ISI Chemistry Server

A versatile source of structural Organic Chemistry information

Matthew A. Kellett
ISI Chemical Production
June 13, 2001

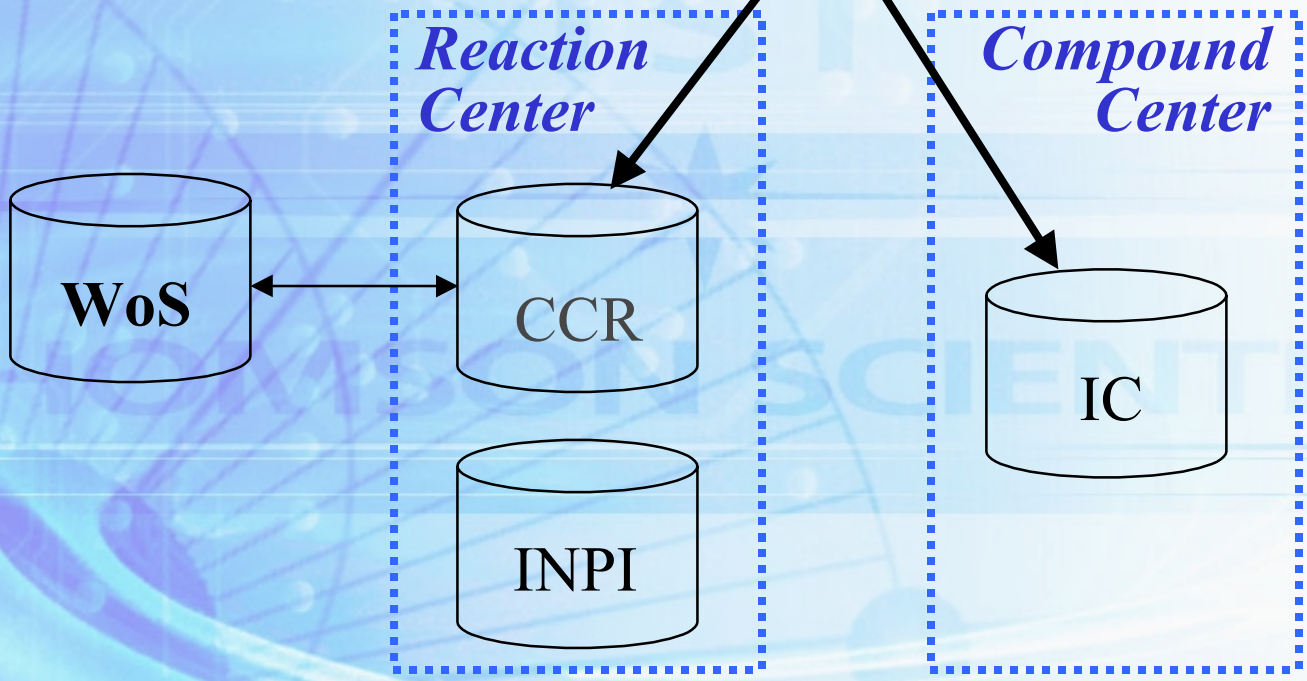
ISI Chemistry Server

- 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 = **W**eb of **S**cience access to ISI Citation Databases
CCR = **C**urrent **C**hemical **R**eactions database
INPI = **I**nstitut National de la **P**ropriete **I**ndustrielle reaction database

IC = **I**ndex **C**hemicus compound database (1996-present)

ISI Chemistry Server

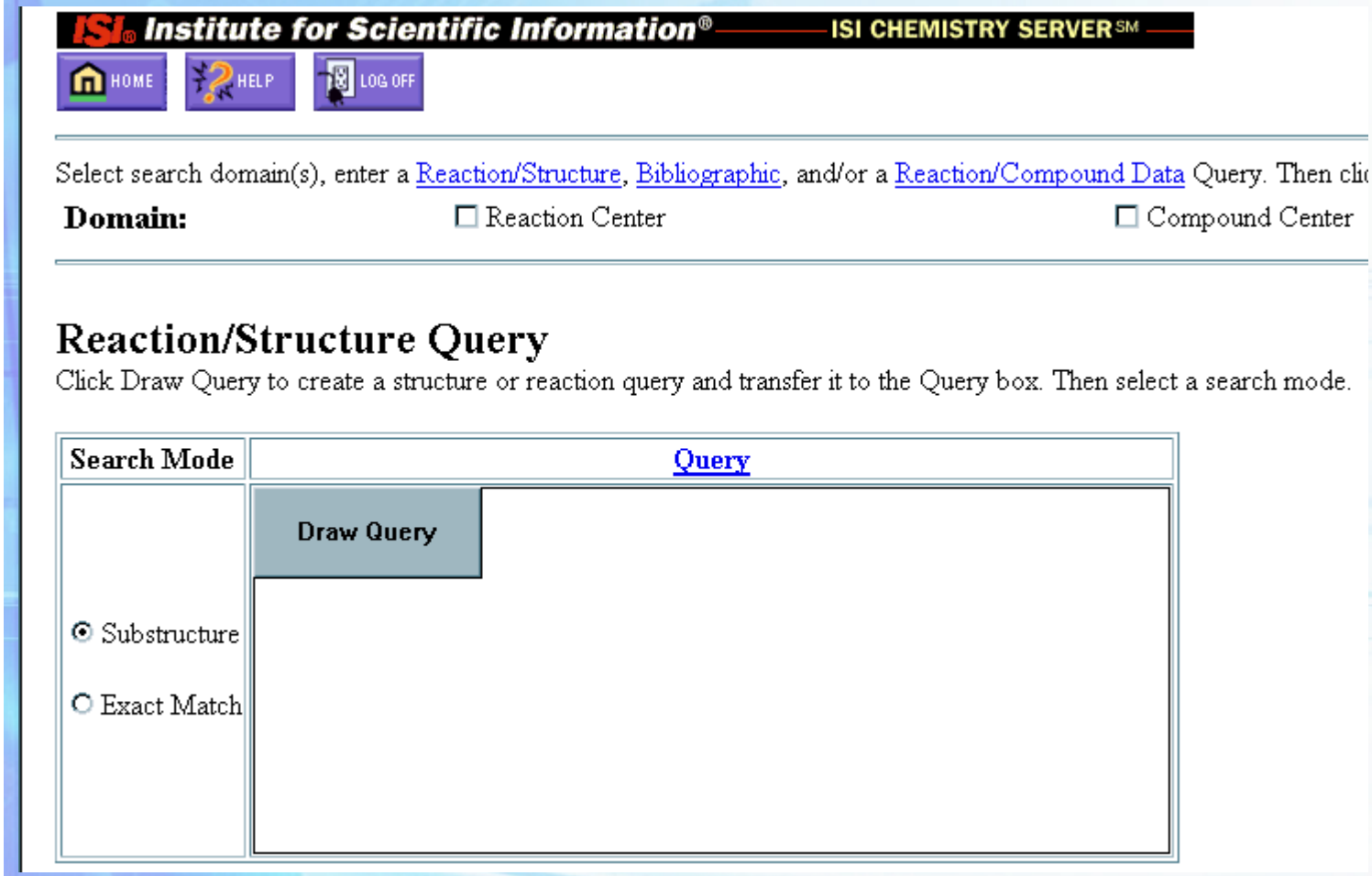
- Over 675,000 reactions (1840-present)
  - Over 535,000 reactions -- ISI (1985-present)
    - Over 45,000 reactions annual growth
  - 140,000 reactions -- INPI (1840-1986)
    - Static file
- Over 1,000,000 compounds (1996-present)
  - Over 180,000 compounds annual growth
  - Over 1,500,000 compounds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

ISI Chemistry Server

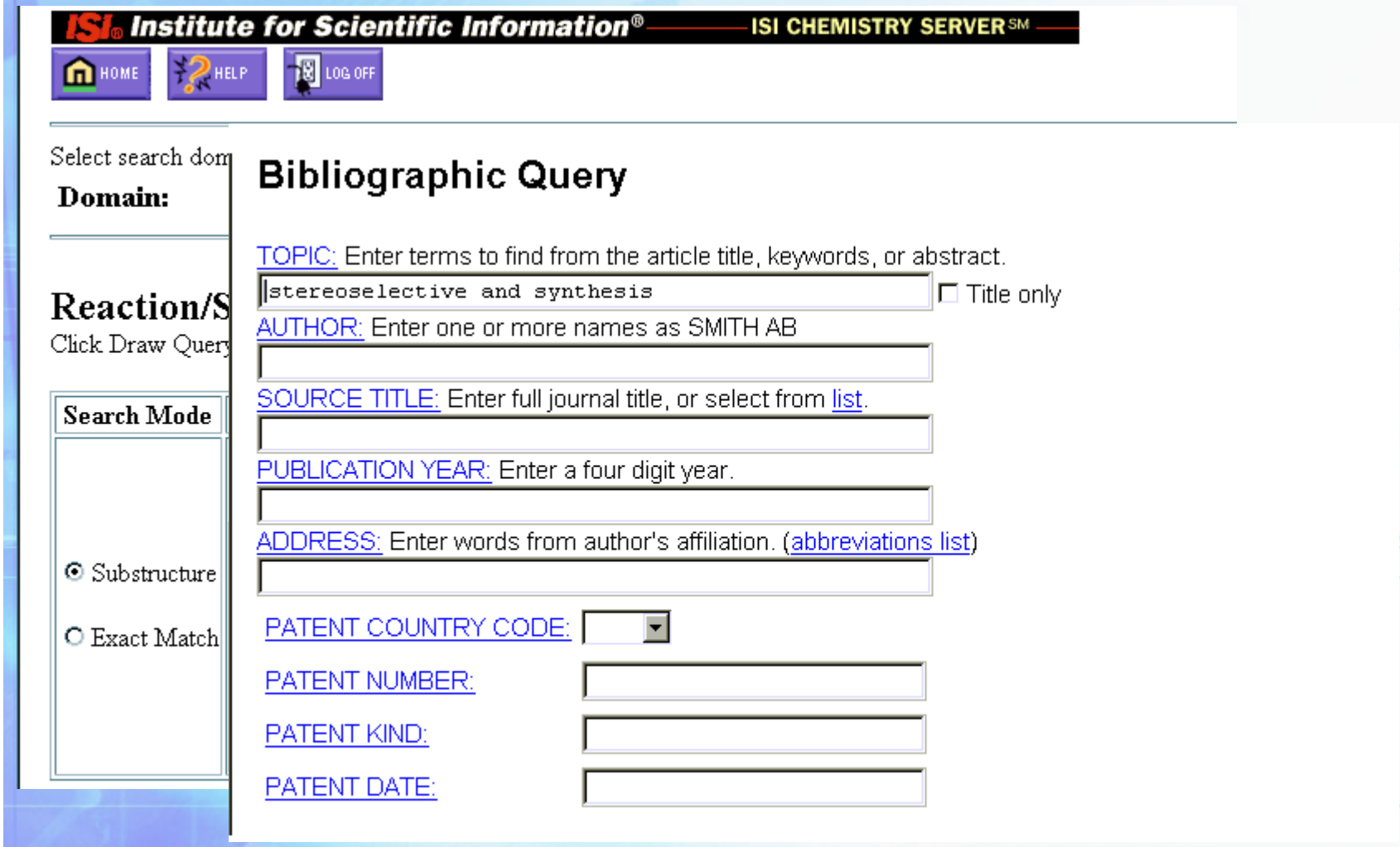
- Flexible Searching Capabilities

- **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)**

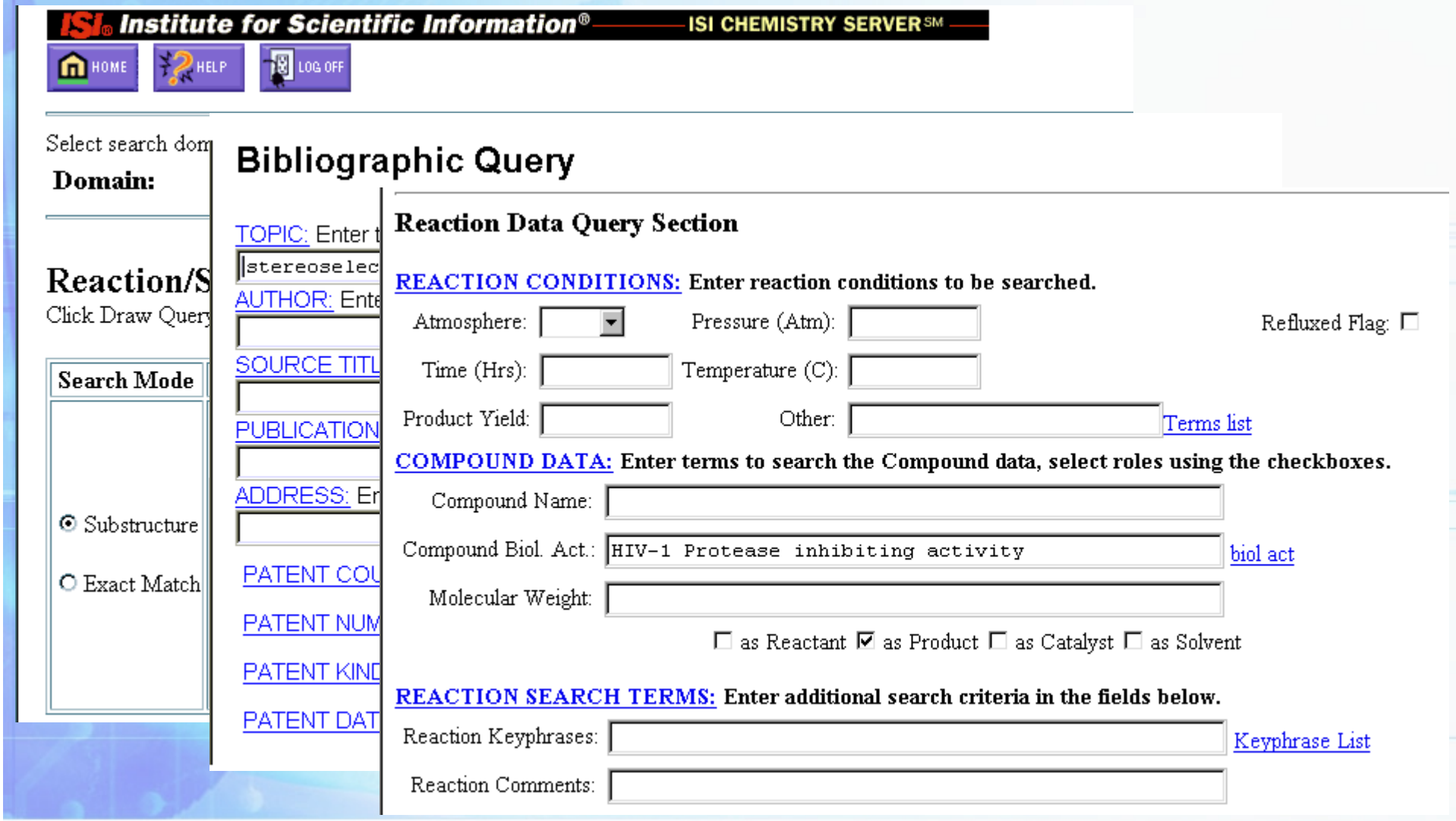
Full Search Strategies available in one step



Full Search Strategies available in one step



Full Search Strategies available in one step



Full Record Display

Complete Bibliographic Information

Article Graphical Summary

Link to the Web of Science

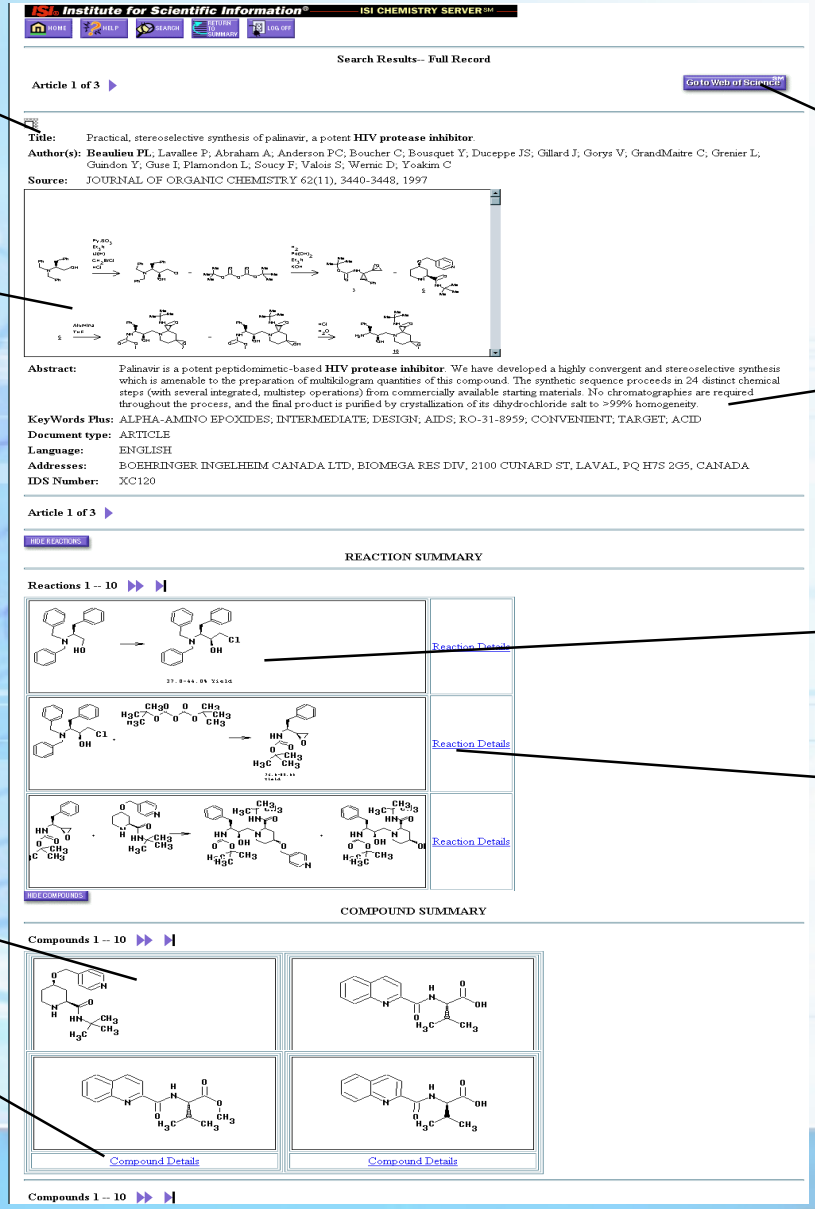
Author Abstract, Address, Keywords

Reaction List

Link to detailed reaction conditions

Compound List

Link to compound information



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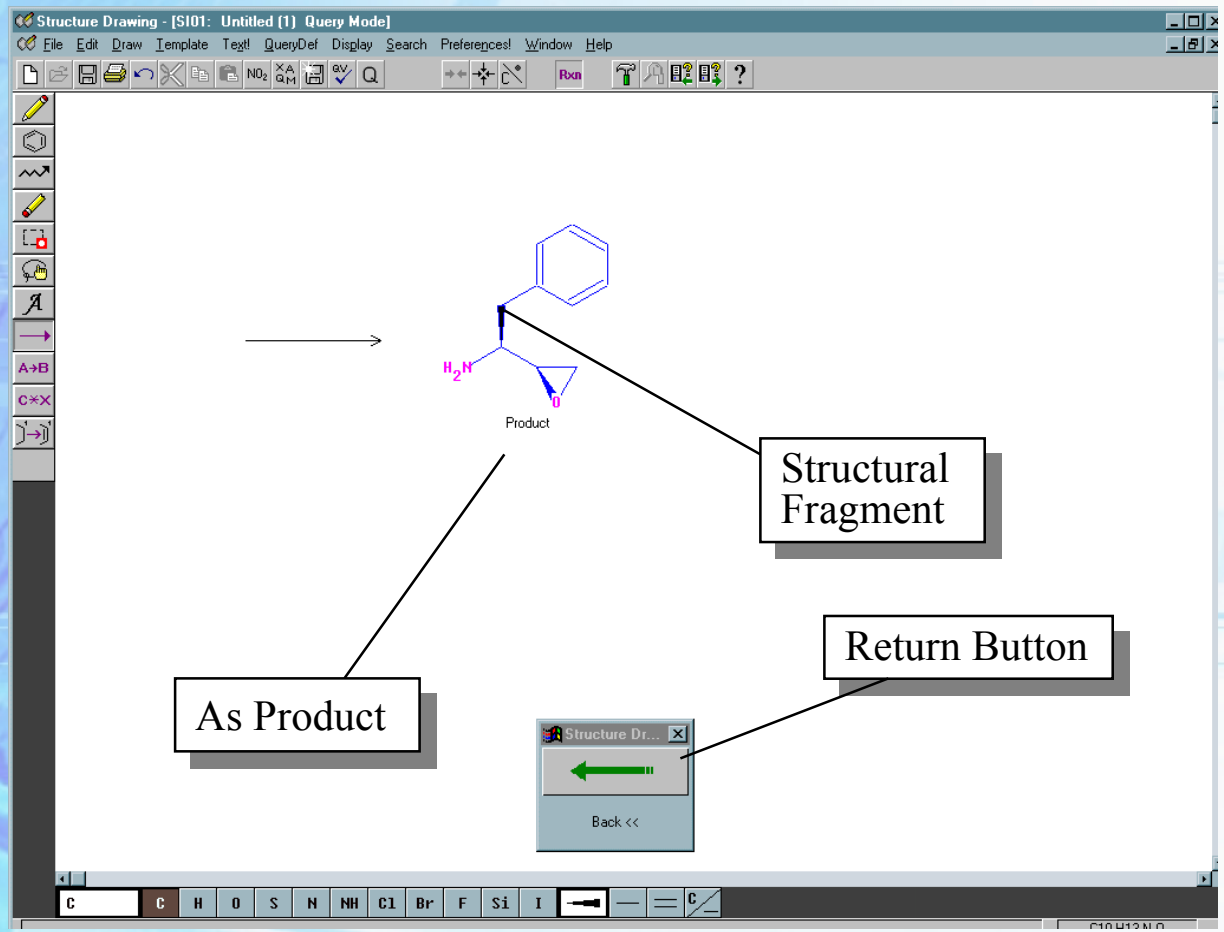
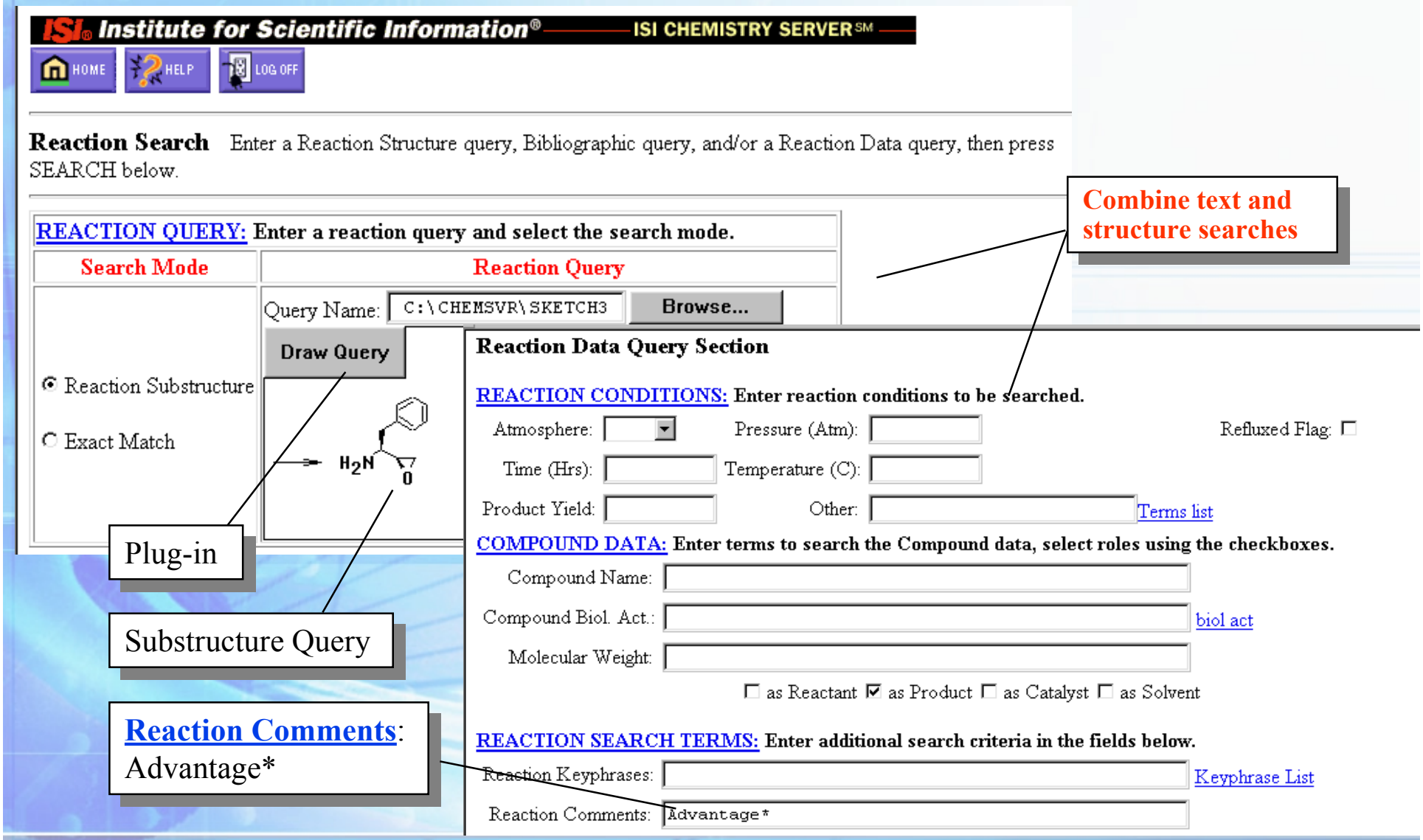
Fully functional structure drawing package



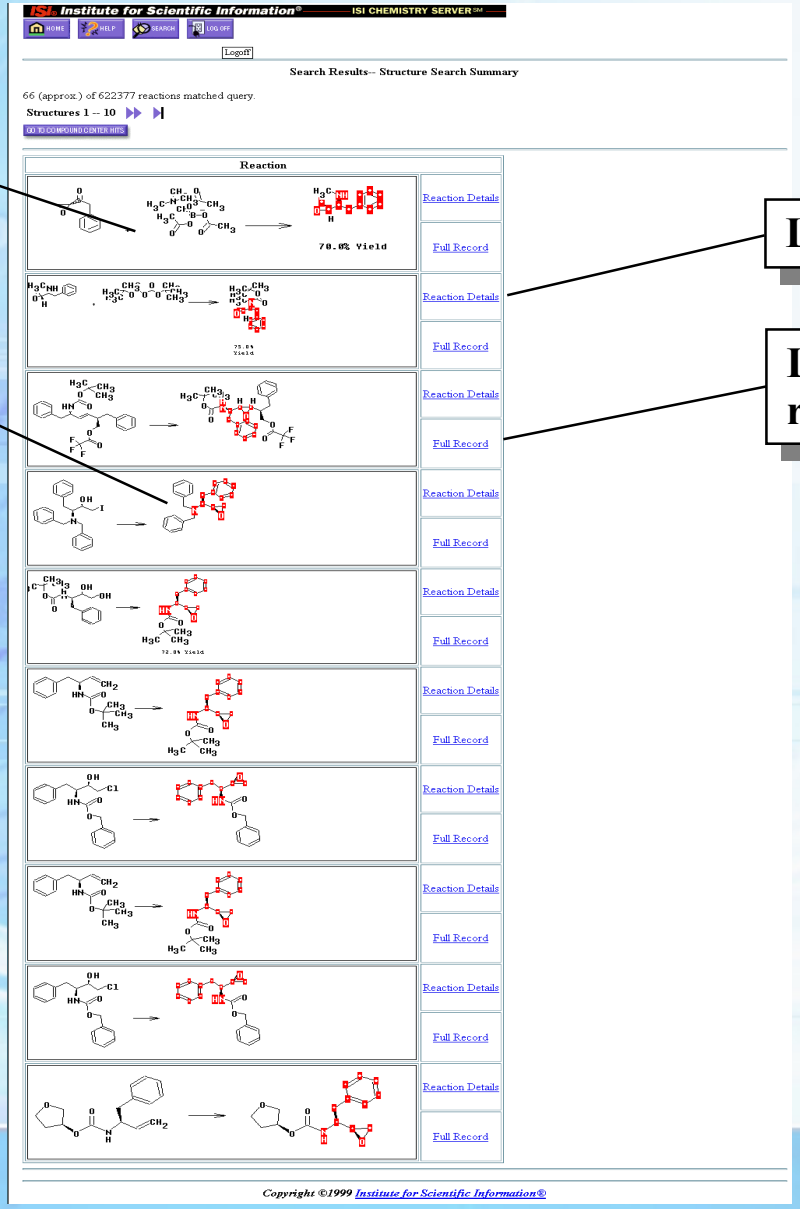
Easily combined searches, with no preset hit limits



Structure Search Summary Screen

Reaction Summary

Initial Query (Red)



Link to Full Record

Link to detailed reaction conditions

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Reaction Details Screen

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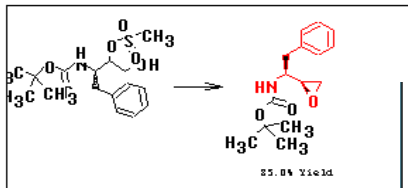
Search Results-- Reaction Details

Green BE; Chen XQ; Norbeck DW; Kempf DJ Convenient synthesis of 1-(S)-(1'-(S)-(t-butyloxycarbonylamino)-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.

INPI Full Record

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Search Results-- Full Record

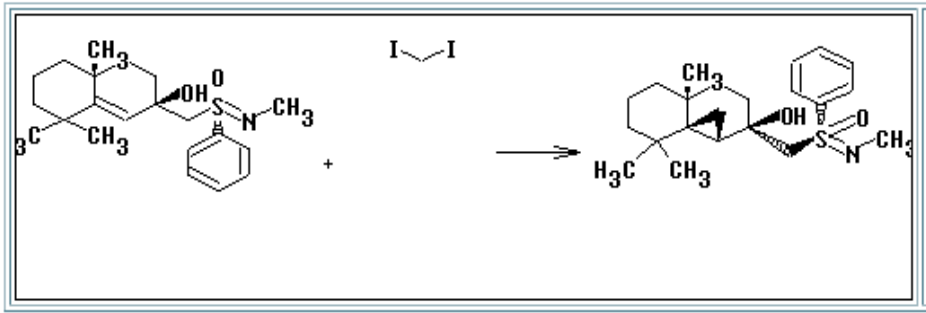
Article 17 of 1319

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



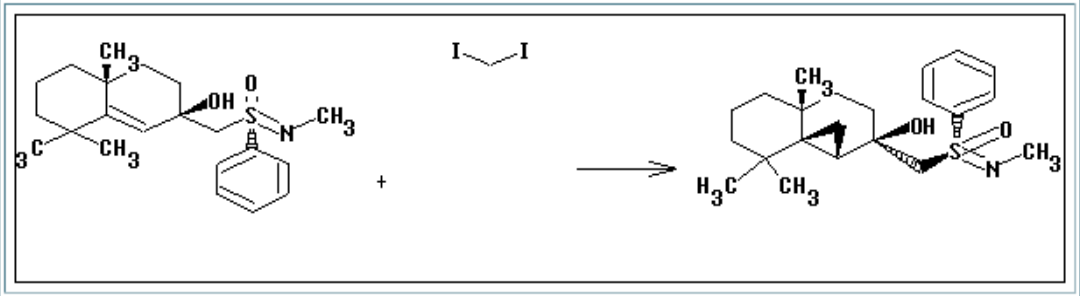
Reaction Details

Reactions 1 -- 1

Search Results-- Reaction Details

JOHNSON CR INPI Reaction

Reaction No:	RCCRB0159001	Path:	A1	Step:	1 Step	KeyRxn:	Yes



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

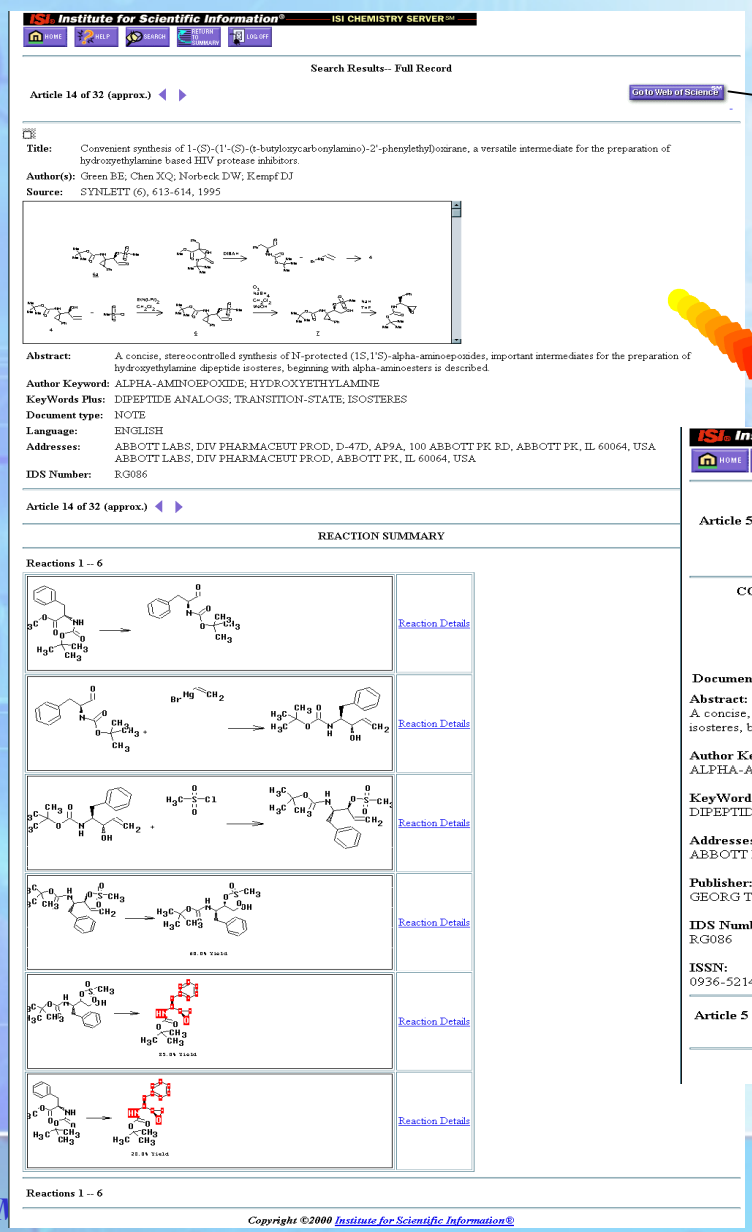
	Symbol	Grade	BioAct	Yield
Reactant(2):	CH2I2			

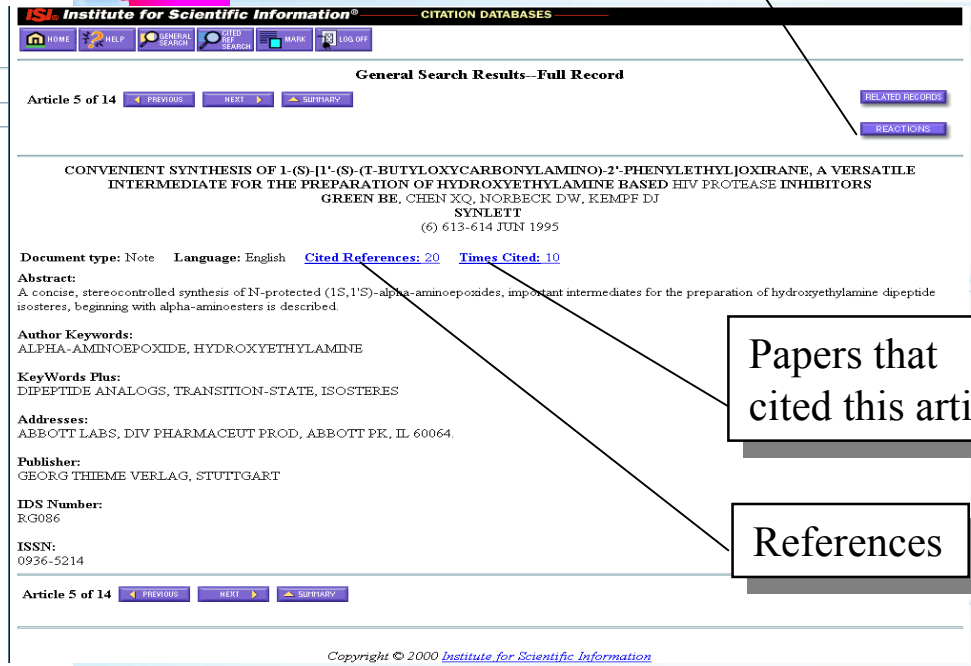
Comments:

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

Direct Linking to the Web of Science





Link to the Web of Science

Link to the Chemistry Server

Papers that cited this article

References

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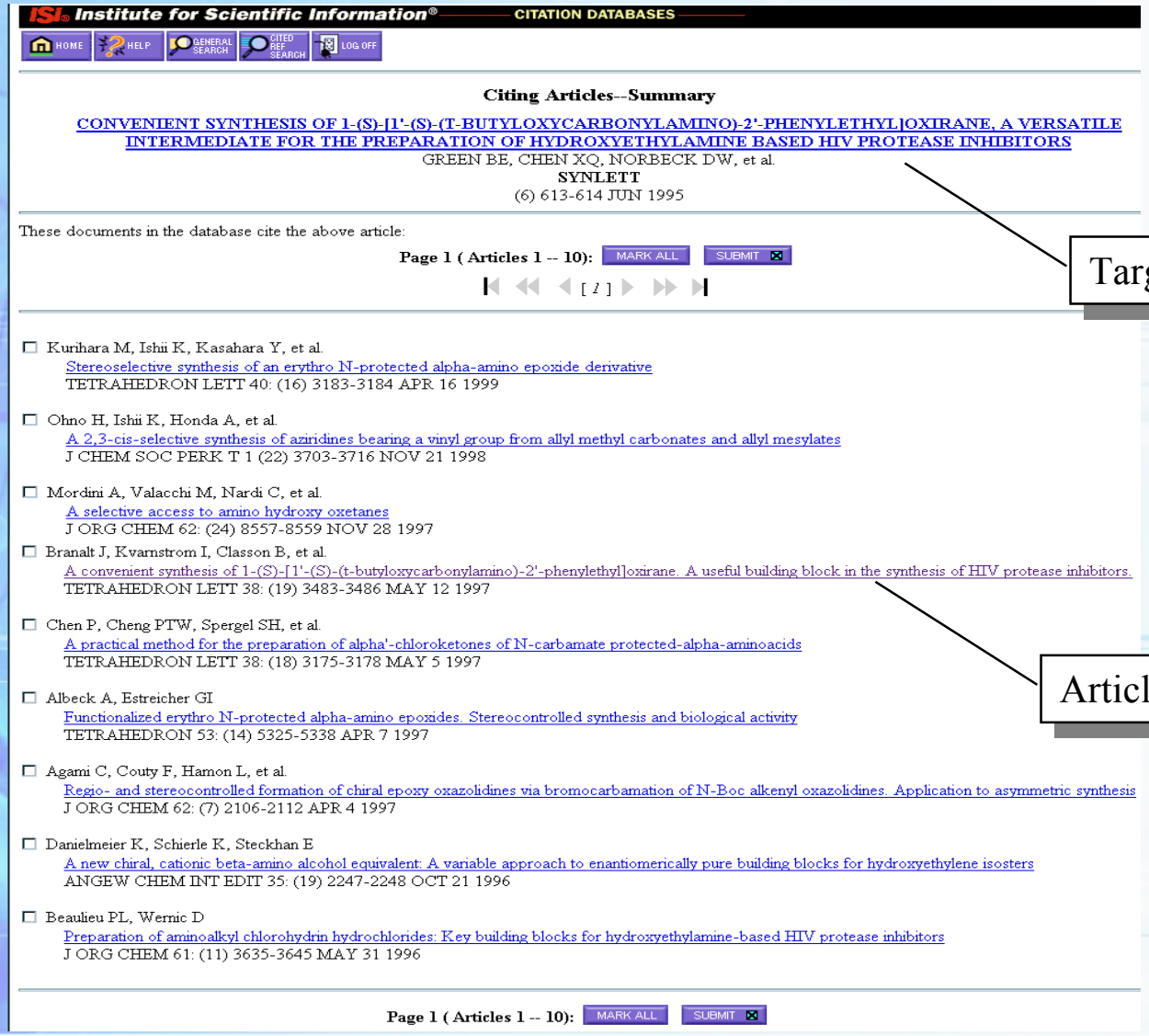
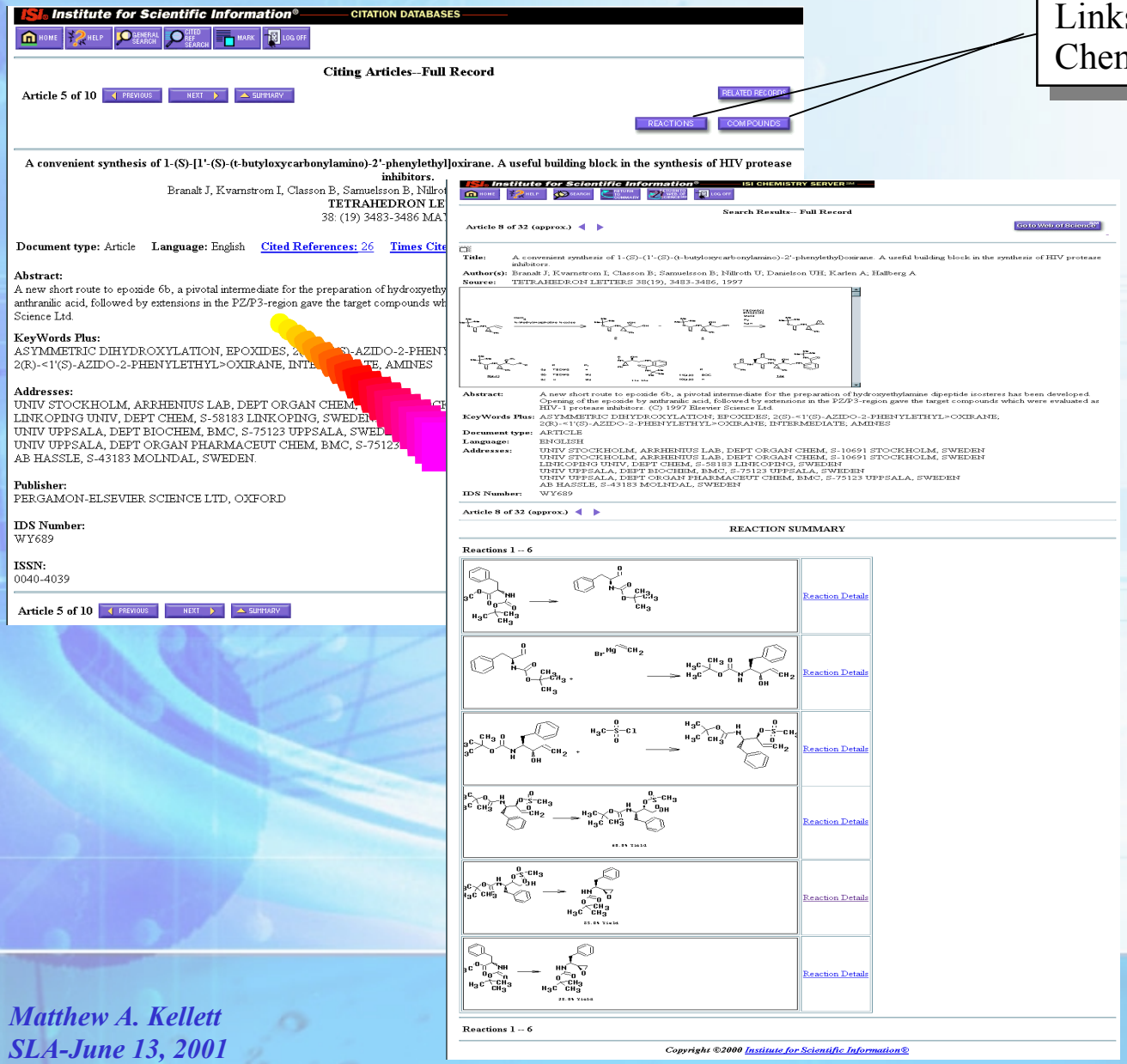
Citation Linking from Web of Science



Citation Linking from Web of Science

Links to the Chemistry Server



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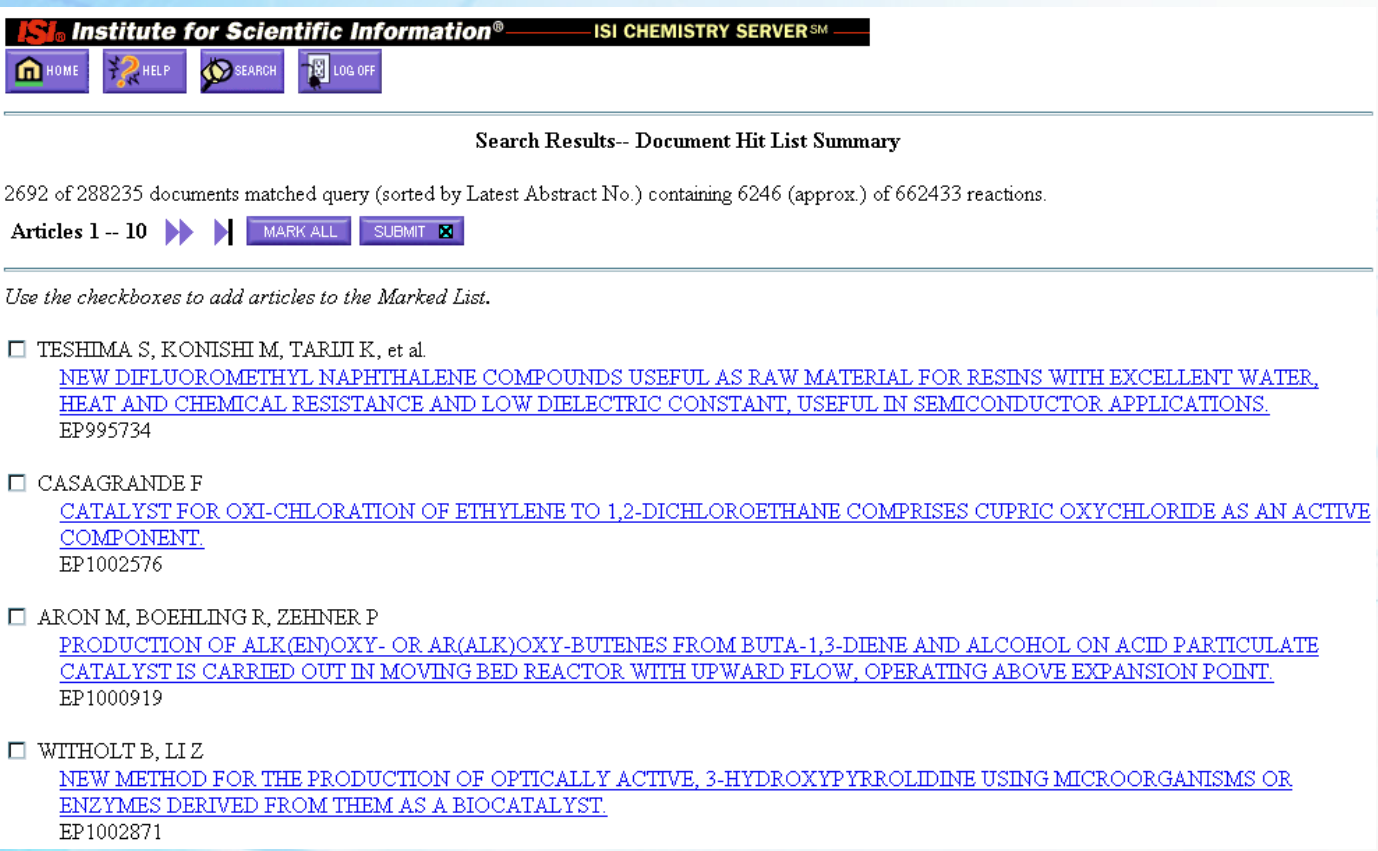
Access to Patent Information in Chemistry Server



Link to additional information in DII via Patent Number

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Search Results-- Full Record

Article 4 of 2692

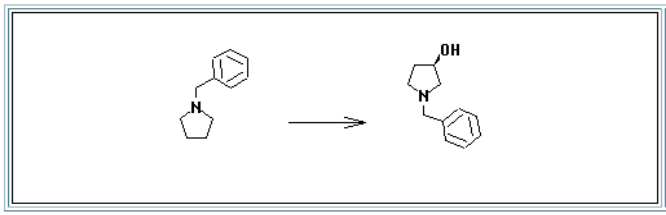
Title:	NEW METHOD FOR THE PRODUCTION OF OPTICALLY ACTIVE, 3-HYDROXYPYRROLIDINE USING MICROORGANISMS OR ENZYMES DERIVED FROM THEM AS A BIOCATALYST.
Author(s):	WITHOLT B; LI Z
Addresses:	EIDGENOESSISCHE TECH HOCHSCHULE ZUERICH
Document type:	PATENT
Source:	EP1002871
Patent Kind:	A1
Patent Date:	5-24-2000
Latest Priority Date:	11-17-1998
Latest Priority Country:	EP
Latest Priority Number:	EP203893

Consistent Patent Number between products

Article 4 of 2692

REACTION SUMMARY

Reactions 1 -- 1



Reaction Details

Reactions 1 -- 1

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General Search

Enter individual search terms, then press SEARCH below.

Set sort option.

SEARCH Search using terms entered below.

TOPIC: Enter terms to find patents based on the title or abstract

☐ Title only

ASSIGNEE: Enter one or more assignee names or codes as XEROX CORP OR XERO

◉ Search name and code ○ Name only ○ Code only

INVENTOR: Enter one or more inventor names as SMITH A* OR JONES D*

PATENT NUMBER: Enter one or more patent numbers as EP797246 OR US5723945-A

EP1002871

DERWENT Innovations Index SM ISI

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General Search Results--Summary Patent Records

Patent Number=ep1002871; Databases= Electrical and Electronic Section, Engineering Section, Chemical Section; Timespan=All Years; (sorted by latest date)

Page 1 (Inventions 1 -- 1): MARK PAGE SUBMIT

[1]

☐ AU200012730-A; **EP1002871-A1**; WO200029606-A1

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

EIDGENOESSISCHE TECH HOCHSCHULE ZUERICH (EIDG-Non-standard)

LI Z, WITHOLT B

Page 1 (Inventions 1 -- 1): MARK PAGE SUBMIT

[1]

DII Full Record Screen

DERWENT Innovations IndexSM

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General Search Results--Full Record

Patent 1 of 1 SHOW DRAWING

Patents Cited by Inventor: 0
Patents Cited by Examiner: 4

Citing Patents: 0

Articles Cited by Inventor: 0
Articles Cited by Examiner: 3

Patent Number(s):
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-0205893	17 Nov 1998
WO200029606-A1	WO-EP09041	15 Nov 1999