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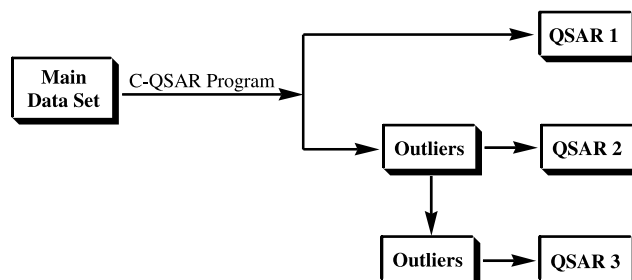
REVIEW

An approach toward the problem of outliers in QSAR

pp 4597–4621

Rajeshwar P. Verma* and Corwin Hansch

Outliers are valuable in defining the limitations under which chemicals act by a common molecular mechanism modeled by one or more descriptors. To explain the peculiar behavior of the outliers, the main data set has been divided according to the figure shown at right.



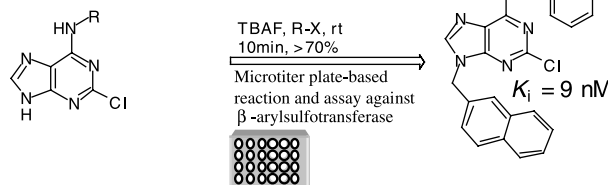
ARTICLES

Tetrabutylammonium fluoride-assisted rapid N⁹-alkylation on purine ring: Application to combinatorial reactions in microtiter plates for the discovery of potent sulfotransferase inhibitors in situ

pp 4622–4626

Ashraf Brik, Chung-Yi Wu, Michael D. Best and Chi-Huey Wong*

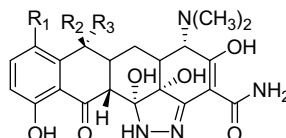
Combinatorial reactions in microtiter plates followed by screening in situ have been developed with the use of tetrabutylammonium fluoride to accelerate the N⁹-alkylation of purine derivatives with organic halides as demonstrated in the discovery of the most potent arylsulfotransferase inhibitor to date.



1,12-Substituted tetracyclines as antioxidant agents

pp 4627–4637

Jittiwud Lertvorachon, Jong-Pyung Kim, Dmitriy V. Soldatov, Jason Boyd,
Gheorghe Roman, Sung Ju Cho, Tomasz Popek, Young-Sik Jung,
Peter C. K. Lau and Yasuo Konishi*

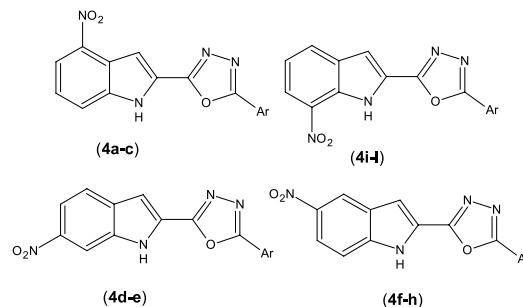


Synthesis of some new biologically active 1,3,4-oxadiazolyl nitroindoles and a modified Fischer indole synthesis of ethyl nitro indole-2-carboxylates

pp 4638–4644

B. Narayana,* B. V. Ashalatha, K. K. Vijaya Raj, J. Fernandes and B. K. Sarojini

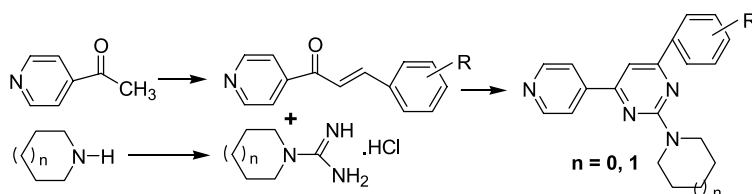
An efficient and modified synthesis of ethyl-4-nitro/5-nitro/6-nitro and 7-nitro-indole-2-carboxylates is described. Carbohydrazides of corresponding ethyl nitroindole-2-carboxylates are converted to 1,3,4-oxadiazolyl nitroindoles and studied for their anti-inflammatory activity.



Synthesis of 2,4,6-trisubstituted pyrimidines as antimalarial agents

pp 4645–4650

Anu Agarwal, Kumkum Srivastava, S. K. Puri and Prem M. S. Chauhan*

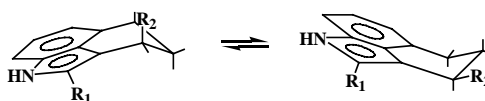


A series of 2,4,6-trisubstituted-pyrimidines were synthesized and evaluated for their in vitro antimalarial activity. Of the 18 compounds synthesized, 14 compounds showed MIC in the range of 0.25–2 µg/mL.

Synthesis and conformational study of 3,4-carbocyclic bridged indole melatonin and serotonin analogues

pp 4651–4657

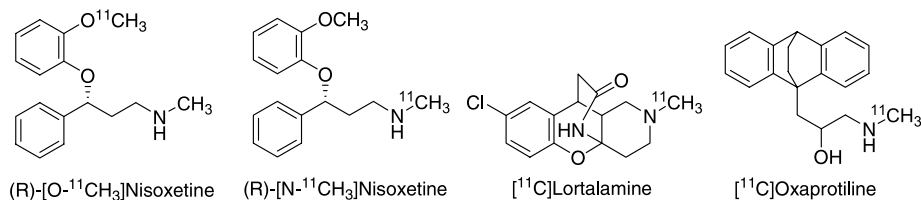
Annalida Bedini, Barbara Di Giacomo, Giuseppe Gatti* and Gilberto Spadoni



Synthesis and C-11 labeling of three potent norepinephrine transporter selective ligands ((R)-nisoxetine, lortalamine, and oxaprotiline) for comparative PET studies in baboons

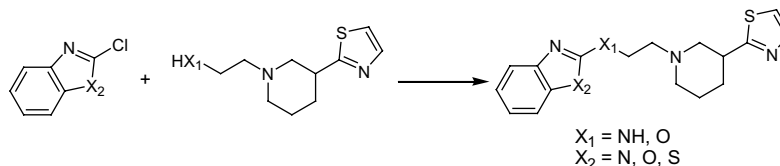
pp 4658–4666

Kuo-Shyan Lin and Yu-Shin Ding*



Synthesis and evaluation of 3-aryl piperidine analogs as potent and efficacious dopamine D₄ receptor agonists pp 4667–4678

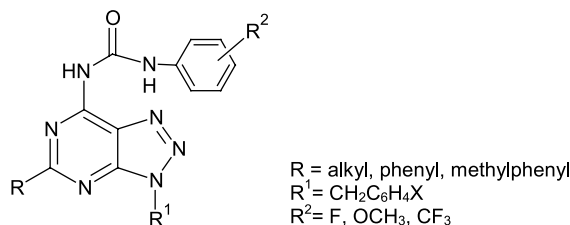
Xueqing Wang,* Pramila A. Bhatia, Jerome F. Daanen, Steve P. Latsaw, Jeffrey Rohde, Teodozyi Kolasa, Ahmed A. Hakeem, Mark A. Matulenko, Masaki Nakane, Marie E. Uchic, Loan N. Miller, Renjie Chang, Robert B. Moreland, Jorge D. Brioni and Andrew O. Stewart



2,9-Disubstituted-*N*⁶-(arylcarbamoyl)-8-azaadenines as new selective A₃ adenosine receptor antagonists: pp 4679–4693

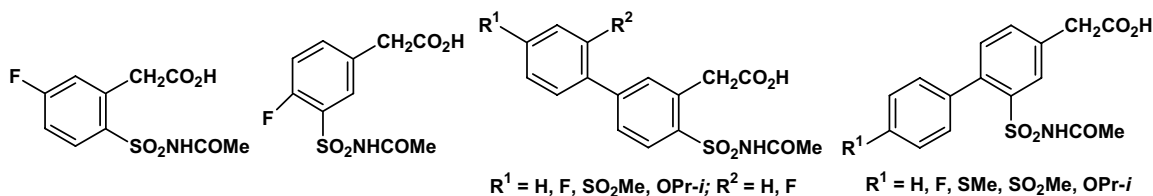
Synthesis, biochemical and molecular modelling studies

Giuliana Biagi, Anna Maria Bianucci, Alessio Coi, Barbara Costa, Laura Fabbrini, Irene Giorgi,* Oreste Livi, Iolanda Micco, Federica Pacchini, Edoardo Santini, Michele Leonardi, Fatena Ahmad Nofal, Oreste LeRoy Salerni and Valerio Scartoni



Design, synthesis, and biological evaluation of *N*-acetyl-2-(or 3)-carboxymethylbenzenesulfonamides as cyclooxygenase isozyme inhibitors pp 4694–4703

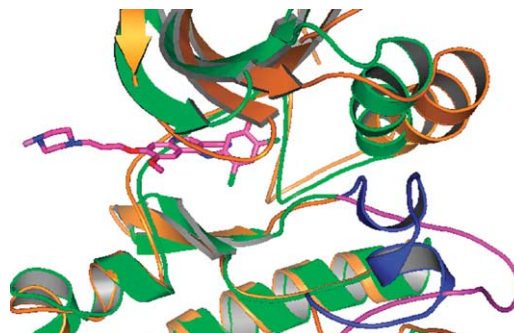
Qiao-Hong Chen, P. N. Praveen Rao and Edward E. Knaus*



3D-QSAR studies on c-Src kinase inhibitors and docking analyses of a potent dual kinase inhibitor of c-Src and c-Abl kinases pp 4704–4712

Ram Thaimattam,* Pankaj R. Daga, Rahul Banerjee and Javed Iqbal

Predictive 3D-QSAR models were developed for a series of quinazoline and quinoline derivatives inhibiting c-Src kinase. A homology model of the active form of c-Src kinase was also constructed. In addition, docking studies of a potent c-Src and c-Abl dual kinase inhibitor (77) were carried out in the active sites of both enzymes to gain insight into the structural requirements for dual activity for this class of molecules.

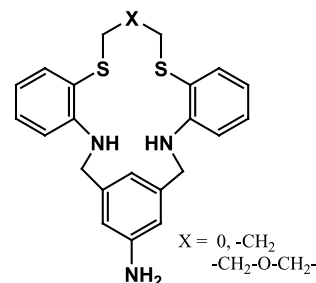


Synthesis and evaluation of bifunctional chelating agents derived from bis(2-aminophenylthio)alkane for radioimaging with ^{99m}Tc

pp 4713–4720

Bhupender S. Chhikara, Nitin Kumar, Vibha Tandon* and Anil K. Mishra*

Synthesis, characterization, and evaluation of novel macrocyclic bifunctional chelating agents for radioimaging with ^{99m}Tc are reported.

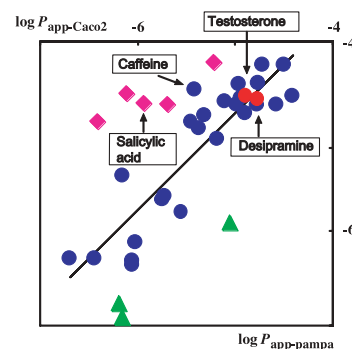


Relationships between structure and high-throughput screening permeability of diverse drugs with artificial membranes: Application to prediction of Caco-2 cell permeability

pp 4721–4732

Masaaki Fujikawa, Rieko Ano, Kazuya Nakao, Ryo Shimizu and Miki Akamatsu*

To evaluate the absorption of drugs with diverse structures across a membrane via the transcellular route, their permeability was measured by the parallel artificial membrane permeation assay (PAMPA). The permeability coefficients obtained by PAMPA were analyzed using a classical quantitative structure–activity relationship approach and 3D-QSAR, VolSurf. The permeability coefficients of the drugs were well correlated with the Caco-2 cell permeability.

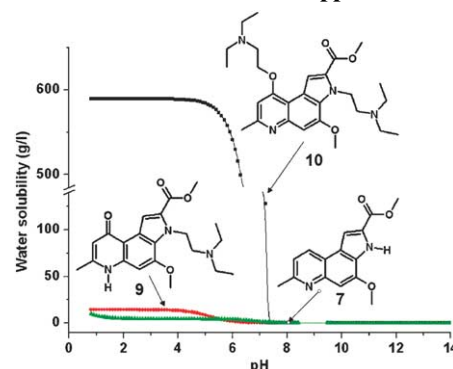


New water soluble pyrroloquinoline derivatives as new potential anticancer agents

pp 4733–4739

Maria Grazia Ferlin,* Christine Marzano, Lisa Dalla Via, Adriana Chilin, Giuseppe Zagotto, Adriano Guiotto and Stefano Moro*

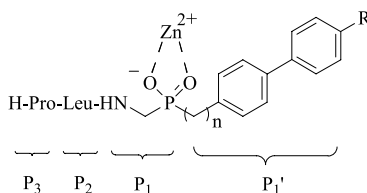
A new class of water soluble 3*H*-pyrrolo[3,2-*f*]quinoline derivatives has been synthesized and investigated as potential anticancer drugs. Water solubility profiles have been used to select the most promising derivatives.



Design, modelling, synthesis and biological evaluation of peptidomimetic phosphinates as inhibitors of matrix metalloproteinases MMP-2 and MMP-8

pp 4740–4749

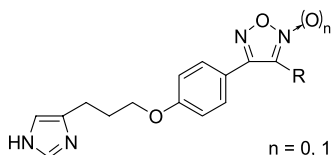
Gianluca Bianchini, Massimiliano Aschi, Giancarlo Cavicchio, Marcello Crucianelli,* Serena Preziuso, Carlo Gallina, Adele Nastari, Enrico Gavuzzo and Fernando Mazza*



Furoxan analogues of the histamine H₃-receptor antagonist imoproxifan and related furazan derivatives

pp 4750–4759

Paolo Tosco, Massimo Bertinaria, Antonella Di Stilo, Clara Cena, Giovanni Sorba, Roberta Fruttero* and Alberto Gasco

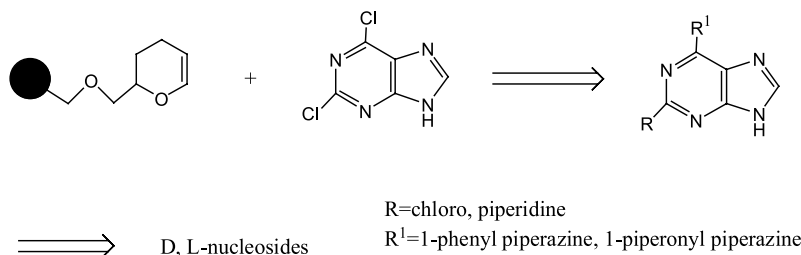


Constrained analogues of imoproxifan containing furazan ($n=0$) and furoxan ($n=1$) systems were synthesised and evaluated in vitro as H₃-antagonists.

A solid-phase approach to novel purine and nucleoside analogs

pp 4760–4766

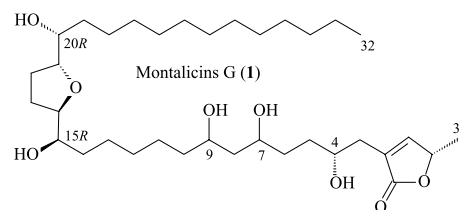
Junbiao Chang,* Chunhong Dong, Xiaohe Guo, Weidong Hu, Senxiang Cheng, Qiang Wang and Rongfeng Chen

**Novel cytotoxic monotetrahydrofuranic Annonaceous acetogenins from *Annona montana***

pp 4767–4776

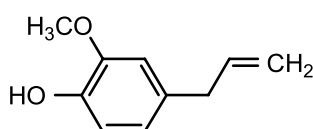
Chih-Chuang Liaw, Fang-Rong Chang, Shu-Li Chen, Chin-Chung Wu, Kuo-Hsiung Lee and Yang-Chang Wu*

Six new Annonaceous acetogenins, montalicens G (1) and H (2), monlicins A (3) and B (4), (+)-monhexocin (5), and (–)-monhexocin (6), as well as three known Annonaceous acetogenins were isolated from the seeds of *Annona montana* by HPLC. The absolute stereochemical structures of new isolates were elucidated and characterized by spectral and chemical methods. Interestingly, these compounds show special cytotoxicity against human hepatoma cells, Hep G2.

**Eugenol and its structural analogs inhibit monoamine oxidase A and exhibit antidepressant-like activity**

pp 4777–4788

Guoxin Tao, Yoshifumi Irie, Dian-Jun Li and Wing Ming Keung*



OTHER CONTENTS

Reviews and Perspectives
Contributors to this issue
Instructions to contributors

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*Corresponding author

i* Supplementary data available via ScienceDirect

COVER

2005: Human liver glycogen phosphorylase A (HLGPa) is an attractive target enzyme for discovering anti-type 2 diabetes drugs. This picture shows the interaction model for a series of indole-2-carboxamides to HLGPa derived from molecular docking simulations [Liu, G.; Zhang, Z.; Luo, X.; Shen, J.; Liu, H.; Shen, X.; Chen, K.; Jiang, H. *Bioorg. Med. Chem.* **2004**, *12*, 4147–4157].



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