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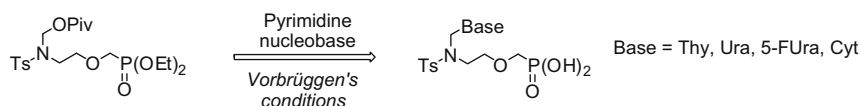
Bioorganic & Medicinal Chemistry Vol. 17, No. 11, 2009

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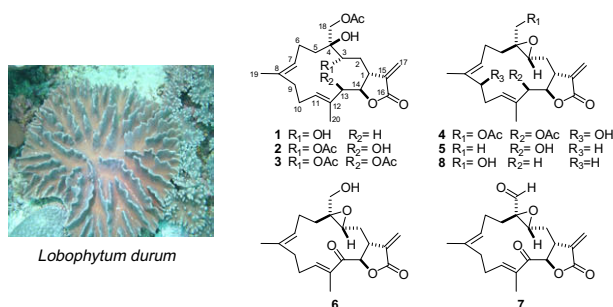
Synthesis and antiviral activity evaluation of acyclic 2'-azanucleosides bearing a phosphonmethoxy function in the side chain pp 3756–3762

Mariola Koszytkowska-Stawińska*, Erik De Clercq, Jan Balzarini



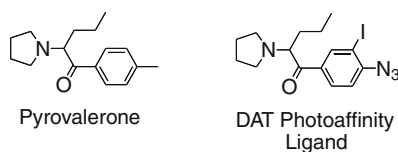
Anti-inflammatory cembranolides from the soft coral *Lobophytum durum* pp 3763–3769

Shi-Yie Cheng, Zhi-Hong Wen, Shang-Kwei Wang, Shu-Fen Chiou, Chi-Hsin Hsu, Chang-Feng Dai, Chang-Yih Duh*



A novel photoaffinity ligand for the dopamine transporter based on pyrovalerone pp 3770–3774

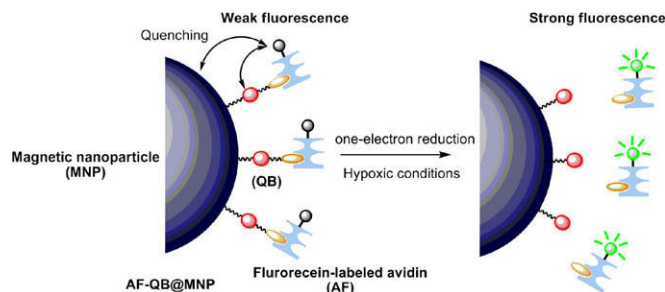
David J. Lapinsky*, Shaili Aggarwal, Yurong Huang, Christopher K. Surratt, John R. Lever, James D. Foster, Roxanne A. Vaughan



Preparation and fluorescence properties of fluorophore-labeled avidin–biotin system immobilized on Fe₃O₄ nanoparticles through functional indolequinone linker

pp 3775–3781

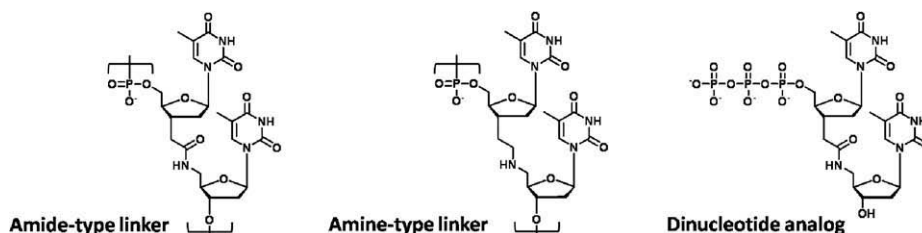
Nao Hirata, Kazuhito Tanabe*, Asako Narita, Kazuo Tanaka, Kensuke Naka, Yoshiki Chujo, Sei-ichi Nishimoto*



Transcription and reverse transcription of artificial nucleic acids involving backbone modification by template-directed DNA polymerase reactions

pp 3782–3788

Masayasu Kuwahara*, Hidetoshi Takeshima, Jun-ichi Nagashima, Satoshi Minezaki, Hiroaki Ozaki, Hiroaki Sawai



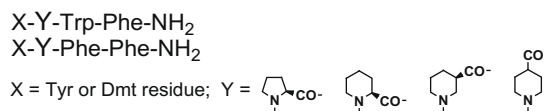
Oligodeoxyribonucleotides (ODN) where the phosphodiester linkage had been replaced with an amide-type linker or an amine-type linker were synthesized to investigate the effect of these backbone modifications on polymerase reactions. A triphosphate analogue of thymidine dinucleotide with the amide-type linker was synthesized and enzymatic insertion into ODN was attempted.



Biological activity of endomorphin and [Dmt¹]endomorphin analogs with six-membered proline surrogates in position 2

pp 3789–3794

Renata Perlikowska, Katarzyna Gach, Jakub Fichna, Geza Toth, Bogdan Walkowiak, Jean-Claude do-Rego*, Anna Janecka*

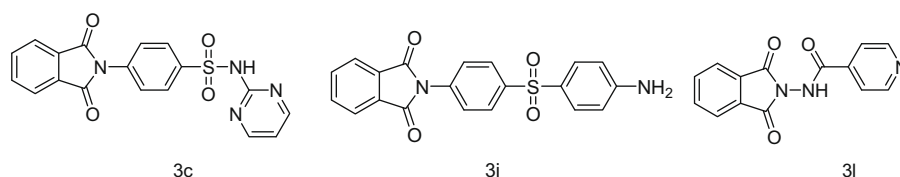


Biological activity of new endomorphin analogs is reported.

Synthesis and in vitro anti *Mycobacterium tuberculosis* activity of a series of phthalimide derivatives

pp 3795–3799

Jean L. Santos*, Paulo R. Yamasaki, Chung Man Chin, Célio H. Takashi, Fernando R. Pavan, Clarice Q. F. Leite

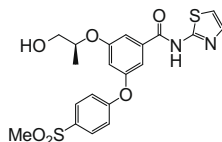


A series of phthalimide derivatives were evaluated against *Mycobacterium tuberculosis* H₃₇Rv and the compounds **3c**, **3i**, and **3l** have the minimum inhibitory concentrations (MICs) of 3.9, 7.8, and 5.0 µg/mL.

Structure–activity relationships of 3,5-disubstituted benzamides as glucokinase activators with potent in vivo efficacy

pp 3800–3809

Tomoharu Iino*, Noriaki Hashimoto, Kaori Sasaki, Sumika Ohyama, Riki Yoshimoto, Hideka Hosaka, Takuro Hasegawa, Masato Chiba, Yasufumi Nagata, Jun-ichi Eiki, Teruyuki Nishimura

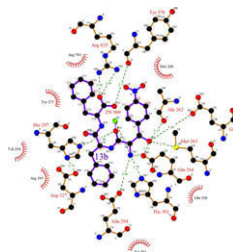


The structure–activity relationships of 3,5-disubstituted benzamide glucokinase activators are described.

**Design and synthesis of novel chloramphenicol amine derivatives as potent aminopeptidase N (APN/CD13) inhibitors**

pp 3810–3817

Kanghui Yang, Qiang Wang, Li Su, Hao Fang*, Xuejian Wang, Jianzhi Gong, Binghe Wang, Wenfang Xu*

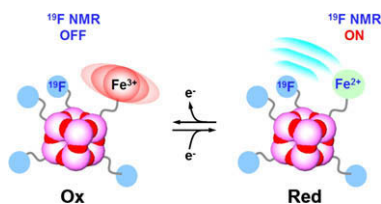


The compound **13b** was built and docked into the active site of APN (PDB code: 2DQM) using SYBYL7.0. The docking result of **13b** is showed by Ligplot.

Reversible signal regulation system of ^{19}F NMR by redox reactions using a metal complex as a switching module

pp 3818–3823

Kazuo Tanaka, Narufumi Kitamura, Yuichi Takahashi, Yoshiki Chujo*

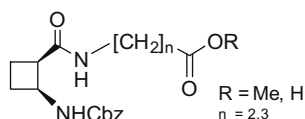


We present the reversible signal regulation system of ^{19}F NMR using the transition metal complex as a switching module. The signal intensities of ^{19}F NMR of the water-soluble fluorinated dendrimers containing ferrocene were reversibly modulated by the oxidation and reduction to the ferrocene moiety.

Cyclobutane-containing peptides: Evaluation as novel metallo-carboxypeptidase inhibitors and modelling of their mode of action

pp 3824–3828

Daniel Fernández, Elisabeth Torres, Francesc X. Avilés, Rosa M. Ortuno*, Josep Vendrell*

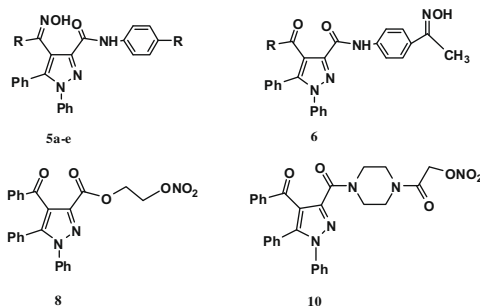


Among other peptides evaluated, these compounds were active and selective. Aromatic stacking plays an important role in the binding to the active site of the target enzymes.

Design, synthesis and biological investigation of certain pyrazole-3-carboxylic acid derivatives as novel carriers for nitric oxide

pp 3829–3837

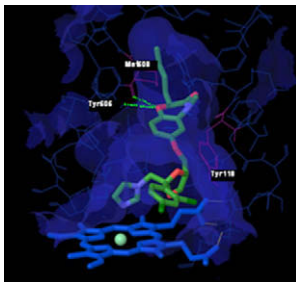
El-Shimaa M. N. Abdel-Hafez, Gamal El-Din A. A. Abu-Rahma*, Mohamed Abdel-Aziz, Mohamed F. Radwan, Hassan H. Farag



Bulky 1,4-benzoxazine derivatives with antifungal activity

pp 3838–3846

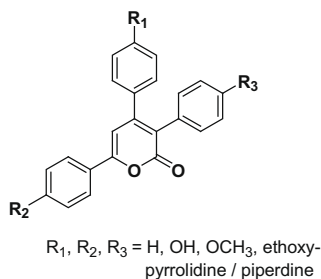
Renata Fringuelli*, Nicola Giacchè, Lara Milanese, Elio Cenci, Antonio Macchiarulo, Anna Vecchiarelli, Gabriele Costantino, Fausto Schiaffella



Synthesis and biological evaluation of 3,4,6-triaryl-2-pyranones as a potential new class of anti-breast cancer agents

pp 3847–3856

Ravi Shankar, Bandana Chakravarti, Uma Sharan Singh, Mohd. Imran Ansari, Shreekanth Deshpande, Shailendra Kumar Dhar Dwivedi, Hemant Kumar Bid, Rituraj Konwar, Geetika Kharkwal, Vishal Chandra, Anila Dwivedi, K. Hajela*

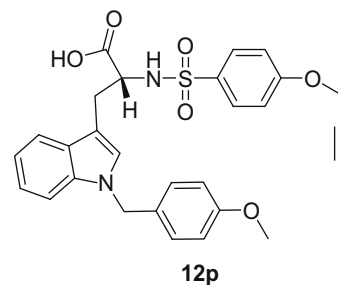


Synthesis and activity of tryptophan sulfonamide derivatives as novel non-hydroxamate TNF-α converting enzyme (TACE) inhibitors

pp 3857–3865

Kaapjoo Park*, Ariamala Gopalsamy, Alexis Aplasca, John W. Ellingboe, Weixin Xu, Yuhua Zhang, Jeremy I. Levin

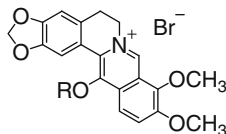
A novel series of non-hydroxamate tryptophan sulfonamide derivatives containing a butynyloxy P1' moiety was identified as inhibitors of TNF-α Converting Enzyme (TACE). The structure activity relationship of the series was examined via substitution on the tryptophan indole ring. Of the compounds investigated, 2-(4-(but-2-ynyloxy)phenylsulfonamido)-3-(1-(4-methoxybenzyl)-1H-indol-3-yl)propanoic acid (**12p**) has the best in vitro potency against isolated TACE enzyme with an IC₅₀ of 80 nM. Compound **12p** also shows good selectivity over MMP-1, -13, -14.



Antibacterial activity of berberine-NorA pump inhibitor hybrids with a methylene ether linking group

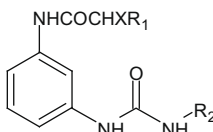
pp 3866–3872

Siritron Samosorn^{*}, Bongkot Tanwirat, Nussara Muhamad, Gabriele Casadei, Danuta Tomkiewicz, Kim Lewis, Apichart Suksamrarn, Therdsak Prammananan, Karina C. Gornall, Jennifer L. Beck, John B. Bremner

**Synthesis and activity evaluation of phenylurea derivatives as potent antitumor agents**

pp 3873–3878

Dan-Qing Song, Na-Na Du, Yue-Ming Wang, Wei-Ying He, En-Zhu Jiang, Shi-Xiang Cheng, Yan-Xiang Wang, Ying-Hong Li, Yu-Ping Wang, Xin Li, Jian-Dong Jiang^{*}



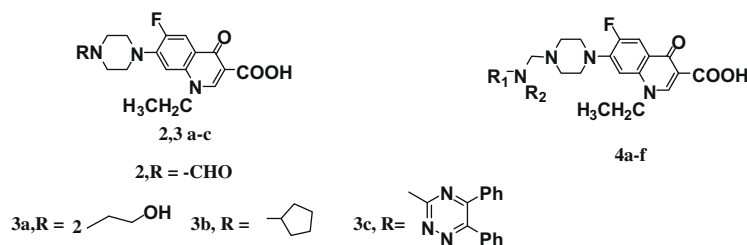
$R_2 = \text{CH}_2\text{CH}_2\text{Cl}, \text{COCH}_2\text{CH}_2\text{Cl}, \text{COCH}_3, \text{CHO}, \text{COCH}_2\text{Br}, \text{COCHBrCH}_3, \text{phenyl},$
 $3,4,5\text{-trimethoxyphenyl}; R_1 = \text{H}, \text{CH}_3; X = \text{Br}, \text{I}$

The phenylurea derivatives were designed, synthesized and evaluated for the anticancer activities as a class of β -tubulin ligands. However, they change the mode of action from tubulin-based mechanism to the one different from their parent compounds.

Design, synthesis, antibacterial activity and physicochemical parameters of novel N-4-piperazinyl derivatives of norfloxacin

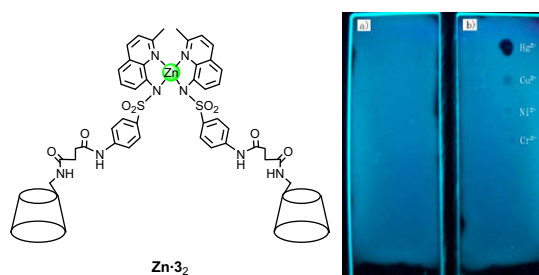
pp 3879–3886

Gamal El-Din A. A. Abu-Rahma^{*}, Hatem. A. Sarhan, Gamal F. M. Gad

**Convenient and highly effective fluorescence sensing for Hg^{2+} in aqueous solution and thin film**

pp 3887–3891

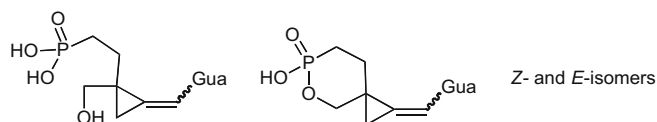
Yu Liu^{*}, Miao Yu, Yong Chen, Ning Zhang



Phosphonate analogues of cyclopropavir phosphates and their *E*-isomers. Synthesis and antiviral activity

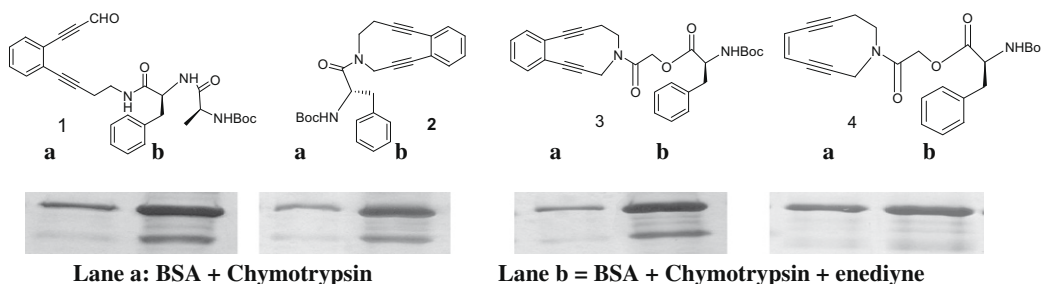
pp 3892–3899

Santosh B. Mhaske, Bashar Ksebati, Mark N. Prichard, John C. Drach, Jiri Zemlicka*

**Design and synthesis of enediynes–peptide conjugates and their inhibiting activity against chymotrypsin**

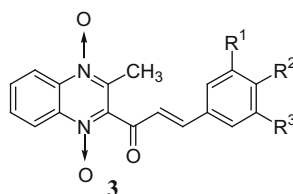
pp 3900–3908

Sansa Dutta, Amit Basak*, Swagata Dasgupta*

**2-(3-Aryl-2-propenoyl)-3-methylquinoxaline-1,4-dioxides: A novel cluster of tumor-specific cytotoxins which reverse multidrug resistance**

pp 3909–3915

Umashankar Das*, Hari N. Pati, Atulya K. Panda, Erik De Clercq, Jan Balzarini, Joseph Molnár, Zoltán Baráth, Imre Ocsóvski, Masami Kawase, Li Zhou, Hiroshi Sakagami, Jonathan R. Dimmock*

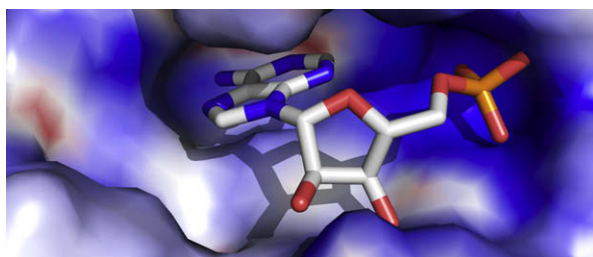


The quinoxaline derivatives **3** possess one or more of the following features, namely antiproliferative activities, selective cytotoxicity to neoplasms than normal cells and MDR-revertant properties.

A library of novel allosteric inhibitors against fructose 1,6-bisphosphatase

pp 3916–3922

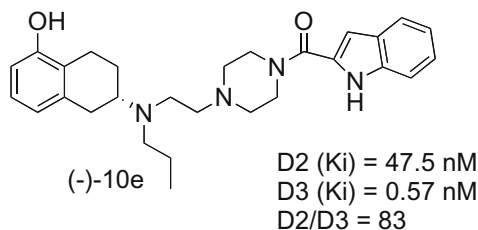
Sabrina Heng, Kimberly R. Gryncel, Evan R. Kantrowitz*



Investigation of various N-heterocyclic substituted piperazine versions of 5/7-[[2-(4-aryl-piperazin-1-yl)-ethyl]-propyl-amino]-5,6,7,8-tetrahydro-naphthalen-2-ol: Effect on affinity and selectivity for dopamine D3 receptor

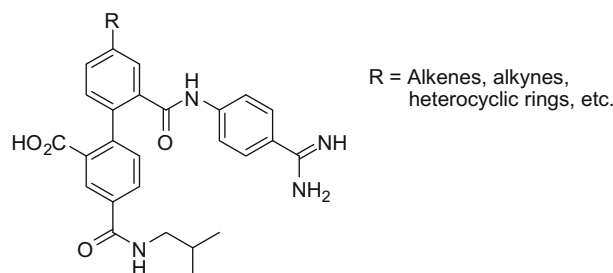
pp 3923–3933

Dennis A. Brown, Manoj Mishra, Suhong Zhang, Swati Biswas, Ingrid Parrington, Tamara Antonio, Maarten E. A. Reith, Alok K. Dutta *

**Design, parallel synthesis, and crystal structures of biphenyl antithrombotics as selective inhibitors of tissue factor FVIIa complex. Part 1: Exploration of S2 pocket pharmacophores**

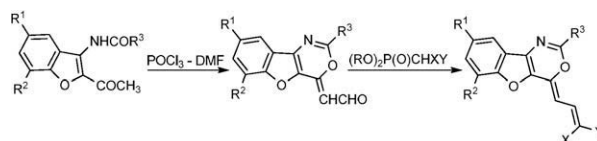
pp 3934–3958

Pravin L. Kotian *, Raman Krishnan, Scott Rowland, Yahya El-Kattan, Surendra K. Saini, Ramanda Upshaw, Shanta Bantia, Shane Arnold, Y. Sudhakar Babu *, Pooran Chand *

**Preparation of novel (Z)-4-ylidenebenzo[b]furo[3,2-d][1,3]oxazines and their biological activity**

pp 3959–3967

Yukako Tabuchi, Yuko Ando, Hidemi Kanemura, Ikuo Kawasaki, Takahiro Ohishi, Masao Koida, Ryo Fukuyama, Hiromichi Nakamuta, Shunsaku Ohta, Kiyoharu Nishide *, Yoshitaka Ohishi *



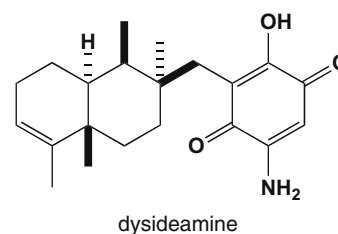
Preparation of novel (Z)-4-ylidenebenzo[b]furo[3,2-d][1,3]oxazines and their biological activities such as anti-osteoclastic bone resorption activity, antagonistic activity of the cysLT1 receptor and growth inhibitory activity for MIA PaCa-2 and MCF-7 are described.

**Dysideamine, a new sesquiterpene aminoquinone, protects hippocampal neuronal cells against iodoacetic acid-induced cell death**

pp 3968–3972

Hideaki Suna, Masayoshi Arai, Yoshie Tsubotani, Asami Hayashi, Andi Setiawan, Motomasa Kobayashi *

Dysideamine (**1**), a new sesquiterpene aminoquinone, was isolated from Indonesian marine sponge of *Dysidea* sp. 05C33. Compound **1** showed neuroprotective effect against iodoacetic acid (IAA)-induced cell death in mouse HT22 hippocampal cells and induced neurite outgrowth against mouse neuroblastoma Neuro 2A cells.

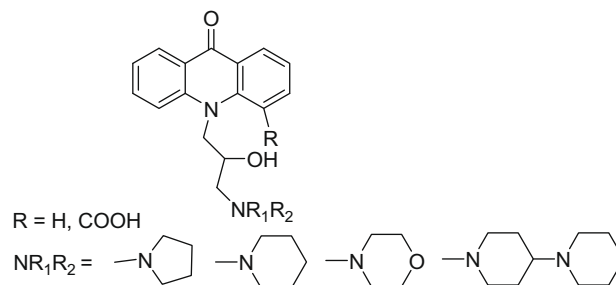


Design, synthesis and evaluations of acridone derivatives using *Candida albicans*—Search for MDR modulators led to the identification of an anti-candidiasis agent

pp 3973–3979

Palwinder Singh*, Jatinder Kaur, Bhawna Yadav, Sneha Sudha Komath*

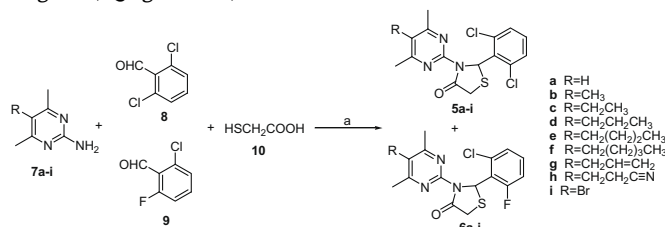
Acridone with piperidino-piperidine at the end of N-10 chain and COOH group at C-4 results in cell wall rupturing of *Candida albicans* and may be a suitable candidate for anti-candidiasis therapy.



Design, microwave-assisted synthesis and HIV-RT inhibitory activity of 2-(2,6-dihalophenyl)-3-(4,6-dimethyl-5-(un)substituted-pyrimidin-2-yl)thiazolidin-4-ones

pp 3980–3986

Hua Chen*, Jie Bai, Lingling Jiao, Zaihong Guo, Qingmei Yin, Xiaoliu Li*

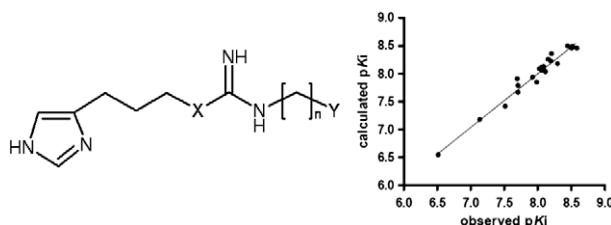


A series of novel thiazolidin-4-ones bearing a hydrophobic substituent at 5-position on the 4,6-dimethyl-pyrimidine ring at N-3 (**5c-i** and **6c-i**) were designed on the prediction of QSAR studies, synthesized in good yields of 60.1–85.3% by improved microwave-assisted one-pot protocol with the combination of using dicyclohexylcarbodiimide (DCC), and evaluated as HIV-1 reverse transcriptases inhibitors.

Clobenpropit analogs as dual activity ligands for the histamine H₃ and H₄ receptors: Synthesis, pharmacological evaluation, and cross-target QSAR studies

pp 3987-3994

Herman D. Lim, Enade P. Istyastono, Andrea van de Stolpe, Giuseppe Romeo, Silvia Gobbi, Marjo Schepers, Roger Lahaye, Wiro M. B. P. Menge, Obbe P. Zuiderveld, Aldo Jongejan, Rogier A. Smits, Remko A. Bakker, Eric E. J. Haaksma, Rob Leurs, Iwan J. P. de Esch *



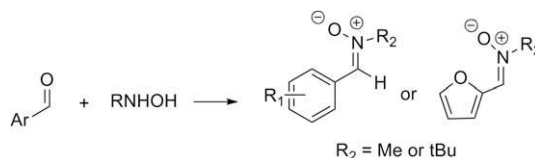
Some clobenpropit analogs were synthesized and pharmacologically characterized as dual activity ligands for the histamine H₃ and H₄ receptors. QSAR models were generated to explain the important properties for the affinities.



N-tert-Butyl and N-methyl nitrones derived from aromatic aldehydes inhibit macromolecular permeability increase induced by ischemia/reperfusion in hamsters

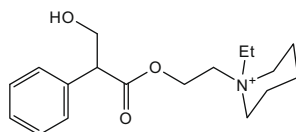
pp 3995–3998

Ayres G. Dias, Carlos E. V. Santos, Fatima Z. G. A. Cyrino, Eliete Bouskela*, Paulo R. R. Costa*



3D-QSAR studies of 2,2-diphenylpropionates to aid discovery of novel potent muscarinic antagonists**pp 3999–4012**

Apurba K. Bhattacharjee*, Jonathan A. Gordon, Elizabeth Marek, Amy Campbell, Richard K. Gordon

(K_i = 2.0 nM, Atropine = 4.4 nM)

We correlated experimental and calculated molecular properties of 15 α -substituted 2,2-diphenylpropionate antimuscarinics using quantum chemical and pharmacophore generation methods and used the model to identify new antimuscarinic in our in-house database. Six new compounds not previously reported as antimuscarinics were characterized. The graphic shows the most potent compound, twofold greater than atropine, which was derived by our pharmacophore model and yet is not a 2,2-diphenylpropionate.

**OTHER CONTENTS****Instructions to contributors****p I**

*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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