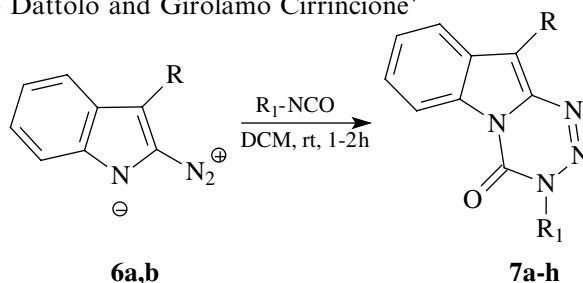


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- Structure-based discovery of human L-xylulose reductase inhibitors from database screening and molecular docking** pp 301–312

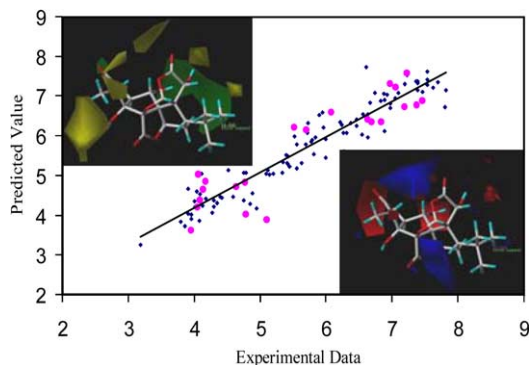
Vincenzo Carbone, Syuhei Ishikura, Akira Hara and Ossama El-Kabbani*

The discovery of novel human L-xylulose reductase inhibitors based on the crystal structure of the holoenzyme and the NCI database is reported.

- QSAR analyses on ginkgolides and their analogues using CoMFA, CoMSIA, and HQSAR** pp 313–322

Weiliang Zhu,* Gang Chen, Lihong Hu, Xiaomin Luo, Chunshan Gui, Cheng Luo, Chum Mok Puah, Kaixian Chen and Hualiang Jiang*

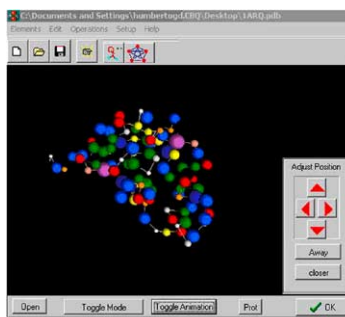
QSAR study was carried out on 117 ginkgolide analogues using the methods of CoMFA, CoMSIA, and HQSAR, for finding new potent substitutes of the natural ginkgolides for treating PAF related diseases. The possible binding mechanism between ginkgolides and human PAF receptor was also deduced based on the QSAR results.



Predicting stability of Arc repressor mutants with protein stochastic moments

pp 323–331

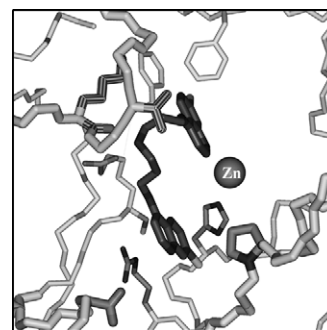
Humberto González-Díaz,* Eugenio Uriarte and Ronal Ramos de Armas

**Conformational sampling of the botulinum neurotoxin serotype a light chain: implications for inhibitor binding**

pp 333–341

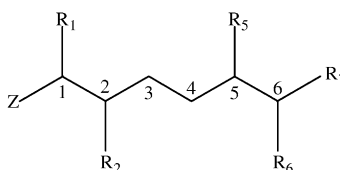
James C. Burnett, James J. Schmidt, Connor F. McGrath, Tam L. Nguyen, Ann R. Hermone, Rekha G. Panchal, Jonathan L. Vennerstrom, Krishna Kodukula, Daniel W. Zaharevitz, Rick Gussio* and Sina Bavari*

Molecular dynamics simulations were used to explore how residue motion in and around the botulinum neurotoxin serotype A light chain (BoNT/A LC) substrate binding cleft might affect inhibitor binding. Results from these studies indicate that surface loop reorientations toward the substrate binding cleft may facilitate small molecule binding by creating additional inhibitor-residue contacts. Based on molecular docking studies, our common pharmacophore model for BoNT/A LC inhibitors has been refined via the inclusion of these potential contact residues.

**CP-MLR directed QSAR studies on the antimycobacterial activity of functionalized alkenols—topological descriptors in modeling the activity**

pp 343–351

Manish K. Gupta, Ram Sagar, Arun K. Shaw and Yenamandra S. Prabhakar*

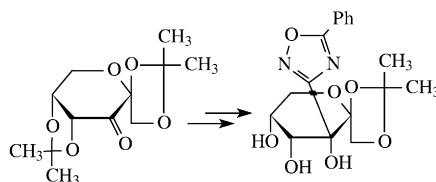


The antimycobacterial activity of nitro/acetamido alkenol derivatives and chloro/amino alkenol derivatives has been analyzed through combinatorial protocol in multiple linear regression (CP-MLR) using different topological descriptors obtained from Dragon software.

**Stereoselective synthesis, structural characterization, and properties of 1,2-O-isopropylidene-3-C-(5-phenyl-1,2,4-oxadiazol-3-yl)-β-D-psicopyranose**

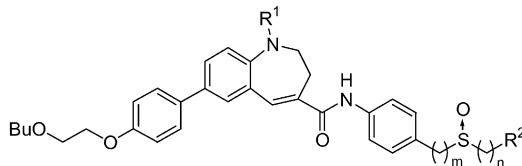
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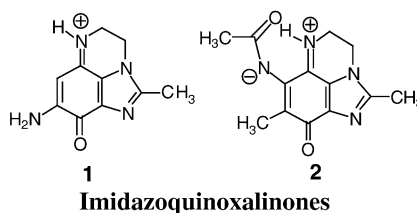
Orally active CCR5 antagonists as anti-HIV-1 agents. Part 3: Synthesis and biological activities of 1-benzazepine derivatives containing a sulfoxide moiety pp 363–386

Masaki Seto,* Naoki Miyamoto, Katsuji Aikawa, Yoshio Aramaki, Naoyuki Kanzaki, Yuji Iizawa, Masanori Baba and Mitsuru Shiraishi



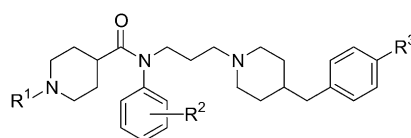
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Daniel V. LaBarbera and Edward B. Skibo*



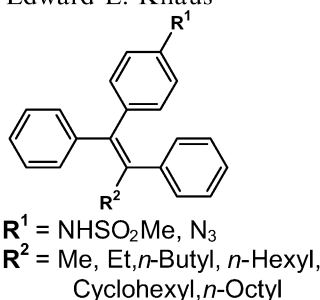
CCR5 antagonists as anti-HIV-1 agents. Part 3: Synthesis and biological evaluation of piperidine-4-carboxamide derivatives pp 397–416

Shinichi Imamura,* Youichi Nishikawa, Takashi Ichikawa, Taeko Hattori, Yoshihiro Matsushita, Shohei Hashiguchi, Naoyuki Kanzaki, Yuji Iizawa, Masanori Baba and Yoshihiro Sugihara



Design and synthesis of (*Z*)-1,2-diphenyl-1-(4-methanesulfonamidophenyl)alk-1-enes and (*Z*)-1-(4-azidophenyl)-1,2-diphenylalk-1-enes: novel inhibitors of cyclooxygenase-2 (COX-2) with anti-inflammatory and analgesic activity pp 417–424

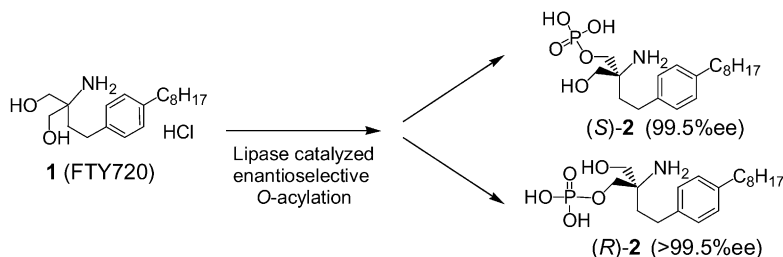
Md. Jashim Uddin, P. N. Praveen Rao and Edward E. Knaus*



Asymmetric synthesis and biological evaluation of the enantiomeric isomers of the immunosuppressive FTY720-phosphate

pp 425–432

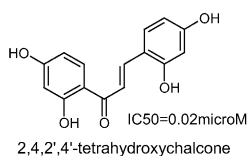
Masatoshi Kiuchi,* Kunitomo Adachi, Ayumi Tomatsu, Masao Chino, Shuzo Takeda, Yoshihito Tanaka, Yasuhiro Maeda, Noriko Sato, Naoko Mitsutomi, Kunio Sugahara and Kenji Chiba



Chalcones as potent tyrosinase inhibitors: the importance of a 2,4-substituted resorcinol moiety

pp 433–441

Soliman Khatib, Ohad Nerya, Ramadan Musa, Maayan Shmuel, Snait Tamir and Jacob Vaya*

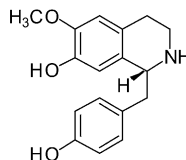


Chalcones with tetra-substituted hydroxyl groups were synthesized and tested as tyrosinase inhibitors towards designing novel whitening agents, resulting with the most potent inhibitor, with IC₅₀ of 0.02 μM concn.

Anti-HIV benzyloisoquinoline alkaloids and flavonoids from the leaves of *Nelumbo nucifera*, and structure–activity correlations with related alkaloids

pp 443–448

Yoshiki Kashiwada,* Akihiro Aoshima, Yasumasa Ikeshiro, Yuh-Pan Chen, Hiroshi Furukawa, Masataka Itoigawa, Toshihiro Fujioka, Kunihide Mihashi, L. Mark Cosentino, Susan L. Morris-Natschke and Kuo-Hsiung Lee*

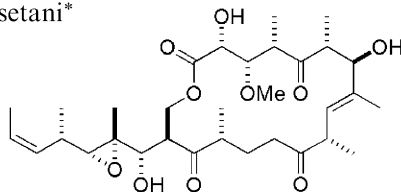


(+)-1(R)-Coclaurine (1) and (–)-1(S)-norcoclaurine (3), together with quercetin 3-O-β-D-glucuronide (4), were isolated from the leaves of *Nelumbo nucifera* (Nymphaeaceae), and identified as anti-HIV principles. These compounds can serve as new leads for further development of anti-AIDS agents.

13-Deoxytedanolide, a marine sponge-derived antitumor macrolide, binds to the 60S large ribosomal subunit

pp 449–454

Shinichi Nishimura, Shigeki Matsunaga, Minoru Yoshida, Hiroshi Hirota, Shigeyuki Yokoyama and Nobuhiro Fusetani*

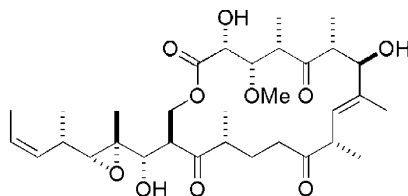


13-deoxytedanolide

By using radiolabeled ligand derived from 13-deoxytedanolide, the ribosome was identified as the target molecule of 13-deoxytedanolide. As expected, 13-deoxytedanolide inhibited polypeptide elongation at low concentration.

Structure–activity relationship study on 13-deoxytedanolide, a highly antitumor macrolide from the marine sponge *Mycale adhaerens* pp 455–462

Shinichi Nishimura, Shigeki Matsunaga, Satoru Yoshida, Yoichi Nakao, Hiroshi Hirota and Nobuhiro Fusetani*



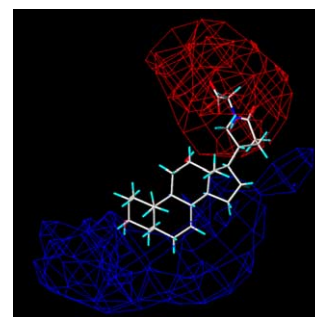
13-deoxytedanolide

Structure–activity relationship of 13-deoxytedanolide showed that the southern and northern hemispheres play independent roles to exhibit potent biological activity.

Application of QSAR analysis to organic anion transporting polypeptide 1a5 (Oatp1a5) substrates pp 463–471

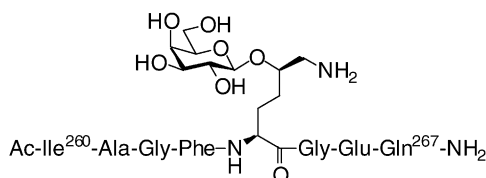
Mine Yarim,* Stefano Moro, Robert Huber, Peter J. Meier, Chosei Kaseda, Toru Kashima, Bruno Hagenbuch and Gerd Folkers

We used three-dimensional quantitative structure–activity relationship (3D-QSAR) techniques to obtain topological information on the substrate binding site of the protein. Based on the derived model we identified new potential Oatp1a5 substrates and confirmed their predicted apparent affinity values experimentally.



Identification of the minimal glycopeptide core recognized by T cells in a model for rheumatoid arthritis pp 473–482

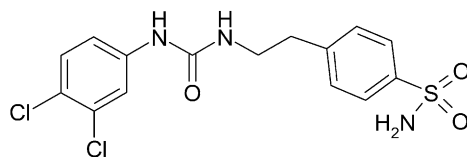
Lotta Holm, Peter Kjellén, Rikard Holmdahl and Jan Kihlberg*



The minimal peptide epitope required for binding to MHC-II molecules associated with arthritis in mice, was determined to be CII260–266. Elongation to give CII260–267 and glycosylation on Hyl 264 gave an epitope that stimulated T-cell hybridomas obtained from arthritic mice.

Carbonic anhydrase inhibitors. Inhibition of *Plasmodium falciparum* carbonic anhydrase with aromatic sulfonamides: towards antimalarials with a novel mechanism of action? pp 483–489

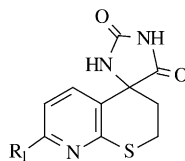
Jerapan Krungkrai,* Andrea Scozzafava, Sutarthip Reungprapavut, Sudaratana R. Krungkrai, Roonglawan Rattanajak, Sumalee Kamchonwongpaisan and Claudiu T. Supuran*



Spirohydantoin derivatives of thiopyrano[2,3-*b*]pyridin-4(4*H*)-one as potent in vitro and in vivo aldose reductase inhibitors

pp 491–499

Federico Da Settimo,* Giampaolo Primofiore, Concettina La Motta, Silvia Salerno, Ettore Novellino, Giovanni Greco, Antonio Lavecchia, Sonia Laneri and Enrico Boldrini

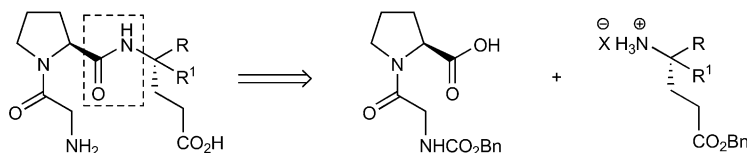

 $R_1 = \text{H, CH}_3$

Spirohydantoin derivatives of thiopyrano[2,3-*b*]pyridin-4(4*H*)-one have been synthesized and examined for their inhibitory activity against aldose reductase.

Synthesis and neuroprotective activity of analogues of glycyl-L-prolyl-L-glutamic acid (GPE) modified at the α -carboxylic acid

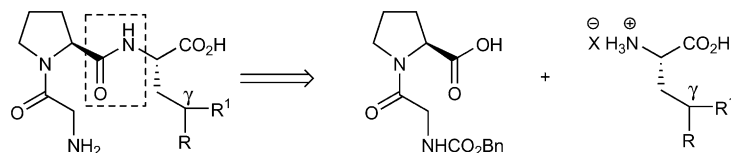
pp 501–517

Nicholas S. Trotter, Margaret A. Brimble,* Paul W. R. Harris, David J. Callis and Frank Sieg


Synthesis and pharmacological evaluation of side chain modified glutamic acid analogues of the neuroprotective agent glycyl-L-prolyl-L-glutamic acid (GPE)

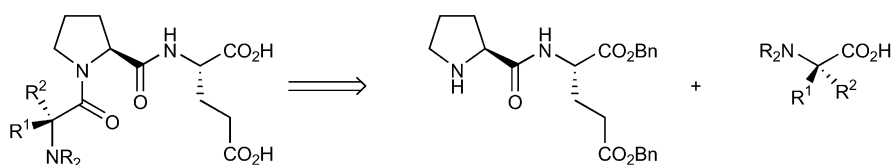
pp 519–532

Margaret A. Brimble,* Nicholas S. Trotter, Paul W. R. Harris and Frank Sieg


Synthesis and pharmacological evaluation of glycine-modified analogues of the neuroprotective agent glycyl-L-prolyl-L-glutamic acid (GPE)

pp 533–548

Michelle Y. H. Lai, Margaret A. Brimble,* David J. Callis, Paul W. R. Harris, Mark S. Levi and Frank Sieg

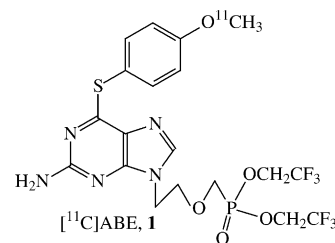


Synthesis of 2-amino-6-(4-[^{11}C]methoxyphenylthio)-9-[2-(phosphonomethoxy)ethyl]purine bis(2,2,2-trifluoroethyl) ester as a novel potential PET gene reporter probe for HBV and HSV-tk in cancers

pp 549–556

Ji-Quan Wang, Xiangshu Fei, Thomas A. Gardner, Gary D. Hutchins and Qi-Huang Zheng*

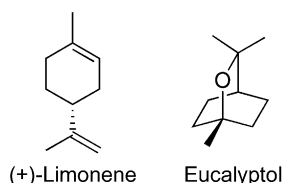
Synthesis of radiolabeled antiviral nucleoside analogue 2-amino-6-(4-[^{11}C]methoxyphenylthio)-9-[2-(phosphonomethoxy)ethyl]purine bis(2,2,2-trifluoroethyl) ester ([^{11}C]ABE) as a novel potential PET reporter probe for hepatitis B virus (HBV) and herpes simplex virus thymidine kinase (HSV-tk) in cancers is reported.



Natural ozone scavenger prevents asthma in sensitized rats

pp 557–562

Ehud Keinan,* Aaron Alt, Gail Amir, Lea Bentur, Haim Bibi and David Shoseyov



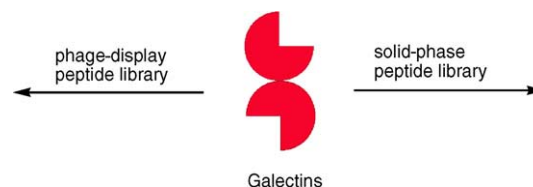
Pulmonary inflammation in asthma may involve a vicious circle of ozone production and recruitment of white blood cells, which produce more ozone. Pulmonary function tests and pathological data using a sensitized rat model with limonene (ozone scavenger) and eucalyptol (control) strongly support the hypothesis.

Identification of peptide ligands for malignancy- and growth-regulating galectins using random phage-display and designed combinatorial peptide libraries

pp 563–573

Sabine André, Christopher J. Arnusch, Ichiro Kuwabara, Roland Russwurm, Herbert Kaltner, Hans-Joachim Gabius and Roland J. Pieters*

Peptide ligands were identified for the medically important galectins by screening on-bead with a synthetic solid-phase peptide library and by screening with a phage-display library. The first method yielded sequences binding at or near the carbohydrate-binding site while the latter yielded a sequence binding at a different site.




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*Corresponding author

* Supplementary data available via ScienceDirect

COVER

Peptide libraries on phage and on solid phase beads were screened as ligands for members of the galectin family of endogenous lectins relevant in e.g. cancer. The phage libraries were screened in microtiter plates whereas the on-bead library hits were identified by a colorimetric method. The galectins normally bind β -galactosides, as exemplified by the space filling models, in each of its two binding sites. The peptides identified from the phage did not bind to the sugar binding site whereas the on-bead library derived peptides did, as illustrated by the arrows pointing to the respective parts of the protein. [André, S.; Arnusch, C. J.; Kuwabara, I.; Russwurm, R.; Kaltner, H.; Gabius, H.-J.; Pieters, R. J. *Bioorg. Med. Chem.* **2005**, *13*, 563–573].

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