

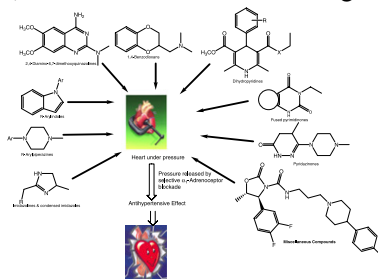
Contents

REVIEW

Recent advances in selective α_1 -adrenoreceptor antagonists as antihypertensive agents

pp 4759–4800

Kishor S. Jain,* Jitender B. Bariwal, Muthu K. Kathiravan, Manisha S. Phoujdar,
Rajkumari S. Sahne, Bishram S. Chauhan, Anamik K. Shah and Mange Ram Yadav

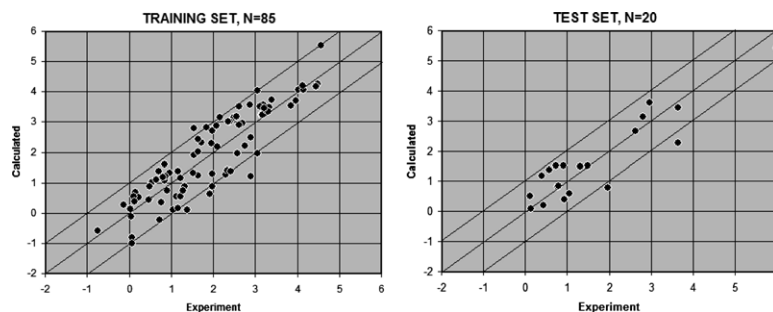


ARTICLES

Additive SMILES-based optimal descriptors in QSAR modelling bee toxicity: Using rare SMILES attributes to define the applicability domain

pp 4801–4809

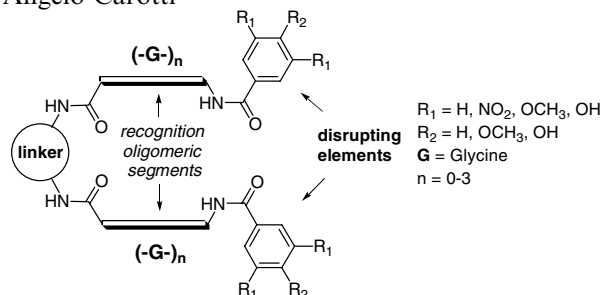
A. A. Toropov* and E. Benfenati



Design, synthesis, and biological evaluation of glycine-based molecular tongs as inhibitors of $A\beta_{1-40}$ aggregation in vitro

pp 4810–4822

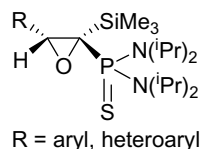
Saverio Cellamare, Angela Stefanachi, Diana A. Stolfa, Teodora Basile, Marco Catto,
Francesco Campagna, Eddy Sotelo, Pasquale Acquafredda and Angelo Carotti*



Thioxophosphoranyl aryl- and heteroaryloxiranes as the representants of a new class of metallocarboxypeptidase inhibitors

pp 4823–4828

Daniel Fernández, Ona Illa, Francesc X. Avilés, Vicenç Branchadell, Josep Vendrell* and Rosa M. Ortuño*

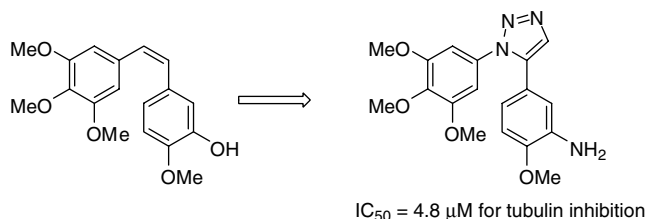


These compounds display strong inhibitory activity toward both bovine CPA and human CPB.

1,5-Disubstituted 1,2,3-triazoles as *cis*-restricted analogues of combretastatin A-4: Synthesis, molecular modeling and evaluation as cytotoxic agents and inhibitors of tubulin

pp 4829–4838

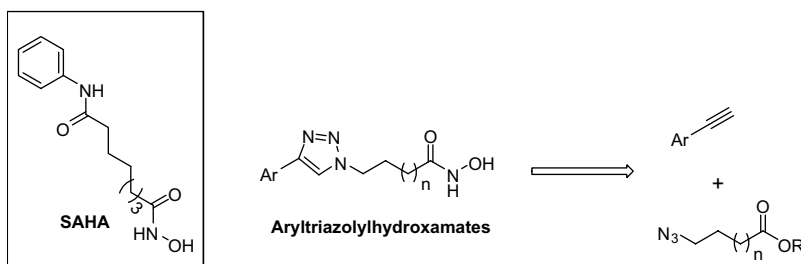
Kristin Odlo, Jean Hentzen, Jérémie Fournier dit Chabert, Sylvie Ducki, Osman A. B. S. M. Gani, Ingebrigt Sylte, Martina Skrede, Vivi Ann Flørenes and Trond Vidar Hansen*



Synthesis and structure–activity relationship of histone deacetylase (HDAC) inhibitors with triazole-linked cap group

pp 4839–4853

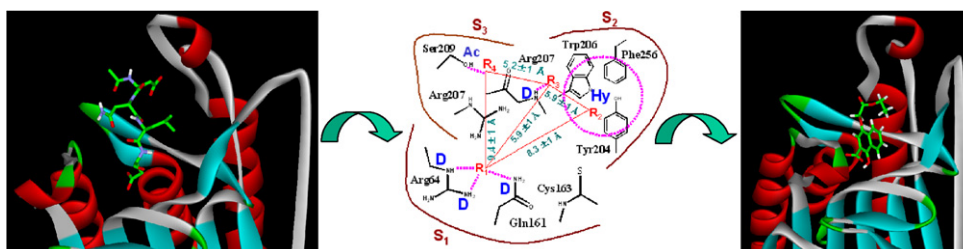
Po C. Chen, Vishal Patil, William Guerrant, Patience Green and Adegboyega K. Oyelere*



Structure-based discovery of a novel non-peptidic small molecular inhibitor of caspase-3

pp 4854–4859

Junichi Sakai, Atsushi Yoshimori, Yasuyo Nose, Akihiko Mizoroki, Naoyuki Okita, Ryoko Takasawa and Sei-ichi Tanuma*

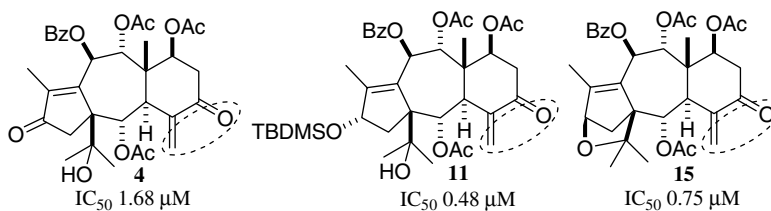


COSMOS : Conversion to small molecules through optimized-peptides strategy

Synthesis, cytotoxic activity, and SAR analysis of the derivatives of taxchinin A and brevifoliol

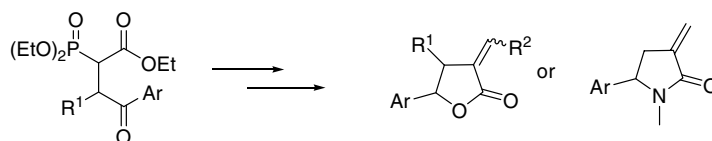
pp 4860–4871

Yu Zhao, Na Guo, Li-Guang Lou, Yu-Wen Cong, Li-Yan Peng and Qin-Shi Zhao*

**Synthesis and cytotoxic activity of γ -aryl substituted α -alkylidene- γ -lactones and α -alkylidene- γ -lactams**

pp 4872–4882

Anna Albrecht, Jacek F. Koszuk, Jakub Modranka, Marek Różalski, Urszula Krajewska, Anna Janecka, Kazimierz Studzian and Tomasz Janecki*

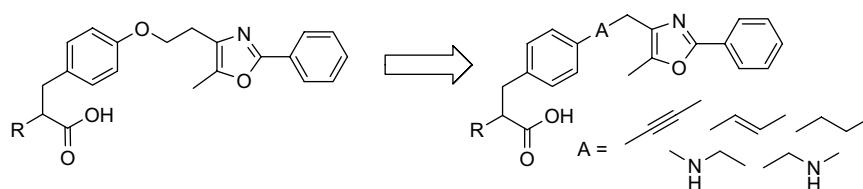


A series of 5-aryl-3-alkylidenedihydrofuran-2(3*H*)-ones and 5-aryl-3-methylidenepyrrolidin-2-ones were synthesized starting from 4-aryl-2-diethoxyphosphoryl-4-oxobutanoates. Target compounds were evaluated for their cytotoxic activity against L-1210, HL-60 and NALM-6 cell lines.

Effects of modifications of the linker in a series of phenylpropanoic acid derivatives: Synthesis, evaluation as PPAR α/γ dual agonists, and X-ray crystallographic studies

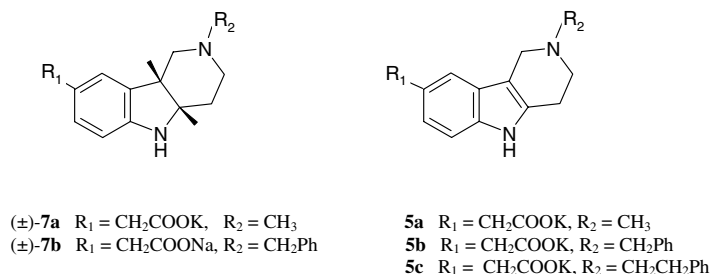
pp 4883–4907

Agustin Casimiro-Garcia,* Christopher F. Bigge, Jo Ann Davis, Teresa Padalino, James Pulaski, Jeffrey F. Ohren, Patrick McConnell, Christopher D. Kane, Lori J. Royer, Kimberly A. Stevens, Bruce J. Auerbach, Wendy T. Collard, Christine McGregor, Stephen A. Fakhoury, Robert P. Schaum and Hairong Zhou

**Carboxymethylated pyridoindole antioxidants as aldose reductase inhibitors: Synthesis, activity, partitioning, and molecular modeling**

pp 4908–4920

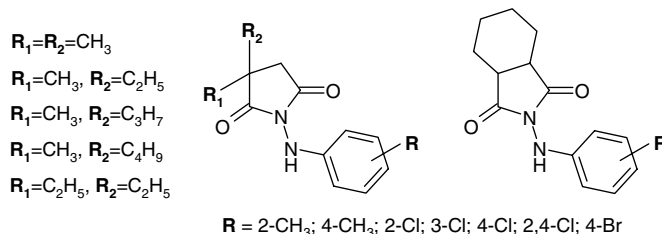
Milan Stefek,* Vladimir Snirc, Paul-Omer Djoubissie, Magdalena Majekova, Vassilis Demopoulos, Lucia Rackova, Zelmira Bezakova, Cimen Karasu, Vincenzo Carbone and Ossama El-Kabbani



Design, synthesis, and anticonvulsant activity of *N*-phenylamino derivatives of 3,3-dialkyl-pyrrolidine-2,5-diones and hexahydro-isoindole-1,3-diones

pp 4921–4931

Krzysztof Kamiński* and Jolanta Obniska

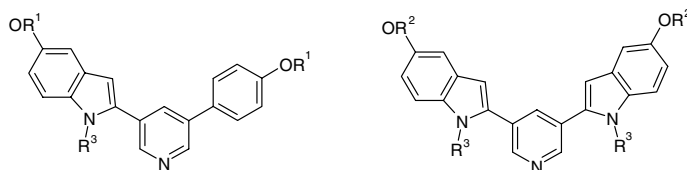


The majority of compounds investigated showed activity in the MES and *sc*PTZ screens the most widely employed seizure models for early identification of candidate anticonvulsants.

Synthesis of 3,5-bis(2-indolyl)pyridine and 3-[(2-indolyl)-5-phenyl]pyridine derivatives as CDK inhibitors and cytotoxic agents

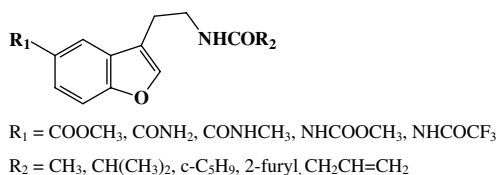
pp 4932–4953

Ulrich Jacquemard, Nathalie Dias, Amélie Lansiaux, Christian Bailly, Cédric Logé, Jean-Michel Robert, Olivier Lozach, Laurent Meijer, Jean-Yves Mèroux and Sylvain Routier*


Design and synthesis of benzofuranic derivatives as new ligands at the melatonin-binding site *MT3*

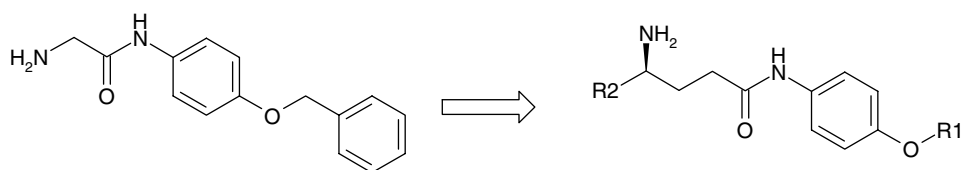
pp 4954–4962

Mohamed Ettaoussi, Basile Péres, Frédérique Klupsch, Philippe Delagrè, Jean-A. Boutin, Pierre Renard, Daniel-H. Caignard, Philippe Chavatte, Pascal Berthelot, Daniel Lesieur and Saïd Yous*


Synthesis of glutamic acid analogs as potent inhibitors of leukotriene *A4* hydrolase

pp 4963–4983

Thomas A. Kirkland,* Marc Adler, John G. Bauman, Ming Chen, Jesper Z. Haeggström, Beverly King, Monica J. Kochanny, Amy M. Liang, Lisa Mendoza, Gary B. Phillips, Marjolein Thunnissen, Lan Trinh, Marc Whitlow, Bin Ye, Hong Ye, John Parkinson and William J. Guilford

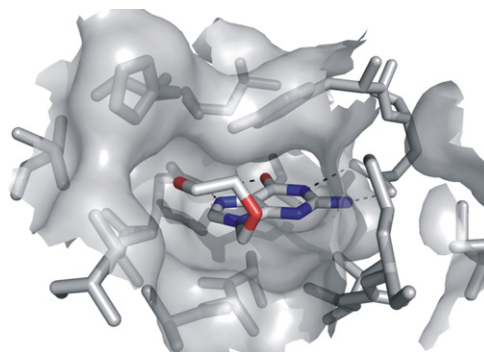


Molecular modeling and dynamics simulations of PNP from *Streptococcus agalactiae*

pp 4984–4993

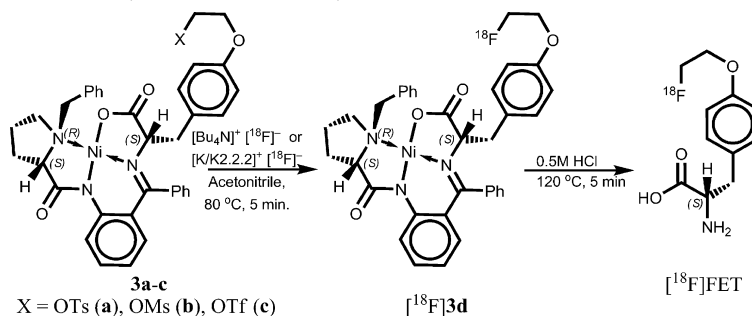
Rafael Andrade Caceres, Luis Fernando Saraiva Timmers,
Raquel Dias, Luiz Augusto Basso,
Diogenes Santiago Santos* and
Walter Filgueira de Azevedo, Jr.*

Six complexes of SaPNP were modeled with six different ligands, molecular dynamics simulations have been performed to evaluate the structural and dynamical properties of SaPNP.

**No carrier added synthesis of *O*-(2'-[¹⁸F]fluoroethyl)-L-tyrosine via a novel type of chiral enantiomerically pure precursor, Ni^{II} complex of a (*S*)-tyrosine Schiff base**

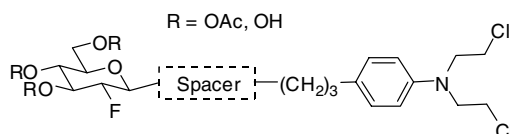
pp 4994–5003

Raisa N. Krasikova,* Olga F. Kuznetsova, Olga S. Fedorova, Victor I. Maleev,
Tatyana F. Saveleva and Yuri N. Belokon

**Synthesis and cytotoxic properties of new fluorodeoxyglucose-coupled chlorambucil derivatives**

pp 5004–5020

Bastien Reux, Valérie Weber,* Marie-Joséphine Galmier, Michèle Borel, Michel Madesclaire,
Jean-Claude Madelmont, Eric Debiton and Pascal Coudert



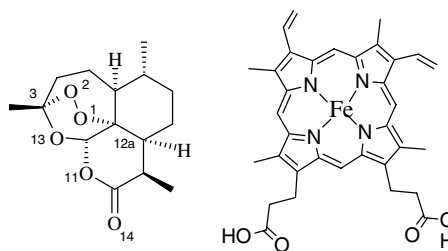
The synthesis and in vitro cytotoxicity of new fluoroglucoconjugates in which chlorambucil is attached to the C-1 position of the FDG skeleton using a variety of linkages are reported.

**Interaction between artemisinin and heme. A Density Functional Theory study of structures and interaction energies**

pp 5021–5029

Jocley Queiroz Araújo, José Walkimar de Mesquita Carneiro,*
Martha Teixeira de Araújo, Franco Henrique Andrade Leite and Alex Gutterres Taranto

Density Functional Theory calculations were employed to calculate interaction energies between the heme group and artemisinin. The results suggest a thermodynamically favorable interaction.

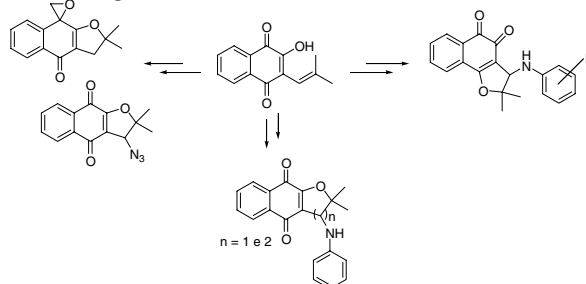


Synthesis and anti-*Trypanosoma cruzi* activity of derivatives from nor-lapachones and lapachones

pp 5030–5038

Eufrânio N. da Silva Júnior, Maria Cecília B. V. de Souza, Michelle C. Fernandes, Rubem F. S. Menna-Barreto, Maria do Carmo F. R. Pinto, Francisco de Assis Lopes, Carlos Alberto de Simone, Carlos Kleber Z. Andrade, Antônio V. Pinto, Vitor F. Ferreira and Solange L. de Castro*

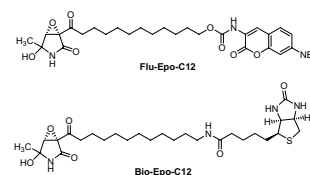
New naphthoquinone derivatives were synthesized and assayed against bloodstream trypomastigote forms of *Trypanosoma cruzi*, the etiological agent of Chagas' disease. From nor-lapachol were prepared five substituted *ortho*-naphthofuranquinones, a non-substituted *para*-naphthofuranquinone, a new oxyrane and an azide and from α -lapachone a new non-substituted *para*-naphthofuranquinone. Other five substituted *ortho*-naphthofuranquinones, recently designed as toxic to cancer lines, were also evaluated.

**Syntheses and applications of fluorescent and biotinylated epolactaene derivatives: Epolactaene and its derivative induce disulfide formation**

pp 5039–5049

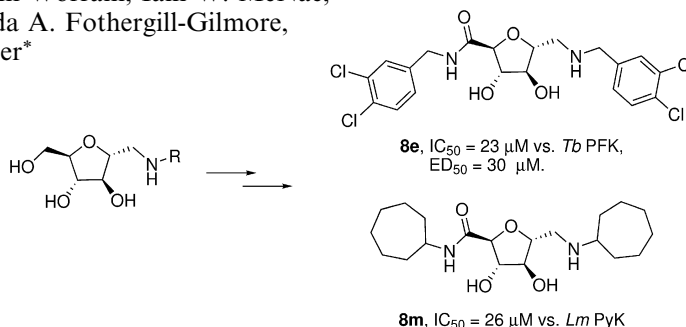
Kouji Kuramochi, Shunsuke Yukizawa, Seiki Ikeda, Takashi Sunoki, Satoshi Arai, Rie Matsui, Akinori Morita, Yoshiyuki Mizushima, Kengo Sakaguchi, Fumio Sugawara, Masahiko Ikekita and Susumu Kobayashi*

Syntheses and applications of fluorescent and biotinylated epolactaene derivatives are described. A hypothetical mechanism of action of epolactaene and its derivatives is proposed.

**Design, synthesis and trypanocidal activity of lead compounds based on inhibitors of parasite glycolysis**

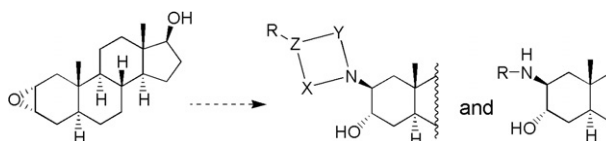
pp 5050–5061

Matthew W. Nowicki, Lindsay B. Tulloch, Liam Worrall, Iain W. McNae, Véronique Hannaert, Paul A. M. Michels, Linda A. Fothergill-Gilmore, Malcolm D. Walkinshaw and Nicholas J. Turner*

**Chemical synthesis of 2 β -amino-5 α -androstane-3 α ,17 β -diol *N*-derivatives and their antiproliferative effect on HL-60 human leukemia cells**

pp 5062–5077

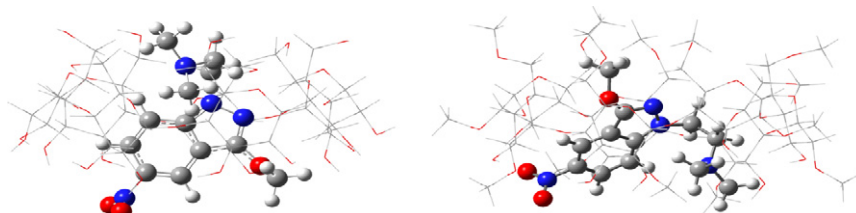
Dominic Thibeault, Jenny Roy, Patrick DeRoy and Donald Poirier*



Characterization, phase-solubility, and molecular modeling of inclusion complex of 5-nitroindazole derivative with cyclodextrins

pp 5078–5084

Carolina Jullian,* Javier Morales-Montecinos, Gerald Zapata-Torres, Benjamín Aguilera, Jorge Rodriguez, Vicente Arán and Claudio Olea-Azar

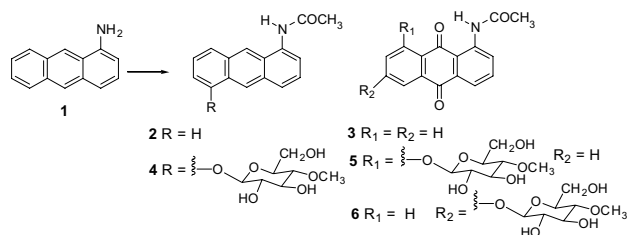


The inclusion properties of 5-nitroindazole into native and (2,6-dimethyl)- β -cyclodextrin were evaluated using phase-solubility studies, electrochemistry, NMR and molecular modeling techniques.

Microbial metabolism of 1-aminoanthracene by *Beauveria bassiana*

pp 5085–5089

Jixun Zhan and A. A. Leslie Gunatilaka*

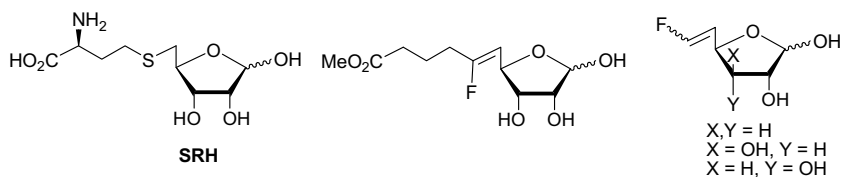


1-Aminoanthracene (**1**) was biotransformed by *Beauveria bassiana* to yield five metabolites **2–6**, the formation of which involved acetylation, oxidation, hydroxylation, and *O*-methylglucosylation reactions.

S-Ribosylhomocysteine analogues with the carbon-5 and sulfur atoms replaced by a vinyl or (fluoro)vinyl unit

pp 5090–5102

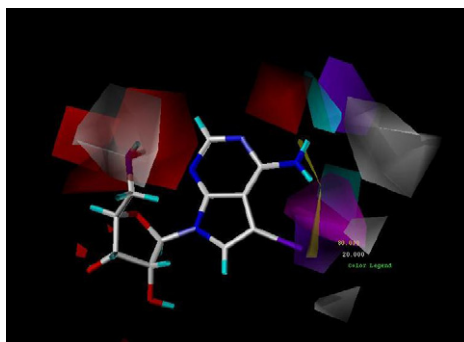
Stanislaw F. Wnuk,* Jennifer Lalama, Craig A. Garmendia, Jenay Robert, Jinge Zhu and Dehua Pei



A CoMSIA study on the adenosine kinase inhibition of pyrrolo[2,3-*d*]pyrimidine nucleoside analogues

pp 5103–5108

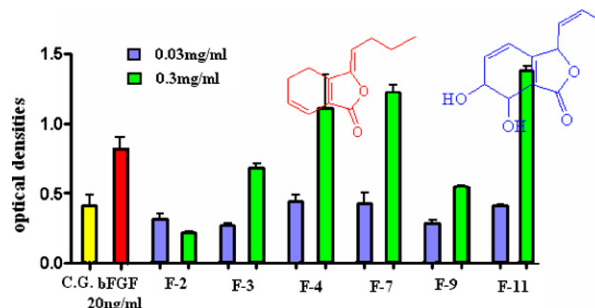
Julio Caballero,* Michael Fernández and Fernando D. González-Nilo



Characterization of chemical components in extracts from *Si-wu* decoction with proliferation-promoting effects on rat mesenchymal stem cells

pp 5109–5114

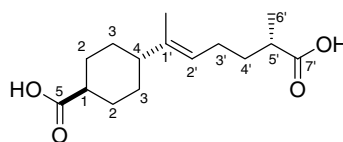
He-Ping Zeng,* Ting-Ting Wang, Wei Chen, Chun-Yan Wang, Dong-Feng Chen and Jian-Gang Shen*



Hymenoic acid, a novel specific inhibitor of human DNA polymerase λ from a fungus of *Hymenochaetaceae* sp.

pp 5115–5122

Masayuki Nishida, Noriko Ida, Mao Horio, Toshifumi Takeuchi, Shinji Kamisuki, Hiroshi Murata, Kouji Kuramochi, Fumio Sugawara, Hiromi Yoshida and Yoshiyuki Mizushima*



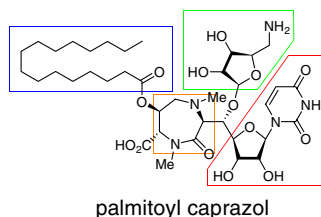
Hymenoic acid

Hymenoic acid (**1**) is a novel sesquiterpene, *trans*-4-[(1'*E*,5'*S*)-5'-carboxy-1'-methyl-1'-hexenyl]cyclohexanecarboxylic acid, isolated from cultures of a fungus, *Hymenochaetaceae* sp., and this compound selectively inhibited the activities of eukaryotic pol λ .

Structure–activity relationship of truncated analogs of caprazamycins as potential anti-tuberculosis agents

pp 5123–5133

Shinpei Hirano, Satoshi Ichikawa* and Akira Matsuda*



palmitoyl caprazol

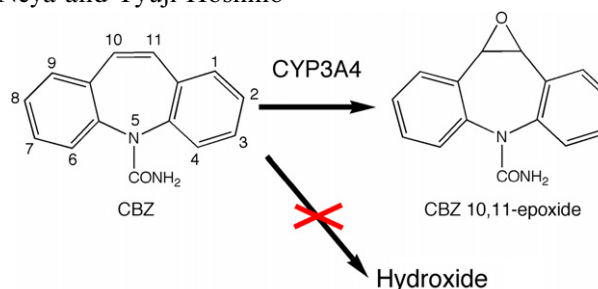
Synthesis and structure–activity relationship studies of caprazamycin (CPZ) analogs, including the aminoribose-truncated and the uridine-truncated one have been carried out.

An epoxidation mechanism of carbamazepine by CYP3A4

pp 5134–5148

Masayuki Hata,* Yoshikazu Tanaka, Naoko Kyoda, Taisuke Osakabe, Hitomi Yuki, Itsuko Ishii, Mitsukazu Kitada, Saburo Neya and Tyuji Hoshino

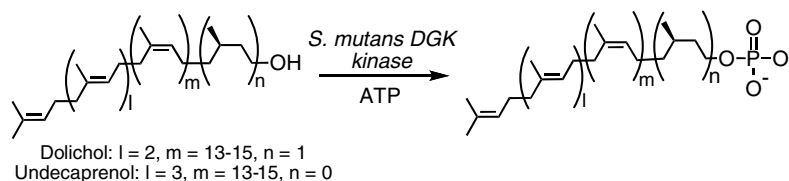
To clarify the reason why CYP3A4 produces an epoxide rather than a hydroxide, the mechanism of epoxidation of carbamazepine (CBZ) by CYP3A4 was investigated by theoretical calculations.



Chemoenzymatic synthesis of polyprenyl phosphates

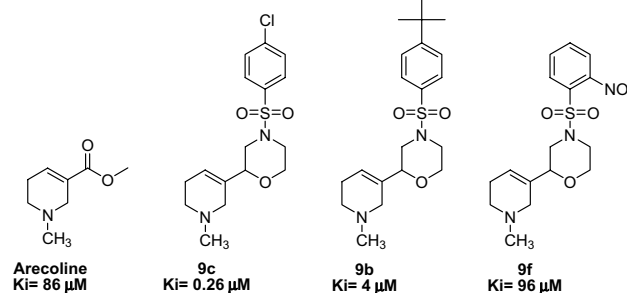
pp 5149–5156

Meredith D. Hartley, Angelyn Larkin and Barbara Imperiali*

**Effect of novel *N*-aryl sulfonamide substituted 3-morpholino arecoline derivatives as muscarinic receptor 1 agonists in Alzheimer's dementia models**

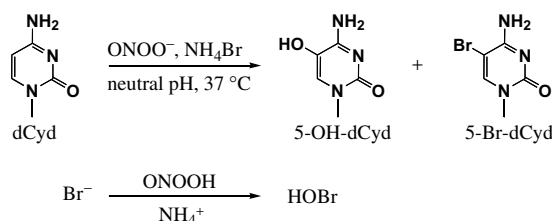
pp 5157–5163

Y. C. Sunil Kumar, Manish Malviya, J. N. Narendra Sharath Chandra, C. T. Sadashiva, C. S. Ananda Kumar, S. B. Benaka Prasad, D. S. Prasanna, M. N. Subhash and K. S. Rangappa*

**Reaction of 2'-deoxycytidine with peroxynitrite in the presence of ammonium bromide**

pp 5164–5170

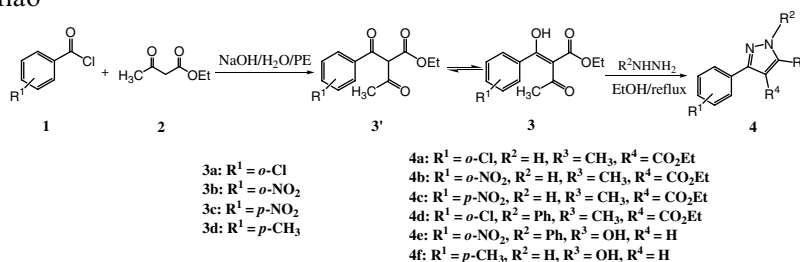
Toshinori Suzuki,* Kazuya Ida, Shinya Uchibe and Michiyo Inukai

**Synthesis and discovery of a novel pyrazole derivative as an inhibitor of apoptosis through modulating integrin β_4 , ROS, and p53 levels in vascular endothelial cells**

pp 5171–5180

Bao-Xiang Zhao,* Lu Zhang, Xing-Shang Zhu, Mao-Sheng Wan, Jing Zhao, Yun Zhang, Shang-Li Zhang and Jun-Ying Miao*

Six novel multi-pyrazole derivatives have been synthesized and characterized by IR, ^1H NMR, mass spectroscopy, and element analysis. Ethyl 3-(*o*-chlorophenyl)-5-methyl-1-phenyl-1*H*-pyrazole-4-carboxylate (MPD) at low concentration ($25 \mu\text{M}$) increased VEC viability and inhibited VEC apoptosis through down-regulating the levels of integrin β_4 , p53, and ROS increased by deprivation of serum and FGF-2 in vascular endothelial cells.

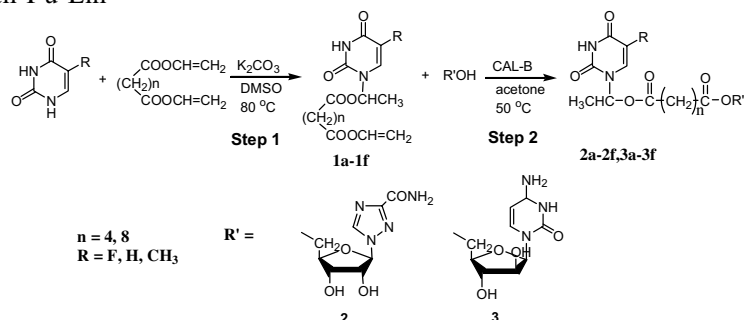


Facile synthesis of novel mutual derivatives of nucleosides and pyrimidines by regioselectively chemo-enzymatic protocol

pp 5181–5188

Xueqi Qian, Bokai Liu, Qi Wu, Deshui Lv and Xian-Fu Lin*

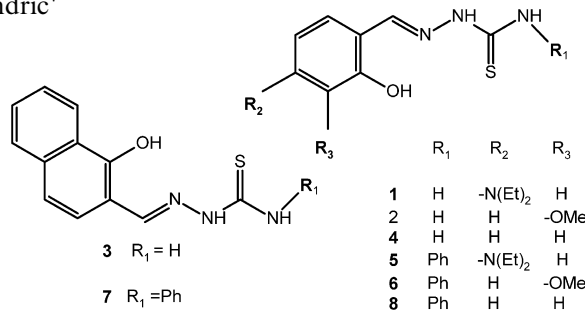
A facile regioselectively chemo-enzymatic synthesis procedure for the preparation of novel mutual derivatives of nucleosides and pyrimidines was developed by sequential Markovnikov addition and acylation.



Novel thiosemicarbazone derivatives as potential antitumor agents: Synthesis, physicochemical and structural properties, DNA interactions and antiproliferative activity

pp 5189–5198

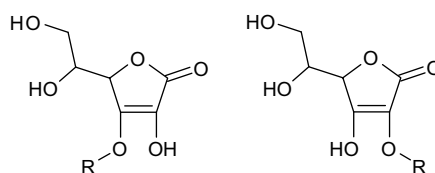
Ivica Dilović, Mirta Rubčić, Višnja Vrdoljak, Sandra Kraljević Pavelić, Marijeta Kralj, Ivo Piantanida* and Marina Cindrić*



Novel antioxidant agents deriving from molecular combination of Vitamin C and NO-donor moieties

pp 5199–5206

Clara Cena, Konstantin Chegae, Silvia Balbo, Loretta Lazzarato, Barbara Rolando, Marta Giorgis, Elisabetta Marini, Roberta Fruttero and Alberto Gasco*



R = NO -donor substructures

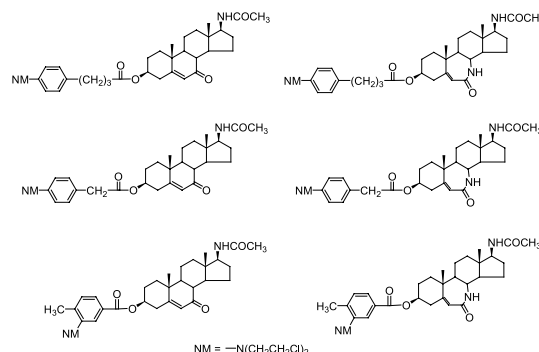
A new class of products in which NO-donor moieties are linked to either the 3-OH or 2-OH group of ascorbic acid was synthesized. Their physico-chemical properties, antioxidant and vasodilator activities are discussed.

Rational design, synthesis, and in vivo evaluation of the antileukemic activity of six new alkylating steroidal esters

pp 5207–5215

Anna I. Koutsourea, Manolis A. Foustieris, Evagelia S. Arsenou, Athanasios Papageorgiou, George N. Pairas and Sotiris S. Nikolaropoulos*

The SAR study of six novel alkylating steroidal esters is described. The 17β-acetamido-B-lactamic steroidal skeleton contributes significantly to the compounds' selectivity toward P388 and L1210 leukemic cells.



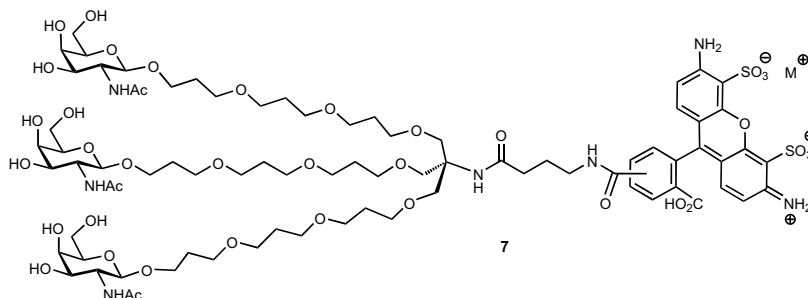
Trivalent, Gal/GalNAc-containing ligands designed for the asialoglycoprotein receptor

pp 5216–5231

Oleg Khorev, Daniela Stokmaier, Oliver Schwardt, Brian Cutting and Beat Ernst*

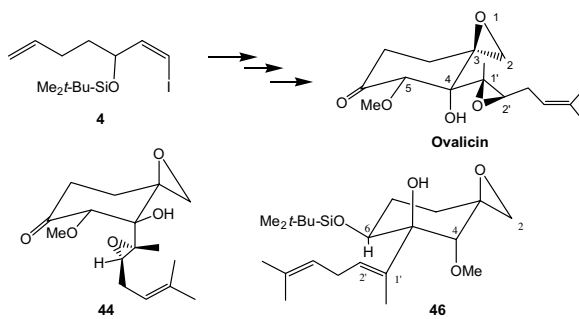
A step closer toward liver-specific drug delivery:

The novel, fluorescent-labeled liver targeting device **7** bearing three GalNAc moieties, and designed for efficient interaction with the asialoglycoprotein receptor (ASGP-R), has been synthesized. It evinced efficient uptake by, and high selectivity for human hepatocytes as could be demonstrated using fluorescence microscopy and flow cytometry.

**Total syntheses of (±)-ovalicin, C4(S*)-isomer, and its C5-analogs and anti-trypanosomal activities**

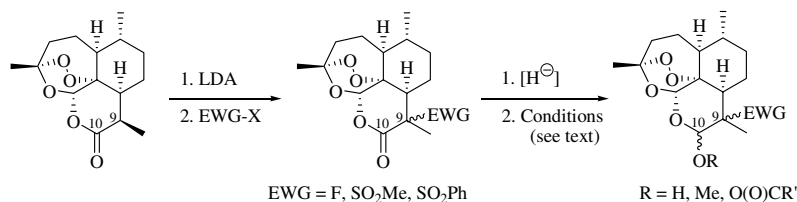
pp 5232–5246

Duy H. Hua,* Huiping Zhao, Srinivas K. Battina, Kaiyan Lou, Ana L. Jimenez, John Desper, Elisabeth M. Perchellet, Jean-Pierre H. Perchellet and Peter K. Chiang

**Electronically stabilized versions of the antimalarial acetal trioxanes artemether and artesunate**

pp 5247–5253

Gary H. Posner,* William A. Maio and Alvin S. Kalinda

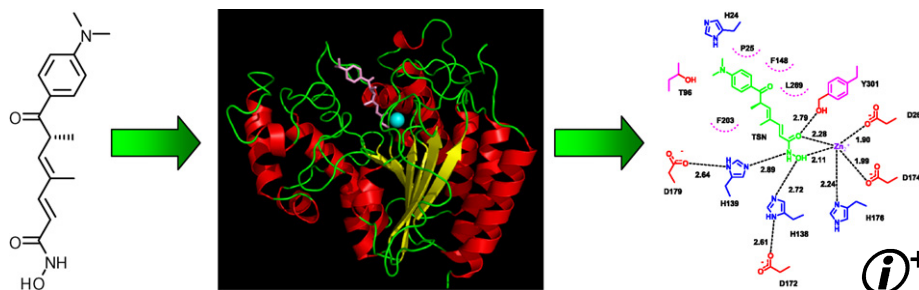
**Structural insights into the *Plasmodium falciparum* histone deacetylase 1 (PfHDAC-1):**

pp 5254–5265

A novel target for the development of antimalarial therapy

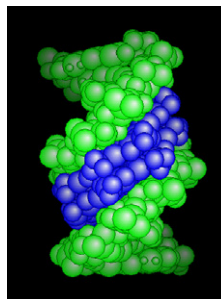
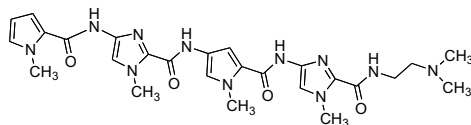
Prasenjit Mukherjee, Anupam Pradhan, Falgun Shah, Babu L. Tekwani and Mitchell A. Avery*

A ligand-refined homology model of *Plasmodium falciparum* histone deacetylase 1 was generated and a predictive docking protocol was established for structure-based drug design applications.



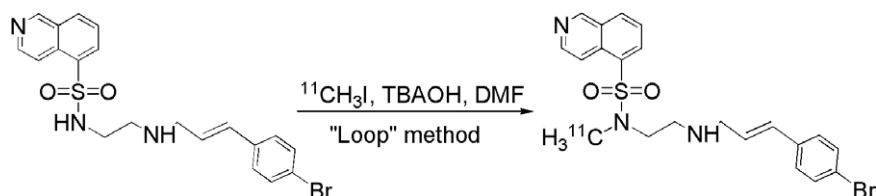
Modifying the N-terminus of polyamides: PyImPyIm has improved sequence specificity over f-ImPyIm pp 5266–5276

Toni Brown, Hilary Mackay, Mark Turlington, Arden Sutterfield, Traci Smith, Alan Sielaff, Laura Westrate, Chrystal Bruce, Jerome Kluza, Caroline O'Hare, Binh Nguyen, W. David Wilson, John A. Hartley and Moses Lee*

**Rationally designed PKA inhibitors for positron emission tomography: Synthesis and cerebral biodistribution of *N*-(2-(4-bromocinnamylamino)ethyl)-*N*-[¹¹C]methyl-isoquinoline-5-sulfonamide**

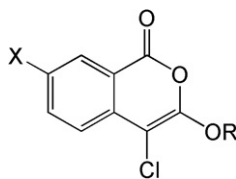
pp 5277–5284

Neil Vasdev,* Frank J. LaRonde, James R. Woodgett, Armando Garcia, Elizabeth A. Rubie, Jeffrey H. Meyer, Sylvain Houle and Alan A. Wilson

**Isocoumarin-based inhibitors of pancreatic cholesterol esterase**

pp 5285–5294

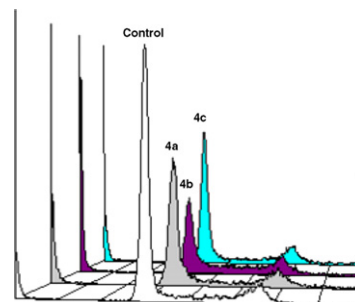
Justin J. Heynekamp, Lucy A. Hunsaker, Thomas A. Vander Jagt, Robert E. Royer, Lorraine M. Deck* and David L. Vander Jagt*

**Synthesis and biological evaluation of thiobenzanilides as anticancer agents**

pp 5295–5302

Wan-Ping Hu, Hsin-Su Yu, Yan-Ren Chen, Yi-Min Tsai, Yin-Kai Chen, Chao-Cheng Liao, Long-Sen Chang and Jeh-Jeng Wang*

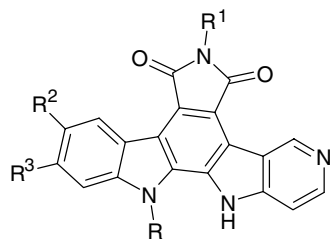
Cell cycle distribution of A375 cells after treating with thiobenzanilides (**4a–c**).



Novel 5-azaindolocarbazoles as cytotoxic agents and Chk1 inhibitors

pp 5303–5321

Myriam Lefoix, Gérard Coudert,* Sylvain Routier, Bruno Pfeiffer, Daniel-Henri Caignard, John Hickman, Alain Pierré, Roy M. Golsteyn, Stéphane Léonce, Céline Bossard and Jean-Yves Mèroux*

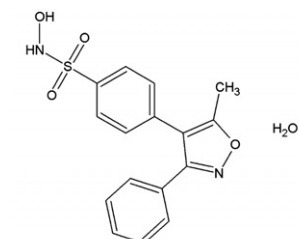


R = H, glucopyranosyl
 R¹ = H, , CH₃, CH₂CH₂N(CH₃)₂
 R² or R³ = H, OH, OBn
 R², R³ = -OCH₂O-

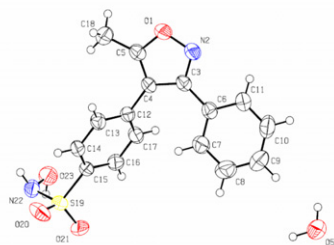
Chemical and biological investigation of *N*-hydroxy-valdecocix: An active metabolite of valdecocix

pp 5322–5330

Péter Erdélyi,* Tamás Fodor, Ágnes Kis Varga, Mátyás Czugler, Anikó Gere and János Fischer

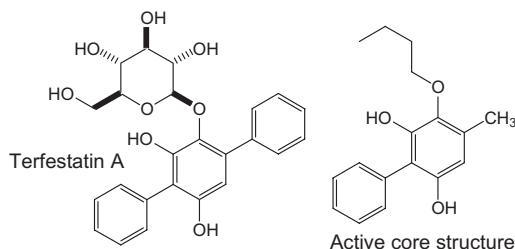


N-Hydroxy-valdecocix monohydrate

**Active core structure of terfestatin A, a new specific inhibitor of auxin signaling**

pp 5331–5344

Ken-ichiro Hayashi,* Atsushi Yamazoe, Yuki Ishibashi, Naoyuki Kusaka, Yutaka Oono and Hiroshi Nozaki

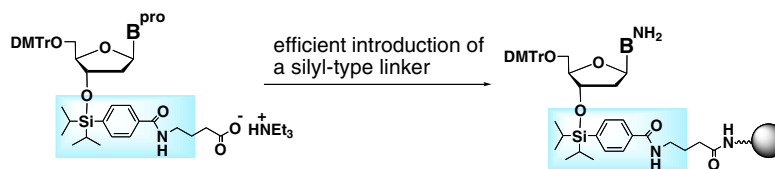


From SAR study of 25 derivatives of terfestatin A, auxin signaling inhibitor, the essential active core structure of terfestatin A was identified.

**Efficient synthesis of functionalized oligodeoxyribonucleotides with base-labile groups using a new silyl linker**

pp 5345–5351

Akihiro Ohkubo, Rintaro Kasuya, Katsufumi Aoki, Akio Kobori, Haruhiko Taguchi, Kohji Seio and Mitsuo Sekine*




We developed new loading reagents with a new silyl-type linker for DNA synthesis. These reagents could increase the efficiency of introduction of 3'-terminal deoxyribonucleoside components into polymer supports to a level of 17–29 $\mu\text{mol/g}$.

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*Corresponding author

+ Supplementary data available via ScienceDirect

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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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