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Bioorganic & Medicinal Chemistry Volume 19, Issue 9, 2011

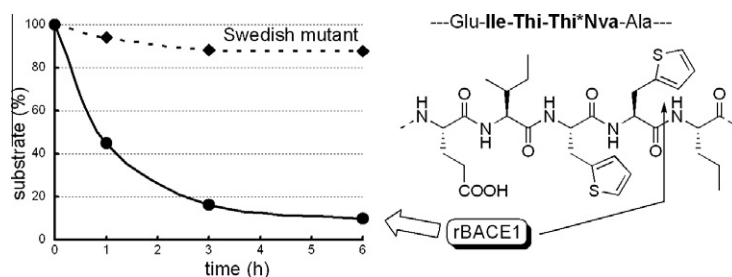
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Evaluation of superior BACE1 cleavage sequences containing unnatural amino acids

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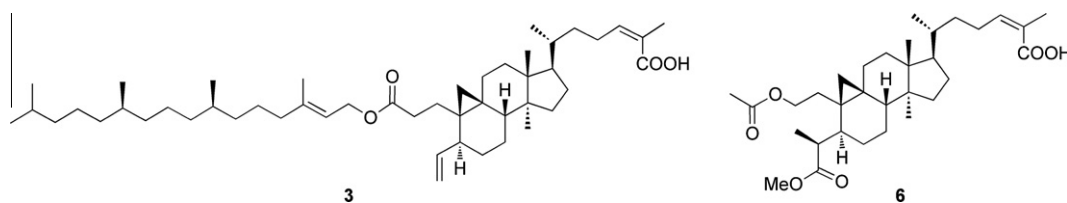
Taeko Kakizawa, Akira Sanjoh, Akane Kobayashi, Yasunao Hattori, Kenta Teruya, Kenichi Akaji*



New 29-nor-cycloartanes with a 3,4-*seco*- and a novel 2,3-*seco*-structure from the leaves of *Sinocalycanthus chinensis*

pp 2790–2796

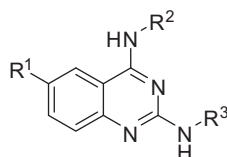
Yoshiki Kashiwada*, Kazuya Nishimura, Shin-ichiro Kurimoto, Yoshihisa Takaishi



Synthesis and biological evaluation of novel quinazoline-derived human Pin1 inhibitors

pp 2797–2807

Lina Zhu, Jing Jin, Chang Liu, Chongjing Zhang, Yan Sun, Yanshen Guo, Decai Fu, Xiaoguang Chen, Bailing Xu*

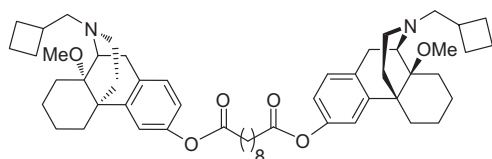
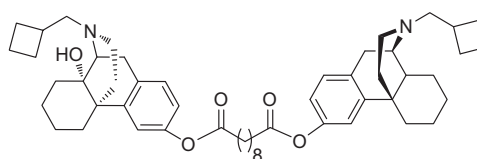


A series of novel 2,4-disubstituted quinazoline derivatives were prepared and their inhibitory activities on hPin1 were evaluated. Of all the synthesized compounds, eight compounds displayed inhibitory activities with IC_{50} value at the level of 10^{-6} mol/L. Preliminary structure–activity relationships were analyzed in details and the binding mode of the titled compounds was predicted using FlexX algorithm.

Synthesis and binding affinity of novel mono- and bivalent morphinan ligands for κ , μ , and δ opioid receptors

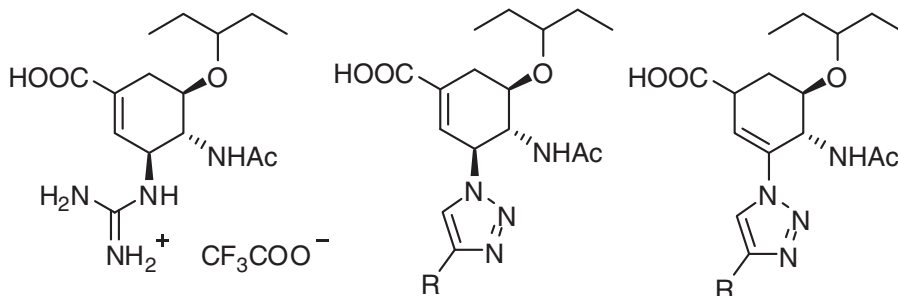
pp 2808–2816

Bin Zhang, Tangzhi Zhang, Anna W. Sromek, Thomas Scrimale, Jean M. Bidlack, John L. Neumeyer*

**9b (MCL-692)**
 $\mu = 0.26 \text{ nM}$
 $\kappa = 0.37 \text{ nM}$
 $\delta = 13 \text{ nM}$
**15b (MCL-695)**
 $\mu = 0.089 \text{ nM}$
 $\kappa = 0.073 \text{ nM}$
 $\delta = 8.0 \text{ nM}$
Inhibitor selectivity of a new class of oseltamivir analogs against viral neuraminidase over human neuraminidase enzymes

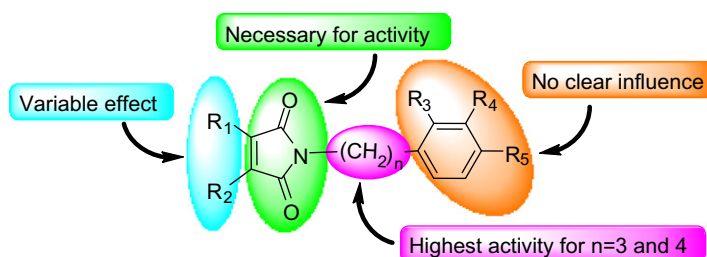
pp 2817–2822

Amgad Albohy, Sankar Mohan, Ruixiang Blake Zheng, B. Mario Pinto, Christopher W. Cairo*

**Antifungal, cytotoxic and SAR studies of a series of *N*-alkyl, *N*-aryl and *N*-alkylphenyl-1,4-pyrrolediones and related compounds**

pp 2823–2834

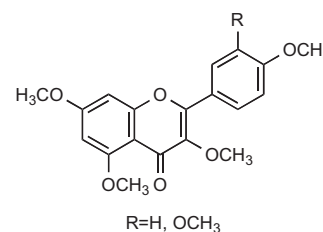
M. Sortino, F. Garibotto, V. Cechinel Filho, M. Gupta, R. Enriz, S. Zacchino*

**Structural requirements of flavonoids for the adipogenesis of 3T3-L1 cells**

pp 2835–2841

Hisashi Matsuda, Yuichiro Kogami, Seikou Nakamura, Tomomi Sugiyama, Tsubasa Ueno, Masayuki Yoshikawa*

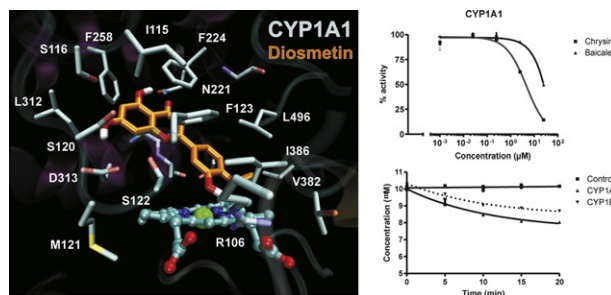
Among the 44 flavonoids, 3,4',7-trimethylkaempferol, tetramethylkaempferol, and pentamethylquercetin concentration-dependently enhanced the adipogenesis of 3T3-L1 cells. With regard to structural requirements of flavonoids for the activity, it was found that: (1) most flavonoids having hydroxy groups lacked the effects; (2) flavonols with methoxy groups showed stronger effects particularly those with a methoxy group at the 3-position; (3) a methoxy group of flavonols at the B ring was also important. Tetramethylkaempferol and pentamethylquercetin significantly increased the amount of adiponectin released into the medium and the uptake of 2-deoxyglucose into the cells. Furthermore, both compounds also increased the mRNA levels of GLUT4, aP2, PPAR γ 2, and C/EBPs, although they did not activate PPAR γ directly in a nuclear receptor cofactor assay.



Comparative CYP1A1 and CYP1B1 substrate and inhibitor profile of dietary flavonoids

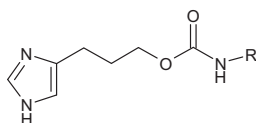
pp 2842–2849

Vasilis P. Androutsopoulos*, Athanasios Papakyriakou, Dionisios Vourloumis, Demetrios A. Spandidos

**N-Alkenyl and cycloalkyl carbamates as dual acting histamine H₃ and H₄ receptor ligands**

pp 2850–2858

Małgorzata Więcek, Tim Kottke, Xavier Ligneau, Walter Schunack, Roland Seifert, Holger Stark, Jadwiga Handzlik, Katarzyna Kieć-Kononowicz*

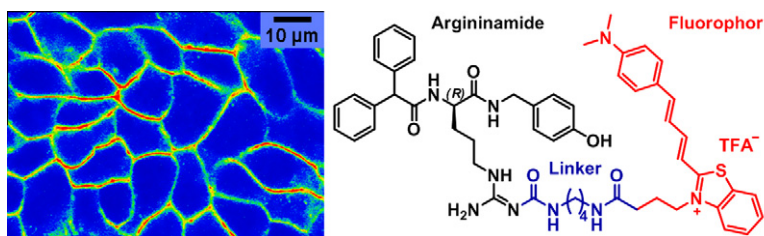


Two series of 3-(1H-imidazol-4-yl)propyl carbamates: a series of unsaturated alkyl derivatives and a series possessing a cycloalkyl group different distances to the carbamate moiety were prepared and tested for their affinities at human histamine H₃ and H₄ receptors. To expand pharmacological profile, compounds were also tested for their H₃ receptor antagonist activity on guinea pig ileum and in vivo after oral administration to mice. Tested compounds exhibited good affinity for the hH₃R and moderate to weak affinity for the hH₄R.

**Red-fluorescent argininamide-type NPY Y₁ receptor antagonists as pharmacological tools**

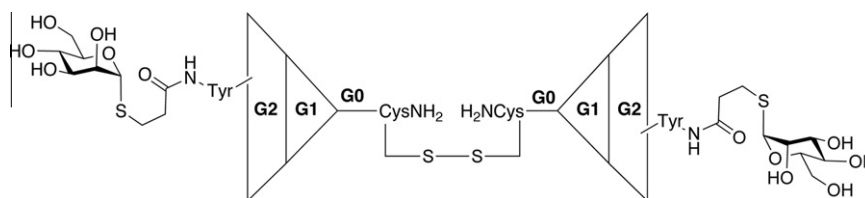
pp 2859–2878

Max Keller, Daniela Erdmann, Nathalie Pop, Nikola Pluym, Shangjun Teng, Günther Bernhardt, Armin Buschauer*

**Synthesis of glycopeptide dendrimers, dimerization and affinity for Concanavalin A**

pp 2879–2887

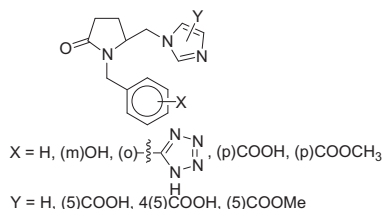
Ronan Euzen*, Jean-Louis Reymond



Synthesis, in silico docking experiments of new 2-pyrrolidinone derivatives and study of their anti-inflammatory activity

pp 2888–2902

Panagiota Moutevelis-Minakakis*, Eleni Papavassilopoulou, George Michas, Kalliopi Georgikopoulou, Maria-Eleni Ragoussi, Niki Neophytou, Panagiotis Zoumpoulakis, Thomas Mavromoustakos, Dimitra Hadjipavlou-Litina

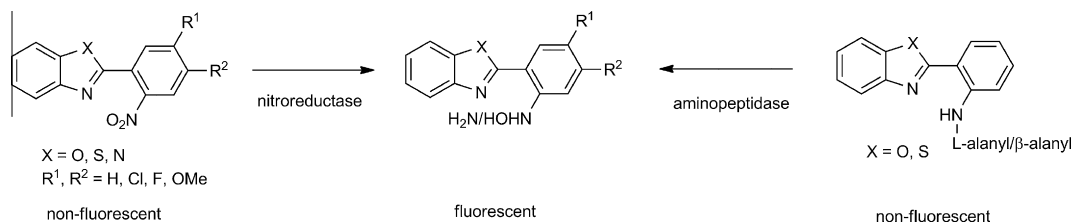


General structure of the target biologically evaluated synthetic compounds.

2-Arylbenzothiazole, benzoxazole and benzimidazole derivatives as fluorogenic substrates for the detection of nitroreductase and aminopeptidase activity in clinically important bacteria

pp 2903–2910

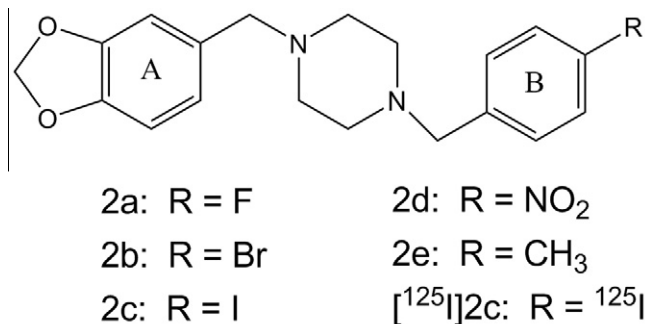
Marie Cellier, Olivier J. Fabrega, Elizabeth Fazackerley, Arthur L. James, Sylvain Orenge, John D. Perry, Vindhya L. Salwatura, Stephen P. Stanforth*



Synthesis and biological evaluation of novel 4-benzylpiperazine ligands for sigma-1 receptor imaging

pp 2911–2917

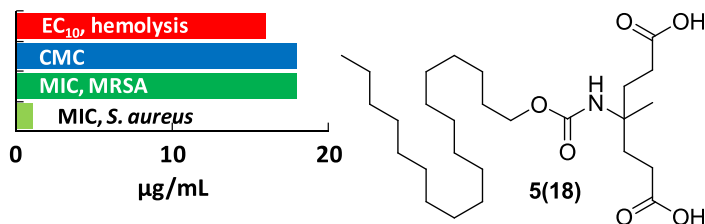
Zi-Jing Li, Hui-Ying Ren, Meng-Chao Cui, Winnie Deuther-Conrad, Rui-Kun Tang, Jörg Steinbach, Peter Brust, Bo-Li Liu, Hong-Mei Jia*



Comparing micellar, hemolytic, and antibacterial properties of di- and tricarboxyl dendritic amphiphiles

pp 2918–2926

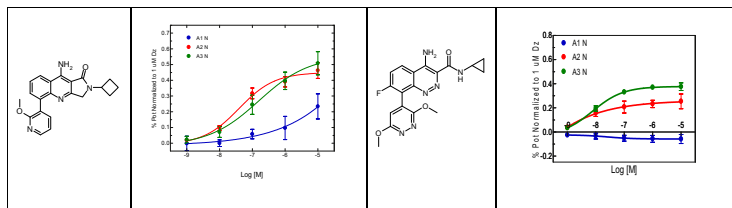
Bhadreshkumar B. Maisuria, Marcelo L. Actis, Shauntrece N. Hardrict, Joseph O. Falkinham III, Michael F. Cole, Ronald L. Cihlar, Stephen M. Peters, Richard V. Macri, Eko W. Sugandhi, André A. Williams, Michael A. Poppe, Alan R. Esker, Richard D. Gandour*



Development and SAR of functionally selective allosteric modulators of GABA_A receptors

pp 2927–2938

Cristobal Alhambra, Chris Becker, Timothy Blake, Amy (Hui-Fang) Chang, James R. Damewood Jr., Thalia Daniels, Bruce T. Dembofsky, David A. Gurley, James E. Hall, Keith J. Herzog, Carey L. Horchler, Cyrus J. Ohnmacht, Richard Jon Schmiesing, Adam Dudley, Maria D. Ribadeneira, Katherine S. Knappenberger, Carla Maciag, Mark M. Stein, Maninder Chopra, Xiaodong F. Liu, Edward P. Christian, Jeffrey L. Arriza, Marc J. Chapdelaine*

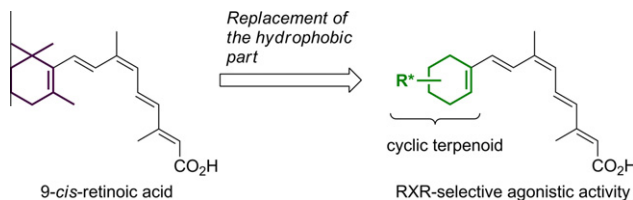


New structural classes of functionally selective benzodiazepine-site allosteric modulators of GABA_A receptors are reported.

**Replacement of the hydrophobic part of 9-*cis*-retinoic acid with cyclic terpenoid moiety results in RXR-selective agonistic activity**

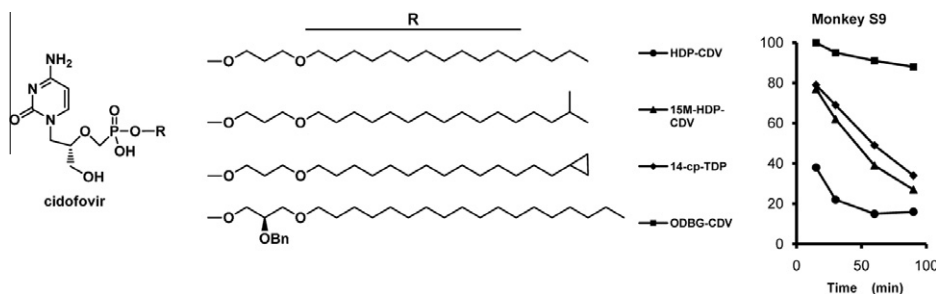
pp 2939–2949

Takashi Okitsu, Kana Sato, Kinya Iwatsuka, Natsumi Sawada, Kimie Nakagawa, Toshio Okano, Shoya Yamada, Hiroki Kakuta, Akimori Wada*

**Synthesis, metabolic stability and antiviral evaluation of various alkoxyalkyl esters of cidofovir and 9-(*S*)-[3-hydroxy-2-(phosphonomethoxy)propyl]adenine**

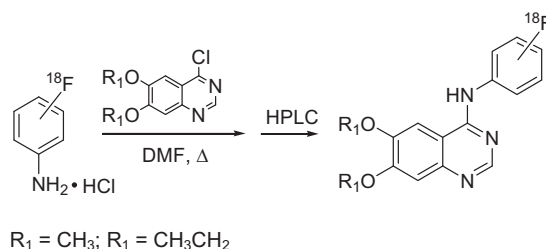
pp 2950–2958

Jacqueline Ruiz, James R. Beadle, R. Mark Buller, Jill Schreiwer, Mark N. Prichard, Kathy A. Keith, Kenneth C. Lewis, Karl Y. Hostetler*

**Metabolic stability of 6,7-dialkoxy-4-(2-, 3- and 4-[¹⁸F]fluoroanilino)quinazolines, potential EGFR imaging probes**

pp 2959–2965

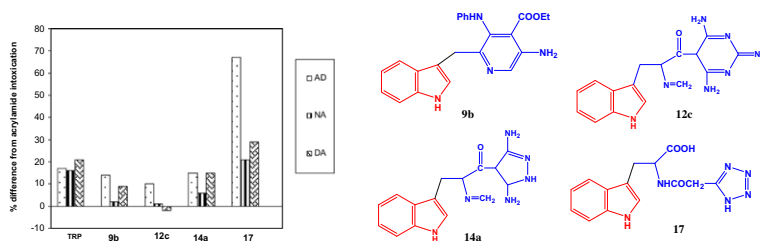
Neil Vasdev, Peter N. Dorff, James P. O'Neil, Frederick T. Chin, Stephen Hanrahan, Henry F. VanBrocklin*



Development of new indole-derived neuroprotective agents

pp 2966–2974

Rafat M. Mohareb, Hanaa H. Ahmed, Gamal A. Elmegeed*, Mervat M. Abd-Elhalim, Reham W. Shafic

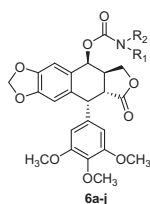


The main goal of the present study was to synthesize new indole derivatives with structures justifying neuroprotective activity. The potential neuroprotective effects of these newly synthesized agents against acrylamide induced neurotoxicity in rats were investigated.

Synthesis of 4β-carbamoyl epipodophyllotoxins as potential antitumour agents

pp 2975–2979

Ahmed Kamal*, B. Ashwini Kumar, Paidakula Suresh, Aarti Juvekar, Surekha Zingde

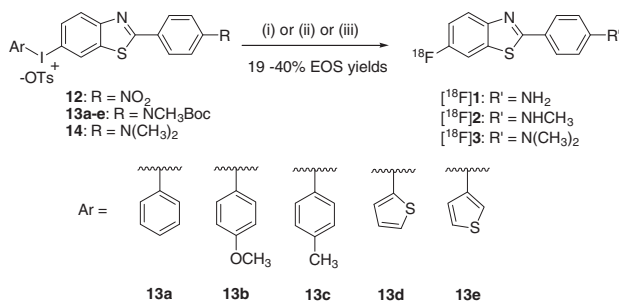


- 6a: R₁ = H, R₂ = propyl
 6b: R₁ = H, R₂ = isopropyl
 6c: R₁ = H, R₂ = cyclopropylmethyl
 6d: R₁ = CH₃, R₂ = CH₃
 6e: R₁ = H, R₂ = 2-methoxyethyl
 6f: R₁ = H, R₂ = prop-2-yn-1-yl
 6g: R₁R₂N = morpholinyl
 6h: R₁ = H, R₂ = 4-trifluoromethylbenzyl
 6i: R₁ = H, R₂ = 3-ethyl-1H-indole
 6j: R₁ = H, R₂ = 2-dimethylaminoethyl

Aromatic radiofluorination and biological evaluation of 2-aryl-6-[¹⁸F]fluorobenzothiazoles as a potential positron emission tomography imaging probe for β-amyloid plaques

pp 2980–2990

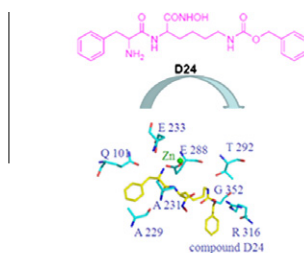
Byung Chul Lee, Ji Sun Kim, Bom Sahn Kim, Ji Yeon Son, Soo Kyung Hong, Hyun Soo Park, Byung Seok Moon, Jae Ho Jung, Jae Min Jeong, Sang Eun Kim*



Engineered *Thermoplasma acidophilum* factor F3 mimics human aminopeptidase N (APN) as a target for anticancer drug development

pp 2991–2996

Jing Su, Qiang Wang, Jinhong Feng, Cong Zhang, Deyu Zhu, Tiandi Wei, Wenfang Xu*, Lichuan Gu*



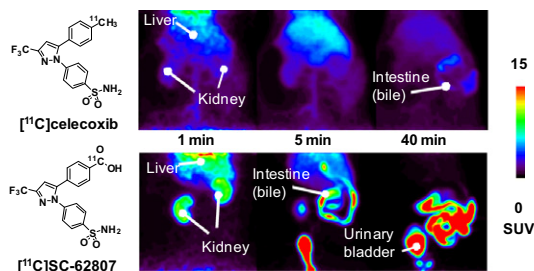
Eight amino acids of engineered *Thermoplasma Acidophilum* factor F3 have interactions with the inhibitors. They are Q101, A229, A231, E233, E288, T292, R316 and G352.



Efficient sequential synthesis of PET Probes of the COX-2 inhibitor [^{11}C]celecoxib and its major metabolite [^{11}C]SC-62807 and in vivo PET evaluation

pp 2997–3004

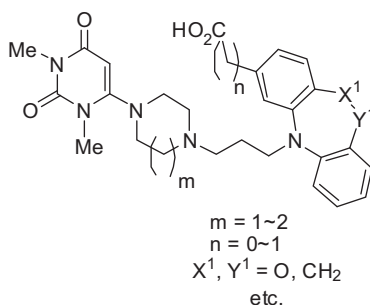
Misato Takashima-Hirano, Tadayuki Takashima, Yumiko Katayama, Yasuhiro Wada, Yuichi Sugiyama, Yasuyoshi Watanabe, Hisashi Doi, Masaaki Suzuki*



Synthesis and structure–activity relationship of tricyclic carboxylic acids as novel anti-histamines

pp 3005–3021

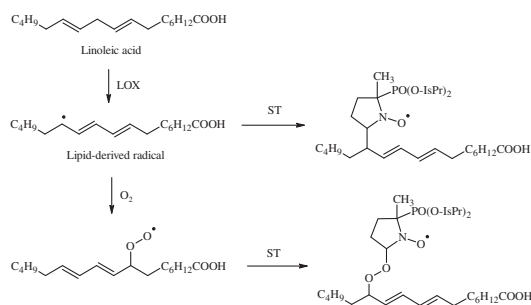
Katsumi Kubota, Hirotaka Kurebayashi, Hirotaka Miyachi, Masanori Tobe, Masako Onishi, Yoshiaki Isobe*



Understanding the radical mechanism of lipoxygenases using ^{31}P NMR spin trapping

pp 3022–3028

Luca Zoia, Raffaella Perazzini, Claudia Crestini, Dimitris S. Argyropoulos*



OTHER CONTENTS

Corrigenda

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*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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