

## Contents

### REVIEW

#### Chemical–biological interactions in human

pp 933–948

Rajeshwar P. Verma, Alka Kurup, Suresh B. Mekapati and Corwin Hansch\*

Chemical–biological interactions in human have been discussed in terms of QSAR (quantitative structure–activity relationships).

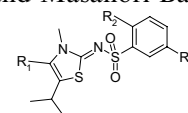
### ARTICLES

#### Studies of non-nucleoside HIV-1 reverse transcriptase inhibitors. Part 2: Synthesis and structure–activity relationships of 2-cyano and 2-hydroxy thiazolidenebenzenesulfonamide derivatives

pp 949–961

Naoyuki Masuda,\* Osamu Yamamoto, Masahiro Fujii, Tetsuro Ohgami, Jiro Fujiyasu, Toru Kontani, Ayako Moritomo, Masaya Orita, Hiroyuki Kurihara, Hironobu Koga, Shunji Kageyama, Mitsuaki Ohta, Hiroshi Inoue, Toshifumi Hatta, Masafumi Shintani, Hiroshi Suzuki, Kenji Sudo, Yasuaki Shimizu, Eiichi Kodama, Masao Matsuoka, Masatoshi Fujiwara, Tomoyuki Yokota, Shiro Shigeta and Masanori Baba

A series of thiazolidenebenzenesulfonamides was prepared and evaluated for their inhibitory effects on the WT, Y181C, and K103N reverse transcriptase (RT) activity and HIV-1 replication. The cyano derivatives **10l** and **18b** (YM-228855) showed extremely potent anti-HIV-1 activity. Compound **11g** (YM-215389) showed the most potent activity against the WT and the two mutant RTs. Furthermore, this compound was also a highly potent inhibitor of HIV-1 replication.

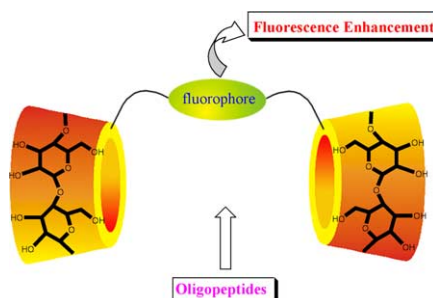


**10l**:  $R_1 = \text{Me}$ ,  $R_2 = \text{CN}$ ,  $R_3 = \text{Cl}$   
**11g** (YM-215389):  $R_1 = \text{Cl}$ ,  $R_2 = \text{OH}$ ,  $R_3 = \text{Br}$   
**18b** (YM-228855):  $R_1 = \text{Me}$ ,  $R_2 = \text{CN}$ ,  $R_3 = \text{CN}$

#### Efficient fluorescent sensors of oligopeptides by dithiobis(2-benzoylamide)-bridged bis( $\beta$ -cyclodextrin)s: structure in solution, binding behavior, and thermodynamic origin

pp 963–971

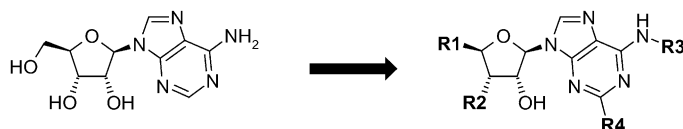
Yu Liu,\* Ying-Wei Yang, Yong Chen and Fei Ding



### Exploring human adenosine A<sub>3</sub> receptor complementarity and activity for adenosine analogues modified in the ribose and purine moiety

pp 973–983

Philippe Van Rompaey, Kenneth A. Jacobson,\* Ariel S. Gross, Zhan-Guo Gao and Serge Van Calenbergh\*

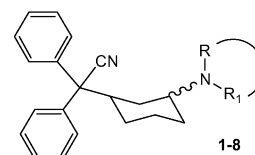


### Diphenylcyclohexylamine derivatives as new potent multidrug resistance (MDR) modulators

pp 985–998

Silvia Dei,\* Roberta Budriesi, Paiwan Sudwan, Marta Ferraroni, Alberto Chiarini, Arlette Garnier-Suillerot, Dina Manetti, Cecilia Martelli, Serena Scapecchi and Elisabetta Teodori

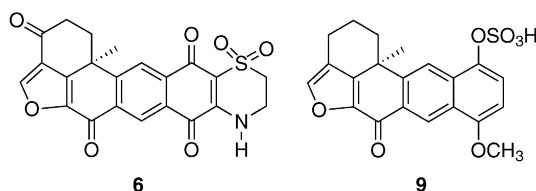
A series of compounds with a diphenylmethyl cyclohexyl skeleton, loosely related to verapamil, has been synthesized and tested as MDR modulators on anthracycline-resistant erythroleukemia K 562 cells. Their residual cardiovascular action (negative inotropic and chronotropic activity as well as vasorelaxant activity) was evaluated on guinea-pig isolated atria preparations and on guinea-pig aortic strip preparations. Most compounds of the series possess a good MDR-reverting activity together with a low cardiovascular action. Among them, three compounds are more potent than verapamil as MDR reverters and lack any cardiovascular action; they can represent useful leads for the development of new safe MDR reversing drugs.



### Halenaquinone and xestoquinone derivatives, inhibitors of Cdc25B phosphatase from a *Xestospongia* sp.

pp 999–1003

Shugeng Cao, Caleb Foster, Marni Brisson, John S. Lazo and David G. I. Kingston\*



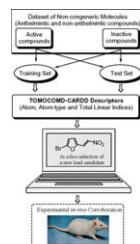
Nine quinones, including the new natural products **6** and **9**, were isolated from a sponge of the genus *Xestospongia*. All the isolated compounds were inhibitory to the dual specificity phosphatase Cdc25B, and five were active at the nanomolar level.



### Atom, atom-type and total molecular linear indices as a promising approach for bioorganic and medicinal chemistry: theoretical and experimental assessment of a novel method for virtual screening and rational design of new lead anthelmintic

pp 1005–1020

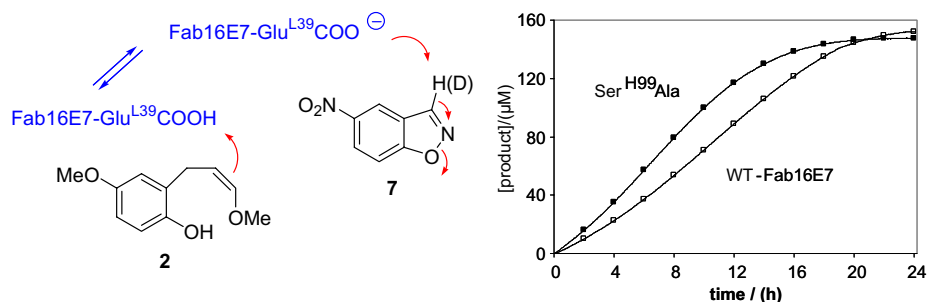
Yovani Marrero-Ponce,\* Juan A. Castillo-Garit, Erelvio Olazabal, Hector S. Serrano, Alcidez Morales, Nilo Castañedo, Froylán Ibarra-Velarde, Alma Huesca-Guillen, Alicia M. Sánchez, Francisco Torrens and Eduardo A. Castro



# Mechanistic study of proton transfer and hysteresis in catalytic antibody 16E7 by site-directed mutagenesis and homology modeling

pp 1021–1029

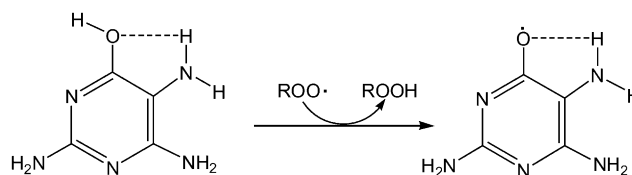
Lei Zheng, Roman Manetsch, Wolf-Dietrich Woggon, Ulrich Baumann and Jean-Louis Reymond\*



# A theoretical study on the structure–activity relationships of metabolites of folates as antioxidants and its implications for rational design of antioxidants

pp 1031–1036

Hong-Fang Ji, Guang-Yan Tang and Hong-Yu Zhang\*

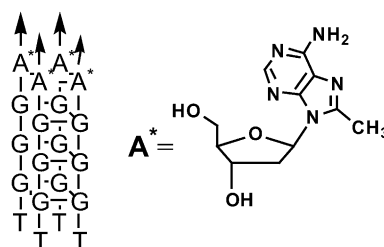


By means of DFT calculation, the structure–activity relationships of metabolites of folates as antioxidants was elucidated and the potential of 4-hydroxypyrimidine as a novel lead antioxidant was evaluated as well.

# Effects of 8-methyl-2'-deoxyadenosine incorporation into quadruplex forming oligodeoxyribonucleotides

pp 1037–1044

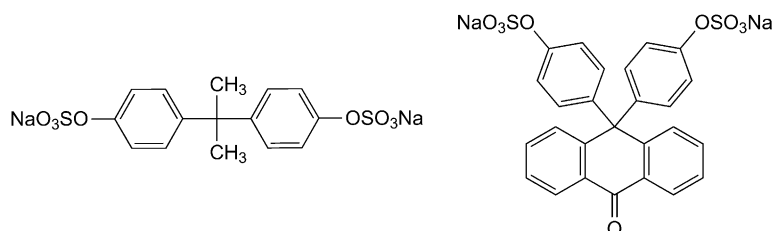
Antonella Virgilio, Veronica Esposito, Antonio Randazzo, Luciano Mayol and Aldo Galeone\*



# Inhibition of classical pathway of complement activation with negative charged derivatives of bisphenol A and bisphenol disulphates

pp 1045–1052

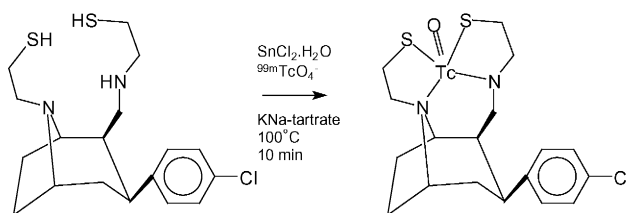
Svetlana Bureeva,\* Julian Andia-Pravdivy, Gennadiy Petrov, Michael Igumnov, Sergey Romanov, Elena Kolesnikova, Alexander Kaplun\* and Leonid Kozlov



**Technetium-99m labelled integrated tropane–BAT as a potential dopamine transporter tracer**

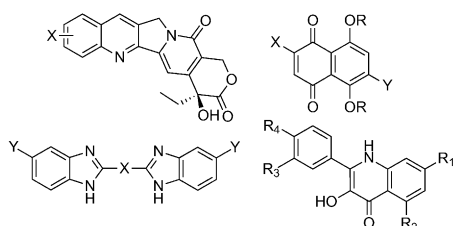
pp 1053–1058

Bernard J. Cleynhens, Tjibbe J. de Groot, Hubert P. Vanbilloen, Davy Kieffer, Luc Mortelmans, Guy M. Bormans and Alfons M. Verbruggen\*

**Understanding topoisomerase I and II in terms of QSAR**

pp 1059–1067

Rajeshwar P. Verma

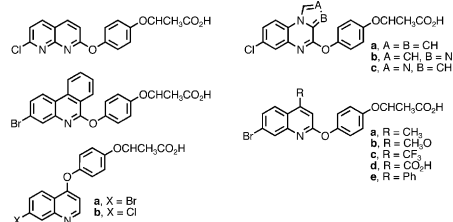


Quantitative structure–activity relationships have been performed for different sets of compounds with respect to their inhibitory activities towards topoisomerase I and II. Activities of these compounds are found to be largely dependent on their hydrophobicity for topoisomerase I and, polarizability and molar volume for topoisomerase II.

**Part 3: Synthesis and biological evaluation of some analogs of the antitumor agents, 2-{4-[(7-chloro-2-quinoxalinyloxy]phenoxy}propionic acid, and 2-{4-[(7-bromo-2-quinolinyloxy]phenoxy}propionic acid**

pp 1069–1081

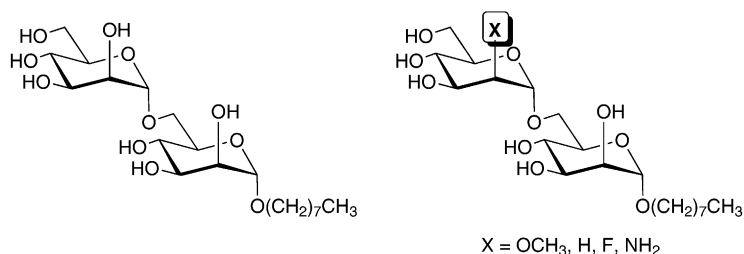
Stuart T. Hazeldine, Lisa Polin, Juiwanna Kushner, Kathryn White, Thomas H. Corbett, Jason Biehl and Jerome P. Horwitz\*



**Modified mannose disaccharides as substrates and inhibitors of a polyprenol monophosphomannose-dependent  $\alpha$ -(1→6)-mannosyltransferase involved in mycobacterial lipoarabinomannan biosynthesis**

pp 1083–1094

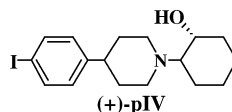
Vinodhkumar Subramaniam, Sudagar S. Gurcha, Gurdyal S. Besra and Todd L. Lowary\*



## In vitro characterization of radioiodinated (+)-2-[4-(4-iodophenyl) piperidino]cyclohexanol [(+)-pIV] as a sigma-1 receptor ligand

pp 1095–1099

Kazuhiro Shiba,\* Kazuma Ogawa and Hirofumi Mori

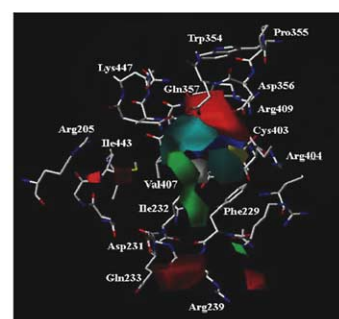
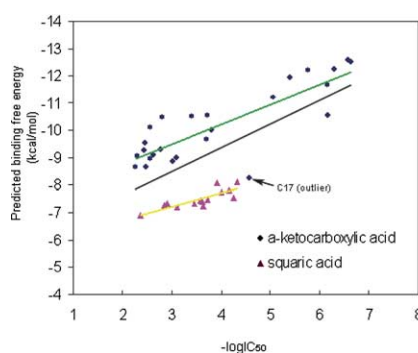


## Molecular docking and 3D-QSAR studies of *Yersinia* protein tyrosine phosphatase YopH inhibitors

pp 1101–1109

Xin Hu and C. Erec Stebbins\*

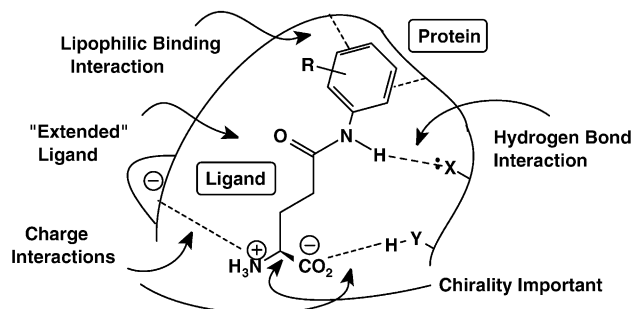
Molecular docking and 3D-QSAR approaches were applied to investigate the interactions of two series of compounds,  $\alpha$ -ketocarboxylic acid and squaric acid, with the target protein *Yersinia* protein tyrosine phosphatase YopH. The studies demonstrate the power of combined docking/QSAR approach to explore the probable binding conformations of YopH inhibitors, and further develop reliable quantitative models for rational drug design.



## $N_\gamma$ -Aryl glutamine analogues as probes of the ASCT2 neutral amino acid transporter binding site

pp 1111–1118

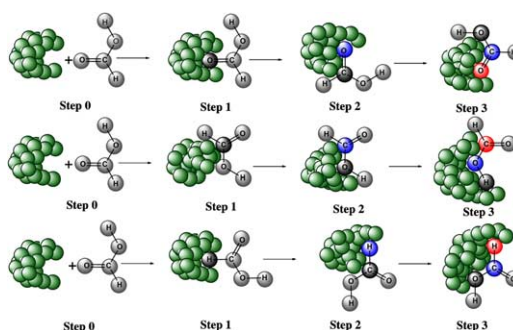
C. Sean Esslinger,\* Kimberly A. Cybulski and Joseph F. Rhoderick



## Predicting multiple drugs side effects with a general drug-target interaction thermodynamic Markov model

pp 1119–1129

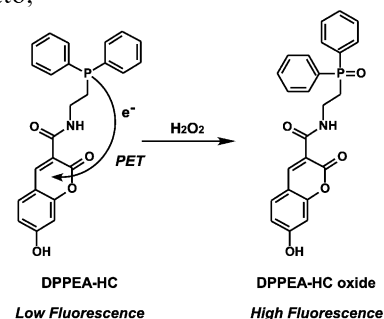
Humberto González-Díaz, Maykel Cruz-Monteaugudo,\* Reinaldo Molina, Esvieta Tenorio and Eugenio Uriarte



## Design and development of a fluorescent probe for monitoring hydrogen peroxide using photoinduced electron transfer pp 1131–1139

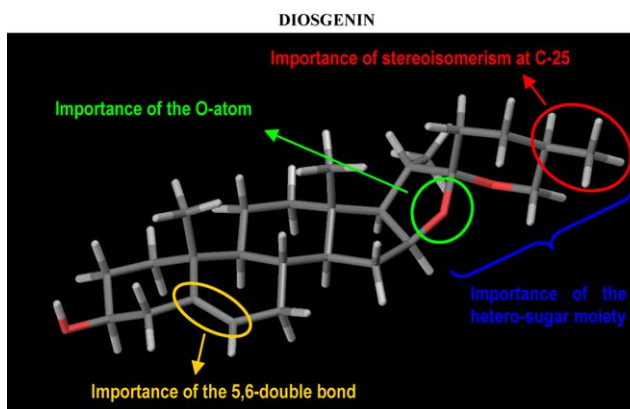
Nobuaki Soh, Osamu Sakawaki, Koji Makihara, Yuka Odo, Tuyoshi Fukaminato, Tsuyoshi Kawai, Masahiro Irie and Toshihiko Imato\*

A novel fluorescent probe for monitoring hydrogen peroxide ( $\text{H}_2\text{O}_2$ ), DPPEA-HC, was developed by utilizing the fluorescence off/on switching mechanism, based on the on/off control of photoinduced electron transfer (PET). DPPEA-HC reacted with  $\text{H}_2\text{O}_2$  to form the strongly-fluorescent DPPEA-HC oxide. Because of the high selectivity for  $\text{H}_2\text{O}_2$  and the greater resistance to autoxidation, the probe is expected to be useful for the detection of  $\text{H}_2\text{O}_2$  in cellular systems.



## Structure–function relationship for saponin effects on cell cycle arrest and apoptosis in the human 1547 osteosarcoma cells: a molecular modelling approach of natural molecules structurally close to diosgenin

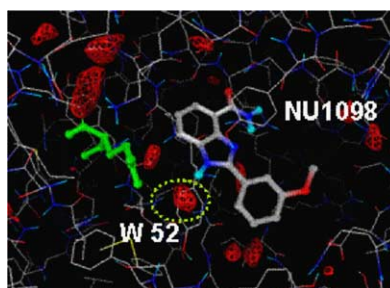
Patrick Trouillas, Cécile Corbière, Bertrand Liagre,\* Jean-Luc Duroux and Jean-Louis Beneytout



pp 1141–1149

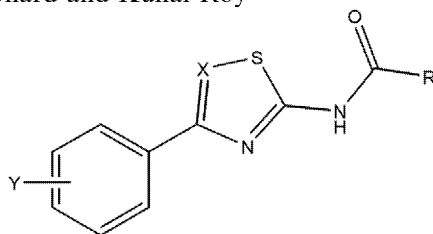
## Docking studies on PARP-1 inhibitors: insights into the role of a binding pocket water molecule pp 1151–1157

Daniele Bellocchi, Antonio Macchiarulo, Gabriele Costantino\* and Roberto Pellicciari



## Exploring QSAR of thiazole and thiadiazole derivatives as potent and selective human adenosine A<sub>3</sub> receptor antagonists using FA and GFA techniques pp 1159–1165

Prosenjit Bhattacharya, J. Thomas Leonard and Kunal Roy\*

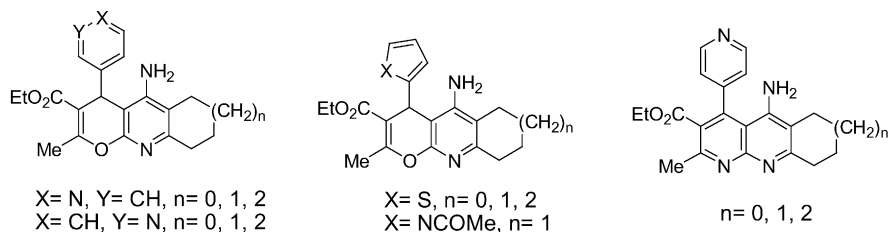


Adenosine  $\text{A}_3$  binding affinity data of thiazole and thiadiazole derivatives have been subjected to QSAR study using factor analysis and genetic function approximation.

**Synthesis, acetylcholinesterase inhibition and neuroprotective activity of new tacrine analogues**

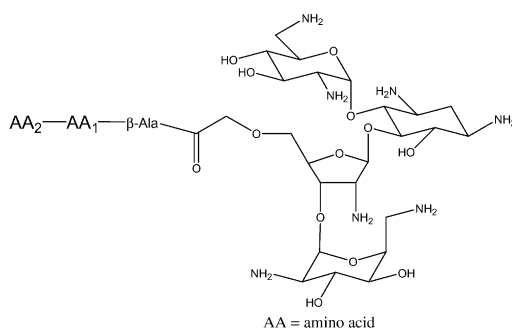
pp 1167–1175

Rafael León, José Marco-Contelles,\* Antonio G. García and Mercedes Villarroya\*

**Library construction of neomycin–dipeptide heteroconjugates and selection against RRE RNA**

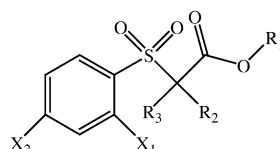
pp 1177–1183

Dae-Ro Ahn and Jaehoon Yu\*

**QSTR with extended topochemical atom indices. Part 5: Modeling of the acute toxicity of phenylsulfonyl carboxylates to *Vibrio fischeri* using genetic function approximation**

pp 1185–1194

Kunal Roy\* and Gopinath Ghosh



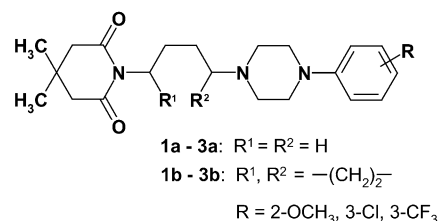
In continuation of our recent efforts to model the acute toxicity of 56 phenylsulfonyl carboxylates to *Vibrio fischeri* using principal component factor analysis, the present paper deals with modeling of the same data set with extended topochemical atom (ETA) indices using genetic function approximation (GFA) as the statistical tool.

**Novel, flexible, and conformationally defined analogs of gepirone: synthesis and 5-HT<sub>1A</sub>, 5-HT<sub>2A</sub>, and D<sub>2</sub> receptor activity**

pp 1195–1200

Maria H. Paluchowska,\* Ryszard Bugno, Andrzej J. Bojarski, Sijka Charakchieva-Minol, Beata Duszyńska, Ewa Tatarczyńska, Aleksandra Kłodzińska, Katarzyna Stachowicz and Ewa Chojnacka-Wójcik

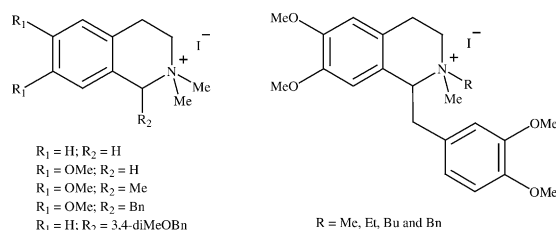
Novel, flexible arylpiperazine gepirone analogs (**1a–3a**) with a mixed 5-HT<sub>1A</sub>/5-HT<sub>2A</sub> receptor profile, low D<sub>2</sub> receptor affinity, and agonistic (**2a**) or partial agonistic (**1a**, **3a**) activity toward 5-HT<sub>1A</sub> receptor sites were synthesized. Their conformationally restricted counterparts (**1b–3b**) were selective 5-HT<sub>1A</sub> ligands (over 5-HT<sub>2A</sub> and D<sub>2</sub> receptors), which turned out to be agonists (**2b**, **3b**), or partial agonist (**1b**) of 5-HT<sub>1A</sub> receptors.



### Synthesis and biological evaluation of *N*-methyl-laundanosine iodide analogues as potential SK channel blockers

pp 1201–1209

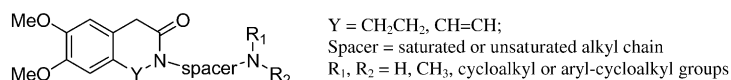
A. Graulich,\* F. Mercier, J. Scuvée-Moreau, V. Seutin and J.-F. Liégeois



### Design, synthesis and preliminary biological evaluation of zatebradine analogues as potential blockers of the hyperpolarization-activated current

pp 1211–1220

Maria Novella Romanelli,\* Elisabetta Cerbai, Silvia Dei, Luca Guandalini, Cecilia Martelli, Elisabetta Martini, Serena Scapecchi, Elisabetta Teodori and Alessandro Mugelli

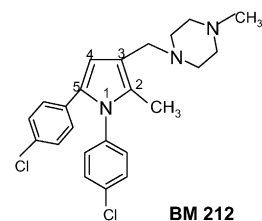


### Antimycobacterial compounds. Optimization of the BM 212 structure, the lead compound for a new pyrrole derivative class

pp 1221–1230

Mariangela Biava,\* Giulio Cesare Porretta, Giovanna Poce, Delia Deidda, Raffaello Pompei, Andrea Tafi and Fabrizio Manetti

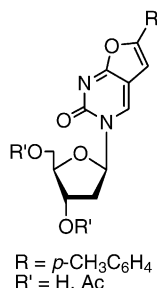
Previously we have identified **BM 212**, a pyrrole derivative with good in vitro activity against mycobacteria and a four-feature pharmacophore model derived from it and many other antimycobacterial compounds synthesized by us. On SAR and molecular modeling considerations, we prepared new pyrrole derivatives in the hope of increasing the activity. The microbiological data showed interesting in vitro activity against *Mycobacterium tuberculosis*.



### NMR conformational analysis of *p*-tolyl furanopyrimidine 2'-deoxyribonucleoside and crystal structure of its 3',5'-di-*O*-acetyl derivative

pp 1231–1238

Noor Esho, Jean-Paul Desautniers, Brian Davies, Helen M.-P. Chui, Meneni Srinivasa Rao, Christine S. Chow, Slawomir Szafert\* and Roman Dembinski\*

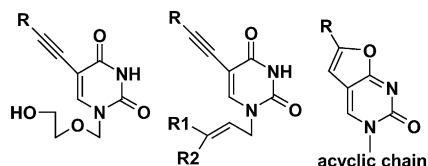




## Synthesis and antiviral activity of novel acyclic nucleosides in the 5-alkynyl- and 6-alkylfuro[2,3-*d*]pyrimidine series

pp 1239–1248

Franck Amblard, Vincent Aucagne, Pierre Guenot, Raymond F. Schinazi and Luigi A. Agrofoglio\*

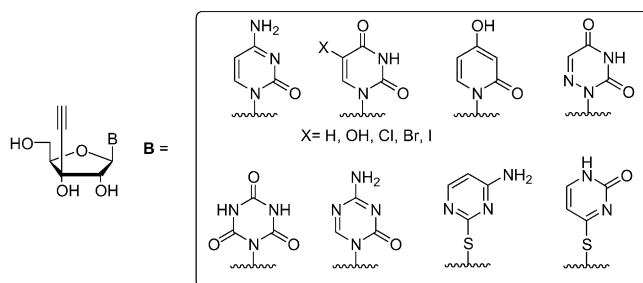


The synthesis of series of *hitherto unknown* 5-alkynyl pyrimidine acyclic nucleosides and their furopyrimidine analogues is described. The in vitro antiviral activity (HIV, HSV-1) and toxicity in different cell lines are reported.

## Synthesis and biological evaluation of nucleobase-modified analogs of the anticancer compounds 3'-C-ethynyluridine (EURd) and 3'-C-ethynylcytidine (ECyd)

pp 1249–1260

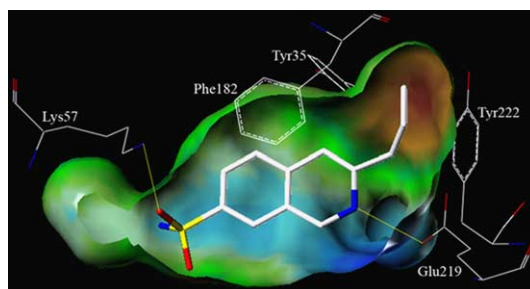
Patrick J. Hrdlicka, Jan S. Jepsen, Claus Nielsen and Jesper Wengel\*



## Exploring the active site of phenylethanolamine *N*-methyltransferase: 3-alkyl-7-substituted-1,2,3,4-tetrahydroisoquinoline inhibitors

pp 1261–1273

Gary L. Grunewald,\* F. Anthony Romero, Alex D. Chieu, Kelcie J. Fincham, Seema R. Bhat and Kevin R. Criscione

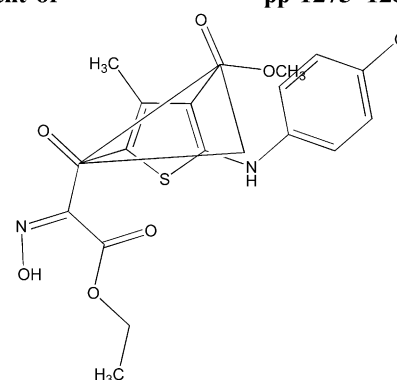


## QSAR studies on some thiophene analogs as anti-inflammatory agents: enhancement of activity by electronic parameters and its utilization for chemical lead optimization

pp 1275–1283

Ajay D. Pillai, Shubha Rani, Parendu D. Rathod, Franklin P. Xavier,  
Kamala K. Vasu,\* Harish Padh and Vasudevan Sudarsanam

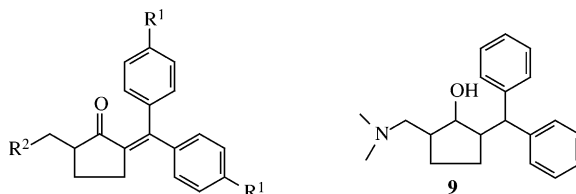
We report the QSAR studies of some thiophene analogs as anti-inflammatory agents. The dominant role played by the electronic parameters,  $E_{\text{LUMO}}$  and dipole moment in the modulation of the biological activity, help us to propose a novel anti-inflammatory pharmacophore where involvement of oxime is well reflected.



### Synthesis and anticancer activity of 2-alkylaminomethyl-5-diaryl-methylenecyclopentanone hydrochlorides and related compounds

pp 1285–1291

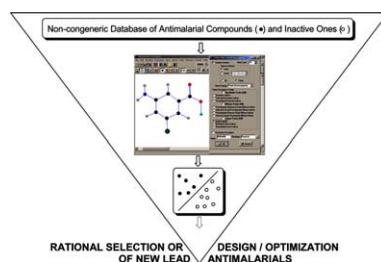
Jingli Wang, Linxiang Zhao, Rui Wang, Min Lu, Duo Chen and Yongkui Jing\*

7a ~ 7d R<sup>1</sup> = H R<sup>2</sup> = dimethylamino, 4-morpholinyl, 1-piperidyl, 1-pyrrolidinyl7e ~ 7h R<sup>1</sup> = CH<sub>3</sub> R<sup>2</sup> = dimethylamino, 4-morpholinyl, 1-piperidyl, 1-pyrrolidinyl

### Non-stochastic and stochastic linear indices of the ‘molecular pseudograph’s atom adjacency matrix’: application to ‘in silico’ studies for the rational discovery of new antimalarial compounds

pp 1293–1304

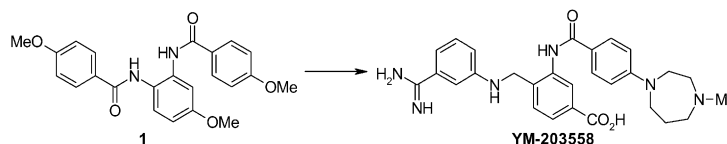
Yovani Marrero-Ponce,\* Alina Montero-Torres, Carlos Romero Zaldivar, Maité Iyarreta Veitia, Mariuchy Mayón Pérez and Rory N. García Sánchez



### Synthesis and biological activity of novel 1,2-disubstituted Benzene derivatives as factor Xa inhibitors

pp 1305–1323

Hiroyuki Koshio,\* Fukushi Hirayama, Tsukasa Ishihara, Ryouta Shiraki, Takeshi Shigenaga, Yuta Taniuchi, Kazuo Sato, Yumiko Moritani, Yoshiyuki Iwatsuki, Seiji Kaku, Naoko Katayama, Tomihisa Kawasaki, Yuzo Matsumoto, Shuichi Sakamoto and Shin-ichi Tsukamoto

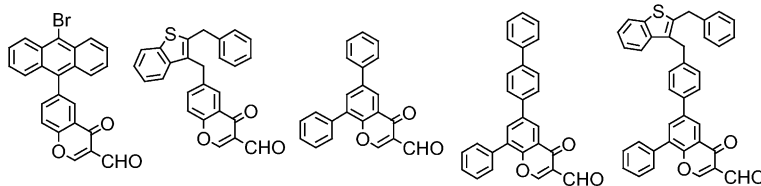


As a result of modification of HTS hit compound **1** to improve both its fXa inhibitory activity and its oral anticoagulant activity, YM-203558 showed nanomolar potency in fXa inhibitory activity and had excellent oral anticoagulant activity.

### Formylchromone derivatives as irreversible and selective inhibitors of human protein tyrosine phosphatase 1B. Kinetic and modeling studies

pp 1325–1332

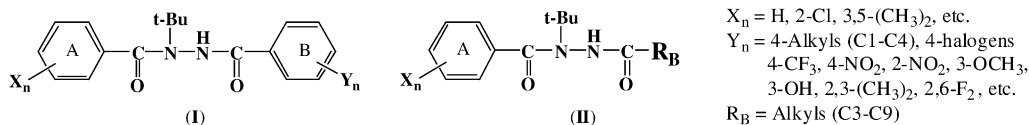
Yi Sup Shim, Ki Chul Kim, Kyung A. Lee, Suja Shrestha, Keun-Hyeung Lee, Chan Kyung Kim and Hyeongjin Cho\*



**Classical and three-dimensional QSAR for the inhibition of [<sup>3</sup>H]ponasterone A binding by diacylhydrazine-type ecdysone agonists to insect Sf-9 cells**

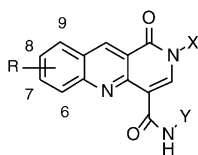
pp 1333–1340

Yoshiaki Nakagawa,\* Kaoru Takahashi, Hidetoshi Kishikawa, Takehiko Ogura, Chieka Minakuchi and Hisashi Miyagawa

**Synthesis and cytotoxic activity of carboxamide derivatives of benzo[*b*][1,6]naphthyridin-(5*H*)ones**

pp 1341–1355

Leslie W. Deady,\* Michael L. Rogers, Li Zhuang, Bruce C. Baguley and William A. Denny\*

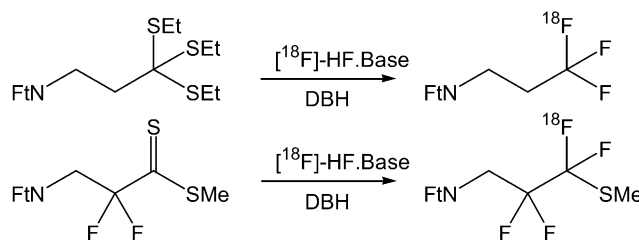


Twenty-six new compounds were prepared and tested. Compound **2t** ( $R = 6\text{-Me}$ ,  $X = 4\text{-FC}_6\text{H}_4$ ,  $Y = (\text{CH}_2)_2\text{NMe}_2$ ) at  $1.8 \text{ mg kg}^{-1}$  was curative against colon 38 tumors in mice.

**Perfluorinated markers for hypoxia detection: synthesis of sulfur-containing precursors and [<sup>18</sup>F]-labelling**

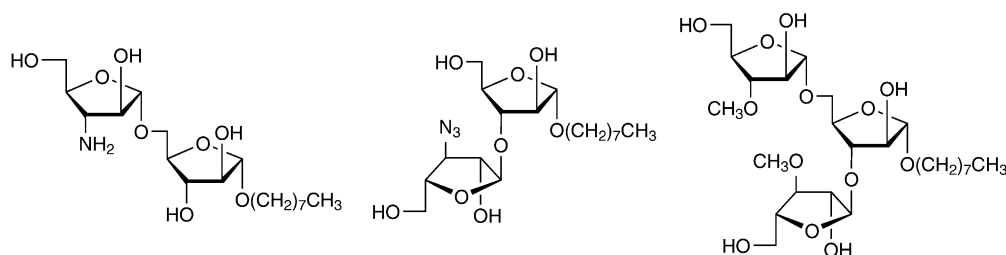
pp 1357–1367

Arnaud Cheguillaume, Jacques Gillart, Daniel Labar, Vincent Grégoire and Jacqueline Marchand-Brynaert\*

**Oligosaccharides as inhibitors of mycobacterial arabinosyltransferases. Di- and trisaccharides containing C-3 modified arabinofuranosyl residues**

pp 1369–1379

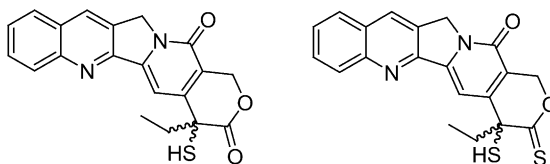
Oana M. Cociorva, Sudagar S. Gurcha, Gurdial S. Besra and Todd L. Lowary\*



**On the role of E-ring oxygen atoms in the binding of camptothecin to the topoisomerase I–DNA covalent binary complex**

pp 1381–1386

Nicolas J. Rahier, Brian M. Eisenhauer, Rong Gao, Shannon J. Thomas and Sidney M. Hecht\*


**Antioxidant activity of differently regioselective chitosan sulfates in vitro**

pp 1387–1392

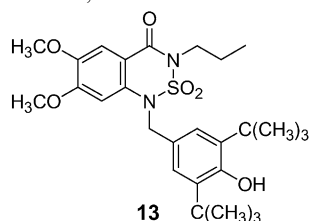
Ronge Xing, Huahua Yu, Song Liu, Weiwei Zhang, Quanbin Zhang, Zhien Li and Pengcheng Li\*

Antioxidant activities of differently regioselective chitosan sulfates in vitro and the relevance of antioxidant activities and their structures were reported.

**Synthesis, biological evaluation and molecular modelling studies on benzothiadiazine derivatives as PDE4 selective inhibitors**

pp 1393–1402

Annalisa Tait,\* Amedeo Luppi, Armin Hatzelmann, Paola Fossa and Luisa Mosti

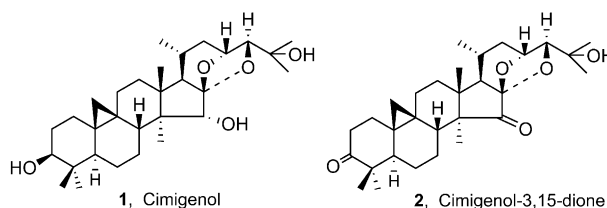


A series of 2,1,3- and 1,2,4-benzothiadiazine derivatives (BTDs) were synthesized and evaluated for their inhibitory activity versus enzymatic isoforms PDE3, PDE4 and PDE7. The antioxidant compound **13** was found active and selective at micromolar level versus PDE4.

**Cancer preventive agents. Part 1: Chemopreventive potential of cimigenol, cimigenol-3,15-dione, and related compounds**

pp 1403–1408

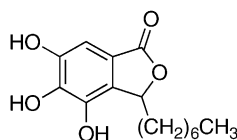
Nobuko Sakurai, Mutsuo Kozuka, Harukuni Tokuda, Teruo Mukainaka, Fumio Enjo, Hoyoku Nishino, Masahiro Nagai, Yojiro Sakurai and Kuo-Hsiung Lee\*



**Cytosporone E: racemic synthesis and preliminary antibacterial testing**

pp 1409–1413

Jeffrey D. Hall, Nathan W. Duncan-Gould, Nasar A. Siddiqi, Jennifer N. Kelly,  
L. Alexis Hoferlin, Susan J. Morrison and Justin K. Wyatt\*

**Cytosporone E**

Cytosporone E was synthesized using the Meyers *ortho*-alkylation of a chiral aromatic oxazoline as the key step to form the phthalide backbone. Antibacterial testing demonstrates activity against Gram-positive bacteria and not Gram-negative bacteria.

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\*Corresponding author

Ⓜ<sup>+</sup> Supplementary data available via ScienceDirect**COVER**

2005: Human liver glycogen phosphorylase A (HLGP<sub>a</sub>) 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 HLGP<sub>a</sub> 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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