

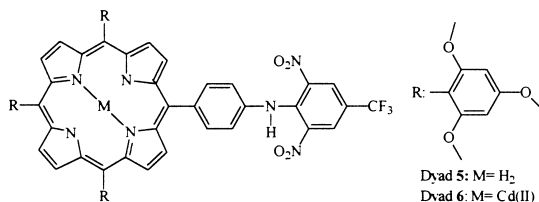
Synthesis and Biological Evaluation of Methoxyphenyl Porphyrin Derivatives as Potential Photodynamic Agents

Bioorg. Med. Chem. 9 (2001) 1943

M. Elisa Milanesio,^a Flavia S. Morán,^b E. Ines Yslas,^b M. Gabriela Alvarez,^b Viviana Rivarola^b and Edgardo N. Durantini^a

^aDepartamento de Química y Física, Universidad Nacional de Río Cuarto, Agencia Postal Nro 3, 5800 Río Cuarto, Argentina

^bDepartamento de Biología Molecular, Universidad Nacional de Río Cuarto, Agencia Postal Nro 3, 5800 Río Cuarto, Argentina



Thermodynamic Quantitative Structure–Activity Relationship

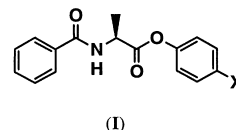
Bioorg. Med. Chem. 9 (2001) 1951

Analysis for Enzyme–Ligand Interactions in Aqueous Phosphate Buffer and Organic Solvent

Ki Hwan Kim

Department of Structural Biology, Abbott Laboratories, Abbott Park, IL 60064-6100, USA

Thermodynamic quantitative structure–activity relationships (QSAR) for chymotrypsin–ligand binding is developed, and the results are compared for the effects of organic solvent on the substrate specificity of the enzymes to those in aqueous phosphate buffer.



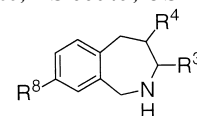
Effects of a 3-Alkyl-, 4-Hydroxy- and/or 8-Aromatic-substituent on the Phenylethanolamine N-Methyltransferase Inhibitor Potency and α_2 -Adrenoceptor Affinity of 2,3,4,5-Tetrahydro-1H-2-benzazepines

Bioorg. Med. Chem. 9 (2001) 1957

Gary L. Grunewald, Vilas H. Dahanukar and Kevin R. Criscione

Department of Medicinal Chemistry, 4060 Malott Hall, School of Pharmacy, University of Kansas, Lawrence, KS 66045, USA

The PNMT-inhibitory activity and selectivity of tetrahydroisogionoline was enhanced by the introduction of a hydrophilic electron-withdrawing 7-substituent and a 3-alkyl-substituent, so a similar study was conducted on tetrahydrobenzazepine.



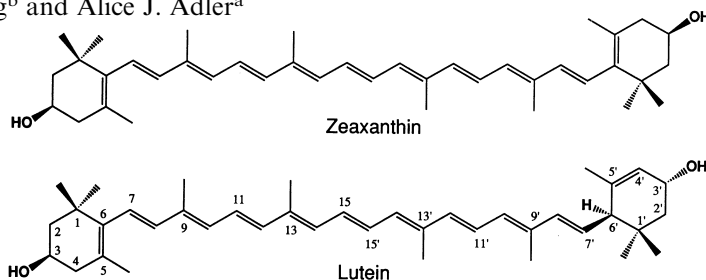
Tubulins in the Primate Retina: Evidence that Xanthophylls may be Endogenous Ligands for the Paclitaxel-Binding Site

Bioorg. Med. Chem. 9 (2001) 1967

Donald V. Crabtree,^a Iwao Ojima,^b Xudong Geng^b and Alice J. Adler^a

^aSchepens Eye Research Institute and Department of Ophthalmology, Harvard Medical School, 20 Staniford Street, Boston, MA 02114, USA

^bDepartment of Chemistry, State University of New York at Stony Brook, Stony Brook, NY 11794, USA

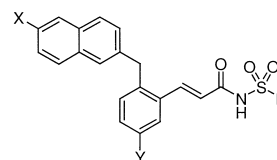


Structure–Activity Relationship of Cinnamic Acylsulfonamide Analogues on the Human EP₃ Prostanoid Receptor

Bioorg. Med. Chem. 9 (2001) 1977

Hélène Juteau, Yves Gareau, Marc Labelle, Claudio F. Sturino, Nicole Sawyer, Nathalie Tremblay, Sonia Lamontagne, Marie-Claude Carrière, Danielle Denis and Kathleen M. Metters
Merck Frosst Canada & Co., PO Box 1005, Pointe-Claire-Dorval, Québec, Canada H9R 4P8

The structure–activity of the cinnamic acylsulfonamide series was conducted. Potent and selective antagonists of the human EP₃ receptor displaying sub-nanomolar K_i values were identified.



Microbial and Reducing Agents Catalyze the Rearrangement of Taxanes

Bioorg. Med. Chem. 9 (2001) 1985

Di-An Sun,^a Anastasia Nikolakakis,^a Françoise Sauriol,^b Orval Mamer^c and Lolita O. Zamir^{a,d}

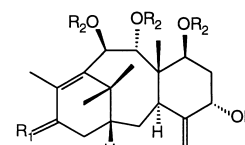
^aHuman Health Research Center, INRS-Institut Armand-Frappier, Université du Québec, 531 Boulevard des Prairies, Laval, Québec, Canada H7V 1B7

^bDepartment of Chemistry, Queen's University, Kingston, Ontario, Canada K7L 3N6

^cBiomedical Mass Spectrometry Unit, McGill University, 1130 Pine Avenue west, Montreal Québec, Canada H3A 1A3

^dMcGill Center for Translational Research in Cancer, Sir Mortimer B. Davis-Jewish General Hospital, 3755 Côte Ste. Catherine Rd., Suite D-127, Montreal, Québec, Canada H3T 1E2

Biotransformation and treatment with zinc of taxane derivatives **1** and **3** gave a similar taxane with a C10–C11 double bond. New 1(15→11)abeo-taxanes are described.



1: R₁ = α-OH, β-H; R₂ = H
3: R₁ = O; R₂ = Ac

Synthesis and QSAR Studies of 4-Substituted Phenyl-2,6-dimethyl-3, 5-Bis-*N*-(substituted Phenyl)carbamoyl-1,4-dihydropyridines as Potential Antitubercular Agents

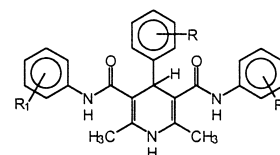
Bioorg. Med. Chem. 9 (2001) 1993

Bhavik Desai,^a Dinesh Sureja,^a Yogesh Naliapara,^a Anamik Shah^a and Anil K. Saxena^b

^aDepartment of Chemistry, Saurashtra University, Rajkot-360 005, India

^bMedicinal Chemistry Division, Central Drug Research Institute, Lucknow-226 001, India

Synthesis and QSAR studies of the title compounds have resulted in the identification of structural and physicochemical parameters (MR, σ^o, σ^m, σ^p) contributing to antitubercular activity. Among these, carbamoyl phenyl ring substituted at 3 and 4 position with NO₂ group or 2 position with Cl or OCH₃ group shows >90% inhibition against H₃₇Rv comparable to other substituted phenyls.



In Vitro Antifungal Evaluation and Structure–Activity Relationships of a New Series of Chalcone Derivatives and Synthetic Analogues, with Inhibitory Properties Against Polymers of the Fungal Cell Wall

Bioorg. Med. Chem. 9 (2001) 1999

Silvia N. López,^a María V. Castelli,^a Susana A. Zacchino,^a José N. Domínguez,^b Gricela Lobo,^b Jaime Charris-Charris,^b Juan C. G. Cortés,^c Juan C. Ribas,^c Cristina Devia,^d Ana M. Rodríguez^d and Ricardo D. Enriz^d

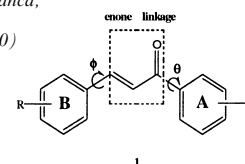
^aFarmacognosia, Facultad de Ciencias Bioquímicas y Farmacéuticas, Universidad Nacional de Rosario, Suipacha 531, (2000) Rosario, Argentina

^bLaboratorio de Síntesis Orgánica, Facultad de Farmacia, Universidad Central de Venezuela, Apartado 40109, Nva. Granada, (1040) Caracas, Venezuela

^cInstituto de Microbiología Bioquímica, Campus 'Miguel de Unamuno', Edificio Departamental #222, C.S.I.C./Universidad de Salamanca, (37007) Salamanca, Spain

^dQuímica General, Facultad de Química, Bioquímica y Farmacia, Universidad Nacional de San Luis, Chacabuco y Pedernera, (5700) San Luis, Argentina

Compounds of the general structure **1** were synthesized and examined for their antifungal properties with cellular and enzymatic assays. Many chalcone derivatives displayed potent activities against dermatophytes. A structure–activity relationship (SAR) study supported by theoretical calculations aided to identify the minimal structural requirements for the antifungal action. Regarding the mode of action, all active structures inhibited β(1,3)-glucan synthase and mainly chitin synthase-1, enzymes that catalyze the synthesis of the two major polymers of the fungal cell wall.



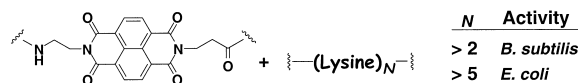
The Synthesis and Screening of 1,4,5,8-Naphthalenetetracarboxylic Diimide–Peptide Conjugates with Antibacterial Activity

Bioorg. Med. Chem. 9 (2001) 2015

Chandra T. Miller,^a Ramal Weragoda,^a Elzbieta Izbicka^b and Brent L. Iverson^a

^aDepartment of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712, USA

^bInstitute for Drug Development, San Antonio, TX 78245, USA



Synthesis and QSAR Studies in 2-(N-aryl-N-aroyle)amino-4,5-dihydrothiazole Derivatives as Potential Antithrombotic Agents

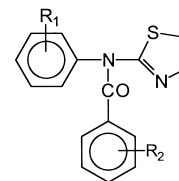
Bioorg. Med. Chem. 9 (2001) 2025

Anil K. Saxena,^a Suresh K. Pandey,^a P. Seth,^b M.P. Singh,^b M. Dikshit^b and A. Carpy^c

^aDivision of Medicinal Chemistry, Central Drug Research Institute, Lucknow-226 001, India

^bDivision of Pharmacology, Central Drug Research Institute, Lucknow-226 001, India

^cLaboratoire de Physico- & Toxic-Chimie (LPTC) des Systèmes Naturels, UMR 5472, CNRS, Université de Bordeaux I, 33405 Talence Cedex, France

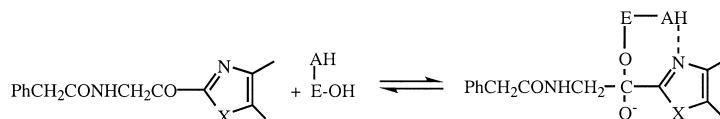


Design, Synthesis, and Evaluation of α -Ketoheterocycles as Class C β -Lactamase Inhibitors

Bioorg. Med. Chem. 9 (2001) 2035

Sanjai Kumar, Andre L. Pearson and R.F. Pratt

Department of Chemistry, Wesleyan University, Middletown, CT 06459, USA



Novel (4-Piperidin-1-yl)-phenyl Sulfonamides as Potent and Selective Human β_3 Agonists

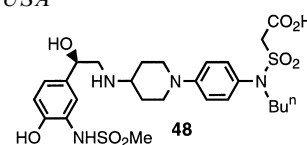
Bioorg. Med. Chem. 9 (2001) 2045

Baihua Hu,^a John Ellingboe,^a Stella Han,^b Elwood Largis,^b Kitae Lim,^a Michael Malamas,^a Ruth Mulvey,^b Chuansheng Niu,^a Alexander Oliphant,^a Jeffrey Pelletier,^a Thiruvikraman Singanallor,^a Fuk-Wah Sum,^a Jeff Tillett^b and Victoria Wong^a

^aChemical Sciences, Wyeth-Ayerst Research, Pearl River, NY 10965, USA

^bCardiovascular/Metabolic Diseases Research, Wyeth-Ayerst Research, Pearl River, NY 10965, USA

(4-Piperidin-1-yl)-phenyl sulfonamide **48** is a potent and selective β_3 agonist.



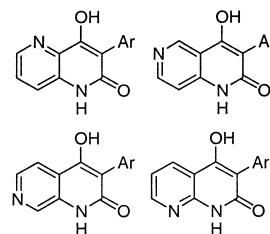
Synthesis and SAR of 5-, 6-, 7- and 8-Aza Analogues of 3-Aryl-4-hydroxyquinolin-2(1H)-one as NMDA/Glycine Site Antagonists

Bioorg. Med. Chem. 9 (2001) 2061

Zhang-Lin Zhou,^{a,b} James M. Navratil,^b Sui Xiong Cai,^a Edward R. Whittemore,^a Stephen A. Espitia,^a Jon E. Hawkinson,^a Minhtam Tran,^a Richard M. Woodward,^a Eckard Weber^a and John F.W. Keana^b

^aCoCensys, Inc., 213 Technology Drive, Irvine, CA 92618, USA

^bDepartment of Chemistry, University of Oregon, Eugene, OR 97403, USA



Toward the Identification of Selective Modulators of Protein Kinase C (PKC) Isozymes: Establishment of a Binding Assay for PKC Isozymes Using Synthetic C1 Peptide Receptors and Identification of the Critical Residues Involved in the Phorbol Ester Binding

Bioorg. Med. Chem. 9 (2001) 2073

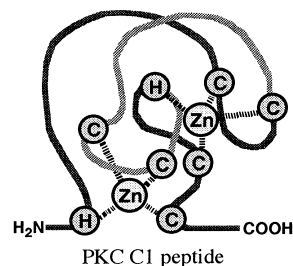
Mayumi Shindo,^a Kazuhiro Irie,^b Akifumi Nakahara,^b Hajime Ohigashi,^b Hiroaki Konishi,^c Ushio Kikkawa,^c Hiroyuki Fukuda^a and Paul A. Wender^d

^aApplied Biosystems Japan Ltd, Tokyo 104-0032, Japan

^bDivision of Applied Life Sciences, Graduate School of Agriculture, Kyoto University, Kyoto 606-8502, Japan

^cBiosignal Research Center, Kobe University, Kobe 657-8501, Japan

^dDepartment of Chemistry, Stanford University, Stanford, CA 94305-5080, USA



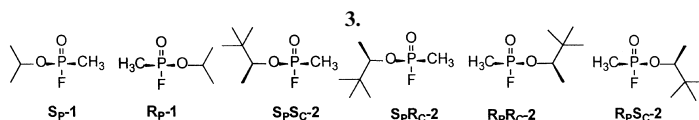
Stereoselective Detoxification of Chiral Sarin and Soman Analogues by Phosphotriesterase

Bioorg. Med. Chem. 9 (2001) 2083

Wen-Shan Li, Karin T. Lum, Misty Chen-Goodspeed, Miguel A. Sogorb and Frank M. Raushel

Department of Chemistry, Texas A&M University, PO Box 30012, College Station, TX 77842-3012, USA

The chemo-enzymatic synthesis and detoxification of chiral analogues of sarin (**1**) and soman (**2**) by mutants of the bacterial phosphotriesterase is reported.



Inhibition of Major Groove DNA Binding bZIP Proteins by Positive Patch Polyamides

Bioorg. Med. Chem. 9 (2001) 2093

Ryan E. Bremer, Nicholas R. Wurtz, Jason W. Szewczyk and Peter B. Dervan

Contribution from the Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, 91125, USA



The Structure of McN-5652

Bioorg. Med. Chem. 9 (2001) 2105

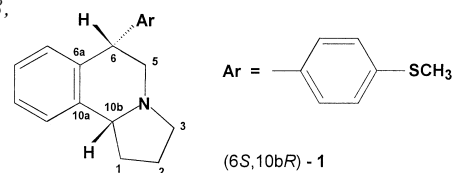
Oliver Schulze,^{a,b} Ulrich Schmidt,^a Jürgen Voss,^a Bruno Nebeling,^b Gunadi Adiwidjaja^c and Klaus Scharwächter^a

^aInstitut für Organische Chemie der Universität Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany

^bUniversitätsklinikum Hamburg-Eppendorf, Klinik und Poliklinik für Radiologie, Abt. für Nuklearmedizin, UKE-Zyklotron, Luruper Chaussee 149, 22761 Hamburg, Germany

^cMineralogisch-Petrographisches Institut der Universität Hamburg, Grindelallee 48, 20146 Hamburg, Germany

The configuration of the diastereoisomers of McN-5652 **1** is determined and unequivocally assigned by NMR spectroscopy (NOE measurements) and an X-ray structural analysis of the *trans* diastereomer.



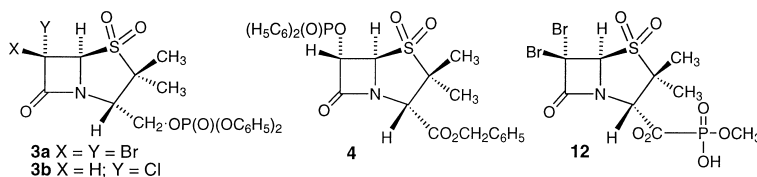
Synthesis and Human Leukocyte Elastase Inhibitory Evaluation of Phosphate Triesters and Acyl Phosphates of Penam Sulfides and Sulfones

Bioorg. Med. Chem. 9 (2001) 2113

María Laborde,^a Germán Pezzinati,^a Patricia Yovaldi,^a Oreste A. Mascaretti,^a Rolando C. Rossi^b and Juan Pablo Rossi^b

^aInstituto de Química Orgánica de Síntesis, Casilla de Correo 991, 2000 Rosario, Argentina

^bDepartamento de Química Biológica-IQUIFIB, Facultad de Farmacia y Bioquímica Universidad de Buenos Aires, Junin 956, 1113 Buenos Aires, Argentina



Synthesis and Pharmacological Activity of Metabolites of the 5-HT₄ Receptor Antagonist SB-207266

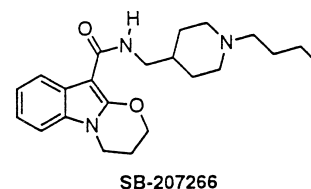
Bioorg. Med. Chem. 9 (2001) 2119

Michael Fedouloff,^a Frank Hossner,^a Martyn Voyle,^a Jennie Ranson,^b Jenifer Powles,^b Graham Riley^b and Gareth Sanger^b

^aDepartment of Synthetic Chemistry, Smithkline Beecham Pharmaceuticals, New Frontiers Science Park, Third Avenue, Harlow, Essex CM19 5AW, UK

^bDepartment of Neuroscience Research, Smithkline Beecham Pharmaceuticals, New Frontiers Science Park, Third Avenue, Harlow, Essex CM19 5AW, UK

Three metabolites of *N*-[1-butyl-4-piperidinyl)methyl]-3,4-dihydro-2*H*-[1,3]-oxazino[3,2-*a*]indole-10-carboxamide SB-207266 were synthesised and their pharmacological activity determined.



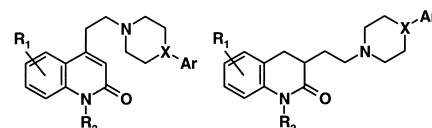
Synthesis and SAR of 3- and 4-Substituted Quinolin-2-ones: Discovery of Mixed 5-HT_{1B}/5-HT_{2A} Receptor Antagonists

Bioorg. Med. Chem. 9 (2001) 2129

Gary McCort,^a Christian Hoornaert,^a Michel Aletru,^a Colombe Denys,^a Olivier Duclos,^a Caroline Cadilhac,^a Eric Guilpain,^a Geneviève Dellac,^a Philip Janiak,^b Anne-Marie Galzin,^b Monique -Delahaye,^b Frédérique Guilbert^b and Stephen O'Connor^b

^aDepartment of Cardiovascular/Thrombosis Medicinal Chemistry, Sanofi-Synthelabo Recherche, 1 Avenue Pierre Brossolette, 91385 Chilly-Mazarin Cedex, France

^bDepartment of Pharmacology, Sanofi-Synthelabo Recherche, 1 Avenue Pierre Brossolette, 91385 Chilly-Mazarin Cedex, France



Design and Synthesis of a Cephalosporin-Retinoic Acid Prodrug Activated by a Monoclonal Antibody- β -Lactamase Conjugate

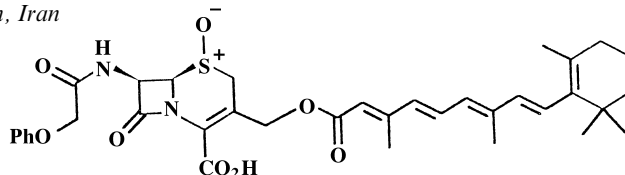
Bioorg. Med. Chem. 9 (2001) 2139

Gholam H. Hakimelahi,^a Tai Wei Ly,^a Sheng-Fa Yu,^a Maryam Zakerinia,^b Ali Khalafi-Nezhad,^b Mohammad N. Soltani,^b Mohsen N. Gorgani,^c Azra R. Chadegani^c and Ali A. Moosavi-Movahedi^c

^aInstitute of Chemistry, Academia Sinica, Taipei, Taiwan 115, Republic of China

^bDepartments of Chemistry and Medicine, Shiraz University, Shiraz, Iran

^cInstitute of Biochemistry-Biophysics, Tehran University, Tehran, Iran



3-Arylsulphonyl-5-arylamino-1,3,4-thiadiazol-2(3H)ones as Anti-inflammatory and Analgesic Agents

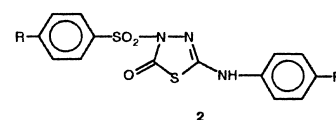
Bioorg. Med. Chem. 9 (2001) 2149

Silvia Schenone,^a Olga Bruno,^a Angelo Ranise,^a Francesco Bondavalli,^a Walter Filippelli,^b Giuseppe Falcone,^b Lucio Giordano^b and Maria Redenta Vitelli^b

^aDipartimento di Scienze Farmaceutiche, Facoltà di Farmacia dell'Università degli Studi di Genova, Viale Benedetto XV, 3, 16132, Genoa, Italy

^bDipartimento di Medicina Sperimentale, sezione di Farmacologia 'L. Donatelli', Facoltà di Medicina e Chirurgia, II Università degli Studi di Napoli, Via S. Andrea delle Dame 8, 80138, Naples, Italy

3-arylsulphonyl-5-arylamino-1,3,4-thiadiazol-2(3H)ones **2** with potential anti-inflammatory and analgesic activity were prepared and tested. Pharmacological results revealed that all the title compounds, endowed with an arylsulphonyl side chain, possess good antalgic activity and fair anti-inflammatory properties. The analgesic profile of the two series, evaluated by the acetic acid writhing test, showed that compounds **2c**, **2f** and **2h**, in particular, were the most active.



Cytotoxic Activities of Novel Hexahydroindolizino[8,7-b]indole Derivatives Prepared by 1,3-Dipolar Cycloaddition Reactions of 3,4-Dihydro- β -carboline Ylides

Bioorg. Med. Chem. 9 (2001) 2155

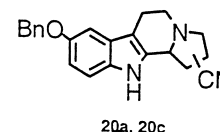
Martial Bertrand,^{a,†} Guillaume Poissonnet,^{a,‡} Marie-Hélène Thérêt-Bettiol,^a Christiane Gaspard,^a Georges H. Werner,^a Bruno Pfeiffer,^b Pierre Renard,^b Stéphane Léonce^c and Robert H. Dodd^a

^aInstitut de Chimie des Substances Naturelles, Centre National de la Recherche Scientifique, 91198 Gif-sur-Yvette Cedex, France

^bA.D.I.R., 1, rue Carle Hébert, 92415 Courbevoie cedex, France

^cInstitut de Recherches Servier, Division de Cancérologie Expérimentale, 11, rue des Moulineaux, 92150 Suresnes, France

The title compounds were synthesized and their cytotoxic properties toward L1210 cancer cells were evaluated in vitro. Compounds **20a** and **20c** displayed IC₅₀'s in the 15 μ M range and were found to stop cancer cell growth at the G2M and 8N stage of the cell cycle. These compounds were also active in a multidrug resistance cancer cell line.



Anti-HIV-1 Activity of an Antisense Phosphorothioate Oligonucleotide Bearing Imidazole and Primary Amine Groups

Bioorg. Med. Chem. 9 (2001) 2165

Kaoru Ushijima,^a Masahiro Shirakawa,^a Koumei Kagoshima,^a Wee-Sung Park,^a Naoko Miyano-Kurosaki^b and Hiroshi Takaku^{a,b,*}

^aDepartment of Industrial Chemistry, Chiba Institute of Technology, 2-17-1 Tsudanuma, Narashino, Chiba 275-0016, Japan

^bHigh Technology Research Center, Chiba Institute of Technology, 2-17-1 Tsudanuma, Narashino, Chiba 275-0016, Japan

The RNA cleaving reagent composed of imidazole and primary amine groups on an antisense phosphorothioate oligonucleotide (Im-anti-s-ODN), was synthesized and evaluated for anti-HIV-1 activity in MT-4 cells.

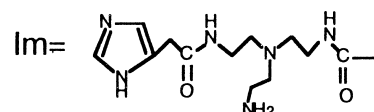
Target site (784-803) of HIV-1 gag-AUG sequence



↑
cleavage site

Im-anti-s-ODN

Im— 5'-cgctctgcacccatctctc-3'



Neuritogenic Cerebrosides from an Edible Chinese Mushroom.

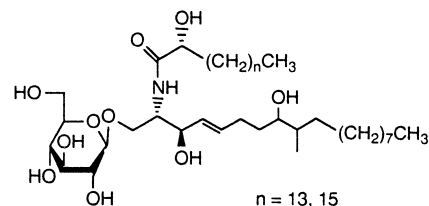
Bioorg. Med. Chem. 9 (2001) 2171

Part 2: Structures of Two Additional Termitomycesphins and Activity Enhancement of an Inactive Cerebroside by Hydroxylation

Jianhua Qi, Makoto Ojika and Youji Sakagami

Graduate School of Bioagricultural Sciences, Nagoya University, Chikusa-ku, Nagoya 464-8601, Japan

The isolation, structures, and neuritogenic activity against PC12 cells of termitomycesphins E and F are described. Di- and tetrahydroxylation of an inactive cerebroside enhanced the neuritogenic activity.



Synthesis and Evaluation of Bifunctional Anti-HIV Agents Based on Specific CXCR4 Antagonists-AZT Conjugation

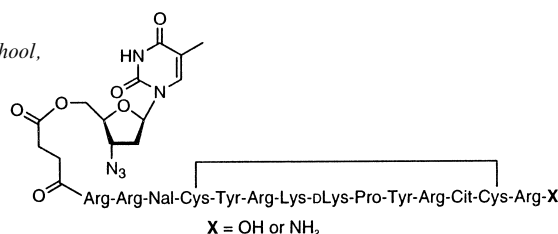
Bioorg. Med. Chem. 9 (2001) 2179

Hirokazu Tamamura,^a Akane Omagari,^a Kenichi Hiramatsu,^a Taisei Kanamoto,^b Kazuyo Gotoh,^b Kenji Kanbara,^b Naoki Yamamoto,^c Hideki Nakashima,^b Akira Otaka^a and Nobutaka Fujii^a

^aGraduate School of Pharmaceutical Sciences, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan

^bDepartment of Microbiology and Immunology, Kagoshima University Dental School, Sakuragaoka, Kagoshima 890-8544, Japan

^cTokyo Medical and Dental University, School of Medicine, Bunkyo-ku, Tokyo 113-8519, Japan



The Influence of Glutathione and Cysteine Levels on the Cytotoxicity of Helenanolide Type Sesquiterpene Lactones Against KB Cells

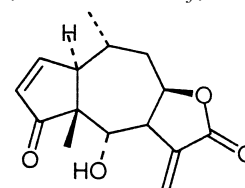
Bioorg. Med. Chem. 9 (2001) 2189

Jörg Heilmann,^a Michael R. Wasescha^a and Thomas J. Schmidt^b

^aDepartement für Angewandte Biowissenschaften, Institut für Pharmazeutische Wissenschaften, Eidgenössische Technische Hochschule (ETH) Zürich, Winterthurerstr. 190, 8057 Zürich, Switzerland

^bInstitut für Pharmazeutische Biologie der Heinrich-Heine-Universität Düsseldorf, Universitätsstrasse 1, 40225 Düsseldorf, Germany

The influence of different L-cysteine (cys) and glutathione (GSH) concentrations on the in-vitro cytotoxicity of the sesquiterpene lactones helenalin, 11 α ,13-dihydrohelenalin acetate and chamissonolide against KB cells were investigated. The observed effects are explained by the different reactivity and equilibrium conditions of the two reactive centers of bifunctional STLs.



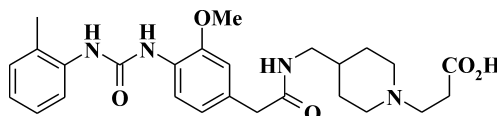
Diamine Containing VLA-4 Antagonists

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The design and synthesis of a library of potential VLA-4 inhibitors has been undertaken, resulting in the identification of antagonists with IC₅₀'s < 10 nM for the binding of fibronectin to ³H RAMOS cells.



Nickel(II) 2,6-Diacetylpyridine Bis(isonicotinoylhydrazonate) and Bis(benzoylhydrazonate) Complexes: Structure and Antimycobacterial Evaluation. Part XI

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Nickel(II) 2,6-diacetylpyridine bis(benzoylhydrazonate) **8b** displayed MIC = 0.025 µg/mL against *Mycobacterium tuberculosis* H37Rv, reaching the activity levels of isoniazid.

