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Symposium-in-Print

Current Perspectives in Marine Bioorganic Chemistry

Edited by:

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Phillip Crews

Dept. of Chemistry and Biochemistry, University of California at Santa Cruz, Santa Cruz, CA, USA

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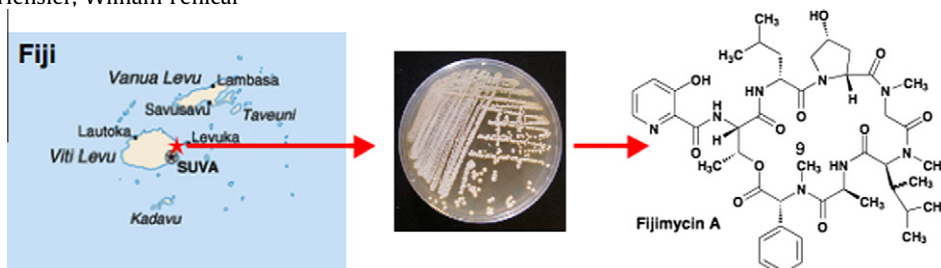
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Guy T. Carter, Phillip Crews*

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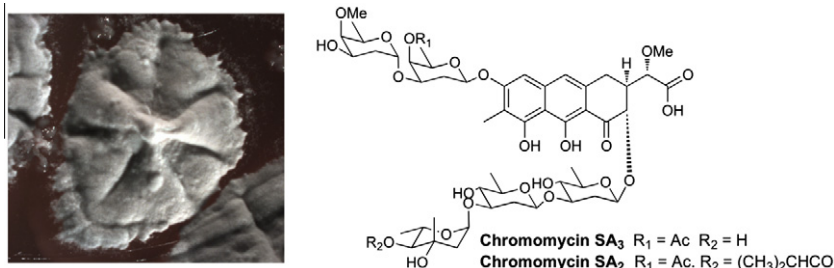


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[Bioorg. Med. Chem. 19 (2011) 5183–5189]

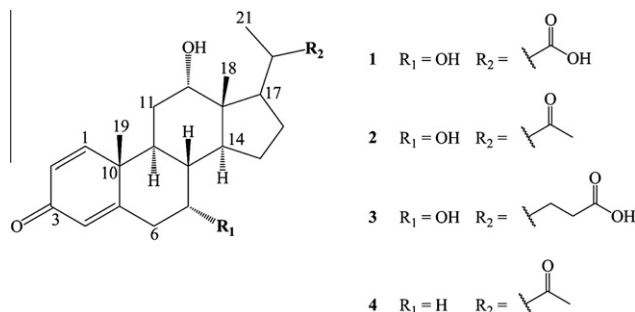
Y. Hu, A. Paula, D.M. Espindola, N.A. Stewart, S. Wei, B.A. Posner, J.B. MacMillan



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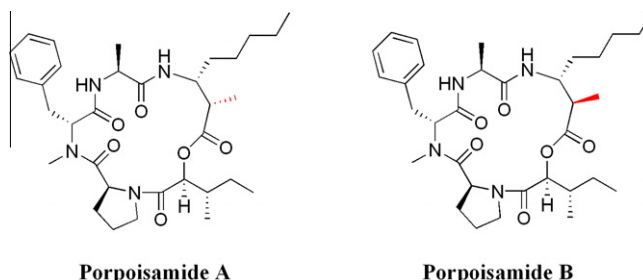
pp 6570–6575

Luke Simmons, Katrin Kaufmann, Ronald Garcia, Gertrud Schwär, Volker Huch, Rolf Müller*

**Porpoisamides A and B, two novel epimeric cyclic depsipeptides from a Florida Keys collection of *Lyngbya* sp.**

pp 6576–6580

Theresa Meickle, Sarath P. Gunasekera, Yanxia Liu, Hendrik Luesch, Valerie J. Paul*

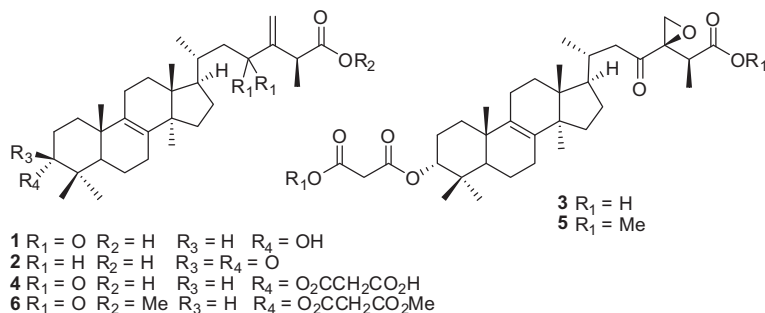


The porpoisamides are two unique cyclic depsipeptides that differ only in the epimeric nature of C-2 of the β -amino acid, 3-amino-2-methyloctanoic acid.

**Daedalols A–C, fungal-derived BACE1 inhibitors**

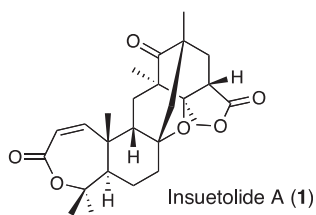
pp 6581–6586

Analia Sorribas, Jorge I. Jiménez, Wesley Y. Yoshida, Philip G. Williams*

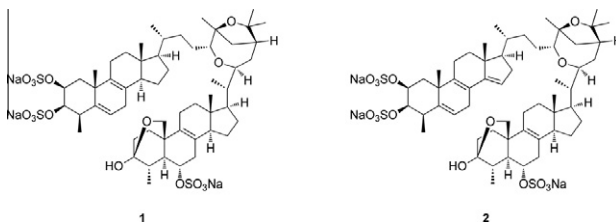
**Novel terpenoids of the fungus *Aspergillus insuetus* isolated from the Mediterranean sponge *Psammocinia* sp. collected along the coast of Israel**

pp 6587–6593

Elazar Cohen, Liat Koch, Kathy Myint Thu, Yocheved Rahamim, Yaniv Aluma, Micha Ilan, Oded Yarden, Shmuel Carmeli*



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Chemical structures of compounds **1** and **2** are shown. Compound **1** is a complex polycyclic molecule with multiple carbonyl groups and numbered atoms (1-21). Compound **2** is a similar polycyclic molecule with a hydroxyl group and a carbonyl group.



pp 6604–6607

Chemical structures of three indole alkaloids are shown, labeled 1, 2, and 3. Each structure features a tryptamine core (indole ring fused to a benzene ring, with an ethylamine side chain) and a quaternary nitrogen atom (N⁺) bonded to a chloride ion (Cl⁻).

- Structure 1:** A tryptamine derivative with a quaternary nitrogen atom (N⁺) bonded to a chloride ion (Cl⁻). The side chain is a 2-hydroxy-3-methylbutyl group. The indole ring is substituted with a bromine atom (Br) at the 5-position.
- Structure 2:** A tryptamine derivative with a quaternary nitrogen atom (N⁺) bonded to a chloride ion (Cl⁻). The side chain is a 2-hydroxy-3-methylbutyl group. The indole ring is substituted with a phenyl group at the 5-position.
- Structure 3:** A tryptamine derivative with a quaternary nitrogen atom (N⁺) bonded to a chloride ion (Cl⁻). The side chain is a 2-hydroxy-3-methylbutyl group. The indole ring is substituted with a phenyl group at the 5-position.



pp 6608–6614

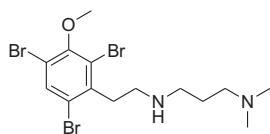
The figure shows a photograph of a coral reef with a ruler and a chemical structure. The ruler is placed horizontally across the middle of the image, showing measurements in centimeters. The coral is orange and yellow. The chemical structure is a complex polycyclic molecule with a long chain and a ring system, labeled with various functional groups like OH, NH, and O.



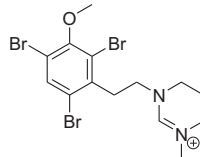
Convolutamines I and J, antitrypanosomal alkaloids from the bryozoan *Amathia tortusa*

pp 6615–6619

Rohan A. Davis, Melissa Sykes, Vicky M. Avery, David Camp, Ronald J. Quinn*



Convolutamine I
 $IC_{50} = 1.1 \mu M$
 (*Trypanosoma brucei brucei*)

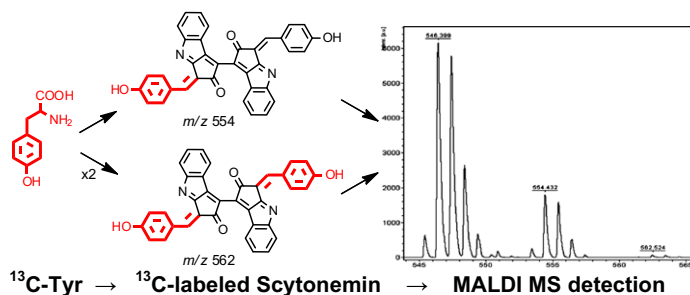


Convolutamine J
 $IC_{50} = 13.7 \mu M$
 (*Trypanosoma brucei brucei*)

**Probing the in vivo biosynthesis of scytonemin, a cyanobacterial ultraviolet radiation sunscreen, through small scale stable isotope incubation studies and MALDI-TOF mass spectrometry**

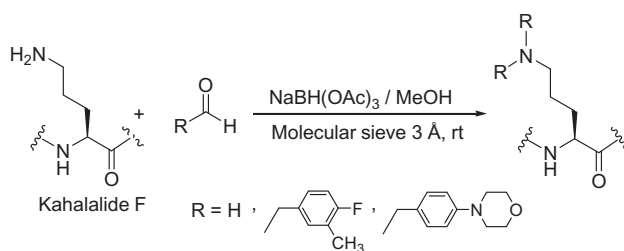
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Carla S. Jones, Eduardo Esquenazi, Pieter C. Dorrestein, William H. Gerwick*

**In vitro and in vivo evaluation of select kahalalide F analogs with antitumor and antifungal activities**

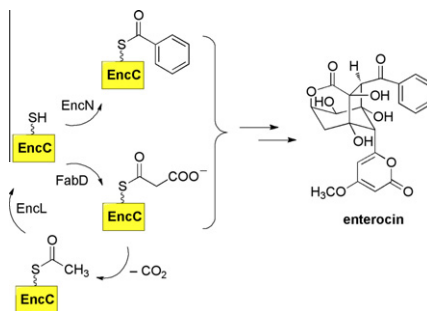
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**Policing starter unit selection of the enterocin type II polyketide synthase by the type II thioesterase EncL**

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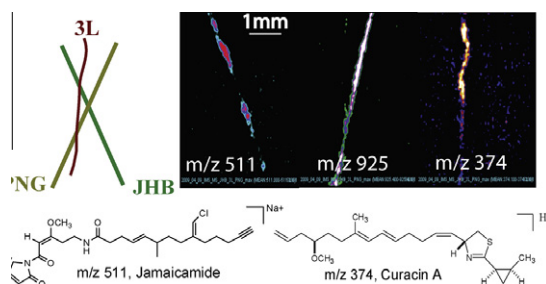
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Ion mobility mass spectrometry enables the efficient detection and identification of halogenated natural products from cyanobacteria with minimal sample preparation

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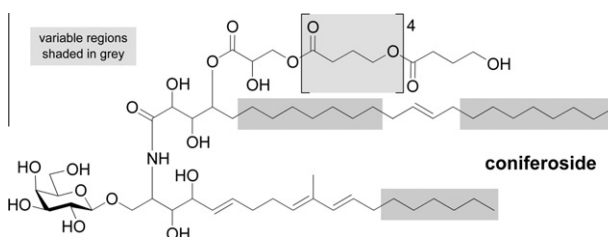
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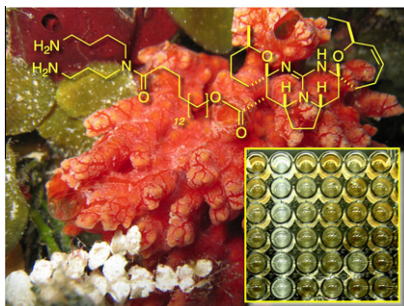
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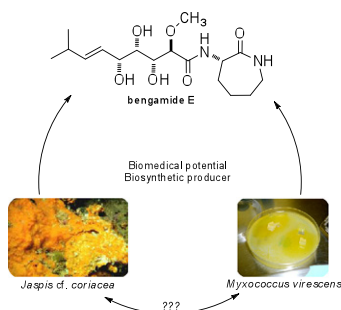
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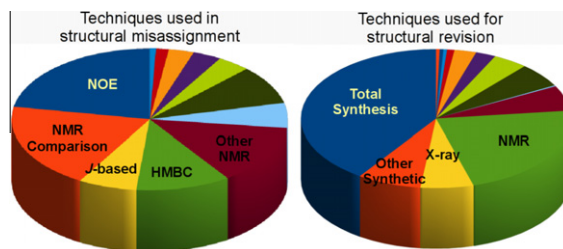
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Survey of marine natural product structure revisions: A synergy of spectroscopy and chemical synthesis

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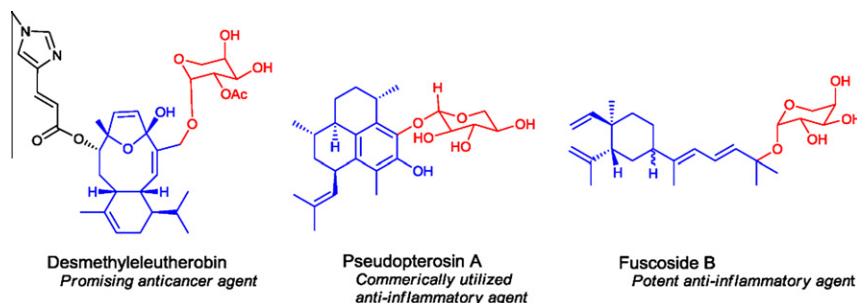
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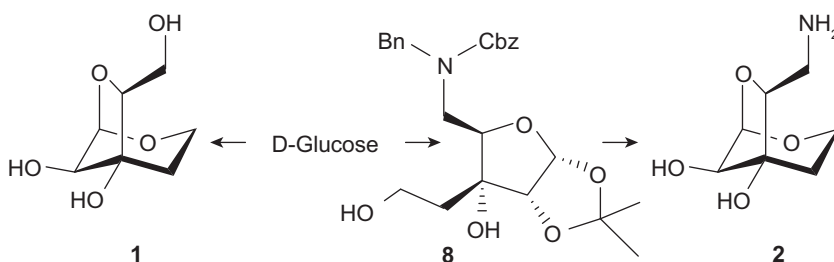


REGULAR ARTICLES

Synthesis of anomeric 1,5-anhydrosugars as conformationally locked selective α -mannosidase inhibitors

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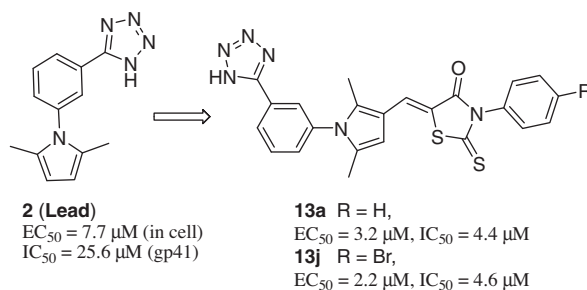
Rajendra S. Mane, Sougata Ghosh, Shailza Singh, Balu A. Chopade, Dilip D. Dhavale*



Design, synthesis and biological evaluation of 3-substituted 2,5-dimethyl-N-(3-(1H-tetrazol-5-yl)phenyl)pyrroles as novel potential HIV-1 gp41 inhibitors

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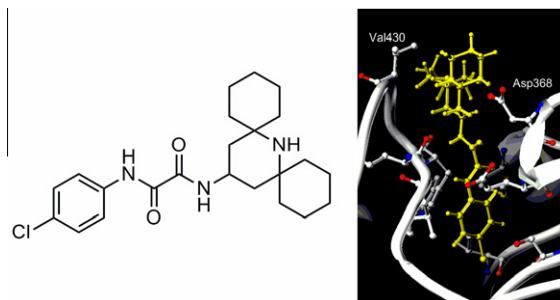
Xiao-Yang He, Peng Zou, Jiayin Qiu, Ling Hou, Shibo Jiang, Shuwen Liu, Lan Xie*



Small molecular CD4 mimics as HIV entry inhibitors

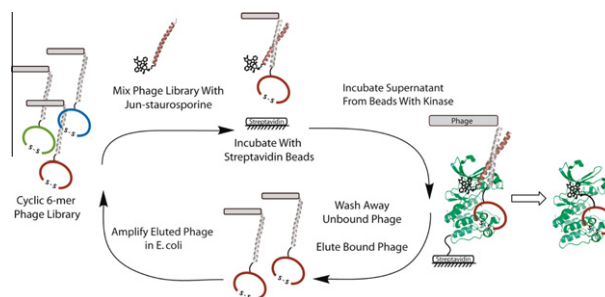
pp 6735–6742

Tetsuo Narumi, Hiroshi Arai, Kazuhisa Yoshimura, Shigeyoshi Harada, Wataru Nomura, Shuzo Matsushita, Hirokazu Tamamura*

**Selection of cyclic-peptide inhibitors targeting Aurora kinase A: Problems and solutions**

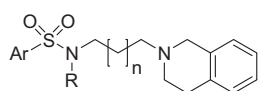
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Carolyn D. Shomin, Elizabeth Restituyo, Kurt J. Cox, Indraneel Ghosh*

**Arene- and quinoline-sulfonamides as novel 5-HT₇ receptor ligands**

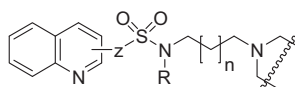
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Paweł Zajdel*, Krzysztof Marciniak, Andrzej Maślankiewicz, Maria H. Paluchowska, Grzegorz Satała, Anna Partyka, Magdalena Jastrzębska-Więsek, Dagmara Wróbel, Anna Wesołowska, Beata Duszyńska, Andrzej J. Bojarski, Maciej Pawłowski



18 - 21

Ar = phenyl, 1-, 2-naphthyl
 n = 0, 1, 2
 R = (CH₂)₂NH₂, (CH₂)₃NH₂



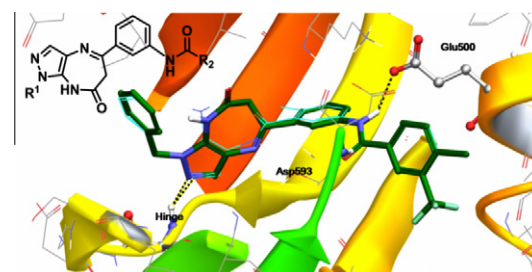
28 - 40, 49 - 55

Amine = 1,2,3,4-tetrahydroisoquinoline, perhydroisoquinoline,
 4,5,6,7-tetrahydrothieno[3,2-c]pyridine, 2-methoxyphenylpiperazine
 R = H, C₂H₅
 z = 3, 6, 7, 8; n = 1, 2, 3

**Syntheses of phenylpyrazolodiazepin-7-ones as conformationally rigid analogs of aminopyrazole amide scaffold and their antiproliferative effects on cancer cells**

pp 6760–6767

Hyangmi Kim, Minjung Kim, Junghun Lee, Hana Yu, Jung-Mi Hah*

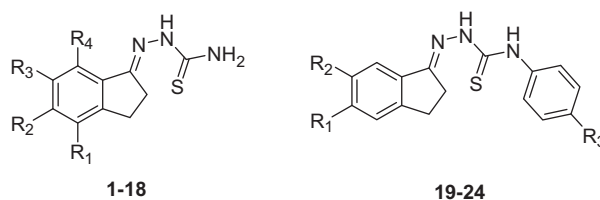


The synthesis of a novel series of phenylpyrazolodiazepin-7-one derivatives **7a–g**, **8a–o** and their antiproliferative activities against A375P melanoma cell line and U937 hematopoietic cell line were described.

Thiosemicarbazones derived from 1-indanones as new anti-*Trypanosoma cruzi* agents

pp 6818–6826

María E. Caputto, Lucas E. Fabian, Diego Benítez, Alicia Merlino, Natalia Ríos, Hugo Cerecetto, Graciela Y. Moltrasio, Albertina G. Moglioni, Mercedes González*, Liliana M. Finkielstein*



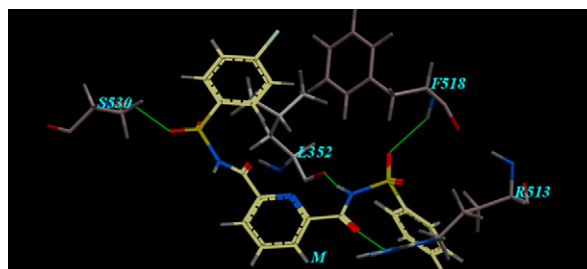
Total 24 thiosemicarbazones were synthesized and screened for in vitro tripanosomicidal activity against the epimastigote form of *Trypanosoma cruzi*. Most of the evaluated compounds displayed remarkable activity with excellent selectivity indexes. Two of these derivatives inhibited cruzipain at the dose assayed. The mode of action was explained using molecular docking studies.



Design, synthesis and biological evaluation of pyridine acyl sulfonamide derivatives as novel COX-2 inhibitors

pp 6827–6832

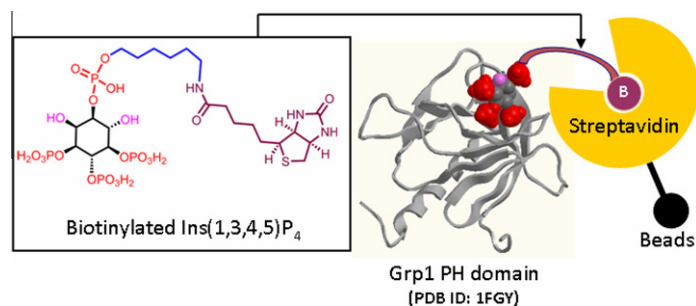
Xiang Lu, Hui Zhang, Xi Li, Guo Chen, Qing-Shan Li, Yin Luo, Ban-Feng Ruan, Xian-Wei Chen, Hai-Liang Zhu*



Design and synthesis of biotinylated inositol 1,3,4,5-tetrakisphosphate targeting Grp1 pleckstrin homology domain

pp 6833–6841

Kensaku Anraku, Teruhiko Inoue, Kenji Sugimoto, Kota Kudo, Yoshinari Okamoto, Takashi Morii, Yasuo Mori, Masami Otsuka*

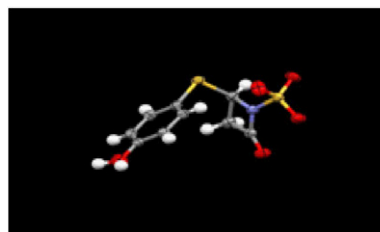
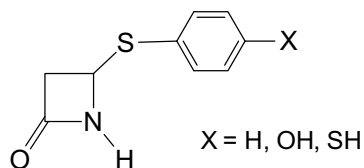


C4-Alkylthiols with activity against *Moraxella catarrhalis* and *Mycobacterium tuberculosis*

pp 6842–6852

Maya B. Kostova, Carey J. Myers, Tim N. Beck, Balbina J. Plotkin, Jacalyn M. Green, Helena I. M. Boshoff, Clifton E. Barry III, Jeffrey R. Deschamps, Monika I. Konaklieva*

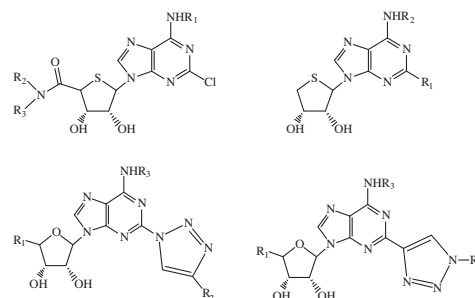
C4 Phenylthio- β -lactams active against *Moraxella catarrhalis* and *Mycobacterium tuberculosis*.



Affinity prediction on A₃ adenosine receptor antagonists: The chemometric approach

Feng Luan, André Melo, Fernanda Borges, M. Natália D. S. Cordeiro*

pp 6853–6859



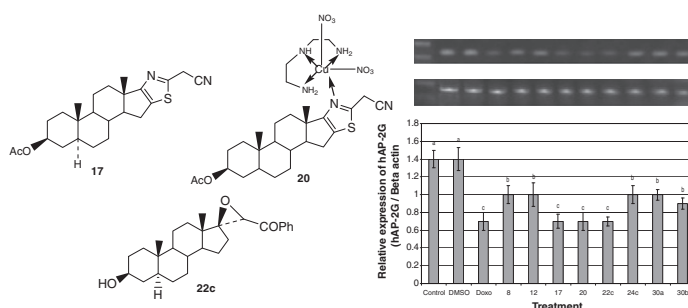
A QSAR method based on 3D-MoRSE descriptors provided a highly robust and predictive model for the binding affinity of a series of potent and selective antagonists of the human A₃ adenosine receptor.



Cytotoxicity and gene expression profiles of novel synthesized steroid derivatives as chemotherapeutic anti-breast cancer agents

pp 6860–6872

Gamal A. Elmegeed*, Wagdy K. B. Khalil, Rafat M. Mohareb, Hanaa H. Ahmed, Mervat M. Abd-Elhalim, Ghada H. Elsayed

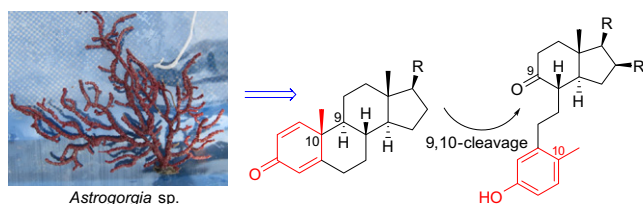


The present study aimed to synthesize and evaluate new potential chemotherapeutic anti-breast cancer agents. Thiazolo-androstane **17** (IC_{50} = 2.5 μ M) exhibited more inhibitory influence on MCF-7 growth than doxorubicin (IC_{50} = 4.5 μ M) after 48 h incubation. All the tested steroid derivatives exhibited significant depletion in gene expression of breast cancer related genes. Noteworthy, compounds **17**, **20** and **22c** showed the most pronounced effect in this respect.

9,10-Secosteroids, protein kinase inhibitors from the Chinese gorgonian *Astrogorgia* sp.

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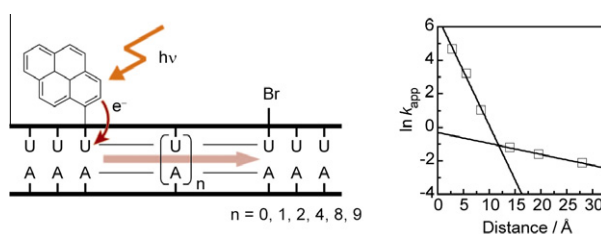
Daowan Lai, Shanjiang Yu, Leen van Ofwegen, Frank Totzke, Peter Proksch, Wenhan Lin*



Electron transfer through RNA: Chemical probing of dual distance dependence

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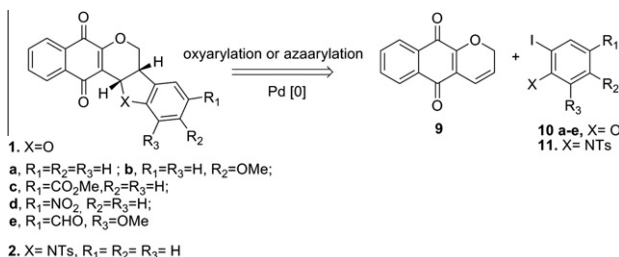
Tadao Takada, Yumiko Otsuka, Mitsunobu Nakamura, Kazushige Yamana*



Pterocarpanquinones, aza-pterocarpanquinone and derivatives: Synthesis, antineoplastic activity on human malignant cell lines and antileishmanial activity on *Leishmania amazonensis*

pp 6885–6891

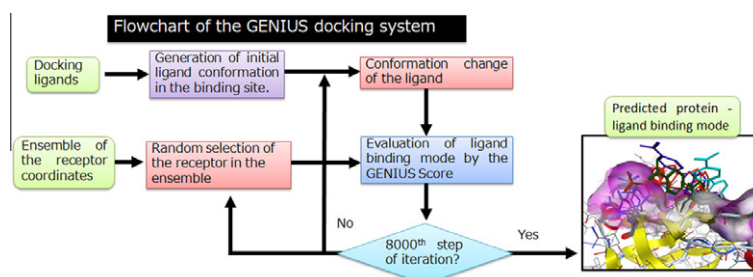
Camilla D. Buarque, Gardenia C. G. Militão, Daisy J. B. Lima, Leticia V. Costa-Lotufo, Cláudia Pessoa, Manoel Odorico de Moraes, Edéio Ferreira Cunha-Junior, Eduardo Caio Torres-Santos, Chaquip D. Netto, Paulo R. R. Costa*



A new method for induced fit docking (GENIUS) and its application to virtual screening of novel HCV NS3-4A protease inhibitors

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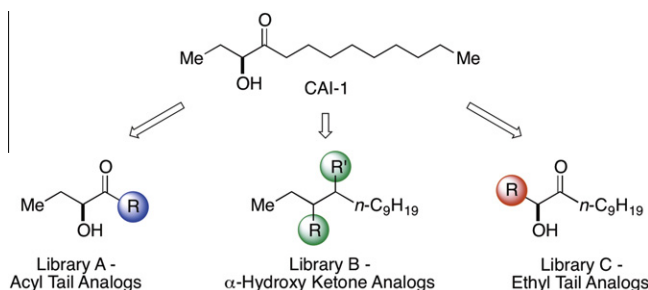
Daisuke Takaya, Atsuya Yamashita, Kazue Kamijo, Junko Gomi, Masahiko Ito, Shinya Maekawa, Nobuyuki Enomoto, Naoya Sakamoto, Yoshiaki Watanabe, Ryoichi Arai, Hideaki Umeyama, Teruki Honma, Takehisa Matsumoto, Shigeyuki Yokoyama*



Small molecule probes of the receptor binding site in the *Vibrio cholerae* CAI-1 quorum sensing circuit

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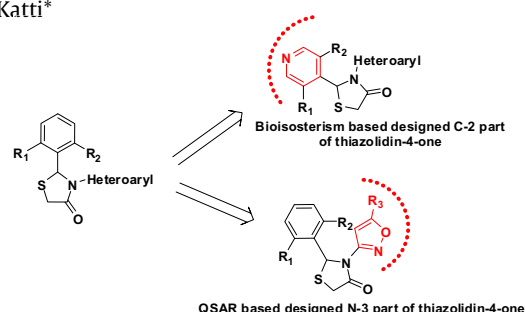
Megan E. Bolitho, Lark J. Perez, Matthew J. Koch, Wai-Leung Ng, Bonnie L. Bassler, Martin F. Semmelhack*



Lead optimization at C-2 and N-3 positions of thiazolidin-4-ones as HIV-1 non-nucleoside reverse transcriptase inhibitors

pp 6919–6926

Vanangamudi Murugesan, Vinay S. Tiwari, Reshu Saxena, Rajkamal Tripathi, Ramesh Paranjape, Smita Kulkarni, Nandini Makwana, Rahul Suryawanshi, Seturam B. Katti*



On the basis of QSAR-based drug design strategy and bioisosteric principle, a series of novel thiazolidin-4-ones bearing different aryl/heteroaryl moieties at position C-2 and N-3 of thiazolidin-4-one were synthesized and evaluated as potent inhibitors of human immunodeficiency virus type-1 (HIV-1).

Synthesis and anticonvulsant activity of *trans*- and *cis*-2-(2,6-dimethylphenoxy)-*N*-(2- or 4-hydroxycyclohexyl)acetamides and their amine analogs

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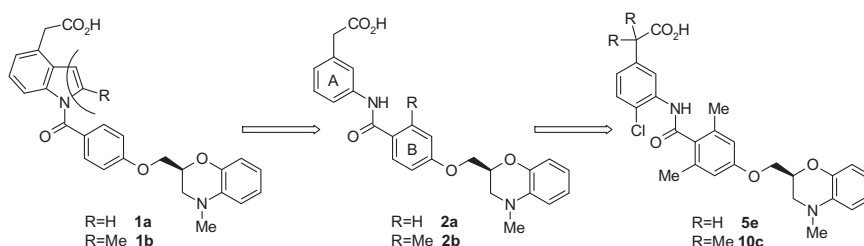
Elżbieta Pękala, Anna M. Waszkielewicz*, Edward Szneler, Maria Walczak, Henryk Marona



Discovery of new orally active prostaglandin D₂ receptor antagonists

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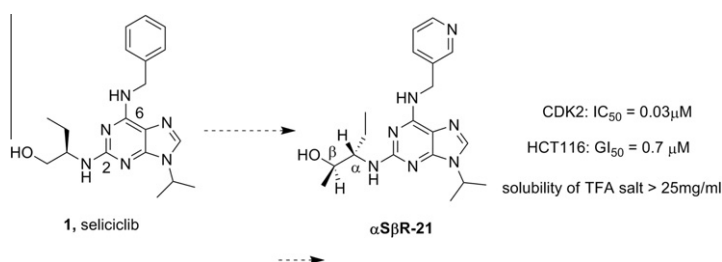
Maki Iwahashi*, Atsushi Naganawa, Atsushi Kinoshita, Atsushi Shimabukuro, Toshihiko Nishiyama, Seiji Ogawa, Yoko Matsunaga, Kohki Tsukamoto, Yutaka Okada, Ryoji Matsumoto, Fumio Nambu, Rie Oumi, Yoshihiko Odagaki, Jun Katagi, Koji Yano, Kousuke Tani, Hisao Nakai, Masaaki Toda

To identify an orally available drug candidate, a series of 3-benzoylaminophenylacetic acids were synthesized and evaluated as prostaglandin D₂ (PGD₂) receptor antagonists.

Design, synthesis and biological evaluation of 6-pyridylmethylaminopurines as CDK inhibitors

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Stuart C. Wilson, Butrus Atrash, Clare Barlow, Susan Eccles, Peter M. Fischer, Angela Hayes, Lloyd Kelland, Wayne Jackson, Michael Jarman, Amin Mirza, Javier Moreno, Bernard P. Nutley, Florence I. Raynaud, Peter Sheldrake, Mike Walton, Robert Westwood, Steven Whittaker, Paul Workman, Edward McDonald*



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*Corresponding author

* Supplementary data available via SciVerse ScienceDirect**COVER**

The molecular structures and information flow depicted on the cover illustrates how current research is “Harnessing the Biosynthetic Capacity of Marine-Derived Organisms.” [Carter, G.T.; Crews, P. *Bioorg. Med. Chem.* **2011**, *19*, 9599.]

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