

CREATIVE TECHNOLOGY-DRIVEN DRUG DISCOVERY

origenis



Mestrelab Research

chemistry software solutions

Cippix – A Patent Search Engine

Dr Manuel Perez – Senior VP

Layout

- Introduction
- Types of searches
- How to use the chemical structure search tab
- How to handle lists and combine chemical searches
- How to search for similar documents
- How to export compounds and structures
- How the tag cloud works
- How to make the most of the chemical search capabilities
- The Cippix Development Environment

Introduction

- Optimised for fast access
- Weekly updated
- Database with different indexes
- LINGO

386

J. Chem. Inf. Model. 2005, 45, 386–393

LINGO, an Efficient Holographic Text Based Method To Calculate Biophysical Properties and Intermolecular Similarities

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Laboratory of Biomolecular NMR, Parc Científic de Barcelona, Josep Samitier, 1-5 08028 Barcelona, Spain, Morphochem AG, Gmunder Strasse 37-37a, 81379 München, Germany, and Departament de Química Orgànica, Universitat de Barcelona, Martí i Franquès, 1-11, 08028 Barcelona, Spain

Received October 21, 2004

Types of Searches

- Exact
- Similar
- Substructure
- Similar Substructure

How to use the chemical structure search tab

Keywords | Chemical Names | **Chemical Structures** | Patent Numbers

Set

H
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Cl
Br
I

Exact Search | Substructure Search

Search Similar Structures Toto 0.6

Search Similar Substructures Toto 0.9

Search only in selected patents

New Results

Enter name, SMILES ...

Replace Old Results (default)

Show Combination (OR)

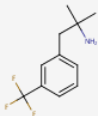
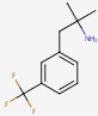
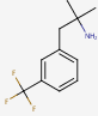
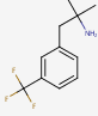
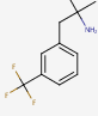
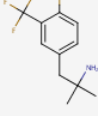

Show Intersection (AND)

Show Exclusive Combination (XOR)

Show Only New (NOT)

Show Only Old (NOT)

Substance Results

Hit No.	Structure	
1		(3'-Trifluoromethylphenyl)-2-methyl-2-aminopropan DE1275530B <chem>CC(C)(N)Cc1cccc(c1)C(F)(F)F</chem>
2		1,1-Dimethyl-2-(3-trifluoromethyl-phenyl)-ethylamin EP1730126B1 EP1577306A1 <chem>CC(C)(N)Cc1cccc(c1)C(F)(F)F</chem>
3		1,1-dimethyl-2-(3-trifluoromethyl-phenyl)-ethylamine JP2007529443T JP4991519B2 US7244728B2 JP2007529443A US2005209227A1 <chem>CC(C)(N)Cc1cccc(c1)C(F)(F)F</chem>
4		2-(3-trifluoromethylphenyl)-1,1-dimethylethylamine US4305951A <chem>CC(C)(N)Cc1cccc(c1)C(F)(F)F</chem>
5		1, 1-Dimethyl-2(3-trifluoromethyl-phenyl)-ethylamin WO2005092870A1 <chem>CC(C)(N)Cc1cccc(c1)C(F)(F)F</chem>
6		2-(4-fluoro-3-trifluoromethyl-phenyl)-1,1-dimethyl-ethylamine JP2007529443T JP4991519B2 US7244728B2 JP2007529443A US2005209227A1 <chem>Fc1ccc(cc1C(F)(F)F)CC(C)(C)N</chem>
7		1-(3'-Trifluoromethylphenyl)-2-methyl-2-methylaminopropan DE1275530B

Name

Patent No

SMILES

Working with Results

0. Structure

zoom export ccr view doc view select

docs sel. docs name structure numbers

Keywords Chemical Names Chemical Structures Patent Numbers

Query: US2004127574A1|JP2002293764A|US6982348B2|EP1362846A1

Search Substances in Patent List

Keywords Chemical Names Chemical Structures Patent Numbers

Query: 4-Chloro-3-(1,1-difluoro-ethyl)-phe

Search Exact Name

Search Similar Names 0.6

Search Similar Name Fragments 0.9

docs sel. docs name structure numbers

transfer patent numbers of selected substances to Keyword Search

Working with Keyword searches

Keywords Chemical Names Chemical Structures Patent Numbers

Query: (

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pn:US2008200445A1 OR
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pn:JP2006505573A OR
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pn:US7700589B2
)
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Keyword Search Help

sort by : fulltext score cippix score hit score first prio

Show only first member of patent family

Show Tag Clouds Show Document Results

Editable
Use of Keywords

You can run simple queries:		
Words (case insensitive)	EP1231212	finds documents with document number or text containing EP1231212
Word Groups	"nuclear receptors"	finds documents containing the word group "nuclear receptors"
Wildcards	nu?lear re?eptor	finds documents containing the word "nuclear" or "nuklear" and "receptor" or "rezeptor"
Wildcards	H4 antagoni*	finds documents containing "H4" and "antagonist" or "antagonists" or "antagonising" or "antagonizing"
You can use Boolean operators:		
AND	"nuclear receptors" AND inhibitors	AND is implicitly assumed and can be omitted
OR	"H4 antagonists" OR "H3 agonists"	OR must be defined
NOT	"H1 antagonists"	set a minus before the term or field you want to exclude
NOT	pa:Biovitrum -in:"Johansson"	find documents where applicant is "Biovitrum" but inventor is NOT "Johansson"
Round Brackets	agonists") AND ("blood brain barrier")	() can be used to define more complex Boolean queries
You can use relevance boosting to highlight and emphasise words:		
^Boostfactor	H3 (agonists OR antagonists^5)	finds documents containing "H3" "agonists" or "antagonists" and give "antagonists" 5 times higher relevance
	(agonists OR antagonists) (H1 OR H2^2 OR H3^3 OR H4^4)	keyword highlighting with different colors due to relevance for "H1", "H2", "H3", and "H4"
You can use near operators:		
~Similarity	pa:Meier~1	finds documents where applicant is within narrow Levenshtein distance 1 of "Meier" (Meir, Maier, Meer, Beier, ...)
~Similarity	pa:Meier~2	finds documents where applicant is within wider Levenshtein distance 2 of "Meier" (Breier, Bemer, Beyer, Peter, ...) in addition to (Meir, Maier, Meer, Beier, ...)
		finds documents for "nuclear" and "receptors" less than 8

Result visualisation
options

Tag Clouds

- In combination with Keywords = Powerful Visualisation

US71058207A20070223) HETEROCYCLIC ASPARTYL PROTEASE INHIBITORS - ZHU ZHAONING; MCKITTRICK BRIAN; SUN ZHONG-YUE; YE YUANZAN C.; VOIGT JOHANNES H.; STRICKLAND COREY O.; SMITH ELIZABETH M.; STAMFORD ANDREW; GREENLEE WILLIAM J.; MOZZOLA ROBERT D.; CALDWELL JOHN P.; CUMMING JARED N.; WANG LINGYAN; WU YUSHENG; ISERLOH ULRICH; LIU XIAOANG; GUO TAO; LE THUY X. E.; SAINOZ KURT W.; BABU SURESH D.; HUNTER RACHAEL C.; MORRIS MICHELLE L.; GU HUIZHONG; QIAN GANG; TADESSE DAWIT; HUANG YING; LI GUOQING; PAN JIANPING; MISIASZEK JEFFREY A.; LAI GAIFA; DUO JINGQI; QU CHUANXING; SHAO YUEFEI - ZHU ZHAONING; MCKITTRICK BRIAN; SUN ZHONG-YUE; YE YUANZAN C.; VOIGT JOHANNES H.; STRICKLAND COREY O.; SMITH ELIZABETH M.; STAMFORD ANDREW; GREENLEE WILLIAM J.; MOZZOLA ROBERT D.; CALDWELL JOHN P.; CUMMING JARED N.; WANG LINGYAN; WU YUSHENG; ISERLOH ULRICH; LIU XIAOANG; GUO TAO; LE THUY X. E.; SAINOZ KURT W.; BABU SURESH D.; HUNTER RACHAEL C.; MORRIS MICHELLE L.; GU HUIZHONG; QIAN GANG; TADESSE DAWIT; HUANG YING; LI GUOQING; PAN JIANPING; MISIASZEK JEFFREY A.; LAI GAIFA; DUO JINGQI; QU CHUANXING; SHAO YUEFEI; PHARMACOEPIA INC.; SCHERING CORPORATION

Disclosed are compounds of the formula I or a stereoisomer, tautomer, or pharmaceutically acceptable salt or solvate thereof, wherein each variable in Formula 1 are as defined in the specification; and pharmaceutical compositions comprising the compounds of formula I. Also disclosed are methods of inhibiting aspartyl protease, and in particular, the methods of treating cardiovascular diseases, cognitive and neurodegenerative diseases, and the methods of inhibiting of Human Immunodeficiency Virus, plasmepsins, cathepsin D and protozoal enzymes. Also disclosed are methods of treating cognitive or neurodegenerative diseases using the compounds of formula I in combination with a cholinesterase inhibitor or a muscarinic m1 agonist or m2 antagonist.

Abstract: Also disclosed are methods of inhibiting aspartyl protease, and in particular, the methods of treating cardiovascular diseases, cognitive and neurodegenerative diseases, and the methods of inhibiting of Human Immunodeficiency Virus, plasmepsins, cathepsin D and protozoal enzymes.; Also disclosed are methods of treating cognitive or neurodegenerative diseases using the compounds of formula I in combination with a cholinesterase inhibitor or a muscarinic m1 agonist or m2 antagonist

Description: [0002] This invention relates to heterocyclic aspartyl protease inhibitors, pharmaceutical compositions comprising said compounds, their use in the treatment of cardiovascular diseases, cognitive and neurodegenerative diseases, and their use as inhibitors of the Human ... plasmepsins, cathepsin D and protozoal enzymes.; It has been linked to numerous diseases including, Alzheimers, disease, connective tissue disease, muscular dystrophy and breast cancer. [0006] Alzheimer's disease (AD) is a progressive neurodegenerative disease that is ultimately fatal. Disease progression is associated with gradual loss of cognitive function related to memory, reasoning, orientation and judgment; Behavioral changes including confusion, depression and aggression also manifest as the disease progresses.; The currently available AD treatments are palliative, and while they ameliorate the cognitive and behavioral disorders, they do not prevent disease progression.; Therefore there is an unmet medical need for AD treatments that halt disease progression.; Thus inhibition of BACE-1 is a therapeutic approach to the ... of AD and other cognitive and neurodegenerative diseases caused by Abeta; [0011] Human immunodeficiency virus (HIV), is the causative agent of acquired immune deficiency syndrome (AIDS).; [0012] In addition, Human T-cell leukemia virus type I (HTLV-I) is a human retrovirus that has been clinically associated with adult T-cell leukemia and other chronic diseases.; [0057] More specifically, the invention comprises: the method of treating a cardiovascular disease such as hypertension, renal failure, or a disease modulated by renin inhibition; the method of treating Human ... of treating a cognitive or neurodegenerative disease such as Alzheimer's Disease; the method of inhibiting plasmepsins I and II ... Cathepsin D for the treatment of Alzheimer's Disease, breast cancer, and ovarian cancer; and the ... of plasmodium falciparum, for the treatment of fungal infections.; In particular, the invention comprises the method of treating Alzheimer's disease comprising administering at least one compound of formula I to a patient in need of such treatment.; [0058] In another aspect, the invention comprises the method of treating Alzheimer's disease comprising administering to a patient I need of ... I and a cholinesterase inhibitor or a muscarinic m.sub.1 agonist or m2 antagonist.; [0059] In a final aspect, the invention relates to a kit comprising in separate containers in a single package pharmaceutical compositions for use in ... container comprises a compound of formula I in a pharmaceutically acceptable carrier and a second container ... being an effective amount to treat a cognitive disease or neurodegenerative disease such as Alzheimer's disease.; Preferably, these combinations are directed to the treatment of Alzheimer's disease.; Preferably, these combinations are directed to the treatment of Alzheimer's disease.;

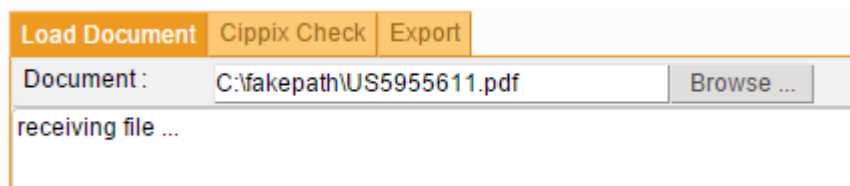
Claims: A method of treating cardiovascular disease, cognitive or neurodegenerative disease, a fungal infection, or a protozoal infection, ... amount of a compound of claim 68, or said tautomer thereof, or a pharmaceutically acceptable salt of said compound or said tautomer.; A method of treating a cognitive or neurodegenerative disease, said method comprising administering to a ... salt of said compound or said tautomer.; A method of claim 73, wherein said cognitive or neurodegenerative disease is Alzheimer's disease.;

fulltext score : 7.26e-3 cinnix score : 440 hit score : 0

Cippix as an Expanding Platform - ChemBio

		<p>US8173650B2 20120608 US78761310A20100526; US18145209P20090627; US2870706P20051217 Bicyclic pyrimidine P3K inhibitor compounds selective for P110 delta, and methods of use - CASTANEDO GEORGETTE; CHAN BRYAN; GOLDSTEIN DAVID; KONDRU RAMA; LUCAS MATTHEW; PALMER WYLLIE; PRICE STEPHEN; SAFINA BRIAN; SAVY PASCAL PIERRE ALEXANDRE; SEWARD EILEEN MARY; SUTHERLIN DANIEL P.; SWEENEY ZACHARY K. - CASTANEDO GEORGETTE; CHAN BRYAN; GOLDSTEIN DAVID; KONDRU RAMA; LUCAS MATTHEW; PALMER WYLLIE; PRICE STEPHEN; SAFINA BRIAN; SAVY PASCAL PIERRE ALEXANDRE; SEWARD EILEEN MARY; SUTHERLIN DANIEL P.; SWEENEY ZACHARY K.; GENENTECH, INC.</p> <p>Formula I (Ia and Ib) compounds wherein (i) X1 is N and X2 is S, (ii) X1 is S, (iii) X1 is N and X2 is NR2, or (iv) X1 is CR7 and X2 is O, including stereoisomers, tautomers, metabolites and pharmaceutically acceptable salts thereof, are useful for inhibiting the delta isoform of PI3K, and for treating disorders mediated by lipid kinases such as inflammation, immunological, and cancer. Methods of using compounds of Formula I for in vitro, in situ, and in vivo diagnosis, prevention or treatment of such disorders in mammalian cells, or associated pathological conditions, are disclosed.</p>	
		<p>US2013040931A1 20130214 US201113522823A20110114; US29641610P20100119; US2011021423W20110114 Amino Heteroaryl Compounds as Beta-Secretase Modulators and Methods of Use - PARAS NICK A.; BROWN JAMES; CHENG YUJIAN; HITCHCOCK STEPHEN A.; JUDD TED; LOPEZ PATRICIA; MINATTI ANA ELENA; NIXEY THOMAS; POWERS TIMOTHY; TEGLEY CHRISTOPHER M.; XUE QIUFEN; YANG BRYANT; ZHONG WENGE - AMGEN INC.; PARAS NICK A.; BROWN JAMES; CHENG YUJIAN; HITCHCOCK STEPHEN A.; JUDD TED; LOPEZ PATRICIA; MINATTI ANA ELENA; NIXEY THOMAS; POWERS TIMOTHY; TEGLEY CHRISTOPHER M.; XUE QIUFEN; YANG BRYANT; ZHONG WENGE</p> <p>The present invention comprises a new class of compounds useful for the modulation of Beta-secretase enzyme activity and for the treatment of Beta-secretase mediated diseases, including Alzheimer's disease (AD) and related conditions. In one embodiment, the compounds have a general Formula (I), wherein ring A, B1, B2, B3, L, R1, R2, ring Z, m and n of Formula I are defined herein. The invention also includes use of these compounds in pharmaceutical compositions for treatment, prophylactic or therapeutic, of disorders and conditions related to the activity of beta-secretase protein. Such disorders include, for example, Alzheimer's Disease (AD), cognitive deficits, cognitive impairment, schizophrenia and other central nervous system conditions related to and/or caused by the formation and/or deposition of plaque on the brain. The invention also comprises further embodiments of Formula (I), intermediates and processes useful for the preparation of compounds of Formula (I).</p>	

Cippix as an Expanding Platform – Cippix Proof



Acknowledgements

Origenis (Michael Thormann)

Mestrelab (Olalla Lema)