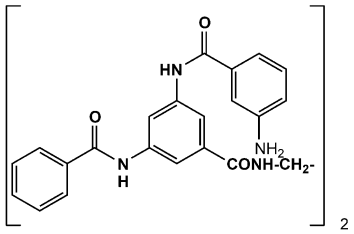
Bioorg. Med. Chem. Lett. 12 (2002) 1

DNA Cleavage by Aromatic Amines

Philip M. Warner,* Jiwei Qi, Bin Meng, Gang Li, Longfei Xie, Ahmed El-Shafey and Graham B. Jones

Department of Chemistry, Northeastern University, 360 Huntington Ave., Boston, MA 02115, USA

A series of dimeric aryl amines was found to induce cleavage of DNA.
Initial investigations suggest this to be a novel mode for DNA cleavage.



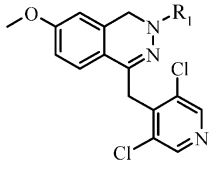
Bioorg. Med. Chem. Lett. 12 (2002) 5

Phthalazine PDE4 Inhibitors. Part 3: The Synthesis and In Vitro Evaluation of Derivatives with a Hydrogen Bond Acceptor

Mauro Napoletano,[a,*] Gabriele Norcini,[c] Franco Pellacini,[a] Francesco Marchini,[b] Gabriele Morazzoni,[a] Raimondo Fattori,[a] Pierpaolo Ferlenga[b] and Lorenzo Pradella[b]

[a]*Inpharzam Ricerche, Zambon Group, Via Ai Soi, 6807 Taverne, Switzerland*
[b]*R&D, Zambon Group SpA, Via Lillo Del Duca 10, 20091 Bresso, Milan, Italy*
[c]*Lamberti SpA, Fine Chemical Lab., Via Piave 18, 21041 Albizzate, Italy*

This communication describes the synthesis and in vitro evaluation of a novel and potent series of phthalazine phosphodiesterase type (IV) (PDE4) inhibitors. The interaction with two distinct polar binding sites allowed us to eliminate the cyclopentyloxy substitution from rolipram-like analogues.



Bioorg. Med. Chem. Lett. 12 (2002) 9

Design, Synthesis and Pharmacological Evaluation of Novel Pyrazolo[3,4-*b*]thieno[2,3-*d*]pyridine Acid Derivatives: a New Class of Anti-inflammatory and Anti-platelet Agents

Carla R. Cardoso,[b] Fernanda C. F. de Brito,[a] Kelli C. M. da Silva,[a] Ana L. P. de Miranda,[a] Carlos A. M. Fraga[a,b] and Eliezer J. Barreiro[a,b,*]

[a]*LASSBio, Faculdade de Farmácia, Universidade Federal do Rio de Janeiro, PO Box 68006, Rio de Janeiro, 21944-970, RJ, Brazil*
[b]*Instituto de Química, Universidade Federal do Rio de Janeiro, Rio de Janeiro, 21949-900, RJ, Brazil*

A series of pyrazolo[3,4-*b*]thieno[2,3-*d*]pyridine alkanoic acid derivatives has been synthesized and evaluated as thromboxane synthetase inhibitors and leukotriene D_4 receptor antagonists. The glutaric acid derivative LASSBio341 (**6**) was shown to be active in arachidonic acid-induced platelet aggregation ($IC_{50} = 0.14\,\mu M$) and inhibition of the contraction of guinea pig tracheal strip induced with LTD_4 ($IC_{50} = 43.7\,\mu M$), displaying still in vivo anti-inflammatory profile.

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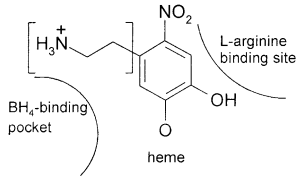
Nitrocatechols versus Nitrocatecholamines as Novel Competitive Inhibitors of Neuronal Nitric Oxide Synthase: Lack of the Aminoethyl Side Chain Determines Loss of Tetrahydrobiopterin-Antagonizing Properties

Anna Palumbo,[a] Alessandra Napolitano[b] and Marco d'Ischia[b,*]

[a]*Laboratory of Biochemistry, Zoological Station "Anton Dohrn", Villa Comunale I-80121 Naples, Italy*
[b]*Department of Organic Chemistry and Biochemistry, University of Naples "Federico II", Via Cinthia 4, I-80126 Naples, Italy*



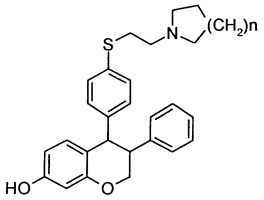
Bioorg. Med. Chem. Lett. 12 (2002) 17

Synthesis and Biological Evaluation of Novel Thio-Substituted Chromanes as High-Affinity Partial Agonists for the Estrogen Receptor

Lise B. Christiansen,* Martin Wenckens, Paul S. Bury, Birgitte Gissel, Birgit S. Hansen, Susan M. Thorpe, Poul Jacobsen, Anders Kanstrup, Anker S. Jørgensen, Lars Nærum and Karsten Wassermann

Health Care Discovery & Preclinical Development, Novo Nordisk A/S, Novo Nordisk Park, DK-2760 Måløv, Denmark

The synthesis and in vitro pharmacological evaluation of the novel partiel estrogen agonists, (±)-*cis*-7-hydroxy-3-phenyl-4-(4-(2-piperidinoethanethio)phenyl)chromane and (±)-*cis*-7-hydroxy-3-phenyl-4-(4-(2-pyrrolidinoethanethio)phenyl)chromane, are described.



Bioorg. Med. Chem. Lett. 12 (2002) 21

Minimal Structural Requirements for Agonist Activity of PAR-2 Activating Peptides

Vincenzo Santagada,[a] Giuseppe Caliendo,[a] Beatrice Severino,[a] Elisa Perissutti,[a] Ferdinando Fiorino,[a] Carla Cicala,[b] Vincenzo De Filippis[c,*] and Giuseppe Cirino[b]

[a]*Department of Pharmaceutical Chemistry, University of Naples 'Federico II', Via D. Montesano 49, 80131 Naples, Italy*
[b]*Department of Experimental Pharmacology, University of Naples 'Federico II', Via D. Montesano 49, 80131 Naples, Italy*
[c]*Department of Pharmaceutical Sciences and CRIBI Biotechnology Center, University of Padua, Via F. Marzolo 5, 35131 Padua, Italy*

In this study we have shown that it is possible to shorten the sequence of rat PAR-2 activating hexapeptide Ser-Leu-Ile-Gly-Arg-Leu-NH_2 down to the dipeptide derivative N^{α}-(*p*-trifluoromethoxy)benzoyl-Arg(NO2)-Leu-NH_2 (**10**), displaying an agonist potency comparable ($EC_{50} = 20 \pm 10$ μM) to that of the full-length hexapeptide ($EC_{50} = 4 \pm 1$ μM).

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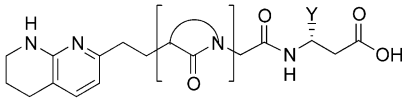
Nonpeptide $\alpha_v\beta_3$ Antagonists. Part 2: Constrained Glycyl Amides Derived from the RGD Tripeptide

Robert S. Meissner,[a,*] James J. Perkins,[a] Le T. Duong,[b] George D. Hartman,[a] William F. Hoffman,[a] Joel R. Huff,[a] Nathan C. Ihle,[a] Chih-Tai Leu,[b] Rose M. Nagy,[b] Adel Naylor-Olsen,[c] Gideon A. Rodan,[b] Sevgi B. Rodan,[b] David B. Whitman,[a] Gregg A. Wesolowski[b] and Mark E. Duggan[a]

[a]*Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA 19486, USA*
[b]*Department of Bone Biology and Osteoporosis Research, Merck Research Laboratories, West Point, PA 19486, USA*
[c]*Department of Molecular Design and Diversity, Merck Research Laboratories, West Point, PA 19486, USA*

Mimetics of the RGD tripeptide are described that are potent, selective antagonists of the integrin receptor $\alpha_v\beta_3$. The use of the 5,6,7,8-tetrahydro[1,8]naphthyridine group as a potency-enhancing N-terminus is demonstrated. Two 3-substituted-3-amino-propionic acids previously contained in $\alpha_{IIb}\beta_3$ antagonists were utilized to enhance binding affinity and functional activity for the targeted receptor.



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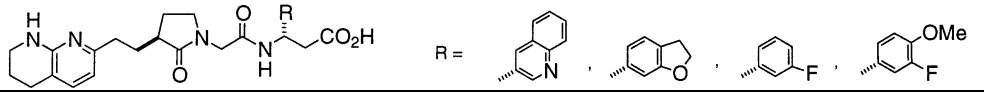
Non-Peptide $\alpha_v\beta_3$ Antagonists. Part 3: Identification of Potent RGD Mimetics Incorporating Novel β-Amino Acids as Aspartic Acid Replacements

Paul J. Coleman,[a,*] Karen M. Brashear,[a] Cecilia A. Hunt,[a] William F. Hoffman,[a] John H. Hutchinson,[a] Michael J. Breslin,[a] Carol A. McVean,[a] Ben C. Askew,[a] George D. Hartman,[a] Sevgi B. Rodan,[b] Gideon A. Rodan,[b] Chih-Tai Leu,[b] Thomayant Prueksaritanont,[c] Carmen Fernandez-Metzler,[c] Bennett Ma,[c] Laura A. Libby,[c] Kara M. Merkle,[c] Gary L. Stump,[d] Audrey A. Wallace,[d] Joseph J. Lynch,[d] Robert Lynch[d] and Mark E. Duggan[a]

[a]*Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA 19486, USA*
[b]*Department of Bone Biology and Osteoporosis Research, Merck Research Laboratories, West Point, PA 19486, USA*
[c]*Department of Drug Metabolism, Merck Research Laboratories, West Point, PA 19486, USA*
[d]*Department of Pharmacology, Merck Research Laboratories, West Point, PA 19486, USA*

Potent non-peptidic $\alpha_v\beta_3$ antagonists have been prepared incorporating various β-amino acids as aspartic acid mimetics. Modification of the β-alanine 3-substituents alters the potency and physicochemical properties of these receptor antagonists and in some cases provides orally bioavailable $\alpha_v\beta_3$ inhibitors.



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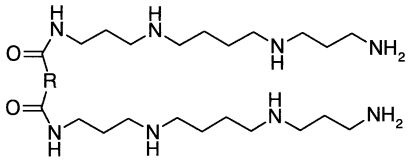
Synthesis of Bis-spermine Dimers that are Potent Polyamine Transport Inhibitors

Gerard F. Graminski,[a,*] C. Lance Carlson,[a] Josh R. Ziemer,[a] Feng Cai,[b] Nicolaas M. J. Vermeulen,[c] Scott M. Vanderwerf[d] and Mark R. Burns[a]

[a]*Oridigm Corporation, 4010 Stone Way North, Suite 220, Seattle, WA 98103, USA*
[b]*Corixa Corporation, 1124 Columbia Street, Suite 200, Seattle, WA 98104, USA*
[c]*Epoch Biosciences, Inc., 21720-23rd Dr., Suite 150, Bothell, WA 98021, USA*
[d]*Oregon Health & Science University, Biochemistry and Molecular Biology, L224, Portland, OR 97201, USA*

A series of potent bis-spermine polyamine transport inhibitors is reported.



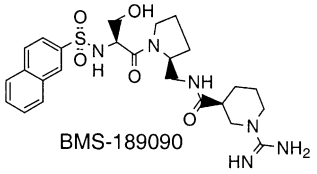
Bioorg. Med. Chem. Lett. 12 (2002) 41

Thrombin Active Site Inhibitors: Chemical Synthesis, In Vitro and In Vivo Pharmacological Profile of a Novel and Selective Agent BMS-189090 and Analogues

Jagabandhu Das,* S. David Kimball, Joyce A. Reid, Tammy C. Wang, Wan F. Lau, Daniel G. M. Roberts, Steven M. Seiler, William A. Schumacher and Martin L. Ogletree

Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ 08543-4000, USA

A novel series of human α-thrombin inhibitors was prepared to elucidate their SAR relationships, selectivity, and activity in vivo. BMS-189090 is identified as a potent, selective and orally active inhibitor which is efficacious in vivo.



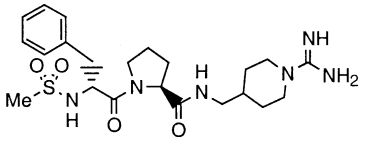
Bioorg. Med. Chem. Lett. 12 (2002) 45

Molecular Design and Structure–Activity Relationships Leading to the Potent, Selective, and Orally Active Thrombin Active Site Inhibitor BMS-189664

Jagabandhu Das,* S. David Kimball,* Steven E. Hall, Wen-Ching Han, Edwin Iwanowicz, James Lin, Robert V. Moquin, Joyce A. Reid, John S. Sack, Mary F. Malley, Chiehying Y. Chang, Saeho Chong, David B. Wang-Iverson, Daniel G. M. Roberts, Steven M. Seiler, William A. Schumacher and Martin L. Ogletree

Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ 08543-4000, USA

A novel series of human α-thrombin inhibitors was prepared to elucidate their SAR relationships, selectivity, and activity in vivo. BMS-189664 is identified as a potent, selective, and orally active inhibitor which is efficacious in vivo.



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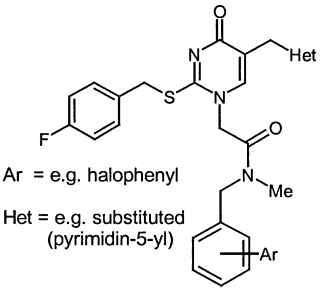
Potent, Orally Active Inhibitors of Lipoprotein-Associated Phospholipase A_2: 1-(Biphenylmethylamidoalkyl)-pyrimidones

Helen F. Boyd, Stephen C. M. Fell, Deirdre M. B. Hickey, Robert J. Ife, Colin A. Leach, Colin H. Macphee, Kevin J. Milliner, Ivan L. Pinto, D. Anthony Rawlings, Stephen A. Smith,* Ian G. Stansfield, Steven J. Stanway, Colin J. Theobald and Caroline M. Whittaker

GlaxoSmithKline, Medicines Research Centre, Gunnell's Wood Road, Stevenage SG1 2NY, UK

A series of 1-(biphenylmethylamidoalkyl)-pyrimidones has been designed as nanomolar inhibitors of recombinant lipoprotein-associated phospholipase A_2 with high potency in whole human plasma. Selected derivatives demonstrate excellent pharmacodynamic profiles which correlate well with their pharmacokinetic effects.

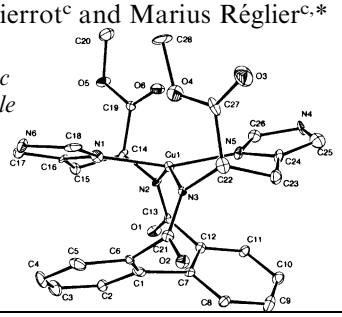


Bioorg. Med. Chem. Lett. 12 (2002) 57

Copper(II)/H_2O_2-Mediated DNA Cleavage: Involvement of a Copper(III) Species in H-Atom Abstraction of Deoxyribose Units

Amina Amine,[a,c] Zidane Atmani,[a] Abdelila El Hallaoui,[b] Michel Giorgi,[c] Marcel Pierrot[c] and Marius Réglier[c,*]

[a]*Université Moulay Ismail, Faculté des Sciences de Meknès, Meknès, Maroc*
[b]*Université Mohamed Benabdellah, Faculté des Sciences et Techniques de Fès Sais, Fès, Maroc*
[c]*Chimie, Biologie et Radicaux Libres, UMR-CNRS 6517, case 432, Universités d'Aix-Marseille 1 et 3, Faculté des Sciences et Techniques de Saint Jérôme, av. Escadrille Normandie-Niemen, F-13397 Marseille Cedex 20, France*



A new bis-amido–copper(II) complex **2** has been prepared. In the presence of hydrogen peroxide, complex **2** exhibited interesting nuclease activities in the 1–10 μM concentration range. For explaining its reactivity, we proposed the occurrence of a bis-amido–copper(III) intermediate and an oxidation mechanism involving a H-atom abstraction of deoxyribose moieties of DNA.

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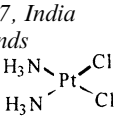
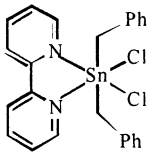
3-D QSAR Studies on New Dibenzyltin(IV) Anticancer Agents by Comparative Molecular Field Analysis (CoMFA)

Purnima M. Samuel,[a] Dick de Vos,[b] D. Raveendra,[c] J. A. R. P. Sarma[c,*] and Sujit Roy[d,*]

[a]*Metallo-Organic Laboratory, Indian Institute of Chemical Technology, Hyderabad 500007, India*
[b]*Medical Department, Pharmachemie BV, PO Box 552, 2003 RN Haarlem, The Netherlands*
[c]*Molecular Modeling Group, Organic Division-I, Indian Institute of Chemical Technology, Hyderabad 500007, India*
[d]*Organometallics & Catalysis Laboratory, Chemistry Department, Indian Institute of Technology, Kharagpur 721302, India*





MCF-7	IC_{50} (μM)	467	2.3
In vivo	LD_{50} (mg/Kg)	31	960

Dibenzyltin(IV) derivatives with N,S-donor ligands show significant cytotoxicity against human cancer cell lines. CoMFA PLS study on 21 complexes show good correlation with high r^2 and r^2_{CV} values.

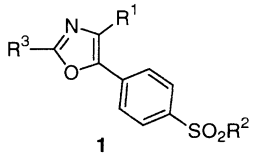
Bioorg. Med. Chem. Lett. 12 (2002) 65

4-Aryl/cycloalkyl-5-phenyloxazole Derivatives as Selective COX-2 Inhibitors

Hiromasa Hashimoto,* Kimiya Maeda, Koichi Ozawa, Jun-ichi Haruta and Korekiyo Wakitani

Central Pharmaceutical Research Institute, JT, Inc., 1-1 Murasaki-cho, Takatsuki, Osaka 569-1125, Japan

A series of 4-aryl/cycloalkyl-5-phenyloxazole derivatives **1** were synthesized and evaluated for their human cyclooxygenase-2 and cyclooxygenase-1 inhibitory activities.



1

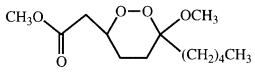
Bioorg. Med. Chem. Lett. 12 (2002) 69

New Readily Accessible Peroxides with High Anti-Malarial Potency

Nobutoshi Murakami,[a] Motoyuki Kawanishi,[a] Sawako Itagaki,[b] Toshihiro Horii[b] and Motomasa Kobayashi[a,*]

[a]*Graduate School of Pharmaceutical Sciences, Osaka University, 1-6 Yamada-oka, Suita, Osaka 565-0871, Japan*
[b]*Research Institute for Microbial Diseases, Osaka University, 3-1 Yamada-oka, Suita, Osaka 565-0871, Japan*

Exploration for new anti-malarial substances using the methyl esters of peroxyplakoric acids A_3 and B_3 as scaffolds led to a new readily accessible peroxide, 6-carbomethoxymethyl-3-methoxy-3-pentyl-1,2-dioxane.

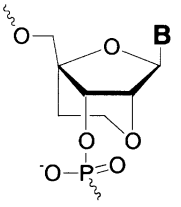


Bioorg. Med. Chem. Lett. 12 (2002) 73

2′-*O*,4′-*C*-Ethylene-Bridged Nucleic Acids (ENA): Highly Nuclease-Resistant and Thermodynamically Stable Oligonucleotides for Antisense Drug

Koji Morita,[a] Chikako Hasegawa,[a] Masakatsu Kaneko,[a] Shinya Tsutsumi,[b] Junko Sone,[b] Tomio Ishikawa,[b] Takeshi Imanishi[c] and Makoto Koizumi[a,*]

[a]*Exploratory Chemistry Research Laboratories, Sankyo Co., Ltd., Tokyo 140-8710, Japan*
[b]*Biomedical Research Laboratories, Sankyo Co., Ltd., Tokyo 140-8710, Japan*
[c]*Graduate School of Pharmaceutical Sciences, Osaka University, Osaka 565-0871, Japan*



ENA

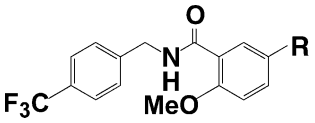
Bioorg. Med. Chem. Lett. 12 (2002) 77

Design, Synthesis and Evaluation of Substituted Phenylpropanoic Acid Derivatives as Peroxisome Proliferator-Activated Receptor (PPAR) Activators: Novel Human PPARα-Selective Activators

Hiroyuki Miyachi,* Masahiro Nomura, Takahiro Tanase, Yukie Takahashi, Tomohiro Ide, Masaki Tsunoda, Koji Murakami and Katsuya Awano

Discovery Research Laboratories, Kyorin Pharmaceutical Co., Ltd., 2399-1 Mitarai, Nogi-machi, Shimotsuga-gun, Tochigi 329-0114, Japan

A series of substituted phenylpropanoic acid derivatives was prepared as part of a search for subtype-selective human peroxisome proliferator-activated receptor (PPAR) activators.



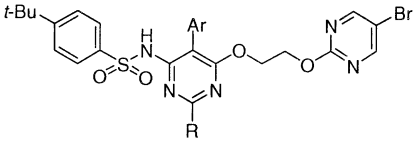
Bioorg. Med. Chem. Lett. 12 (2002) 81

Modifications and Structure–Activity Relationships at the 2-Position of 4-Sulfonamidopyrimidine Derivatives as Potent Endothelin Antagonists

Hiroshi Morimoto, Hideshi Shimadzu, Toshihiro Hosaka, Yasushi Kawase, Kosuke Yasuda, Kohei Kikkawa, Rikako Yamauchi-Kohno and Koichiro Yamada*

Discovery Research Laboratory, Tanabe Seiyaku Co. Ltd., 2-2-50 Kawagishi, Toda, Saitama 335-8505, Japan

Modifications at the 2-position of the nucleus pyrimidine of a series of potent ET_A antagonists, which showed extremely high affinity for ET_A receptor in porcine aortic membrane, were performed by efficient synthetic methods to examine structure–activity relationship.



Ar = 4-methylphenyl, (2-methoxy)phenoxy

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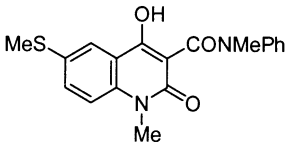
Synthesis and Antinephritic Activities of Quinoline-3-carboxamides and Related Compounds

Kiyoshi Tsuji,[a,*] Glen W. Spears,[a] Katsuya Nakamura,[a] Takashi Tojo,[a] Nobuo Seki,[c] Aiko Sugiyama[b] and Masaaki Matsuo[b]

[a]*Medicinal Chemistry Research Laboratories, Fujisawa Pharmaceutical Co., Ltd, 1-6, Kashima 2-chome, Yodogawa-ku, Osaka 532-8514, Japan*
[b]*Research Information Management, Fujisawa Pharmaceutical Co., Ltd, 1-6, Kashima 2-chome, Yodogawa-ku, Osaka 532-8514, Japan*
[c]*Exploratory Research Laboratories, Fujisawa Pharmaceutical Co., Ltd, 2-3, Tokodai 5-chome, Tsukuba, Ibaraki 300-2698, Japan*

A series of linomide-related quinoline-3-carboxamides and their analogues was prepared and evaluated for antinephritic activities. The 6-MeS derivative **7a** was highly effective in both chronic graft-versus-host disease and autoimmune MRL/l mice.



7a

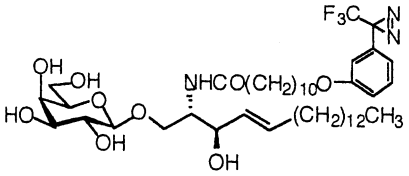
Bioorg. Med. Chem. Lett. 12 (2002) 89

Versatile Synthesis of Phenoxydiazirine-Based Fatty Acid Analogues and Photoreactive Galactosylceramide

Makoto Hashimoto,[a,*] Yasumaru Hatanaka[b] and Kensuke Nabeta[a]

[a]*Department of Bioresource Science, Obihiro University of Agriculture and Veterinary Medicine, Inada-cho, Obihiro 080-8555, Hokkaido, Japan*
[b]*Faculty of Pharmaceutical Sciences, Toyama Medical and Pharmaceutical University, 2360 Sugitani, Toyama 930-0194, Japan*

The synthesis of the phenoxydiazirinyl fatty acids and galactosylceramide are reported.



Bioorg. Med. Chem. Lett. 12 (2002) 93

Combinatorial Synthesis of 3-(Amidoalkyl) and 3-(Aminoalkyl)-2-arylindole Derivatives: Discovery of Potent Ligands for a Variety of G-protein Coupled Receptors

Christopher A. Willoughby,[a,*] Steven M. Hutchins,[a] Keith G. Rosauer,[a] Madhumeeta J. Dhar,[a] Kevin T. Chapman,[a] Gary G. Chicchi,[b] Sharon Sadowski,[b] David H. Weinberg,[c] Smita Patel,[d] Lorraine Malkowitz,[b] Jerry Di Salvo,[c] Stephen G. Pacholok[b] and Kang Cheng[c]

[a]*Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ 07065, USA*
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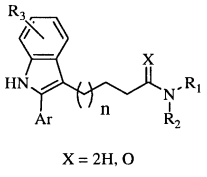

X = 2H, O

The synthesis of a combinatorial library of indole derivatives is reported. Several compounds were discovered to have high affinity/selectivity for various G-protein coupled receptors. These compounds serve as potential leads for further drug development.

Bioorg. Med. Chem. Lett. 12 (2002) 97

2-Amino-7-deazaadenine Forms Stable Base Pairs with Cytosine and Thymine

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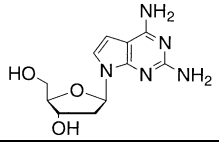
2-Amino-7-deazaadenine (^{AD}A) was incorporated into oligodeoxynucleotides and their base-pairing properties with natural nucleobases were investigated. ^{AD}A acts as a superior degenerate base to form a stable base pair with both cytosine and thymine.



Bioorg. Med. Chem. Lett. 12 (2002) 101

Potent P1′ Biphenylmethyl Substituted Aggrecanase Inhibitors

Wenqing Yao,[a,*] Michael Chao,[a] Zelda R. Wasserman,[a] Rui-Qin Liu,[b] Maryanne B. Covington,[b] Robert Newton,[b] David Christ,[c] Ruth R. Wexler[a] and Carl P. Decicco[a]

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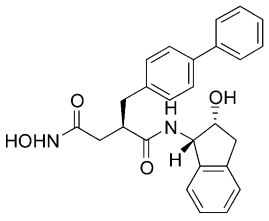

Bioorg. Med. Chem. Lett. 12 (2002) 105

Synthesis of Highly Functionalised Dibenzylglycine Derivatives Via the Suzuki–Miyaura Coupling Reaction

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