



Bioorganic & Medicinal Chemistry Volume 19, Issue 1, 2011

Contents

Editor's Note

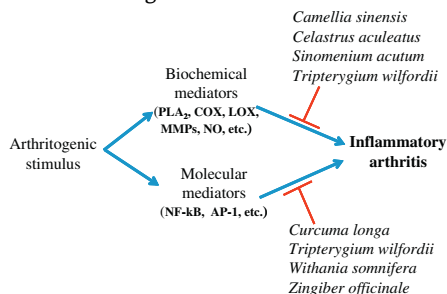
p 20

REVIEW

Herbal medicinal products target defined biochemical and molecular mediators of inflammatory autoimmune arthritis

pp 21–29

Shivaprasad H. Venkatesha, Brian M. Berman, Kamal D. Moudgil*



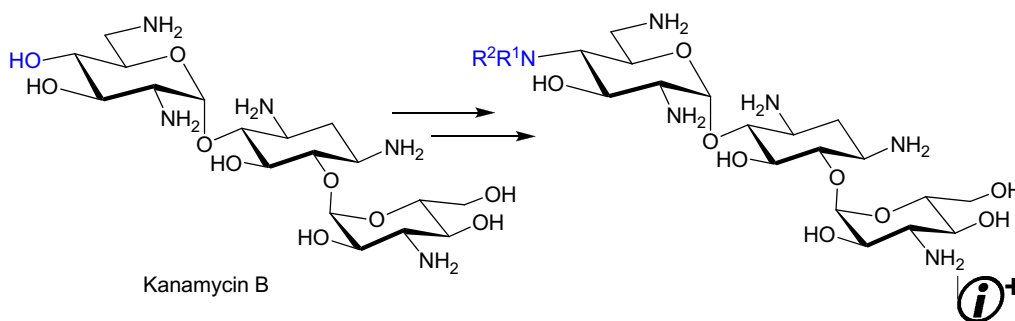
ARTICLES

Rational design and synthesis of potent aminoglycoside antibiotics against resistant bacterial strains

pp 30–40

Ri-Bai Yan, Min Yuan, Yanfen Wu, Xuefu You, Xin-Shan Ye*

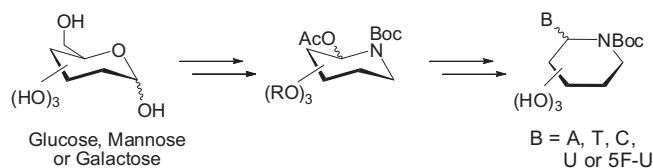
Kanamycin B analogues were rationally designed and synthesized. Some synthetic compounds exhibited good to excellent antibiotic activity against drug-resistant bacteria.



Synthesis and in vitro anti-hepatitis B virus activity of six-membered azanucleoside analogues

pp 41–51

Dan Wang, Yu-Huan Li, Yu-Ping Wang, Rong-Mei Gao, Li-He Zhang, Xin-Shan Ye*



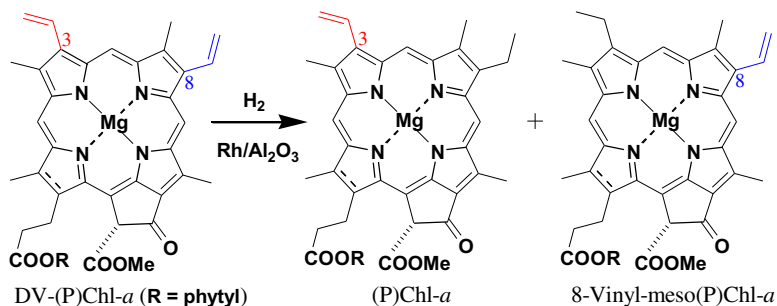
Fifteen novel six-membered azanucleoside derivatives were prepared and evaluated for their anti-hepatitis B virus activity and cytotoxicity in human hepatoblastoma-derived liver Hep-G2 cells.



Reduction of vinyl groups in naturally occurring chlorophylls-*a*

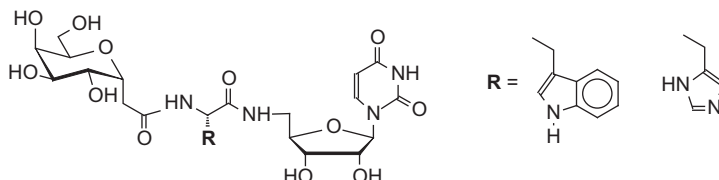
pp 52–57

Hitoshi Tamiaki*, Daisuke Takekoshi, Tadashi Mizoguchi

**Synthesis of sugar–amino acid–nucleosides as potential glycosyltransferase inhibitors**

pp 58–66

Kannan Vembaiyan, Jean A. Pearcey, Milan Bhasin, Todd L. Lowary, Wei Zou*

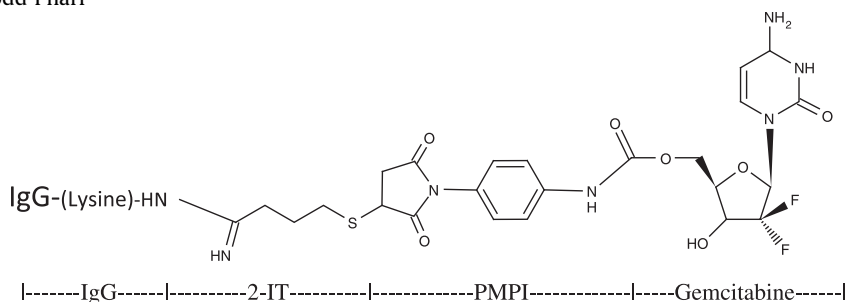


Potential galactosyltransferase inhibitors were synthesized by replacing the diphosphate moiety in sugar donor with a basic amino acid. Analogues containing tryptophan and histidine showed moderate inhibition against mycobacterial GlfT2, which we suggest may arise by mimicking the interaction between the diphosphate metal ion complex with the carboxylate residues present in the active site of the enzyme.

**Synthesis of a covalent gemcitabine-(carbamate)-[anti-HER2/*neu*] immunochemotherapeutic and its cytotoxic anti-neoplastic activity against chemotherapeutic-resistant SKBr-3 mammary carcinoma**

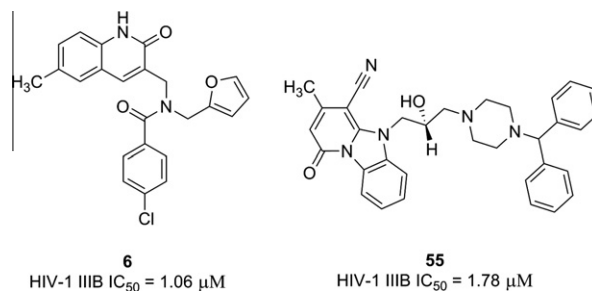
pp 67–76

C. P. Coyne*, Toni Jones, Todd Pharr

**Virtual screening based identification of novel small-molecule inhibitors targeted to the HIV-1 capsid**

pp 77–90

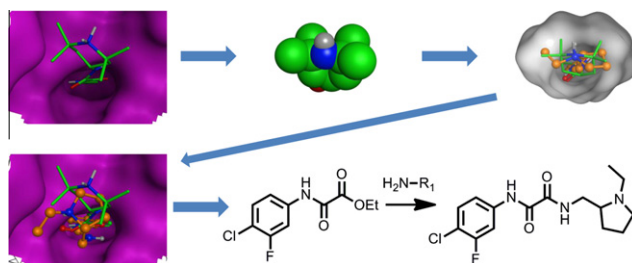
Francesca Curreli, Hongtao Zhang, Xihui Zhang, Ilya Pyatkin, Zagorodnikov Victor, Andrea Altieri, Asim K. Debnath*



Design, synthesis and biological evaluation of small molecule inhibitors of CD4-gp120 binding based on virtual screening

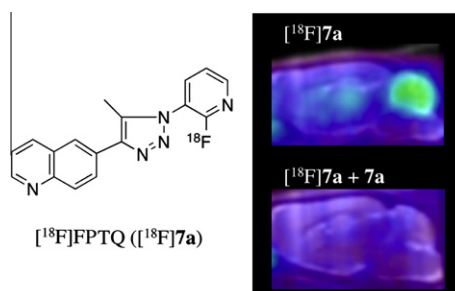
pp 91–101

Judith M. LaLonde*, Mark A. Elban, Joel R. Courter, Akihiro Sugawara, Takahiro Soeta, Navid Madani, Amy M. Princiotta, Young Do Kwon, Peter D. Kwong, Arne Schön, Ernesto Freire, Joseph Sodroski, Amos B. Smith III

**Synthesis and evaluation of 6-[1-(2-[¹⁸F]fluoro-3-pyridyl)-5-methyl-1H-1,2,3-triazol-4-yl]quinoline for positron emission tomography imaging of the metabotropic glutamate receptor type 1 in brain**

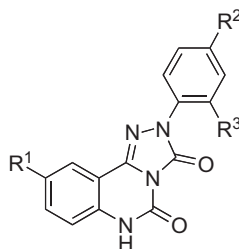
pp 102–110

Masayuki Fujinaga, Tomoteru Yamasaki, Kazunori Kawamura, Katsushi Kumata, Akiko Hatori, Joji Yui, Kazuhiko Yanamoto, Yuichiro Yoshida, Masanao Ogawa, Nobuki Nengaki, Jun Maeda, Toshimitsu Fukumura, Ming-Rong Zhang*

**Triazoloquinazolinones as novel high affinity ligands for the benzodiazepine site of GABA_A receptors**

pp 111–121

Jakob Nilsson, Ritha Gidlöf, Elsebet Østergaard Nielsen, Tommy Liljefors, Mogens Nielsen, Olov Sterner*

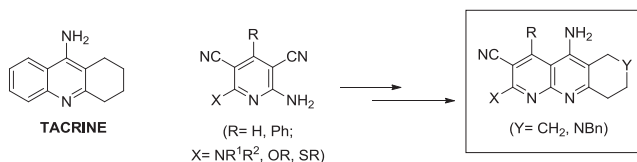


2-Aryl-2,6-dihydro[1,2,4]triazolo[4,3-c]quinazoline-3,5-diones were designed based on a pharmacophore model, synthesized and evaluated for their affinity for the benzodiazepine binding site of GABA_A receptors.

**Cholinergic and neuroprotective drugs for the treatment of Alzheimer and neuronal vascular diseases. II. Synthesis, biological assessment, and molecular modelling of new tacrine analogues from highly substituted 2-aminopyridine-3-carbonitriles**

pp 122–133

Abdelouahid Samadi, Carolina Valderas, Cristóbal de los Ríos, Agatha Bastida, Mourad Chioua, Laura González-Lafuente, Inés Colmena, Luis Gandía, Alejandro Romero, Laura del Barrio, María D. Martín-de-Saavedra, Manuela G. López, Mercedes Villarroja, José Marco-Contelles*

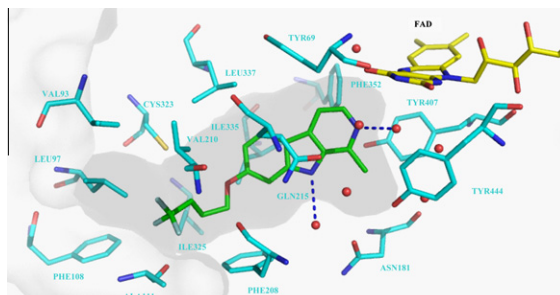


The structures of tacrine, the 2-aminopyridine-3,5-dicarbonitrile precursors, and the new tacrine analogues.

Synthesis and evaluation of β -carboline derivatives as potential monoamine oxidase inhibitors

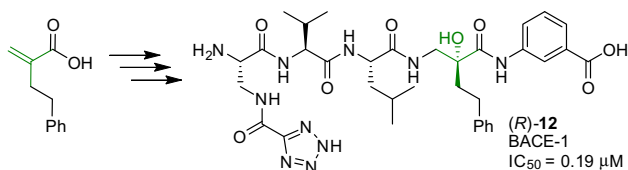
pp 134–144

J. Reniers, S. Robert, R. Frederick, B. Masereel, S. Vincent, J. Wouters*

**Investigation of α -phenylnorstatine and α -benzylnorstatine as transition state isostere motifs in the search for new BACE-1 inhibitors**

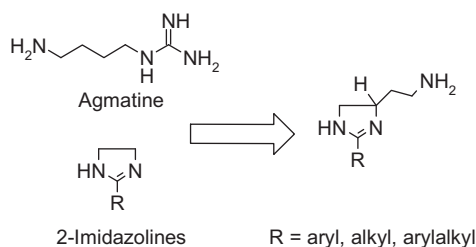
pp 145–155

Fredrik Wängsell, Patrik Nordeman, Jonas Sävmarker, Rikard Emanuelsson, Katarina Jansson, Jimmy Lindberg, Åsa Rosenquist, Bertil Samuelsson, Mats Larhed*

**New imidazoline/ α_2 -adrenoceptors affecting compounds—4(5)-(2-aminoethyl)imidazoline (dihydrohistamine) derivatives. Synthesis and receptor affinity studies**

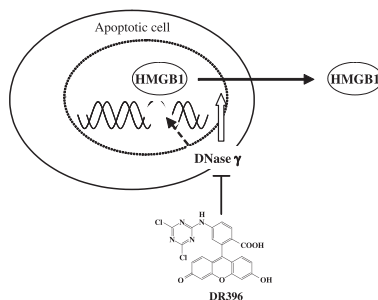
pp 156–167

Adam P. Treder*, Ryszard Andruszkiewicz*, Włodzimierz Zgoda, Aleksandra Walkowiak, Celeste Ford, Alan L. Hudson

Series of imidazoline 2,4(5)-derivatives, analogues of agmatine and known 2-imidazolines are described. Synthesis and α_2 -adrenergic, I₁, I₂ receptor affinity studies are reported.**DR396, an apoptotic DNase γ inhibitor, attenuates high mobility group box 1 release from apoptotic cells**

pp 168–171

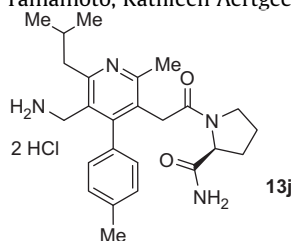
Yoichiro Yamada, Taku Fujii, Rei Ishijima, Haruki Tachibana, Natsuki Yokoue, Ryoko Takasawa, Sei-ichi Tanuma*



Design and synthesis of 3-pyridylacetamide derivatives as dipeptidyl peptidase IV (DPP-4) inhibitors targeting a bidentate interaction with Arg125

pp 172–185

Yasufumi Miyamoto*, Yoshihiro Banno, Tohru Yamashita, Tatsuhiko Fujimoto, Satoru Oi, Yusuke Moritoh, Tomoko Asakawa, Osamu Kataoka, Koji Takeuchi, Nobuhiro Suzuki, Koji Ikeda, Takuo Kosaka, Shigetoshi Tsubotani, Akiyoshi Tani, Miyuki Funami, Michiko Amano, Yoshio Yamamoto, Kathleen Aertgeerts, Jason Yano, Hironobu Maezaki

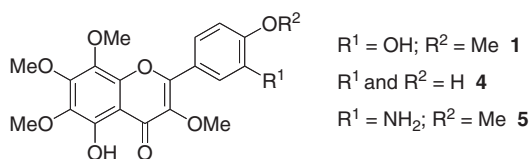


Synthesis and biological evaluation of our dipeptidyl peptidase IV (DPP-4) inhibitor were performed, and compound **13j** with the potent activity were identified.

Synthesis of antiproliferative flavones from calycoperin, major flavonoid of *Calycopteris floribunda* Lamk.

pp 186–196

Guy Lewin*, Narayan Bhat Shridhar, Geneviève Aubert, Sylviane Thoret, Joëlle Dubois, Thierry Cresteil



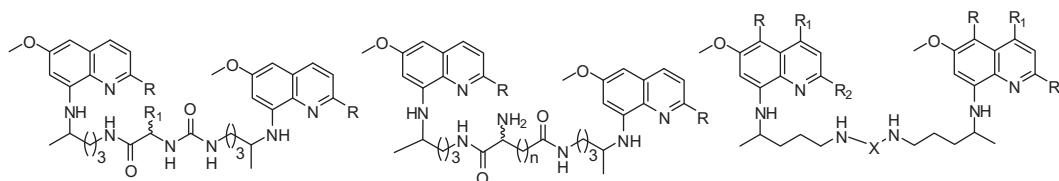
Eighteen new analogues of the potent natural cytotoxic and antimitotic flavone **1** were synthesized from calycoperin **4**. One of them, the 3'-amino analogue **5** displayed almost same activity as **1**.



Synthesis, antiprotozoal, antimicrobial, β -hematin inhibition, cytotoxicity and methemoglobin (MetHb) formation activities of bis(8-aminoquinolines)

pp 197–210

Kirandeep Kaur, Meenakshi Jain, Shabana I. Khan, Melissa R. Jacob, Babu L. Tekwani, Savita Singh, Prati Pal Singh, Rahul Jain*

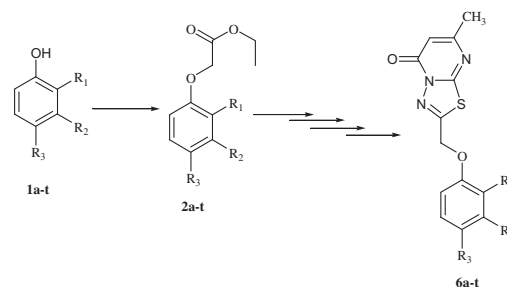


Synthesis and xanthine oxidase inhibitory activity of 7-methyl-2-(phenoxyethyl)-5H-[1,3,4]thiadiazolo[3,2-a]pyrimidin-5-one derivatives

pp 211–220

K. R. Sathisha, Shaikath A. Khanum, J. N. Narendra Sharath Chandra, F. Ayisha, S. Balaji, Gopal K. Marathe, Shubha Gopal*, K. S. Rangappa

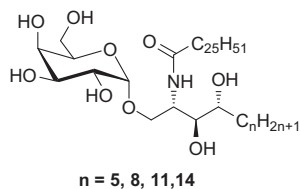
Synthesized title compounds **6a–t** are characterized by spectroscopic techniques and elemental analysis. Four (**6a**, **6b**, **6d** and **6f**) out of 20 synthesized molecules in this class showed good inhibition against three different sources of xanthine oxidase, which were more potent than allopurinol based on their respective IC_{50} values.



Synthesis of truncated analogues of the iNKT cell agonist, α -galactosyl ceramide (KRN7000), and their biological evaluation

pp 221–228

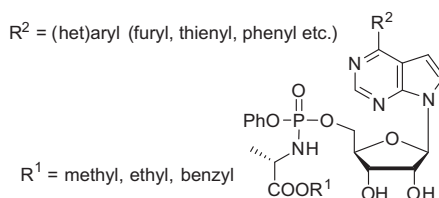
Natacha Veerapen, Faye Reddington, Mariolina Salio, Vincenzo Cerundolo, Gurdial S. Besra*



Phosphoramidate pronucleotides of cytostatic 6-aryl-7-deazapurine ribonucleosides

pp 229–242

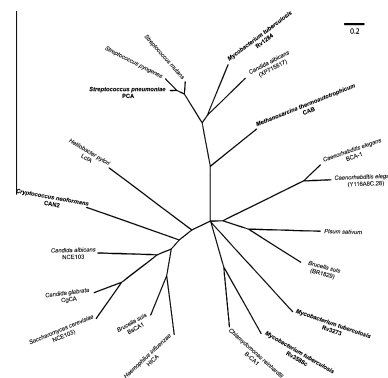
Pavla Perlíková, Radek Pohl, Ivan Votruba, Robert Shih, Gabriel Birkuš, Tomáš Cihlář, Michal Hocek*



Inhibition of the β -carbonic anhydrase from *Streptococcus pneumoniae* by inorganic anions and small molecules: Toward innovative drug design of antiinfectives?

pp 243–248

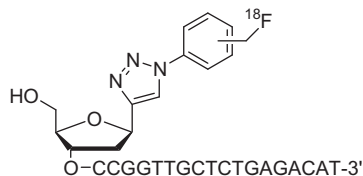
Peter Burghout, Daniela Vullo, Andrea Scozzafava, Peter W. M. Hermans, Claudiu T. Supuran*



Stoichiometry-focused ^{18}F -labeling of alkyne-substituted oligodeoxynucleotides using azido(^{18}F fluoromethyl)benzenes by Cu-catalyzed Huisgen reaction

pp 249–255

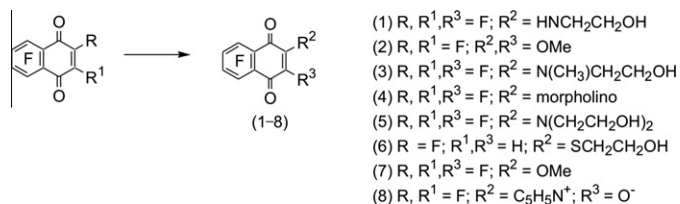
Takeshi Kuboyama, Motoi Nakahara, Masafumi Yoshino, Yilong Cui, Takeo Sako, Yasuhiro Wada, Takeshi Imanishi, Satoshi Obika*, Yasuyoshi Watanabe*, Masaaki Suzuki*, Hisashi Doi



Cytotoxicity of new polyfluorinated 1,4-naphthoquinones with diverse substituents in the quinone moiety

pp 256–260

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

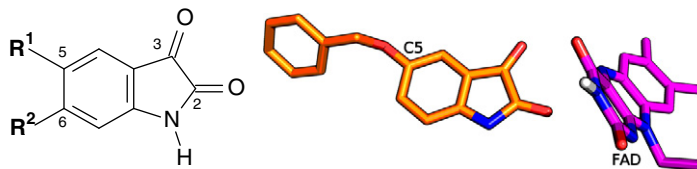


Eight new derivatives of polyfluoro-1,4-naphthoquinone were synthesized and their cytotoxicity in human myeloma (RPMI 8226), human mammary adenocarcinoma (MCF-7), mouse fibroblasts (LMTK), and primary mouse fibroblast cells (PMF) were studied. It was shown that average efficiency of suppressing of two lines of tumor cells decrease from **1** to **8** compound and all compounds are less toxic toward LMTK and PMF cells.

Inhibition of monoamine oxidase by selected C5- and C6-substituted isatin analogues

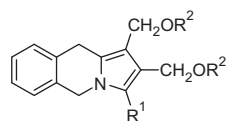
pp 261–274

Clarina I. Manley-King, Jacobus J. Bergh, Jacobus P. Petzer*

**Novel bifunctional alkylating agents, 5,10-dihydropyrrolo[1,2-*b*]isoquinoline derivatives, synthesis and biological activity**

pp 275–286

Ravi Chaniyara, Naval Kapuriya, Huajin Dong, Pei-Chih Lee, Sharda Suman, Bhavin Marvania, Ting-Chao Chou, Te-Chang Lee, Rajesh Kakadiya, Anamik Shah, Tsann-Long Su*

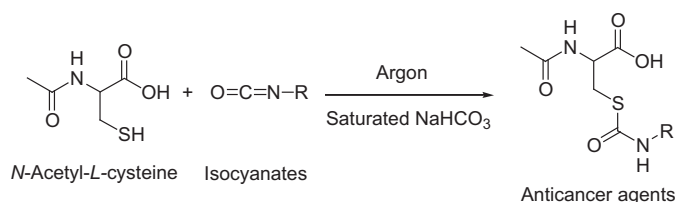


R¹ = Alkyl or substituted phenyl
 R² = H, CONHMe, CONHEt, or CONH-*i*-Pr

Design, synthesis, and biological evaluation of *N*-acetyl-*S*-(*p*-chlorophenylcarbamoyl)cysteine and its analogs as a novel class of anticancer agents

pp 287–294

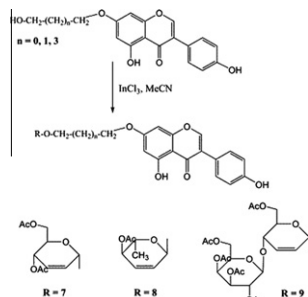
Wei Chen, Teresa Seefeldt, Alan Young, Xiaoying Zhang, Xiangming Guan*



Synthetic conjugates of genistein affecting proliferation and mitosis of cancer cells

pp 295–305

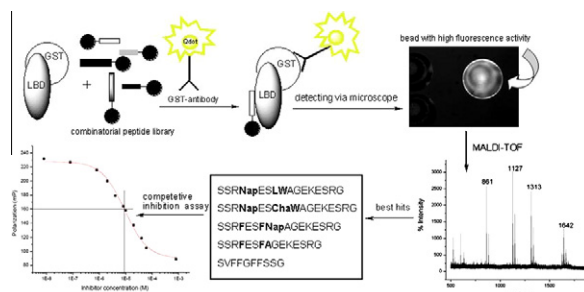
Aleksandra Rusin*, Jadwiga Zawisza-Puchałka, Katarzyna Kujawa, Agnieszka Gogler-Piğłowska, Joanna Wietrzyk, Marta Świtalska, Magdalena Głowala-Kosińska, Aleksandra Gruca, Wiesław Szeja, Zdzisław Krawczyk, Grzegorz Grynkiewicz



An on-bead assay for the identification of non-natural peptides targeting the Androgen Receptor–cofactor interaction

pp 306–311

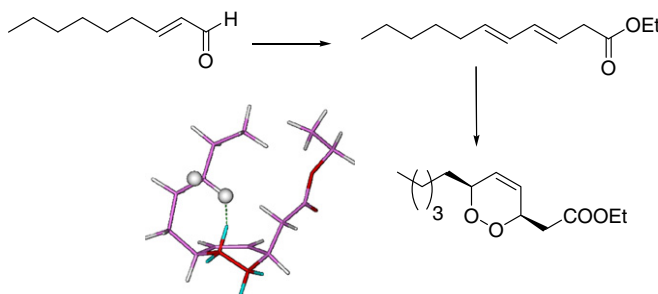
Hülya Göksel, Dorothee Wasserberg, Sabine Möcklinghoff, Belen Vaz Araujo, Luc Brunsveld*



Antimalarials based on the dioxane scaffold of plakortin. A concise synthesis and SAR studies

pp 312–320

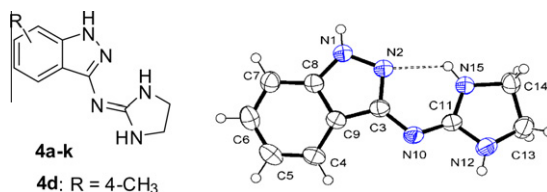
Caterina Fattorusso, Marco Persico, Nicoletta Basilico, Donatella Taramelli, Ernesto Fattorusso, Fernando Scala, Orazio Tagliatela-Scafati*



3-[(Imidazolidin-2-yl)imino]indazole ligands with selectivity for the α_2 -adrenoceptor compared to the imidazoline I₁ receptor

pp 321–329

Franciszek Sączewski*, Anita Kornicka*, Alan L. Hudson, Shayna Laird, Mika Scheinin, Jonne M. Laurila, Apolonia Rybczyńska, Konrad Boblewski, Artur Lehmann, Maria Gdaniec



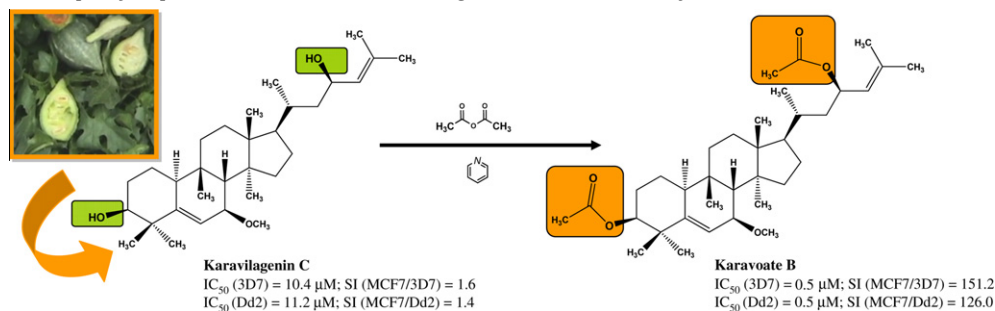
3-[(Imidazolidin-2-yl)imino]indazole derivatives **4a–k** were synthesized as positional analogues of marsanidine. Compound **4d** proved to be partial α_2 -adrenoceptor agonist with high α_2 -adrenoceptor selectivity relative to the imidazoline I₁ receptor and was shown to possess pronounced hypotensive activity.



Karavilagenin C derivatives as antimalarials

pp 330–338

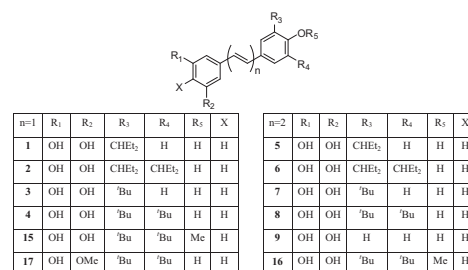
Cátia Ramalhete, Dinora Lopes, Joseph Molnár, Silva Mulhovo, Virgílio E. Rosário, Maria-José U. Ferreira*

Karavilagenin C, a major constituent of the African plant medicinal plant *Momordica balsamina*, as lead for the development of new antimalarials.**New hydroxystilbenoid derivatives endowed with neuroprotective activity and devoid of interference with estrogen and aryl hydrocarbon receptor-mediated transcription**

pp 339–351

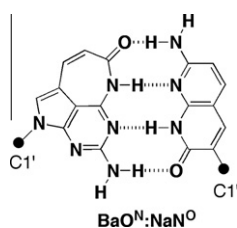
Carolina Villalonga-Barber, Aggeliki K. Meligova, Xanthippi Alexi, Barry R. Steele, Constantinos E. Kouzinos, Constantinos G. Screttas, Efrosini S. Katsanou, Maria Micha-Screttas*, Michael N. Alexis*

A series of hydroxystilbenoid derivatives were synthesized and screened positive for neuroprotective activity and lack of interference with estrogen and aryl hydrocarbon receptor-mediated transcription.

**Synthesis and characterization of oligodeoxynucleotides containing a novel tetraazabenzoc[cd]azulene:naphthyridine base pair**

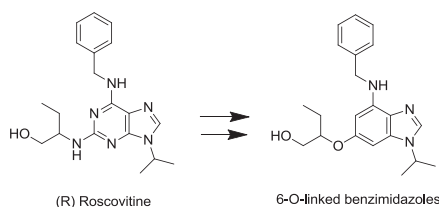
pp 352–358

Yasuyuki Hirama, Noriaki Minakawa*, Akira Matsuda

**Design, synthesis, and testing of an 6-O-linked series of benzimidazole based inhibitors of CDK5/p25**

pp 359–373

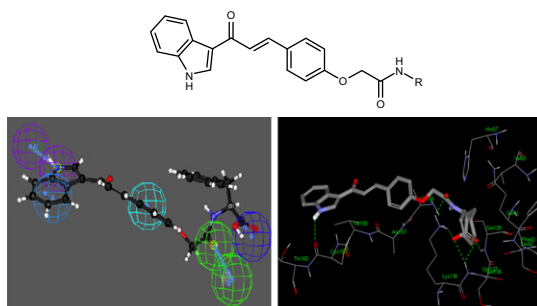
Prashi Jain, Patrick T. Flaherty*, Shuyan Yi, Ishveen Chopra, Gwentyth Bleasdel, Josh Lipay, Yoan Ferandin, Laurent Meijer, Jeffry D. Madura



Beginning with the structure of Roscovitine, a moderately selective CDK5 the design, synthesis, and testing of a series of 1-isopropyl-4-aminobenzyl-6-ether-linked benzimidazoles is presented.

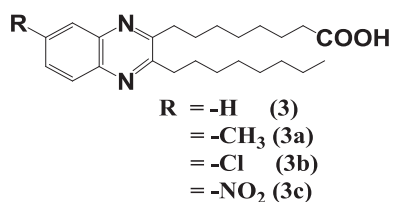
Molecular modeling based approach, synthesis and in vitro assay to new indole inhibitors of hepatitis C NS3/4A serine protease pp 374–383

Nasser S. M. Ismail*, Masao Hattori



Antioxidant, anti-inflammatory and anti-hyperglycaemic activities of heterocyclic homoprostanoid derivatives pp 384–392

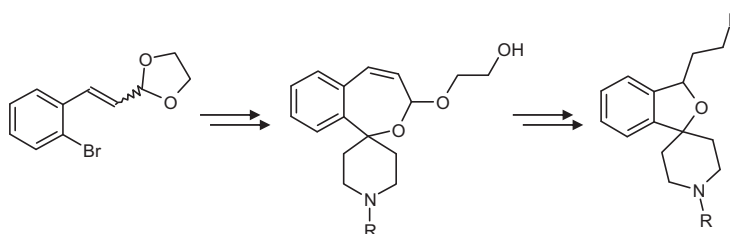
S. A. Manohara Reddy*, Jayesh Mudgal, Punit Bansal, S. G. Vasanthraju, K. K. Srinivasan, C. Mallikarjuna Rao, N. Gopalan Kutty



A series of 19 heterocyclic homoprostanoids were synthesized from easily available oleic and ricinoleic acid and evaluated for their antioxidant, anti-inflammatory and anti-hyperlipidaemic activities. Heterocyclic homoprostanoids with quinoxaline ring and their derivatives (**3**, **3a**, **3b** and **3c**) have shown good anti-inflammatory and anti-hyperglycaemic activity.

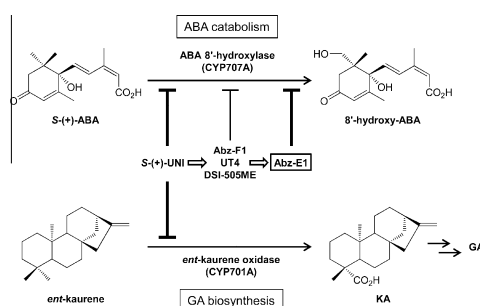
Synthesis, pharmacological activity and structure affinity relationships of spirocyclic σ_1 receptor ligands with a (2-fluoroethyl) residue in 3-position pp 393–405

Eva Große Mastrup, Christian Wiese, Dirk Schepmann, Peter Brust, Bernhard Wunsch*



Abscinazole-E1, a novel chemical tool for exploring the role of ABA 8'-hydroxylase CYP707A pp 406–413

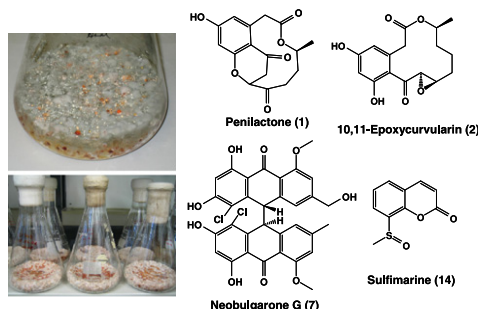
Mariko Okazaki, Hataitip Nimitkeatkai, Taku Muramatsu, Hikaru Aoyama, Kotomi Ueno, Masaharu Mizutani, Nobuhiro Hirai, Satoru Kondo, Toshiyuki Ohnishi, Yasushi Todoroki*



NF kappa B inhibitors and antitrypanosomal metabolites from endophytic fungus *Penicillium* sp. isolated from *Limonium tubiflorum*

pp 414–421

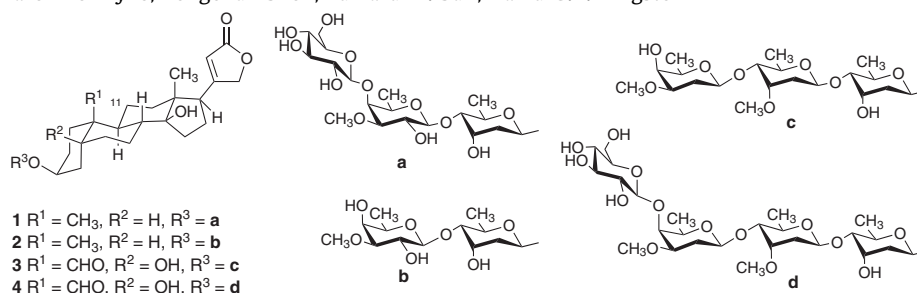
Amal H. Aly*, Abdessamad Debbab, Carol Clements, RuAngelie Edrada-Ebel, Barbora Orlikova, Marc Diederich, Victor Wray, WenHan Lin, Peter Proksch*



Cardenolides of *Leptadenia madagascariensis* from the Madagascar dry forest

pp 422–428

Ende Pan, Liva Harinantenaina, Peggy J. Brodie, Martin Callmänder, Stephan Rakotonandrasana, Etienne Rakotobe, Vincent E. Rasamison, Karen TenDyke, Yongchun Shen, Edward M. Suh, David G. I. Kingston*

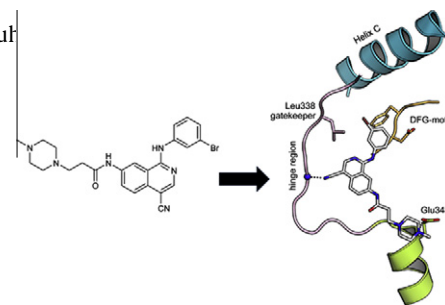


Synthesis and biological evaluation of 7-substituted-1-(3-bromophenylamino)isoquinoline-4-carbonitriles as inhibitors of myosin light chain kinase and epidermal growth factor receptor

pp 429–439

Haridas B. Rode, Martin L. Sos, Christian Grütter, Stefanie Heynck, Jeffrey R. Simard, Daniel Raulf

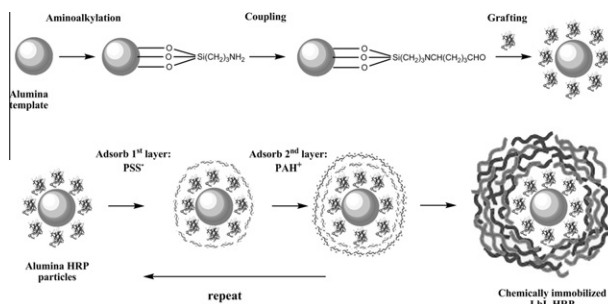
The nature of substituents at the 7-position of 1-(3-bromophenylamino)isoquinoline-4-carbonitriles modulates potency for MLCK and EGFR.



A novel and efficient oxidative functionalization of lignin by layer-by-layer immobilised Horseradish peroxidase

pp 440–447

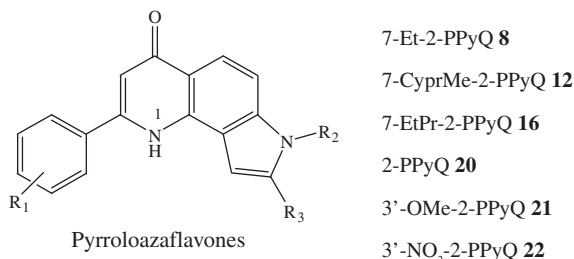
Raffaella Perazzini, Raffaele Saladino, Melissa Guazzaroni, Claudia Crestini*



Synthesis, in vitro and in vivo preliminary evaluation of anti-angiogenic properties of some pyrroloazaflavones

pp 448–457

Maria Grazia Ferlin*, Maria Teresa Conconi, Luca Urbani, Barbara Oselladore, Diego Guidolin, Rosa Di Liddo, Pier Paolo Parnigotto

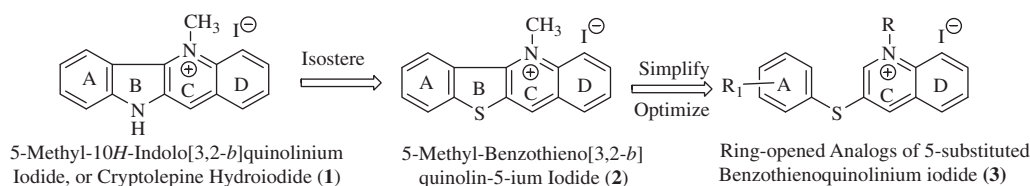


Pyrroloazaflavones or 2-phenyl-1*H*-pyrrolo[2,3-*h*]quinolin-4(7*H*)-ones show in vitro and in vivo anti-angiogenic activity and counteract the pro-angiogenic effects of FGF-2 at non-cytotoxic concentrations.

**Benzothieno[3,2-*b*]quinolinium and 3-(phenylthio)quinolinium compounds: Synthesis and evaluation against opportunistic fungal pathogens**

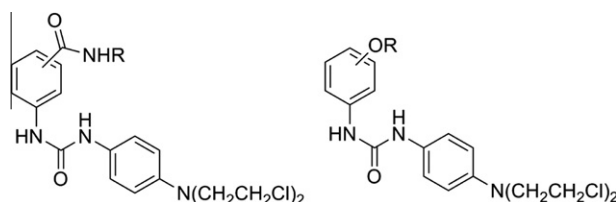
pp 458–470

Comfort A. Boateng, Suresh V. K. Eyunni, Xue Y. Zhu, Jagan R. Etukala, Barbara A. Bricker, M. K. Ashfaq, Melissa R. Jacob, Shabana I. Khan, Larry A. Walker, Seth Y. Ablordepey*

**Design, synthesis, and biological evaluation of novel water-soluble *N*-mustards as potential anticancer agents**

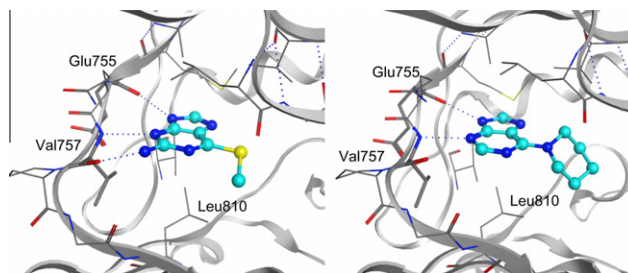
pp 471–485

Naval Kapuriya, Rajesh Kakadiya, Huajin Dong, Amit Kumar, Pei-Chih Lee, Xiuguo Zhang, Ting-Chao Chou, Te-Chang Lee, Ching-Huang Chen, King Lam, Bhavin Marvania, Anamik Shah, Tsann-Long Su*

**Identification of novel ASK1 inhibitors using virtual screening**

pp 486–489

Masako Okamoto, Nae Saito, Hirotatsu Kojima, Takayoshi Okabe, Kohsuke Takeda, Hidenori Ichijo, Toshio Furuya, Tetsuo Nagano*



Predicted binding modes of novel ASK1 inhibitors identified by virtual screening.

pp 490–497

1 CC(C)=CC/C=C\C/C=C\CCSC[C@H](NC(=O)OCC)C(=O)OC **2:** $n = 0$ **3:** $n = 1$ CC(C)=CC/C=C\C/C=C\CCSC[C@H](NC(=O)OCC)C(=O)OC



D

RC757
(MAT α)



H

LM102
(MAT α)



pp 498–503

pp 504–512



(±)-*threo*-Methylphenidate
(Ritalin, Concerta)



DAT Photoaffinity Ligand

pp 513–523

4c
 IC_{50} vs. *T. b. rhodesiense* = 11 nM

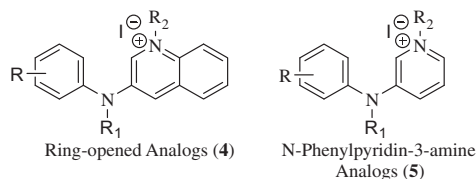
5a
 IC_{50} vs. *T. b. rhodesiense* = 13 nM

5c
 IC_{50} vs. *T. b. rhodesiense* = 14 nM



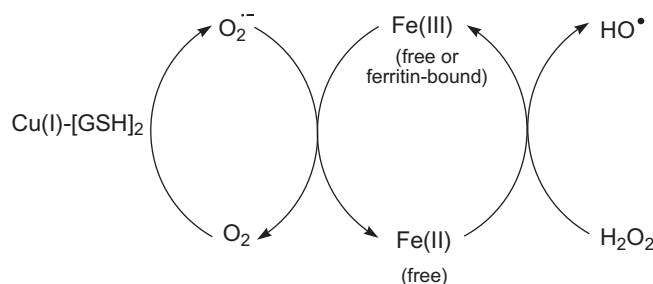
Identification of 3-phenylaminoquinolinium and 3-phenylaminopyridinium salts as new agents against opportunistic fungal pathogens pp 524–533

Tryphon K. Mazu, Jagan R. Etukala, Xue Y. Zhu, Melissa R. Jacob, Shabana I. Khan, Larry A. Walker, Seth Y. Ablordeppey*



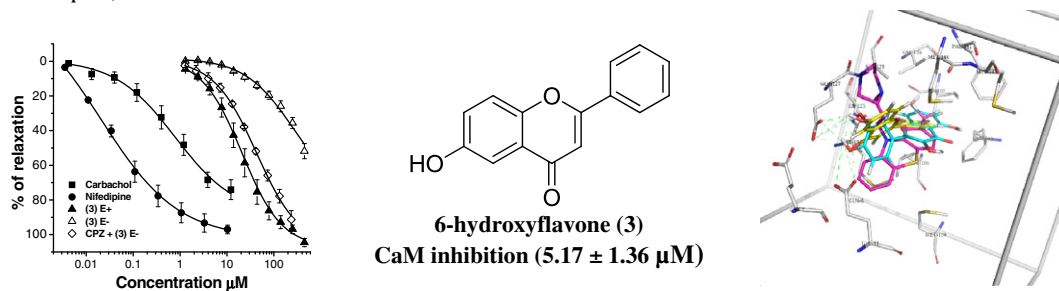
Superoxide-dependent reduction of free Fe^{3+} and release of Fe^{2+} from ferritin by the physiologically-occurring Cu(I)–glutathione complex pp 534–541

Margarita E. Aliaga, Catalina Carrasco-Pozo, Camilo López-Alarcón, Claudio Olea-Azar, Hernán Speisky*



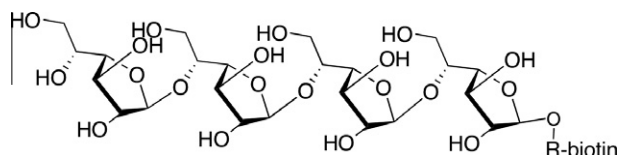
Vasorelaxant effect of flavonoids through calmodulin inhibition: Ex vivo, in vitro, and in silico approaches pp 542–546

Mariana Torres-Piedra, Mario Figueroa*, Oswaldo Hernández-Abreu, Maximiliano Ibarra-Barajas, Gabriel Navarrete-Vázquez, Samuel Estrada-Soto*



Synthetic biotinylated tetra $\beta(1 \rightarrow 5)$ galactofuranoside for in vitro aspergillosis diagnosis pp 547–555

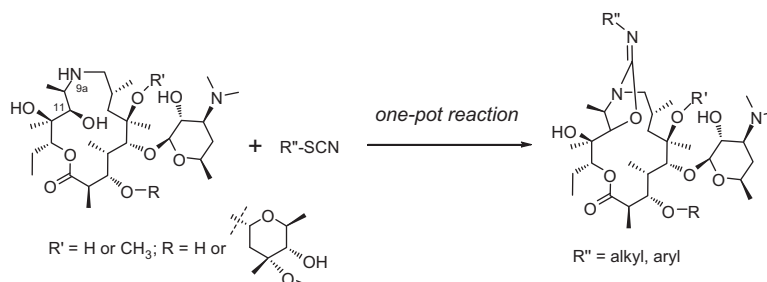
Laurent Cattiaux, Boualem Sendid, Mayeul Collot, Emeline Machez, Daniel Poulain, Jean-Maurice Mallet*



Novel 9a,11-bridged azalides: One-pot synthesis of N'-substituted 2-imino-1,3-oxazolidines condensed to an azalide aglycone

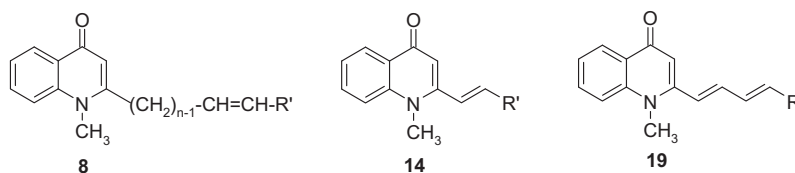
pp 556–566

Zorica Marušić Ištuk, Ana Čikoš, Dubravka Gembarovski, Gorjana Lazarevski, Ivica Đilović, Dubravka Matković-Čalogović, Goran Kragol*

**Design, synthesis and antimycobacterial activities of 1-methyl-2-alkenyl-4(1H)-quinolones**

pp 567–579

Abraham A. Wube, Antje Hübner, Christina Thomaschitz, Martina Blunder, Manfred Kollroser, Rudolf Bauer, Franz Bucar*

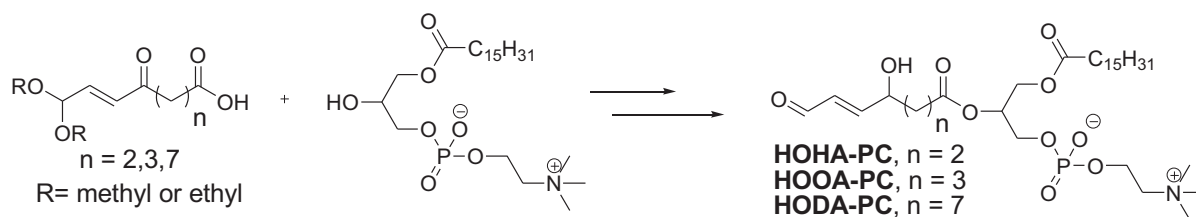


A series of new 1-methyl-2-alkenyl-4(1H)-quinolones lacking carboxyl, fluorine and piperazinyl at position-3, -6 and -7, respectively, have been synthesized and tested in vitro against fast growing species of mycobacteria.

An efficient synthesis of γ -hydroxy- α,β -unsaturated aldehydic esters of 2-lysophosphatidylcholine

pp 580–587

Jaewoo Choi, James M. Laird, Robert G. Salomon*

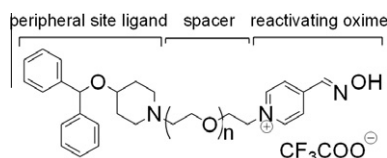


Herein, we report efficient total synthesis of HOOA-, HODA-, and HOHA-phosphatidylcholines.

**Peripheral site ligand–oxime conjugates: A novel concept towards reactivation of nerve agent-inhibited human acetylcholinesterase**

pp 588–594

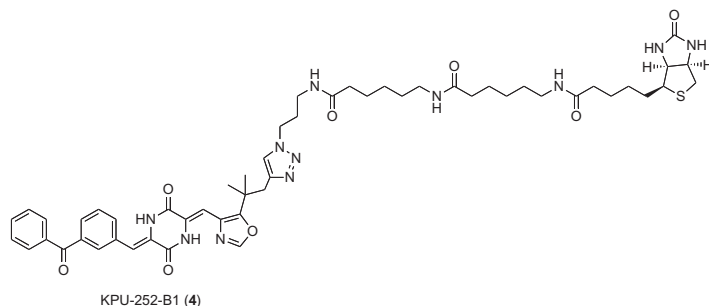
M. C. de Koning*, M. J. A. Joosen, D. Noort, A. van Zuylen, M. C. Tromp



Tubulin photoaffinity labeling study with a plinabulin chemical probe possessing a biotin tag at the oxazole

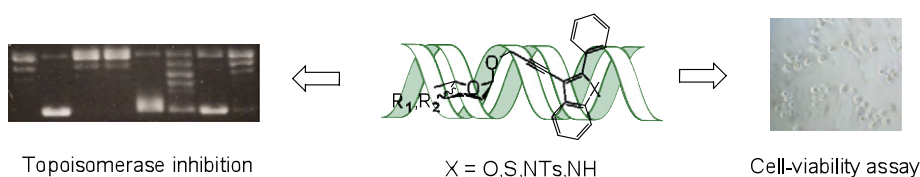
pp 595–602

Yuri Yamazaki, Yui Kido, Koushi Hidaka, Hiroyuki Yasui, Yoshiaki Kiso, Fumika Yakushiji, Yoshio Hayashi*

**Cytotoxicity and topoisomerase I/II inhibition of glycosylated 2-phenyl-indoles, 2-phenyl-benzo[b]thiophenes and 2-phenyl-benzo[b]furans**

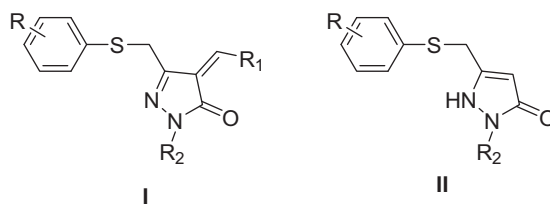
pp 603–612

Wei Shi, Sandra L. Marcus, Todd L. Lowary*

**Arylsulfanyl pyrazolones block mutant SOD1-G93A aggregation. Potential application for the treatment of amyotrophic lateral sclerosis**

pp 613–622

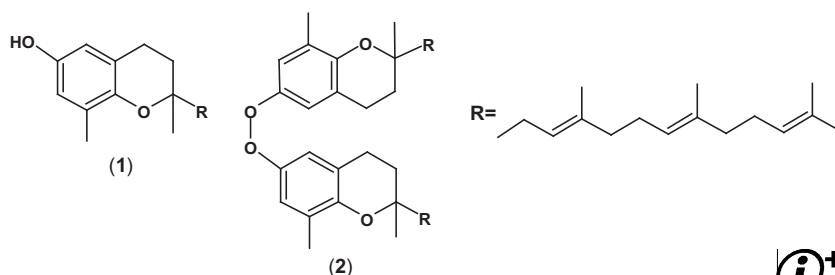
Tian Chen, Radhia Benmohamed, Anthony C. Arvanites, Hantamalala Ralay Ranaivo, Richard I. Morimoto, Robert J. Ferrante, D. Martin Watterson, Donald R. Kirsch, Richard B. Silverman*

**Cytotoxicity of δ -tocotrienols from *Kielmeyera coriacea* against cancer cell lines**

pp 623–630

Mariana Laundry de Mesquita, Renata Mendonça Araújo, Daniel Pereira Bezerra, Raimundo Braz Filho, José Elias de Paula, Edilberto Rocha Silveira, Cláudia Pessoa, Manoel Odorico de Moraes, Letícia Veras Costa Lotufo, Laila Salmen Espindola*

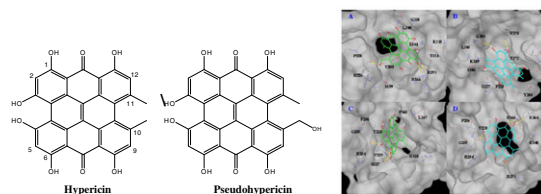
A mixture of δ -tocotrienol (1) and its peroxy-dimer (2) from the hexane root bark extract of the *Kielmeyera coriacea* was obtained as part of an effort to discover new anticancer drugs from Brazilian Cerrado plants.



Hypericins and thioredoxin reductase: Biochemical and docking studies disclose the molecular basis for effective inhibition by naphthodianthrone

pp 631–641

Francesca Sorrentino, Anastasia Karioti, Paola Gratter, Maria Pia Rigobello, Guido Scutari, Luigi Messori, Alberto Bindoli*, Matteo Chioccioli, Chiara Gabbiani, Maria Camilla Bergonzi, Anna Rita Bilia*



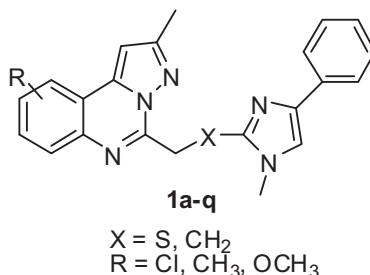
IC₅₀ values of pseudohypericin (4.40 μM) towards TrxR1 is noticeably higher than that of hypericin (157.08 μM), in accordance with the modeling results. IC₅₀ values measured towards TrxR2 were 7.45 μM for pseudohypericin and 43.12 μM for hypericin.



Synthesis and SAR study of new phenylimidazole-pyrazolo[1,5-c]quinazolines as potent phosphodiesterase 10A inhibitors

pp 642–649

Battistina Asproni*, Gabriele Murineddu, Amedeo Pau, Gérard A. Pinna, Morten Langgård, Claus Tornby Christoffersen, Jacob Nielsen, Jan Kehler*

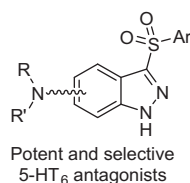


Synthesis, inhibition of PDE10A activity of new phenylimidazole-pyrazolo[1,5-c]quinazolines (**1**) are described.

Identification of 3-sulfonylindazole derivatives as potent and selective 5-HT₆ antagonists

pp 650–662

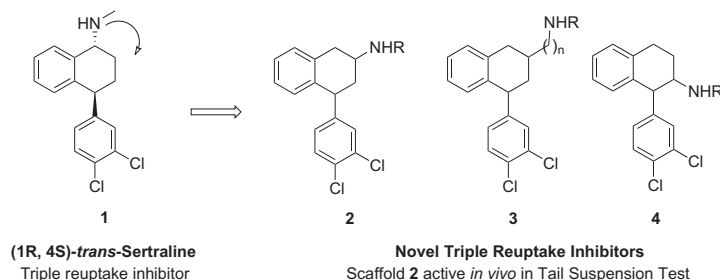
Kevin G. Liu*, Albert J. Robichaud*, Alexander A. Greenfield, Jennifer R. Lo, Cristina Grosanu, James F. Mattes, Yanxuan Cai, Guo Ming Zhang, Jean Y. Zhang, Dianne M. Kowal, Deborah L. Smith, Li Di, Edward H. Kerns, Lee E. Schechter, Thomas A. Comery



Synthesis and pharmacological evaluation of 4-(3,4-dichlorophenyl)-N-methyl-1,2,3,4-tetrahydronaphthalenyl amines as triple reuptake inhibitors

pp 663–676

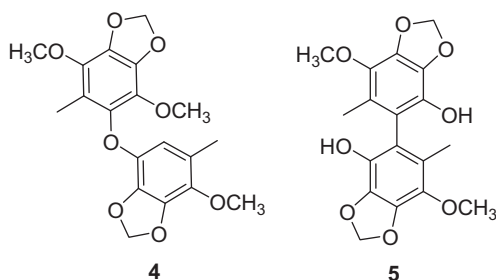
Liming Shao*, Fengjiang Wang, Scott C. Malcolm, Jianguo Ma, Michael C. Hewitt, Una C. Campbell, Larry R. Bush, Nancy A. Spicer, Sharon R. Engel, Lakshmi D. Saraswat, Larry W. Hardy, Patrick Koch, Rudy Schreiber, Kerry L. Spear, Mark A. Varney



Biologically active constituents from the fruiting body of *Taiwanofungus camphoratus*

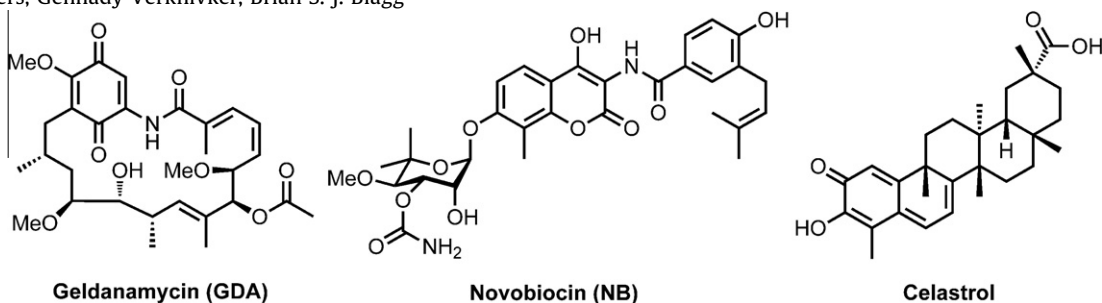
pp 677–683

Li-Shian Shi, Chih-Hua Chao, De-Yang Shen, Hsiu-Hui Chan, Chou-Hsiung Chen, Yu-Ren Liao, Shwu-Jen Wu, Yann-Lii Leu, Yuh-Chiang Shen, Yao-Haur Kuo, E-Jian Lee, Keduo Qian, Tian-Shung Wu*, Kuo-Hsiung Lee*

**A systematic protocol for the characterization of Hsp90 modulators**

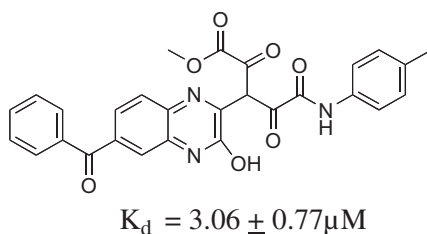
pp 684–692

Robert L. Matts, Gary E. L. Brandt, Yuanming Lu, Anshuman Dixit, Mehdi Mollapour, Suiquan Wang, Alison C. Donnelly, Leonard Neckers, Gennady Verkhivker, Brian S. J. Blagg*

**Benzopyrazine derivatives: A novel class of growth factor receptor bound protein 7 antagonists**

pp 693–701

Nigus D. Ambaye, Menachem J. Gunzburg, Reece C. C. Lim, John T. Price, Matthew C. J. Wilce, Jacqueline A. Wilce*

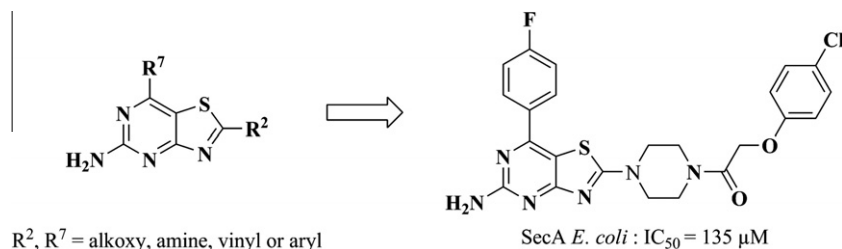


A succession of computational ligand design regimes followed by experimental binding affinity measurements was conducted to identify a novel class of Grb7 antagonists.

Synthesis of novel 5-amino-thiazolo[4,5-d]pyrimidines as *E. coli* and *S. aureus* SecA inhibitors

pp 702–714

Mi-Yeon Jang, Steven De Jonghe, Kenneth Segers, Jozef Anné, Piet Herdewijn*



OTHER CONTENT**Bioorganic & Medicinal Chemistry Reviews and Perspectives****pp I–III**

*Corresponding author

+ Supplementary data available via ScienceDirect**COVER**

The known veterinary anthelmintic and proton ionophore, closantel, was recently discovered to also exhibit potent chitinase inhibition activity and inhibit molting in the parasitic nematode, *Onchocerca volvulus*, the causative agent of the neglected tropical disease onchocerciasis. [C. Gloeckner, A. L. Garner, F. Mersha, Y. Oksov, N. Tricoche, L. M. Eubanks, S. Lustigman, G. F. Kaufmann, K. D. Janda, Repositioning of an existing drug for the neglected tropical disease Onchocerciasis, *Proc. Natl. Acad. Sci., U.S.A.* **2010**, 107, 3424.]

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