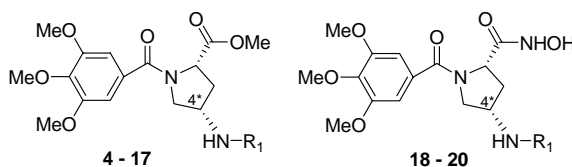


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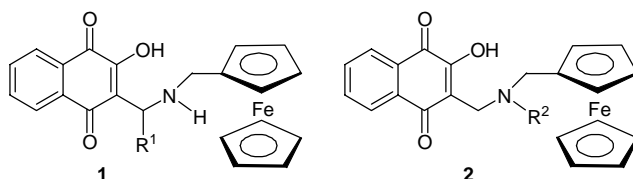
- Design, synthesis, and evaluation of novel galloyl pyrrolidine derivatives as potential anti-tumor agents** pp 1287–1293
Xun Li, Yalin Li and Wenfang Xu*



A series of novel C-2 substituted carbomethoxy (**4–17**) and hydroxamic acid (**18–20**) derivatives of galloyl pyrrolidine were synthesized and evaluated for their in vitro inhibitory activities against gelatinase (MMP-2, -9) and in vivo anti-tumor activities.

- Synthesis and in vitro activities of ferrocenic aminohydroxynaphthoquinones against *Toxoplasma gondii* and *Plasmodium falciparum*** pp 1294–1302

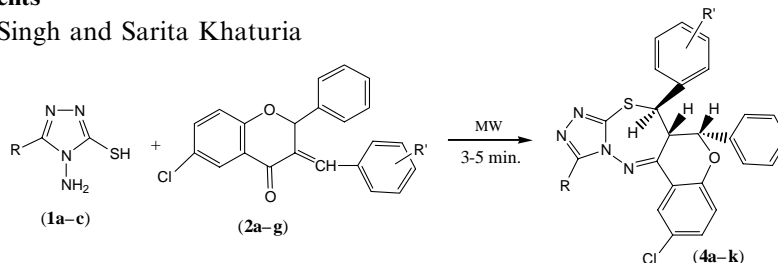
Apiwat Baramée, Alexandra Coppin, Marlène Mortuaire, Lydie Pelinski,*
Stanislas Tomavo* and Jacques Brocard



Ferrocenyl atovaquone derivatives **1** and **2** were synthesized from the hydroxynaphthoquinone core and tested for their in vitro activity against *Toxoplasma gondii* and *Plasmodium falciparum*, including resistant strains to atovaquone and chloroquine.

- Microwave enhanced solid support synthesis of fluorine containing benzopyrano-triazolo-thiadiazepines** pp 1303–1308
as potent anti-fungal agents

Anshu Dandia,* Ruby Singh and Sarita Khaturia

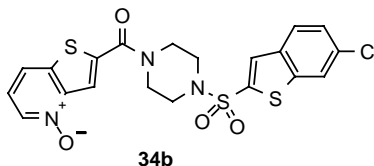


An efficient and environmentally benign synthesis of benzopyrano[4,3-*e*][1,2,4]-triazolo[3,4-*b*][1,3,4]-thiadiazepines is described from 4-amino-5-alkyl-3-mercaptotriazole and substituted 3-arylidene flavanones under microwave irradiation using basic alumina as solid support.

Design, synthesis, and biological activity of novel factor Xa inhibitors: Improving metabolic stability by S1 and S4 ligand modification

pp 1309–1330

Satoshi Komoriya,* Shozo Kobayashi, Ken Osanai, Toshiharu Yoshino, Tsutomu Nagata, Noriyasu Haginoya, Yumi Nakamoto, Akiyoshi Mochizuki, Takayasu Nagahara, Makoto Suzuki, Takashi Shimada, Kengo Watanabe, Yumiko Isobe and Taketoshi Furugoori

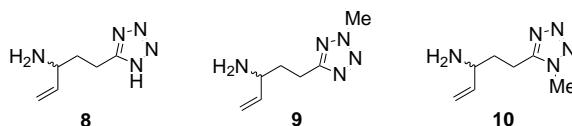


A novel fXa inhibitor **34b** was reported. Compound **34b** exhibited selective anti-fXa activity, excellent anti-coagulation activity, and good anti-thrombotic effect in an in vivo model after oral administration.

New substrates and inhibitors of γ -aminobutyric acid aminotransferase containing bioisosteres of the carboxylic acid group: Design, synthesis, and biological activity

pp 1331–1338

Hai Yuan and Richard B. Silverman*


Stereoselective synthesis and anti-inflammatory activities of 6- and 7-membered dioxacycloalkanes

pp 1339–1347

Keli Gu, Lanrong Bi, Ming Zhao,* Chao Wang, Cheryl Dolan, Michael C. Kao, Jeffrey B.-H. Tok* and Shiqi Peng*

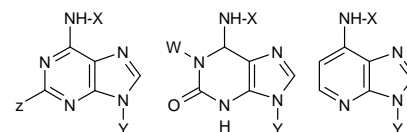
A class of 5-trifluoroacetyl-amino-1,3-dioxacycloalkanes, 5-benzoylamino-1,3-dioxacycloalkanes, and 5-amino-1,3-dioxacycloalkane compounds were stereoselectively synthesized as potential anti-inflammatory drug candidates. The anti-inflammatory activities of these compounds were tested using the xylene-induced mouse ear edema model, from which multiple compounds possessing anti-inflammatory properties which surpass aspirin were identified; these compounds were then compared to establish structure–activity relationships.

Affinity prediction on A₁ adenosine receptor agonists: The chemometric approach

pp 1348–1363

Paola Fossa,* Luisa Mosti, Francesco Bondavalli, Silvia Schenone, Angelo Ranise, Chiara Casolino and Michele Forina

In this paper, we are presenting a quantitative-structure–activity relationship study performed on 21 selective A₁ adenosine receptor agonists plus the endogenous substrate, adenosine, so as to identify those predictors which play a key role in describing the binding of the ligand with the A₁ receptor. This in silico approach could be useful for the screening of large libraries of compounds and in the rational design of new selective agonists.



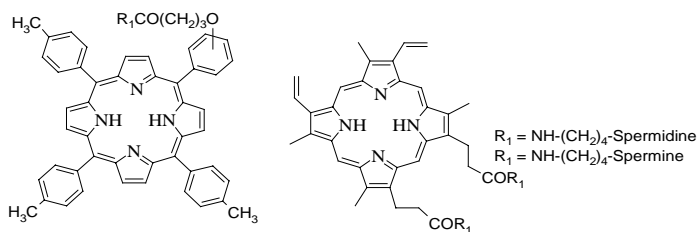
Polyamine conjugates of *meso*-tritolypporphyrin and protoporphyrin

pp 1364–1377

IX: Potential agents for photodynamic therapy of cancers

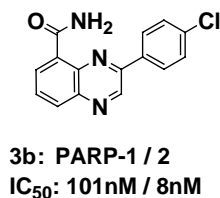
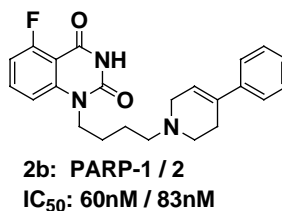
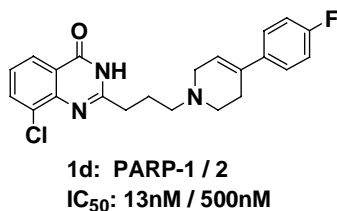
Vincent Sol, François Lamarche, Michaela Enache, Guillaume Garcia, Robert Granet, Michel Guilloton, J.C. Blais and Pierre Krausz*

Biological tests were realised on K562 cells.

**Discovery of potent and selective PARP-1 and PARP-2 inhibitors: SBDD analysis via a combination of X-ray structural study and homology modeling**

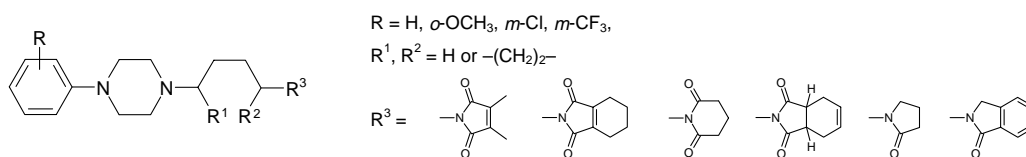
pp 1378–1390

Junya Ishida, Hirofumi Yamamoto, Yoshiyuki Kido, Kazunori Kamijo, Kenji Murano, Hiroshi Miyake, Mitsuru Ohkubo, Takayoshi Kinoshita, Masaichi Warizaya, Akinori Iwashita, Kayoko Mihara, Nobuya Matsuoka and Kouji Hattori*

**Structure–intrinsic activity relationship studies in the group of 1-imido/amido substituted 4-(4-arylpiperazin-1-yl)cyclohexane derivatives; new, potent 5-HT_{1A} receptor agents with anxiolytic-like activity**

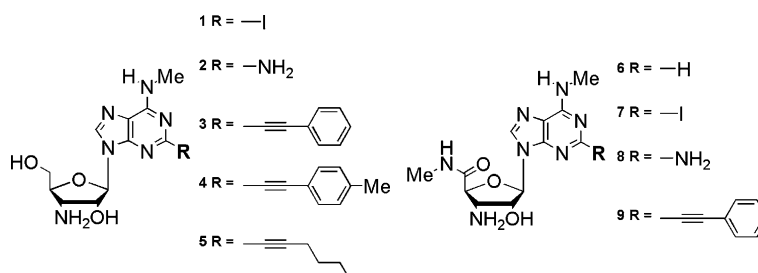
pp 1391–1402

Andrzej J. Bojarski,* Maria H. Paluchowska, Beata Duszyńska, Ryszard Bugno, Aleksandra Kłodzińska, Ewa Tatarczyńska and Ewa Chojnacka-Wójcik

**Synthesis of hypermodified adenosine derivatives as selective adenosine A₃ receptor ligands**

pp 1403–1412

Liesbet Cosyn, Zhan-Guo Gao, Philippe Van Rompaey, Changrui Lu, Kenneth A. Jacobson* and Serge Van Calenbergh*

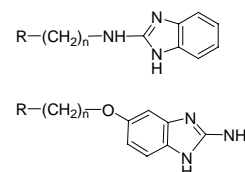


Synthesis and biological evaluation of new non-imidazole H₃-receptor antagonists of the 2-aminobenzimidazole series

pp 1413–1424

Mirko Rivara, Valentina Zuliani, Giuseppe Cocconcelli, Giovanni Morini, Mara Comini, Silvia Rivara, Marco Mor,* Fabrizio Bordi, Elisabetta Barocelli, Vigilio Ballabeni, Simona Bertoni and Pier Vincenzo Plazzi

The synthesis and biological evaluation of a new class of non-imidazole H₃-receptor antagonists, characterized by a 2-aminobenzimidazole fragment connected to a basic or a lipophilic group through an alkyl spacer, are reported. The best affinity values were observed when the 2-aminobenzimidazole was connected to a tertiary amino group at appropriate distance.

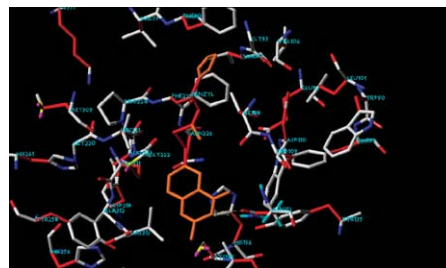


The 3D-QSAR analysis of 4(3H)-quinazolinone derivatives with dithiocarbamate side chains on thymidylate synthase

pp 1425–1430

Shiying Liu, Feng Liu, Xiaoqing Yu, Guoyu Ding, Ping Xu, Jian Cao and Yuyang Jiang*

The binding model of 14 nonclassical lipophilic antifolates of 4(3H)-quinazolinone derivatives with dithiocarbamate side chains was examined using molecular simulation method—FlexiDock and SCORE2.0.

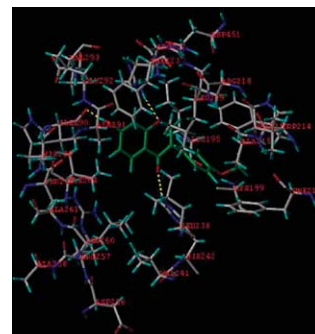


Human serum albumin interaction with formononetin studied using fluorescence anisotropy, FT-IR spectroscopy, and molecular modeling methods

pp 1431–1436

Ying Li, WenYing He, YuMing Dong, Fenling Sheng and ZhiDe Hu*

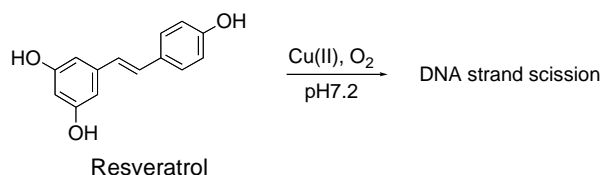
The interaction mode between formononetin and HSA.



Structural basis for DNA-cleaving activity of resveratrol in the presence of Cu(II)

pp 1437–1443

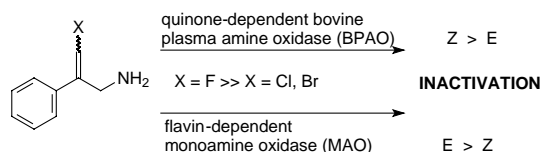
Kiyoshi Fukuhara,* Maki Nagakawa, Ikuo Nakanishi, Kei Ohkubo, Kohei Imai, Shiro Urano, Shunichi Fukuzumi, Toshihiko Ozawa, Nobuo Ikota, Masataka Mochizuki, Naoki Miyata and Haruhiro Okuda



Inactivation of bovine plasma amine oxidase by haloallylamines

pp 1444–1453

Jisook Kim, Yuming Zhang, Chongzhao Ran and Lawrence M. Sayre*

**Classification of dopamine antagonists using functional feature hypothesis and topological descriptors**

pp 1454–1461

Hye-Jung Kim, Yong Seo Cho, Hun Yeong Koh, Jae Yang Kong, Kyoung Tai No and Ae Nim Pae*

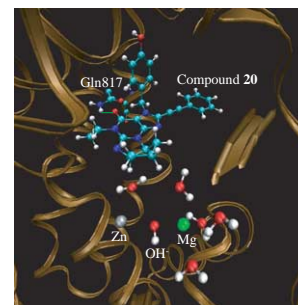
Two-dimensional topological descriptors and three-dimensional pharmacophore hypothesis were used to investigate and compare different classes of dopamine antagonists. Molconn-Z and BCUT topological descriptors were employed to develop a classification model for 1475 dopamine antagonists from MDDR database. The combining both of classification using topological descriptors and functional feature hypotheses could be a useful tool to predict selective antagonists.

**Understanding the structure–activity and structure–selectivity correlation of cyclic guanine derivatives as phosphodiesterase-5 inhibitors by molecular docking, CoMFA and CoMSIA analyses**

pp 1462–1473

Guang-Fu Yang,* Hai-Ting Lu, Ying Xiong and Chang-Guo Zhan*

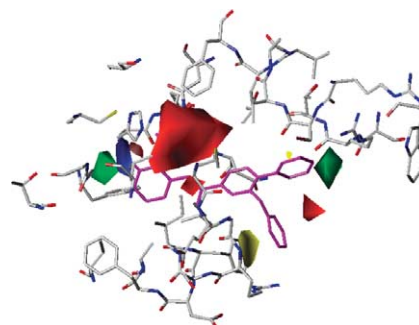
Understanding the structure–activity and structure–selectivity correlation of cyclic guanine derivatives as phosphodiesterase-5 inhibitors by molecular docking, CoMFA and CoMSIA analyses

**A combined approach of docking and 3D QSAR study of β -ketoacyl-acyl carrier protein synthase III (FabH) inhibitors**

pp 1474–1482

Ali Ashek and Seung Joo Cho*

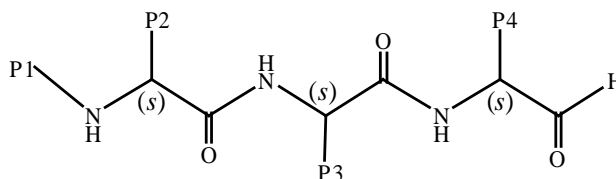
We performed CoMFA and CoMSIA based on the docking conformations of benzoylaminobenzoic acid derivatives into the active site of FabH enzyme. Mapping the 3D QSAR models into the active site of FabH provides a useful perspective for the active site of FabH.



3D-QSAR studies on tripeptide aldehyde inhibitors of proteasome using CoMFA and CoMSIA methods

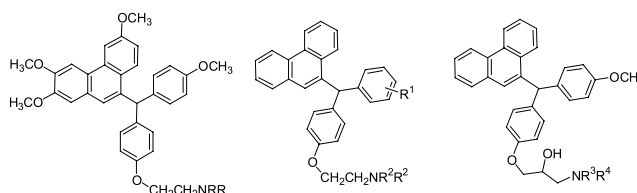
pp 1483–1496

Yong-Qiang Zhu, Jian-Feng Pei, Zhen-Ming Liu, Lu-Hua Lai,* Jing-Rong Cui and Run-Tao Li*


Substituted phenanthrenes with basic amino side chains: A new series of anti-breast cancer agents

pp 1497–1505

Shagufta, Ajay Kumar Srivastava, Ramesh Sharma, Rajeev Mishra, Anil Kumar Balapure, Puvvada S. R. Murthy and Gautam Panda*


Direct observation (NMR) of the efficacy of glucagon receptor antagonists in murine liver expressing the human glucagon receptor

pp 1506–1517

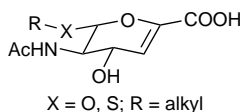
Sheila M. Cohen, Joseph L. Duffy,* Corin Miller, Brian A. Kirk, Mari Rios Candelore, Victor D. H. Ding, Gregory Kaczorowski, Laurie M. Tota, Jeffrey G. Werrmann, Michael Wright, Emma R. Parmee, James R. Tata and Bei B. Zhang

The biosynthesis of [^{13}C]glycogen from [^{13}C]pyruvate via the gluconeogenic pathway is monitored in surgically removed perfused livers by ^{13}C NMR. The rapid breakdown of [^{13}C]glycogen (glycogenolysis) following the addition of 50 pM exogenous glucagon is then monitored in real time using this technique. The concentration-dependent inhibition of glucagon-mediated glycogenolysis is demonstrated for both the peptidyl glucagon antagonist **1** and structurally diverse synthetic glucagon antagonists **2–7**. Perfused livers were obtained from a transgenic mouse strain that exclusively expresses the functional human glucagon receptor, conferring human relevance to the activity observed with these antagonists.

Modelling, synthesis and biological evaluation of novel glucuronide-based probes of *Vibrio cholerae* sialidase

pp 1518–1537

Maretta C. Mann, Robin J. Thomson, Jeffrey C. Dyason, Sarah McAtamney and Mark von Itzstein*



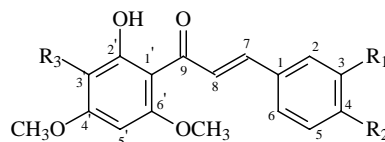
Glucuronide-Based Neu5Ac2en Mimetics

The synthesis and biological evaluation of a series of glucuronide-based Neu5Ac2en mimetics are presented.

Synthesis of chalcone analogues with increased antileishmanial activity

pp 1538–1545

Paula Boeck, Camila Alves Bandeira Falcão, Paulo César Leal, Rosendo Augusto Yunes, Valdir Cechinel Filho, Eduardo Caio Torres-Santos and Bartira Rossi-Bergmann*



10 R₁ = NO₂, R₂ = H, R₃ = H

12 R₁ = H, R₂ = F, R₃ = H

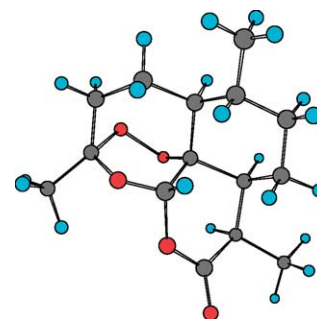
19 R₁ = NO₂, R₂ = H, R₃ = Br

DFT study of the reductive decomposition of artemisinin

pp 1546–1557

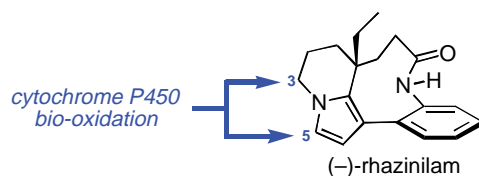
Alex Gutterres Taranto, José Walkimar de Mesquita Carneiro* and Martha Teixeira de Araujo

The DFT B3LYP method was employed to calculate the mechanism for the reductive decomposition of artemisinin. A set of radical anions and neutral species supposed to be relevant in the mechanism of action of artemisinin were calculated. Primary and secondary radicals centered on C₄ were found as the most stable species.

**In vitro oxidative metabolism study of (–)-rhazinilam**

pp 1558–1564

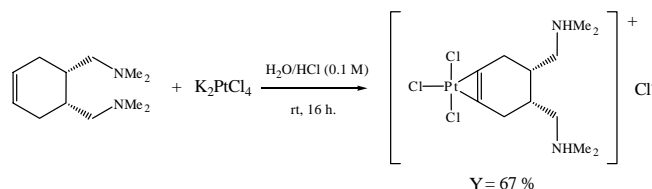
Anne Décor, Delphine Bellocq, Odile Thoison, Nicolas Lekieffre, Angèle Chiaroni, Jamal Ouazzani, Thierry Cresteil, Françoise Guéritte and Olivier Baudoin*


Studies of interaction of trichloro{η²-cis-*N,N*-dimethyl-1-[6-(*N,N*-dimethyl-ammoniummethyl)-cyclohex-3-ene-1-yl]-methylammonium}platinum(II) chloride with DNA: Effects on secondary and tertiary structures of DNA. Cytotoxic assays on human ovarian cancer cell lines, resistant and non-resistant to cisplatin

pp 1565–1572

Marina Gay, Ángel M. Montaña,* Virtudes Moreno,* María-José Prieto, José Manuel Pérez and Carlos Alonso

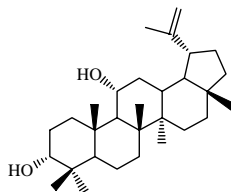
The ability of this new platinum complex to modify secondary DNA structure was explored by circular dichroism (CD). Electrophoretic mobility showed changes in tertiary DNA structure, and atomic force microscopy (AFM) revealed morphological changes of plasmid DNA (pBR322). A lower cytotoxicity but also a lower resistant factor was observed for the here described organometallic compound than for cisplatin, against A2780 and A2780cisR ovarian cancer cell lines.



Activity of lupane triterpenoids from *Maytenus* species as inhibitors of nitric oxide and prostaglandin E₂

pp 1573–1579

Carolina P. Reyes, Marvin J. Núñez, Ignacio A. Jiménez, Jérôme Busserolles, María J. Alcaraz and Isabel L. Bazzocchi*

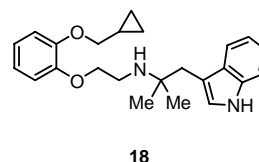
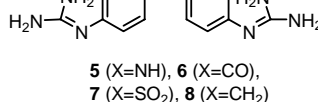
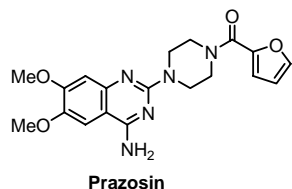


Three new lupane triterpenes, in addition to 16 known ones, were isolated from *Maytenus* species. These compounds and four derivatives have been tested for potential anti-inflammatory activity. Some of them exhibited potent inhibitory effects on NO and prostaglandin E₂ production in mouse macrophages.

Theoretical proton affinities of $\alpha 1$ adrenoceptor ligands

pp 1580–1587

Gemma K. Kinsella, Graeme W. Watson and Isabel Rozas*

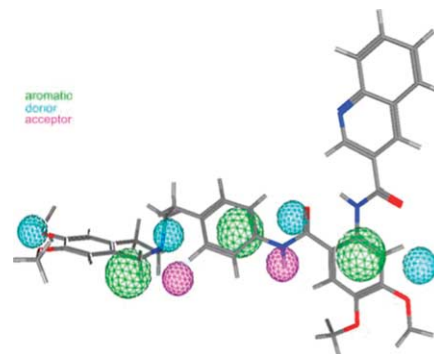


The figure illustrates some of the $\alpha 1$ -adrenoceptor ligand objects of this study. Their proton affinity have been theoretically computed at the B3LYP/6-31G* level.

Structure–activity relationships of a series of tariquidar analogs as multidrug resistance modulators

pp 1588–1598

Christoph Globisch, Ilza K. Pajeva and Michael Wiese*

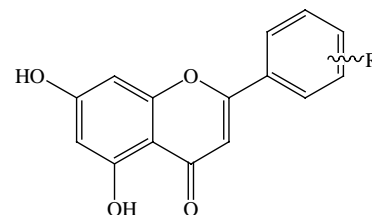


Synthesis and biological evaluation of a series of flavone derivatives as potential radioligands for imaging the multidrug resistance-associated protein 1 (ABCC1/MRP1)

pp 1599–1607

Sylvie Mavel,* Branko Dikic, Somchit Palakas, Patrick Emond, Ivan Greguric, Adrienne Gomez de Gracia, Filomena Mattner, Manuel Garrigos, Denis Guilloteau and Andrew Katsifis

5 Flavone derivatives were synthesized, and their cytotoxic activity and MDR-reversing capacity using hMRP1 or hMDR1 overexpressing cell lines were determined by in vitro assays. These derivatives constituted a class of hMRP1-related MDR modulators, making them potential PET or SPECT radiotracers in the field of MDR imaging.

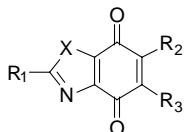


R = 4-Br, 3-Br, 4-I, 4-O-(CH₂)₉-F, 4-O-(CH₂)₁₀-F

The development of 3D-QSAR study and recursive partitioning of heterocyclic quinone derivatives with antifungal activity

pp 1608–1617

Su-Young Choi, Jae Hong Shin, Chung Kyu Ryu, Ky-Youb Nam,
Kyoung Tai No and Hea-Young Park Choo*

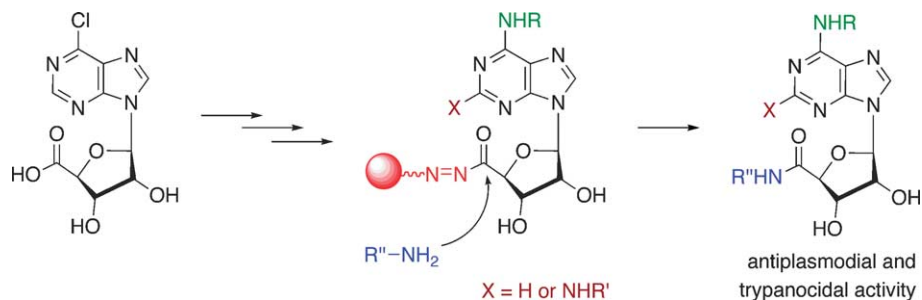


Quantitative structure–activity relationship studies for antifungal 1,4-quinone derivatives using comparative molecular field analysis (CoMFA) and recursive partitioning (RP) analysis are reported.

Solid phase synthesis and antiprotozoal evaluation of di- and trisubstituted 5'-carboxamidoadenosine analogues

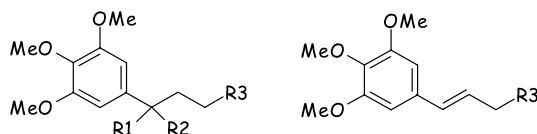
pp 1618–1629

Boris Rodenko, Remko J. Detz, Victorine A. Pinas, Catia Lambertucci, Reto Brun,
Martin J. Wanner and
Gerrit-Jan Koomen*

**3D QSAR study of hypolipidemic asarones by comparative molecular surface analysis**

pp 1630–1643

Tomasz Magdziarz, Bożena Łozowicka, Rafał Gieleciak, Andrzej Bąk,
Jarosław Polański* and Zdzisław Chilmonczyk

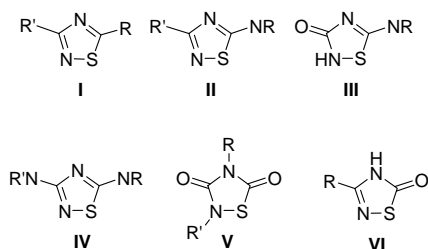


Several novel hypolipidemic α -asarones have been synthesized and 3D QSAR has been modeled.

Advances in the synthesis and recent therapeutic applications of 1,2,4-thiadiazole heterocycles

pp 1644–1652

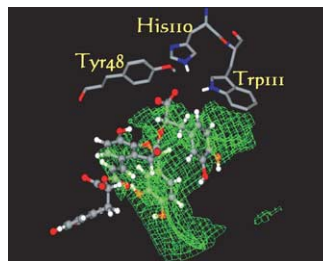
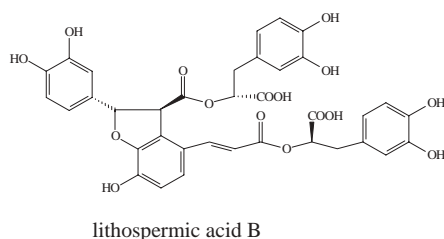
Ana Castro, Tania Castaño, Arantxa Encinas, Williams Porcal and Carmen Gil*



Evaluation of aldose reductase inhibition and docking studies of some secondary metabolites, isolated from *Origanum vulgare* L. ssp. *hirtum*

pp 1653–1659

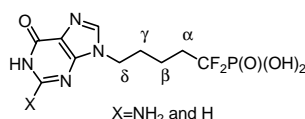
Catherine Koukoulitsa,* Chariklia Zika, George D. Geromichalos,
Vassilis J. Demopoulos and Helen Skaltsa



Synthesis and biological evaluation of 9-(5',5'-difluoro-5'-phosphonopentyl)guanine derivatives for PNP-inhibitors

pp 1660–1670

Sadao Hikishima, Machiko Isobe, Satoru Koyanagi, Shinji Soeda, Hiroshi Shimeno,*
Shiroshi Shibuya and Tsutomu Yokomatsu*



9-(5',5'-Difluoro-5'-phosphonopentyl)guanine and its hypoxanthin analogue were modified by introducing a methyl group to all possible positions (α - to γ -position) of the linker connecting a purine and a difluoromethylenephosphonic acid moiety to evaluate the effects of the methyl group on inhibition against purine nucleoside phosphorylase.

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Corrigendum

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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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