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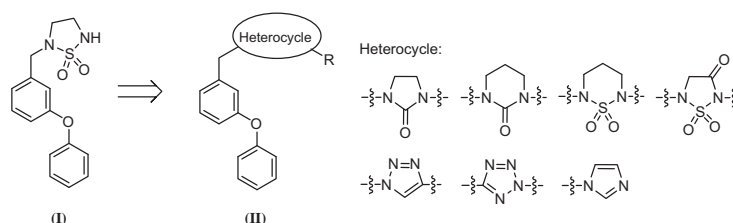
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ARTICLES

Design and synthesis of inhibitors of noroviruses by scaffold hopping

pp 5749–5755

Dengfeng Dou, Sivakoteswara Rao Mandadapu, Kevin R. Alliston, Yunjeong Kim, Kyeong-Ok Chang, William C. Groutas*

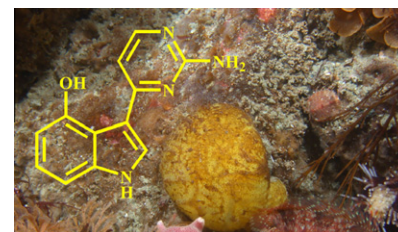


A scaffold hopping strategy was employed to identify new chemotypes that inhibit noroviruses. The replacement of the cyclosulfamide scaffold by an array of heterocyclic scaffolds lead to the identification of additional series of compounds that possessed anti-norovirus activity in a cell-based replicon system.

CNS and antimalarial activity of synthetic meridianin and psammopemmin analogs

pp 5756–5762

Matthew D. Lebar, Kristopher N. Hahn, Tina Mutka, Patrick Maignan, James B. McClintock, Charles D. Amsler, Alberto van Olphen, Dennis E. Kyle, Bill J. Baker*



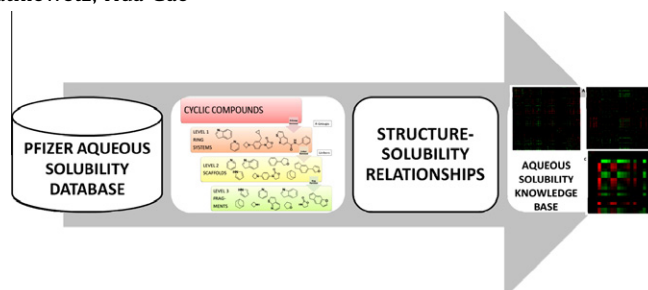
The marine invertebrate-derived meridianin A, the originally proposed structure for psammopemmin A, and several related 3-pyrimidylindole analogs were synthesized and subsequently investigated for central nervous system, antimalarial, and cytotoxic activity. A Suzuki coupling of an indoleborate ester to the pyrimidine electrophile was utilized to form the natural product and derivatives thereof. The 3-pyrimidineindoles were found to prevent radioligand binding to several CNS receptors and transporters, most notably, serotonin receptors ($<0.2 \mu\text{M}$ K_i for 5HT_{2B}). Two compounds also inhibited the human malaria parasite *Plasmodium falciparum* (IC_{50} $<50 \mu\text{M}$). Only the natural product was cytotoxic toward A549 cells ($\text{IC}_{50} = 15 \mu\text{M}$).



Deep understanding of structure–solubility relationship for a diverse set of organic compounds using matched molecular pairs

pp 5763–5770

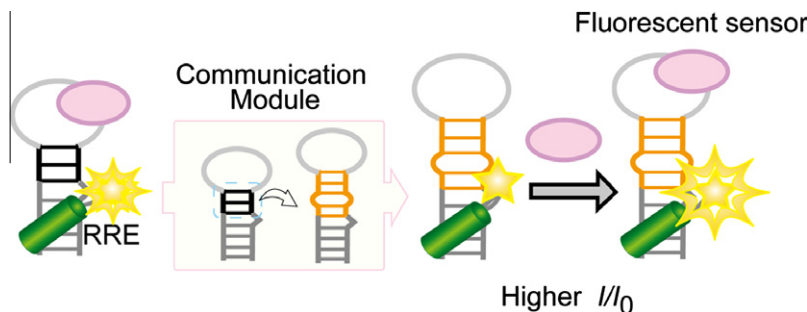
Liying Zhang, Hongyao Zhu, Alan Mathiowetz, Hua Gao*



A ribonucleopeptide module for effective conversion of an RNA aptamer to a fluorescent sensor

pp 5771–5775

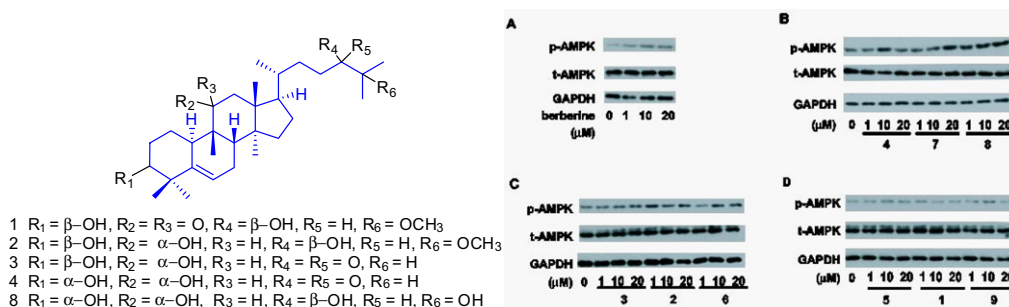
Fong Fong Liew, Hironori Hayashi, Shun Nakano, Eiji Nakata, Takashi Morii*



Potential AMPK activators of cucurbitane triterpenoids from *Siraitia grosvenorii* Swingle

pp 5776–5781

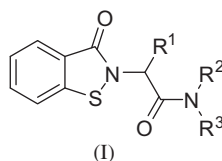
Xu-bing Chen, Jing-jing Zhuang, Jun-hua Liu, Min Lei, Lei Ma, Jing Chen*, Xu Shen, Li-hong Hu*



Antifungal activity of a series of 1,2-benzisothiazol-3(2H)-one derivatives

pp 5782–5787

Dengfeng Dou, Deepu Alex, Bingfan Du, Kok-Chuan Tiew, Sridhar Aravapalli, Sivakoteswara Rao Mandadapu, Richard Calderone, William C. Groutas*

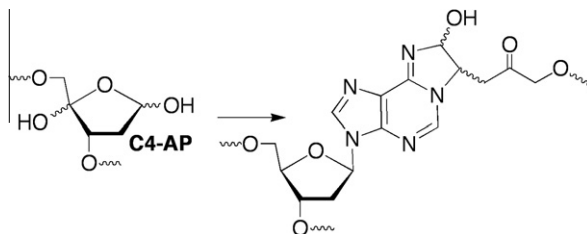


A series of broad-spectrum antifungal agents based on the 1,2-benzisothiazol-3(2H)-one scaffold is reported.

Probing DNA interstrand cross-link formation by an oxidized abasic site using nonnative nucleotides

pp 5788–5793

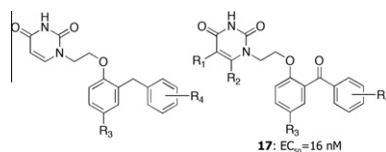
Jonathan T. Szczepanski, Christine N. Hiemstra, Marc M. Greenberg*



1-[2-(2-Benzoyl- and 2-benzylphenoxy)ethyl]uracils as potent anti-HIV-1 agents

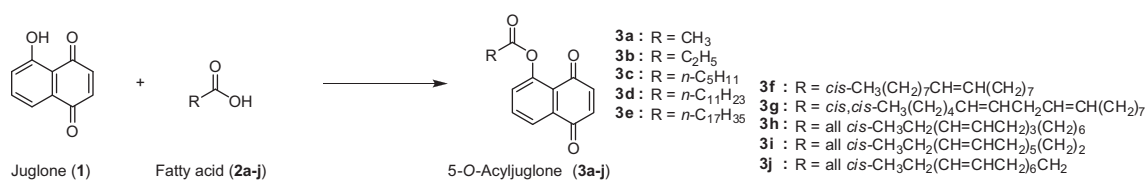
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**Inhibitory effect of novel 5-O-acyl juglones on mammalian DNA polymerase activity, cancer cell growth and inflammatory response**

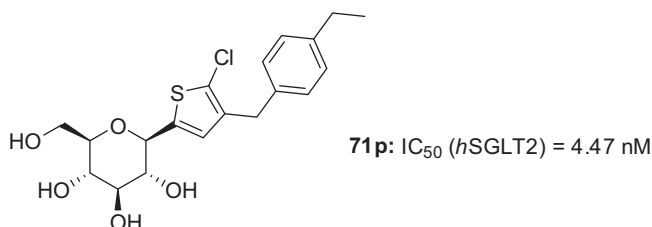
pp 5803–5812

Sayako Maruo, Isoko Kuriyama, Kouji Kuramochi*, Kazunori Tsubaki, Hiromi Yoshida, Yoshiyuki Mizushina*

**Novel thiophenyl C-aryl glucoside SGLT2 inhibitors as potential antidiabetic agents**

pp 5813–5832

Suk Ho Lee, Kwang-Seop Song, Jong Yup Kim, Misuk Kang, Jun Sung Lee, Seung-Hwan Cho, Hyun-Ju Park, Jeongmin Kim, Jinhwa Lee*



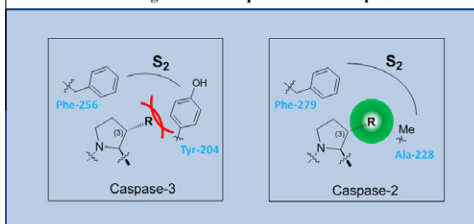
Novel thiophene C-aryl glucoside SGLT2 inhibitors were designed and synthesized. Two different types of thiophene derivatives were readily prepared. Among the compounds tested, ethylphenyl at the distal ring **71p** showed the best in vitro inhibitory activity in this series to date (IC₅₀ = 4.47 nM) against SGLT2.

Exploiting differences in caspase-2 and -3 S₂ subsites for selectivity: Structure-based design, solid-phase synthesis and in vitro activity of novel substrate-based caspase-2 inhibitors

pp 5833–5851

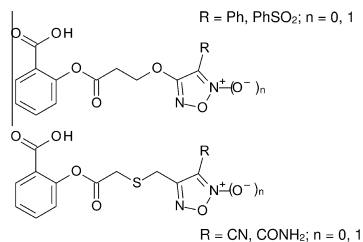
Michel C. Maillard*, Frederick A. Brookfield, Stephen M. Courtney, Florence M. Eustache, Mark J. Gemkow, Rebecca K. Handel, Laura C. Johnson, Peter D. Johnson, Mark A. Kerry, Florian Krieger, Mirco Meniconi, Ignacio Muñoz-Sanjuán, Jordan J. Palfrey, Hyunsun Park, Sabine Schaertl, Malcolm G. Taylor, Derek Weddell, Celia Dominguez

Structure-based design of selective proline-based caspase-2 inhibitors



Searching for new NO-donor aspirin-like molecules: Furoxanylacyl derivatives of salicylic acid and related furazans pp 5852–5860

Loretta Lazzarato, Clara Cena, Barbara Rolando, Elisabetta Marini, Marco Lucio Lolli, Stefano Guglielmo, Elena Guaita, Giuseppina Morini, Gabriella Coruzzi, Roberta Fruttero*, Alberto Gasco

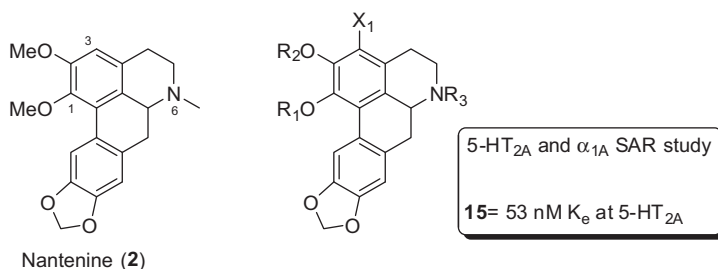


A new group of derivatives of salicylic acid containing NO-donor furoxans, and the related des-NO-furazans, were synthesized and evaluated as new aspirin-like molecules.

New aporphinoid 5-HT_{2A} and α_{1A} antagonists via structural manipulations of nantenine

pp 5861–5868

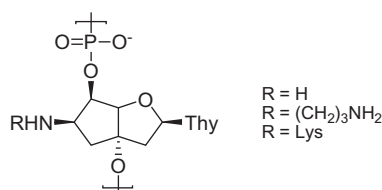
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Synthesis, binding and cellular uptake properties of oligodeoxynucleotides containing cationic bicyclo-thymidine residues

pp 5869–5875

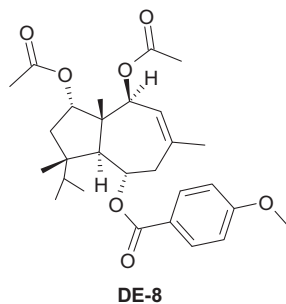
Jory Lietard, Damian Ittig, Christian J. Leumann*



Natural daucane sesquiterpenes with antiproliferative and proapoptotic activity against human tumor cells

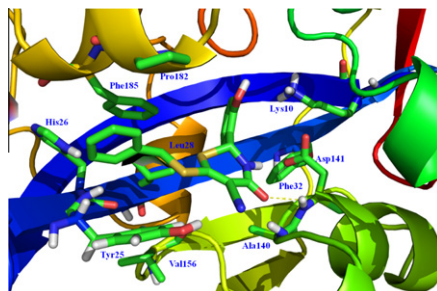
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Stefano Dall'Acqua, Maria Antonella Linardi, Filippo Maggi, Marcello Nicoletti, Valentina Petitto, Gabbriella Innocenti, Giuseppe Basso, Giampietro Viola*



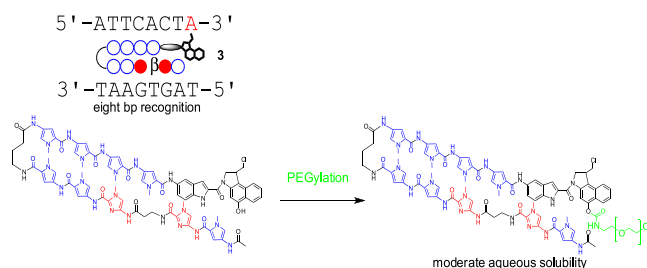
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M. Tang, S. I. Odejinmi, Y. M. Allette, H. Vankayalapati, K. Lai*



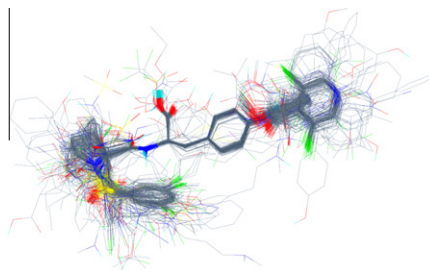
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Toshiki Takagaki, Toshikazu Bando*, Masaaki Kitano, Kaori Hashiya, Gengo Kashiwazaki, Hiroshi Sugiyama*



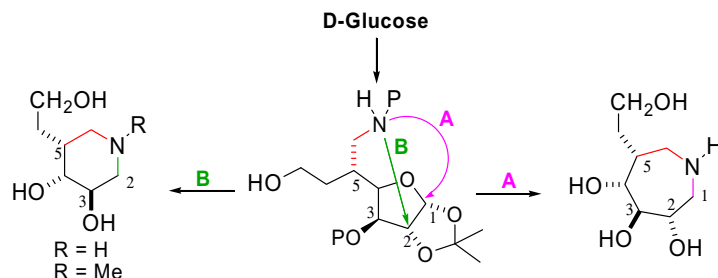
Modeling the molecular basis for $\alpha 4\beta 1$ integrin antagonism pp 5903–5911

Oliver E. Hutt, Simon Saubern, David A. Winkler*




Synthesis of new six- and seven-membered 1-N-iminosugars as promising glycosidase inhibitors pp 5912–5915

Amit M. Jabgunde, Navnath B. Kalamkar, Sanjay T. Chavan, Sushma G. Sabharwal, Dilip D. Dhavale*



*Corresponding author

 Supplementary data available via SciVerse 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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