



# Bioorganic & Medicinal Chemistry Volume 19, Issue 24, 2011

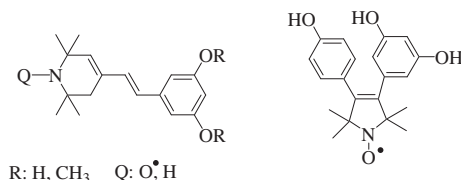
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### ARTICLES

#### Synthesis and study of new paramagnetic resveratrol analogues

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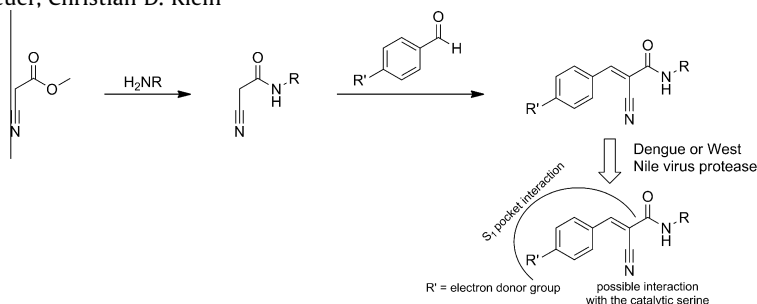
Tamás Kálai, Erzsébet Borza, Csenge Antus, Balázs Radnai, Gergely Gulyás-Fekete, Andrea Fehér, Balázs Sümegi, Kálmán Hideg\*



#### Arylcynoacrylamides as inhibitors of the Dengue and West Nile virus proteases

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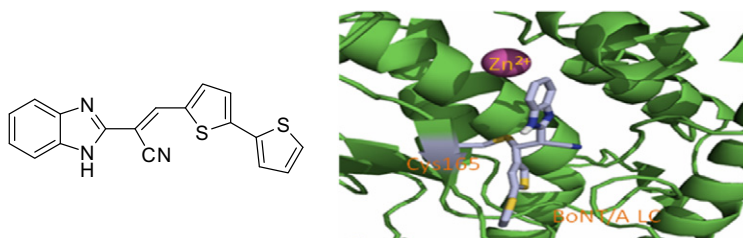
Christoph Nitsche, Christian Steuer, Christian D. Klein\*



#### Time-dependent botulinum neurotoxin serotype A metalloprotease inhibitors

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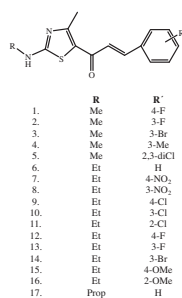
Bing Li\*, Steven C. Cardinale, Michelle M. Butler, Ramdas Pai, Jonathan E. Nuss, Norton P. Peet, Sina Bavari, Terry L. Bowlin



**Novel (*E*)-1-(4-methyl-2-(alkylamino)thiazol-5-yl)-3-arylprop-2-en-1-ones as potent antimicrobial agents**

pp 7349–7356

K. Liaras, A. Geronikaki\*, J. Glamočlija, A. Ćirić, M. Soković

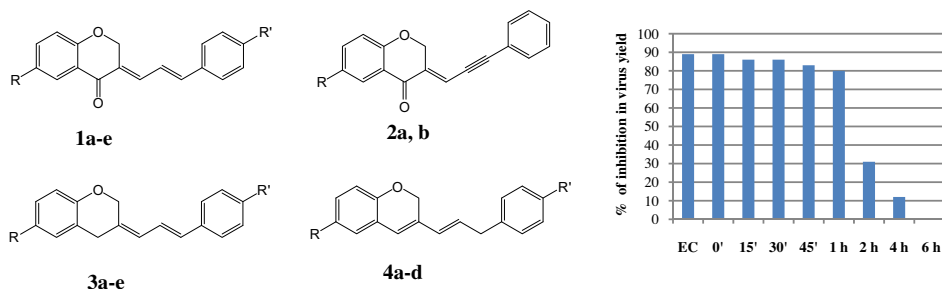


A series of novel (*E*)-1-(4-methyl-2-(alkylamino)thiazol-5-yl)-3-arylprop-2-en-1-ones were synthesized and evaluated for their antibacterial and antifungal activity.

**Design, synthesis and in vitro evaluation of novel chroman-4-one, chroman, and 2*H*-chromene derivatives as human rhinovirus capsid-binding inhibitors**

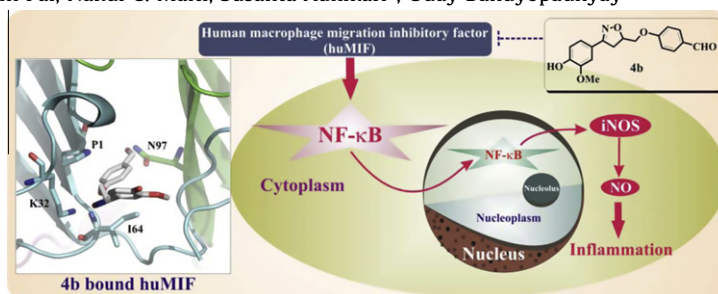
pp 7357–7364

Cinzia Conti, Luca Proietti Monaco, Nicoletta Desideri\*

**Synthesis and bio-evaluation of human macrophage migration inhibitory factor inhibitor to develop anti-inflammatory agent**

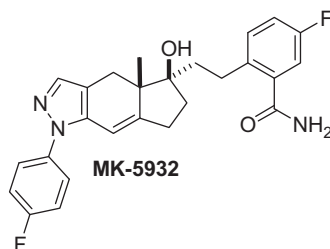
pp 7365–7373

Athar Alam, Chinmay Pal, Manish Goyal, Milan Kumar Kundu, Rahul Kumar, Mohd Shameel Iqbal, Sumanta Dey, Samik Bindu, Souvik Sarkar, Uttam Pal, Nakul C. Maiti, Susanta Adhikari\*, Uday Bandyopadhyay\*

**Discovery of selective glucocorticoid receptor modulator MK-5932**

pp 7374–7386

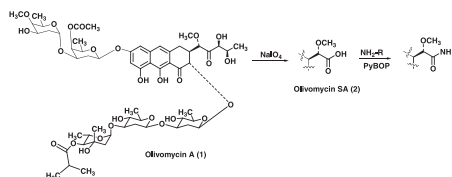
Christopher J. Bungard\*, George D. Hartman, Jesse J. Manikowski, James J. Perkins, Chang Bai, Philip E. Brandish, Danielle H. Euler, James C. Hershey, Azriel Schmidt, Yulin Fang, Ryan T. Norcross, Tom H. Rushmore, Charles D. Thompson, Robert S. Meissner



### Modification of olivomycin A at the side chain of the aglycon yields the derivative with perspective antitumor characteristics

pp 7387–7393

Anna N. Tevyashova, Alexander A. Shtil, Eugenia N. Olsufyeva, Yury N. Luzikov, Marina I. Reznikova, Lyubov G. Dezhenkova, Elena B. Isakova, Vladimir M. Bukhman, Nikita A. Durandin, Alexander M. Vinogradov, Vladimir A. Kuzmin, Maria N. Preobrazhenskaya\*



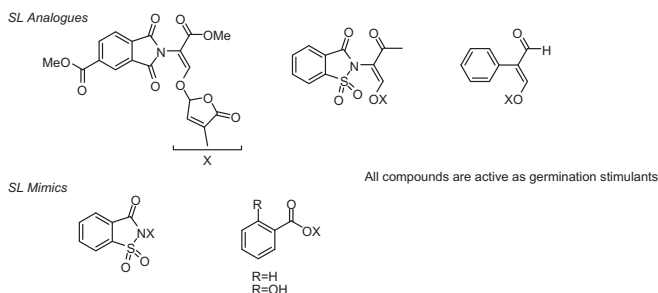
Interaction of olivomycin A with sodium periodate produced the key acid derivative called olivomycin SA (86% yield). *N,N*-Dimethylaminoethylamide of olivomycin SA showed a pronounced antitumor effect and a remarkably high binding constant to double stranded DNA.



### Strigolactone analogues and mimics derived from phthalimide, saccharine, *p*-tolylmalondialdehyde, benzoic and salicylic acid as scaffolds

pp 7394–7400

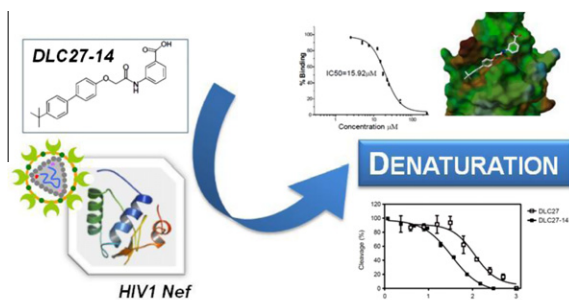
Binne Zwanenburg\*, Alinanuswe S. Mwakaboko



### A specific protein disorder catalyzer of HIV-1 Nef

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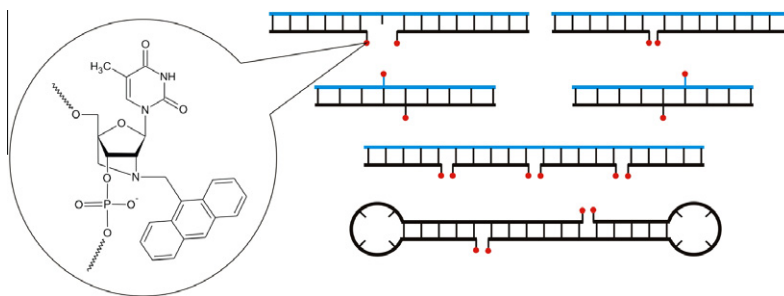
Adrien Lugari, Sebastian Breuer, Thibault Coursindel, Sandrine Opi, Audrey Restouin, Xiaoli Shi, Alexis Nazabal, Bruce E. Torbett, Jean Martinez, Yves Collette, Isabelle Parrot, Stefan T. Arold\*, Xavier Morelli\*



### Photoligation of self-assembled DNA constructs containing anthracene-functionalized 2'-amino-LNA monomers

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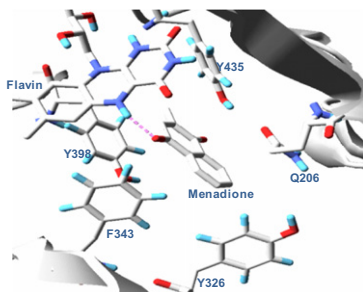
Karol Pasternak, Anna Pasternak, Pankaj Gupta, Rakesh N. Veedu, Jesper Wengel\*



### Molecular insights into human monoamine oxidase (MAO) inhibition by 1,4-naphthoquinone: Evidences for menadione (vitamin K3) acting as a competitive and reversible inhibitor of MAO

pp 7416–7424

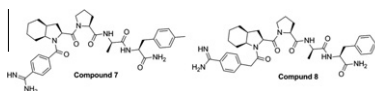
Eduardo Coelho Cerqueira, Paulo Augusto Netz, Cristiane Diniz, Vanessa Petry do Canto, Cristian Follmer\*



### Conformationally restricted analogs of the direct thrombin inhibitor FM 19

pp 7425–7434

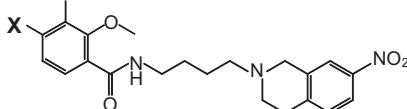
Elizabeth A. Girnys, Vanessa R. Porter, Henry I. Mosberg\*



### Electron-donating *para*-methoxy converts a benzamide-isoquinoline derivative into a highly Sigma-2 receptor selective ligand

pp 7435–7440

Abdol R. Hajipour, Lian-Wang Guo\*, Arindam Pal, Timur Mavlyutov, Arnold E. Ruoho\*



X = OCH<sub>3</sub>  
5e

$\sigma_2$  Ki = 26.78 nM  
 $\sigma_1$  Ki = 10,320 nM  
 $\sigma_1/\sigma_2$  = 385

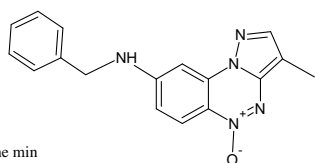
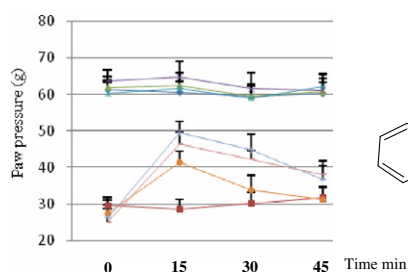
X = H  
5f

$\sigma_2$  Ki = 12,930 nM  
 $\sigma_1$  Ki = 7,870 nM  
 $\sigma_1/\sigma_2$  = 0.61

### Development of ligands at $\gamma$ -aminobutyric acid type A (GABA<sub>A</sub>) receptor subtype as new agents for pain relief

pp 7441–7452

Gabiella Guerrini\*, Giovanna Ciciani, Fabrizio Bruni, Silvia Selleri, Claudia Martini, Simona Daniele, Carla Ghelardini, Lorenzo Di Cesare Mannelli, Annarella Costanzo



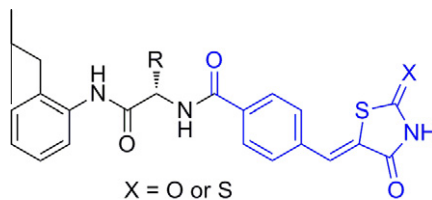
11  
Antihyperalgesic at 3 mg/kg



**New cholesterol esterase inhibitors based on rhodanine and thiazolidinedione scaffolds**

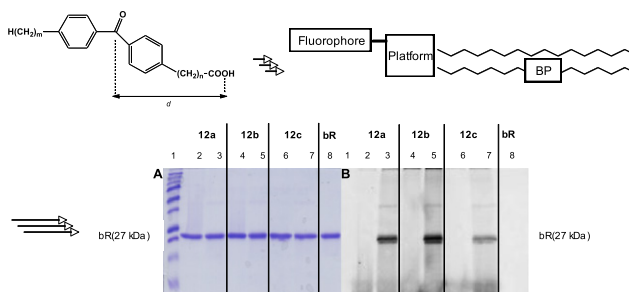
pp 7453–7463

Sabrina Heng, William Tieu, Stephanie Hautmann, Kevin Kuan, Daniel Sejer Pedersen, Markus Pietsch, Michael Gütschow, Andrew D. Abell\*

**Benzophenone-containing fatty acids and their related photosensitive fluorescent new probes: Design, physico-chemical properties and preliminary functional investigations**

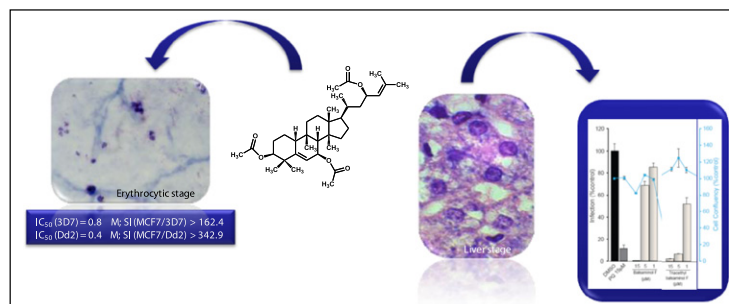
pp 7464–7473

Benoît Hilbold, Marie Perrault, Christophe Ehret, Song-Lin Niu, Benoît Frisch, Eve-Isabelle Pécheur\*, Line Bourel-Bonnet\*

**Triterpenoids as inhibitors of erythrocytic and liver stages of *Plasmodium* infections**

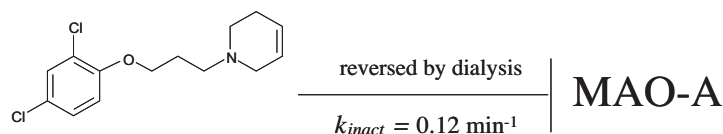
pp 7474–7481

Cátia Ramalhete, Filipa P. da Cruz, Dinora Lopes, Silva Mulhovo, Virgílio E. Rosário, Miguel Prudêncio, Maria-José U. Ferreira\*

**Time-dependent slowly-reversible inhibition of monoamine oxidase A by N-substituted 1,2,3,6-tetrahydropyridines**

pp 7482–7492

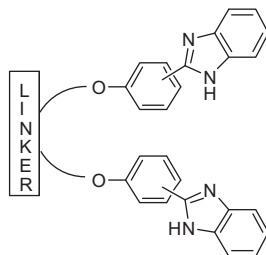
Wisut Wichitnithad, James P. O'Callaghan, Diane B. Miller, Brian C. Train, Patrick S. Callery\*



**Bis(oxyphenylene)benzimidazoles: A novel class of anti-*Plasmodium falciparum* agents**

pp 7493–7500

Annie Mayence, Jean Jacques Vanden Eynde\*, Marcel Kaiser, Reto Brun, Nigel Yarlett, Tien L. Huang\*

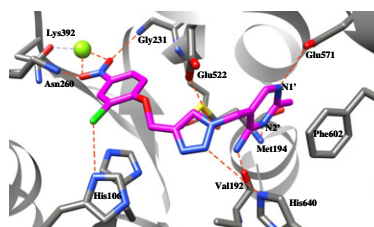


Eight derivatives out of a newly prepared small library of twenty-six bisbenzimidazoles emerged as promising effective agents against *Plasmodium falciparum*. They were characterized by  $IC_{50}$  values ranging from 190 to 450 nM and selectivity indexes ranging from 92 to more than 450.

**Structure-based rational design of novel hit compounds for pyruvate dehydrogenase multienzyme complex E1 components from *Escherichia coli***

pp 7501–7506

Yanliang Ren, Junbo He, Lingling Feng, Xun Liao, Jing Jin, Yongjian Li, Yi Cao, Jian Wan\*, Hongwu He\*



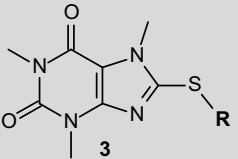
Four novel hit compounds with high inhibitory activity against PDHC-E1 from *Escherichia coli* have been designed, synthesized and tested, the best one of these compounds exhibit an  $IC_{50}$  value of 6.88  $\mu$ M, the binding model of this compound was obtained by molecular docking, as shown in Figure 2.

**Thio- and aminocaffeine analogues as inhibitors of human monoamine oxidase**

pp 7507–7518

Hermanus P. Booysen, Christina Moraal, Gisella Terre'Blanche, Anél Petzer, Jacobus J. Bergh, Jacobus P. Petzer\*

The human MAO inhibition potencies of a synthetic series of sulfanylcaffeine (**3**) and aminocaffeine analogues are reported.

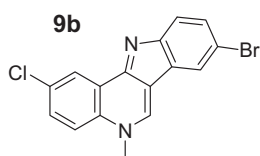
|  | R                     | $IC_{50}$ MAO-A | $IC_{50}$ MAO-B |
|-------------------------------------------------------------------------------------|-----------------------|-----------------|-----------------|
|                                                                                     |                       | $\mu$ M         | $\mu$ M         |
| <b>3c</b>                                                                           | $-(CH_2)_2-C_6H_5$    | 20.5            | 0.223           |
| <b>3d</b>                                                                           | $-(CH_2)_2-O-C_6H_5$  | 15.5            | 0.332           |
| <b>3e</b>                                                                           | $-CH_2-(4-Cl-C_6H_4)$ | 2.77            | 0.192           |
| <b>3f</b>                                                                           | $-CH_2-(4-Br-C_6H_4)$ | 2.62            | 0.167           |

The human MAO inhibition potencies of a synthetic series of sulfanylcaffeine (**3**) and aminocaffeine analogues are reported.

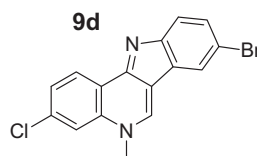
**Synthesis and antimalarial evaluation of novel isocryptolepine derivatives**

pp 7519–7525

Louise R. Whittell, Kevin T. Batty, Rina P. M. Wong, Erin M. Bolitho, Simon A. Fox, Timothy M. E. Davis, Paul E. Murray\*



$IC_{50}$  (*P. falciparum*) = 85 nM

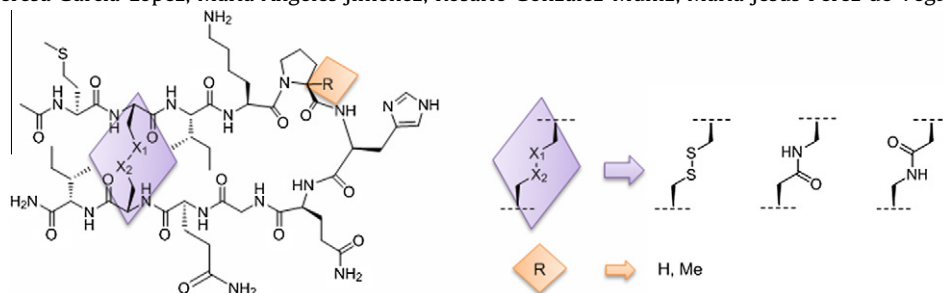


$IC_{50}$  (*P. falciparum*) = 100 nM

A novel series of mono- and di-substituted analogues of isocryptolepine have been synthesized and evaluated for in vitro antimalarial activity and cytotoxicity.

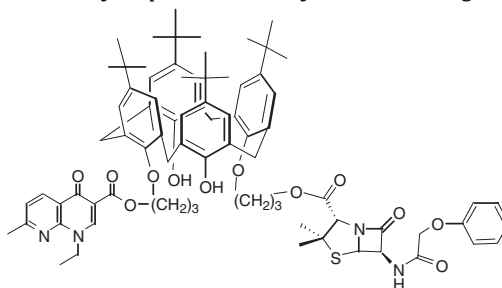
### Disulfide and amide-bridged cyclic peptide analogues of the VEGF<sub>81–91</sub> fragment: Synthesis, conformational analysis and biological evaluation pp 7526–7533

María Isabel García-Aranda, Yasmina Mirassou, Benoit Gautier, Mercedes Martín-Martínez, Nicolas Inguibert, Michel Vidal, María Teresa García-López, María Angeles Jiménez, Rosario González-Muñiz, María Jesús Pérez de Vega\*



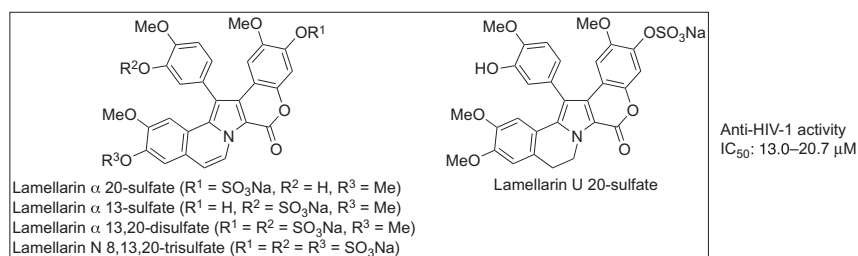
### Molecular drug-organiser: Synthesis, characterization and biological evaluation of penicillin V and/or nalidixic acid calixarene-based podands pp 7534–7540

Adel Ben Salem, Guillaume Sautrey, Stéphane Fontanay, Raphaël E. Duval, Jean-Bernard Regnouf-de-Vains\*



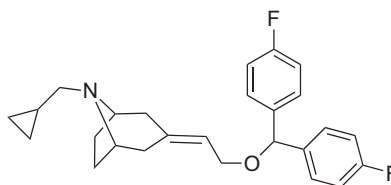
### Synthesis, structure–activity relationships, and mechanism of action of anti-HIV-1 lamellarin $\alpha$ 20-sulfate analogues pp 7541–7550

Haruka Kamiyama, Yoshinao Kubo\*, Hironori Sato, Naoki Yamamoto, Tsutomu Fukuda, Fumito Ishibashi, Masatomo Iwao\*



### Further structure–activity relationship studies on 8-substituted-3-[2-(diarylmethoxyethylidenyl)]-8-azabicyclo[3.2.1]octane derivatives at monoamine transporters pp 7551–7558

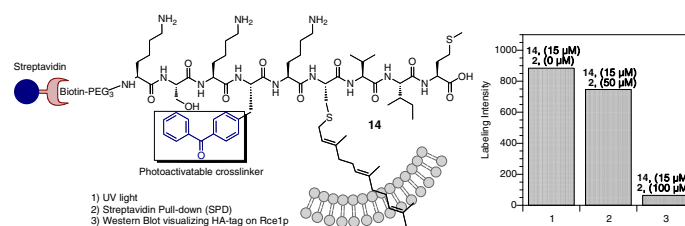
Shaine A. Cararas, Sari Izenwasser, Dean Wade, Amy Housman, Abha Verma, Stacey A. Lomenzo, Mark L. Trudell\*



### Photoaffinity labeling of Ras converting enzyme using peptide substrates that incorporate benzoylphenylalanine (Bpa) residues: Improved labeling and structural implications

pp 7559–7569

Kelly Kyro, Surya P. Manandhar, Daniel Mullen, Walter K. Schmidt, Mark D. Distefano\*



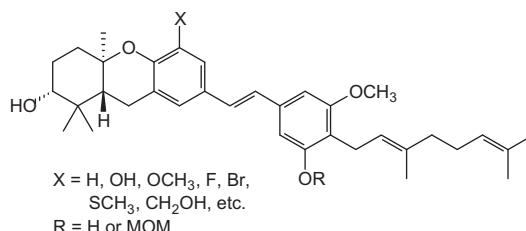
14: Above compound, 2: Farnesylated competitor without photoactive group.



### Relevance of the C-5 position to schweinfurthin induced cytotoxicity

pp 7570–7581

Joseph J. Topczewski, Michael P. Callahan, John G. Kodet, Jerry D. Inbarasu, Nolan R. Mente, John A. Beutler, David F. Wiemer\*

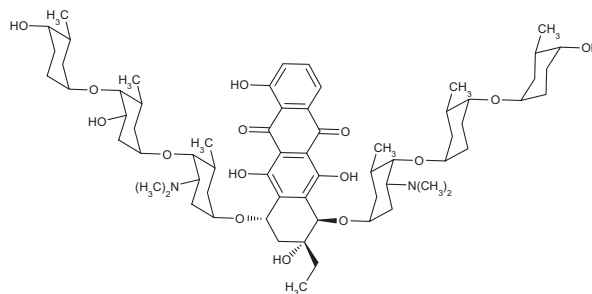


### Cosmomycin C inhibits signal transducer and activator of transcription 3 (STAT3) pathways in MDA-MB-468 breast cancer cell

pp 7582–7589

Jihoon Kim, Yu-Jin Lee, Dae-Seop Shin, Sun-Hee Jeon, Kwang-Hee Son, Dong Cho Han, Seung-Nam Jung, Tae-Kwang Oh, Byoung-Mog Kwon\*

Cosmomycin C inhibited phosphorylation of STAT3 activity and down-regulated expression of STAT3 target genes. And cosmomycin C induced apoptosis of the cells by down regulation of STAT3 target genes.

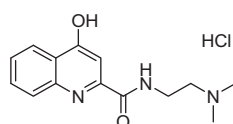


### Synthesis and biological effects of some kynurenic acid analogs

pp 7590–7596

K. Nagy, I. Plangár, B. Tuka, L. Gellért, D. Varga, I. Demeter, T. Farkas, Zs. Kis, M. Marosi, D. Zádori, P. Klivényi, F. Fülöp, I. Szatmári, L. Vécsei, J. Toldi\*

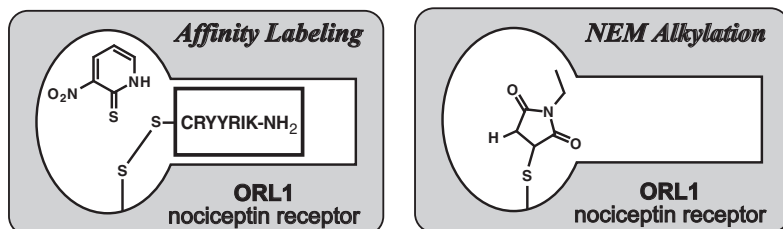
#### KYNA-1



This paper reports the synthesis of 10 new KYNA amides (KYNA-1–KYNA10) and on the effectiveness of this molecule as an inhibitor of excitatory synaptic transmission in the CA1 region of the hippocampus. The most effected molecule is newly synthesized KYNA-analogue (KYNA-1).

**Capturing of the free cysteine residue in the ligand-binding site by affinity labeling of the ORL1 nociceptin receptor** pp 7597–7602

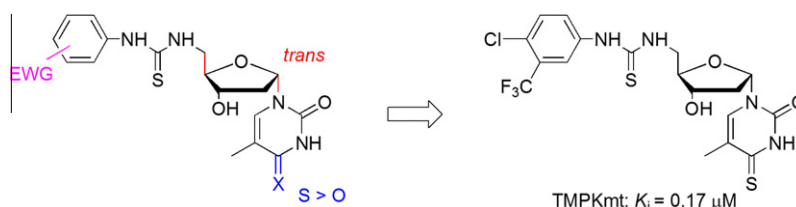
Ayami Matsushima, Hirokazu Nishimura, Shogo Inamine, Shiho Uemura, Yasuyuki Shimohigashi\*



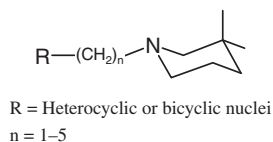
The ORL1 nociceptin receptor was found to consist of a free Cys- $\beta$ -thiol group by affinity labeling with Cys(Npys)-RYRIK-NH<sub>2</sub>, an SNpys-containing antagonist peptide, and also by C–S thioether-forming alkylation with *N*-ethylmaleimide.

**Synthesis and inhibitory activity of thymidine analogues targeting *Mycobacterium tuberculosis* thymidine monophosphate kinase** pp 7603–7611

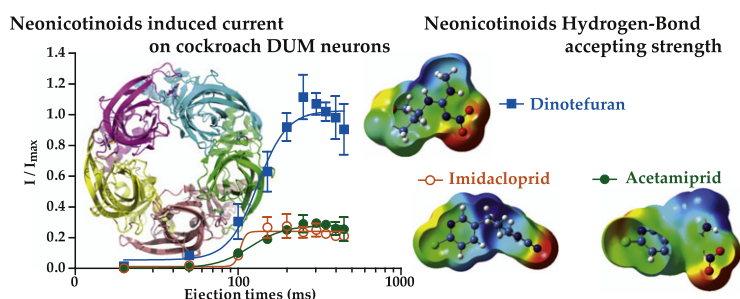
Sara Van Poecke, Hélène Munier-Lehmann, Olivier Helynck, Matheus Froeyen, Serge Van Calenbergh\*

**Synthesis and binding assays of novel 3,3-dimethylpiperidine derivatives with various lipophilicities as  $\sigma_1$  receptor ligands** pp 7612–7622

Savina Ferorelli, Carmen Abate, Maria P. Pedone, Nicola A. Colabufo, Marialessandra Contino, Roberto Perrone, Francesco Berardi\*

**New insights on the molecular features and electrophysiological properties of dinotefuran, imidacloprid and acetamiprid neonicotinoid insecticides** pp 7623–7634

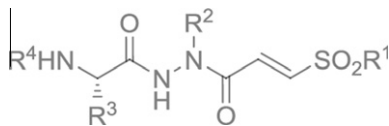
Jean-Yves Le Questel\*, Jérôme Graton, José P. Cerón-Carrasco, Denis Jacquemin, Aurélien Planchat, Steeve H. Thany\*



**Aza vinyl sulfones: Synthesis and evaluation as antiplasmodial agents**

pp 7635–7642

Paulo M. C. Glória, Jiri Gut, Lídia M. Gonçalves, Philip J. Rosenthal, Rui Moreira, Maria M. M. Santos\*

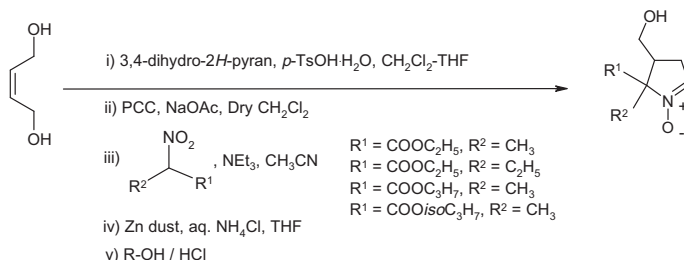


The design, synthesis and evaluation of aza vinyl sulfones as antiplasmodial agents is described. A number of the new compounds effectively inhibited the *in vitro* development of *Plasmodium falciparum*. Compounds containing a squaramide group were the most active, with IC<sub>50</sub> values between 0.95 and 4.5 μM, suggesting that these are potential lead compounds for the development of new antimalarial agents.

**Synthesis and characterization of 5-alkoxycarbonyl-4-hydroxymethyl-5-alkyl-pyrroline N-oxide derivatives**

pp 7643–7652

Anjan Patel, Natascha Rohr-Udilova, Thomas Rosenau, Klaus Stolze\*

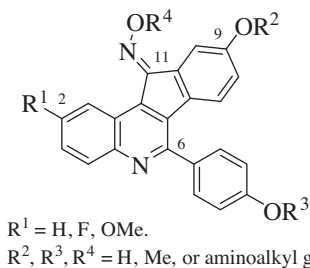


Syntheses, analytical data, and spin trapping properties of 5-ethoxycarbonyl-4-hydroxymethyl-5-methylpyrroline N-oxide and three of its homologues are reported.

**Synthesis and antiproliferative evaluation of 6-aryl-11-iminoindeno[1,2-*c*]quinoline derivatives**

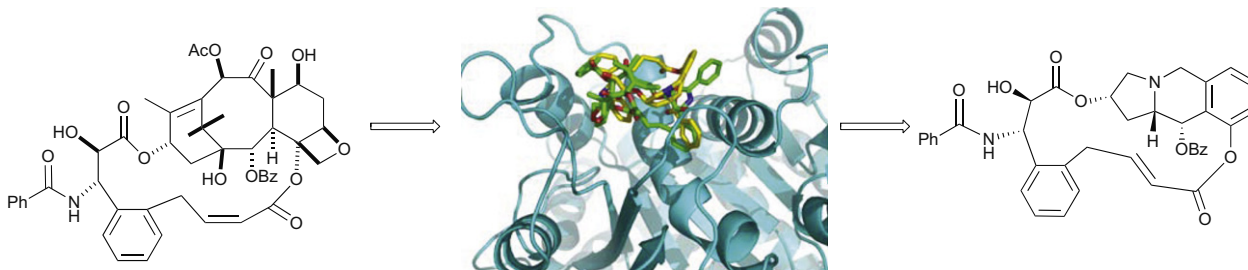
pp 7653–7663

Chih-Hua Tseng, Cherng-Chyi Tzeng, Kuin-Yu Chung, Chai-Lin Kao, Chih-Yao Hsu, Chih-Mei Cheng, Keng-Shiang Huang, Yeh-Long Chen\*

**Design and synthesis of simplified taxol analogs based on the T-Taxol bioactive conformation**

pp 7664–7678

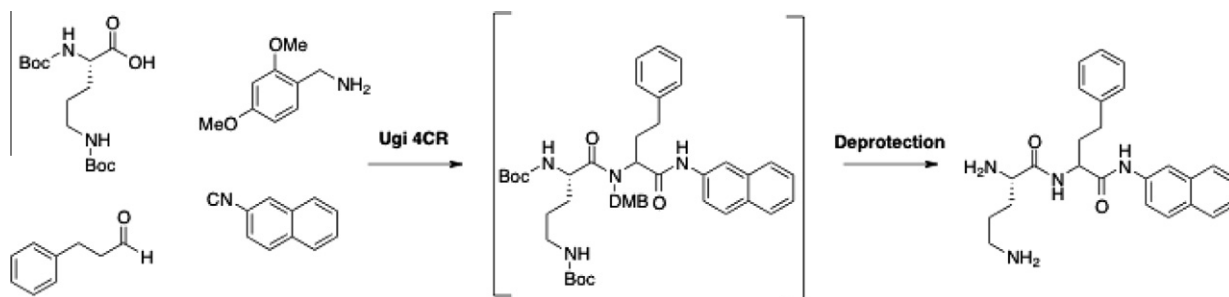
Jielu Zhao, Susan Bane, James P. Snyder, Haipeng Hu, Kamalika Mukherjee, Carla Slebodnick, David G. I. Kingston\*



**Synthesis and evaluation of inhibitors of bacterial drug efflux pumps of the major facilitator superfamily**

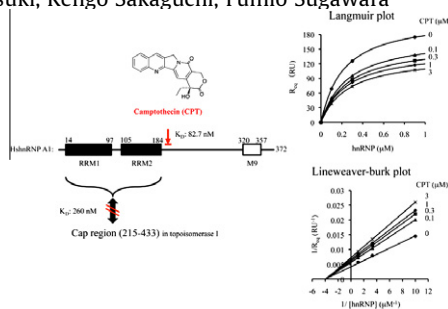
pp 7679–7689

Babajide O. Okandeji, Daniel M. Greenwald, Jessica Wroten, Jason K. Sello\*

**Camptothecin (CPT) directly binds to human heterogeneous nuclear ribonucleoprotein A1 (hnRNP A1) and inhibits the hnRNP A1/topoisomerase I interaction**

pp 7690–7697

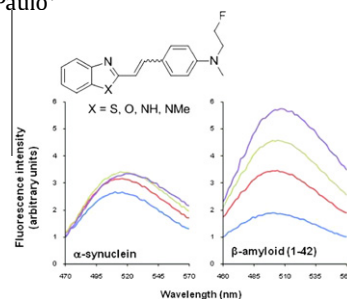
Daisuke Manita, Yuzuru Toba, Yoichi Takakusagi, Yuki Matsumoto, Tomoe Kusayanagi, Kaori Takakusagi, Senko Tsukuda, Kazunori Takada, Yoshihiro Kanai, Shinji Kamisuki, Kengo Sakaguchi, Fumio Sugawara\*

**Synthesis and in vitro evaluation of fluorinated styryl benzazoles as amyloid-probes**

pp 7698–7710

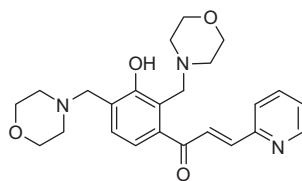
Goreti Ribeiro Morais, Hugo Vicente Miranda, Isabel C. Santos, Isabel Santos, Tiago F. Outeiro\*, Antonio Paulo\*

Novel fluorinated styryl benzazoles have been synthesized and evaluated in vitro as amyloid-probing agents. The compounds interact with fibrillary species with a red-shift in the excitation wavelengths along with an increase in the fluorescence emission intensity, appearing as good candidates to design  $^{18}\text{F}$ -labelled amyloid radioprobes.

**Structure–activity relationships of chalcone analogs as potential inhibitors of ADP- and collagen-induced platelet aggregation**

pp 7711–7719

M. Vijaya Bhaskar Reddy, Wei-Jern Tsai, Keduo Qian, Kuo-Hsiung Lee, Tian-Shung Wu\*



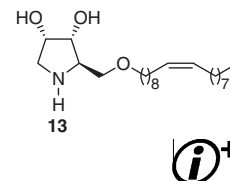
57

**Anti-cancer activity of 5-O-alkyl 1,4-imino-1,4-dideoxyribitols**

pp 7720–7727

Claudia Bello, Giovanna Dal Bello, Michele Cea, Aimable Nahimana, Dominique Aubry, Anna Garuti, Giulia Motta, Eva Moran, Floriana Fruscione, Paolo Pronzato, Francesco Grossi, Franco Patrone, Alberto Ballestrero, Marc Dupuis, Bernard Sordat, Kaspar Zimmermann, Jacqueline Loretan, Markus Wartmann, Michel A. Duchosal, Alessio Nencioni, Pierre Vogel\*

The oleyl derivative **13** ( $IC_{50} \sim 2$  M) is cytotoxic toward SKBR3 (breast cancer) cells. **13** also inhibits ( $IC_{50} \sim 8$  M) growth of JURKAT (acute lymphoblastic leukemia) cells.



\*Corresponding author

**i**<sup>+</sup> Supplementary data available via SciVerse 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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