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# Bioorganic & Medicinal Chemistry

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## Bioorganic & Medicinal Chemistry Volume 19, Issue 11, 2011

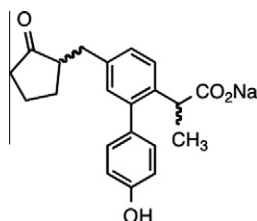
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##### Synthesis and biological evaluation of loxoprofen derivatives

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Naoki Yamakawa, Shintaro Suemasu, Masaaki Matoyama, Ken-ichiro Tanaka, Takashi Katsu, Keishi Miyata, Yoshinari Okamoto, Masami Otsuka, Tohru Mizushima\*



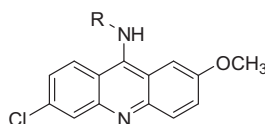
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##### Exploration of acridine scaffold as a potentially interesting scaffold for discovering novel multi-target VEGFR-2 and Src kinase inhibitors

pp 3312–3319

Xudong Luan, Chunmei Gao, Nannan Zhang, Yuzong Chen, Qinsheng Sun, Chunyan Tan, Hongxia Liu, Yibao Jin, Yuyang Jiang\*



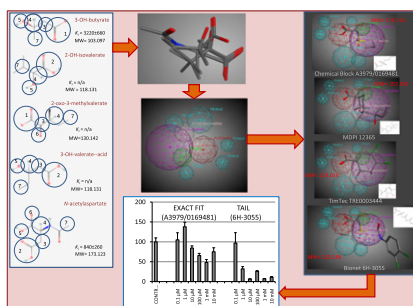
A series of 21 acridine derivatives have been discovered and synthesized as potent VEGFR-2 and Src inhibitors.



##### Elucidation of common pharmacophores from analysis of targeted metabolites transported by the multispecific drug transporter—Organic anion transporter1 (Oat1)

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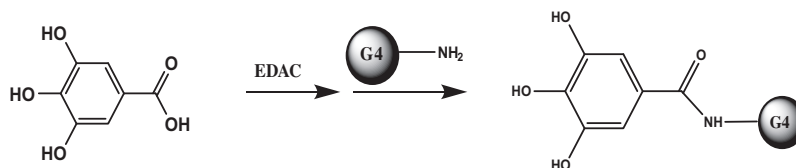
Valentina L. Kouznetsova, Igor F. Tsigelny, Megha A. Nagle, Sanjay K. Nigam\*



**Surface modified dendrimers: Synthesis and characterization for cancer targeted drug delivery**

pp 3341–3346

Anupama Sharma, Surya Prakash Gautam, Arun Kumar Gupta\*

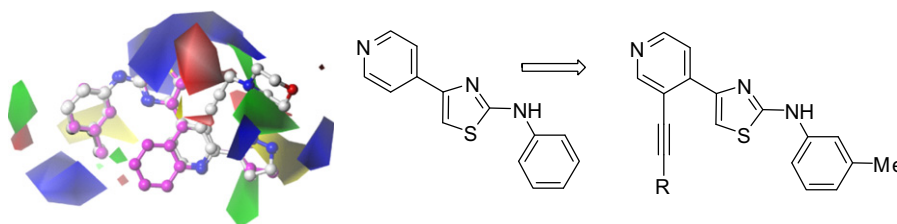


4.0 G PAMAM dendrimer was conjugated with Gallic acid [GA] and characterized through UV, IR,  $^1\text{H}$  NMR and mass spectroscopy.

**SAR studies of 4-pyridyl heterocyclic anilines that selectively induce autophagic cell death in von Hippel-Lindau-deficient renal cell carcinoma cells**

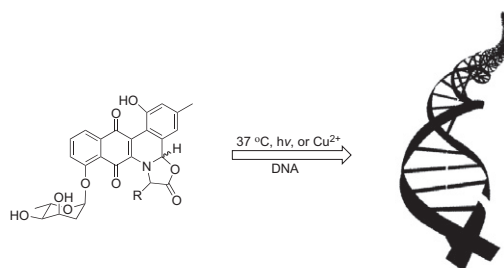
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Muriel Bonnet, Jack U. Flanagan, Denise A. Chan, Edwin W. Lai, Phuong Nguyen, Amato J. Giaccia, Michael P. Hay\*

**Copper-mediated nuclease activity of jadomycin B**

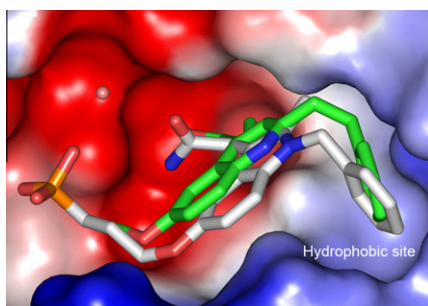
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Susan M. A. Monro, Krista M. Cottreau, Colin Spencer, Jason R. Wentzell, Cathy L. Graham, Charles N. Borissow, David L. Jakeman, Sherri A. McFarland\*

**Quinoline-4-methyl esters as human nonpancreatic secretory phospholipase A<sub>2</sub> inhibitors**

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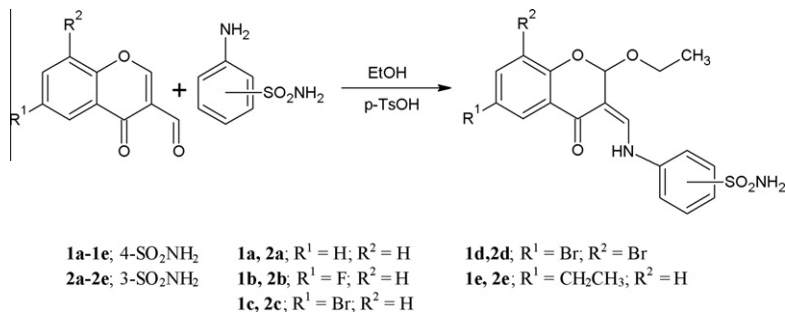
Yiran Wu, Zheng Chen, Ying Liu\*, Lanlan Yu, Lu Zhou, Suijia Yang, Luhua Lai\*



**Discovery of new chromone containing sulfonamides as potent inhibitors of bovine cytosolic carbonic anhydrase**

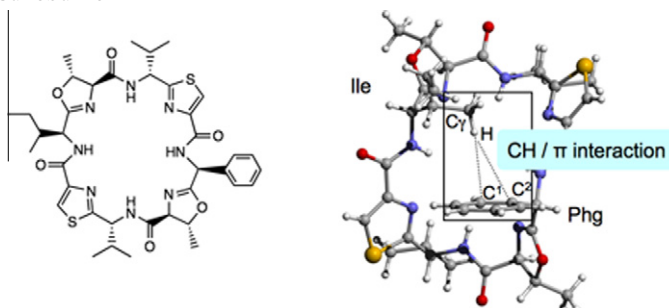
pp 3367–3371

Mariya al-Rashida\*, Muhammad Ashraf, Bushra Hussain, Saeed Ahmad Nagra, Ghulam Abbas

**The square conformation of phenylglycine-incorporated ascidiacyclamide is stabilized by CH/π interactions between amino acid side chains**

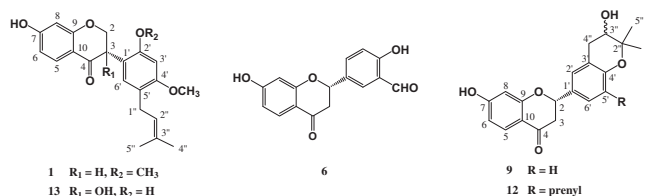
pp 3372–3377

Akiko Asano\*, Takeshi Yamada, Mitsunobu Doi

**New 5-deoxyflavonoids and their inhibitory effects on protein tyrosine phosphatase 1B (PTP1B) activity**

pp 3378–3383

Phi Hung Nguyen, Trong Tuan Dao, Jayeon Kim, Do Tuan Phong, Derek Tantoh Ndinteh, Joseph Tanyi Mbafor, Won Keun Oh\*

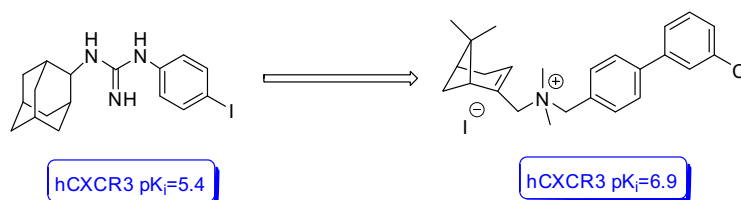


Five new 5-deoxyflavonoids along with eight known analogues were isolated from an EtOAc-soluble extract of the root bark of *Erythrina abyssinica*. All compounds showed dose-dependent inhibitory effects on the enzyme activity of protein tyrosine phosphatase 1B (PTP1B) in an in vitro assay with IC<sub>50</sub> values ranging from 14.9 ± 1.6 to 72.9 ± 9.7 μM. Compounds with prenyl and methoxy groups on the B ring possessed higher activity than those bearing the 2,2-dimethylpyrano ring in the structure.

**CXCR3 antagonists: Quaternary ammonium salts equipped with biphenyl- and polycycloaliphatic-anchors**

pp 3384–3393

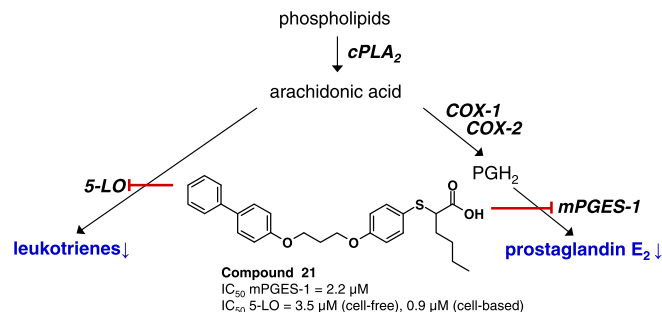
Maikel Wijtmans, Dennis Verzijl, Serge Bergmans, Michael Lai, Leontien Bosch, Martine J. Smit, Iwan J. P. de Esch, Rob Leurs\*



## Identification of 2-mercaptohexanoic acids as dual inhibitors of 5-lipoxygenase and microsomal prostaglandin E<sub>2</sub> synthase-1

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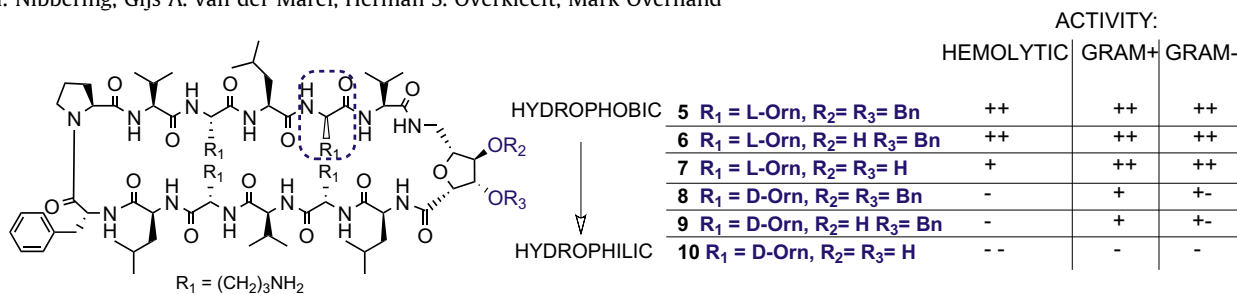
Christine Greiner, Heiko Zettl, Andreas Koeberle, Carlo Pergola, Hinnak Northoff, Manfred Schubert-Zsilavecz, Oliver Werz\*



## Synthesis and evaluation of strand and turn modified ring-extended gramicidin S derivatives

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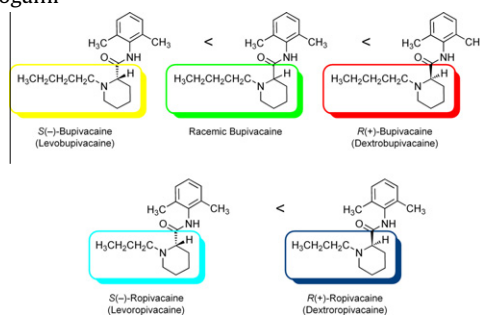
Annemiek D. Knijnenburg, Varsha V. Kapoor, Gijsbert M. Grotenbreg, Emile Spalburg, Albert J. de Neeling, Roos H. Mars-Groenendijk, Daan Noort, José M. Otero, Antonio L. Llamas-Saiz, Mark J. van Raaij, Bep Ravensbergen, Peter H. Nibbering, Gijs A. van der Marel, Herman S. Overkleeft, Mark Overhand\*



## Stereostructure-based differences in the interactions of cardiotoxic local anesthetics with cholesterol-containing biomimetic membranes

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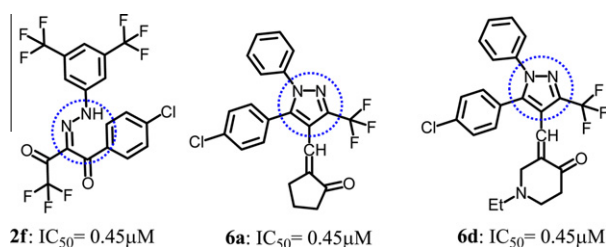
Hironori Tsuchiya\*, Takahiro Ueno, Maki Mizogami



## Design, synthesis, and biological evaluation of substituted hydrazone and pyrazole derivatives as selective COX-2 inhibitors: Molecular docking study

pp 3416–3424

Magda A.-A. El-Sayed, Naglaa I. Abdel-Aziz\*, Alaa A.-M. Abdel-Aziz, Adel S. El-Azab, Yousif A. Asiri, Kamal E. H. ElTahir

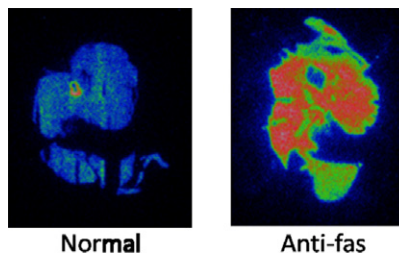


A series of hydrazone and pyrazole derivatives were prepared and evaluated for their anti-inflammatory activities and selectivity as COX-2 inhibitor.

**Synthesis and preliminary evaluation of radiolabeled bis(zinc(II)–dipicolylamine) coordination complexes as cell death imaging agents**

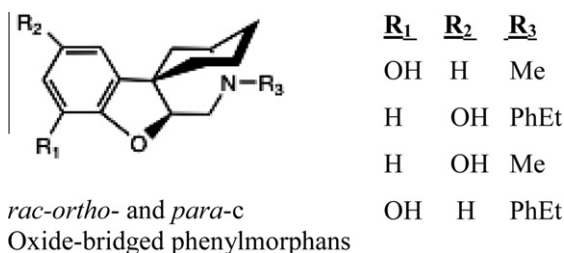
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Leonie wyffels, Brian D. Gray, Christy Barber, James M. Woolfenden, Koon Y. Pak, Zhonglin Liu\*

Autoradiograms of  $^{99m}\text{Tc}$ -HYNIC-1 uptake in normal or anti-Fas treated liver.**Probes for narcotic receptor mediated phenomena. Part 42: Synthesis and in vitro pharmacological characterization of the *N*-methyl and *N*-phenethyl analogues of the racemic *ortho*-c and *para*-c oxide-bridged phenylmorphans**

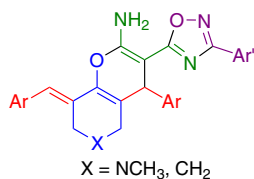
pp 3434–3443

Jin-Hee Kim, Jeffrey R. Deschamps, Richard B. Rothman, Christina M. Dersch, John E. Folk, Kejun Cheng, Arthur E. Jacobson, Kenner C. Rice\*

**Antimycobacterial activity of novel 1,2,4-oxadiazole-pyranopyridine/chromene hybrids generated by chemoselective 1,3-dipolar cycloadditions of nitrile oxides**

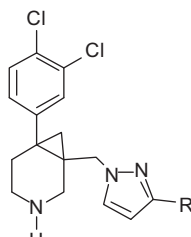
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Raju Ranjith Kumar, Subbu Perumal\*, J. Carlos Menéndez\*, Perumal Yogeewari, Dharmarajan Sriram

**1-Heteroaryl-6-(3,4-dichlorophenyl)-3-azabicyclo[4.1.0]heptane: Further insights into a class of triple re-uptake inhibitors**

pp 3451–3461

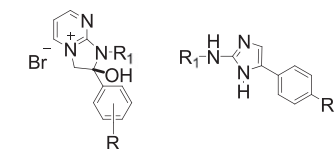
Fabrizio Micheli\*, Paolo Cavanni, Michela Bettati, Giorgio Bonanomi, Romano Di Fabio, Elettra Fazzolari, Carla Marchioro, Maja Rosic, Luca Tarsi, Filippo Visentini, Laura Zonzini, Angela Worby



### Structure–activity relationship of 2-hydroxy-2-aryl-2,3-dihydro-imidazo[1,2-*a*]pyrimidinium salts and 2*N*-substituted 4(5)-aryl-2-amino-1*H*-imidazoles as inhibitors of biofilm formation by *Salmonella Typhimurium* and *Pseudomonas aeruginosa*

pp 3462–3473

Hans P. L. Steenackers, Denis S. Ermolat'ev, Bharat Savaliya, Ami De Weerd, David De Coster, Anamik Shah, Erik V. Van der Eycken, Dirk E. De Vos, Jozef Vanderleyden, Sigrid C. J. De Keersmaecker\*



R<sub>1</sub> = n-alkyl, cyclo-alkyl, aromatic group

R = H, -Cl, -Br, -F, -I, -NO<sub>2</sub>, -OMe, -Ph, Biphenyl, ...

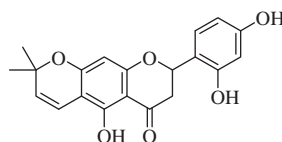
A library of 80 2-hydroxy-2-aryl-2,3-dihydro-imidazo[1,2-*a*]pyrimidinium salts and 54 2*N*-substituted 4(5)-aryl-2-aminoimidazoles was synthesized and tested for the antagonistic effect against biofilm formation by *Salmonella Typhimurium* and *Pseudomonas aeruginosa*.



### Tyrosinase inhibitory activity of a 6-isoprenoid-substituted flavanone isolated from *Dalea elegans*

pp 3474–3482

María Eugenia Chiari, Domingo Mariano A. Vera, Sara María Palacios, María Cecilia Carpinella\*



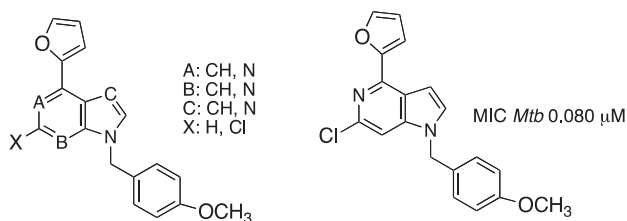
With the aim of finding new anti-tyrosinase agents, the extract from *Dalea elegans* was submitted to fractionation yielding 5,2',4'-trihydroxy-2'',2''-dimethylchromene-(6,7:5'',6'')-flavanone which showed notable activity at inhibiting tyrosinase.



### Synthesis and antimycobacterial activities of non-purine analogs of 6-aryl-9-benzylpurines: Imidazopyridines, pyrrolopyridines, benzimidazoles, and indoles

pp 3483–3491

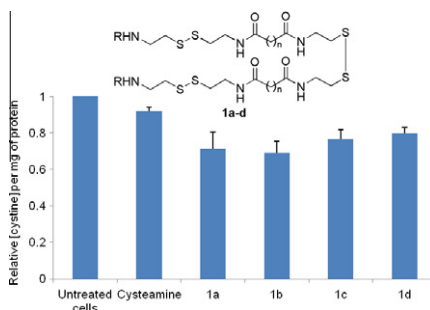
Abhijit Datta Khoje, Colin Charnock, Baojie Wan, Scott Franzblau, Lise-Lotte Gundersen\*



### Synthesis and in vitro evaluation of novel pro-drugs for the treatment of nephropathic cystinosis

pp 3492–3496

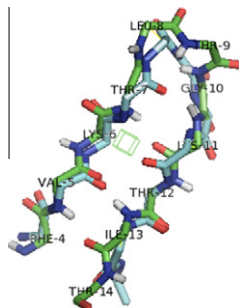
Ziad Omran\*, Kevin A. Moloney, Amina Benylles, Graeme Kay, Rachel M. Knott, Donald Cairns



**Hairpin conformation of an 11-mer peptide**

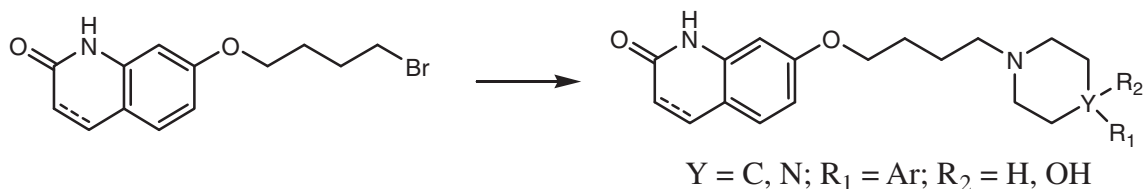
pp 3497–3501

Chong Geok Mei, Nicole Jahr, David Singer, Stefan Berger\*

**Synthesis and characterization of selective dopamine D<sub>2</sub> receptor ligands using aripiprazole as the lead compound**

pp 3502–3511

Suwanna Vangveravong, Zhanbin Zhang, Michelle Taylor, Melissa Bearden, Jinbin Xu, Jinquan Cui, Wei Wang, Robert R. Luedtke, Robert H. Mach\*

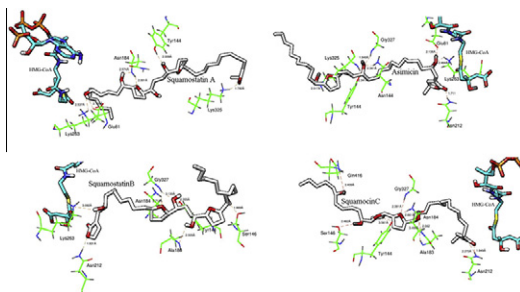


A series of structural congeners of aripiprazole was synthesized and found to have a high affinity and selectivity for dopamine D<sub>2</sub> versus D<sub>3</sub> and D<sub>4</sub> receptors. These compounds were found to be partial agonists at the D<sub>2</sub> receptor.

**Specific inhibitions of annonaceous acetogenins on class II 3-hydroxy-3-methylglutaryl coenzyme A reductase from *Streptococcus pneumoniae***

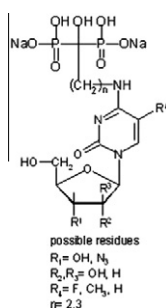
pp 3512–3519

Lingling Feng\*, Li Zhou, Yao Sun, Jie Gui, Xiaofeng Wang, Ping Wu, Jian Wan\*, Yanliang Ren, Shengxiang Qiu, Xiaoyi Wei, Jun Li

**N<sup>4</sup>-[Alkyl-(hydroxyphosphono)phosphonate]-cytidine—New drugs covalently linking antimetabolites (5-FdU, araU or AZT) with bone-targeting bisphosphonates (alendronate or pamidronate)**

pp 3520–3526

Herbert Schott\*, Daniel Goltz, Timm C. Schott, Claudia Jauch, Reto A. Schwendener

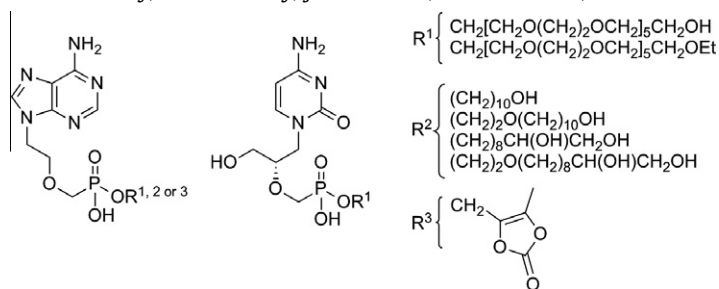


New cytostatic antimetabolite-bisphosphonates.

### New prodrugs of Adefovir and Cidofovir

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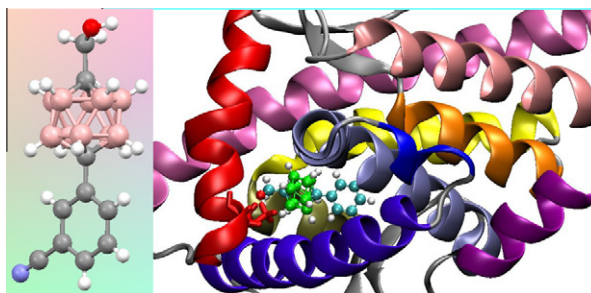
Tomáš Tichý\*, Graciela Andrei, Martin Dračinský, Antonín Holý, Jan Balzarini, Robert Snoeck, Marcela Krečmerová



### Crystal structure, docking study and structure–activity relationship of carborane-containing androgen receptor antagonist 3-(12-hydroxymethyl-1,12-dicarba-closo-dodecaboran-1-yl)benzonitrile

pp 3540–3548

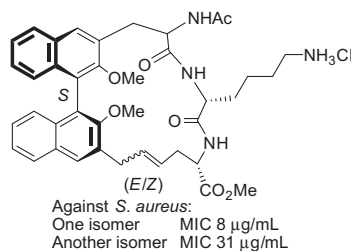
Kiminori Ohta, Tokuhito Goto, Shinya Fujii, Masatoshi Kawahata, Akifumi Oda, Shigeru Ohta, Kentaro Yamaguchi, Shuichi Hirono, Yasuyuki Endo\*



### Synthesis and antibacterial activity of some binaphthyl-supported macrocycles containing a cationic amino acid

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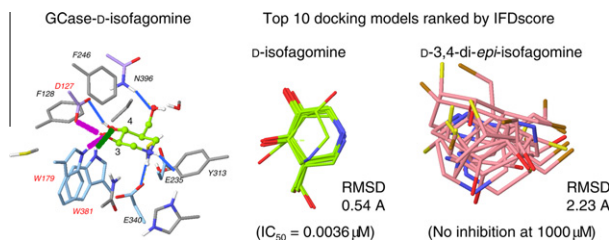
Daniel R. Coghlan, John B. Bremner\*, Paul A. Keller\*, Stephen G. Pyne\*, Dorothy M. David, Kittiya Somphol, Dean Baylis, Jonathan Coates, John Deadman, David I. Rhodes, Alan D. Robertson

Twelve macrocyclic derivatives with anti-bacterial activity against *Staphylococcus aureus* are reported.

### Docking and SAR studies of D- and L-isofagomine isomers as human β-glucocerebrosidase inhibitors

pp 3558–3568

Atsushi Kato\*, Saori Miyauchi, Noriko Kato, Robert J. Nash, Yuichi Yoshimura, Izumi Nakagome, Shuichi Hirono, Hiroki Takahata, Isao Adachi



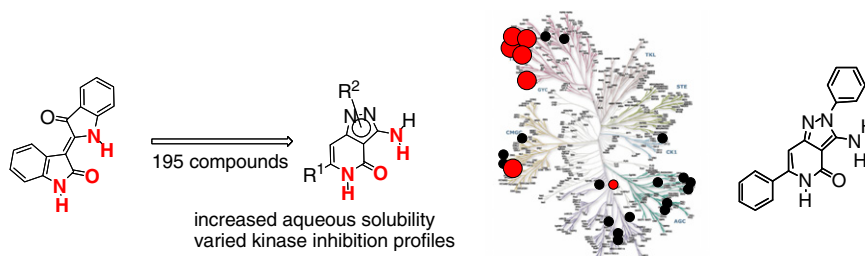
A molecular docking study revealed that D-3-*epi*-isofagomine missed the hydrogen bond interactions between Asp127 and the 3-OH group and between Trp179 and the 3-OH group. Furthermore, the top 10 docking models ranked by IFDscore suggested that D-3,4-di-*epi*-isofagomine can not bind to β-glucocerebrosidase (Gcase) at a stable interaction mode.



**Design and evaluation of 3-aminopyrazolopyridinone kinase inhibitors inspired by the natural product indirubin**

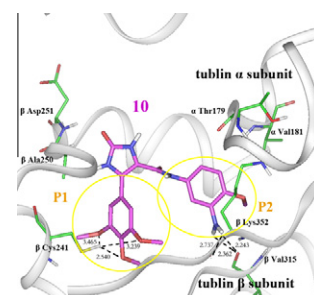
pp 3569–3578

Lynette A. Smyth, Thomas P. Matthews, Ian Collins\*

**Imidazolone–amide bridges and their effects on tubulin polymerization in *cis*-locked vinylogous combretastatin-A4 analogues: Synthesis and biological evaluation**

pp 3579–3584

Yao-Wu Li, Jia Liu, Na Liu, Duo Shi, Xiao-Tian Zhou, Jia-Guo Lv, Ju Zhu, Can-Hui Zheng\*, You-Jun Zhou\*

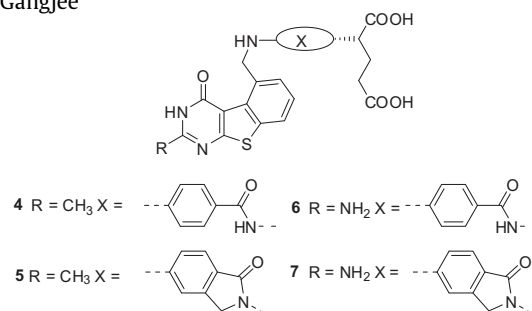


Several CA-4 analogues bearing an imidazolone–amide moiety showed cytotoxicity and tubulin polymerization inhibitory activity. The binding mode of compound **10** with optimal bioactivity to tubulin was obtained by molecular docking.

**Design, synthesis, biological evaluation and X-ray crystal structure of novel classical 6,5,6-tricyclic benzo[4,5]thieno[2,3-*d*]pyrimidines as dual thymidylate synthase and dihydrofolate reductase inhibitors**

pp 3585–3594

Xin Zhang, Xilin Zhou, Roy L. Kisliuk, Jennifer Piraino, Vivian Cody, Aleem Gangjee\*



\*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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