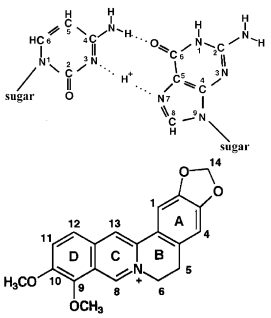
Protonated Forms of Poly[d(G-C)] and Poly(dG).poly(dC) and Their Interaction with Berberine

Bioorg. Med. Chem. 11 (2003) 4861

Gopinatha Suresh Kumar, Suman Das, Kakali Bhadra and Motilal Maiti*

Biophysical Chemistry Laboratory, Indian Institute of Chemical Biology, 4, Raja S.C. Mullick Road, Kolkata 700 032, India

Interaction of berberine with protonated structures of homo- and hetero-polymers of G.C sequences clearly established that berberine can be used as a probe for the detection of left-handed Hoogsteen base-paired structure that may potentiate its use in regulatory roles in biological functions.

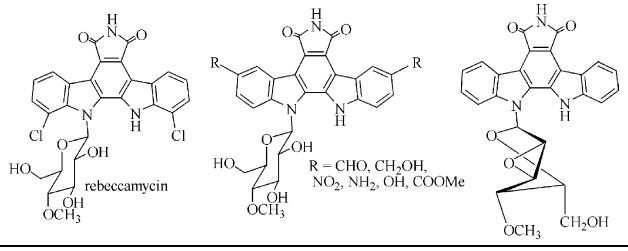


Semi-Synthesis, Topoisomerase I and Kinases Inhibitory Properties, and Antiproliferative Activities of New Rebeccamycin Derivatives

Bioorg. Med. Chem. 11 (2003) 4871

Pascale Moreau,[a] Nathalie Gaillard,[a] Christelle Marminon,[a] Fabrice Anizon,[a] Nathalie Dias,[b] Brigitte Baldeyrou,[b] Christian Bailly,[b] Alain Pierré,[c] John Hickman,[c] Bruno Pfeiffer,[d] Pierre Renard[d] and Michelle Prudhomme[a,*]

[a]*Université Blaise Pascal, Synthèse et Etude de Systèmes à Intérêt Biologique, UMR 6504, 63177 Aubière, France*
[b]*INSERM U-524 et Laboratoire de Pharmacologie Antitumorale du Centre Oscar Lambret, IRCL, 59045 Lille, France*
[c]*Institut de Recherches SERVIER, Division Recherche Cancérologie, 125 Chemin de ronde, 78290 Croissy sur Seine, France*
[d]*Les Laboratoires SERVIER, 1 Rue Carle Hébert, 92415 Courbevoie, France*

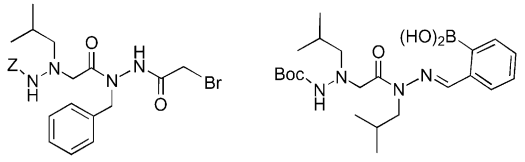


Hydrazino-Aza and *N*-Azapeptoids with Therapeutic Potential as Anticancer Agents

Bioorg. Med. Chem. 11 (2003) 4881

Karine Bouget,[a] Sandrine Aubin,[a] Jean-Guy Delcros,[b] Yannick Arlot-Bonnemains[c,*] and Michèle Baudy-Floc'h[a,*]

[a]*Laboratoire de Synthèse et Electrosynthèse Organiques (SESO), CNRS UMR 6510, Université de Rennes I, Avenue du Général Leclerc, F-35042 Rennes Cédex, France*
[b]*Groupe de Recherche en Thérapeutique Anticancéreuse (GRETAC), Faculté de Médecine, Université de Rennes I, 2 Avenue du Pr Leon Bernard, CS 34317, 35043 Rennes Cedex, France*
[c]*Groupe Cycle Cellulaire, CNRS UMR 6061 Génétique et Développement, IFR 97 Génomique Fonctionnelle et Santé, Faculté de Médecine, Université Rennes I, 2 Avenue du Pr Leon Bernard, CS 34317, 35043 Rennes Cedex, France*



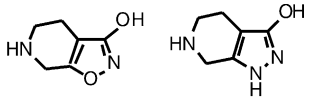
Aza-THIP and Related Analogues of THIP as $GABA_C$ Antagonists

Bioorg. Med. Chem. 11 (2003) 4891

Dorte Krehan,[a] Bente Frølund,[a] Bjarke Ebert,[b] Birgitte Nielsen,[a] Povl Krogsgaard-Larsen,[a,*] Graham A.R. Johnston[c] and Mary Chebib[d]

[a]*Centre for Drug Design and Transport, Department of Medicinal Chemistry, The Danish University of Pharmaceutical Sciences, DK 2100 Copenhagen, Denmark*
[b]*Department of Neurobiology, H. Lundbeck A/S, DK 2500 Valby, Denmark*
[c]*Adrien Albert Laboratory of Medicinal Chemistry, Department of Pharmacology, Sydney, NSW 2006, Australia*
[d]*Department of Pharmacy, The University of Sydney, Sydney, NSW 2006, Australia*

A series of eight compounds structurally related with THIP has been characterized pharmacologically using homomeric $GABA_C$ ρ_1 receptors expressed in *Xenopus* oocytes. The eight compounds were shown to be either inactive or competitive antagonists. Within this series of $GABA_C$ antagonists, only Aza-THIP was a selective and moderately potent $GABA_C$ antagonist showing no detectable interaction with $GABA_A$ receptors.

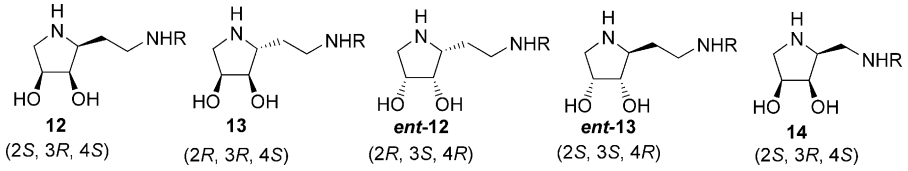


Bioorg. Med. Chem. 11 (2003) 4897

Synthesis and Glycosidase Inhibitory Activities of 2-(aminoalkyl)pyrrolidine-3,4-diol Derivatives

Ana T. Carmona,[a] Florence Popowycz,[b] Sandrine Gerber-Lemaire,[b] Eliazar Rodríguez-García,[b] Catherine Schütz,[b] Pierre Vogel[b,*] and Inmaculada Robina[a,*]

[a]*Departamento de Química Orgánica, Facultad de Química, Universidad de Sevilla, E-41071 Seville, Spain*
[b]*Institut de chimie moléculaire et biologique, Ecole Polytechnique Fédérale de Lausanne, BCH, 1015 Lausanne, Switzerland*



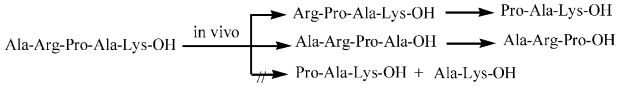
Bioorg. Med. Chem. 11 (2003) 4913

Identification, Synthesis and Bioassay for the Metabolites of P6A

Ming Zhao, Chao Wang, Jian Yang, Jiangyuan Liu, Youxuan Xu, Yanfen Wu and Shiqi Peng*

College of Pharmaceutical Sciences, Peking University, Beijing 100083, China

The metabolites Ala-Arg-Pro-Ala-OH, Ala-Arg-Pro-OH, Arg-Pro-Ala-Lys-OH and Pro-Ala-Lys-OH were identified by HPLC/ESI/MS from the in vivo blood of Ala-Arg-Pro-Ala-Lys-OH received mice. In the in vivo thrombolytic assay Ala-Arg-Pro-Ala-OH and Ala-Arg-Pro-OH exhibited no activity, Arg-Pro-Ala-Lys-OH exhibited the comparable potency to Ala-Arg-Pro-Ala-Lys-OH, and an enhanced activity was observed for Pro-Ala-Lys-OH.

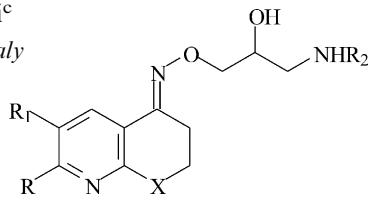


Bioorg. Med. Chem. 11 (2003) 4921

Synthesis and β-Blocking Activity of (*R*,*S*)-(*E*)-Oximeethers of 2,3-Dihydro-1,8-naphthyridine and 2,3-Dihydrothiopyrano[2,3-*b*]pyridine: Identification of β_3-Antagonists

Giuseppe Saccomanni,[a] Muwaffag Badawneh,[b] Barbara Adinolfi,[c] Vincenzo Calderone,[c] Tiziana Cavallini,[a] Pier Luigi Ferrarini,[a,*] Rosamiria Greco,[c] Clementina Manera[a] and Lara Testai[c]

[a]*Dipartimento di Scienze Farmaceutiche, Università di Pisa, via Bonanno 6, 56126 Pisa, Italy*
[b]*Philadelphia University, PO Box 1101 Sweileh-Jordan, Philadelphia, USA*
[c]*Dipartimento di Psichiatria, Neurobiologia, Farmacologia e Biotecnologie, Università di Pisa, sez. via Bonanno 6, 56126 Pisa, Italy*



Synthesis and the biological results in vitro towards β-adrenergic receptors of (*R*,*S*)-(*E*)-oxyiminoethers of 2,3-dihydro-1,8-naphthyridine and of 2,3-dihydrothiopyrano[2,3-*b*]pyridine.

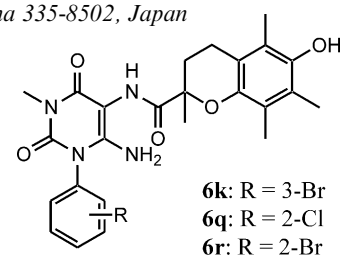
Bioorg. Med. Chem. 11 (2003) 4933

Structure and Activity Relationships of Novel Uracil Derivatives as Topical Anti-Inflammatory Agents

Yoshiaki Isobe, Masanori Tobe, Yoshifumi Inoue, Masakazu Isobe, Masami Tsuchiya and Hideya Hayashi*

Pharmaceuticals and Biotechnology Laboratory, Japan Energy Corporation, Toda-shi, Saitama 335-8502, Japan

Compounds **6k**, **6q**, and **6r** exhibited most potent inhibitory activities against picryl chloride-induced contact hypersensitivity reaction by topical application. Inhibitory potencies of these compounds were almost equipotent with that of Tacrolimus, a potent immunosuppressant.



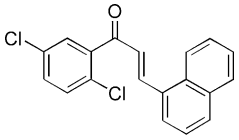
6k: R = 3-Br
6q: R = 2-Cl
6r: R = 2-Br

Bioorg. Med. Chem. 11 (2003) 4941

Screening of *Plasmodium falciparum* Iron Superoxide Dismutase Inhibitors and Accuracy of the SOD-Assays

Laurent Soulère,[a] Patrick Delplace,[b] Elisabeth Davioud-Charvet,[c] Sandrine Py,[c] Christian Sergheraert,[c] Jacques Périé,[a] Isabelle Ricard,[b] Pascal Hoffmann[a,*] and Daniel Dive[b,*]

[a]*UMR/CNRS 5068, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse cedex 4, France*
[b]*INSERM U547, Institut Pasteur, 1 rue du Professeur Calmette, BP 245, 59019 Lille cedex, France*
[c]*UMR/CNRS 8525/Lille2, Institut de Biologie de Lille, Campus Pasteur, 1 rue du Professeur Calmette, BP 447, 59021 Lille cedex, France*



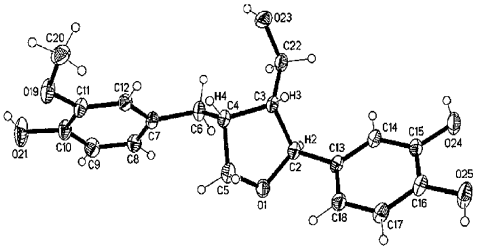
IC_{50} = 18 μM

Bioorg. Med. Chem. 11 (2003) 4945

Absolute Configuration and Anticancer Activity of Taxiresinol and Related Lignans of *Taxus wallichiana*

Sunil K. Chattopadhyay,[a,*] T. R. Santha Kumar,[a] Prakas R. Maulik,[b] Sachin Srivastava,[a] Ankur Garg,[a] Ashoke Sharon,[b] Arvind S. Negi[a] and Suman Preet S. Khanuja[a]

[a]*Central Institute of Medicinal and Aromatic Plants (CIMAP), PO CIMAP, Lucknow-226 015, India*
[b]*Central Drug Research Institute, Chattar Manzil Palace, Lucknow-226 001, India*

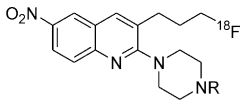


Bioorg. Med. Chem. 11 (2003) 4949

Syntheses and Binding Affinities of 6-Nitroquipazine Analogues for Serotonin Transporter: Part 3. A Potential 5-HT Transporter Imaging Agent, 3-(3-[^{18}F]Fluoropropyl)-6-nitroquipazine

Byoung Se Lee,[a] Soyoung Chu,[a] Kyo Chul Lee,[a] Bon-Su Lee,[a] Dae Yoon Chi,[a,*] Yearn Seong Choe,[b,*] Sang Eun Kim,[b] Yun Seon Song[c] and Changbae Jin[c]

[a]*Department of Chemistry, Inha University, 253 Yonghyundong Namgu, Inchon 402-751, South Korea*
[b]*Department of Nuclear Medicine, Samsung Medical Center, Sungkyunkwan University School of Medicine, 50 Ilwon-dong Kangnam-ku, Seoul 135-710, South Korea*
[c]*Bioanalysis & Biotransformation Research Center, Korea Institute of Science and Technology, PO Box 131, Cheongryang, Seoul 130-650, South Korea*

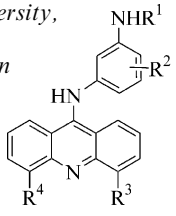


Bioorg. Med. Chem. 11 (2003) 4959

New Analogues of AHMA as Potential Antitumor Agents: Synthesis and Biological Activity

Jang-Yang Chang,[c] Chyun-Feng Lin,[a,b] Wen-Yu Pan,[c] Valeriy Bacherikov,[a] Ting-Chao Chou,[d] Ching-Huang Chen,[a] Huajin Dong,[d] Shu-Yun Cheng,[a] Tsong-Jen Tasi,[a] Yi-Wen Lin,[a] Kuo-Tung Chen,[b] Li-Tzong Chen[c] and Tsann-Long Su[a,*]

[a]*Laboratory of Bioorganic Chemistry, Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan*
[b]*Department of Medicinal Chemistry, College of Pharmacy, Taipei Medical University, Taipei, Taiwan*
[c]*Division of Cancer Research, National Health Research Institutes, Taipei, Taiwan*
[d]*Molecular Pharmacology and Chemistry Program, Memorial Sloan-Kettering Cancer Center, New York, NY 10021, USA*



R^1 = H, COOEt
R^2 = CH_2COO-alkyl
$CONH(CH_2)_nNMe_2$
Me
R^3, R^4 = H, Me,
$CONH(CH_2)_2NMe_2$

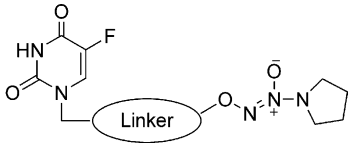
Bioorg. Med. Chem. 11 (2003) 4971

Synthesis and Cytotoxicity of 5-Fluorouracil/Diazeniumdiolate Conjugates

Tingwei Bill Cai,[a] Xiaoping Tang,[a] Janet Nagorski,[b] Paul G. Brauschweiger[b] and Peng George Wang[a,*]

[a]*Departments of Biochemistry and Chemistry, The Ohio State University, OH 43210, USA*
[b]*Department of Radiation Oncology, University of Miami, Miami, FL 33136, USA*

5-Fluorouracil/diazeniumdiolate conjugates were first synthesized, and showed greater cytotoxicities than fluorouracil.

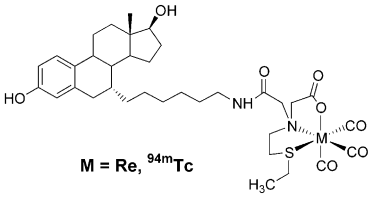


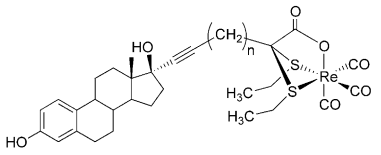
Bioorg. Med. Chem. 11 (2003) 4977

7α- and 17α-Substituted Estrogens Containing Tridentate Tricarbonyl Rhenium/Technetium Complexes: Synthesis of Estrogen Receptor Imaging Agents and Evaluation Using MicroPET with Technetium-94m

Leonard G. Luyt,[a] Heather M. Bigott,[b] Michael J. Welch[b] and John A. Katzenellenbogen[a,*]

[a]*Department of Chemistry, University of Illinois, 600 South Mathews Avenue, Urbana, IL 61801, USA*
[b]*Mallinckrodt Institute of Radiology, Washington University School of Medicine, 510 S. Kingshighway, Campus Box 8225, St. Louis, MO 63110, USA*





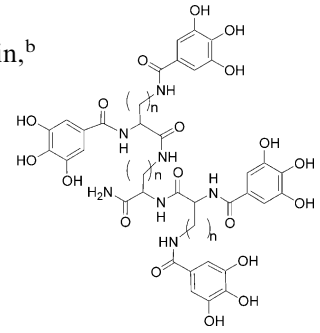
Bioorg. Med. Chem. 11 (2003) 4991

Identification of Novel Small-Molecule *Ulex Europaeus* I Mimetics for Targeted Drug Delivery

Christa Hamashin,[a] Lisa Spindler,[a] Shannon Russell,[a] Amy Schink,[a] Imelda Lambkin,[b] Daniel O'Mahony,[b] Richard Houghten[a] and Clemencia Pinilla[a,*]

[a]*Mixture Sciences, Inc., 3550 General Atomics Court, San Diego, CA 92121, USA*
[b]*Elan Drug Delivery, Biotechnology Building, Trinity College, Dublin 2, Ireland*

Lectin mimetics have been identified that may have potential application towards targeted drug delivery. Synthetic multivalent polygalloyl constructs effectively competed with *Ulex europaeus* agglutinin I (UEA1) for binding to intestinal Caco-2 cell membranes.

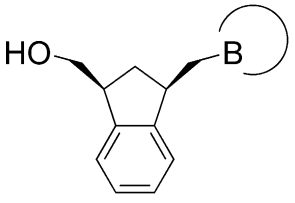


Bioorg. Med. Chem. 11 (2003) 4999

Synthesis and QSAR Study of the Anticancer Activity of Some Novel Indane Carbocyclic Nucleosides

S.-W. Yao,[a] V. H. C. Lopes,[a] F. Fernández,[b] X. García-Mera,[b,*] M. Morales,[b] J. E. Rodríguez-Borges[c] and M. N. D. S. Cordeiro[a,*]

[a]*REQUIMTE/Departamento de Química, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal*
[b]*Departamento de Química Orgánica, Facultade de Farmacia, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain*
[c]*CIQ/Departamento de Química, Faculdade de Ciências, Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal*



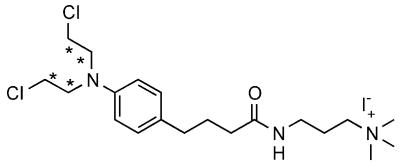
Bioorg. Med. Chem. 11 (2003) 5007

Synthesis and Pharmacokinetic Profile of a Quaternary Ammonium Derivative of Chlorambucil, a Potential Anticancer Drug for the Chemotherapy of Chondrosarcoma

Maryse Rapp,* Isabelle Giraud, Jean-Claude Maurizis and Jean-Claude Madelmont

INSERM UMR 484, Rue Montalembert, BP 184, 63005 Clermont-Ferrand Cedex, France

A quaternary ammonium (QA) conjugate of chlorambucil was synthesized and labeled with ^{14}C. The results obtained after pharmacokinetic studies show that the introduction of the QA moiety on chlorambucil allows the molecule to be carried selectively to cartilaginous tissues.



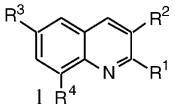
Bioorg. Med. Chem. 11 (2003) 5013

Synthesis and Biological Evaluation of Substituted Quinolines: Potential Treatment of Protozoal and Retroviral Co-infections

Mohammed A. Fakhfakh,[a] Alain Fournet,[a,b] Eric Prina,[c] Jean-François Mouscadet,[d] Xavier Franck,[a] Reynald Hocquemiller[a] and Bruno Figadère[a,*]

[a]*Laboratoire de Pharmacognosie (associé au CNRS-BioCIS), Faculté de Pharmacie, Université Paris-Sud, rue J.B. Clément, 92296 Châtenay-Malabry, France*
[b]*Institut de Recherche pour le Développement (IRD), 213 rue Lafayette, 75480 Paris, France*
[c]*Institut Pasteur, Unité d'Immunophysiologie et Parasitisme Intracellulaire, 25 rue du Dr. Roux, 75724 Paris cedex 15, France*
[d]*Laboratoire de Physicochimie et de Pharmacologie des Macromolécules Biologiques, URA 147 CNRS, PRII, Institut Gustave Roussy, 39 rue Camille Desmoulins, 94805 Villejuif, France*

Fourty nine substituted quinolines were synthesized and evaluated against several strains of leishmania, African trypanosomiasis, Chagas' disease, and against HIV-1 infected cells.



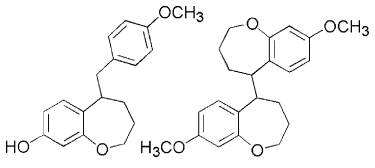
Bioorg. Med. Chem. 11 (2003) 5025

Structure-Based Drug Design: Synthesis, Crystal Structure, Biological Evaluation and Docking Studies of Mono- and Bis-benzo[*b*]oxepines as Non-steroidal Estrogens

Sanjay Sarkhel,[a] Ashoke Sharon,[a] Vishal Trivedi,[a] Prakas R. Maulik,[a,*] Man Mohan Singh,[b] Paloth Venugopalan[d] and Suprabhat Ray[c]

[a]*Molecular and Structural Biology Division, Central Drug Research Institute, Lucknow 226001, India*
[b]*Endocrinology Division, Central Drug Research Institute, Lucknow 226001, India*
[c]*Medicinal Chemistry Division, Central Drug Research Institute, Lucknow 226001, India*
[d]*Department of Chemistry, Punjab University, Chandigarh 160014, India*

Mono- and bis-benzo[*b*]oxepine derivatives have been rationally synthesized to meet the molecular requirement for interaction with estrogen receptor. Bis-benzo[*b*]oxepines (**7** and **9**) and mono-benzo [*b*]oxepine derivatives (**10**) acquire geometry with phenolic groups disposed in a fashion to stimulate estrogen receptor. Structural-based investigation, in vivo activity and docking studies have been described and correlated to demonstrate a practical approach for suitable ligand design.



Bioorg. Med. Chem. 11 (2003) 5035

Analysis of Structural Features of Bis-Quaternary Ammonium Antimicrobial Agents 4,4′-(α,ω-Polymethylenedithio)bis(1-alkylpyridinium Iodide)s Using Computational Simulation

Kazuto Ohkura,[a,b] Akiko Sukeno,[a] Keiko Yamamoto,[a] Hideaki Nagamune,[a] Takuya Maeda[a] and Hiroki Kourai[a,*]

[a]*Department of Biological Science and Technology, Faculty of Engineering, University of Tokushima, 2-1 Minamijosanjima-cho, Tokushima 770-8506, Japan*
[b]*Bioagricultural Science, Nagoya University, Furo-cho, Chikusa-ku, Aichi 464-8601, Japan*

Most of the median lethal dose (LD_{50}) values in acute cytotoxic assays of these bis-QACs were in the order of $10^{-6}\sim10^{-5}$ M, and tended to be lower than those of benzalkonium chloride (Bz).

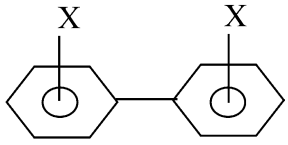
Bioorg. Med. Chem. 11 (2003) 5045

QSAR Study on Bioconcentration Factor (BCF) of Polyhalogented Biphenyls Using the PI Index

Padmakar V. Khadikar,[a,*] Shalini Singh,[a] Dheeraj Mandloi,[b] Sheela Joshi[c] and Amrit V. Bajaj[c]

[a]*Research Division, Laxmi Fumigation & Pest Control Pvt. Ltd., 3 Khatipura, Indore 452007, India*
[b]*Institute of Engineering & Technology, D.A. University, Indore 452017, India*
[c]*School of Chemical Sciences, D.A. University, Indore 452017, India*

The accuracy, predictive power, and domain of application of the PI (Padmakar–Ivan) index for modeling bioconcentration factor (BCF) of polyhalogenated biphenyls is discuss. Relative potential of PI index is investigated by comparing the results obtained using this index with those obtained from Wiener (W) and Szeged (Sz) indices. We observed that these indices gave better results for modeling log BCF than logP.



X = cl or Br

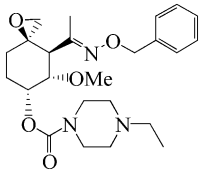
Bioorg. Med. Chem. 11 (2003) 5051

Design, Synthesis and Evaluation of a Series of Novel Fumagillin Analogues

Maria Fardis,[a,*] Hyung-Jung Pyun,[a] James Tario,[a] Haolun Jin,[a] Choung U. Kim,[a] Judy Ruckman,[b] Yun Lin,[c] Louis Green[c] and Brian Hicke[d]

[a]*Department of Medicinal Chemistry, Gilead, 333 Lakeside Dr., Foster City, CA 94404, USA*
[b]*CBR International Corp., 2905 Wilderness Place, Suite 202, Boulder, CO 80301, USA*
[c]*Replidyne Inc., 1450 Infinite Dr., Louisville, CO 80027, USA*
[d]*SomaLogic Inc., 1775 38th Street, Boulder, CO 80301, USA*

A series of fumagillin analogues targeted at understanding tolerability of MetAP2 toward substitution at C4 and C6 were synthesized. Initially, the C6 side chain was maintained as cinnamoyl ester and C4 was modified. It was concluded that replacing the natural C4 of fumagillin with a benzyl oxime at C4 resulted in moderate loss of activity toward binding to MetAP2. Placement of a primary or secondary carbamate at C6 did not improve the potency of compounds toward inhibition of MetAP2. However, the inhibitory activity against MetAP2 was gained back by placing polar groups such as piperazinyl carbamate at C6. Small alkyl substituents on the amine of piperazinyl carbamate were well tolerated.

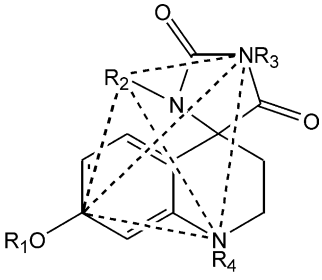


Bioorg. Med. Chem. 11 (2003) 5059

Application of a Novel Design Paradigm to Generate General Nonpeptide Combinatorial Scaffolds Mimicking Beta Turns: Synthesis of Ligands for Somatostatin Receptors

Dona Chianelli,[a] Yong-Chul Kim,[a] Dmitriy Lvovskiy[b] and Thomas R. Webb[a,b,*]

[a]*ChemBridge Research Labs., LLC, 16981 Via Tazon, San Diego, CA 92127, USA*
[b]*ChemBridge Corporation, 16981 Via Tazon, San Diego, CA 92127, USA*



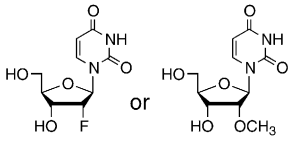
Bioorg. Med. Chem. 11 (2003) 5069

A Specific Substrate-Inhibitor, a 2′-Deoxy-2′-fluorouridine-Containing Oligoribonucleotide, against Human RNase L

Yoshihito Ueno, Yuuki Yamada, Masayuki Nakanishi and Yukio Kitade*

Department of Biomolecular Science, Faculty of Engineering, Gifu University, Yanagido, Gifu 501-1193, Japan

5'-r(CCC CCC CCC CC**N** **N**CC CCC CC)-3' **N** =



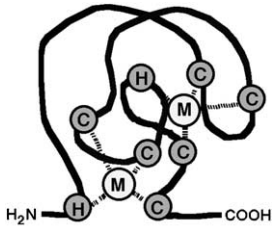
Bioorg. Med. Chem. 11 (2003) 5075

Analysis of the Non-covalent Interaction Between Metal Ions and the Cysteine-Rich Domain of Protein Kinase C Eta by Electrospray Ionization Mass Spectrometry

Mayumi Shindo,[a] Kazuhiro Irie,[b,*] Hiroyuki Fukuda[a] and Hajime Ohigashi[b]

[a]*Applied Biosystems Japan Ltd., 4-5-4Hacchobori, Chuo-ku, Tokyo 104-0032, Japan*
[b]*Division of Food Science and Biotechnology, Graduate School of Agriculture, Kyoto University, Kitashirakawa Oiwake-cho, Sakyo-ku, Kyoto 606-8502, Japan*

Effect of zinc and other metal ions on the folding of the protein kinase C surrogate peptide (PKC_{η}-C1B) was analyzed by the electrospray ionization mass spectrometry.



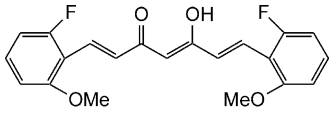
PKC C1 domain

Bioorg. Med. Chem. 11 (2003) 5083

Antitumor Agents 222. Synthesis and Anti-androgen Activity of New Diarylheptanoids

Hironori Ohtsu,[a] Hideji Itokawa,[a] Zhiyan Xiao,[a] Ching-Yuan Su,[b] Charles C.-Y. Shih,[b] Tzuying Chiang,[c] Eugene Chang,[c] YiFen Lee,[c] Shang-Yi Chiu,[c] Chawnshang Chang[c] and Kuo-Hsiung Lee[a,*]

[a]*Natural Products Laboratory, School of Pharmacy, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599-7360, USA*
[b]*AndroScience Corporation, 11175 Flintkote Avenue, Suite F, San Diego, CA 92121, USA*
[c]*George Whipple Laboratory for Cancer Research, Department of Pathology, Urology and Biochemistry, University of Rochester Medical Center, 601 Elmwood Avenue, Box 626, Rochester, NY 14642, USA*



10

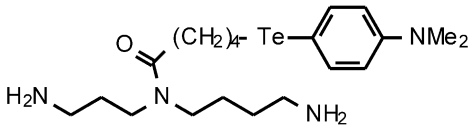
Bioorg. Med. Chem. 11 (2003) 5091

Thioredoxin Reductase and Cancer Cell Growth Inhibition by Organotellurium Compounds that Could Be Selectively Incorporated into Tumor Cells

Lars Engman,[a,*] Nawaf Al-Maharik,[a] Michael McNaughton,[a] Anne Birmingham[b] and Garth Powis[b]

[a]*Department of Organic Chemistry, Institute of Chemistry, Uppsala University, PO Box 599, S-751 24, Uppsala, Sweden*
[b]*Arizona Cancer Center, University of Arizona, Tucson, AZ 85724-5024, USA*

Organotellurium steroid, lipid, amino acid, nucleic base and polyamine derivatives were prepared and evaluated for their thioredoxin/thioredoxin reductase and cancer cell growth inhibiting capacity.

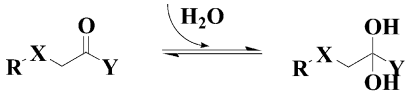


Bioorg. Med. Chem. 11 (2003) 5101

Use of Classical and 3-D QSAR to Examine the Hydration State of Juvenile Hormone Esterase Inhibitors

Craig E. Wheelock,[a,b] Yoshiaki Nakagawa,*[a] Miki Akamatsu[c] and Bruce D. Hammock[b]

[a]*Division of Applied Life Sciences, Graduate School of Agriculture, Kyoto University, Kyoto 606-8502, Japan*
[b]*Department of Entomology and Cancer Research Center, University of California, Davis, CA 95616, USA*
[c]*Division of Environmental Science and Technology, Graduate School of Agriculture, Kyoto University, Kyoto 606-8502, Japan*



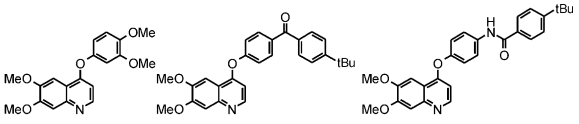
X = CH_2, S, S(O), $S(O)_2$, alkene, alkyne
Y = CF_3, CF_2H, CFH_2, CH_3
R = aliphatic, aromatic, juvenile hormone mimic

Bioorg. Med. Chem. 11 (2003) 5117

Synthesis and Structure–Activity Relationship for New Series of 4-Phenoxyquinoline Derivatives as Specific Inhibitors of Platelet-derived Growth Factor Receptor Tyrosine Kinase

Kazuo Kubo,* Shin-ichi Ohyama, Toshiyuki Shimizu, Atsuya Takami, Hideko Murooka, Tsuyoshi Nishitoba, Shinichiro Kato, Mikio Yagi, Yoshiko Kobayashi, Noriko Iinuma, Toshiyuki Isoe, Kazuhide Nakamura, Hiroshi Iijima, Tatsushi Osawa and Toshio Izawa

Pharmaceutical Research Laboratories, Kirin Brewery Co., Ltd., 3 Miyahara-cho, Takasaki-shi, Gunma 370-1295, Japan



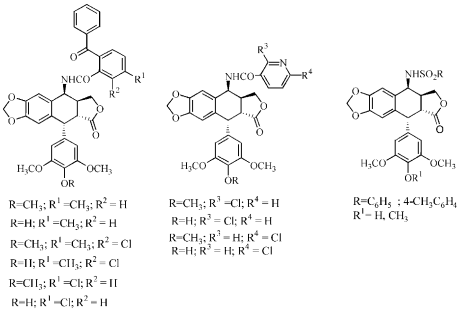
1 (Ki6783) **2** (Ki6896) **3** (Ki6945)

Bioorg. Med. Chem. 11 (2003) 5135

Synthesis of 4β-Amido and 4β-Sulphonamido Analogues of Podophyllotoxin as Potential Antitumour Agents

Ahmed Kamal,[a,*] B. Ashwini Kumar,[a] M. Arifuddin[a] and Sunanda G. Dastidar[b]

[a]*Division of Organic Chemistry, Indian Institute of Chemical Technology, Hyderabad-500007, India*
[b]*Ranbaxy Research Laboratories, Gurgaon-122001, Haryana, India*



R=CH_3; R^1=CH_3; R^2 = H
R=H; R^1=CH_3; R^2 = H
R=CH_3; R^1=CH_3; R^2 = Cl
R=H; R^1=CH_3; R^2 = Cl
R=CH_3; R^1=Cl; R^2 = H
R=H; R^1=Cl; R^2 = H

R=CH_3; R^3=Cl; R^4 = H
R=H; R^3 = Cl; R^4 = H
R=CH_3; R^3 = H; R^4 = Cl
R=H; R^3 = H; R^4 = Cl

R=C_6H_5 ; 4-$CH_3C_6H_4$
R^1= H, CH_3

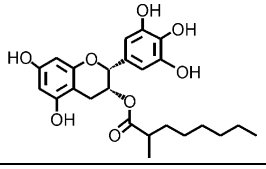
Bioorg. Med. Chem. 11 (2003) 5143

Tumor Chemopreventive Activity of 3-*O*-Acylated (−)-epigallocatechins

Ayako Kumagai,[a] Yasuo Nagaoka,[a,b] Tomoko Obayashi,[a] Yasuhiro Terashima,[a] Harukuni Tokuda,[c] Yukihiko Hara,[d] Teruo Mukainaka,[c] Hoyoku Nishino,[c] Hiroshi Kuwajima[e] and Shinichi Uesato[a,b,*]

[a]*Department of Biotechnology, Faculty of Engineering, Kansai University, Suita, Osaka 564-8680, Japan*
[b]*Organization for Research and Development of Innovative Science and Technology, Kansai University, Suita, Osaka 564-8680, Japan*
[c]*Department of Biochemistry and Molecular Biology, Kyoto Prefectural University of Medicine, Kawaramachi-Hirokoji, Kamigyo-ku, Kyoto 602-0841, Japan*
[d]*Central Research Laboratories, Tokyo Food techno Co., LTD., Miyabara, Fujieda, Shizuoka 426-0133, Japan*
[e]*Faculty of Pharmaceutical Sciences, Kinki University, 3-4-1 Kowakae, Higashiosaka, Osaka 577-8502, Japan*

(−)-Epigallocatechin derivatives possessing a 2-methyloctanoyl-chain inhibited papilloma formation more strongly than (−)-epigallocatechin gallate, well established antitumor promoter, in a two-stage mouse skin carcinogenesis assay.



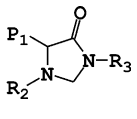
Bioorg. Med. Chem. 11 (2003) 5149

Noncovalent Inhibitors of Human Leukocyte Elastase Based on the 4-Imidazolidinone Scaffold

Liuqing Wei, Xiangdong Gan, Jiaying Zhong, Kevin R. Alliston and William C. Groutas*

Department of Chemistry, Wichita State University, Wichita, KS 67260, USA

Substituted 4-imidazolidinones were found to be competitive inhibitors of human leukocyte elastase.

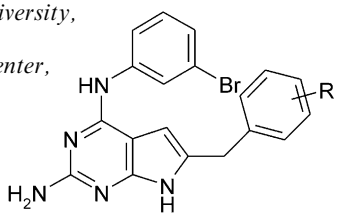


Bioorg. Med. Chem. 11 (2003) 5155

Antiangiogenic and Antitumor Agents: Design, Synthesis, and Evaluation of Novel 2-Amino-4-(3-bromoanilino)-6-benzylsubstituted Pyrrolo[2,3-*d*] pyrimidines as Inhibitors of Receptor Tyrosine Kinases

Aleem Gangjee,[a,*] Jie Yang,[a] Michael A. Ihnat[b] and Shekhar Kamat[b]

[a]*Division of Medicinal Chemistry, Graduate School of Pharmaceutical Sciences, Duquesne University, Pittsburgh, PA 15282, USA*
[b]*Department of Cell Biology, School of Medicine, University of Oklahoma Health Sciences Center, Oklahoma City, OK 73104, USA*



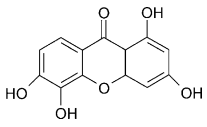
Bioorg. Med. Chem. 11 (2003) 5171

Relationship between Protective Effect of Xanthone on Endothelial Cells and Endogenous Nitric Oxide Synthase Inhibitors

De-Jian Jiang,[a] Gao-Yun Hu,[b] Jun-Lin Jiang,[a] Hong-Lin Xiang,[b] Han-Wu Deng[a] and Yuan-Jian Li[a,*]

[a]*Department of Pharmacology, School of Pharmaceutical Sciences, Central South University, Changsha 410078, China*
[b]*Department of Medicinal Chemistry, School of Pharmaceutical Sciences, Central South University, Changsha 410078, China*

1,3,5,6-tetrahydroxyxanthone was synthesized. The relationship between protective effect of xanthone on endothelial cells and endogenous nitric oxide synthase inhibitors was investigated.

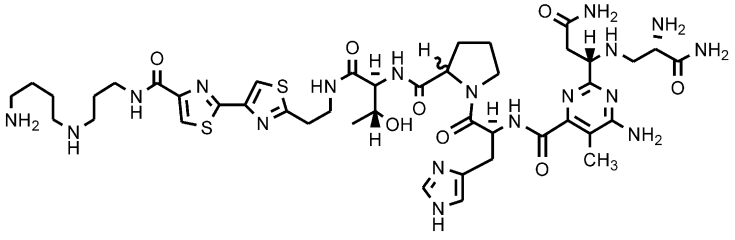


Bioorg. Med. Chem. 11 (2003) 5179

Solid-Phase Synthesis and Biochemical Evaluation of Conformationally Constrained Analogues of Deglycobleomycin A_5

Ali Cagir, Zhi-Fu Tao, Steven J. Sucheck and Sidney M. Hecht*

Departments of Chemistry and Biology, University of Virginia, Charlottesville, VA 22901, USA

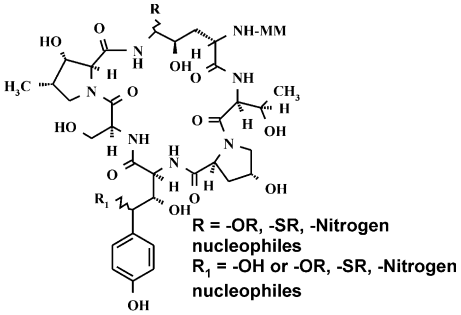


Bioorg. Med. Chem. 11 (2003) 5189

Semisynthetic Modifications of Hemiaminal Function at Ornithine Unit of Mulundocandin, Towards Chemical Stability and Antifungal Activity

Bansi Lal,[a,*] Vitthal Genbhau Gund,[a,c] Ashok Kumar Gangopadhyay,[a] S.R. Nadkarni,[b] Vidula Dikshit,[b] D.K. Chatterjee[b] and R. Shirvaikar[b]

[a]*Department of Medicinal Chemistry, Quest Institute of LifeSciences, Nicholas Piramal India Limited, Mulund (w). Mumbai 4000 80, India*
[b]*Department of Natural Products, Quest Institute of LifeSciences, Nicholas Piramal India Limited, Mulund (w). Mumbai 4000 80, India*
[c]*Department of Chemistry, University of Sherbrooke, 2500 Boul. University, Sherbrooke-J1K 2R1, Quebec, Canada*

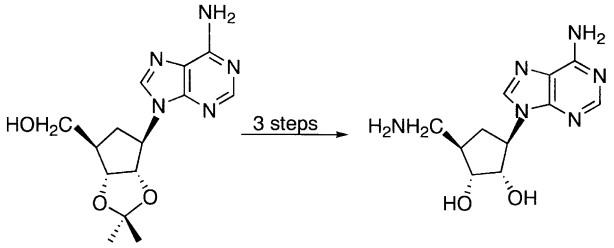


Bioorg. Med. Chem. 11 (2003) 5199

5′-Amino-5′-deoxyaristeromycin and Its Antiviral Properties

Vasanthakumar P. Rajappan and Stewart W. Schneller*

Department of Chemistry, Auburn University, Auburn, AL 36849, USA



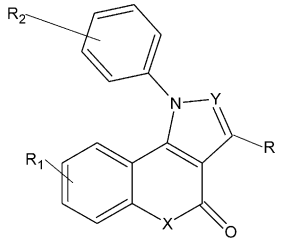
Bioorg. Med. Chem. 11 (2003) 5203

Topological Modeling of Benzodiazepine Receptor Binding

Abhilash Thakur,[a] Mamta Thakur[b] and Padmakar Khadikar[c,*]

[a]*Department of Chemistry, Bhopal institute of Technology & Science, Bhopal, India*
[b]*School of Chemical Sciences, D.A.V.V Indore 452009, India*
[c]*Research Division, Laxmi Fumigation Pest Control, Pvt. Ltd., 3 Khatipura, Indore 452007, India*

QSAR study was performed using physicochemical properties on some benzodiazepine receptor ligands for giving statistically significant models better than previously proposed models.

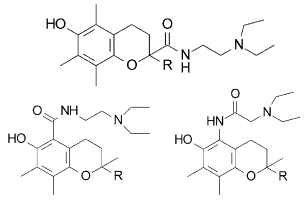


Bioorg. Med. Chem. 11 (2003) 5209

Bifunctional Agents for Reperfusion Arrhythmias: Novel Hybrid Vitamin E/Class I Anti-arrhythmics

Maria Koufaki,[a,*] Theodora Calogeropoulou,[a] Eleni Rekka,[b] Michael Chryselis,[b] Panagiota Papazafiri,[c] Catherine Gaitanaki[c] and Alexandros Makriyannis[d,*]

[a]*Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., 116 35 Athens, Greece*
[b]*Department of Pharmaceutical Chemistry, School of Pharmacy, Aristotelian University of Thessaloniki, 54124 Thessaloniki, Greece*
[c]*Department of Animal & Human Physiology, School of Biology, University of Athens, Panepistimiopolis, 15784 Athens, Greece*
[d]*Center for Drug Discovery and Departments of Pharmaceutical Sciences and Molecular & Cell Biology, University of Connecticut, 372 Fairfield Road, U 92, Storrs, CT 06269-2092, USA*

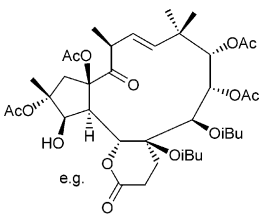


Bioorg. Med. Chem. 11 (2003) 5221

Modified Jatrophane Diterpenes as Modulators of Multidrug Resistance from *Euphorbia Dendroides* L.

Gabriella Corea,[a] Ernesto Fattorusso,[a] Virginia Lanzotti,[b,*] Orazio Taglialatela-Scafati,[a] Giovanni Appendino,[c] Mauro Ballero,[d] Pierre-Noël Simon,[e] Charles Dumontet[f] and Attilio Di Pietro[g]

[a]*Dipartimento di Chimica delle Sostanze Naturali, Università di Napoli 'Federico II', Via D. Montesano 49, I-80131 Napoli, Italy*
[b]*DISTAAM, Università degli Studi del Molise, Via F. De Sanctis, I-86100 Campobasso, Italy*
[c]*DISCAFF, Università del Piemonte Orientale, V.le Ferrucci 33, 28100 Novara, Italy*
[d]*Dipartimento di Scienze Botaniche, Viale San Ignazio 13, 09123 Cagliari, Italy*
[e]*Département de Pharmacognosie de la Faculté de Pharmacie de Lyon, 8 Avenue Rockefeller, 69880 Lyon, France*
[f]*INSERM U590, 8 Avenue Rockefeller, 69880 Lyon, France*
[g]*Institut de Biologie et Chimie des Proteines, UMR 5086 CNRS/Université Claude Bernard-Lyon I et IFR 128, Passage du Vercors 7, 69367 Lyon Cedex 07, France*

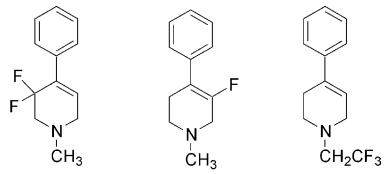


Bioorg. Med. Chem. 11 (2003) 5229

Synthesis and In Vitro Biological Evaluation of Fluoro-Substituted-4-phenyl-1,2,3,6-tetrahydropyridines as Monoamine Oxidase B Substrates

Aaron B. Beeler,[a] Rama Sarma V. S. Gadepalli,[a] Salome Steyn,[b] Neal Castagnoli, Jr[b] and John M. Rimoldi[a,*]

[a]*Department of Medicinal Chemistry and Laboratory for Applied Drug Design and Synthesis, University of Mississippi, University MS, 38677 USA*
[b]*Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061 USA*



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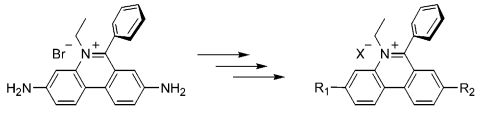
Bioorg. Med. Chem. 11 (2003) 5235

Synthesis, Photophysical Properties, and Nucleic Acid Binding of Phenanthridinium Derivatives Based on Ethidium

Nathan W. Luedtke,* Qi Liu and Yitzhak Tor*

Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA 92093-0358, USA



Ethidium Bromide

$R_1 = NH_2$, $NHCO_2CH_2Ph$, NC_4H_4, etc.
$R_2 = NHC(NH)NH_2$, $NHC(O)NH_2$, etc.

Bioorg. Med. Chem. 11 (2003) 5249

Identification of Structural Components Associated with Cytostatic Activity in MCF-7 but not in MDA-MB-231 Cells

Albert R. Cunningham,[a,*] Suzanne L. Cunningham[a,c] and Billy W. Day[b,c]

[a]*Department of Environmental Studies, Louisiana State University, Baton Rouge, LA 70803, USA*
[b]*Departments of Pharmaceutical Sciences and of Chemistry, University of Pittsburgh, Pittsburgh, PA 15261, USA*
[c]*Department of Environmental and Occupational Health, University of Pittsburgh, Pittsburgh, PA 15260, USA*

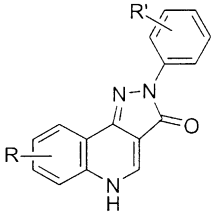
We report a novel SAR modeling approach based on a subtractive protocol to develop mechanistically informative models that describe cell type-specific molecular descriptors of cytotoxicity. We surmise the outgrowth of this method can facilitate the development of models with sufficient clarity to identify chemical moieties associated with antiproliferative activity to selective individual cancer types while being innocuous to other cell types.

Bioorg. Med. Chem. 11 (2003) 5259

High Affinity Central Benzodiazepine Receptor Ligands. Part 3: Insights Into the Pharmacophore and Pattern Recognition Study of Intrinsic Activities of Pyrazolo[4,3-*c*]quinolin-3-ones

Andrea Carotti,[a] Cosimo Altomare,[a,*] Luisa Savini,[b] Luisa Chiasserini,[b] Cesare Pellerano,[b] Maria P. Mascia,[c] Elisabetta Maciocco,[c] Fabio Busonero,[c] Manuel Mameli,[c] Giovanni Biggio[c] and Enrico Sanna[c]

[a]*Dipartimento Farmaco Chimico, Università degli Studi, Via E. Orabona 4, I-70125 Bari, Italy*
[b]*Dipartimento Farmaco Chimico Tecnologico, Università degli Studi, Via A. Moro, I-53100 Siena, Italy*
[c]*Dipartimento di Biologia Sperimentale, Università degli Studi, Via Palabanda 12, I-09123 Cagliari, Italy*



2

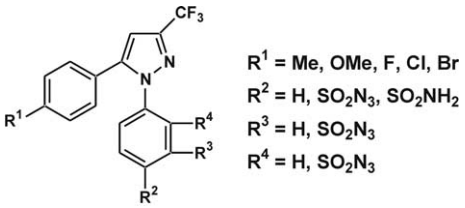
A number of high affinity CBR ligands of general structure **2** were synthesized. They allowed us to gain new insights into the pharmacophore. A pattern recognition study (especially linear discriminant analysis) proved to be useful in classifying more than fifty ligands **2** having different intrinsic activities.

Bioorg. Med. Chem. 11 (2003) 5273

Design and Synthesis of Novel Celecoxib Analogues as Selective Cyclooxygenase-2 (COX-2) Inhibitors: Replacement of the Sulfonamide Pharmacophore by a Sulfonylazide Bioisostere

Md. Jashim Uddin, P. N. Praveen Rao and Edward E. Knaus*

Faculty of Pharmacy and Pharmaceutical Sciences, University of Alberta, Edmonton, Alberta, Canada T6G 2N8



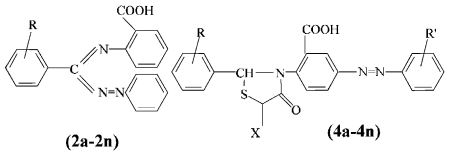
Bioorg. Med. Chem. 11 (2003) 5281

Synthesis of Some Newer Derivatives of 2-Amino Benzoic Acid as Potent Anti-inflammatory and Analgesic Agents

Ashok Kumar,* Deepti Bansal, Kiran Bajaj, Shalabh Sharma, Archana and V. K. Srivastava

Medicinal Chemistry Division, Department of Pharmacology, L.L.R.M. Medical College, Meerut (U.P) 250004, India

2-Amino benzoic acid derivatives were designed and prepared as potent anti-inflammatory and analgesic agents. Pharmacological evaluation were performed on the synthesized compounds.



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Some New 2,3,6-Trisubstituted Quinazolinones as Potent Anti-inflammatory, Analgesic and COX-II Inhibitors

Ashok Kumar,* Shalabh Sharma, Archana, Kiran Bajaj, Shipra Sharma, Hemant Panwar, Tripti Singh and V. K. Srivastava

Medicinal Chemistry Division, Department of Pharmacology, L.L.R.M Medical College, Meerut (U.P.)-250004, India

Some 2-(substitutedphenylmethyleneimino)aminoacetylmethylene-3-(2′-substitutedindol-3′-yl)-halosubstituted-4(3H)quinazolinones (**5a**–**5i**) and 2-(substituted phenylaminomethyleneacetyl-4′-oxo-1′-thiazolidinyl-3-(2″-substitutedindol-3″-yl)-4(3H)-quinazolinones (**6a**–**6i**) have been synthesized. Compound 2-(*o*-Methoxyphenylaminomethylacetyl-4′-oxo-1′-thiazolidinyl)-3-(indol-3″-yl)-6-iodo-4(3H)-quinazolinone (**6d**) was found to be the most potent compound of the present study.