Bioorganic & Medicinal Chemistry 16 (2008) 9627–9634

Contents lists available at ScienceDirect

Bioorganic & Medicinal Chemistry

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

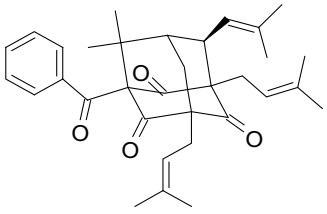
Bioorganic & Medicinal Chemistry Vol. 16, No. 22, 2008

Contents

ARTICLES

The contribution of plukenetione A to the anti-tumoral activity of Cuban propolis **pp 9635–9643**

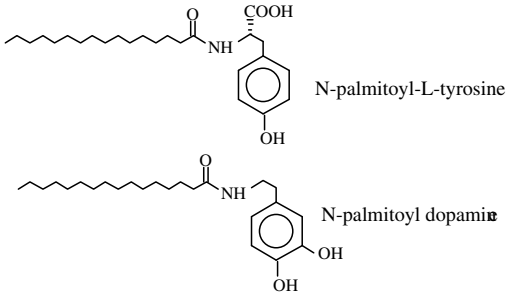
David Díaz-Carballo*, Sascha Malak, Walter Bardenheuer, Michael Freistuehler, H. Peter Reusch



Here, we are reporting for the first time the anti-tumoral activity of Plukenetione A, isolated from propolis, which exerts its anti-cancer properties inhibiting both topoisomerase I and DNA polymerase.

Acylamido analogs of endocannabinoids selectively inhibit cancer cell proliferation **pp 9644–9651**

Sumner Burstein*, Rebecca Salmonsen

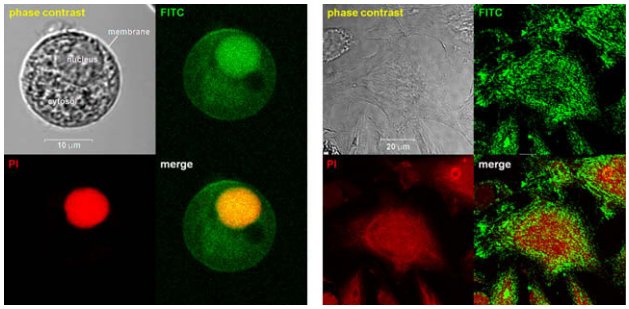


A series of amide derivatives of long-chain fatty acids has been studied for their effects on the proliferation of cancer cells in vitro. Two analogs showed a high degree of specificity in matched breast cancer (tumor vs normal) cell lines obtained from the same donor. *N*-palmitoyl dopamine and *N*-palmitoyl tyrosine each demonstrated complete specificity of action at a concentration of 10 μM and were highly efficacious in both cases.

Time-dependent intracellular trafficking of FITC-conjugated epigallocatechin-3-*O*-gallate in L-929 cells **pp 9652–9659**

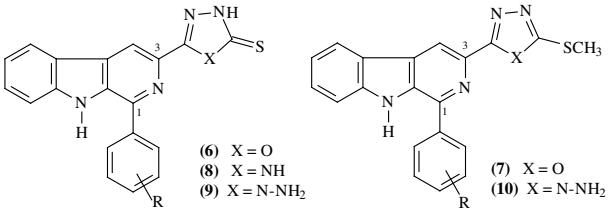
Dong-Wook Han, Kazuaki Matsumura, Bongju Kim, Suong-Hyu Hyon*

In the present study, epigallocatechin-3-*O*-gallate (EGCG) was conjugated with fluorescein-4-isothiocyanate (FITC) via the 3″-OH or 5″-OH group on the gallate ring of EGCG. We demonstrated the binding of FITC-conjugated EGCG onto membranes, its incorporation into cytoplasm and subsequent translocation into nucleus in suspended (left) and cultured (right) L-929 cells after 4 h and 8 h of treatment, respectively.



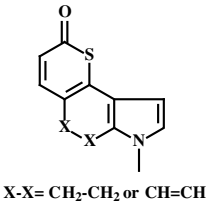
Synthesis and antitumoral activity of novel 3-(2-substituted-1,3,4-oxadiazol-5-yl) and 3-(5-substituted-1,2,4-triazol-3-yl) β-carboline derivatives **pp 9660–9667**

Anelise S. Nazari Formagio, Lilian T. Düsman Tonin, Mary Ann Foglio, Christiana Madjarof, João Ernesto de Carvalho, Willian Ferreira da Costa, Flávia P. Cardoso, Maria Helena Sarragiotto *



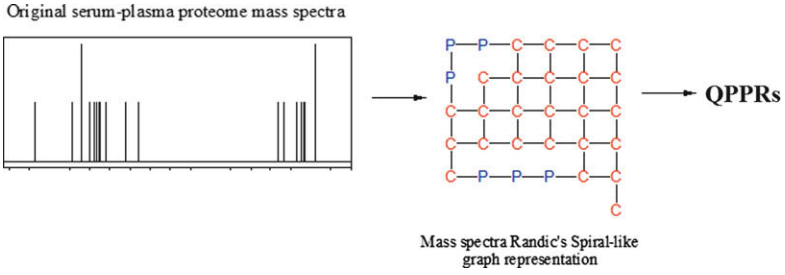
Thiopyrano[2,3-*e*]indol-2-ones: Angelicin heteroanalogues with potent photoantiproliferative activity **pp 9668–9683**

Paola Barraja, Patrizia Diana, Alessandra Montalbano, Anna Carbone, Girolamo Cirrincione *, Giampietro Viola, Alessia Salvador, Daniela Vedaldi, Francesco Dall'Acqua



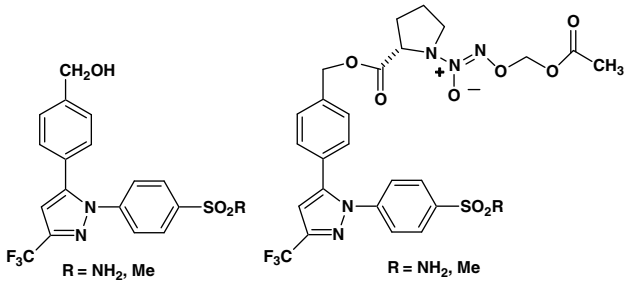
Quantitative Proteome–Property Relationships (QPPRs). Part 1: Finding biomarkers of organic drugs with mean Markov connectivity indices of spiral networks of blood mass spectra **pp 9684–9693**

Maykel Cruz-Monteagudo, Cristian Robert Munteanu, Fernanda Borges, M. Natália D. S. Cordeiro, Eugenio Uriarte, Humberto González-Díaz *



Diazen-1-ium-1,2-diolated nitric oxide donor ester prodrugs of 5-(4-hydroxymethylphenyl)-1-(4-aminosulfonylphenyl)-3-trifluoromethyl-1*H*-pyrazole and its methanesulfonyl analog: Synthesis, biological evaluation and nitric oxide release studies **pp 9694–9698**

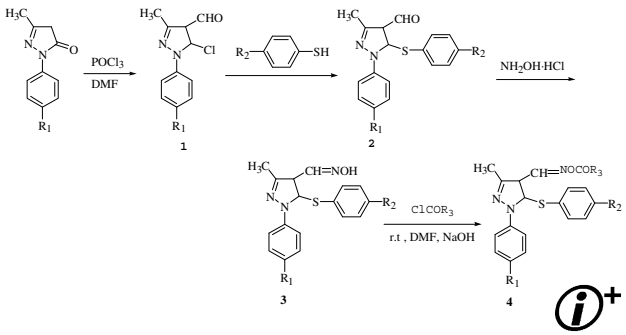
Khaled R. A. Abdellatif, Morshed Alam Chowdhury, Ying Dong, Carlos Velázquez, Dipankar Das, Mavanur R. Suresh, Edward E. Knaus *



Synthesis and antiviral activity of novel pyrazole derivatives containing oxime esters group **pp 9699–9707**

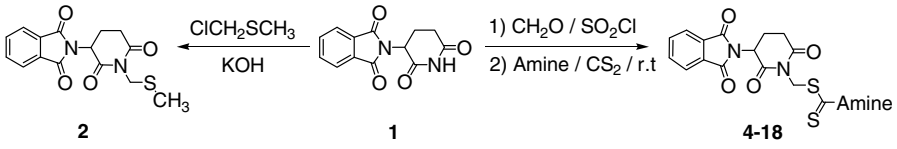
Guiping Ouyang, Zhuo Chen, Xue-Jian Cai, Bao-An Song *, Pinaki S. Bhadury, Song Yang, Lin-Hong Jin, Wei Xue, De-Yu Hu, Song Zeng

1-Substituted-5-substitutedphenylthio-4-pyrazolaldoxime ester derivatives **4a**–**4n**, were synthesized from the starting material 1-substitutedphenyl-3-methyl-5-substitutedphenylthio-4- pyrazolaldoximes **3** by treatment with acyl chloride. The bioassay results showed that title compounds possessed weak to good anti-TMV bioactivity with **4l** showing significant enhancement of disease resistance in tobacco leaves with high affinity for TMV CP.



Design, synthesis and antitumor evaluation of novel thalidomide dithiocarbamate and dithioate analogs against Ehrlich ascites carcinoma-induced solid tumor in Swiss albino mice **pp 9708–9718**

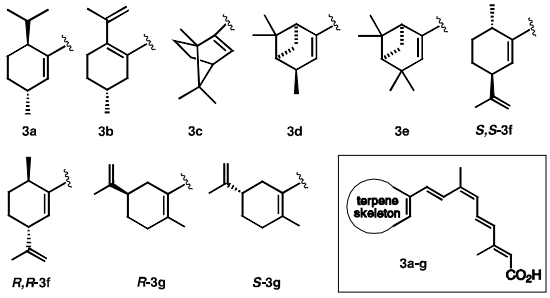
Magdy A.-H. Zahran *, Tarek A.-R. Salem, Rehab M. Samaka, Hussein S. Agwa, Ayman R. Awad



Synthesis of 16 novel thalidomide sulfur analogs is discussed and their apoptotic, necrotic, antimitotic, antioxidant, cytotoxic, antiproliferative and anti-angiogenic effects on Ehrlich ascites carcinoma-induced solid tumor in Swiss albino mice were evaluated.

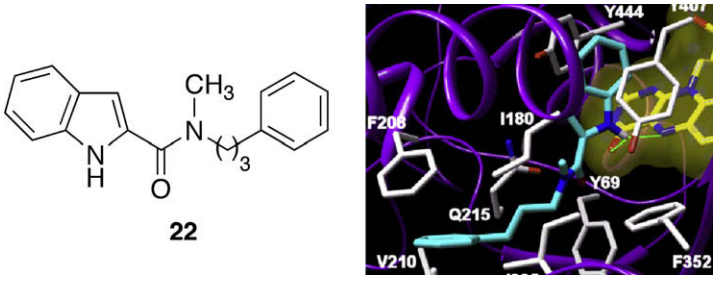
New retinoid chemotypes: 9-*cis*-Retinoic acid analogs with hydrophobic rings derived from terpenes as selective RAR agonists **pp 9719–9728**

Susana Álvarez, Yolanda Pazos-Randulfe, Harshal Khanwalkar, Pierre Germain, Rosana Álvarez, Hinrich Gronemeyer *, Ángel R. de Lera *

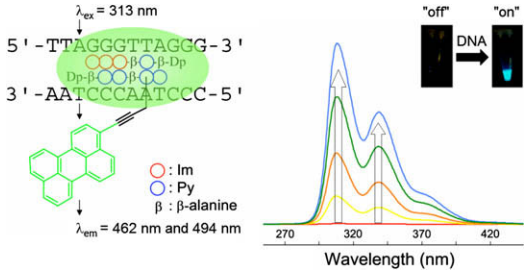


Synthesis, structure–activity relationships and molecular modeling studies of new indole inhibitors of monoamine oxidases A and B **pp 9729–9740**

Giuseppe La Regina, Romano Silvestri *, Valerio Gatti, Antonio Lavecchia *, Ettore Novellino, Olivia Befani, Paola Turini, Enzo Agostinelli

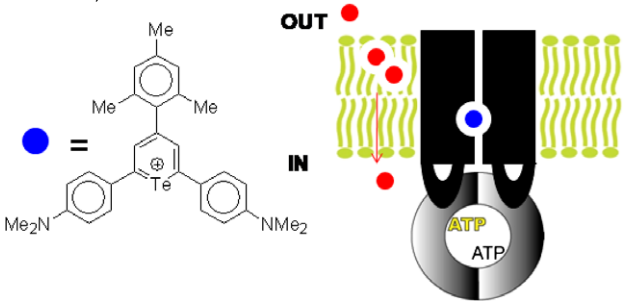


Perylene-conjugated pyrrole polyamide as a sequence-specific fluorescent probe **pp 9741–9744**
Jun Fujimoto, Toshikazu Bando *, Masafumi Minoshima, Gengo Kashiwazaki, Shigeki Nishijima, Ken-ichi Shinohara, Hiroshi Sugiyama *

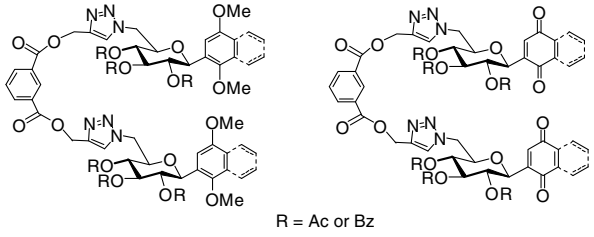


Chalcogenopyrylium dyes as inhibitors/modulators of P-glycoprotein in multidrug-resistant cells **pp 9745–9756**
Geri A. Sawada, Thomas J. Raub, J. William Higgins, Nancy K. Brennan, Teiah M. Moore, Gregory Tombline, Michael R. Detty *

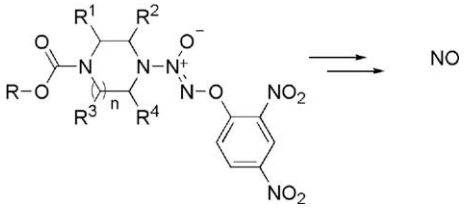
A series of chalcogenopyrylium compounds were evaluated as inhibitors/modulators of P-glycoprotein in lipid-activated protein, inside-out membrane vesicles, and in human MDCKIIMDR1 cells.



Synthesis of triazole-linked β-*C*-glycosyl dimers as inhibitors of PTP1B **pp 9757–9763**
Li Lin, Qiang Shen, Guo-Rong Chen *, Juan Xie *

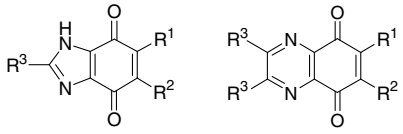


Synthesis, mechanistic studies, and anti-proliferative activity of glutathione/glutathione *S*-transferase-activated nitric oxide prodrugs **pp 9764–9771**
Harinath Chakrapani *, Ravi C. Kalathur, Anna E. Maciag, Michael L. Citro, Xinhua Ji, Larry K. Keefer, Joseph E. Saavedra *



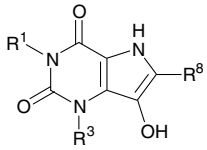
A number of structural analogues of JS-K, an anti-cancer lead compound, were prepared and their chemical and biological properties were compared.

3D-QSAR studies of heterocyclic quinones with inhibitory activity on vascular smooth muscle cell proliferation using pharmacophore-based alignment **pp 9772–9779**
Chung-Kyu Ryu *, Yoonji Lee, Seul-gi Park, Hea-Jung You, Ra-Young Lee, Seung-Yon Lee, Sun Choi *

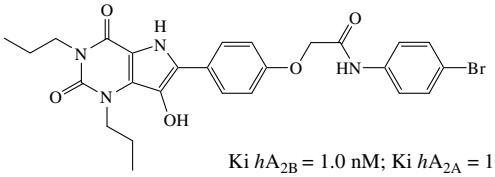


Synthesis and 3D-QSAR studies of quinoxaline-5,8-diones and 1H-benzo[*d*]imidazole-4,7-diones with antiproliferative activity on vascular smooth muscle cells using Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Indices Analysis (CoMSIA) after pharmacophore-based alignment are reported.

1,3-Dialkyl-8-(hetero)aryl-9-OH-9-deazaxanthines as potent A_{2B} adenosine receptor antagonists: Design, synthesis, structure–affinity and structure–selectivity relationships **pp 9780–9789**
Angela Stefanachi, Orazio Nicolotti, Francesco Leonetti, Saverio Cellamare, Francesco Campagna, Maria Isabel Loza, Jose Manuel Brea, Fernando Mazza, Enrico Gavuzzo, Angelo Carotti *

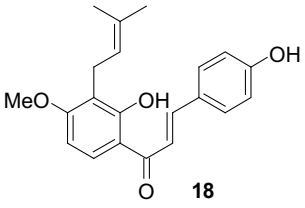


R^1=R^3= Me, Pr
R^1=Pr and R^3= Me
R^8= Aryl or Heteroaryl

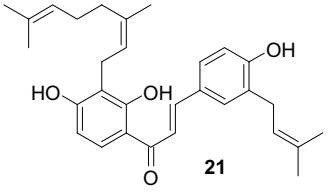


Ki hA_{2B} = 1.0 nM; Ki hA_{2A} = 100 nM
Ki hA_1 = 79 nM; Ki hA_3 = 1290 nM

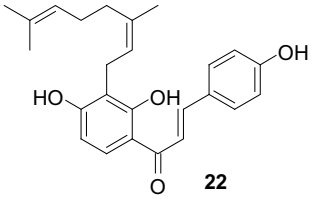
Structure–activity relationship of antibacterial chalcones **pp 9790–9794**
Hugo Pereira Ávila, Elza de Fátima Albino Smânia, Franco Delle Monache, Artur Smânia Júnior *



18
4-hydroxyderricin



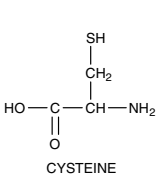
21
2',4,4'-trihydroxy-3-prenyl-3'-geranylchalcone



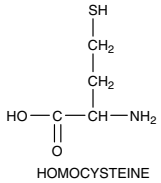
22
2',4,4'-trihydroxy-3'-geranylchalcone

The antibacterial activity of thirty-one chalones is described. Some of the tested compounds showed fair to significant activity against Gram-positive bacteria.

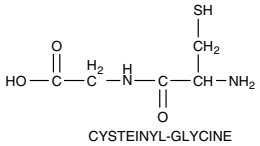
Double edge redox-implications for the interaction between endogenous thiols and copper ions: In vitro studies **pp 9795–9803**
Catalina Carrasco-Pozo *, Margarita E. Aliaga, Claudio Olea-Azar, Hernán Speisky



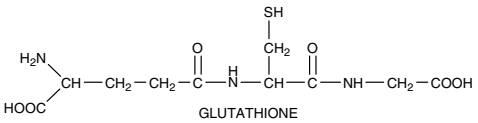
CYSTEINE



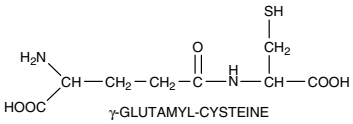
HOMOCYSTEINE



CYSTEINYL-GLYCINE

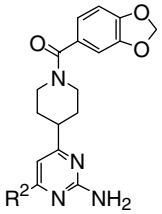


GLUTATHIONE



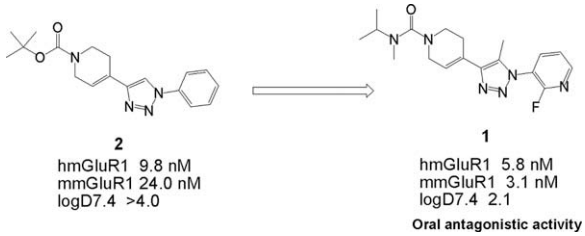
γ-GLUTAMYL-CYSTEINE

Novel piperidinylpyrimidine derivatives as inhibitors of HIV-1 LTR activation **pp 9804–9816**
Norio Fujiwara *, Takashi Nakajima, Yutaka Ueda, Hitoshi Fujita, Hajime Kawakami



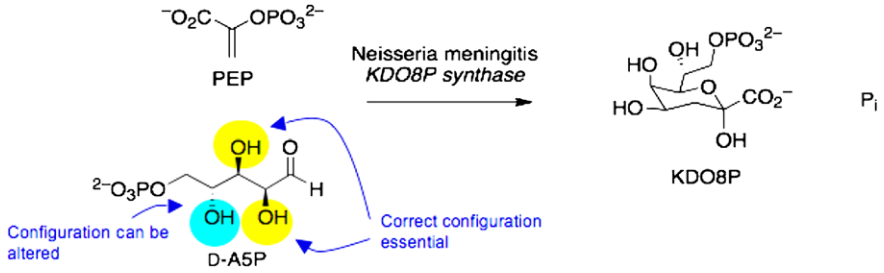
Piperidinylpyrimidine derivatives were found to inhibit HIV-1 LTR transactivation. SAR indicated that the piperonyloyl on the nitrogen of piperidine and lipophilic substitution at pyrimidine C(6)-position are important for this inhibition.

Discovery and biological profile of 4-(1-aryltriazol-4-yl)-tetrahydropyridines as an orally active new class of metabotropic glutamate receptor 1 antagonist **pp 9817–9829**
Satoru Ito *, Atsushi Satoh, Yasushi Nagatomi, Yukari Hirata, Gentaroh Suzuki, Toshifumi Kimura, Akio Satow, Shunsuke Maehara, Hirohiko Hikichi, Mikiko Hata, Hiroshi Kawamoto, Hisashi Ohta

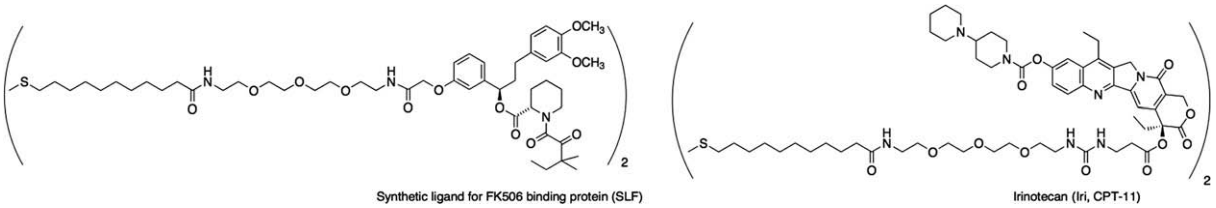


4-(1-Aryltriazol-4-yl)-tetrahydropyridines were designed and synthesized as novel mGluR1 antagonists.

Arabinose 5-phosphate analogues as mechanistic probes for *Neisseria meningitidis* 3-deoxy-D-*manno*-octulosonate 8-phosphate synthase **pp 9830–9836**
Meekyung Ahn, Fiona C. Cochrane, Mark L. Patchett, Emily J. Parker *

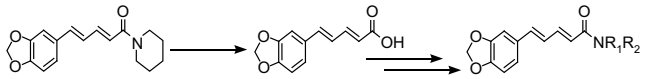


Efficient one-cycle affinity selection of binding proteins or peptides specific for a small-molecule using a T7 phage display pool **pp 9837–9846**
Yoichi Takakusagi, Kouji Kuramochi, Manami Takagi, Tomoe Kusayanagi, Daisuke Manita, Hiroko Ozawa, Kanako Iwakiri, Kaori Takakusagi, Yuka Miyano, Atsuo Nakazaki, Susumu Kobayashi *, Fumio Sugawara *, Kengo Sakaguchi *



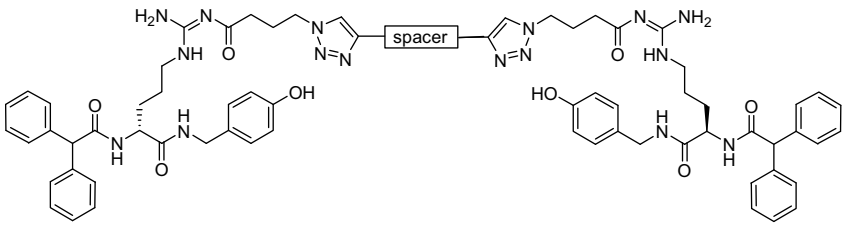
An effective T7 phage display environment for small-molecules using a T7 phage display system and a cuvette type 27-MHz quartz-crystal microbalance (QCM) apparatus was further introduced a self-assembled monolayer (SAM) as a means of small-molecule attachment for the sensor chip. In this approach, one-cycle affinity selection of binding proteins or peptides specific for small-molecules has efficiently been achieved.

Piperine analogs as potent *Staphylococcus aureus* NorA efflux pump inhibitors **pp 9847–9857**
Payare L. Sangwan, Jawahir L. Koul*, Surrinder Koul*, Mallepally V. Reddy, Niranjan Thota, Inshad A. Khan, Ashwani Kumar, Nitin P. Kalia, Ghulam N. Qazi

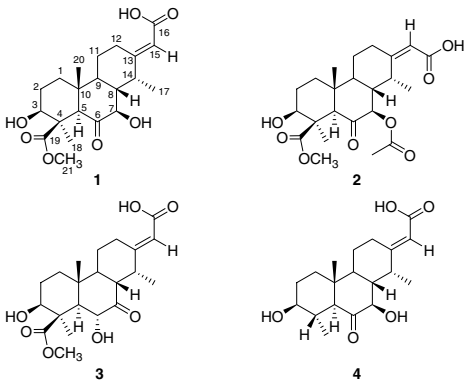


Piperine analogs derived from piperine have been shown to possess potent efflux pump inhibitory activity against NorA system of *Staphylococcus aureus* having better potentiation activity than known EPIs.

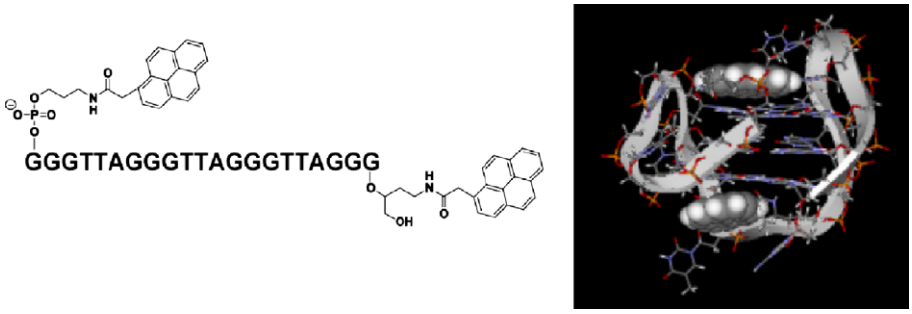
Modular synthesis of non-peptidic bivalent NPY Y_1 receptor antagonists **pp 9858–9866**
Stefan Weiss, Max Keller, Günther Bernhardt, Armin Buschauer, Burkhard König*



New diterpenoids and the bioactivity of *Erythrophleum fordii* **pp 9867–9870**
Chuan-Chung Tsao, Yuh-Chiang Shen, Chung-Ren Su, Chia-Ying Li, Meei-Jen Liu, Nguyen-Xuan Dung, Tian-Shung Wu*



Interactions of sodium and potassium ions with oligonucleotides carrying human telomeric sequence and pyrene moieties at both termini **pp 9871–9881**
Hirohisa Hayashida, Jan Paczesny, Bernard Juskowiak, Shigeori Takenaka*



OTHER CONTENTS

Instructions to contributors **p I**

*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

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].

Indexed/Abstracted in: Beilstein, Biochemistry & Biophysics Citation Index, CANCERLIT, Chemical Abstracts, Chemistry Citation Index, Current Awareness in Biological Sciences/BIOBASE, Current Contents: Life Sciences, EMBASE/Excerpta Medica, MEDLINE, PASCAL, Research Alert, Science Citation Index, SciSearch, TOXFILE

ELSEVIER

ISSN 0968-0896