DiscoveryGate

One place for the answers you need

Library Connect, Malaysia

Presented by: Doreen Tan
Title: Product Sales Manager, Life Science
Date: 14 July 2005, Thursday

DiscoveryGate

Key Challenge:

Scientific information is scattered and is typically accessed by multiple applications.

The DiscoveryGate Solution

- *Connects* scientists to many information sources, giving them the perspective needed to decide what to do next.
- Integrates, indexes and links the three types of content sources necessary for answering discovery questions
- A single login

Integrated, Indexed, Linked – Content and Services

Primary Literature: Journals & Patents

Secondary Databases

Pharmacology, synthetic methodology, bioactivity, sourcing, ADME/T

Single login & Single search accross a huge chemical index

DiscoveryGate®

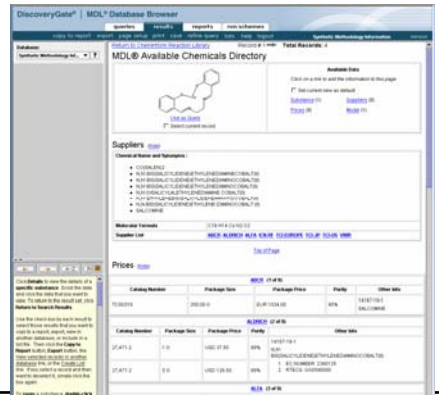
Powerful Administration Environment and Software Deployment

Authoritative Major Reference Works

We handle maintenance, security and support - you can focus on research

Integration, Indexing and Linking

Access to Integrated Content – Single Interface



Chemistry Reference

- CrossFire Beilstein (not indexed in Compound Index)
- CrossFire Gmelin (not indexed in Compound Index)
- MDL Patent Chemistry Database
- OHS Pure Substance MSDS Database
- ISI Index Chemicus

Bioactivity

- MDL Data Drug Report
- MDL Metabolite Database
- MDL Toxicity Database
- National Cancer Institute Databases
- MDL Comprehensive Medicinal Chemistry
- xPharm

Chemical Sourcing and Logistics

- MDL Available Chemicals Directory
- MDL Screening Compounds Directory

Synthetic Methodology

- ChemInform Reaction Library
- Current Synthetic Methodology
- Derwent Journal of Synthetic Methods
- ORGSYN Database
- MDL Solid-Phase Organic Reactions
- MDL Reference Library of Synthetic Methodology
- ISI Current Chemical Reactions
- Integrated Major References Works

Patent sources

- Derwent World Patent Index

- Structures are indexed in Compound Index.
- Hyperlink to 3rd party application to view detailed data

DiscoveryGate 2.0

Faster

- First 12 hits returned as soon as found
- ~8 fold improvement in time to first hits for most searches

Simpler

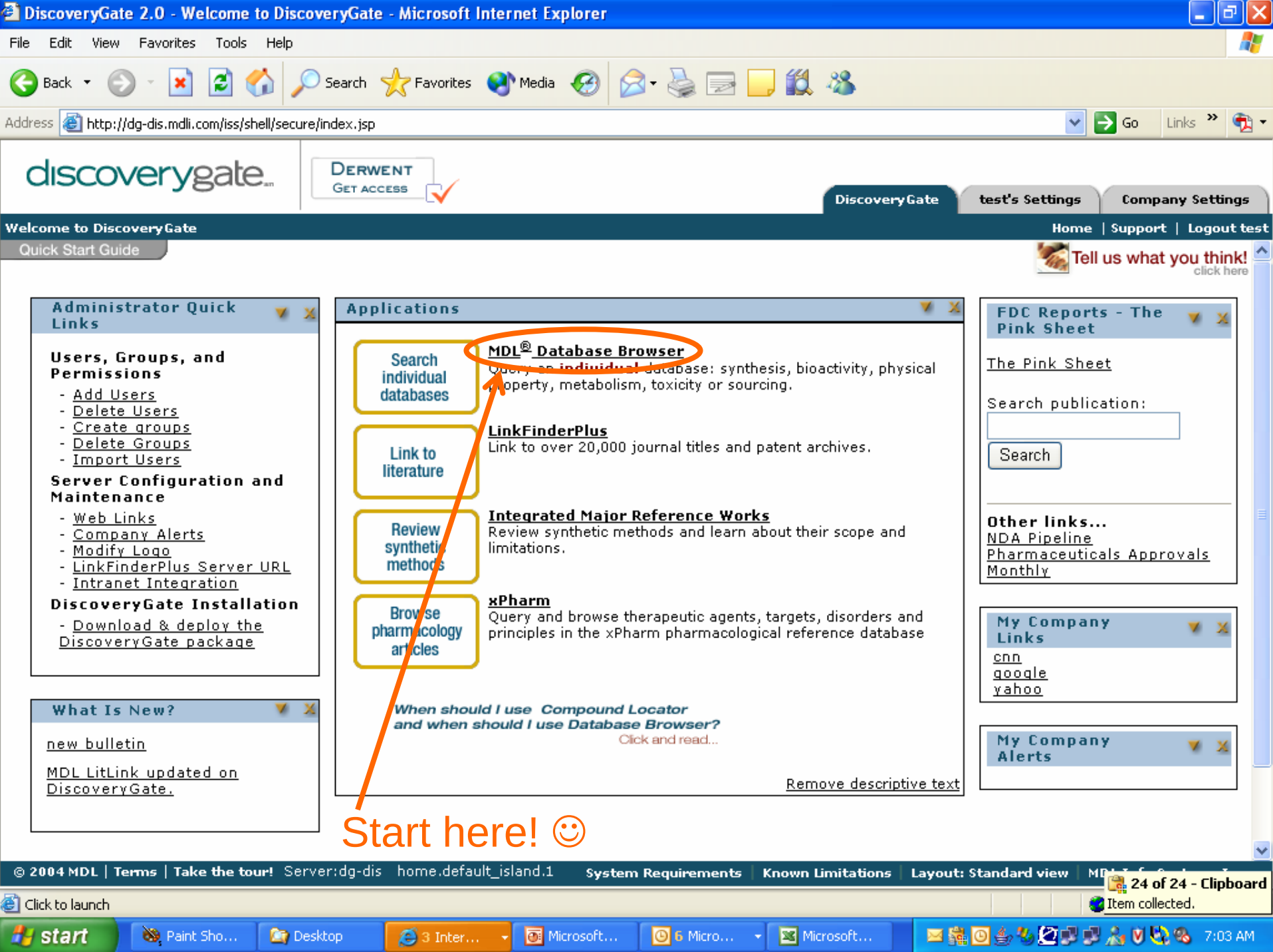
- Fewer windows, fewer clicks
- Retire Compound Locator
- Database pick list as pull down menu in DB Browser

Better Usability

- Exploit Indexed content with “Also Found In” links
- Circumvents need to directly search Compound Index

New Capabilities

- Query highlighting
- Form logic delivers specific queried data
- List handling (save, combine and export/import)
- Export RDFile, table files from all databases
- Grid display of Compound Index searches
- Database View of Compound Index results in DB Browser
- Properties View of Compound Index results in DB Browser


DiscoveryGate 2.0 - Welcome to DiscoveryGate - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites Media
Address http://dg-dis.mdli.com/iss/shell/secure/index.jsp
Go Links
discoverygate
DERWENT GET ACCESS
DiscoveryGate
test's Settings
Company Settings
Welcome to DiscoveryGate
Home | Support | Logout test
Quick Start Guide
Tell us what you think! click here
Administrator Quick Links
Users, Groups, and Permissions
- Add Users
- Delete Users
- Create groups
- Delete Groups
- Import Users
Server Configuration and Maintenance
- Web Links
- Company Alerts
- Modify Logo
- LinkFinderPlus Server URL
- Intranet Integration
DiscoveryGate Installation
- Download & deploy the DiscoveryGate package
What Is New?
new bulletin
MDL LitLink updated on DiscoveryGate.
Applications
Search individual databases
MDL® Database Browser
Query an individual database: synthesis, bioactivity, physical property, metabolism, toxicity or sourcing.
Link to literature
LinkFinderPlus
Link to over 20,000 journal titles and patent archives.
Review synthetic methods
Integrated Major Reference Works
Review synthetic methods and learn about their scope and limitations.
Browse pharmacology articles
xPharm
Query and browse therapeutic agents, targets, disorders and principles in the xPharm pharmacological reference database
When should I use Compound Locator and when should I use Database Browser?
Click and read...
Remove descriptive text
Start here! ☺
FDC Reports - The Pink Sheet
The Pink Sheet
Search publication:
Search
Other links...
NDA Pipeline
Pharmaceuticals Approvals Monthly
My Company Links
cnn
google
yahoo
My Company Alerts
© 2004 MDL | Terms | Take the tour! Server:dg-dis home.default_island.1 System Requirements | Known Limitations | Layout: Standard view
24 of 24 - Clipboard
Item collected.
Click to launch
start
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3 Inter...
Microsoft...
6 Micro...
Microsoft...
7:03 AM

MDL Database Browser - Microsoft Internet Explorer

DiscoveryGate® | MDL® Database Browser

queries | results | reports | rxn schemes

start search | import | save | clear query | help | logout | CrossFire Beilstein | Version

Database:

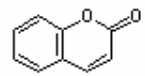
CrossFire Beilstein ?

- CrossFire Beilstein
- CrossFire Gmelin
- MDL® Patent Chemistry Database
- MDL® Compound Index
- MDL® Comprehensive Medicinal Chem
- MDL® Drug Data Report
- National Cancer Institute Database
- Chemical Sourcing and Logistics Inform
- MDL® Available Chemicals Directory
- MDL® Screening Compounds Director
- Synthetic Methodology Information
- ChemInform Reaction Library
- Current Synthetic Methodology
- Derwent Journal of Synthetic Methods
- ORGSYN Database
- MDL® Reference Library of Synthetic M
- MDL® Solid-Phase Organic Reactions
- MDL® Metabolite Database
- MDL® Toxicity Database
- OHS Database
- Derwent World Patents Index
- IC Database
- CCR Database

Drop down pick list for changing database to search

Structure

Find this compound and its properties



Query Highlighting

- Substitution as drawn, exclude tautomers
- Substitution as drawn, include tautomers
- Unlimited substitution on all atoms, exclude tautomers

Allow:
- Multi-component substances
- Ring closure through substitution
- Isotopes Charges Radicals
- Keep fragments separate

Search Stereoinformation: As drawn

Reset Delete Info

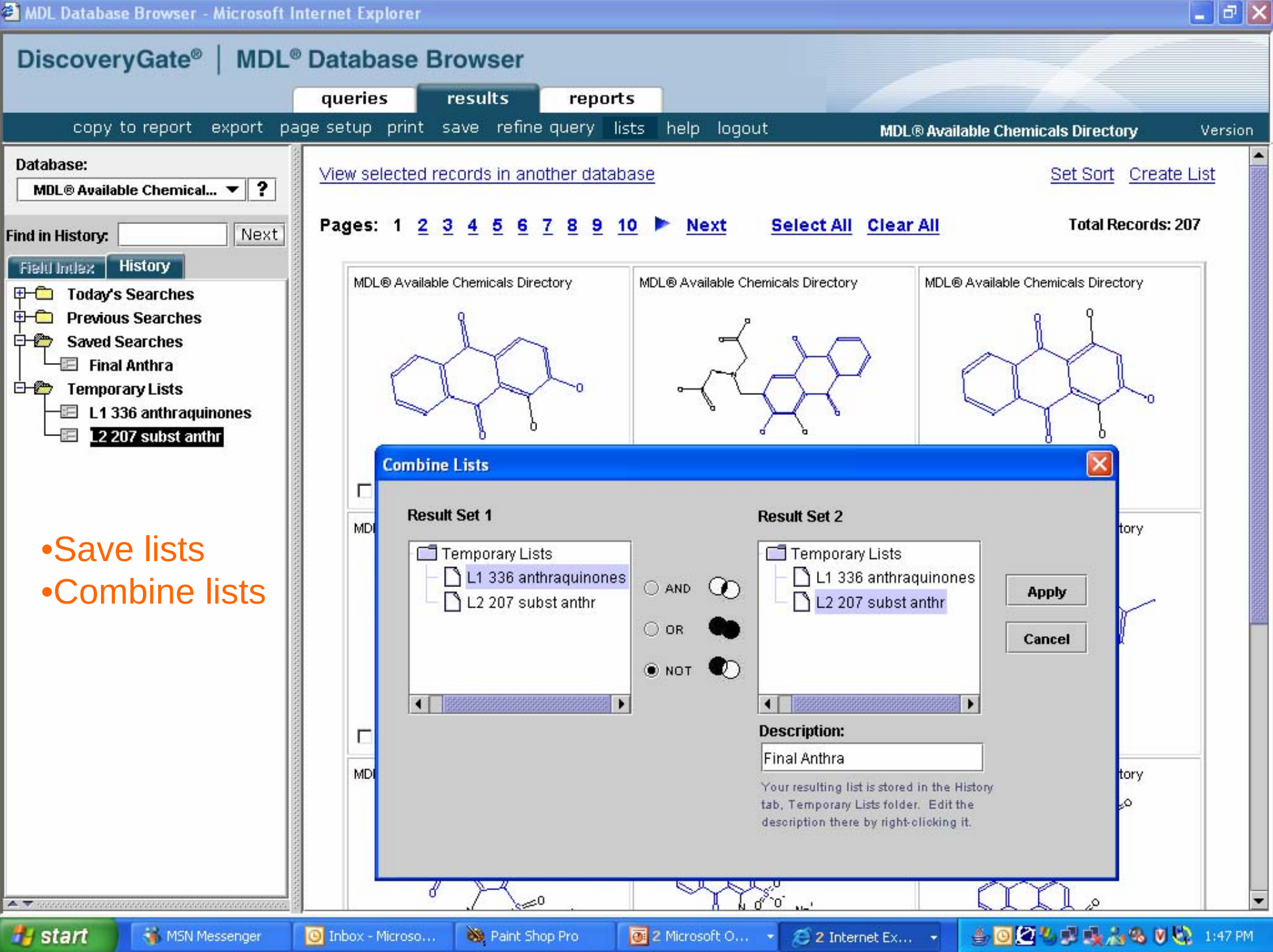
AND | Pharmacological data exists | Delete Duplicate Info

Pharmacological Data

AND	Effect	Contains	genetic tox (Data Lookup...)	Delete Duplicate Info
AND	Species	Contains	mouse (Data Lookup...)	Delete Duplicate Info
AND	Route of Application	Contains	(Data Lookup...)	Delete Duplicate Info
AND	Type (IC50, LD50)	Contains	(Data Lookup...)	Delete Duplicate Info

start search

start | MSN Messenger | Inbox - Microso... | Paint Shop Pro | 2 Microsoft O... | 2 Internet Ex... | 1:35 PM


MDL Database Browser - Microsoft Internet Explorer
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queries
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logout
MDL® Available Chemicals Directory
Version
Database:
MDL® Available Chemical...
Find in History:
Next
Field Index
History
Today's Searches
Previous Searches
Saved Searches
Final Anthra
Temporary Lists
L1 336 anthraquinones
L2 207 subst anthr
View selected records in another database
Set Sort
Create List
Pages: 1 2 3 4 5 6 7 8 9 10
Next
Select All
Clear All
Total Records: 207
MDL® Available Chemicals Directory
MDL® Available Chemicals Directory
MDL® Available Chemicals Directory
Combine Lists
Result Set 1
Temporary Lists
L1 336 anthraquinones
L2 207 subst anthr
AND
OR
NOT
Result Set 2
Temporary Lists
L1 336 anthraquinones
L2 207 subst anthr
Apply
Cancel
Description:
Final Anthra
Your resulting list is stored in the History tab, Temporary Lists folder. Edit the description there by right-clicking it.
•Save lists
•Combine lists
start
MSN Messenger
Inbox - Microso...
Paint Shop Pro
2 Microsoft O...
2 Internet Ex...
1:47 PM

MDL Database Browser - Microsoft Internet Explorer

DiscoveryGate® | MDL® Database Browser

queries | results | reports | rxn schemes

copy to report | export | page setup | print | save | refine query | lists | help | logout | ORGSYN Database | Version

Database: ORGSYN Database ?

Find in History: Next

Field Index | History

- Today's Searches
  - Search #1
  - Search #2
  - Search #3
  - Search #4
  - Search #5
- Previous Searches
  - Feb 13, 2005
- Saved Searches
- Temporary Lists

Indexed databases linked based on common structures

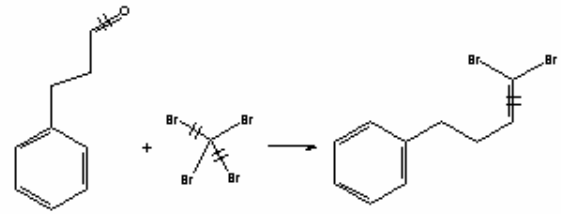
Return to Search Results | View selected records in another database | Find Similar Reactions | Record #

1 **Total Records:** 1

Also found in: ACD SCD TOX NCI CSM DJSM METAB REFLIB SPORE CIRX OHSPURE DWPI IC CCR

Commercial availability

ORGSYN Database



Use as Query

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

Reaction Details (1) Reactant (2) Product (1)

Reaction Details (hide)

RORG00175674 **Reaction Variation 1 of 1**

Product no.	% Yield	Grade	%cs	%ds	%de	%ee
1	96	34.75 g				

Reactant no.	Reactant Grade
1	16.4 mL, 16.7 g, 124.3 mmol
2	82.46 g, 248.64 mmol

Step no.	Catalysts and Solvents	Catalyst ID click ID for details	Solvent ID click ID for details

start | MSN Messenger | Inbox - Micro... | Paint Shop Pro | 2 Microsoft ... | 2 Internet E... | 1:58 PM

MDL Database Browser - Microsoft Internet Explorer

DiscoveryGate® | MDL® Database Browser

queries | results | reports | rxn schemes

copy to report | export | page setup | print | save | refine query | lists | help | logout | ORGSYN Database | Version

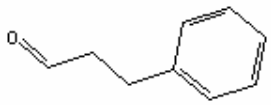
Database: ORGSYN Database ?

View Supplier data for reaction components with a single click!

Return to reaction Db with another click

Return to ORGSYN Record # 3 **Total Records:** 3

MDL® Available Chemicals Directory



Use as Query

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

Substance (1) Suppliers (27)

Prices (27) Model (1)

Prices (hide)

ABCR (1 of 27)

Catalog Number	Package Size	Package Price	Purity	Other Info
AV10367	50.00 G	EUR 14.90	97%	104-53-0 3-PHENYLPROPIONALDEHYDE 1. EINECS: 203-211-8
AV10367	250.00 G	EUR 63.20	97%	
AV10367	1.00 KG	EUR 210.80	97%	

ACROS (2 of 27)

Catalog Number	Package Size	Package Price	Purity	Other Info
24051-0050	5 G	USD 16.80	95%	104-53-0 3-PHENYLPROPIONALDEHYDE 1. AIR SENSITIVE 2. AVAILABLE IN USA AND EUROPE 3. EINECS: 203-211-8 4. RTECS: MW4890000
24051-1000	100 G	USD 57.50	95%	

start | MSN Messenger | 3 Microsoft ... | Paint Shop Pro | 2 Microsoft ... | 2 Internet E... | 2:55 PM

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queries | results | reports | rxn schemes

copy to report | export | page setup | print | save | refine query | lists | help | logout | ORGSYN Database | Version

Database: ORGSYN Database ?

Find in History: Next

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- Today's Searches
  - Search #1
  - Search #2
  - Search #3
  - Search #4
  - Search #5
- Previous Searches
  - Feb 13, 2005
- Saved Searches
- Temporary Lists

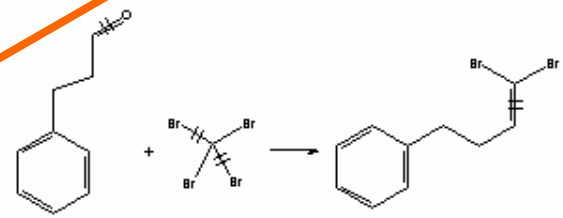
"Find similar reactions" links synthetic methods across all content

Return to Search Results | View selected records in another database | Find Similar Reactions | Record #

1 **Total Records:** 1

Also found in: ACD | SCD | TOX | NCI | CSM | DJSM | METAB | REFLIB | SPORE | CIRX | OHSPURE | DWPI | IC | CCR

ORGSYN Database



Use as Query

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

Reaction Details (1) | Reactant (2) | Product (1)

Reaction Details (hide)

RORG00175674 **Reaction Variation 1 of 1**

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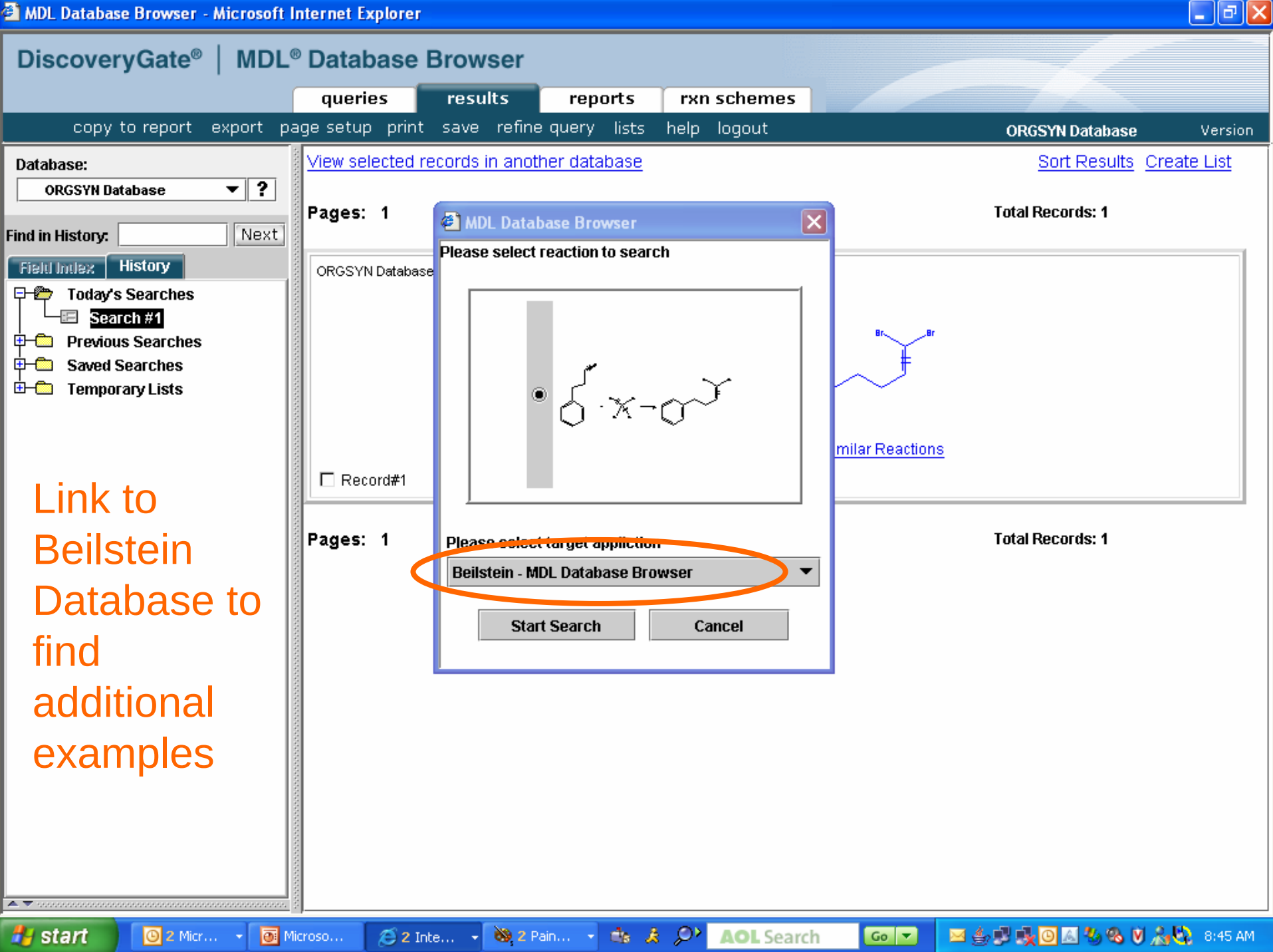
start | MSN Messenger | Inbox - Micro... | Paint Shop Pro | 2 Microsoft ... | 2 Internet E... | 1:58 PM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Temporary Lists
View selected records in another database
Sort Results
Create List
Pages: 1
Total Records: 1
ORGSYN Database
Record#1
milar Reactions
MDL Database Browser
Please select reaction to search
Please select target application
Beilstein - MDL Database Browser
Start Search
Cancel
Pages: 1
Total Records: 1
Link to Beilstein Database to find additional examples
start
AOL Search
Go
8:45 AM

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queries | results | reports | rxn schemes

copy to report | export | page setup | print | save | refine query | lists | help | logout

MDL® Patent Chemistry Database Version

Database: MDL® Patent Chemistry ...

Find in History: Next

Field Index | History

- Today's Searches
  - Search #1
  - Search #2
  - Search #3
- Previous Searches
- Saved Searches
- Temporary Lists

Markush structures included in patent records

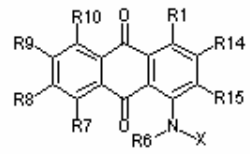
Patent-Specific Data (hide)

Patent-Specific Data record 1 of 2	
Citation Number	670
Citation	Patent; Ciba Specialty Chemicals Corporation; Publ.: US6355783 B1 (2002/03/12), Appl.: US2000-735081 (2000/09/07)
Compound Status in Patent	prophetic product
Entry Date	2003/12/24

Patent-Specific Data record 2 of 2	
Citation Number	253839
Citation	Patent; UNTEGRATED DNA TECHNOLOGIES, INC.; Publ.: WO2004/26804 A1 (2004/04/01), Appl.: WO2003-US29324 (2003/09/19)
Related Markush Structure (PRN)	3818074
Entry Date	2004/08/20

Top of Page

Related Markush Structure 3818074 (hide)



Label	Value	Size	Attributes	Substituted by	Frequency
R1	R15				

start | MSN Messenger | 3 Microsoft ... | Paint Shop Pro | 2 Microsoft ... | 2 Internet E... | 3:29 PM

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queries | results | reports

copy to report | export | page setup | print | save | refine query | lists | help | logout

MDL® Compound Index Version

Database: MDL® Compound Index ?

Find in History: Next

Field Index | History

- Today's Searches
- Previous Searches
- Saved Searches
- Temporary Lists

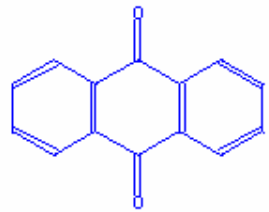
Compound Index Searched using Database Browser

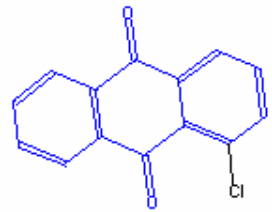
Grid view of results

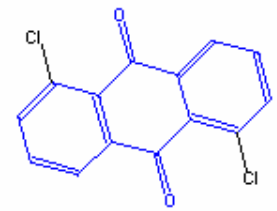
Grid View | Database View | Properties View | Create List

View selected records in another database

Pages: 1 ▶ Next | Select All | Clear All | Total Records: Get Count


Details
Record#1


Details
Record#2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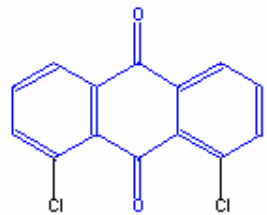
Record#3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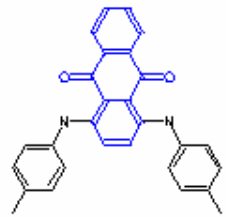
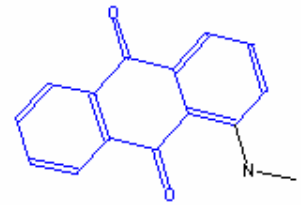
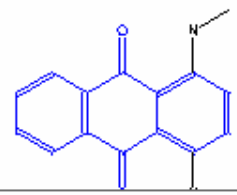
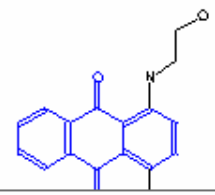
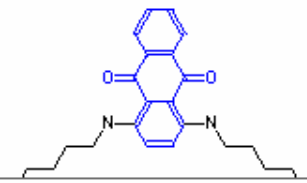

Details
Record#5


Details
Record#6







start | MSN Messenger | 3 Microsoft ... | Paint Shop Pro | 2 Microsoft ... | 2 Internet E... | 3:15 PM

MDL Database Browser - Microsoft Internet Explorer

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queries | results | reports

copy to report | export | page setup | print | save | refine query | lists | help | logout

MDL® Compound Index Version

Database: MDL® Compound Index ?

Find in History: Next

Field Index | History

- Today's Searches
- Previous Searches
- Saved Searches
- Temporary Lists

Compound Index Searched using Database Browser

Database view

Click to see row summary

Grid View | Database View | Properties View

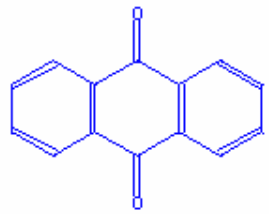
Create List

View selected records in another database

Pages: 1 ▶ Next Select All Clear All

Total Records: Get Count

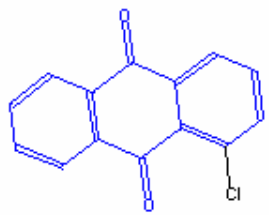
1



Select Record # 1

CIRX CSM
DJSM DWPI
ACD Metabolite
REFLIB SCD
Toxicity NCI
OHS MSDS ORGSYN
CCR

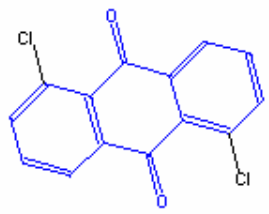
2



Select Record # 2

CIRX CSM
DJSM DWPI
ACD REFLIB
SCD Toxicity
NCI ORGSYN
CCR

3



Select Record # 3

CIRX CSM
ACD SCD
Toxicity NCI
OHS MSDS CCR

start | MSN Messenger | 3 Microsoft ... | Paint Shop Pro | 2 Microsoft ... | 2 Internet E... | 3:22 PM

Database:

MDL® Compound Index ?

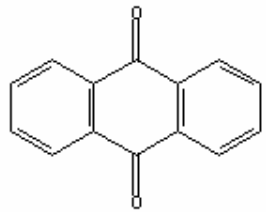
Click through databases to see all relevant data for indexed record

Return to Compound Index

CCR CIRX DJSM DWPI METAB NCI OHSPURE ORGSYN REFLIB SCD TOX

Record # 1 → **Total Records:** 308

MDL® Available Chemicals Directory



Use as Query

Select current record

Available Data

Click on a link to add the information to this page

Set current view as default

Substance (1) Suppliers (38)

Prices (38) Model (1)

Substance (hide)

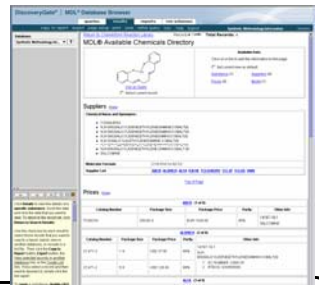
ACD Registry Number	1153
MDL Number	MFCD00001188
CAS Registry Number	84-65-1

Chemical Name and Synonyms :

- 'LGC' (1601)
- 'LGC' (2410)
- 9,10-ANTHRAQUINONE
- 9,10-DIHYDRO-9,10-ANTHRACENEDIONE
- 9,10-DIOXOANTHRACENE
- ALPHA RAXIL CA
- ANTHRAQUINONE
- CORBIT
- CORBIT(R)
- GAUCHO BLE
- MORKIT

Linking from Scopus into CrossFire Commander

From Scopus to CrossFire Commander



Chemistry Reference
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- CrossFire Gmelin (not indexed in Compound Index)
- MDL Patent Chemistry Database
- OHS Pure Substance MSDS Database
- ISI Index Chemicus

Bioactivity
- MDL Data Drug Report
- MDL Metabolite Database
- MDL Toxicity Database
- National Cancer Institute Databases
- MDL Comprehensive Medicinal Chemistry
- xPharm

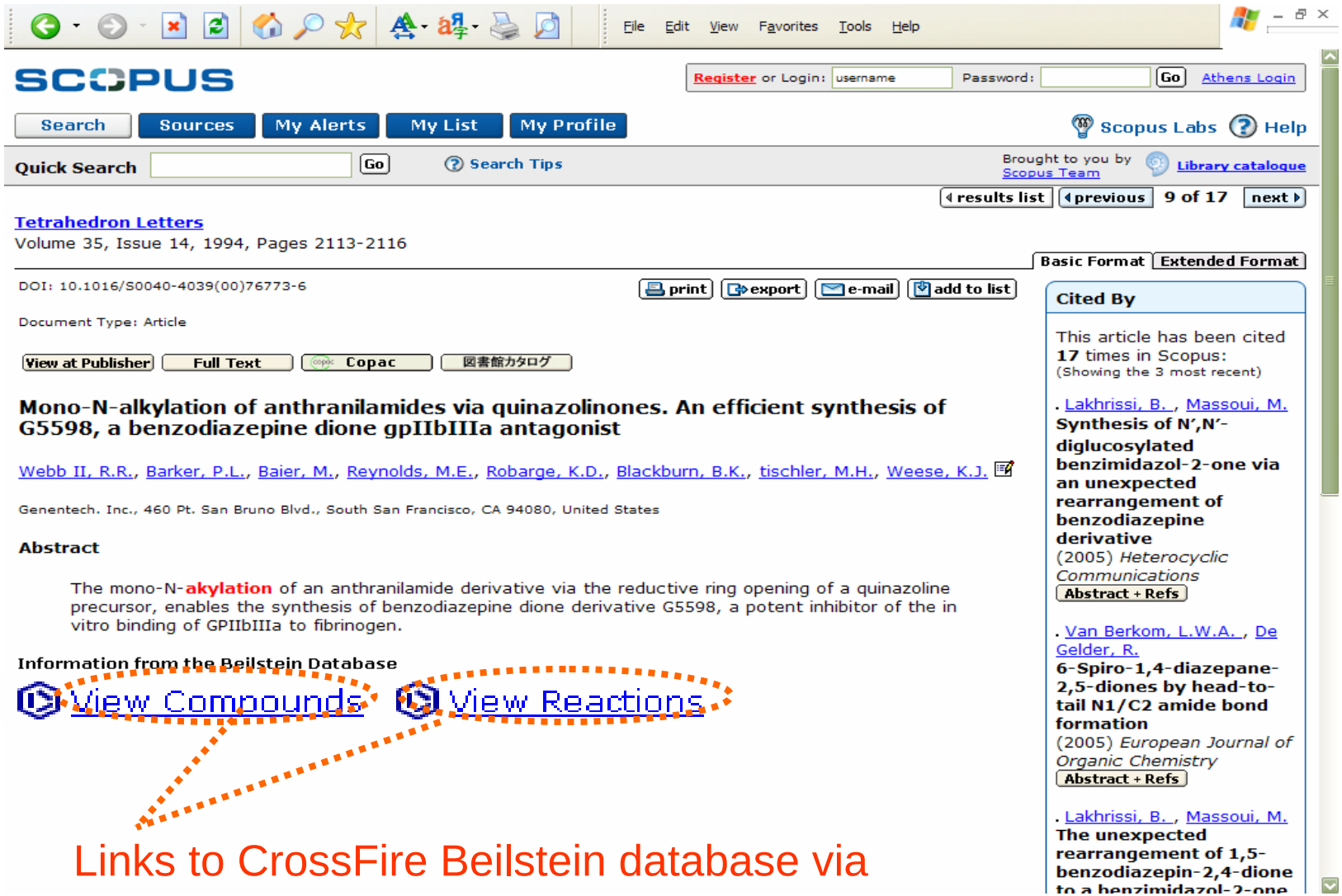
Chemical Sourcing and Logistics
- MDL Available Chemicals Directory
- MDL Screening Compounds Directory

Synthetic Methodology
- ChemInform Reaction Library
- Current Synthetic Methodology
- Derwent Journal of Synthetic Methods
- ORGSYN Database
- MDL Solid-Phase Organic Reactions
- MDL Reference Library of Synthetic Methodology
- ISI Current Chemical Reactions
- Integrated Major References Works

Patent sources
- Derwent World Patent Index

Accessible via CrossFire Commander as well.

From Scopus to CrossFire Commander



Links to CrossFire Beilstein database via CrossFire Commander

From Scopus to CrossFire Commander:

Compound Summary Page

http://scopus-ls.mdli.com - Scopus - Chemical Compounds - Microsoft Internet Explorer

The following information is from th

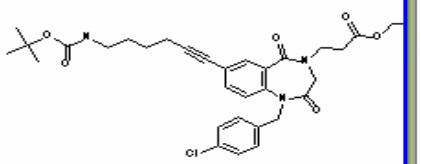
Webb, Robert R., II; Barker, Peter L

Mono-N-Alkylation of Anthranyla
Benzodiazepine Dione GpIIbIIIa A

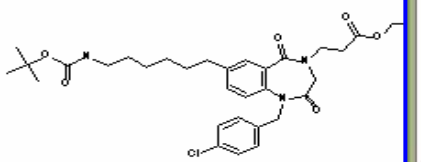
1994, *Tetrahedron Lett.*, **35** (14), p

49 Chemical Compounds View re

1.



2.



http://scopus-ls.mdli.com - Scopus - Chemical Compounds - Microsoft Internet Explorer

The following information is from the Beilstein Database ©

Help close

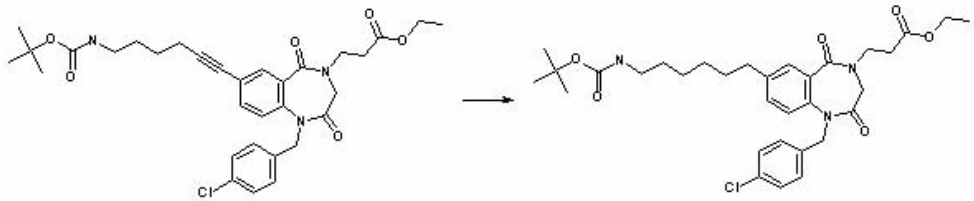
Webb, Robert R., II; Barker, Peter L.; Baier, Mark; Reynolds, Mark E.; Robarge, Kirk D.; et al.

Mono-N-Alkylation of Anthranylamides via Quinazolinones. An Efficient Synthesis of G5598, A Benzodiazepine Dione GpIIbIIIa Antagonist

1994, *Tetrahedron Lett.*, **35** (14), pp. 2113-2116

32 Chemical Reactions View compounds (49) Results 1 to 32

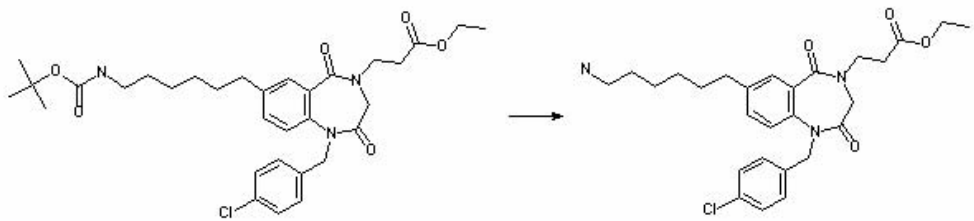
1.



Reaction number	Reaction conditions
3689284	H2 PtO2 ethanol

For more information access the Beilstein Database via:
CrossFire Commander

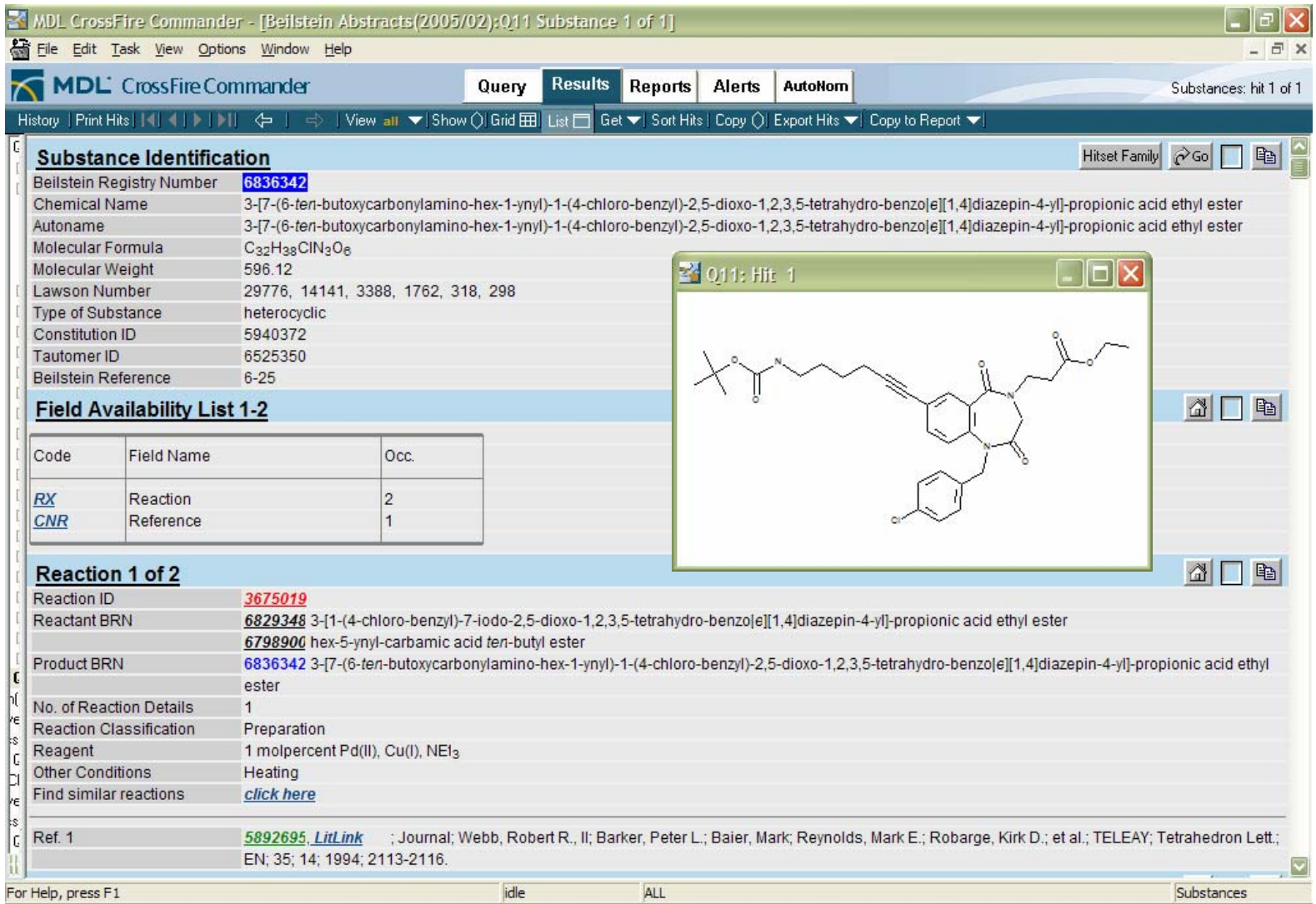
2.



Done Internet

MDL

View Full Record in CrossFire Commander



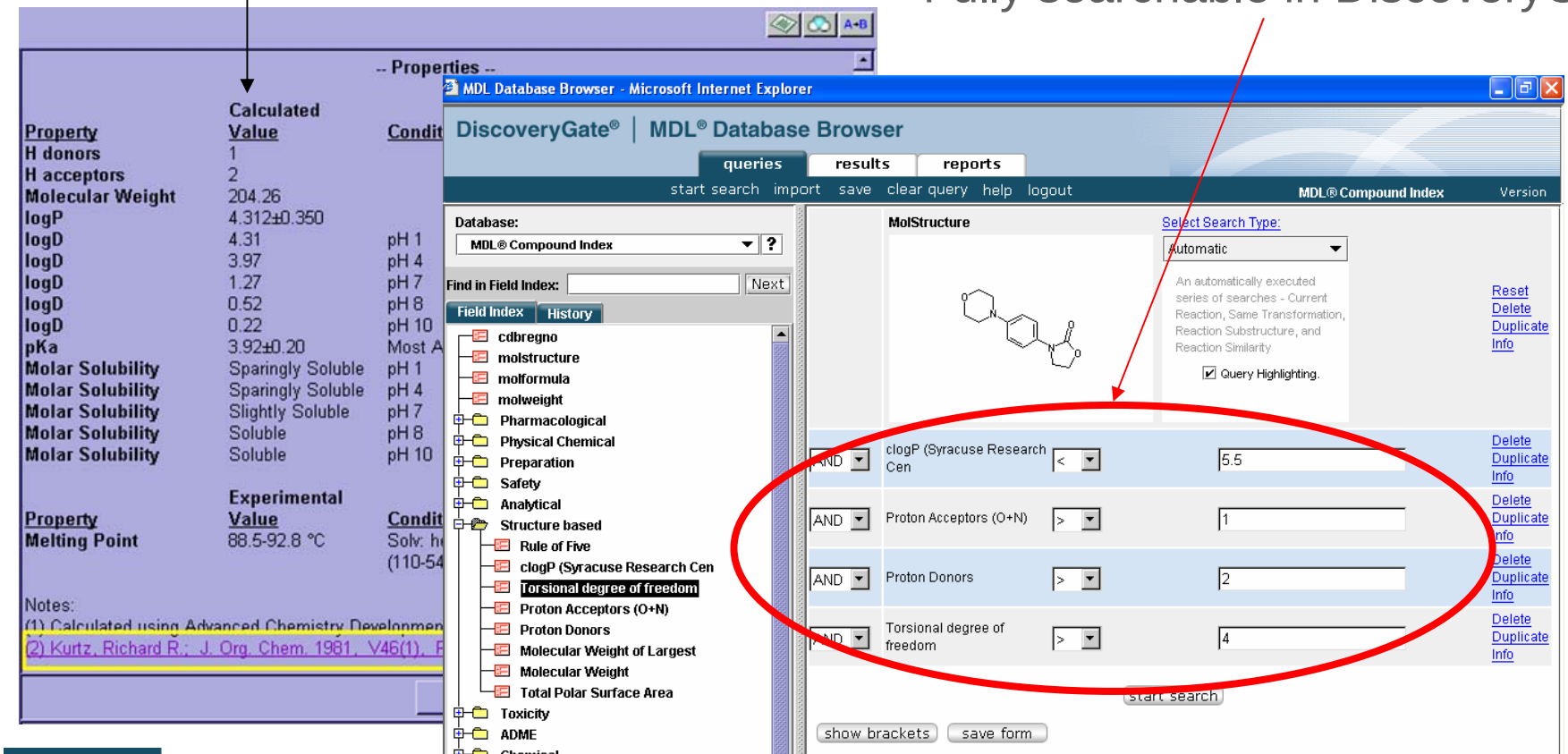
Benefits for the Information Specialist

- Factual data is searchable in DiscoveryGate
  - SciFinder displays static properties tables
- More than150,000,000 explicitly searchable data records
- Used to find and compare facts from multiple literature or patent records

Benefits for the Information Specialist

SciFinder property data not searchable

Fully searchable in DiscoveryGate



SciFinder: See data of interest *if* you find relevant records
DiscoveryGate: *Use* data of interest *to* find relevant records

Benefits for the Information Specialist

- DiscoveryGate is used in daily workflows to solve problems
  - SciFinder provides pointers to literature

- DiscoveryGate solutions include
  - Chemical Sourcing and Safety
  - Chemical Properties
  - Chemical Synthesis
  - Pharmacology and Bioactivity
  - Major Reference Works

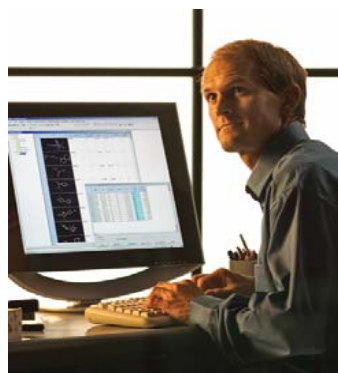
- DiscoveryGate Indexes and links to third party databases
  - Derwent, ISI, Springer, Thieme

Benefits for the IT Specialist

- DiscoveryGate has powerful, easy to use administration tools
  - Access to DiscoveryGate content is configurable
  - Assign data sources to specific user groups
  - Secure online administration interface

- DiscoveryGate eases IT burden
  - No server needed
  - No database maintenance or updates

- DiscoveryGate integrates with local applications and 3rd party vendors
  - Internal applications- Send-to, Hop-into, and ClassCodes
  - Derwent, ISI, Springer, Thieme



Benefits for Research Management

- DiscoveryGate offers more information for your dollar
  - Unlimited usage with annual per user pricing
- DiscoveryGate provides the big picture – better decision making
  - Can create compound profiles. Not able to do this with SciFinder
- DiscoveryGate maps to scientist's workflows
  - From lead identification to synthesis planning to ADME/Tox
- Easily get the information you need from DiscoveryGate
  - Fewer applications to access scientific content
  - No need to learn multiple systems
  - Mine unfamiliar data sources without training
  - Simple queries lead to clear picture of related information

DiscoveryGate in 2005

MDL Elsevier's Life Science Portal Is Now

→ Easier to install and setup

→ Easier to use

→ Faster

Averages 8 times faster to see first hits

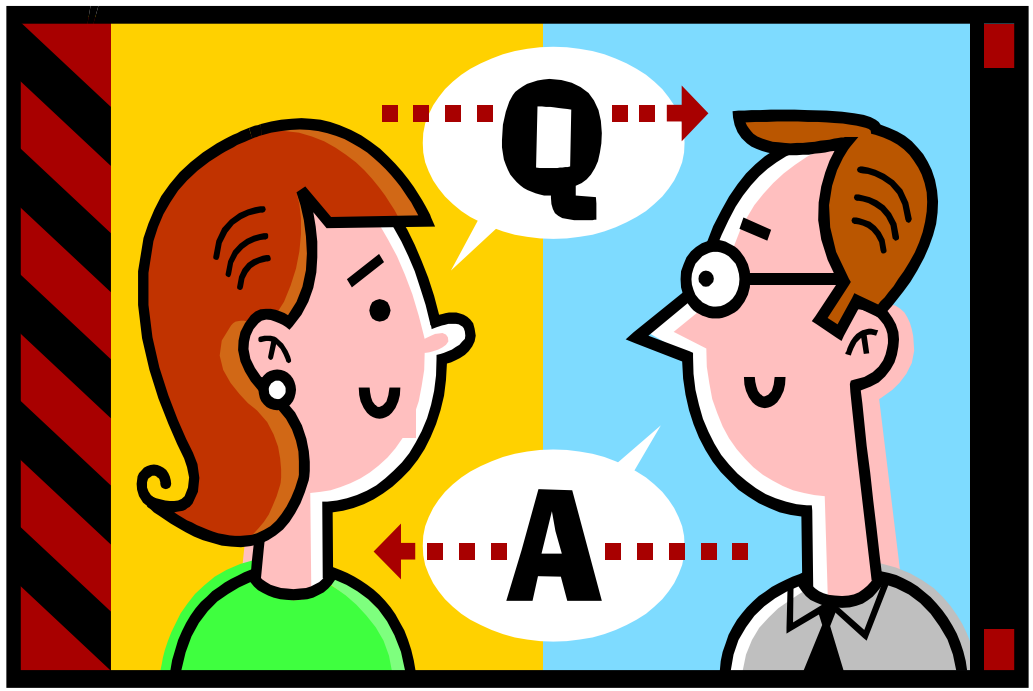
Easy administration – centralized authentication

Link common records from different sources

Fewer windows & clicks, easier & more intuitive

Markush structures in Patent Chemistry Database

Hit set manipulation`


Q
A

Learning More…

- Visit www.discoverygate.com or www.mdl.com