



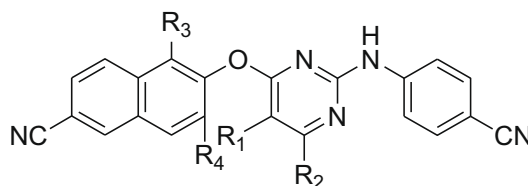
Bioorganic & Medicinal Chemistry Volume 18, Issue 13, 2010

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Synthesis and anti-HIV activity of 2-naphthyl substituted DAPY analogues as non-nucleoside reverse transcriptase inhibitors pp 4601–4605

Yong-Hong Liang, Qiu-Qin He, Zhao-Sen Zeng, Zhi-Qian Liu, Xiao-Qing Feng, Fen-Er Chen*, Jan Balzarini, Christophe Pannecouque, Erik De Clercq

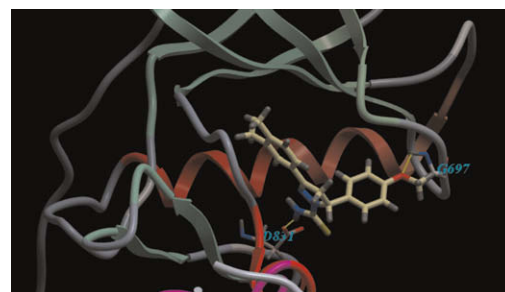


Nine newly 6-cyano-2-naphthyl substituted DAPY analogues were synthesized and evaluated as inhibitors of the HIV-1 wild-type and double mutant (K103N+Y181C) strains in this paper.

Synthesis and biological evaluation of pyrazole derivatives containing thiourea skeleton as anticancer agents pp 4606–4614

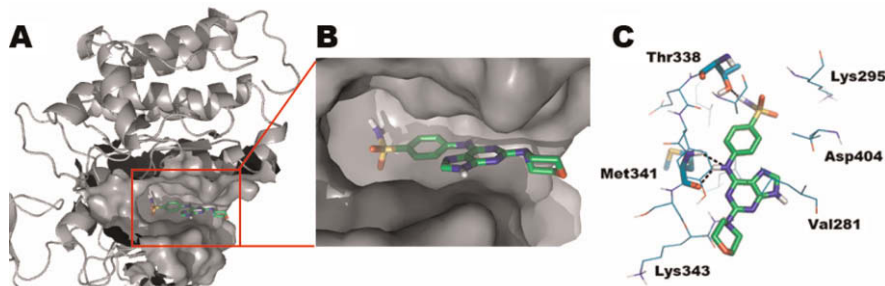
Peng-Cheng Lv, Huan-Qiu Li, Juan Sun, Yang Zhou, Hai-Liang Zhu*

Compound **C5** exhibited the most potent EGFR inhibitory activity with IC_{50} of 0.07 μ M, which was comparable to the positive control erlotinib. Docking simulation was performed to position compound **C5** into the EGFR active site to determine the probable binding model. Besides, compound **C5** showed significant antiproliferative activity against MCF-7 with IC_{50} of 0.08 μ M, which would be a potential anticancer agent.



Discovery of novel purine derivatives with potent and selective inhibitory activity against c-Src tyrosine kinase pp 4615–4624

He Huang, Jingui Ma, Jianmei Shi, Linghua Meng*, Hualiang Jiang, Jian Ding, Hong Liu*



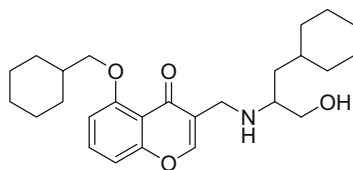
We report novel purine derivatives with potent and selective inhibitory activity against c-Src tyrosine kinase by adopting a strategy integrating focused combinatorial library design, virtual screening, chemical synthesis, and bioassay.



Design and synthesis of novel hydroxyalkylaminomethylchromones for their IL-5 inhibitory activity

pp 4625–4629

P. Thanigaimalai, Ki-Cheul Lee, Vinay K. Sharma, Jun-Ho Yun, Youngsoo Kim, Sang-Hun Jung*

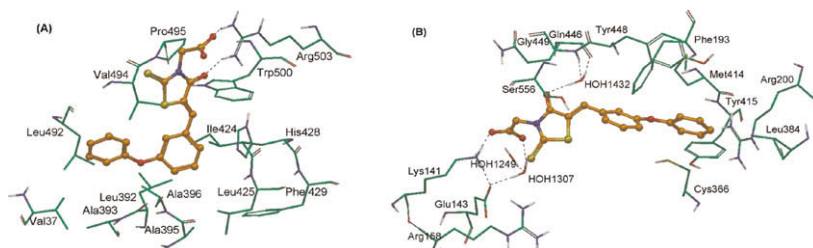
**3d**, IC₅₀ = 17.5 μM

A new series of hydroxyalkylaminomethylchromones **3(a–p)** were synthesized and demonstrated for their activity against interleukin-5. The most active analog **3d** inhibited interleukin-5 activity with an IC₅₀ of 17.5 μM.

Structure-based virtual screening, synthesis and SAR of novel inhibitors of hepatitis C virus NS5B polymerase

pp 4630–4638

Tanaji T. Talele*, Payal Arora, Shridhar S. Kulkarni, Maulik R. Patel, Satyakam Singh, Maksim Chudayeu, Neerja Kaushik-Basu*

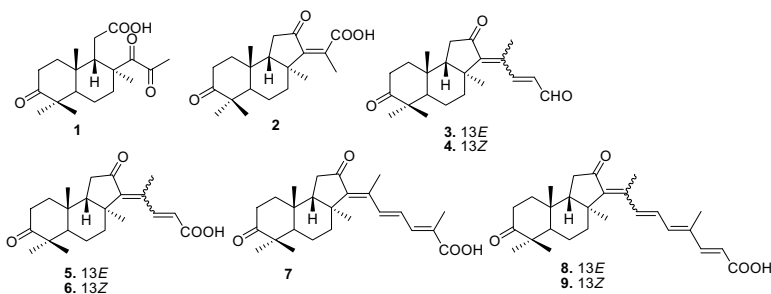


A total of 25 inhibitors belonging to the rhodanine scaffold with IC₅₀ values in the range of 7.7–68.0 μM were identified through a combined use of virtual screening, SAR analysis, synthesis and biological evaluation.

**Globostelletins A–I, cytotoxic isomalabaricane derivatives from the marine sponge *Rhabdastrella globostellata***

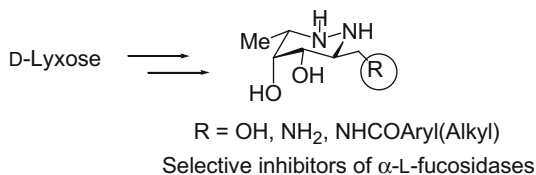
pp 4639–4647

Jin Li, Bo Xu, Jinrong Cui, Zhiwei Deng, Nicole J. de Voogd, Peter Proksch, Wenhan Lin*

**Synthesis and inhibitory activities of novel C-3 substituted azafagomines: A new type of selective inhibitors of α-L-fucosidases**

pp 4648–4660

Elena Moreno-Clavijo, Ana T. Carmona*, Antonio J. Moreno-Vargas, Miguel A. Rodríguez-Carvajal, Inmaculada Robina*



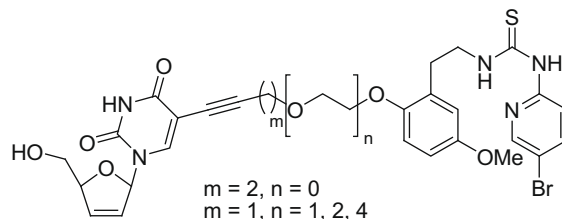
A series of novel C-3 substituted L-fuco-azafagomines has been synthesized. These compounds showed selective inhibition towards α-L-fucosidase in the low micromolar range.



[d4U]-Spacer-[HI-236] double-drug inhibitors of HIV-1 reverse-transcriptase

pp 4661–4673

Yassir Younis, Roger Hunter*, Clare I. Muhanji, Ian Hale, Rajinder Singh, Christopher M. Bailey, Todd J. Sullivan, Karen S. Anderson



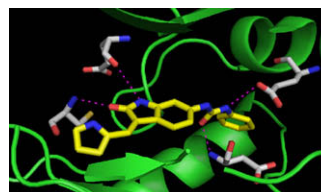
[d4U]-Spacer-[HI-236] bifunctional double-drug inhibitors against HIV-1 RT of the type shown below have been synthesized and evaluated in both cell-culture as well as in vitro against the enzyme, returning some nanomolar EC_{50} and IC_{50} 's.

**Synthesis and structure–activity relationship of 6-aryureido-3-pyrrol-2-ylmethylideneindolin-2-one derivatives as potent receptor tyrosine kinase inhibitors**

pp 4674–4686

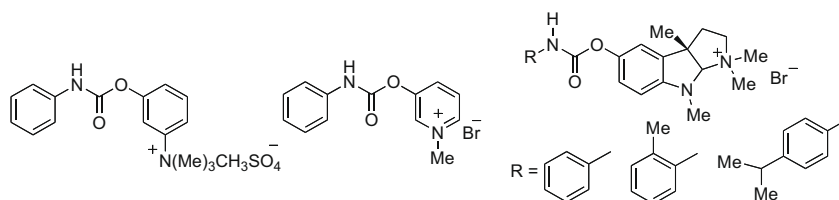
Rahul R. Khanwelkar, Grace Shiahuiy Chen, Hsiao-Chun Wang, Chao-Wu Yu, Chiung-Hua Huang, On Lee, Chih-Hung Chen, Chrong-Shiong Hwang, Ching-Huai Ko, Nien-Tzu Chou, Mai-Wei Lin, Ling-mei Wang, Yen-Chun Chen, Tzong-Hsiung Hseu, Chia-Ni Chang, Hui-Chun Hsu, Hui-Chi Lin, Ying-Chu Shih, Shuen-Hsiang Chou, Hsiang-Wen Tseng, Chih-Peng Liu, Chia-Mu Tu, Tsan-Lin Hu, Yuan-Jang Tsai, Ji-Wang Chern*

A series of 6-ureido-substituted 3-pyrrolemethylidene-2-oxindole derivatives were synthesized and identified as potent inhibitors of the vascular endothelial growth factor receptor and platelet-derived growth factor receptor families of receptor tyrosine kinases.

**Long-acting anticholinesterases for myasthenia gravis: synthesis and activities of quaternary phenylcarbamates of neostigmine, pyridostigmine and physostigmine**

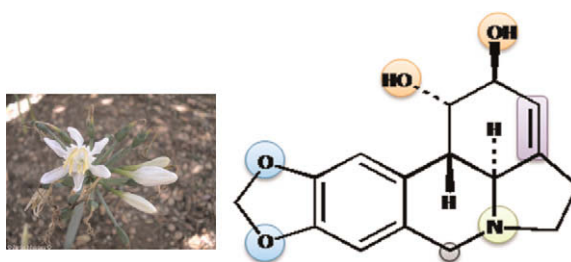
pp 4687–4693

Qian-sheng Yu, Harold W. Holloway, Weiming Luo, Debomoy K. Lahiri, Arnold Brossi, Nigel H. Greig*

**Synthesis and antiparasmodial activity of lycorine derivatives**

pp 4694–4701

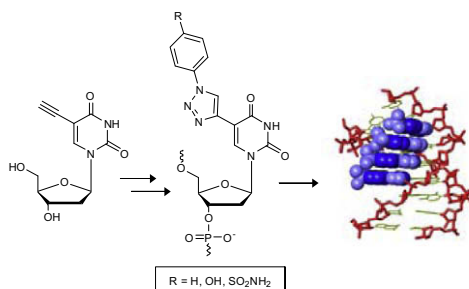
Juan C. Cedrón, David Gutiérrez, Ninoska Flores, Ángel G. Ravelo*, Ana Estévez-Braun*



Efficient RNA-targeting by the introduction of aromatic stacking in the duplex major groove via 5-(1-phenyl-1,2,3-triazol-4-yl)-2'-deoxyuridines

pp 4702–4710

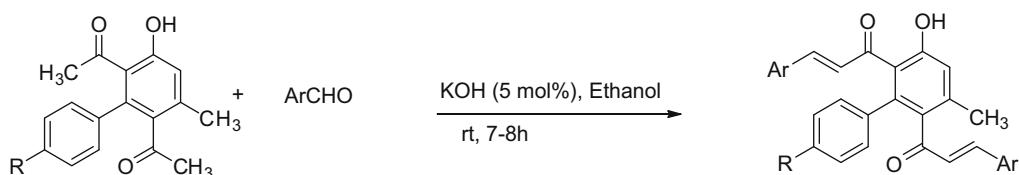
Nicolai Krog Andersen, Navneet Chandak, Lucie Brulíková, Pawan Kumar, Michael Dalager Jensen, Frank Jensen, Pawan K. Sharma*, Poul Nielsen*



Synthesis and anti breast cancer activity of biphenyl based chalcones

pp 4711–4720

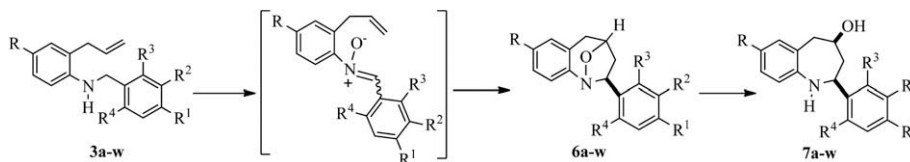
Anindra Sharma, Bandana Chakravarti, Munna Prasad Gupt, Jawed A. Siddiqui, Rituraj Konwar, Rama P. Tripathi*



Synthesis, structural elucidation and in vitro antiparasitic activity against *Trypanosoma cruzi* and *Leishmania chagasi* parasites of novel tetrahydro-1-benzazepine derivatives

pp 4721–4739

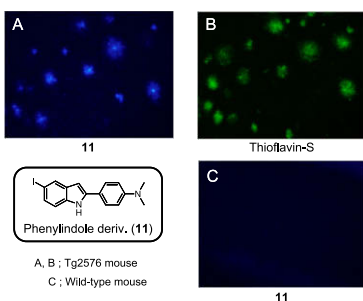
Sandra Gómez-Ayala, Julián A. Castrillón, Alirio Palma*, Sandra M. Leal, Patricia Escobar, Alí Bahsas



Synthesis and characterization of novel phenylindoles as potential probes for imaging of β -amyloid plaques in the brain

pp 4740–4746

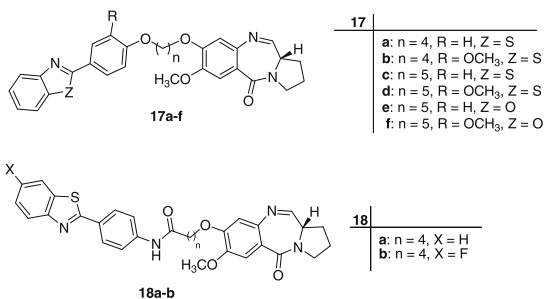
Hiroyuki Watanabe, Masahiro Ono*, Mamoru Haratake, Nobuya Kobashi, Hideo Saji, Morio Nakayama*



Synthesis, DNA-binding ability and anticancer activity of benzothiazole/benzoxazole–pyrrolo[2,1-c][1,4]benzodiazepine conjugates

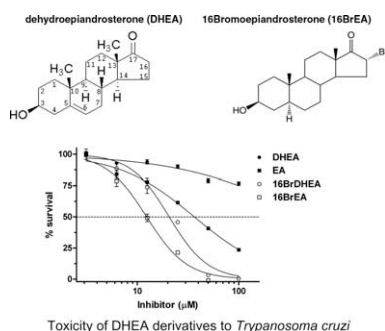
pp 4747–4761

Ahmed Kamal*, K. Srinivasa Reddy, M. Naseer A. Khan, Rajesh V. C. R. N. C. Shetti, M. Janaki Ramaiah, S. N. C. V. L. Pushpavalli, Chatla Srinivas, Manika Pal-Bhadra, Mukesh Chourasia, G. Narahari Sastry, Aarti Juvekar, Surekha Zingde, Madan Barkume

**16-Bromoepiandrosterone, an activator of the mammalian immune system, inhibits glucose 6-phosphate dehydrogenase from *Trypanosoma cruzi* and is toxic to these parasites grown in culture**

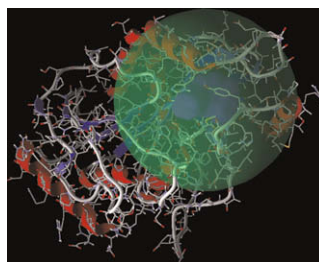
pp 4762–4768

Artur T. Cordeiro*, Otavio H. Thiemann

**Crystallographic and docking studies of purine nucleoside phosphorylase from *Mycobacterium tuberculosis***

pp 4769–4774

Rodrigo G. Ducati, Luiz A. Basso, Diógenes S. Santos*, Walter F. de Azevedo Jr.*

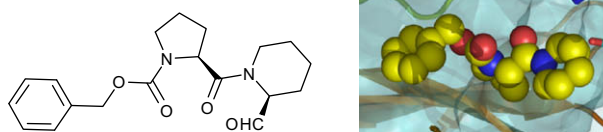


We describe here the structure of purine nucleoside phosphorylase from *Mycobacterium tuberculosis* (MtPNP) in complex with sulfate and its natural substrate, 2'-deoxyguanosine, and its application to virtual screening.

**Inhibition of prolyl oligopeptidase with a synthetic unnatural dipeptide**

pp 4775–4782

Daugirdas Tomas Racys, Dean Rea, Vilmos Fülöp*, Martin Wills*



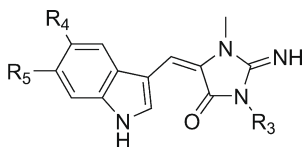
The synthesis of a new inhibitor of prolyl oligopeptidase, containing a piperidine ring, together with an X-ray structure of its complex with the enzyme, is described. This provides evidence that covalent inhibitors of POP do not have to be limited to structures containing five-membered N-containing heterocyclic rings.



Synthesis and structure–affinity relationships of novel small molecule natural product derivatives capable of discriminating between serotonin 5-HT_{1A}, 5-HT_{2A}, 5-HT_{2C} receptor subtypes

pp 4783–4792

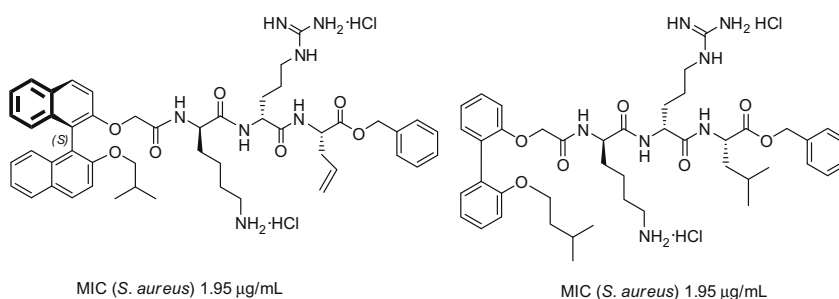
David F. Cummings, Diana C. Canseco, Pratikkumar Sheth, James E. Johnson, John A. Schetz*



Synthesis and antibacterial studies of binaphthyl-based tripeptoids. Part 2

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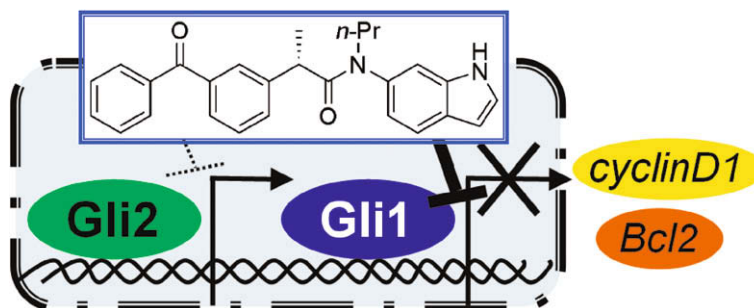
John B. Bremner*, Paul A. Keller*, Stephen G. Pyne*, Timothy P. Boyle, Zinka Brkic, Jody Morgan, Kittiya Somphol, Jonathan A. Coates, John Deadman, David I. Rhodes



Amide conjugates of ketoprofen and indole as inhibitors of Gli1-mediated transcription in the Hedgehog pathway

pp 4801–4811

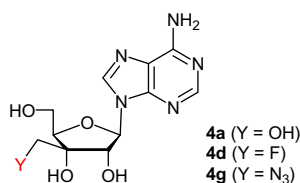
Neeraj Mahindroo, Michele C. Connelly, Chandanamali Punchihewa, Lei Yang, Bing Yan, Naoaki Fujii*



Synthesis and anti-hepatitis C virus (HCV) activity of 3'-C-substituted-methyl pyrimidine and purine nucleosides

pp 4812–4820

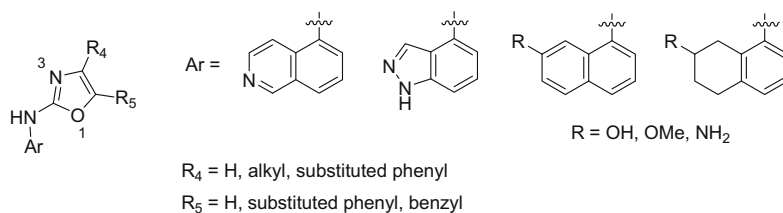
Won Jun Choi, Yu Min Kim, Hea Ok Kim, Hyuk Woo Lee, Dong-Eun Kim, Kwang-su Park, Youhoon Chong, Lak Shin Jeong*



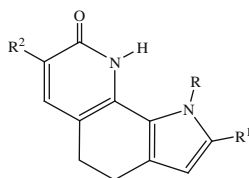
3'-C-Substituted-methyl-ribofuranosyl pyrimidine and purine nucleosides were designed and synthesized from D-xylose. Among these, adenine analogues, **4a**, **4d**, and **4g** showed significant anti-HCV activity in a replicon-based cell assay irrespective of the substituent (Y = OH, F, or N₃) at the 3'-C-substituted-methyl position although they are cytotoxic.

Synthesis and biological evaluation of 5-substituted and 4,5-disubstituted-2-arylamino oxazole TRPV1 antagonists pp 4821–4829

Richard J. Perner*, John R. Koenig, Stanley DiDomenico, Arthur Gomtsyan, Robert G. Schmidt, Chih-Hung Lee, Margaret C. Hsu, Heath A. McDonald, Donna M. Gauvin, Shailen Joshi, Teresa M. Turner, Regina M. Reilly, Philip R. Kym, Michael E. Kort

**Synthesis of pyrrolo[3,2-*h*]quinolinones with good photochemotherapeutic activity and no DNA damage** pp 4830–4843

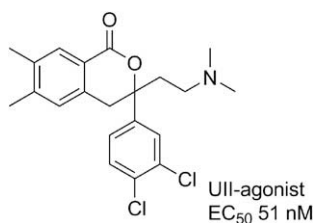
Paola Barraja, Libero Caracausi, Patrizia Diana, Anna Carbone, Alessandra Montalbano, Girolamo Cirrincione*, Paola Brun, Giorgio Palù, Ignazio Castagliuolo, Francesco Dall'Acqua, Daniela Vedaldi, Alessia Salvador



A series of pyrrolo[3,2-*h*]quinolinones, angelicin heteroanalogues, were conveniently synthesized. Three derivatives showed improved photoantiproliferative effect compared to angelicin without inducing DNA damage.

Optimization of isochromanone based urotensin II receptor agonists pp 4844–4854

Fredrik Lehmann, Erika A. Currier, Roger Olsson, Jian-Nong Ma, Ethan S. Burstein, Uli Hacksell, Kristina Luthman*



*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].

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ISSN 0968-0896