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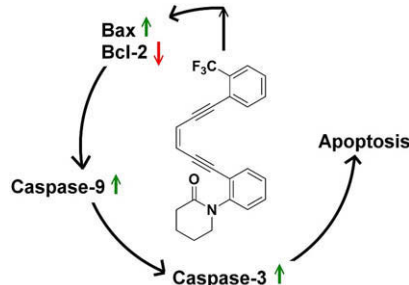
Bioorganic & Medicinal Chemistry Volume 17, Issue 21, 2009

Contents

ARTICLES

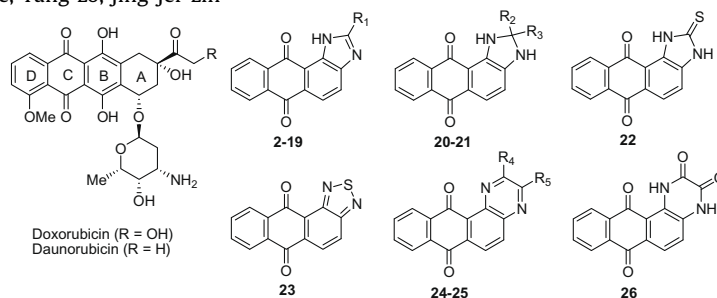
1-(2-((Z)-6-(2-(Trifluoromethyl)phenyl)hexa-3-en-1,5-diynyl)phenyl)piperidin-2-one as a new potent apoptosis agent pp 7412–7417

Yu-Sheng Tu, Tsai-Hui Duh, Chen-Yi Tseng, Ying-Ting Lin, Yu-Hsiang Lo, Yi-Ling Hu, Chen-Hung Chen, Ching-Ming Chien, Sheng-Huei Yang, Shinne-Ren Lin, Shyh-Chyun Yang, Ming-Jung Wu *



Synthesis, cytotoxicity and human telomerase inhibition activities of a series of 1,2-heteroannulated anthraquinones and anthra[1,2-d]imidazole-6,11-dione homologues pp 7418–7428

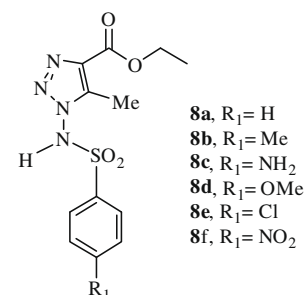
Hsu-Shan Huang *, Tsung-Chih Chen, Ruei-Huei Chen, Kuo-Feng Huang, Fong-Chun Huang, Jing-Ru Jhan, Chun-Liang Chen, Chia-Chung Lee, Yang Lo, Jing-Jer Lin *



Synthesis, biological, and theoretical evaluations of new 1,2,3-triazoles against the hemolytic profile of the *Lachesis muta* snake venom pp 7429–7434

Vinícius R. Campos, Paula A. Abreu, Helena C. Castro, Carlos R. Rodrigues, Alessandro K. Jordão, Vitor F. Ferreira, Maria C. B. V. de Souza, Fernanda da C. Santos, Laura A. Moura, Thaisa S. Domingos, Carla Carvalho, Eládio F. Sanchez, André L. Fuly *, Anna C. Cunha *

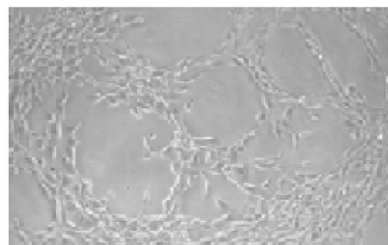
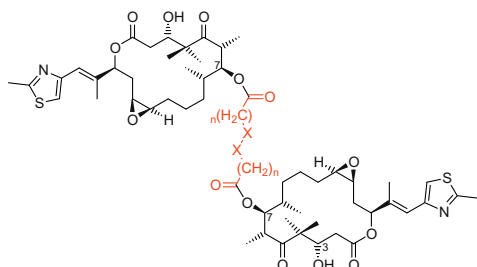
This paper describes the synthesis, pharmacological and theoretical evaluation of new 1-arylsulfonylamino-5-methyl-1H-[1,2,3]-triazole-4-carboxylic acid ethyl esters **8a–f** against the hemolytic profile of the *Lachesis muta* snake venom. All the compounds were able to neutralize hemolytic property of venom.



Synthesis and biological evaluation of epothilone A dimeric compounds

pp 7435–7440

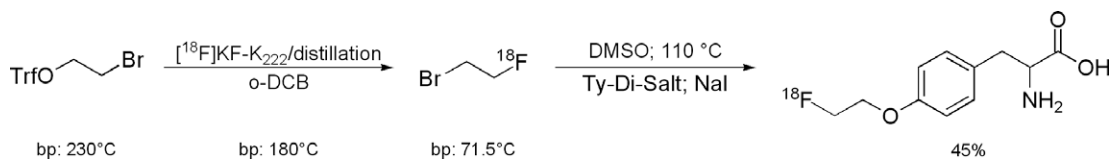
Daniele Passarella ^{*}, Daniela Comi, Graziella Cappelletti, Daniele Cartelli, Juerg Gertsch, Ana R. Quesada, Jurgen Borlak, Karl-Heinz Altmann



New approach for the synthesis of [¹⁸F]fluoroethyltyrosine for cancer imaging: Simple, fast, and high yielding automated synthesis

pp 7441–7448

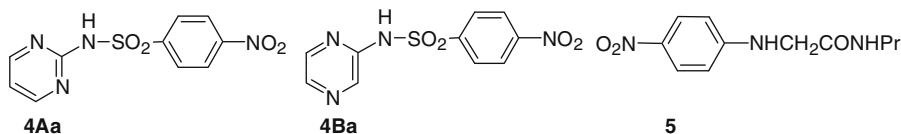
M. Zuhayra ^{*}, A. Alfteimi, C. Von Forstner, U. Lützen, B. Meller, E. Henze



In vivo and in vitro anti-leishmanial activities of 4-nitro-*N*-pyrimidin- and *N*-pyrazin-2-ylbenzenesulfonamides, and *N*²-(4-nitrophenyl)-*N*¹-propylglycinamide

pp 7449–7456

M. Auxiliadora Dea-Ayuela, Encarna Castillo, Marta Gonzalez-Alvarez, Celeste Vega, Miriam Rolón, Francisco Bolás-Fernández, Joaquín Borrás, M. Eugenia González-Rosende ^{*}

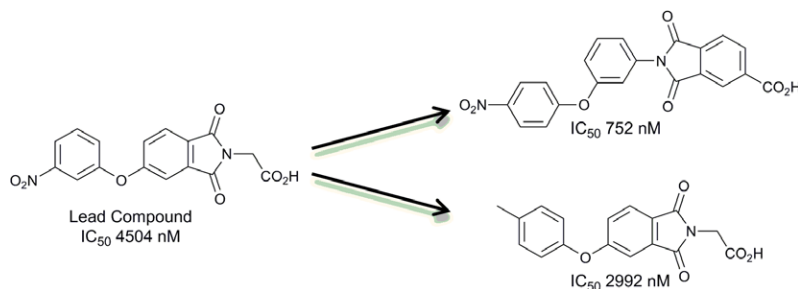


4-Nitrobenzene derivatives **4Aa**, **4Ba** and **5** represent possible candidates for leishmanicidal drugs as they exhibit good in vivo and in vitro activities against *Leishmania infantum* without toxicity to J774 macrophages.

Structure-based drug design identifies novel LPA₃ antagonists

pp 7457–7464

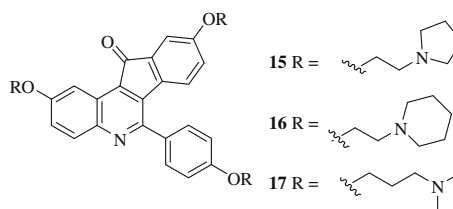
James I. Fells, Ryoko Tsukahara, Jianxiong Liu, Gabor Tigyi, Abby L. Parrill ^{*}



Synthesis and antiproliferative evaluation of 6-arylindeno[1,2-c]quinoline derivatives

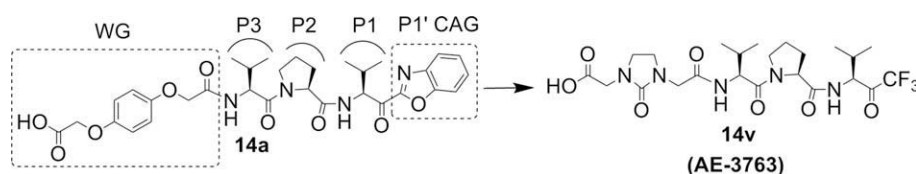
pp 7465–7476

Chih-Hua Tseng, Yeh-Long Chen, Kuin-Yu Chung, Chih-Mei Cheng, Chi-Huei Wang, Cherng-Chyi Tzeng *

**Development of a highly water-soluble peptide-based human neutrophil elastase inhibitor; AE-3763 for treatment of acute organ injury**

pp 7477–7486

Yasunao Inoue *, Tomoki Omodani, Ryotaro Shiratake, Hiroshi Okazaki, Akemi Kuromiya, Taeko Kubo, Fuminori Sato

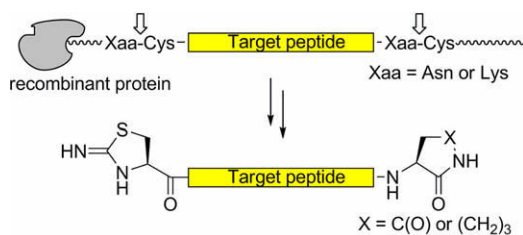


We present the SAR results of a series of peptide-based transition-state HNE inhibitors and the development of a highly water-soluble candidate **14v** (**AE-3763**) for treatment of acute organ injury, from the lead compound **14a**.

**Bioorganic synthesis of end-capped anti-HIV peptides by simultaneous cyanocysteine-mediated cleavages of recombinant proteins**

pp 7487–7492

Michinori Tanaka, Kazumi Kajiwarra, Rei Tokiwa, Kentaro Watanabe, Hiroaki Ohno, Hiroko Tsutsumi, Yoji Hata, Kazuki Izumi, Eiichi Kodama, Masao Matsuoka, Shinya Oishi *, Nobutaka Fujii *

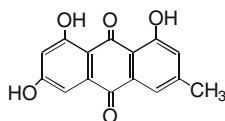


Anti-HIV fusion inhibitory peptides with N- and C-terminal end-capping groups was synthesized by two simultaneous S-cyanocysteine-mediated cleavages of recombinant proteins.

**Characterization of emodin metabolites in Raji cells by LC-APCI-MS/MS**

pp 7493–7499

Junko Koyama *, Atsuko Takeuchi, Izumi Morita, Yu Nishino, Maki Shimizu, Munetaka Inoue, Norihiro Kobayashi

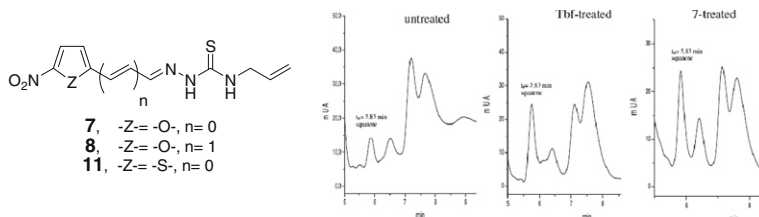


In addition to the major metabolite 8-O-methyl emodin, ω -hydroxyemodin, 3-O-methyl- ω -hydroxyemodin, 3-O-methylemodin, and chrysophanol were detected as emodin metabolites by LC-APCI-MS/MS method in Raji cells.

5-Nitrofuranes and 5-nitrothiophenes with anti-*Trypanosoma cruzi* activity and ability to accumulate squalene

pp 7500–7509

Alejandra Gerpe, Guzmán Álvarez, Diego Benítez, Lucía Boiani, Martín Quiroga, Paola Hernández, Maximiliano Sortino, Susana Zacchino, Mercedes González*, Hugo Cerecetto*



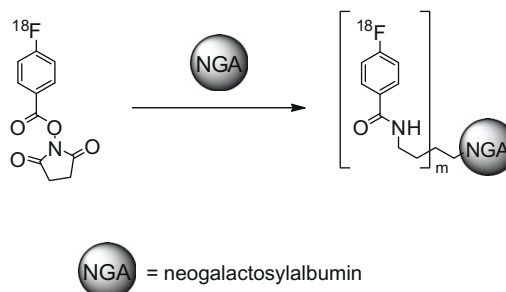
New 5-nitrofuran and 5-nitrothiophene derivatives have been synthesized and evaluated for their in vitro anti-*Trypanosoma cruzi* activities and squalene-accumulation capabilities.



Fluorine-18 labeled galactosyl-neoglycoalbumin for imaging the hepatic asialoglycoprotein receptor

pp 7510–7516

Wenjiang Yang, Tiantian Mou, Cheng Peng, Zhanhong Wu, Xianzhong Zhang^{*}, Fang Li, Yunchuan Ma

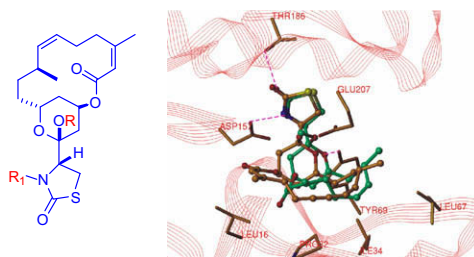


NGA was labeled with ^{18}F through active ester intermediate [^{18}F]SFB to coupling the ϵ -amide of lysine residue.

Semisynthetic latrunculin B analogs: Studies of actin docking support a proposed mechanism for latrunculin bioactivity

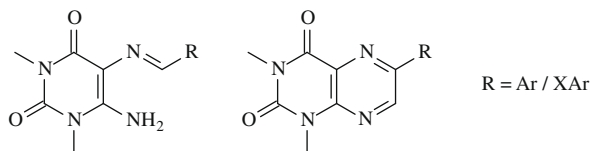
pp 7517–7522

Sucheta Kudrimoti, Safwat A. Ahmed, Pankaj R. Daga, Amir E. Wahba, Sherief I. Khalifa, Robert J. Doerksen, Mark T. Hamann*



Synthesis and in vitro evaluation of pteridine analogues as monoamine oxidase B and nitric oxide synthase inhibitors

pp 7523-7530

Louis H. A. Prins, Jacobus P. Petzer, Sarel F. Malan^{*}

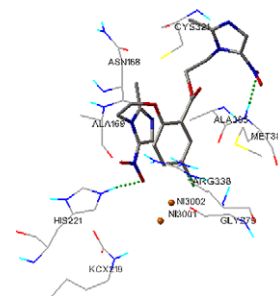
A series of pteridine-2,4-dione analogues were synthesised and evaluated as inhibitors of monoamine oxidase B (MAO-B) and nitric oxide synthase (NOS).

Synthesis, molecular docking and biological evaluation of metronidazole derivatives as potent *Helicobacter pylori* urease inhibitors

pp 7531–7536

Wen-Jun Mao, Peng-Cheng Lv, Lei Shi, Huan-Qiu Li, Hai-Liang Zhu *

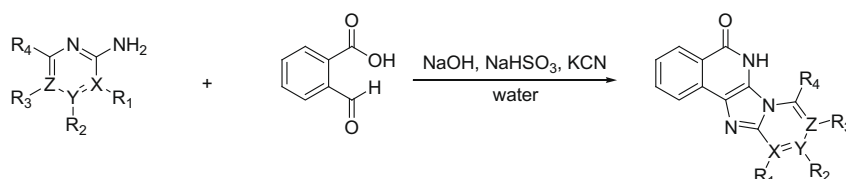
Fourteen metronidazole derivatives (compounds **3a–f** and **4b–h**) have been synthesized by coupling of metronidazole and salicylic acid derivatives. All of them are reported for the first time. Their chemical structures are characterized by ^1H NMR, MS, and elemental analysis. The inhibitory activities against *Helicobacter pylori* urease have been investigated in vitro and many compounds have showed promising potential inhibitory activities of *H. pylori* urease. The effect of compounds **4b** ($\text{IC}_{50} = 26 \mu\text{M}$) and **4g** ($\text{IC}_{50} = 12 \mu\text{M}$) was comparable with that of acetohydroxamic acid, a well known *H. pylori* urease inhibitor used as a positive control. The experimental values of IC_{50} showed that inhibitor was potent urease inhibitor. A docking analysis using the autodock 4.0 program could explain the inhibitory activities of compound **4g** against *H. pylori* urease.



Synthesis of isoquinolinone-based tetracycles as poly (ADP-ribose) polymerase-1 (PARP-1) inhibitors

pp 7537–7541

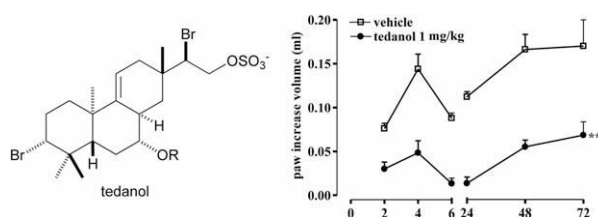
Hee-Kyung Rhee, So Yun Lim, Mi-Ja Jung, Youngjoo Kwon, Myung-Hwa Kim, Hea-Young Park Choo *



Tedanol: A potent anti-inflammatory *ent*-pimarane diterpene from the Caribbean Sponge *Tedania ignis*

pp 7542–7547

Valeria Costantino *, Ernesto Fattorusso, Alfonso Mangoni, Cristina Perinu, Giuseppe Cirino, Luana De Gruttola, Fiorentina Roviezzo



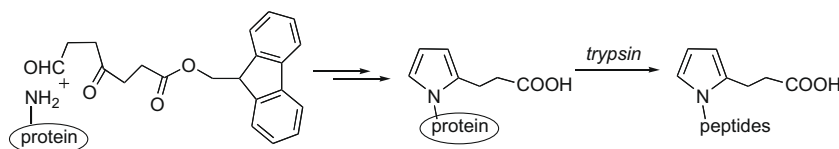
Tedanol, a new brominated and sulfated pimarane diterpene from the Caribbean sponge *Tedania ignis*, showed a potent in vivo anti-inflammatory activity at 1 mg/kg in a mouse model of inflammation.



Synthesis and structural characterization of carboxyethylpyrrole-modified proteins: mediators of age-related macular degeneration

pp 7548–7561

Liang Lu, Xiaorong Gu, Li Hong, James Laird, Keeve Jaffe, Jaewoo Choi, John Crabb, Robert G. Salomon *



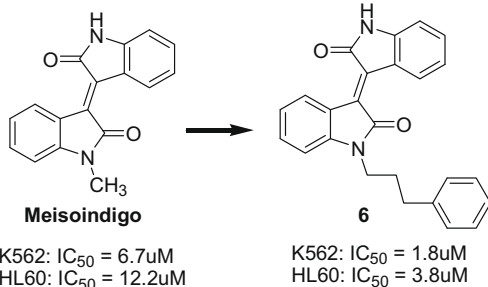
Proteins in which the ϵ -amino groups of lysyl residues are incorporated into 2-(ω -carboxyethyl)-pyrroles are mediators of age-related macular degeneration. We report an efficient synthesis that accommodates a wide variety of CEP:protein ratios. Reaction of proteins with 4,7-dioxoheptanoic acid 9-fluorenylmethyl ester, and in situ deprotection with DBU provides CEP-proteins without causing denaturation. The structures of tryptic peptides derived from CEP-proteins were also determined.



Synthesis and evaluation of functionalized isoindigos as antiproliferative agents

pp 7562–7571

Xi Kai Wee, Wee Kiang Yeo, Bing Zhang, Vincent B. C. Tan, Kian Meng Lim, Tong Earn Tay, Mei-Lin Go *



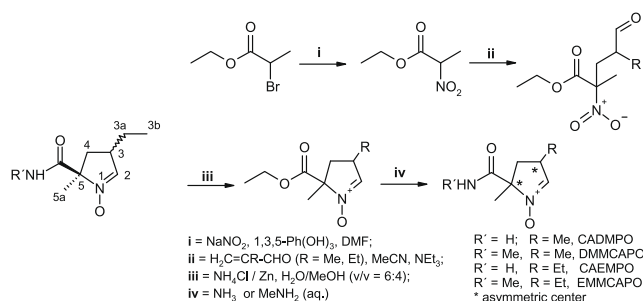
Lead modification of meisoindigo at position 1 of the isoindigo scaffold yield more potent analogs of meisoindigo that have low micromolar antiproliferative activities against K562 and HL60 leukemic cell lines.



Synthesis and characterization of several carbamoyl- and methylcarbamoyl-substituted EMPO derivatives

pp 7572–7584

Klaus Stolze *, Natascha Rohr-Udilova, Andreas Hofinger, Thomas Rosenau

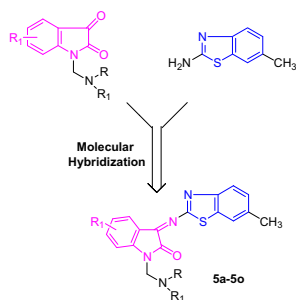


Synthesis and spin trapping properties of a series of carbamoyl- and methylcarbamoyl-substituted nitrones is reported.

Hybrid pharmacophore design and synthesis of isatin-benzothiazole analogs for their anti-breast cancer activity

pp 7585–7592

V. Raja Solomon, Changkun Hu, Hoyun Lee *

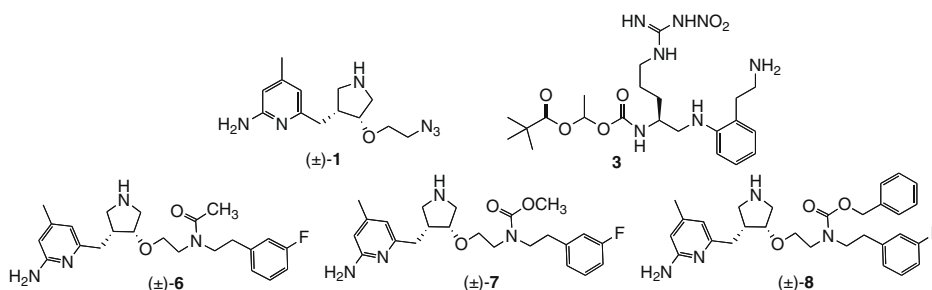


Here we report the designing, synthesis, and examination of isatin-benzothiazole analogs on breast cancer and matching non-cancer cells.

Effect of potential amine prodrugs of selective neuronal nitric oxide synthase inhibitors on blood–brain barrier penetration

pp 7593–7605

Richard B. Silverman *, Graham R. Lawton, Hantamalala Ralay Ranaivo, Laura K. Chico, Jiwon Seo, D. Martin Watterson



pp 7606–7614

$R = \text{CH}_3, \text{C}_2\text{H}_5, \text{CH}_3\text{CO}. R^1 = \text{COCH}_3, \text{COC}_2\text{H}_5.$
 $R^2 = \text{COCH}_3, \text{COC}_2\text{H}_5, \text{PhCO}, 4\text{-F-C}_6\text{H}_4\text{SO}_2, \text{iC}_3\text{H}_7\text{SO}_2,$
 $\text{PhCH}_2\text{CO}, \text{PhNHCO}, \text{PhOCO}. m = 0, 1; n = 1, 2$

pp 7615–7621

[illegible]

 ⁺ Supplementary data available via ScienceDirect

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*, 12722–12727 and S. Wetzel, H. Waldmann, Cheminformatic analysis of natural products and their chemical space, *Chimia* **2007**, *61*(6), 355–360].

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