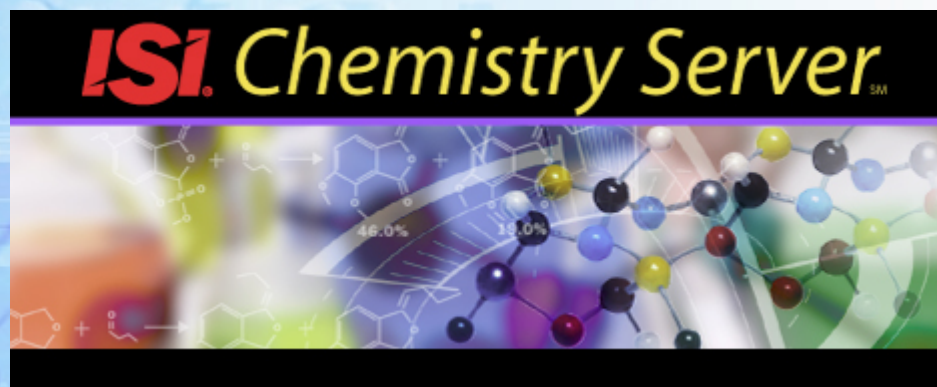


ISI Chemistry Server



*A versatile source of structural
Organic Chemistry information*

Matthew A. Kellett
ISI Chemical Production
June 13, 2001

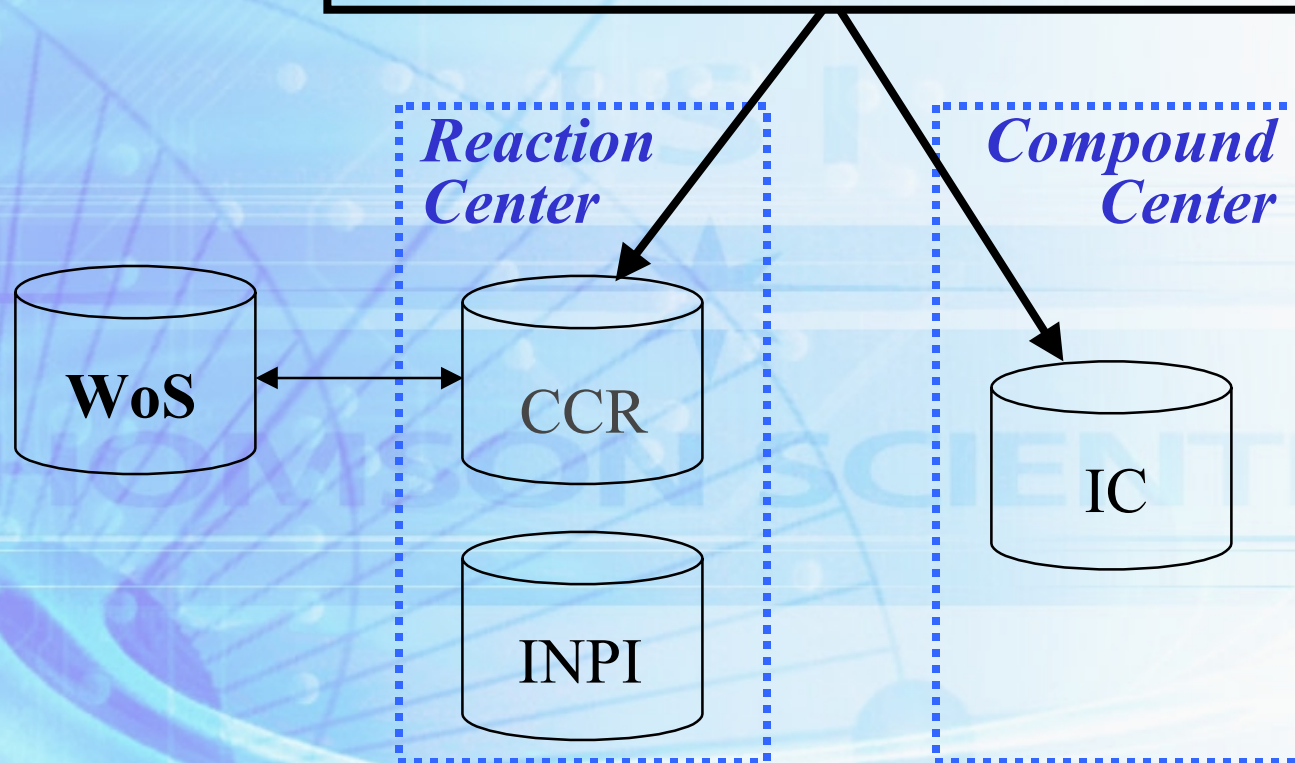
Matthew A. Kellett
SLA-June 13, 2001

ISI
THOMSON SCIENTIFIC™

ISI Chemistry Server

- *Comprised of two databases*
- *Reaction Center*
 - *A fully substructure searchable reaction database, accessible with a simple Web browser*
 - *Dynamic linking with other information resources (via the Web of Science)*
- *Compound Center*
 - *Up-to-date source of new organic compounds*
 - *Fully substructure searchable current awareness product*

ISI Chemistry Server



WoS = Web of Science access to ISI Citation Databases
CCR = Current Chemical Reactions database
INPI = Institut National de la Propriete Industrielle reaction database

IC = Index Chemicus compound database (1996-present)

ISI Chemistry Server

- Over **675,000** reactions (1840-present)
 - Over 535,000 reactions -- ISI (1985-present)
 - Over 45,000 reactions annual growth
 - 140,000 reactions -- INPI (1840-1986)
 - Static file
- Over **1,000,000** compounds (1996-present)
 - Over 180,000 compounds annual growth
 - Over 1,500,000 compounds (1991-present)
 - available on CD
 - Over 3,800,000 compounds (1960-1987)
 - available in print

ISI Chemistry Server

- Flexible Searching Capabilities

– Text searching

- **Bibliographic information**
- **Patent data**
- **Reaction conditions**

– Substructure searching

- **Complete reaction diagram**
- **Incomplete reaction (as product/reactant)**
- **General substructure searching**

– Combined searching (Text + Structure)

Full Search Strategies available in one step

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Select search domain(s), enter a [Reaction/Structure](#), [Bibliographic](#), and/or a [Reaction/Compound Data](#) Query. Then click


Domain:

Reaction Center

Compound Center

Reaction/Structure Query

Click Draw Query to create a structure or reaction query and transfer it to the Query box. Then select a search mode.

Search Mode	Query
<input checked="" type="radio"/> Substructure	
<input type="radio"/> Exact Match	

Full Search Strategies available in one step

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Select search domain

Domain:

Reaction/S

Click Draw Query

Search Mode

Substructure

Exact Match

Bibliographic Query

TOPIC: Enter terms to find from the article title, keywords, or abstract.

stereoselective and synthesis

Title only

AUTHOR: Enter one or more names as SMITH AB

SOURCE TITLE: Enter full journal title, or select from [list](#).

PUBLICATION YEAR: Enter a four digit year.

ADDRESS: Enter words from author's affiliation. ([abbreviations list](#))

PATENT COUNTRY CODE:

PATENT NUMBER:

PATENT KIND:

PATENT DATE:

Full Search Strategies available in one step

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Select search domain

Domain:

Reaction/Structure

Click Draw Query

Search Mode

Substructure

Exact Match

Bibliographic Query

[TOPIC:](#) Enter text

[AUTHOR:](#) Enter text

[SOURCE TITLE:](#) Enter text

[PUBLICATION:](#) Enter text

[ADDRESS:](#) Enter text

[PATENT COUNTRY:](#) Enter text

[PATENT NUMBER:](#) Enter text

[PATENT KIND:](#) Enter text

[PATENT DATE:](#) Enter text

Reaction Data Query Section

[REACTION CONDITIONS:](#) Enter reaction conditions to be searched.

Atmosphere:

Pressure (Atm):

Refluxed Flag:

Time (Hrs):

Temperature (C):

Product Yield:

Other:

[Terms list](#)

[COMPOUND DATA:](#) Enter terms to search the Compound data, select roles using the checkboxes.

Compound Name:

Compound Biol. Act.: [biol act](#)

Molecular Weight:

as Reactant as Product as Catalyst as Solvent

[REACTION SEARCH TERMS:](#) Enter additional search criteria in the fields below.

Reaction Keyphrases: [Keyphrase List](#)

Reaction Comments:

Full Record Display

Complete Bibliographic Information

Article Graphical Summary

Link to the Web of Science

Author Abstract, Address, Keywords

Reaction List

Link to detailed reaction conditions

Compound List

Link to compound information

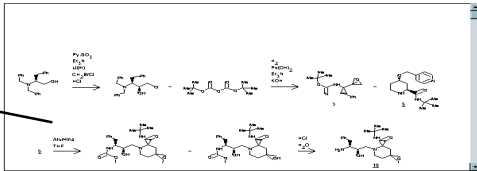
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Search Results - Full Record [Go to Web of Science™](#)

Article 1 of 3 ▶

Title: Practical, stereoselective synthesis of palinavir, a potent HIV protease inhibitor.
Author(s): Beaulieu PL, Lavallee P, Abraham A, Anderson PC, Boucher C, Bouquet Y, Duceppe JS, Gillard J, Gorys V, GrandMaitre C, Grenier L, Gaudon Y, Guse I, Plamondon L, Soucy F, Valois S, Wernic D, Yoakim C
Source: JOURNAL OF ORGANIC CHEMISTRY 62(11), 3440-3443, 1997



Abstract: Palinavir is a potent peptidomimetic-based HIV protease inhibitor. We have developed a highly convergent and stereoselective synthesis which is amenable to the preparation of multikilogram quantities of this compound. The synthetic sequence proceeds in 24 distinct chemical steps (with several integrated, multistep operations) from commercially available starting materials. No chromatographies are required throughout the process, and the final product is purified by crystallization of its dihydrochloride salt to >99% homogeneity.

KeyWords Plus: ALPHA-AMINO EPOXIDES; INTERMEDIATE; DESIGN; AIDS; RO-31-8959; CONVENIENT; TARGET; ACID

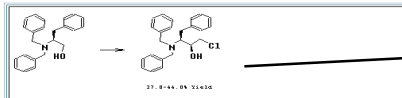
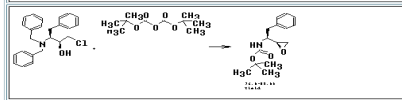
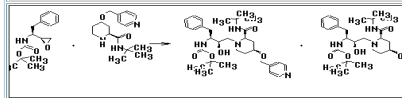
Document type: ARTICLE
Language: ENGLISH
Addresses: BOEHRINGER INGELHEIM CANADA LTD, BIOMEGA RES DIV, 2100 CUNARD ST, LAVAL, PQ H7S 2G5, CANADA
IDS Number: XC120

Article 1 of 3 ▶

REACTATIONS

REACTION SUMMARY

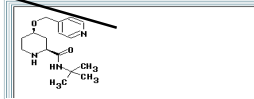
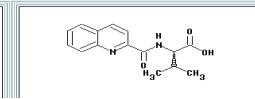
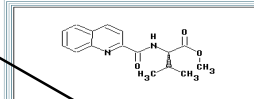
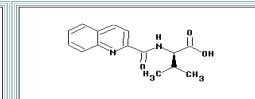
Reactions 1 -- 10 ▶▶

	Reaction Details
	Reaction Details
	Reaction Details

COMPOUNDS

COMPOUND SUMMARY

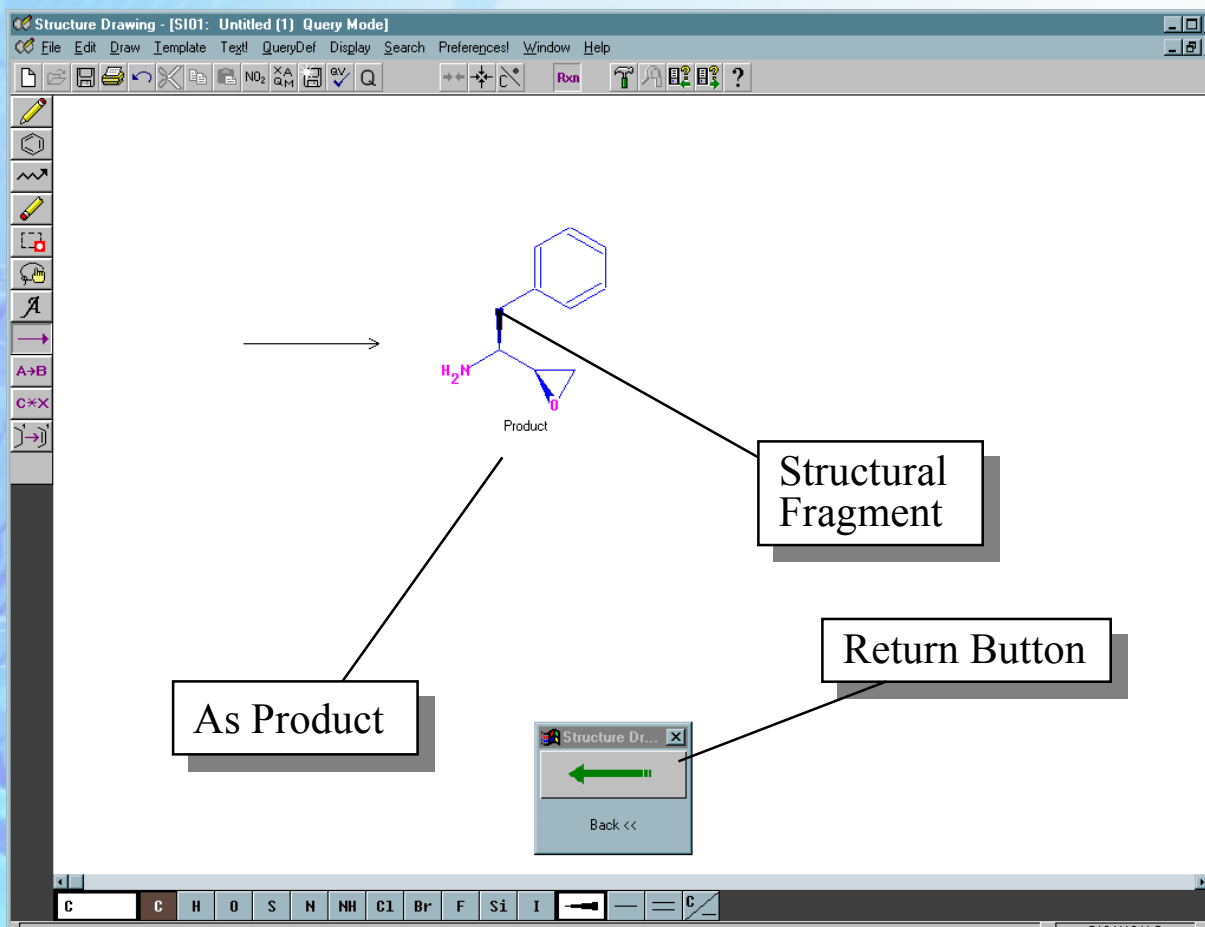
Compounds 1 -- 10 ▶▶

Compounds 1 -- 10 ▶▶

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SLA-June 13, 2001

Fully functional structure drawing package



Easily combined searches, with no preset hit limits

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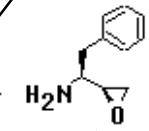


Reaction Search Enter a Reaction Structure query, Bibliographic query, and/or a Reaction Data query, then press SEARCH below.

REACTION QUERY: Enter a reaction query and select the search mode.

Search Mode	Reaction Query
	Query Name: <input type="text" value="C:\CHEMSVR\SKETCH3"/> <input type="button" value="Browse..."/>

Reaction Substructure
 Exact Match



NC(=O)c1ccccc1

Plug-in

Substructure Query

Reaction Comments:
Advantage*

Reaction Data Query Section

REACTION CONDITIONS: Enter reaction conditions to be searched.

Atmosphere: Pressure (Atm): Refluxed Flag:
Time (Hrs): Temperature (C):
Product Yield: Other: [Terms list](#)

COMPOUND DATA: Enter terms to search the Compound data, select roles using the checkboxes.

Compound Name:
Compound Biol. Act.: [biol act](#)
Molecular Weight:
 as Reactant as Product as Catalyst as Solvent

REACTION SEARCH TERMS: Enter additional search criteria in the fields below.

Reaction Keyphrases: [Keyphrase List](#)
Reaction Comments:

Combine text and structure searches

Structure Search Summary Screen

Reaction Summary

Initial Query (Red)

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Search Results - Structure Search Summary

66 (approx.) of 622377 reactions matched query.

Structures 1 - 10

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Reaction	Reaction Details
 70.0% Yield	Reaction Details Full Record
	Reaction Details Full Record
	Reaction Details Full Record
	Reaction Details Full Record
	Reaction Details Full Record
	Reaction Details Full Record
	Reaction Details Full Record
	Reaction Details Full Record
	Reaction Details Full Record
	Reaction Details Full Record

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Link to Full Record

Link to detailed reaction conditions

Reaction Details Screen

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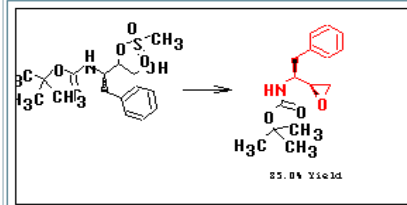
Search Results-- Reaction Details



Green BE; Chen XQ; Norbeck DW; Kempf DJ [Convenient synthesis of 1-\(S\)-\(1'-\(S\)-\(t-butylloxycarbonylamino\)-2'-phenylethyl\)oxirane, a versatile intermediate for the preparation of hydroxyethylamine based HIV protease inhibitors.](#)

Reaction 5 of 6 ◀ ◁ ▷ ▶

Reaction No: RCCR08893405 Path: A1 Step: 5 of 5 KeyRxn: No



REACTION CONDITIONS

Atmosphere: Pressure: Time: 3.66667 HR. Temp: 25.0 DEG C
Refluxed: D Other:

CATALYST AND SOLVENT DATA

	Symbol	Grade
Catalyst(1):	NaH	4.4 mmol
Solvent(1):	THF	dry

REACTANT AND PRODUCT DATA

	Symbol	Grade	BioAct	Yield
Reactant(1):		4.4 mmol		
Product(1):				85.0%

Comments: Advantages: 1) simple, short, and convenient method, 2) good stereocontrol, and 3) high overall yields.

Keyphrases:

Reaction 5 of 6 ◀ ◁ ▷ ▶

Comments:

Advantages: 1) simple, short, and convenient method, 2) good stereocontrol, and 3) high overall yields.

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INPI Full Record

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Search Results-- Full Record

Article 17 of 1319 ◀ ▶

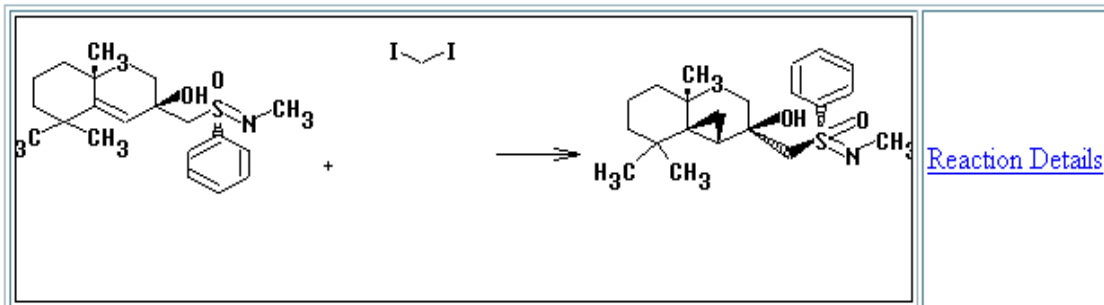


Title: INPI Reaction
Author(s): JOHNSON CR
Source: TETRAHEDRON LETT 104, 4290, 1982
Document type: ARTICLE

Article 17 of 1319 ◀ ▶

REACTION SUMMARY

Reactions 1 -- 1

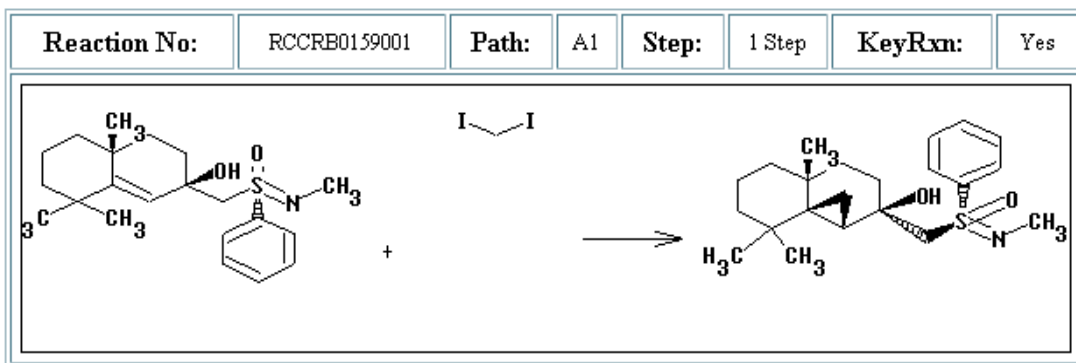


Reactions 1 -- 1

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Search Results-- Reaction Details

JOHNSON CR [INPI Reaction](#)



REACTION CONDITIONS

Atmosphere: Pressure: Time: Temp: 35.0 DEG C
 Refluxed: Other: Zn-Ag Et2O Rf 72h

CATALYST AND SOLVENT DATA

	Symbol	Grade
Catalyst(1):	Zn-Ag	
Solvent(1):	Et2O	

REACTANT AND PRODUCT DATA

	Symbol	Grade	BioAct	Yield
Reactant(2):	CH2I2			

Comments:

Keyphrases: CARBENE INTERMEDIATE, DIASTEREOSELECTIVE, CYCLOADDITION

*INPI Records
have full reaction
details and
represent proven
methods that have
been compiled by
research scientists
working in the
laboratory*

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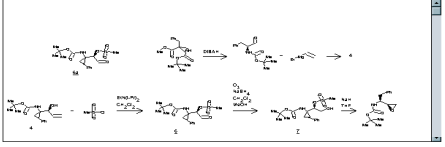
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Article 14 of 32 (approx.) < > [Go to Web of Science®](#)

Title: Convenient synthesis of 1-(S)-(1'-(S)-(t-butylloxycarbonylamino)-2'-phenylethyl)oxirane, a versatile intermediate for the preparation of hydroxyethylamine based HIV protease inhibitors.

Author(s): Green BE, Chen XQ, Norbeck DW, Kempf DJ

Source: SYNLETT (6), 613-614, 1995



Abstract: A concise, stereocontrolled synthesis of N-protected (1S,1'S)-alpha-aminoepoxides, important intermediates for the preparation of hydroxyethylamine dipeptide isosteres, beginning with alpha-aminoesters is described.

Author Keyword: ALPHA-AMINOEPoxide, HYDROXYETHYLAMINE

KeyWords Plus: DIPEPTIDE ANALOGS, TRANSITION-STATE, ISOSTERES

Document type: NOTE

Language: ENGLISH

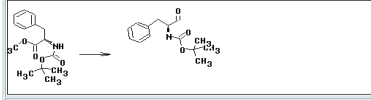
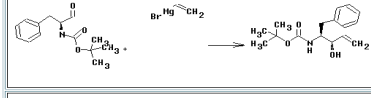
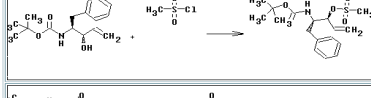
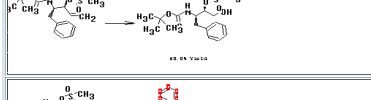
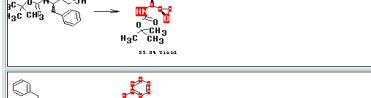

Addresses: ABBOTT LABS, DIV PHARMACEUT PROD, D-47D, AP9A, 100 ABBOTT PK RD, ABBOTT PK, IL 60064, USA
ABBOTT LABS, DIV PHARMACEUT PROD, ABBOTT PK, IL 60064, USA

IDS Number: RG086

Article 14 of 32 (approx.) < >

REACTION SUMMARY

Reactions 1 - 6

	Reaction Details
	Reaction Details
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	Reaction Details
	Reaction Details

Reactions 1 - 6

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CONVENIENT SYNTHESIS OF 1-(S)-(1'-(S)-(T-BUTYLOXYCARBONYLAMINO)-2'-PHENYLETHYL)OXIRANE, A VERSATILE INTERMEDIATE FOR THE PREPARATION OF HYDROXYETHYLAMINE BASED HIV PROTEASE INHIBITORS
GREEN BE, CHEN XQ, NORBECK DW, KEMPF DJ
SYNLETT
(6) 613-614 JUN 1995

Document type: Note **Language:** English **Cited References:** 20 **Times Cited:** 10

Abstract: A concise, stereocontrolled synthesis of N-protected (1S,1'S)-alpha-aminoepoxides, important intermediates for the preparation of hydroxyethylamine dipeptide isosteres, beginning with alpha-aminoesters is described.

Author Keywords: ALPHA-AMINOEPoxide, HYDROXYETHYLAMINE

KeyWords Plus: DIPEPTIDE ANALOGS, TRANSITION-STATE, ISOSTERES

Addresses: ABBOTT LABS, DIV PHARMACEUT PROD, ABBOTT PK, IL 60064.

Publisher: GEORG THIEME VERLAG, STUTTGART

IDS Number: RG086

ISSN: 0936-5214

Article 5 of 14 < PREVIOUS NEXT > SUPPLEMENTARY

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GREEN BE, CHEN XQ, NORBECK DW, et al.
SYNLETT
(6) 613-614 JUN 1995

These documents in the database cite the above article:

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⏪ ⏩ ⏴ ⏵ []

- Kurihara M, Ishii K, Kasahara Y, et al.
[Stereoselective synthesis of an erythro N-protected alpha-amino epoxide derivative](#)
TETRAHEDRON LETT 40: (16) 3183-3184 APR 16 1999
- Ohno H, Ishii K, Honda A, et al.
[A 2,3-cis-selective synthesis of aziridines bearing a vinyl group from allyl methyl carbonates and allyl mesylates](#)
J CHEM SOC PERK T 1 (22) 3703-3716 NOV 21 1998
- Mordini A, Valacchi M, Nardi C, et al.
[A selective access to amino hydroxy oxetanes](#)
J ORG CHEM 62: (24) 8557-8559 NOV 28 1997
- Branalt J, Kvarnstrom I, Classon B, et al.
[A convenient synthesis of 1-\(S\)-\[1'-\(S\)-\(t-butyloxycarbonylamino\)-2'-phenylethyl\]oxirane. A useful building block in the synthesis of HIV protease inhibitors.](#)
TETRAHEDRON LETT 38: (19) 3483-3486 MAY 12 1997
- Chen P, Cheng PTW, Spergel SH, et al.
[A practical method for the preparation of alpha'-chloroketones of N-carbamate protected-alpha-aminoacids](#)
TETRAHEDRON LETT 38: (18) 3175-3178 MAY 5 1997
- Albeck A, Estreicher GI
[Functionalized erythro N-protected alpha-amino epoxides. Stereocontrolled synthesis and biological activity](#)
TETRAHEDRON 53: (14) 5325-5338 APR 7 1997
- Agami C, Couty F, Hamon L, et al.
[Regio- and stereocontrolled formation of chiral epoxy oxazolidines via bromocarbamation of N-Boc alkenyl oxazolidines. Application to asymmetric synthesis](#)
J ORG CHEM 62: (7) 2106-2112 APR 4 1997
- Danielmeier K, Schierle K, Steckhan E
[A new chiral, cationic beta-amino alcohol equivalent: A variable approach to enantiomerically pure building blocks for hydroxyethylene isomers](#)
ANGEW CHEM INT EDIT 35: (19) 2247-2248 OCT 21 1996
- Beaulieu PL, Wernic D
[Preparation of aminoalkyl chlorohydrin hydrochlorides: Key building blocks for hydroxyethylamine-based HIV protease inhibitors](#)
J ORG CHEM 61: (11) 3635-3645 MAY 31 1996

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RELATED RECORDS

REACTIONS COMPOUNDS

A convenient synthesis of 1-(S)-[1'-(S)-(t-butyloxycarbonylamino)-2'-phenylethyl]oxirane. A useful building block in the synthesis of HIV protease inhibitors.
Branalt J, Kvanstrom I, Classon B, Samuelsson B, Nilroth U, Danielson UH, Karlen A, Hallberg A
TETRAHEDRON LETTERS 38: (19) 3483-3486 MA

Document type: Article **Language:** English **Cited References:** 26 **Times Cited:** 1

Abstract:
A new short route to epoxide 6b, a pivotal intermediate for the preparation of hydroxyethyl antiraminic acid, followed by extensions in the PZ/P3-region gave the target compounds with Science Ltd.

KeyWords Plus:
ASYMMETRIC DIHYDROXYLATION, EPOXIDES, 2-(S)-[1'-(S)-AZIDO-2-PHENYLETHYL]OXIRANE, INTERMEDIATE, AMINES

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ISSN:
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Article 8 of 32 (approx.)

Title:
A convenient synthesis of 1-(S)-[1'-(S)-(t-butyloxycarbonylamino)-2'-phenylethyl]oxirane. A useful building block in the synthesis of HIV protease inhibitors.

Author(s):
Branalt J, Kvanstrom I, Classon B, Samuelsson B, Nilroth U, Danielson UH, Karlen A, Hallberg A

Source:
TETRAHEDRON LETTERS 38(19), 3483-3486, 1997

Abstract:
A new short route to epoxide 6b, a pivotal intermediate for the preparation of hydroxyethylamine dipeptide isosteres has been developed. Opening of the epoxide by sulfuric acid, followed by extensions in the PZ/P3-region gave the target compound which were evaluated as HIV-1 protease inhibitors (C) 1997 Elsevier Science Ltd.

KeyWords Plus:
ASYMMETRIC DIHYDROXYLATION, EPOXIDES, 2-(S)-[1'-(S)-AZIDO-2-PHENYLETHYL]OXIRANE, INTERMEDIATE, AMINES

Document type: ARTICLE

Language: ENGLISH

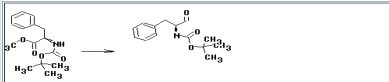
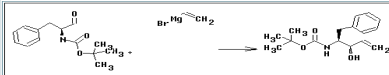
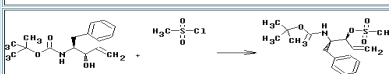
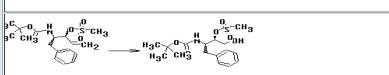
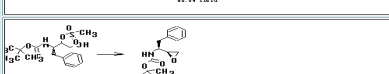

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LINKOPING UNIV, DEPT CHEM, S-58183 LINKOPING, SWEDEN
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IDS Number:
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Article 8 of 32 (approx.)

REACTION SUMMARY

Reactions 1 -- 6

	Reaction Details
	Reaction Details
	Reaction Details
	Reaction Details
	Reaction Details
	Reaction Details

Reactions 1 -- 6

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SLA-June 13, 2001

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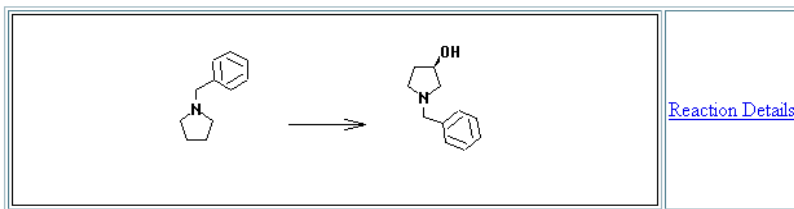
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Author(s): WITHOLT B; LI Z
Addresses: EIDGENOESSISCHE TECH HOCHSCHULE ZUERICH
Document type: PATENT
Source: EP1002871
Patent Kind: A1
Patent Date: 5-24-2000
Latest Priority Date: 11-17-1998
Latest Priority Country: EP
Latest Priority Number: EP203893

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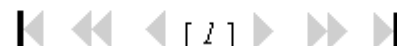
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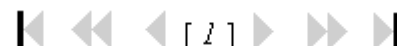
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EIDGENOESSISCHE TECH HOCHSCHULE ZUERICH (EIDG-Non-standard)

LI Z, WITHOLT B

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AU200012730-A; EP1002871-A1; WO200029606-A1

Title:

New method for the production of optically active 3-hydroxypyrrolidine using microorganisms or enzymes derived from them as a biocatalyst

Inventor Name(s):

LI Z, WITHOLT B

Patent Assignee Name(s) and Code(s):

EIDGENOESSISCHE TECH HOCHSCHULE ZUERICH (EIDG-Non-standard)

R3 = hydrogen, a linear, cyclic or branched alkyl, alkenyl, aryl except phenyl, heterocyclic aryl, benzyl, aralkyl or heterocyclic aralkyl group, containing 1 - 20 carbon atoms, optionally with substitution

EP1002871-A1 EP-0205895 17 NOV 1998

WO200029606-A1 WO-EP09041 15 Nov 1999

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SE; SI

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G; MK;
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