CREATIVE TECHNOLOGY-DRIVEN DRUG DISCOVERY

origenis

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Cippix – A Patent Search Engine

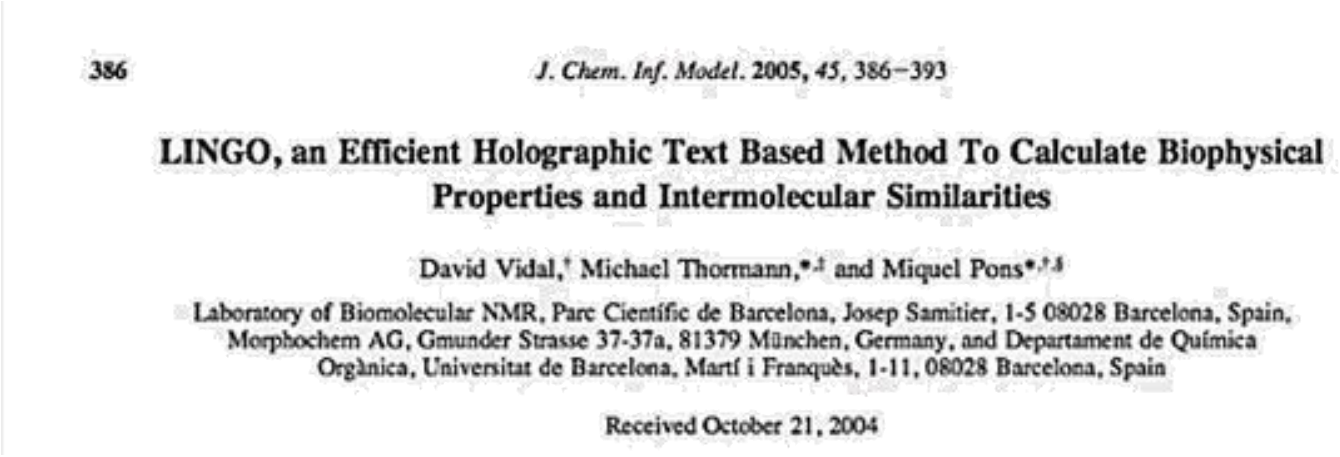
Dr Manuel Perez – Senior VP

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

David Vidal,† Michael Thormann,*,‡ and Miquel Pons*,†,§

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

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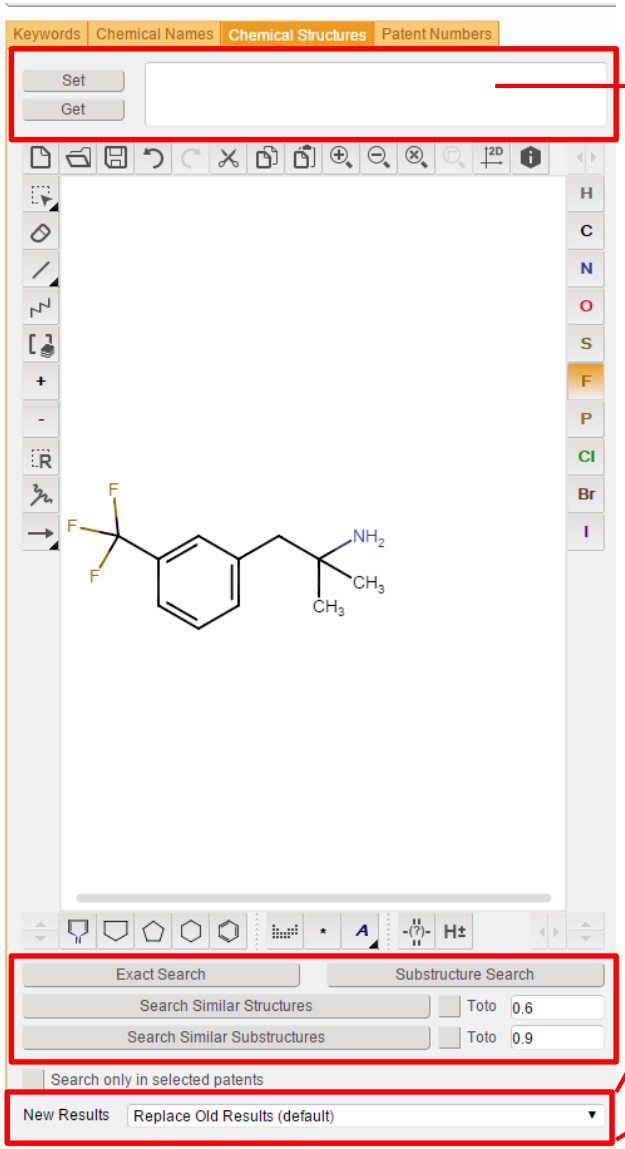
How to use the chemical structure search tab



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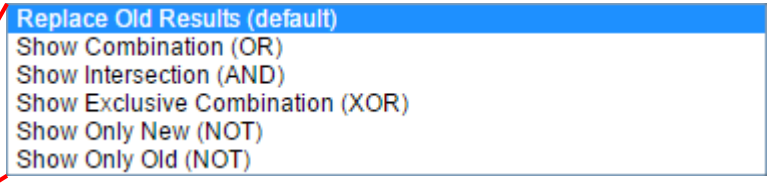

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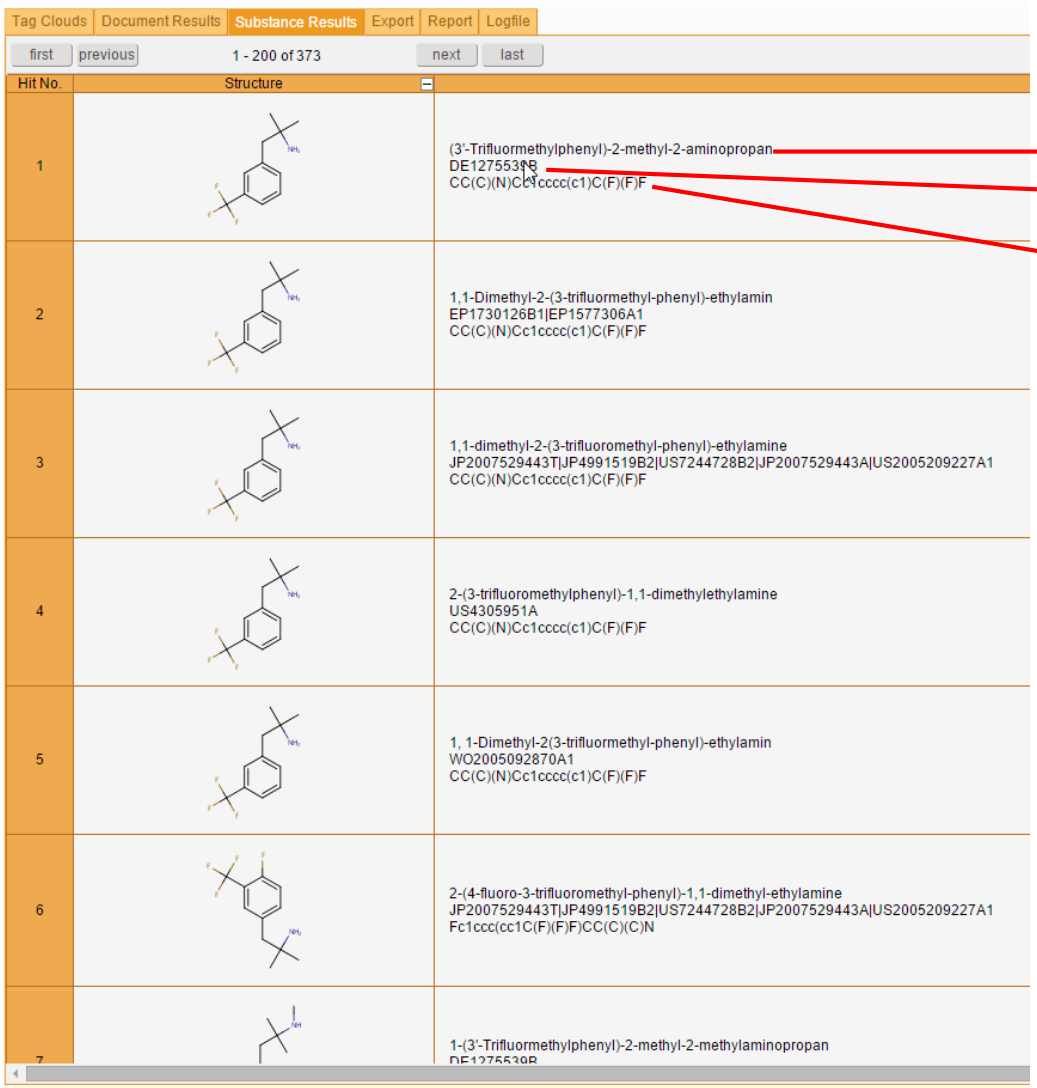
Substance Results

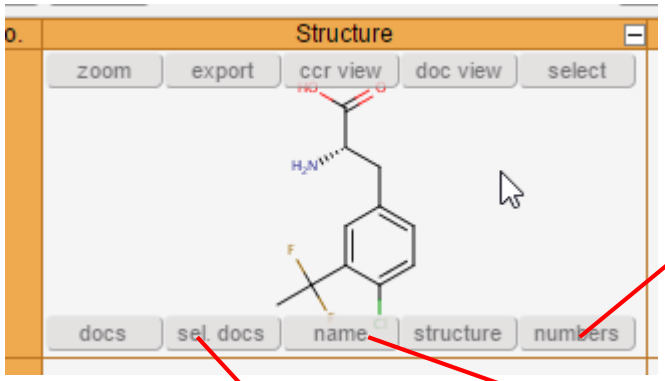


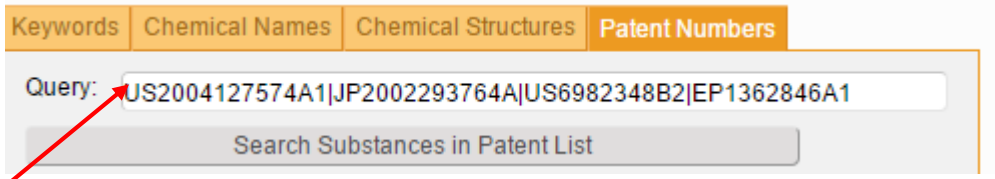
Name

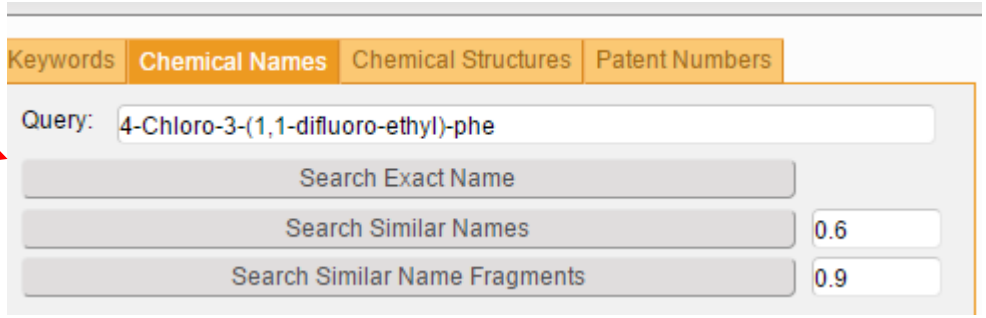
Patent No

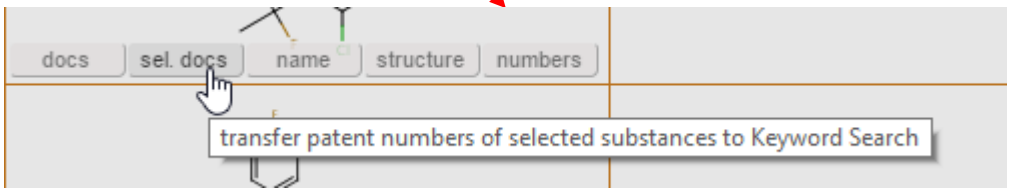
SMILES

Working with Results









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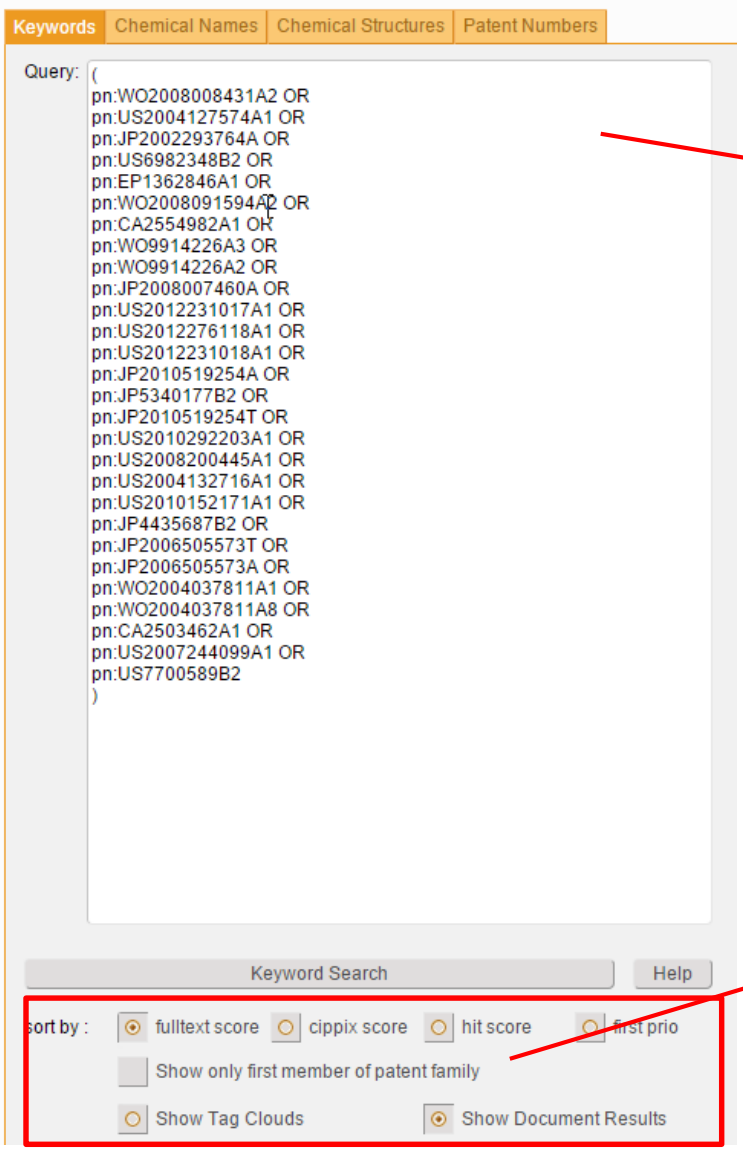
Working with Keyword searches



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" -ketotifen	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	("H4 antagonists" OR "H3 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 XIAOIANG; 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 XIAOIANG; 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; PHARMACOPEIA 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, plasmepins, 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.

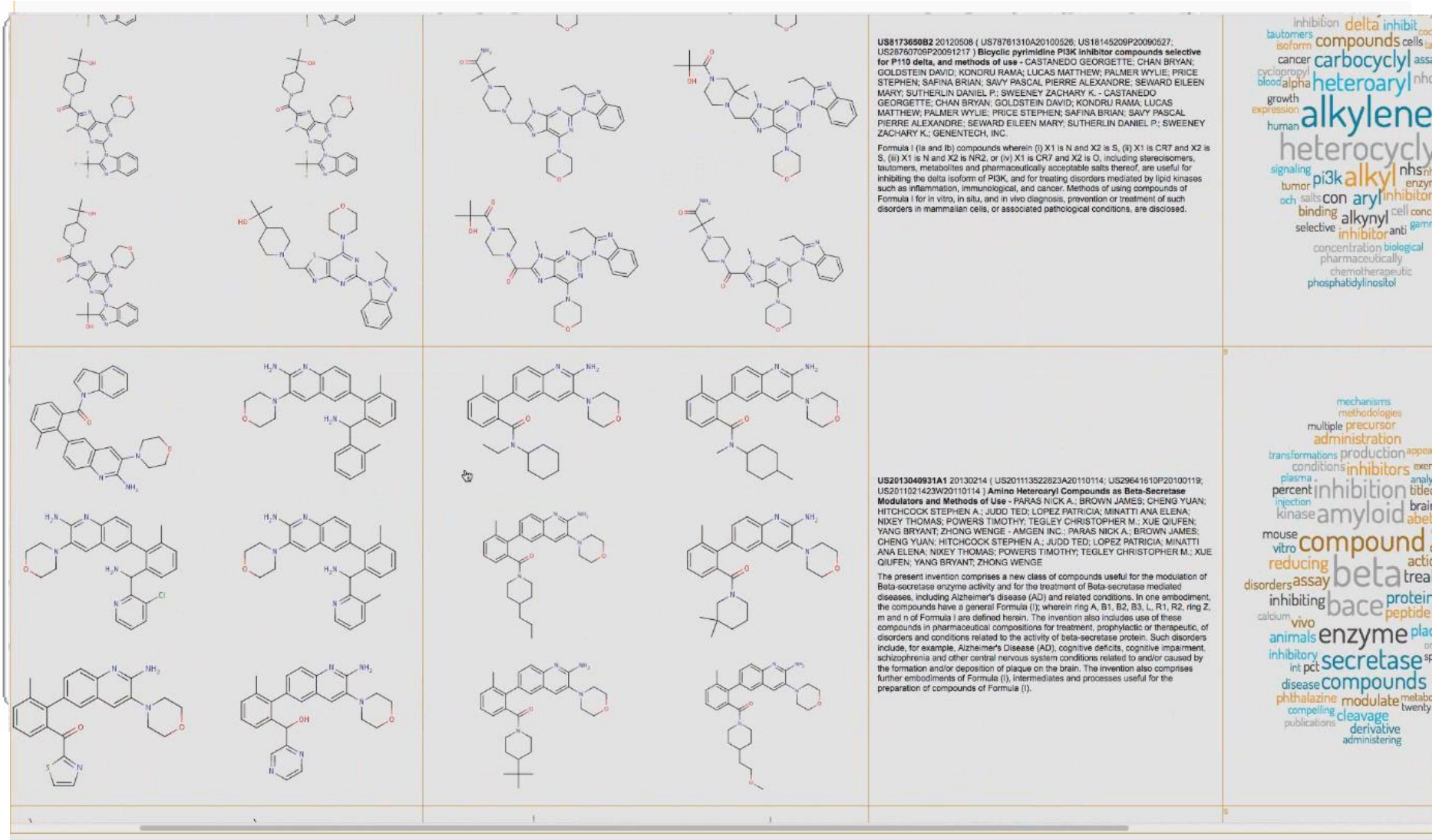
Abstract: Also disclosed are methods of inhibiting aspartyl protease, and in particular, the methods of treating cardiovascular diseases, cognitive and neurodegenerative diseases, and the methods of inhibiting of Human Immunodeficiency Virus, plasmepins, cathepsin D and protozoal enzymes.; Also disclosed 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, Alzheimer's, 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 plasmepins I and II ... Cathepsin D for the treatment of Alzheimer's Disease, breast cancer, and ovarian cancer; and the ... of plasmodium falciparnum, 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.;

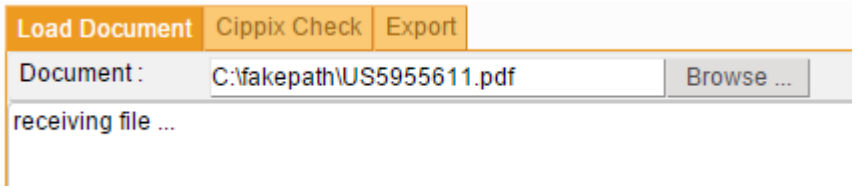
Claims: A method of treating cardiovascular disease, cognitive or neurodegenerative disease, a fungal infection, or a protozoal infection, ... amount of a compound of claim 68, or said tautomer thereof, or a pharmaceutically acceptable salt of said compound or said tautomer.; A method of treating a cognitive 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 , cippix score : 440 , hit score : 0

Cippix as an Expanding Platform - ChemBio



Cippix as an Expanding Platform – Cippix Proof



Acknowledgements

Origenis (Michael Thormann)

Mestrelab (Olalla Lema)