

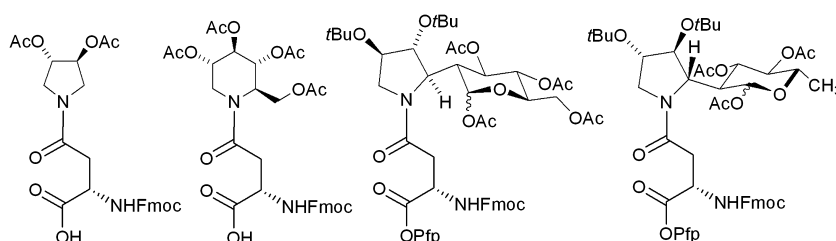
Contents

ARTICLES

Fmoc-protected iminosugar modified asparagine derivatives as building blocks for glycomimetics-containing peptides

pp 3965–3973

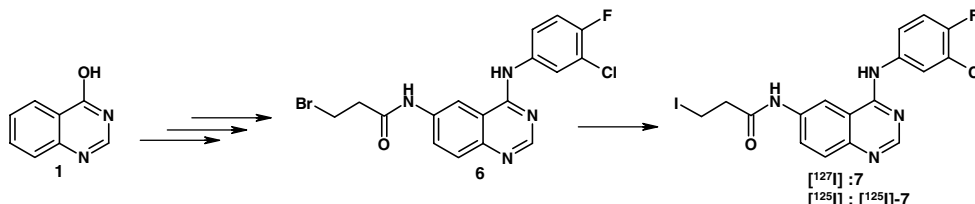
Francesca Nuti, Ilaria Paolini, Francesca Cardona, Mario Chelli, Francesco Lolli, Alberto Brandi, Andrea Goti, Paolo Rovero and Anna M. Papini*



Radioiodination of new EGFR inhibitors as potential SPECT agents for molecular imaging of breast cancer

pp 3974–3980

Célia Fernandes, Cristina Oliveira, Lurdes Gano, Athanasia Bourkoulou, Ioannis Pirmettis and Isabel Santos*

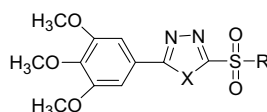


[¹²⁵I]-N-{4-[(3-Chloro-4-fluorophenyl)amino]quinazolin-6-yl}-3-iodopropionamide ([¹²⁵I]-7), a potential EGFR-TK inhibitor, was synthesised from 4-hydroxyquinazoline **1** and was in vitro evaluated for inhibitory activity of EGFR.

Synthesis and antifungal activities of 5-(3,4,5-trimethoxyphenyl)-2-sulfonyl-1,3,4-thiadiazole and 5-(3,4,5-trimethoxyphenyl)-2-sulfonyl-1,3,4-oxadiazole derivatives

pp 3981–3989

Cai-Jun Chen, Bao-An Song,* Song Yang, Guang-Fang Xu, Pinaki S. Bhadury, Lin-Hong Jin, De-Yu Hu, Qian-Zhu Li, Fang Liu, Wei Xue, Ping Lu and Zhuo Chen



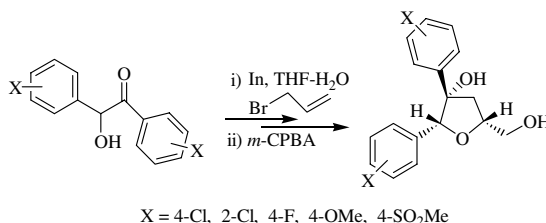
A new series of sulfone derivatives containing trimethoxyphenyl substituted 1,3,4-thiadiazole and 1,3,4-oxadiazole moiety (**9a–9i**, **10a–10q**) were synthesized and evaluated for antifungal activities against *Gibberella zeae*, *Botrytis cinerea*, and *Sclerotinia sclerotiorum*. These compounds are shown to be fungicidally active. Title compounds **10i** and **10j** can inhibit mycelia growth by approximately 50% (EC₅₀) at 2.9–93.3 µg/mL in vitro against 10 kinds of fungus.



2,3,5-Substituted tetrahydrofurans as cancer chemopreventives. Part 1: Synthesis and anti-cancer activities of 5-hydroxymethyl-2,3-diaryl-tetrahydro-furan-3-ols

pp 3990–3996

Palwinder Singh,* Anu Mittal and Subodh Kumar*



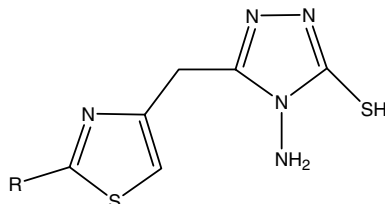
5-Hydroxymethyl-2,3-diaryl-tetrahydro-furan-3-ols have been diastereoselectively synthesized and tested for their anti-cancer activities at 59 human tumor cell lines.



Synthesis of new S-derivatives of clubbed triazolyl thiazole as anti-*Mycobacterium tuberculosis* agents

pp 3997–4008

Mahendra Ramesh Shiradkar,* Kiran Kumar Murahari, Hanimi Reddy Gangadasu, Tatikonda Suresh, Chakravarthy Akula Kalyan, Dolly Panchal, Ranjit Kaur, Prashant Burange, Jyoti Ghogare, Vinod Mokale and Mayuresh Raut

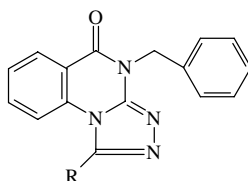


The synthesis of a new series of triazolyl-thiazole derivatives under microwave assisted organic synthesis is described. They were tested as antimycobacterial agents. It was also observed that **8f** and **8g** have shown promising activity, while compounds **8e** and **8h** have shown appreciable antimycobacterial potency. Few compounds were good inhibitors while others were inactive.

Synthesis and pharmacological investigation of novel 4-benzyl-1-substituted-4H-[1,2,4]triazolo[4,3-a]quinazolin-5-ones as new class of H₁-antihistaminic agents

pp 4009–4015

V. Alagarsamy,* V. R. Solomon and M. Murugan

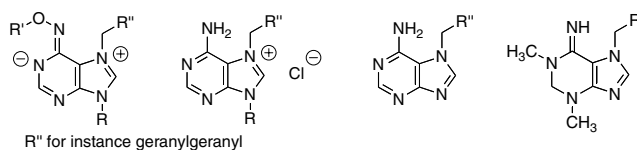


In the present study, a new series of 4-benzyl-1-substituted-4H-[1,2,4]triazolo[4,3-a]quinazolin-5-ones were synthesized and pharmacological screening studies of their H₁-antihistaminic and sedative-hypnotic activity are described.

Antimicrobial and cytotoxic activity of agelasine and agelasimine analogs

pp 4016–4037

Anders Vik, Erik Hedner, Colin Charnock, Linda W. Tangen, Ørjan Samuelsen, Rolf Larsson, Lars Bohlin and Lise-Lotte Gundersen*

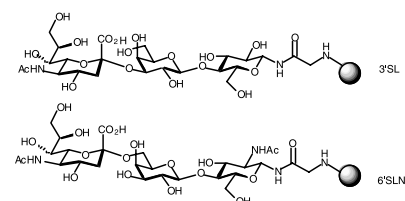


Probing the receptor interactions of an H5 avian influenza virus using a baculovirus expression system and functionalised poly(acrylic acid) ligands

pp 4038–4047

Wendy S. Barclay, Ian M. Jones, Helen M. I. Osborn,* Louisa Phillipson, Junyuan Ren, Guadalupe A. Talevera and Catherine I. Thompson

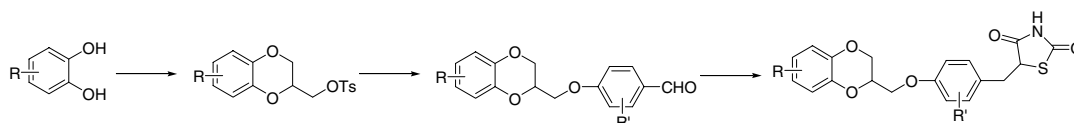
Carbohydrate functionalised poly(acrylic acid) polymers have been utilised to investigate the receptor specificity of an H5 avian influenza virus haemagglutinin protein, and validate the utility of a baculovirus expression system for facile and safe analysis of the Neu5Ac binding specificity of mutants of H5 HA.



Synthesis and glycogen phosphorylase inhibitor activity of 2,3-dihydrobenzo[1,4]dioxin derivatives

pp 4048–4056

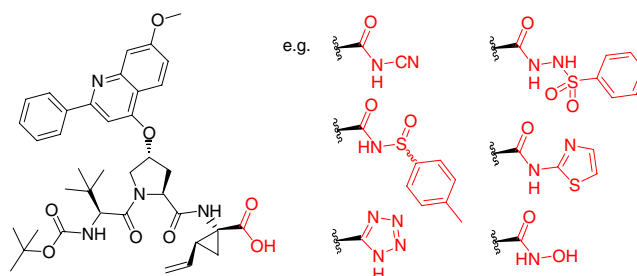
László Juhász,* Tibor Docsa, Attila Brunyászi, Pál Gergely and Sándor Antus



Evaluation of a diverse set of potential P₁ carboxylic acid bioisosteres in hepatitis C virus NS3 protease inhibitors

pp 4057–4068

Robert Rönn, Thomas Gossas, Yogesh A. Sabnis, Hanna Daoud, Eva Åkerblom, U. Helena Danielson and Anja Sandström*

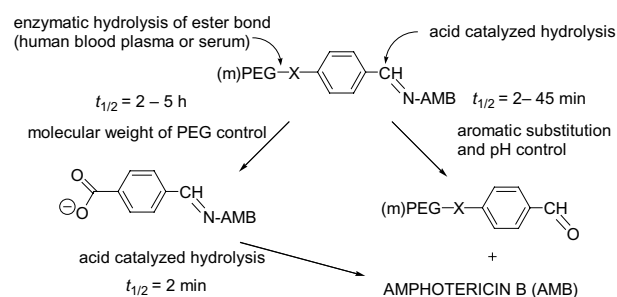


Synthesis of pH-sensitive amphotericin B–poly(ethylene glycol) conjugates and study of their controlled release in vitro

pp 4069–4076

Miloš Sedlák,* Martin Pravda, Frantisek Staud, Lenka Kubicová, Kateřina Týčová and Karel Ventura

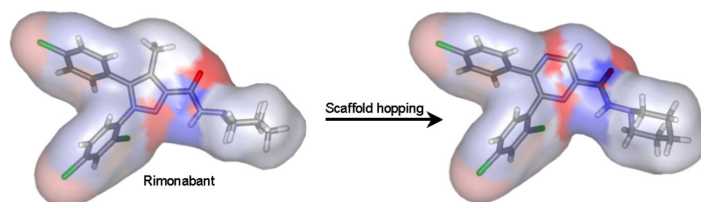
The prepared conjugates of amphotericin B with poly(ethylene glycols) represent a new system of two-stage independent release of AMB from polymeric carrier.



Scaffold hopping, synthesis and structure–activity relationships of 5,6-diaryl-pyrazine-2-amide derivatives: A novel series of CB1 receptor antagonists

pp 4077–4084

Jonas Boström,* Kristina Berggren, Thomas Elebring, Peter J. Greasley and Michael Wilstermann

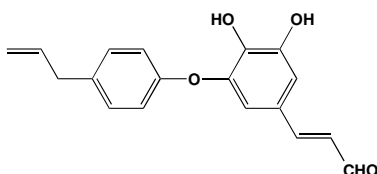


Using a shape-based scaffold hopping approach a novel class of cannabinoid (CB1) receptor antagonists has been identified, which incorporate a six-membered pyrazine ring instead of the five-membered methylpyrazole as central fragment.


Inhibitory effect of obovatal on the migration and invasion of HT1080 cells via the inhibition of MMP-2

pp 4085–4090

Su-Kyung Lee, Hyo Kon Chun, Jae Young Yang, Dong Cho Han, Kwang-Hee Son and Byoung-Mog Kwon*

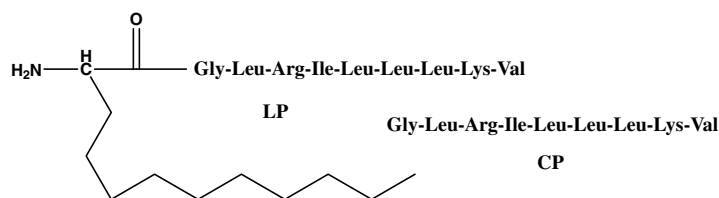


Obovatal was isolated from the leaves of *Magnolia obovata*. Obovatal strongly inhibited MMP-2 activity and the migration and invasion of HT1080 cells.

Novel cationic lipophilic peptides for oligodeoxynucleotide delivery

pp 4091–4097

Enoch Chan, Michael Amon, Robert J. Marano, Norbert Wimmer, Philip S. Kearns, Nicholas Manolios, P. Elizabeth Rakoczy and Istvan Toth*

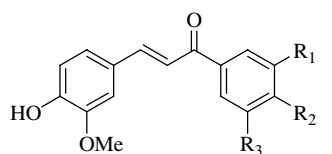


CP and particularly its lipophilic analogue LP have the potential to be used as oligodeoxynucleotide delivery systems.

Synthesis of 1,3-diphenyl-2-propen-1-one derivatives and evaluation of their biological activities

pp 4098–4105

Soyong Jang, Jae-Chul Jung and Seikwan Oh*



$R_1=R_2=R_3=H$, alkyl, halogens, alkoxy

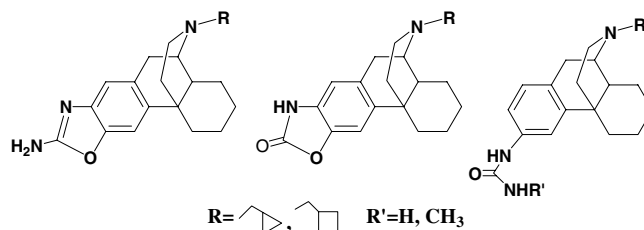
A simple synthesis and biological properties of 1,3-diphenyl-2-propen-1-ones **18–22** and **25–26** are described.

In-vitro investigation of oxazol and urea analogues of morphinan at opioid receptors

pp 4106–4112

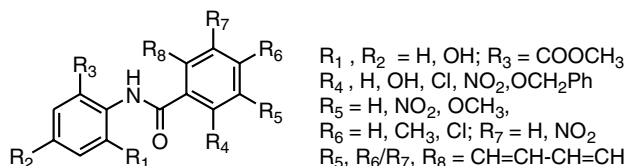
Xuemei Peng, Brian I. Knapp, Jean M. Bidlack and John L. Neumeyer*

A series of 2-amino-oxazole and 2-one-oxazole analogs and ureas were synthesized and evaluated in-vitro by their binding affinity at opioid receptors. The orientation of 2'-amino group in the oxazole and thiozole series contributes to their binding affinity.

**Synthesis, antimicrobial, and QSAR studies of substituted benzamides**

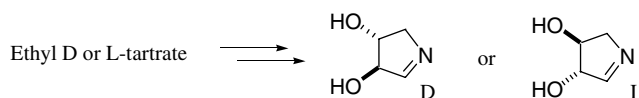
pp 4113–4124

Anil Kumar, Balasubramanian Narasimhan and Devinder Kumar*

**Synthesis and evaluation of amino-threoses in D- and L-series: Are five membered ring amino-sugars more potent glycosidase inhibitors than the six membered ones?**

pp 4125–4135

Carine Chevrier, Albert Defoin* and Céline Tarnus



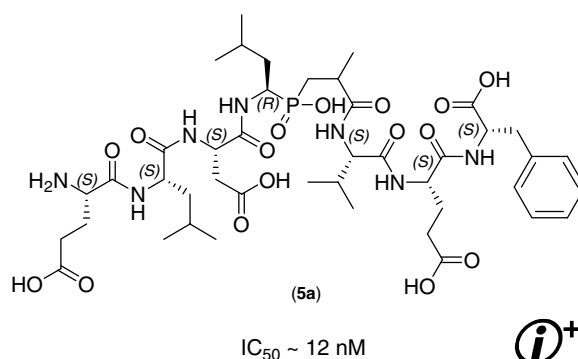
4-Amino-4-deoxy-D- and L-threose were synthesised from ethyl D- and L-tartrate, respectively, and evaluated against glycosidases. From these data as well as the inhibition potencies of others 4-amino-4-deoxy-tetroses, contribution of binding of each functionality of the 5 and 6 membered ring amino-sugars toward the various glycosidases is discussed.

Synthesis and biological evaluation of phosphino dipeptide isostere inhibitor of human β -secretase (BACE1)

pp 4136–4143

Florian Manzenrieder, Andreas O. Frank, Timo Huber, Cornelia Dorner-Ciossek and Horst Kessler*

Phosphino peptide **5a** was synthesized and appeared as a highly active inhibitor of BACE1.

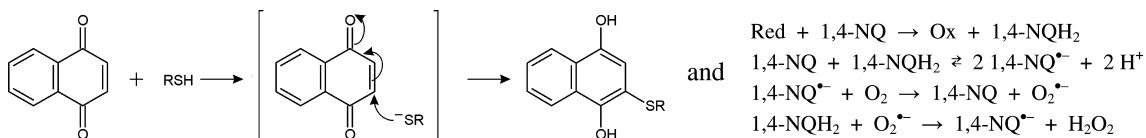


Double mode of inhibition-inducing interactions of 1,4-naphthoquinone with urease:

pp 4144–4151

Arylation versus oxidation of enzyme thiols

Barbara Krajewska* and Wiesława Zaborska

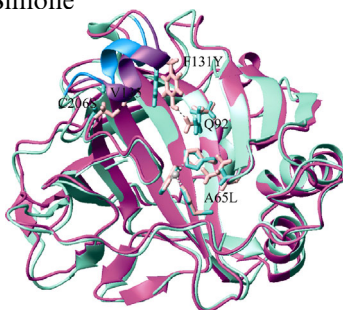


1,4-Naphthoquinone inhibits urease by a mixed mechanism that involves direct arylation of enzyme thiol groups and their oxidation by redox cycling-generated H_2O_2 .

Molecular modeling study for the binding of zonisamide and topiramate to the human mitochondrial carbonic anhydrase isoform VA

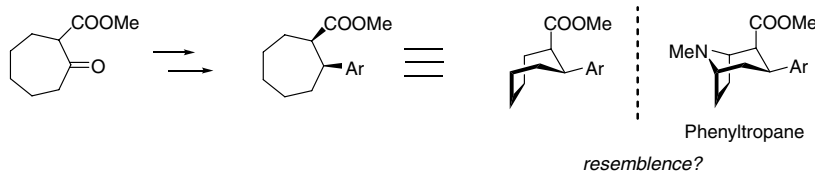
pp 4152–4158

Rosa Maria Vitale, Carlo Pedone, Pietro Amodeo, Jochen Antel, Michael Wurl, Andrea Scozzafava, Claudiu T. Supuran* and Giuseppina De Simone*

**Synthesis, inhibition and binding of simple non-nitrogen inhibitors of monoamine transporters**

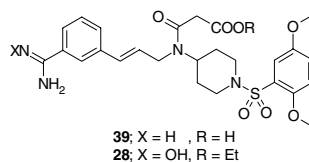
pp 4159–4174

Mikkel Due Petersen, Søren Valdgård Boye, Erik Holm Nielsen, Jeanette Willumsen, Steffen Sinning, Ove Wiborg and Mikael Bols*

**Prodrug-based design, synthesis, and biological evaluation of N-benzenesulfonylpiperidine derivatives as novel, orally active factor Xa inhibitors**

pp 4175–4192

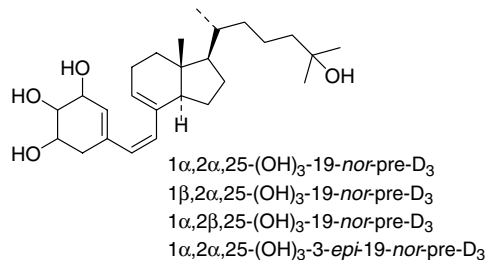
Tsukasa Ishihara,* Norio Seki, Fukushi Hirayama, Masaya Orita, Hiroyuki Koshio, Yuta Taniuchi, Yumiko Sakai-Moritani, Yoshiyuki Iwatsuki, Seiji Kaku, Tomihisa Kawasaki, Yuzo Matsumoto and Shin-ichi Tsukamoto



Parallel synthesis identified potent and selective fXa inhibitors with a benzenesulfonyl group as an S4 binding element. Masking of their hydrophilic groups led to related prodrugs with oral anticoagulant effects.

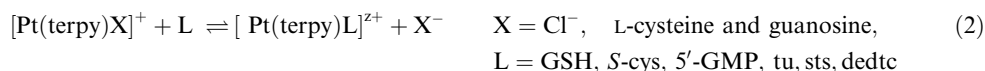
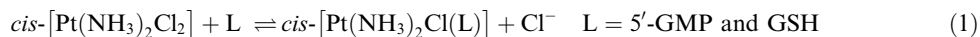
Synthesis and biological evaluation of new 6-*s-cis* locked 1,2,25-trihydroxyprevitamin D₃ analogues pp 4193–4202

Laura Sánchez-Abella, Susana Fernández, Annemieke Verstuyf, Lieve Verlinden, Miguel Ferrero* and Vicente Gotor*

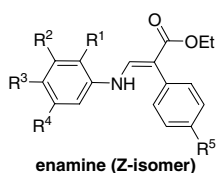
**Studies of interactions between platinum(II) complexes and some biologically relevant molecules** pp 4203–4211

Dejan Petrović, Biljana Stojimirović, Biljana Petrović, Zorica M. Bugarčić and Živadin D. Bugarčić*

The substitution reactions of Pt(II) complexes with some biologically relevant molecules were studied using UV–vis, stopped-flow spectrophotometry and ¹H NMR spectroscopy.

**Synthesis, structure, and structure–activity relationship analysis of enamines as potential antibacterials** pp 4212–4219

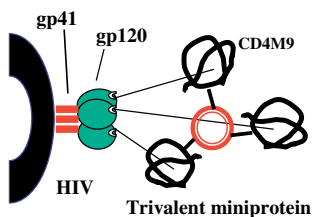
Zhu-Ping Xiao, Jia-Yu Xue, Shu-Hua Tan, Huan-Qiu Li and Hai-Liang Zhu*



The tested enamines were shown more effective to inhibiting growth of bacteria than fungi. An *E*-isomer exhibited higher antibacterial activity than the corresponding *Z*-isomer and four compounds (**9b**, **11b**, **12b** and **15b**) showed considerable antibacterial activities against *Staphylococcus aureus*.

Synthesis and anti-HIV activity of trivalent CD4-mimetic miniproteins pp 4220–4228

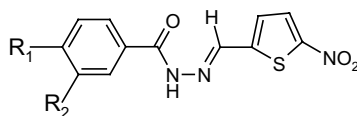
Hengguang Li, Yongjun Guan, Agnieszka Szczepanska, Antonio J. Moreno-Vargas, Ana T. Carmona, Inmaculada Robina, George K. Lewis and Lai-Xi Wang*



A new class of nifuroxazide analogs: Synthesis of 5-nitrothiophene derivatives with antimicrobial activity against multidrug-resistant *Staphylococcus aureus*

pp 4229–4236

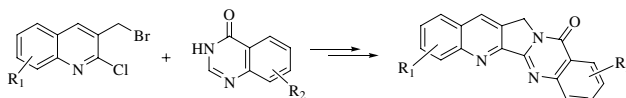
Andrea Masunari* and Leoberto Costa Tavares



In this study it was evaluated the antibacterial activity of 14 acid [(5-nitro-thiophen-2-yl)-methylene]-hydrazides (Fig. 1) against multidrug-resistant (3SP/R33) *Staphylococcus aureus* strain. Compounds were designed according to physicochemical properties and all of them exhibited significant bacteriostatic activity. It was observed bactericidal activity for some compounds tested. These new compounds confirming the potential of nifuroxazide analogs as antimicrobial agents and represent an alternative for the development of promising antibacterial drugs.

Synthesis and topoisoemerase poisoning activity of A-ring and E-ring substituted luotonin A derivatives

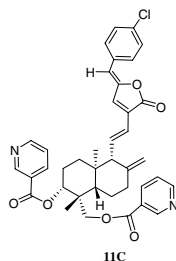
pp 4237–4246

Kassoum Nacro, Conxiang (Charles) Zha, Peter R. Guzzo, R. Jason Herr,*
Denise Peace and Thomas D. Friedrich

Synthesis of andrographolide derivatives: A new family of α -glucosidase inhibitors

pp 4247–4255

Xu Hai-Wei, Dai Gui-Fu, Liu Gai-Zhi, Wang Jun-Feng and Liu Hong-Min*



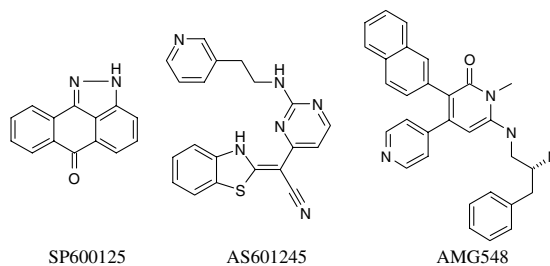
A novel family of α -glucosidase inhibitors were prepared. Among them, **11c** was a very potent inhibitor against α -glucosidase with an IC_{50} value of 6 μ M.

Assessing potency of c-Jun N-terminal kinase 3 (JNK3) inhibitors using 2D molecular descriptors and binary QSAR methodology

pp 4256–4264

Ismail Ijjaali,* François Petit, Elodie Dubus, Olivier Barberan and André Michel

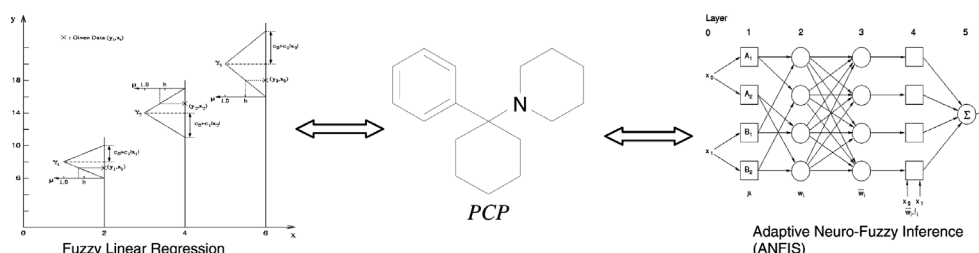
Two-dimensional molecular descriptors in combination with binary QSAR methodology were used to build classification models of JNK3 ligands. The best model was obtained at 100 nM IC_{50} activity threshold with van der Waals surface based descriptors and reached an overall accuracy of 98%.



Adaptive neuro-fuzzy inference system (ANFIS): A new approach to predictive modeling in QSAR applications: A study of neuro-fuzzy modeling of PCP-based NMDA receptor antagonists

pp 4265–4282

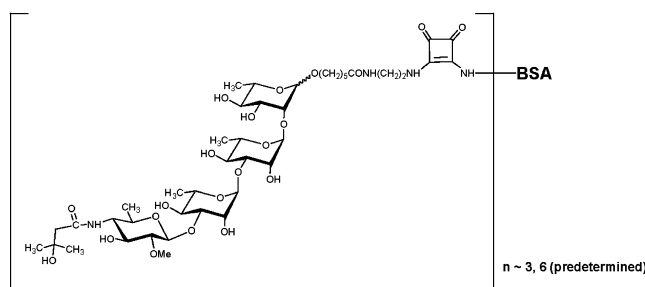
Erdem Buyukbingol,* Arzu Sisman, Murat Akyildiz, Ferda Nur Alparslan and Adeboye Adejare



Immunogens related to the synthetic tetrasaccharide side chain of the *Bacillus anthracis* exosporium

pp 4283–4310

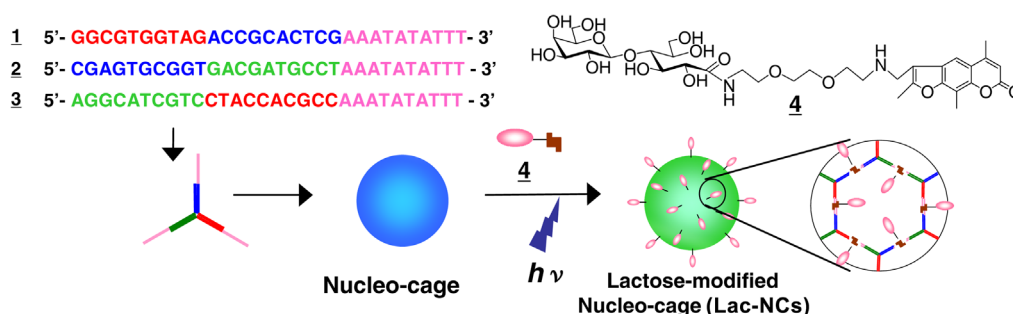
Rina Saksena, Roberto Adamo and Pavol Kováč*



Binding of lectins to DNA micro-assemblies: Modification of nucleocages with lactose-conjugated psoralen

pp 4311–4317

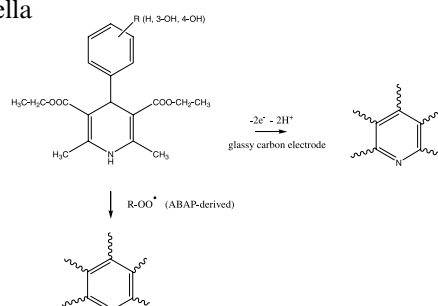
Kwonil Kim, Kazunori Matsuura* and Nobuo Kimizuka*



Oxidation of C4-hydroxyphenyl 1,4-dihydropyridines in dimethylsulfoxide and its reactivity towards alkylperoxyl radicals in aqueous medium


pp 4318–4326

Luis J. Núñez-Vergara,* R. Salazar, C. Camargo, J. Carbajo, B. Conde, P. A. Navarrete-encina and J. A. Squella



OTHER CONTENTS**Summary of instructions to authors****p I**

*Corresponding author

+ Supplementary data available via ScienceDirect**COVER**

Sunshine is a significant source of vitamin D₃, recognized as important biological metabolite for therapeutic applications. To investigate the mechanism of action of the later, locked previtamin D₃ analogues have been synthesized. Potency in inhibiting cell proliferation and binding to VDR and BDP were evaluated [Sánchez-Abella, L.; Fernández, S.; Verstuyf, A.; Verlinden, L.; Ferrero, M.; Gotor, V. *Bioorg. Med. Chem.* **2007**, 15, 4193–4202].

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