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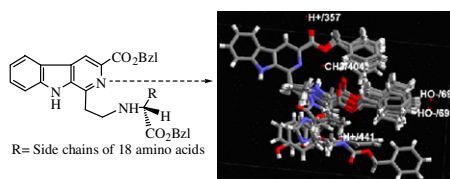
Bioorganic & Medicinal Chemistry Volume 18, Issue 17, 2010

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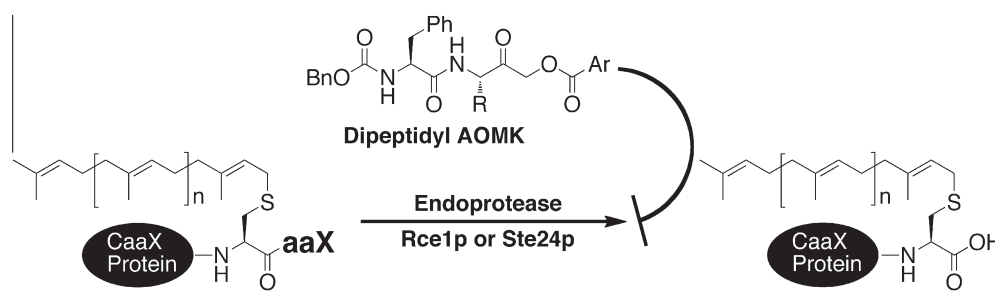
A class of novel carboline intercalators: Their synthesis, in vitro anti-proliferation, in vivo anti-tumor action, and 3D QSAR analysis pp 6220–6229

Jianhui Wu, Chunyu Li, Ming Zhao*, Wenjing Wang, Yuji Wang, Shiqi Peng*



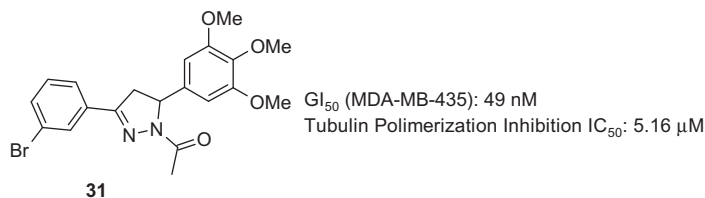
Modulation of the inhibitor properties of dipeptidyl (acyloxy)methyl ketones toward the CaaX proteases pp 6230–6237

Anne-Marie R. Dechert, James P. MacNamara, Sarah R. Breevoort, Emily R. Hildebrandt, Ned W. Hembree, Adam C. Rea, Duncan E. McLain, Stephen B. Porter, Walter K. Schmidt*, Timothy M. Dore*



Synthesis and in vitro antitumor activity of new 4,5-dihydropyrazole derivatives pp 6238–6248

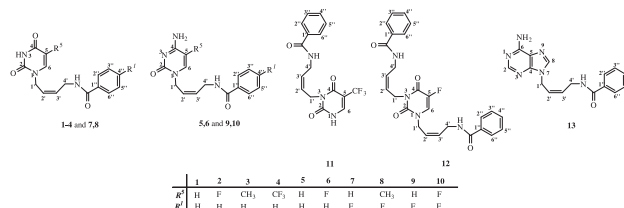
Cenzo Congiu*, Valentina Onnis, Loredana Vesci, Massimo Castorina, Claudio Pisano



The unsaturated acyclic nucleoside analogues bearing a sterically constrained (Z)-4'-benzamido-2'-butenyl moiety: Synthesis, X-ray crystal structure study, cytostatic and antiviral activity evaluations

pp 6249–6257

Krešimir Benci, Karlo Wittine, Malajka Radan, Mario Cetina, Mirela Sedić, Sandra Kraljević Pavelić, Krešimir Pavelić, Erik De Clercq, Mladen Mintas*



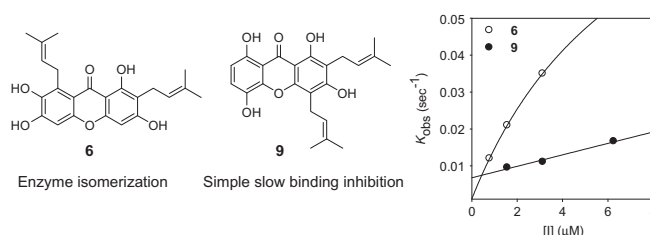
A series of the novel acyclic unsaturated pyrimidine (**1–12**) and adenine (**13**) nucleoside analogues bearing conformationally restricted (Z)-2'-butenyl moiety were synthesized and evaluated for their antiviral and cytostatic activity potency. The N-1 4'-fluoro-substituted-benzamide uracil derivative (**7**) showed inhibitory activity against the growth of MCF-7 cells at a concentration of 2.7 μ M and no cytotoxic effect on normal fibroblasts WI38. The X-ray crystal structure analysis **11–13** revealed supramolecular self-assemblies, in which infinite chains or dimers built two- and three-dimensional networks.



Xanthonones with neuraminidase inhibitory activity from the seedcases of *Garcinia mangostana*

pp 6258–6264

Hyung Won Ryu, Marcus J. Curtis-Long, Sunin Jung, Young Min Jin, Jung Keun Cho, Young Bae Ryu, Woo Song Lee*, Ki Hun Park*



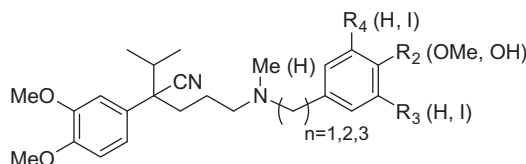
Xanthonones show different kinetic inhibition mechanism depending upon the arrangement of hydroxyl groups in B ring.



Iodination of verapamil for a stronger induction of death, through GSH efflux, of cancer cells overexpressing MRP1

pp 6265–6274

Régis Barattin, Thomas Perrotton, Doriane Trompier, Doriane Lorendeau, Attilio Di Pietro, Amaury du Moulinet d'Hardemare, Hélène Baubichon-Cortay*

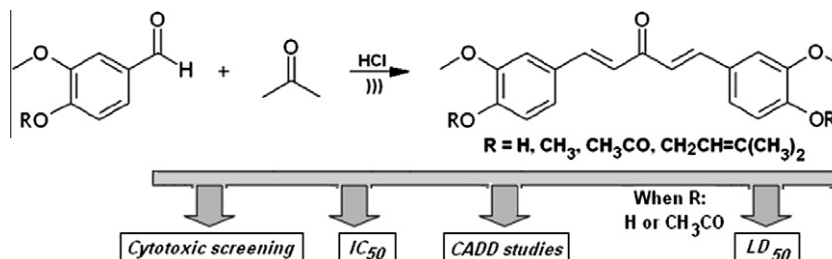


A series of iodinated derivatives of verapamil were synthesized and tested on cells overexpressing the MRP1 drug transporter in order to design novel anti-cancer compounds targeting and killing resistant cancer cells.

New antitumoral agents I: In vitro anticancer activity and in vivo acute toxicity of synthetic 1,5-bis(4-hydroxy-3-methoxyphenyl)-1,4-pentadien-3-one and derivatives

pp 6275–6281

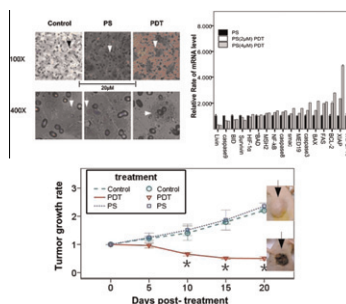
José Agustín Quincoces Suarez*, Daniela Gonçalves Rando, Reginaldo Pereira Santos, Carolina Passarelli Gonçalves, Elizabeth Ferreira, João Ernesto de Carvalho*, Luciana Kohn, Durvanei Augusto Maria, Fernanda Faião-Flores, Dirk Michalik, Maria Cristina Marcucci, Christian Vogel



Studies on preparation and photodynamic mechanism of chlorin P6-13,15-*N*-(cyclohexyl)cycloimide (Chlorin-H) and its antitumor effect for photodynamic therapy in vitro and in vivo

pp 6282–6291

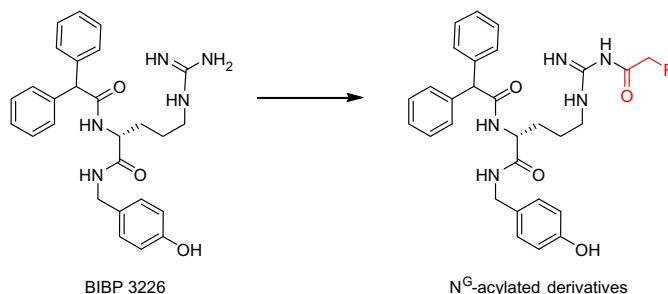
Yi-jia Yan, Mei-zhen Zheng, Zhi-long Chen*, Xin-hai Yu*, Xiao-xia Yang, Zhi-lou Ding, Li Xu



N^G-Acyl-argininamides as NPY Y₁ receptor antagonists: Influence of structurally diverse acyl substituents on stability and affinity

pp 6292–6304

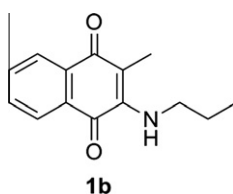
Stefan Weiss, Max Keller, Günther Bernhardt, Armin Buschauer, Burkhard König*



Synthesis and biological evaluation of vitamin K derivatives as angiogenesis inhibitor

pp 6305–6309

Tomoko Kayashima, Masaharu Mori, Ryo Mizutani, Kazuyuki Nishio, Kouji Kuramochi, Kazunori Tsubaki, Hiromi Yoshida, Yoshiyuki Mizushima, Kiminori Matsubara*

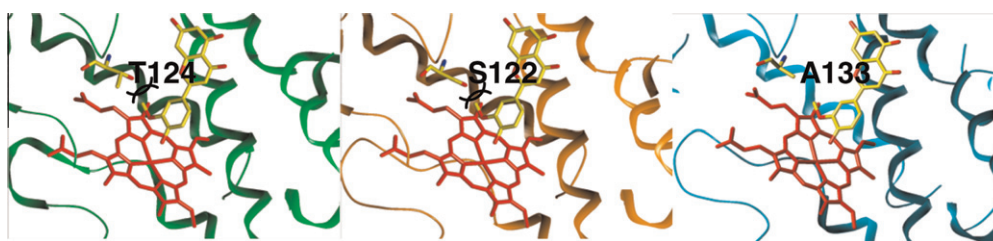


Among the vitamin K derivatives synthesized, **1b** showed the strongest anti-angiogenic effect under both ex vivo and in vitro conditions. Longer alkyl chains weaken anti-angiogenic activity.

Selective inhibition of methoxyflavonoids on human CYP1B1 activity

pp 6310–6315

Hitomi Takemura, Toshimasa Itoh, Keiko Yamamoto, Hiroyuki Sakakibara, Kayoko Shimoi*

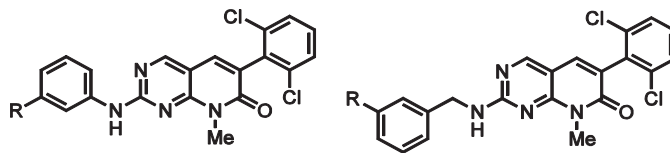


Molecular docking study suggested selective inhibition of human CYP1B1 by methoxyflavonoids.

New effective inhibitors of the Abelson kinase

pp 6316–6321

George A. Kraus*, Vinayak Gupta, Marjan Mokhtarian, Samir Mehanovic, Marit Nilsen-Hamilton

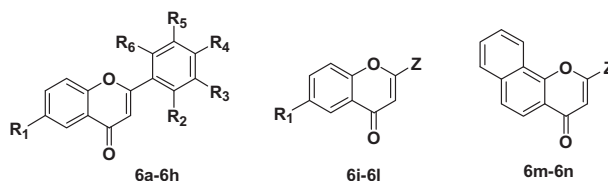


The preparation and testing of several PD173955 analogs is described. Despite its decreased affinity for Abl compared with PD, the PDC analog exhibits a K_i very similar to that reported for Imatinib.

**New synthetic flavone derivatives induce apoptosis of hepatocarcinoma cells**

pp 6322–6328

Huachen Liu, Aijun Dong, Chunmei Gao, Chunyan Tan, Zhenhua Xie, Xuyu Zu, Long Qu, Yuyang Jiang*

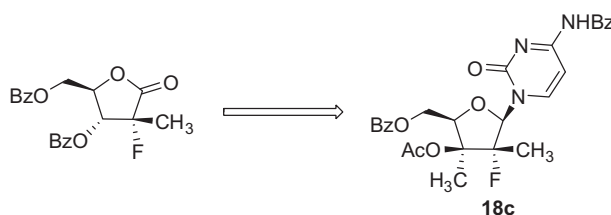


A novel series of flavone derivatives were synthesized and evaluated as potent antitumor activities. Structure–activity relationships and induction of apoptosis are also studied.

Novel nucleosides as potent influenza viral inhibitors

pp 6329–6339

Manohar Sharma Vedula*, Sreenu Jennepalli, Ratnakar Aryasomayajula, Subhash Reddy Rondla, Madanmohan Reddy Musku, Rathnakar Reddy Kura, Parthasaradhi Reddy Bandi

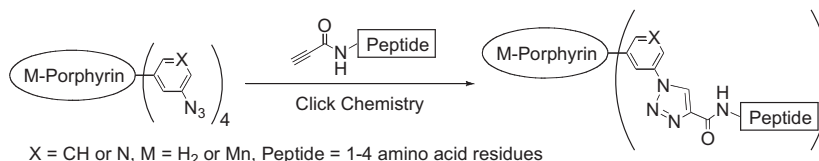


Novel nucleosides were synthesized from di benzoyl fluoro lactone (1) and evaluated their anti-influenza viral activity. Compound (18c) showed the best antiviral activity among the compounds synthesized.

**Facile synthesis of peptide–porphyrin conjugates: Towards artificial catalase**

pp 6340–6350

Naoki Umezawa*, Nobuyoshi Matsumoto, Shinsuke Iwama, Nobuki Kato, Tsunehiko Higuchi*

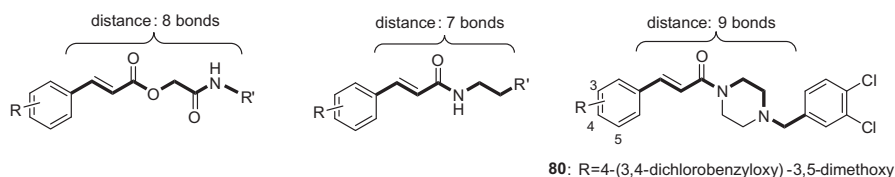


A facile synthetic method for peptide–porphyrin conjugates using click chemistry was developed and used to synthesize nine peptide–porphyrin conjugates, which were evaluated for catalase- and peroxidase-like activities.



Synthesis, biological evaluation, and structure–activity relationship study of novel cytotoxic aza-caffeic acid derivatives pp 6351–6359

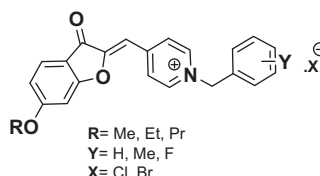
Hongbin Zou, Hao Wu, Xiangnan Zhang, Yu Zhao, Joachim Stöckigt, Yijia Lou*, Yongping Yu*



Three series of aza-caffeic acid derivatives were designed and synthesized with potent cytotoxicity especially compound **80** which shows significant cytotoxicity to several cancer cell lines and mitochondria-dependent apoptosis activity in suppressing K562 cell proliferation.

Design, synthesis and anticholinesterase activity of a novel series of 1-benzyl-4-((6-alkoxy-3-oxobenzofuran-2(3H)-ylidene) methyl) pyridinium derivatives pp 6360–6366

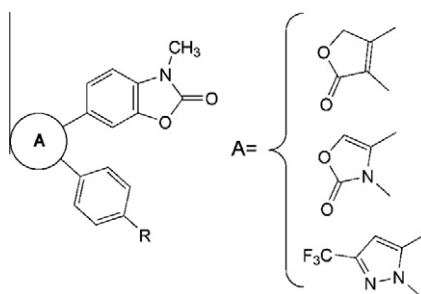
Hamid Nadri, Morteza Pirali-Hamedani, Maryam Shekarchi, Mohammad Abdollahi, Vahid Sheibani, Massoud Amanlou, Abbas Shafiee, Alireza Foroumadi*



A novel series of benzofuranone-ylidene-methyl benzylpyridinium derivatives were synthesized as acetylcholinesterase inhibitors.

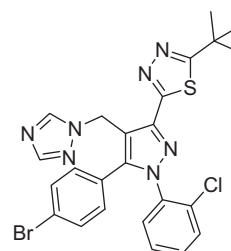
Synthesis, biological evaluation, and docking studies of novel heterocyclic diaryl compounds as selective COX-2 inhibitors pp 6367–6376

Gökçen Eren*, Serdar Ünlü, Maria-Teresa Nuñez, Luis Labeaga, Francisco Ledo, Antonio Entrena, Erden Banoğlu, Gabriele Costantino, M. Fethi Şahin

**Discovery of 2-((1H-1,2,4-triazol-1-yl)methyl)-5-(4-bromophenyl)-1-(2-chlorophenyl)-1H-pyrazol-3-yl)-5-tert-butyl-1,3,4-thiadiazole (GCC2680) as a potent, selective and orally efficacious cannabinoid-1 receptor antagonist** pp 6377–6388

Jinhwa Lee*, Hee Jeong Seo, Suk Ho Lee, Jeongmin Kim, Myung Eun Jung, Sung-Han Lee, Kwang-Seop Song, Junwon Lee, Suk Youn Kang, Min Ju Kim, Mi-Soon Kim, Eun-Jung Son, MinWoo Lee, Ho-Kyun Han

2-((1H-1,2,4-Triazol-1-yl)methyl)-5-(4-bromophenyl)-1-(2-chlorophenyl)-1H-pyrazol-3-yl)-5-tert-butyl-1,3,4-thiadiazole **17s** (GCC2680), a CB1 receptor ligand, has been selected as a preclinical candidate for the treatment of obesity.



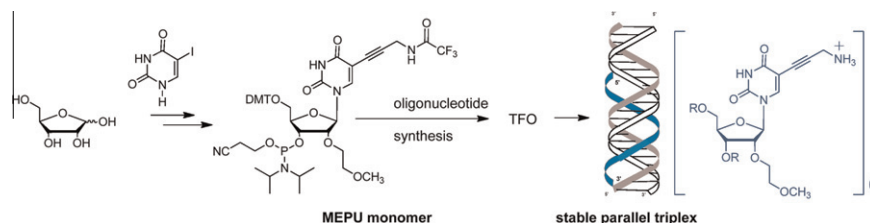
17s (GCC2680)
IC₅₀ = 0.681 nM, rCB1
hCB2/rCB1 = 807



Synthesis and properties of triplex-forming oligonucleotides containing 2'-O-(2-methoxyethyl)-5-(3-aminoprop-1-ynyl)-uridine

pp 6389–6397

Chenguang Lou, Qiang Xiao, Lavinia Brennan, Mark E Light, Nuria Vergara-Irigaray, Elizabeth M. Atkinson, Lindy M. Holden-Dye, Keith R. Fox, Tom Brown*



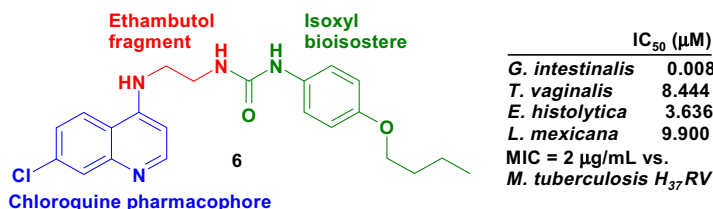
MEPU was synthesized and incorporated into TFOs which formed very stable triplexes with target duplexes.



Design, synthesis, and in vitro antiprotozoal, antimycobacterial activities of N-[2-[(7-chloroquinolin-4-yl)amino]ethyl]ureas

pp 6398–6403

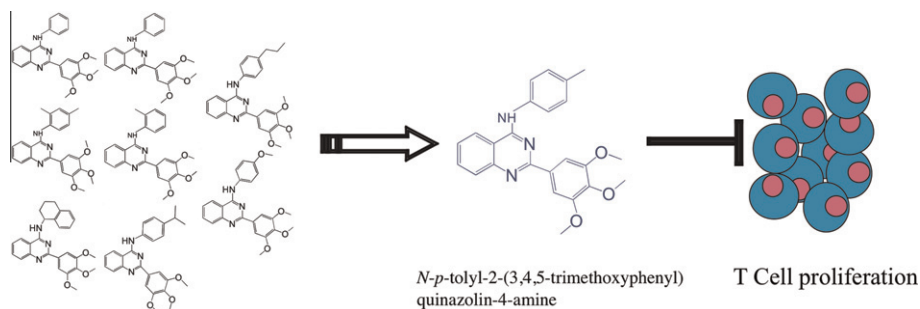
Carlos Nava-Zuazo, Samuel Estrada-Soto, Jorge Guerrero-Álvarez, Ismael León-Rivera, Gloria María Molina-Salinas, Salvador Said-Fernández, Manuel Jesús Chan-Bacab, Roberto Cedillo-Rivera, Rosa Moo-Puc, Gumersindo Mirón-López, Gabriel Navarrete-Vazquez*



Design, synthesis, and evaluation of quinazoline T cell proliferation inhibitors

pp 6404–6413

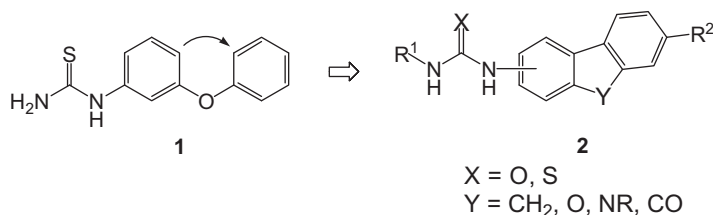
Idit Sagiv-Barfi, Ester Weiss, Alexander Levitzki*



Synthesis, activity, and pharmacokinetic properties of a series of conformationally-restricted thiourea analogs as novel hepatitis C virus inhibitors

pp 6414–6421

Iou-Jiun Kang, Li-Wen Wang, Teng-Kuang Yeh, Chung-Chi Lee, Yen-Chun Lee, Sheng-Ju Hsu, Yen-Shian Wu, Jing-Chyi Wang, Yu-Sheng Chao, Andrew Yueh*, Jyh-Haur Chern*

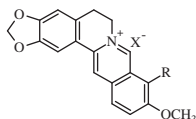


A series of novel conformationally-restricted thiourea analogs were designed, synthesized, and evaluated for their anti-HCV activity and pharmacokinetic properties.

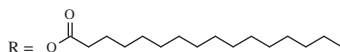
Design, synthesis, and cholesterol-lowering efficacy for prodrugs of berberrubine

pp 6422–6428

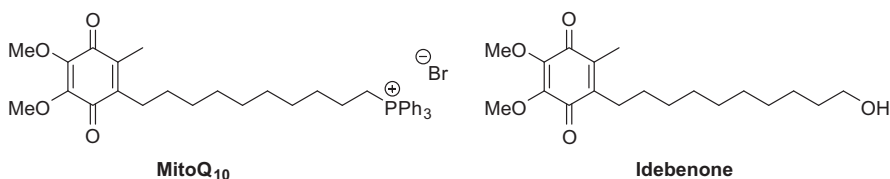
Ying-Hong Li, Yi Li, Peng Yang, Wei-Jia Kong, Xue-Fu You, Gang Ren, Hong-Bin Deng, Yue-Ming Wang, Yan-Xiang Wang, Jian-Dong Jiang*, Dan-Qing Song*



R = Aliphatic ester, aromatic ester, aliphatic acyloxymethylenoxy, aromatic acyloxymethylenoxy.

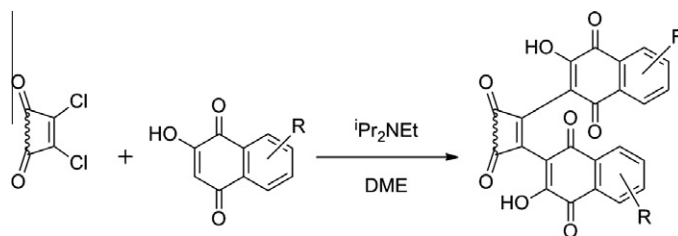
Compound **5g**: Reducing CHO and LDL-c by 35.8% and 45.5% ($p < 0.01$) (100 mg/kg/d, 28 days).**Synthesis and characterization of mitoQ and idebenone analogues as mediators of oxygen consumption in mitochondria** pp 6429–6441

Damien Y. Duveau, Pablo M. Arce, Robert A. Schoenfeld, Nidhi Raghav, Gino A. Cortopassi*, Sidney M. Hecht*

**Antiviral agents 2. Synthesis of trimeric naphthoquinone analogues of conocurvone and their antiviral evaluation against HIV**

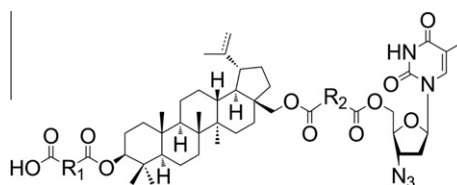
pp 6442–6450

Ian T. Crosby*, David G. Bourke, Eric D. Jones, Paula J. de Bruyn, David Rhodes, Nick Vandegraaff, Susan Cox, Jonathan A. V. Coates, Alan D. Robertson

**Conjugates of betulin derivatives with AZT as potent anti-HIV agents**

pp 6451–6469

Juan Xiong, Yoshiki Kashiwada*, Chin-Ho Chen, Keduo Qian, Susan L. Morris-Natschke, Kuo-Hsiung Lee*, Yoshihisa Takaishi

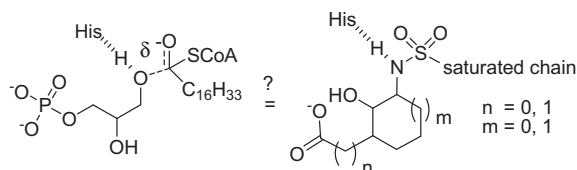


Fourteen novel conjugates of 3,28-di-O-acyl-betulins with AZT were prepared as anti-HIV agents. Among them, nine conjugates were equipotent or more potent than bevirimat, which is currently in Phase IIb anti-AIDS clinical trial.

Design, synthesis, and biological evaluation of conformationally constrained glycerol 3-phosphate acyltransferase inhibitors

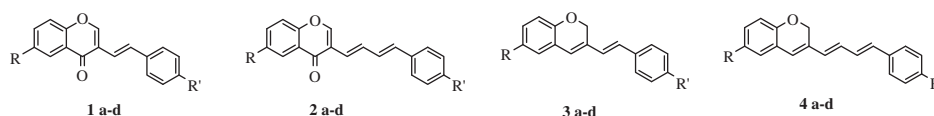
pp 6470–6479

Edward A. Wydysh, Aravinda Vadlamudi, Susan M. Medghalchi, Craig A. Townsend*

**New 4H-chromen-4-one and 2H-chromene derivatives as anti-picornavirus capsid-binders**

pp 6480–6488

Cinzia Conti, Nicoletta Desideri*

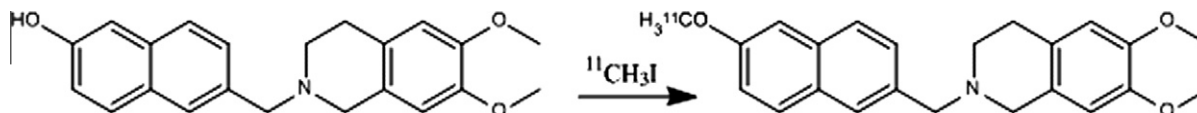


3-Styryl and 3-phenylbuta-1,3-dienyl chromen-4-ones and 2H-chromenes were synthesized and evaluated in cell cultures against human rhinovirus serotype 1B and 14 and enterovirus 71. The new compounds interfered with the replication of picornaviruses dose-dependently, although considerable differences were observed in sensitivity of each virus.

Radiosynthesis and in vivo evaluation of [^{11}C]MC80 for P-glycoprotein imaging

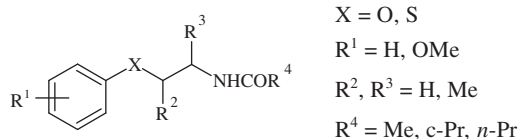
pp 6489–6495

Sylvie De Bruyne*, Leonie wyffels, Lieselotte Moerman, Johan Sambre, Nicola A. Colabufo, Francesco Berardi, Roberto Perrone, Filip De Vos

**Design, synthesis, and pharmacological effects of structurally simple ligands for MT₁ and MT₂ melatonin receptors**

pp 6496–6511

Alessia Carocci*, Alessia Catalano, Angelo Lovece, Giovanni Lentini, Andrea Duranti, Valeria Lucini, Marilou Pannacci, Francesco Scaglione, Carlo Franchini

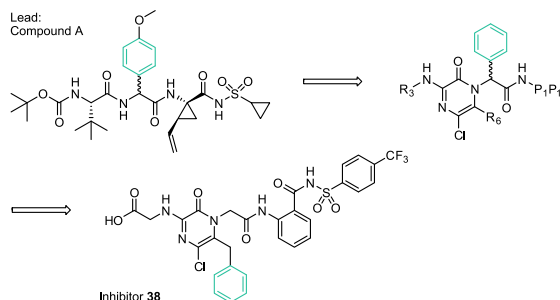


A novel series of phenoxyalkyl and phenylthioalkyl amides were synthesized and their structure–affinity and structure–intrinsic activity relationships for MT₁ and MT₂ receptors were investigated.

Discovery of achiral inhibitors of the hepatitis C virus NS3 protease based on 2(1H)-pyrazinones

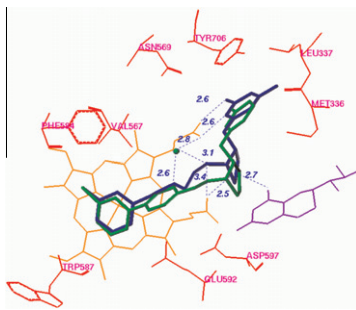
pp 6512–6525

Pernilla Örtqvist, Johan Gising, Angelica E. Ehrenberg, Aparna Vema, Anneli Borg, Anders Karlén, Mats Larhed, U. Helena Danielson, Anja Sandström*

**Structure-based design, synthesis, and biological evaluation of lipophilic-tailed monocationic inhibitors of neuronal nitric oxide synthase**

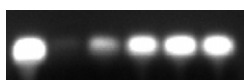
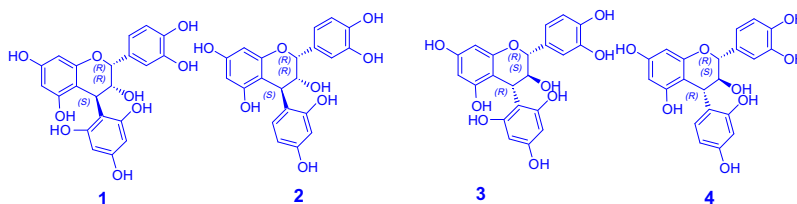
pp 6526–6537

Fengtian Xue, Jinwen Huang, Haitao Ji, Jianguo Fang, Huiying Li, Pavel Martásek, Linda J. Roman, Thomas L. Poulos*, Richard B. Silverman*

**Synthesis and ribonuclease A inhibition activity of resorcinol and phloroglucinol derivatives of catechin and epicatechin: Importance of hydroxyl groups**

pp 6538–6546

Sansa Dutta, Amit Basak*, Swagata Dasgupta*

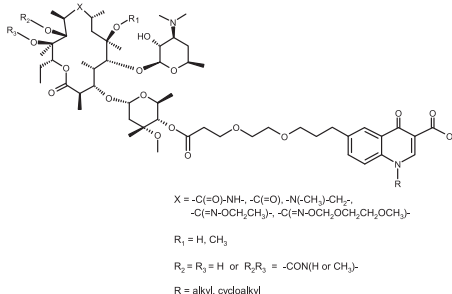
A 1 2 3 4 5 6**B** 1 2 3 4 5

(A) Lane 1: RNA, Lane 2: RNase A + RNA, Lane 3: RNase A + Epicatechin + RNA, Lane 4: RNase A + **2** + RNA, Lane 5: RNase A + **1** + RNA, Lane 6: RNase A + 3'-CMP + RNA. (B) Lane 1: RNA, Lane 2: RNase A + RNA, Lane 3: RNase A + Catechin + RNA, Lane 4: RNase A + **3** + RNA, Lane 5: RNase A + **4** + RNA.

**Synthesis and biological activity of 4''-O-acyl derivatives of 14- and 15-membered macrolides linked to ω-quinolone-carboxylic unit**

pp 6547–6558

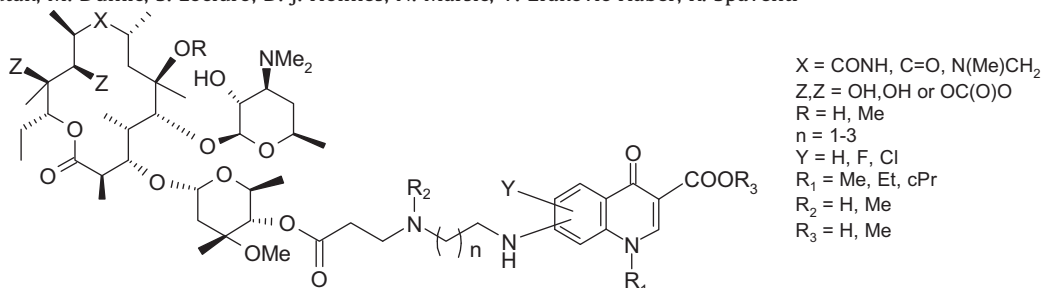
Maja Matanović Škugor*, Vlado Štimac, Ivana Palej, Đurđica Lugarić, Hana Čipčić Paljetak, Darko Filić, Marina Modrić, Ivica Đilović, Dubravka Gembarovski, Stjepan Mutak, Vesna Eraković Haber, David J. Holmes, Zrinka Ivezić-Schoenfeld, Sulejman Alihodžić



4''-O-(ω -Quinolylamino-alkylamino)propionyl derivatives of selected macrolides with the activity against the key erythromycin resistant respiratory pathogens

pp 6559–6568

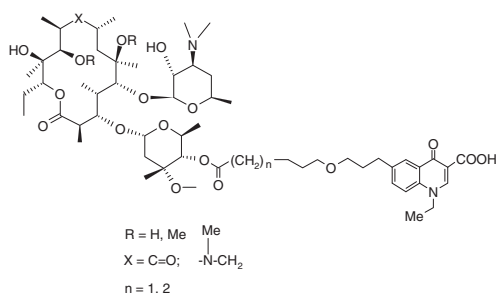
A. Fajdetić*, H. Čipčić Paljetak, G. Lazarevski, A. Hutinec, S. Alihodžić, M. Đerek, V. Štimac, D. Andreotti, V. Šunjić, J. M. Berge, S. Mutak, M. Dumić, S. Lociuro, D. J. Holmes, N. Maršić, V. Eraković Haber, R. Spaventi



6-Alkylquinolone-3-carboxylic acid tethered to macrolides synthesis and antimicrobial profile

pp 6569–6577

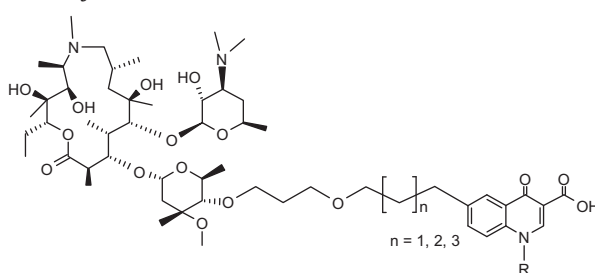
Samra Kapić*, Hana Čipčić Paljetak, Sulejman Alihodžić, Roberto Antolović, Vesna Eraković Haber, Richard L. Jarvest, David J. Holmes, John P. Broskey, Eric Hunt



Synthesis and properties of macrolones characterized by two ether bonds in the linker

pp 6578–6588

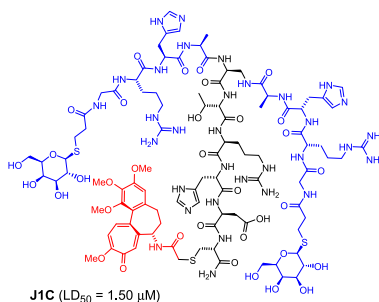
Ivana Palej Jakopović, Goran Kragol, Andrew K. Forrest, Catherine S. V. Frydrych, Vlado Štimac, Samra Kapić, Maja Matanović Škugor, Marina Ilijaš, Hana Čipčić Paljetak, Dubravko Jelić, David J. Holmes, Deirdre M. B. Hickey, Donatella Verbanac, Vesna Eraković Haber, Sulejman Alihodžić*



Glycopeptide dendrimer colchicine conjugates targeting cancer cells

pp 6589–6597

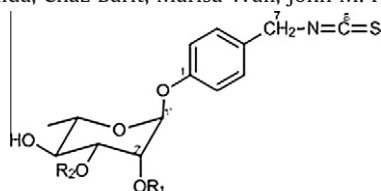
Emma M. V. Johansson, Joëlle Dubois, Tamis Darbre, Jean-Louis Reymond*



Potential anti-inflammatory phenolic glycosides from the medicinal plant *Moringa oleifera* fruits

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1; $R_1 = \text{Ac}$, $R_2 = \text{H}$ 2; $R_1 = \text{H}$, $R_2 = \text{Ac}$

Bioassay-guided isolation and purification of the ethyl acetate extract of *Moringa oleifera* fruits yielded three new phenolic glycosides; 4-[(2'-O-acetyl- α -L-rhamnosyloxy)benzyl]isothiocyanate (**1**), 4-[(3'-O-acetyl- α -L-rhamnosyloxy)benzyl]isothiocyanate (**2**), and S-methyl-N-{4-[(α -L-rhamnosyloxy)benzyl]}thiocarbamate (**3**). The anti-inflammatory activity of isolated compounds were investigated on lipopolysaccharide (LPS)-induced murine macrophage in RAW 264.7 cell line.



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Supplementary data available via ScienceDirect

COVER

Crystal lattice is shown in CPK model, target compound is shown in green and yellow and solvent molecules are in atom colored mode. Small pictures shown in the upper right and lower left corner are target molecule and parent azithromycin shown as Connolly surface colored by lipophilic potential (lipophilic-green, polar- pink). [Škugor, M. M.; Štimac, V.; Palej, I.; Lugarić, D.; Paljetak, H. C.; Filić, D.; Modrić, M.; Dilović, I.; Gembarovski, D.; Mutak, S.; Eraković Haber, V.; Holmes, D.J.; Ivezić-Schoenfeld, Z.; Alihodžić, S. *Bioorg. Med. Chem.* **2010**, *18*, 6547–6558].

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