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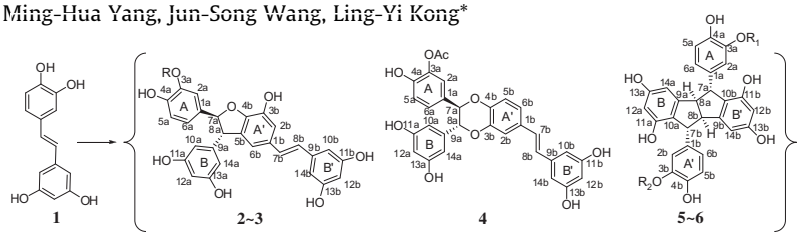
ARTICLES

Dimerization of piceatannol by *Momordica charantia* peroxidase and α-glucosidase inhibitory activity of the biotransformation products **pp 5085–5092**

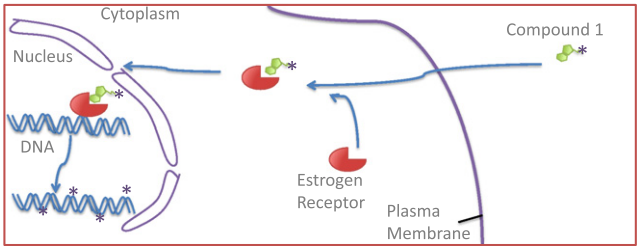
Xiang Wan, Xiao-Bing Wang, Ming-Hua Yang, Jun-Song Wang, Ling-Yi Kong*



Biotransformation of piceatannol by *Momordica charantia* peroxidase (MCP) resulted in eight dimers, including five new ones, which exhibited powerful in vitro α-glucosidase inhibitory effects.

DNA site-specific N3-adenine methylation targeted to estrogen receptor-positive cells **pp 5093–5102**

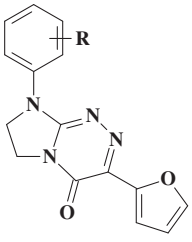
Rigel J. Kishton, Sean E. Miller, Heather Perry, Tera Lynch, Mayur Patel, Vinayak K. Gore, Giridhar R. Akkaraju, Sridhar Varadarajan*



Synthesis, structure elucidation, determination of the lipophilicity and identification of antitumour activities in vitro of novel 3-(2-furanyl)-8-aryl-7,8-dihydroimidazo[2,1-*c*][1,2,4]triazin-4(6*H*)-ones with a low cytotoxicity towards normal human skin fibroblast cells **pp 5103–5116**

Krzysztof Sztanke*, Tomasz Tuzimski, Małgorzata Sztanke, Jolanta Rzymowska, Kazimierz Pasternak

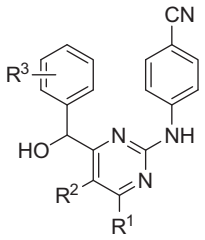
Synthesis, structure elucidation, determination of the lipophilicity and antitumour activities in vitro of eleven novel 3-(2-furanyl)-8-aryl-7,8-dihydroimidazo[2,1-*c*][1,2,4]triazin-4(6*H*)-ones (**12**–**22**) are presented. Among them, compounds **13**, **15**, **16**, **18** and **22** demonstrate remarkable antiproliferative activities and selective toxicities for cancer cells over normal cells. Therefore these ones may be considered as lead structures for the design of novel useful non-toxic (**13**, **15** and **16**) and low toxic (**18** and **22**) antitumour agents.



R = H, 2-CH_3, 4-CH_3, 2,3-$(CH_3)_2$, 2-OCH_3, 4-OCH_3, 2-Cl, 3-Cl, 4-Cl, 3,4-Cl_2, 2,6-Cl_2

Synthesis and structure–activity relationship of novel diarylpyrimidines with hydromethyl linker (*CH*(*OH*)-DAPYs) as HIV-1 NNRTIs **pp 5117–5124**

Shuang-Xi Gu, Qiu-Qin He, Shi-Qiong Yang, Xiao-Dong Ma, Fen-Er Chen*, Erik De Clercq, Jan Balzarini, Christophe Pannecouque

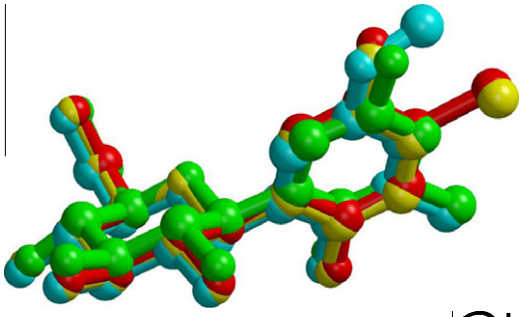


***CH(OH)*-DAPYs**

IC_{50} : 9.870 - 0.008 μ M (wild-type HIV-1)

Halogen-substituted (*C*-β-D-glucopyranosyl)-hydroquinone regioisomers: Synthesis, enzymatic evaluation and their binding to glycogen phosphorylase **pp 5125–5136**

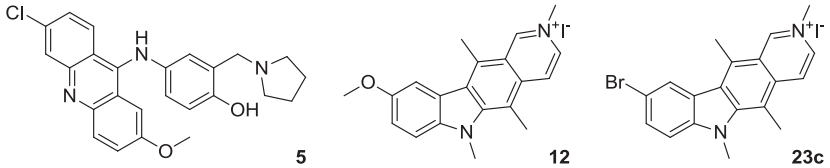
Kyra-Melinda Alexacou, Yun Zhi Zhang, Jean-Pierre Praly*, Spyros E. Zographos, Evangelia D. Chrysina, Nikos G. Oikonomakos, Demetres D. Leonidas*



The catalytic site of muscle glycogen phosphorylase b (GPb) has been probed with four (C-β-D-glucopyranosyl)-hydroquinone regioisomers. The best of these inhibitors displays an IC_{50} value of 39.8 μM.

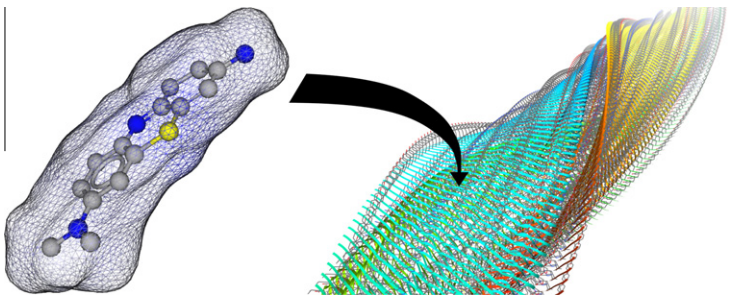
Ellipticines and 9-acridinylamines as inhibitors of D-alanine:D-alanine ligase **pp 5137–5146**

Blaž Vehar, Martina Hrast, Andreja Kovač, Janez Konc, Katherine Mariner, Ian Chopra, Alex O'Neill, Dušanka Janežič, Stanislav Gobec*

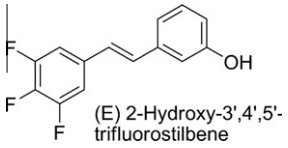


Ligand polarizability contributes to tau fibril binding affinity **pp 5147–5154**

Jordan R. Jensen, Katryna Cisek, Nicolette S. Honson, Jeff Kuret*

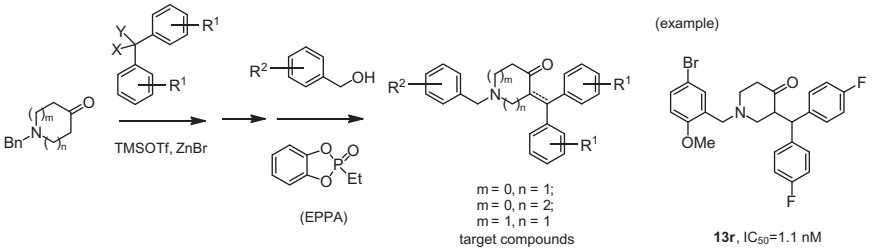


Synthesis and antimicrobial activity of (*E*) stilbene derivatives **pp 5155–5166**
Sabrina Albert, Ralf Horbach, Holger B. Deising, Bianka Siewert, René Csuk*



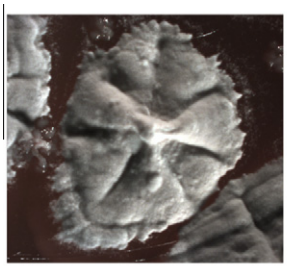
Functionalized polystyrene supports for solid-phase synthesis of glycyl-, alanyl-, and isoleucyl-RNA conjugates as hydrolysis-resistant mimics of peptidyl-tRNAs **pp 5167–5174**
Jessica Steger, Ronald Micura*

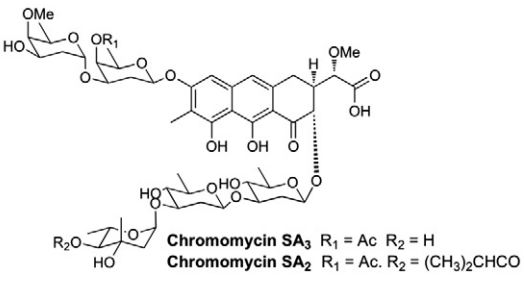
3-Benzhydryl-4-piperidones as novel neurokinin-1 receptor antagonists and their efficient synthesis **pp 5175–5182**
Junya Shirai*, Minoru Nakamura, Naoki Tarui, Tadatoshi Hashimoto, Yoshinori Ikeura



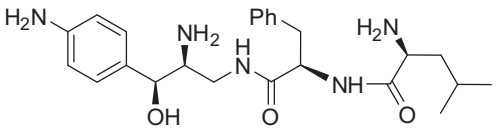
Discovery of novel and potent 3-benzhydryl-4-piperidone tachykinin NK_1 receptor antagonists and their efficient synthesis are reported. This skeleton can be useful for chemical library targeting G-protein coupled receptors.

Chromomycin SA analogs from a marine-derived *Streptomyces* sp. **pp 5183–5189**
Youcai Hu, Ana Paula D. M. Espindola, Nathan A. Stewart, Shuguang Wei, Bruce A. Posner, John B. MacMillan*





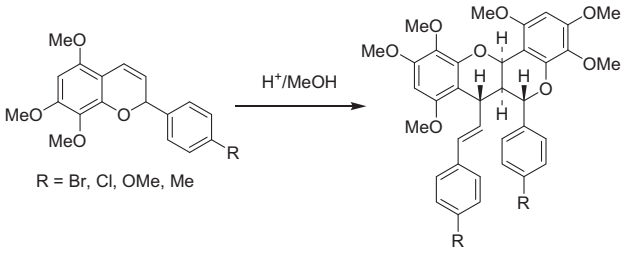
Novel aminopeptidase N (APN/CD13) inhibitors derived from chloramphenicol amine **pp 5190–5198**
Meirong Jia, Kanghui Yang, Hao Fang, Yingying Xu, Siwei Sun, Li Su, Wenfang Xu*



10e

A series of compounds derived from (1*S*,2*S*)-2-amino-1-(4-nitrophenyl) propane-1,3-diol have been designed, synthesized as potential APN inhibitors.

Synthesis and antimalarial evaluation of novel benzopyrano[4,3-*b*]benzopyran derivatives **pp 5199–5206**
Ruth Devakaram, David StC. Black, Katherine T. Andrews, Gillian M. Fisher, Rohan A. Davis, Naresh Kumar*



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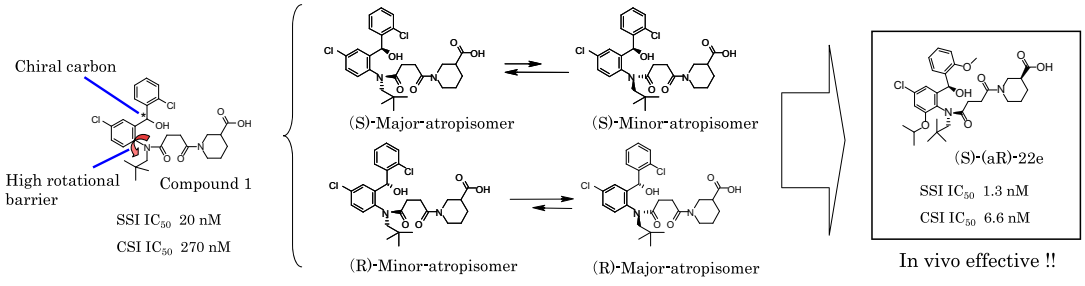
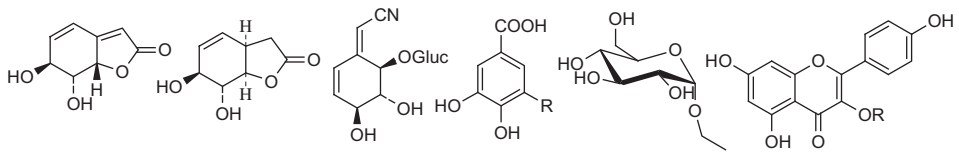
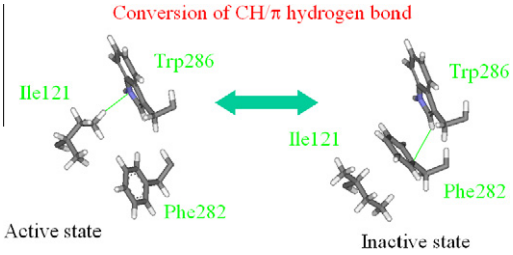
Masanori Ichikawa*, Aki Yokomizo, Masao Itoh, Noriyasu Haginoya, Kazuyuki Sugita, Hiroyuki Usui, Koji Terayama, Akira Kanda



***Tylosema esculentum* extractives and their bioactivity** **pp 5225–5230**
Ofentse Mazimba, Runner R. T. Majinda*, Ceciliah Modibedi, Ishmael B. Masesane, Avrelija Cencič, Walter Chingwaru

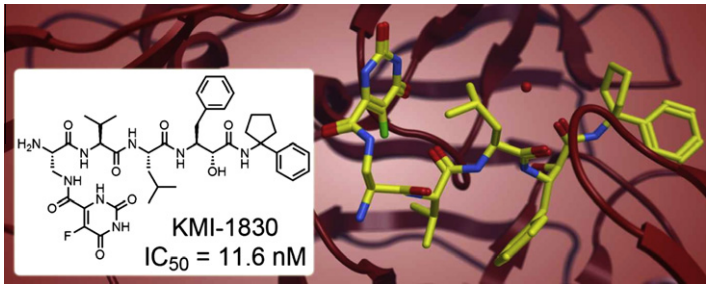


CH/π hydrogen bonds play a role in ligand recognition and equilibrium between active and inactive states of the β2 adrenergic receptor: An ab initio fragment molecular orbital (FMO) study **pp 5231–5237**
Tomonaga Ozawa*, kosuke Okazaki, Kazuo kitaura

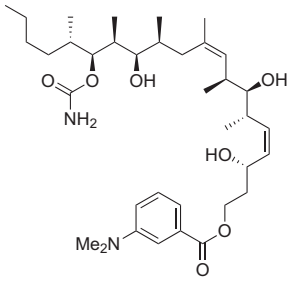


Conversion of CH/π hydrogen bond between active and inactive states.

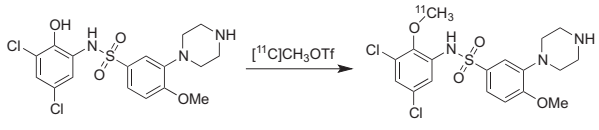
Structure-guided design and synthesis of P_1' position 1-phenylcycloalkylamine-derived pentapeptidic BACE1 inhibitors **pp 5238–5246**
Harichandra D. Tagad, Yoshio Hamada, Jeffrey-Tri Nguyen, Koushi Hidaka, Takashi Hamada, Youhei Sohma, Tooru Kimura, Yoshiaki Kiso*



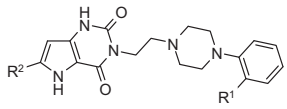
Design, synthesis and biological evaluation of a simplified fluorescently labeled discodermolide as a molecular probe to study the binding of discodermolide to tubulin **pp 5247–5254**
Jun Qi, Adam R. Blanden, Susan Bane, David G. I. Kingston*

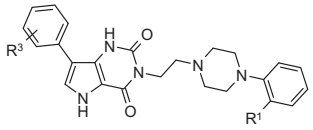


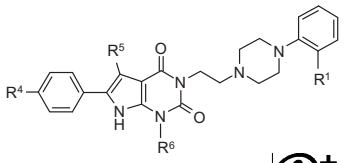
Synthesis and in vivo evaluation of [*O*-methyl-^{11}C] *N*-[3,5-dichloro-2-(methoxy)phenyl]-4-(methoxy)-3-(1-piperazinyl)benzenesulfonamide as an imaging probe for 5-HT_6 receptors **pp 5255–5259**
Fei Liu, Vattoly J. Majo, Jaya Prabhakaran, Matthew S. Milak, J. John Mann, Ramin V. Parsey, J. S. Dileep Kumar*



Synthesis and molecular modeling of 1*H*-pyrrolopyrimidine-2,4-dione derivatives as ligands for the α_1-adrenoceptors pp 5260–5276
Valeria Pittalà*, Maria A. Siracusa*, Maria N. Modica, Loredana Salerno, Alessandro Pedretti, Giulio Vistoli, Alfredo Cagnotto, Tiziana Mennini, Giuseppe Romeo







A series of new 1*H*-pyrrolopyrimidine-2,4-diones were prepared and evaluated for their affinities at α_1-adrenoceptors and 5-HT_{1A} receptors. Binding data were used in computational studies aimed at clarifying molecular requirements for the design of high-selective ligands.

OTHER CONTENTS

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*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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