Structure–activity relationships of new inhibitors of breast cancer resistance protein (ABCG2)**

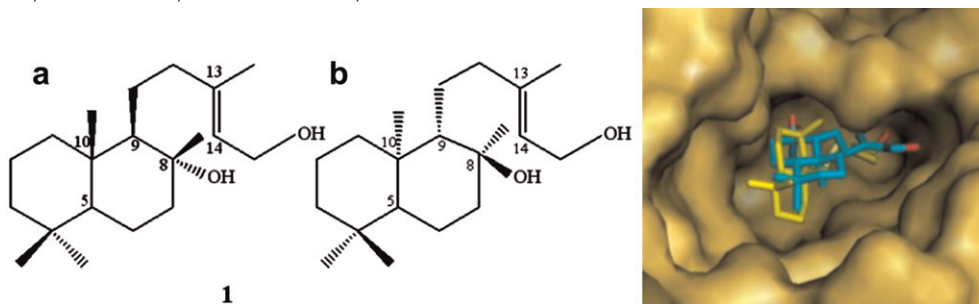
pp 8224–8236

Anne Pick, Henrik Müller, Michael Wiese^{*}

**Comparative docking studies of labdane-type diterpenes with forskolin at the active site of adenylyl cyclase**

pp 8237–8243

Catherine Koukoulitsa^{*}, Maria Zervou, Costas Demetzos, Thomas Mavromoustakos^{*}

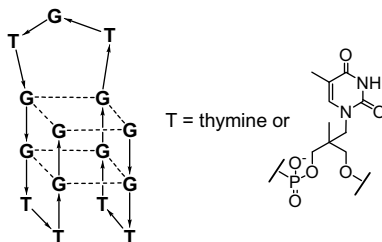


Best binding poses of the two enantiomers of labd-13(*E*)-ene-8a,15-diol (**1a**, colored yellow, and **1b**, colored blue) in the forskolin binding site of AC.

Synthesis, structural studies and biological properties of new TBA analogues containing an acyclic nucleotide

pp 8244–8253

Teresa Coppola, Michela Varra*, Giorgia Oliviero, Aldo Galeone, Giuliana D'Isa, Luciano Mayol, Elena Morelli, Maria-Rosaria Bucci, Valentina Vellecco, Giuseppe Cirino, Nicola Borbone

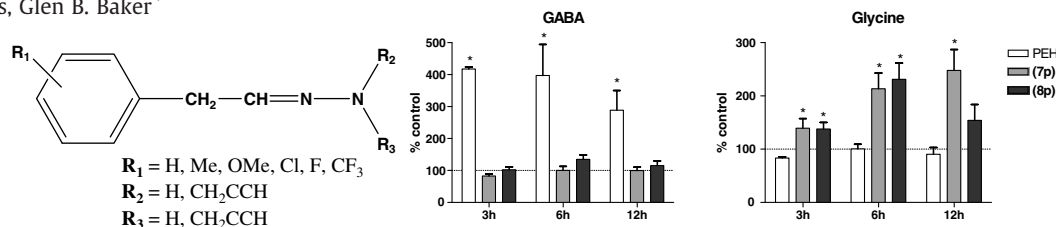


A series of new modified thrombin binding aptamers was synthesized by substitution, one at the time, of the T residues with a new acyclic nucleotide. The structural properties and the thrombin inhibitory activities of the new aptamers have been evaluated.

N-Propynyl analogs of β -phenylethylidenhydrazines: Synthesis and evaluation of effects on glycine, GABA, and monoamine oxidas

pp 8254–8263

Erin M. MacKenzie, Afshin Fassihi, Asghar Davood, Qiao-Hong Chen, Gillian Rauw, Gail Rauw, Edward E. Knaus, Glen B. Baker*

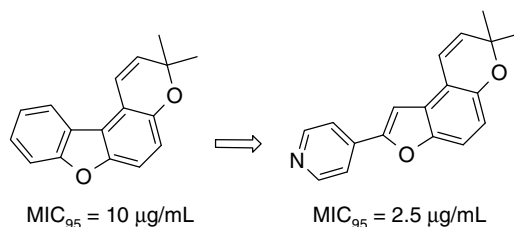


Analogues of β -phenylethylidenhydrazine (PEH) were synthesized and screened in vitro. **7p** ($R_1=H$, $R_2=CH_2CCH$, $R_3=CH_2CCH$) and **8p** ($R_1=H$, $R_2=H$, $R_3=CH_2CCH$) were tested ex vivo for effects on rat brain levels of amino acids (above) and enzyme activity.

A new synthetic access to furo[3,2-f]chromene analogues of an antimycobacterial

pp 8264–8272

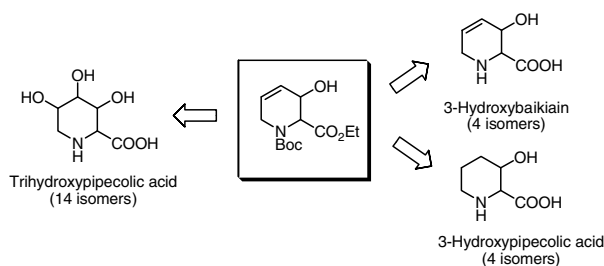
Luke Alvey, Soizic Prado, Valérie Huteau, Brigitte Saint-Joanis, Sylvie Michel, Michel Koch, Stewart T. Cole, François Tillequin, Yves L. Janin*



Synthesis of both enantiomers of hydroxypipercolic acid derivatives equivalent to 5-azapyranuronic acids and evaluation of their inhibitory activities against glycosidases

pp 8273–8286

Yuichi Yoshimura, Chiaki Ohara, Tatsushi Imahori, Yukako Saito, Atsushi Kato, Saori Miyauchi, Isao Adachi, Hiroki Takahata*



COVER

An insight into biologically relevant chemical space showing the scaffolds of potential natural-product based inhibitors orbiting their target, the protein structure of protein 11-beta steroid dehydrogenase (PDB code 1xu7). Graphic produced using Pymol (<http://www.pymol.org>). [M. A. Koch, A. Schuffenhauer, M. Scheck, S. Wetzel, M. Casaulta, A. Odermatt, P. Ertl, H. Waldmann, Charting biologically relevant chemical space: A structural classification of natural products (SCONP), *PNAS* **2005**, 102, 17272–17277 and S. Wetzel, H. Waldmann, Cheminformatic analysis of natural products and their chemical space, *Chimia* **2007**, 61(6), 355–360].

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