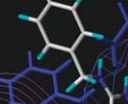
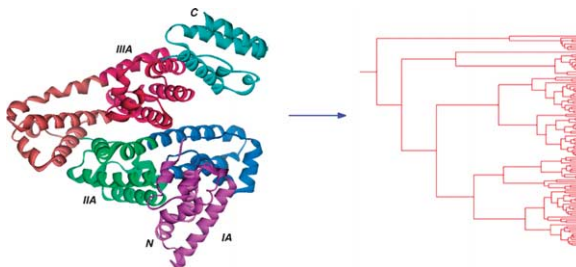


Wei Li, Yun Tang,* You-Li Zheng and Zhui-Bai Qiu*

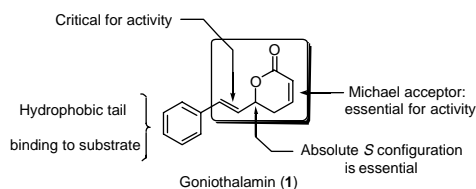


Jianzhong Liu,* Liu Yang, Yi Li, Dahua Pan and Anton J. Hopfinger



Cluster analysis and 4D-MS were used to explore the human serum albumin (HSA) binding affinity prediction.

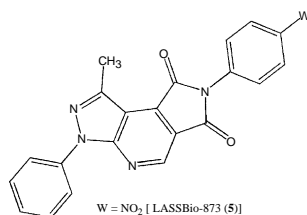
Ângelo de Fátima, Luciana K. Kohn, João Ernesto de Carvalho and Ronaldo A. Pilli*



Design, synthesis, and pharmacological evaluation of new neuroactive pyrazolo [3,4-*b*]pyrrolo[3,4-*d*]pyridine derivatives with in vivo hypnotic and analgesic profile

pp 632–640

Ricardo Menegatti, Gilberto M. S. Silva, Gisele Zapata-Sudo, Juliana M. Raimundo, Roberto T. Sudo, Eliezer J. Barreiro and Carlos A. M. Fraga*



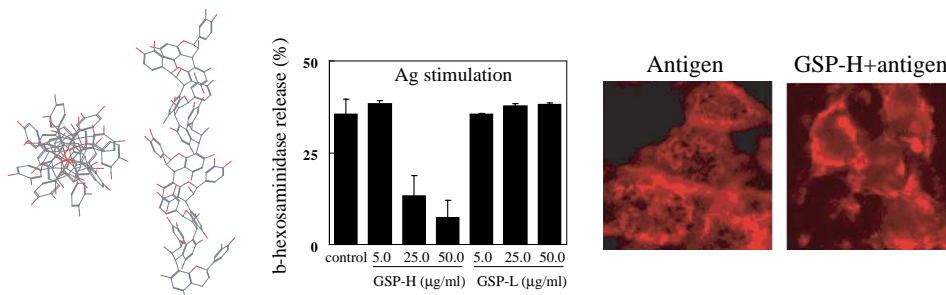
The new powerful central-acting heterotricyclic analgesic agent LASSBio-873 (5) is reported.



Polymeric grape-seed procyanidins, but not monomeric catechins and oligomeric procyanidins, impair degranulation and membrane ruffling in RBL-2H3 cells

pp 641–649

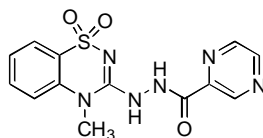
Kazunari Kondo,* Riichiro Uchida, Shoichi Tokutake and Tamio Maitani



Anti-tubercular agents. Part 3. Benzothiadiazine as a novel scaffold for anti-*Mycobacterium* activity

pp 650–658

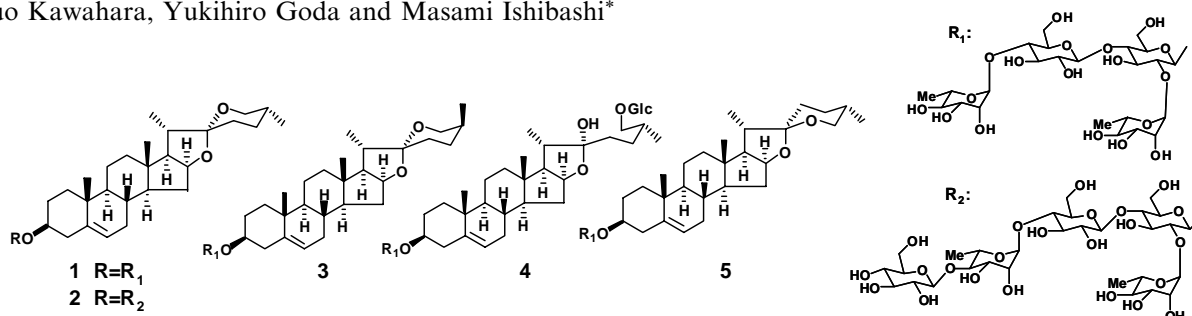
Ahmed Kamal,* K. Srinivasa Reddy, S. Kaleem Ahmed, M. Naseer A. Khan, Rakesh K. Sinha, J. S. Yadav and Sudershan K. Arora



Steroidal saponins from *Calamus insignis*, and their cell growth and cell cycle inhibitory activities

pp 659–665

Takashi Ohtsuki, Masaaki Sato, Takashi Koyano, Thaworn Kowithayakorn, Nobuo Kawahara, Yukihiro Goda and Masami Ishibashi*



Putative drug binding conformations of monoamine transporters

pp 666–675

Aina Westrheim Ravna,* Ingebrigt Sylte, Kurt Kristiansen and Svein G. Dahl

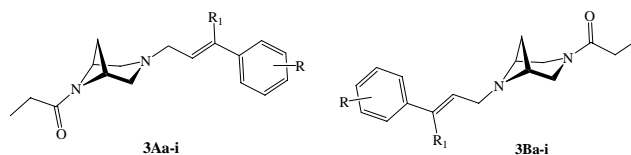


Models of monoamine transporters have been constructed, and *S*-citalopram, cocaine, and *S*-amphetamine have been docked into their putative binding sites using molecular modeling techniques.

Synthesis of 3,6-diazabicyclo[3.1.1]heptanes as novel ligands for the opioid receptors

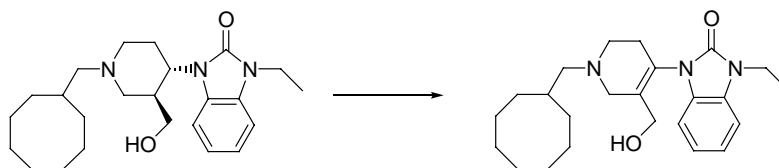
pp 676–691

Giovanni Loriga, Ilaria Manca, Gabriele Murineddu, Giorgio Chelucci, Stefania Villa, Stefania Gessi, Lucio Toma, Giorgio Cignarella and Gerard A. Pinna*

**Identification of an achiral analogue of J-113397 as potent nociceptin/orphanin FQ receptor antagonist**

pp 692–704

Claudio Trapella, Remo Guerrini,* Laura Piccagli, Girolamo Calo', Giacomo Carra', Barbara Spagnolo, Samantha Rubini, Giulia Fanton, Christopher Hebbes, John McDonald, David G. Lambert, Domenico Regoli and Severo Salvadori

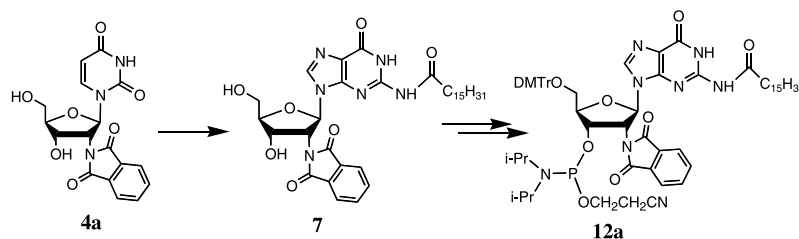


The compound coded as Trap-101 is an achiral analogue of the nociceptin/orphanin FQ receptor antagonist J-113397 that combines a pharmacological profile similar to that of the parent compound with a practical, high-yielding preparation.

Improved synthesis of 2'-amino-2'-deoxyguanosine and its phosphoramidite

pp 705–713

Qing Dai, Shirshendu K. Deb, James L. Hougland and Joseph A. Piccirilli*

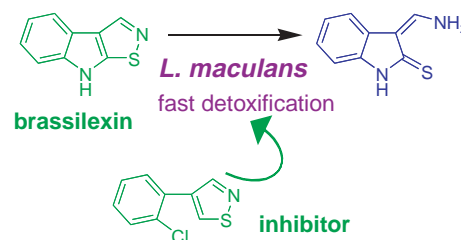


Design, synthesis, and antifungal activity of inhibitors of brassilexin detoxification in the plant pathogenic fungus *Leptosphaeria maculans*

pp 714–723

M. Soledade, C. Pedras* and Mojmir Suchy

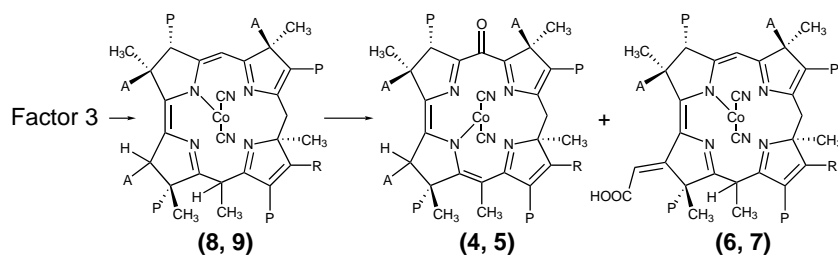
Potential detoxification inhibitors were designed and synthesized based on the planar heteroaromatic structure of isothiazolo[5,4-*b*]indole. 4-(2-Chlorophenyl)-isothiazole had the largest inhibitory effect on the rate of brassilexin detoxification.



Structural characterization of novel cobalt corrinoids synthesized by enzymes of the vitamin B₁₂ anaerobic pathway

pp 724–731

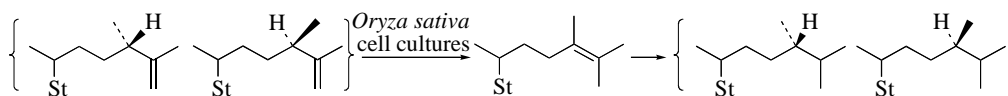
Patricio J. Santander,* Yasuhiro Kajiwar, Howard J. Williams and A. Ian Scott*



Metabolic conversion of 24-methyl- Δ^{25} -cholesterol to 24-methylcholesterol in higher plants

pp 732–738

Kyoko Takahashi,* Kozue Nasu, Tadahiko Mashino, Masuo Morisaki, Noriyuki Hara and Yoshinori Fujimoto

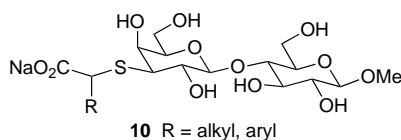


Feeding of [27-¹³C]codisterol, [27-¹³C]24-epicodisterol, [23,24-²H₂]codisterol, and [26,27-²H₆]24-methyl-desmosterol to *Oryza sativa* cell cultures revealed that both (24*R*)- and (24*S*)-epimers of 24-methyl- Δ^{25} -cholesterol were converted to dihydrobrassicasterol/campesterol via the common intermediate 24-methyl-desmosterol.

The synthesis and biological evaluation of lactose-based sialylmimetics as inhibitors of rotaviral infection

pp 739–757

Angela Liakatos, Milton J. Kiefel, Fiona Fleming, Barbara Coulson and Mark von Itzstein*



The synthesis and biological evaluation of a series of lactose-based sialylmimetics of the general structure **10** is presented.

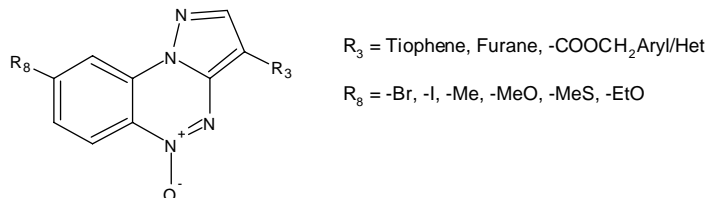


Benzodiazepine receptor ligands. 8: Synthesis and pharmacological evaluation of new pyrazolo[5,1-*c*] [1,2,4]benzotriazine 5-oxide 3- and 8-disubstituted: High affinity ligands endowed with inverse-agonist pharmacological efficacy

pp 758–775

Gabriella Guerrini,* Annarella Costanzo, Giovanna Ciciani, Fabrizio Bruni, Silvia Selleri, Camilla Costagli, François Besnard, Barbara Costa, Claudia Martini, Gaetano De Siena and Petra Malmberg-Aiello

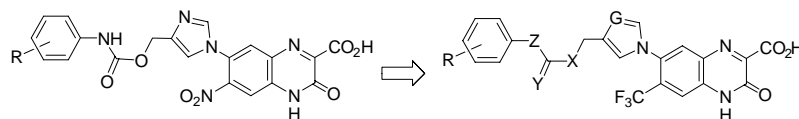
The synthesis, biological and pharmacological investigation on new 3-arylesters and 3-heteroarylpyrazolo[5,1-*c*] [1,2,4]benzotriazine 5-oxide 8-substituted are reported. The structure–activity relationships for these compounds are discussed. Compounds **4d** and **6d** emerge for their inverse-agonist profile from in vivo tests.



Design and synthesis of novel 7-heterocycle-6-trifluoromethyl-3-oxoquinoxaline-2-carboxylic acids bearing a substituted phenyl group as superior AMPA receptor antagonists with good physicochemical properties

pp 776–792

Yasuo Takano,* Futoshi Shiga, Jun Asano, Wataru Hori, Kazunori Fukuchi, Tsuyoshi Anraku and Takashi Uno

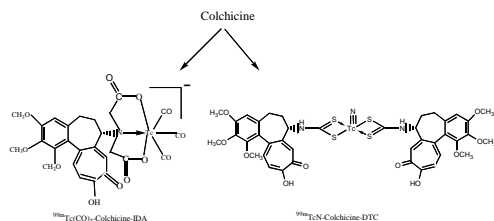


We describe the design, synthesis, and physicochemical properties and biological properties of a novel series of 7-heterocycle-6-trifluoromethyl-3-oxoquinoxaline-2-carboxylic acids which bear a substituted phenyl group through a urethane or urea linkage at the 7 position.

$^{99\text{m}}\text{Tc}$ -labeling of colchicine using $[^{99\text{m}}\text{Tc}(\text{CO})_3(\text{H}_2\text{O})_3]^+$ and $[^{99\text{m}}\text{Tc}\equiv\text{N}]^{2+}$ core for the preparation of potential tumor-targeting agents

pp 793–799

Aruna Korde, Drishti Satpati, Anupam Mathur, Madhava Mallia, Sharmila Banerjee,* Kanchan Kothari, H. D. Sarma, Pradeep Choudhari and Meera Venkatesh



The binding of DNA intercalating and non-intercalating compounds to A-form and protonated form of poly(rC)·poly(rG): Spectroscopic and viscometric study

pp 800–814

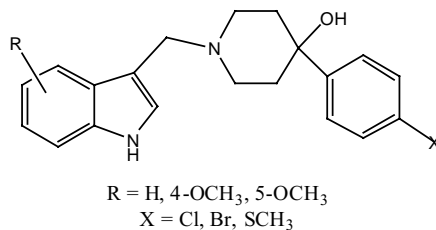
Rangana Sinha, Md. M. Islam, Kakali Bhadra, Gopinatha Suresh Kumar,* Anamika Banerjee and Motilal Maiti

Interaction of DNA intercalators (ethidium, actinomycin D, and methylene blue), partial intercalator (berberine), and groove binder (distamycin A) with A-form and protonated form of poly(rC)·poly(rG) structures clearly established that the complex of ethidium-A-form and methylene blue-protonated form occurred by intercalation process, while partial intercalation was observed in berberine-protonated form complexation. Actinomycin D does not bind to either of the polynucleotide structures. The complexation of ethidium-protonated form, methylene blue-A-form, berberine-A-form, distamycin A-protonated, and A-form is formed by non-intercalative mechanism.

Synthesis and characterization of selective dopamine D₂ receptor antagonists

pp 815–825

Suwanna Vangveravong, Elizabeth McElveen, Michelle Taylor, Jinbin Xu, Zhude Tu, Robert R. Luedtke and Robert H. Mach*

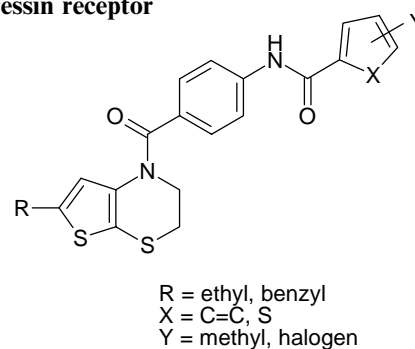


A series of indole analogs having a high affinity for dopamine D₂ versus D₃ and D₄ receptors is reported. These compounds were found to function as antagonists of the D₂ receptor.


Studies on the chemistry of thienoanellated *O,N*- and *S,N*-containing heterocycles. Part 30: Synthesis and pharmacological properties of thieno[2,3-*b*][1,4]thiazines with potential vasopressin receptor antagonistic activity

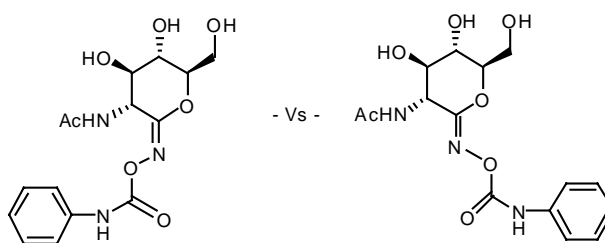
pp 826–836

Maria E. Galanski, Thomas Erker,* Norbert Handler, Rosa Lemmens-Gruber, Majidreza Kamyar and Christian R. Studenik

**Inhibition of *O*-GlcNAcase by PUGNAc is dependent upon the oxime stereochemistry**

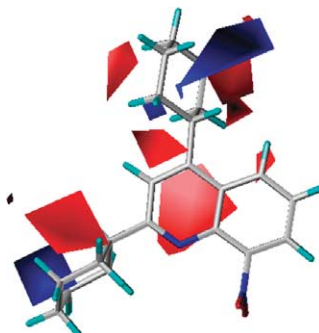
pp 837–846

Melissa Perreira, Eun Ju Kim, Craig J. Thomas* and John A. Hanover

**3D-QSAR study of ring-substituted quinoline class of anti-tuberculosis agents**

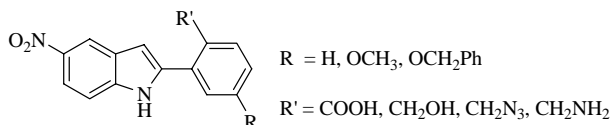
pp 847–856

Amit Nayyar, Alpeshkumar Malde, Rahul Jain* and Evans Coutinho*



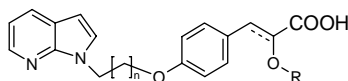
Synthesis of functionalised 2-aryl-5-nitro-1*H*-indoles and their activity as bacterial NorA efflux pump inhibitors pp 857–865

Siritron Samosorn, John B. Bremner,* Anthony Ball and Kim Lewis



Synthesis and evaluation of azaindole- α -alkyloxyphenylpropionic acid analogues as PPAR α/γ agonists pp 866–874

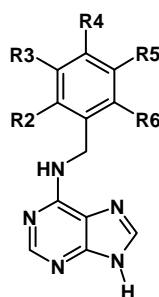
Zhefeng Cai, Jun Feng, Yanshen Guo, Pingping Li, Zhufang Shen, Fengming Chu and Zongru Guo*



A series of azaindole- α -alkyloxyphenylpropionic acid analogues was synthesized and evaluated for PPAR agonist activities. Structure–activity relationship was developed for PPAR α/γ dual agonism. One of the synthesized compounds **7a** was identified as a potent, selective PPAR α/γ dual agonist.

Preparation and biological activity of 6-benzylaminopurine derivatives in plants and human cancer cells pp 875–884

Karel Doležal,* Igor Popa, Vladimír Kryštof, Lukáš Spíchal, Martina Fojtíková, Jan Holub, René Lenobel, Thomas Schmülling and Miroslav Strnad



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Summary of instructions to authors

p I

*Corresponding author

Supplementary data available via ScienceDirect

COVER

2006: The cover figure shows a synthetic multifunctional pore that is composed of rigid-rod staves (para-octiphenyls, tan) and beta-sheet hoops (arrows) and can be activated with external ligands (fullerenes, golden spheres) and closed with internal blockers (alpha-helix, red ribbon) [Gorteau, V.; Bollot, G.; Mareda, J.; Pasini, D.; Tran, D.-H.; Lazar, A. N.; Coleman, A. W.; Sakai, N.; Matile, S. *Bioorg. Med. Chem.* **2005**, *13*, 5171–5180].



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