DiscoveryGate

One place for the answers you need

Chulalongkorn University, Thailand

Presented by: Doreen Tan
Title: Product Sales Manager, Life Science
Date: 1 Sep 2005

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

Three Content Sources

- Primary Content - Original Literature Sources
  - Publications containing detailed descriptions, methodology and scientific results (journals, patents, proprietary original work)
- Secondary Content—Databases
  - Synthesis, bioactivity, physical property, metabolism, toxicity and sourcing databases
- Tertiary Content—Authoritative Reference Works
  - Well regarded core knowledge summarizing a particular topic

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

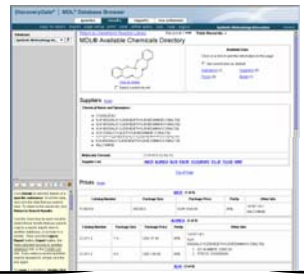
We handle maintenance, security and support - you can focus on research

Integration, Indexing and Linking

DiscoveryGate content

15 Chemistry databases
+ 2 integrated Major Reference Works

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

Content Description – Chemistry Reference

1. CrossFire Beilstein

- World's largest compilation of chemical facts in small molecular organic chemistry;
- Indexes three primary data domains: substances, reactions, and literature;
- Stores structural information with all associated facts and literature references, including chemical, physical, and bioactivity data;
- Details the preparation of substances, enabling scientists to investigate specific reaction pathways with reaction search queries;
- literature domain includes citations, titles, and abstracts, which are hyperlinked to the substance and reaction domain entries;
- Unique coverage runs from 1771 to today.

Content Description – Chemistry Reference 2

2. CrossFire Gmelin

- World's most comprehensive data collection in organometallic and inorganic chemistry, covering literature from the year 1772 to today.
- Contains over 2.2 million compounds, more than 1.6 million reactions, and 1.1 million citations, including titles and abstracts from 1995.
- Fully searchable by structures, substructures, and reactions.
- Answers informatics needs in the material science, catalyst, and semiconductor industries.
- Complements CrossFire Beilstein with organometallic and inorganic content.

Content description – BioActivity 1

3. MDL Drug Data Report

- Contains over 132,000 biologically relevant compounds and well-defined derivatives;
- Covers patent literature, journals, meetings and congresses.
- Produced by MDL and Prous Science,
- Updates adds about 10,000 a year to the database.

4. MDL Toxicity Database

- Structure-searchable bioactivity database of toxic chemical substances.
- Contains data from *in vivo* and *in vitro* studies of acute toxicity, mutagenicity, skin and eye irritation, tumorigenicity and carcinogenicity, reproductive effects and multiple dose effects.
- Information covered includes species of organism studied, tissue studied, route of administration, dose, endpoint, toxic effects descriptors, severity of response, CAS Registry Numbers, Beilstein Registry Numbers, chemical names and synonyms, molecular formula and molecular weight;

Content description - BioActivity 2

5. MDL Metabolite Database

- uses information from multiple studies to assemble structural metabolic database entries for particular parent compounds.

6. MDL Comprehensive Medicinal Chemistry

- Derived from the Drug Compendium in Pergamon's Comprehensive Medicinal Chemistry;

- Provides 3D models and important biochemical properties including drug class, logP, and pKa values for over 8,400 pharmaceutical compounds (1900-present).

– Updated annually with compounds identified for the first time in the United States Approved Names (USAN) list.

7. National Cancer Institute Databases

- Contains over 213,000 structures with corresponding 3D models generated using CORINA 2.4 from Molecular Networks GmbH.

- Four publicly available National Cancer Institute databases were consolidated to produce this data set.

Content Description
- Chemical Sourcing & Logisitics

8. MDL Available Chemicals Directory

- A database of over 400,000 unique chemical entities, representing over one million purchasable products;

- Aggregates catalog information from 658 suppliers of chemical and biological reagents for the pharmaceutical, biotech, and chemical industries;

- Structure-searchable format, includes quantities, purities, and pricing, along with ordering details for each supplier.

- the de facto standard in pharmaceutical, biotechnology, chemical and agrochemical companies worldwide.

9. MDL Screening Chemicals Directory

- Consolidates catalog data from 48 suppliers with product lines targeting High-Throughput Screening programs.

- Contains over 2 million unique structures in over 4 million products, and includes supplier information necessary for ordering.

Content Description - Synthetic Methodology 1

10. ChemInform Reaction Library

- Compilation of 100 years of chemical literature citations;
- Contains reactions of current interest to synthetic chemists, with an emphasis on novel methodology;
- Abstracted, and organized by FIZ CHEMIE Berlin and then classified according to reaction type using InfoChem's reaction classification technology;
- Provides convenient access to full reaction schemes.

11. Current Synthetic Methodology

- Contains the most innovative and significant reactions since 1992;
- Emphasizes new synthetic methodologies, reactions that use new reagents or an important modification of known reagents, and regio-, chemo-, and stereoselective reactions carried out on multifunctional substrates.
- Abstracted, and organized by FIZ CHEMIE Berlin.

Content Description - Synthetic Methodology 2

12.Derwent Journal of Synthetic Methods

- Compilation of chemical reaction literature from international journals and patent sources;

- Contains detailed information about new synthetic methods, high-yield functional group transformations, improvements to existing methodologies, and reactions representing the most significant new patents.

13. ORGSYN Database

- An electronic version of the entire series of *Organic Syntheses* (first published in 1921)

- Offers access to new general synthetic methods and proven compound preparations;

- Contains information on product purity, product yield, and hazards, as well as references to the original procedures and journal sources.

Content Description - Synthetic Methodology 3

14. MDL Solid-Phase Organic Reactions

- Contains reactions of small organic molecules on solid support;
- Designed to meet the needs of combinatorial chemistry groups;
- Includes extensive data on solid-phase organic chemistry, such as information on polymeric materials, linkers, solid supports, and protecting groups;
- Abstracted, and organized by FIZ CHEMIE Berlin

15. Reference Library of Synthetic Methodology

- Broad collection of novel organic synthetic methodologies
- Covers functional group transformations, metal-mediated chemistry, and asymmetric syntheses, as well as reactions;
- Abstracted from Dr. William Theilheimer's *Synthetic Methods of Organic Chemistry.*

Content Description- Integrated Major Reference Works

16. Comprehensive Asymmetric Catalysis (Springer)

- Provides a definitive presentation of the state of the art in synthetic chemistry;

- Find the basic principles, mechanisms, and basis for stereoinduction; the scope and limitations of these reactions; and strategies for future development in this area of chemistry.

- Addresses catalytic availability, preparation, handling, efficiency, loading, recovery, toxicity, as well as special conditions and equipment, and scale and safety issues.

17. Comprehensive Organic Functional Group Transformation (Elsevier)

- Offers comprehensive review of the preparation and transformation of functional groups that forms the basis of all chemical and biological activity;

- Employs rigorous, logical and formal treatment of the structural basis of reactions;

- Provides detailed analysis of all known (and in some cases, unknown) functional groups and the methods of their construction, introduction, and interconversion.

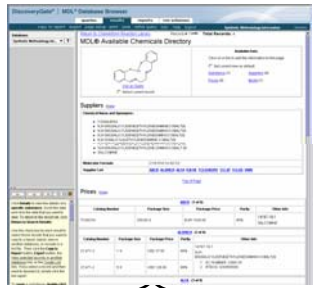
3rd Party Databases

- Derwent World Patent Index
- ISI Current Chemical Reactions
- ISI Index Chemicus

*Only summary information from these databases are displayed on DiscoveryGate. Further details are subject to institutional access rights.

Compound Index Re-ordering

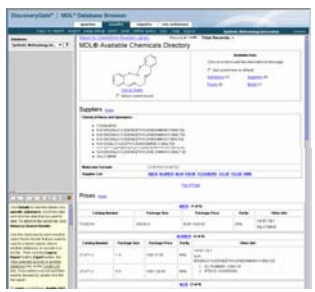
- Before



Newest hits last in Results List

Compound Index: Old → Newest

- With DiscoveryGate 2.0



First shown:
- Newest
- Found in most native databases (most references)

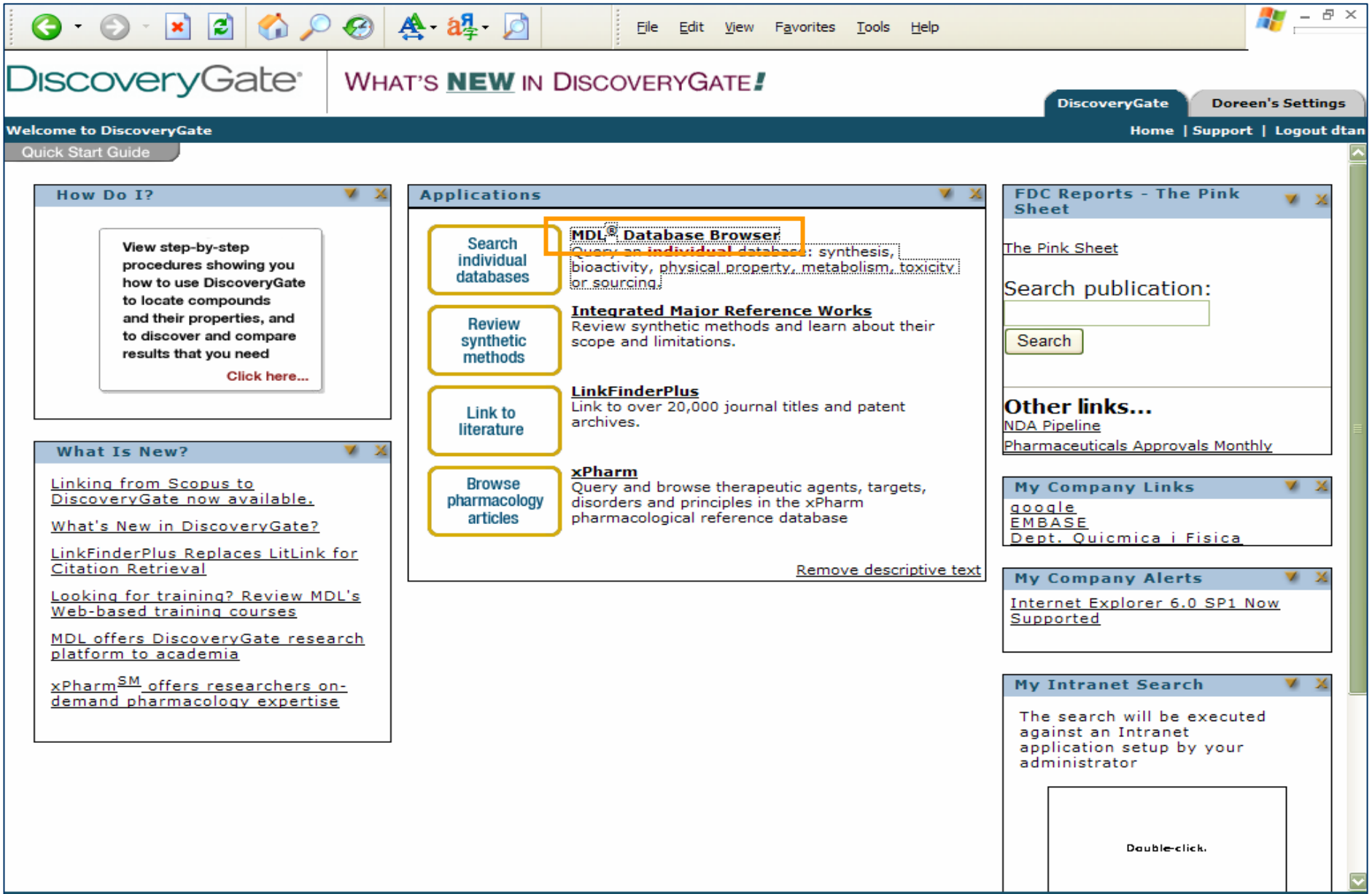
Compound Index

Newest + Most references	All other records
Sorted based on Rule of Five	Sorted based on Rule of Five

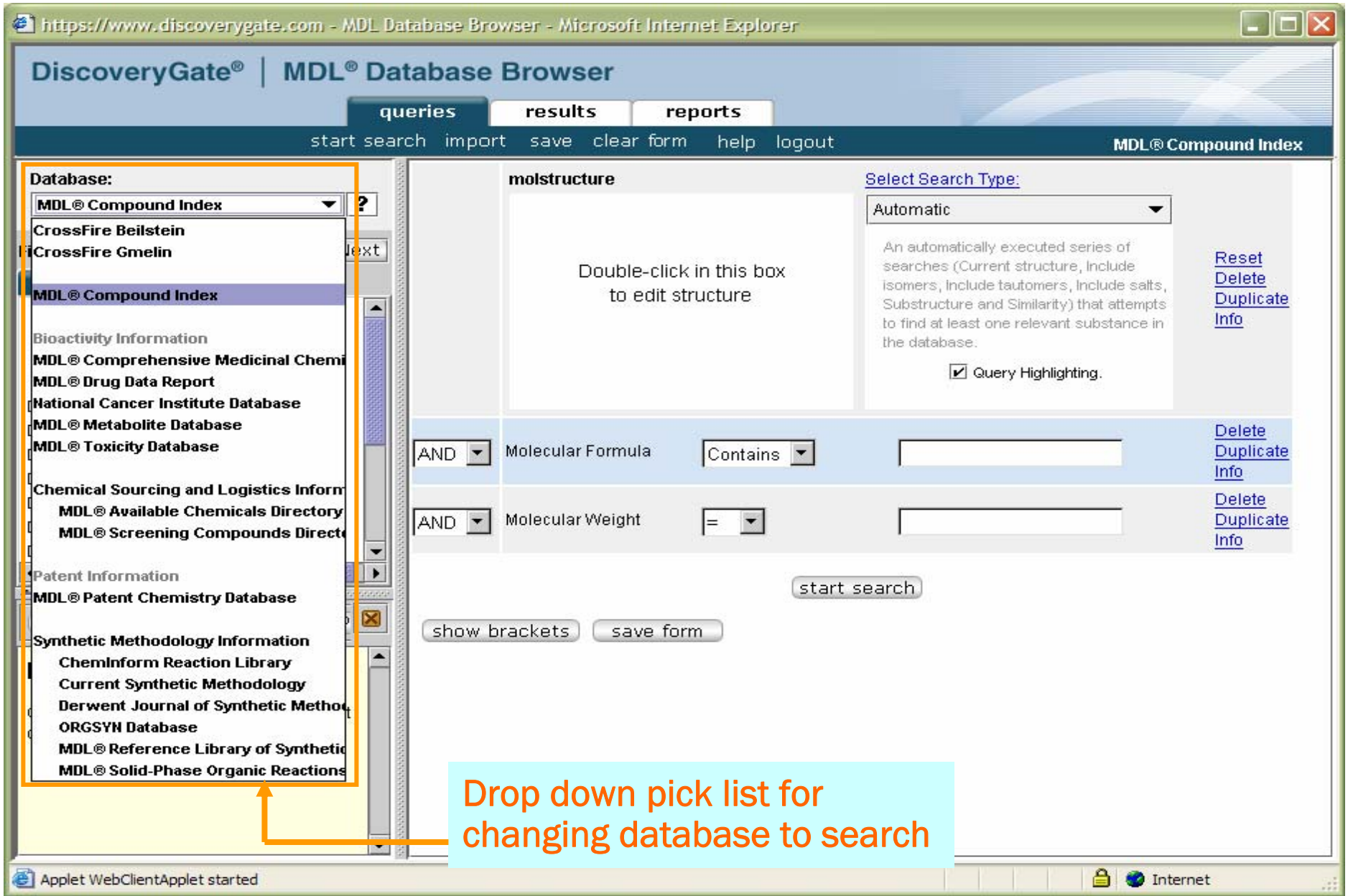
DiscoveryGate 2.0

SCREEN SHOTS

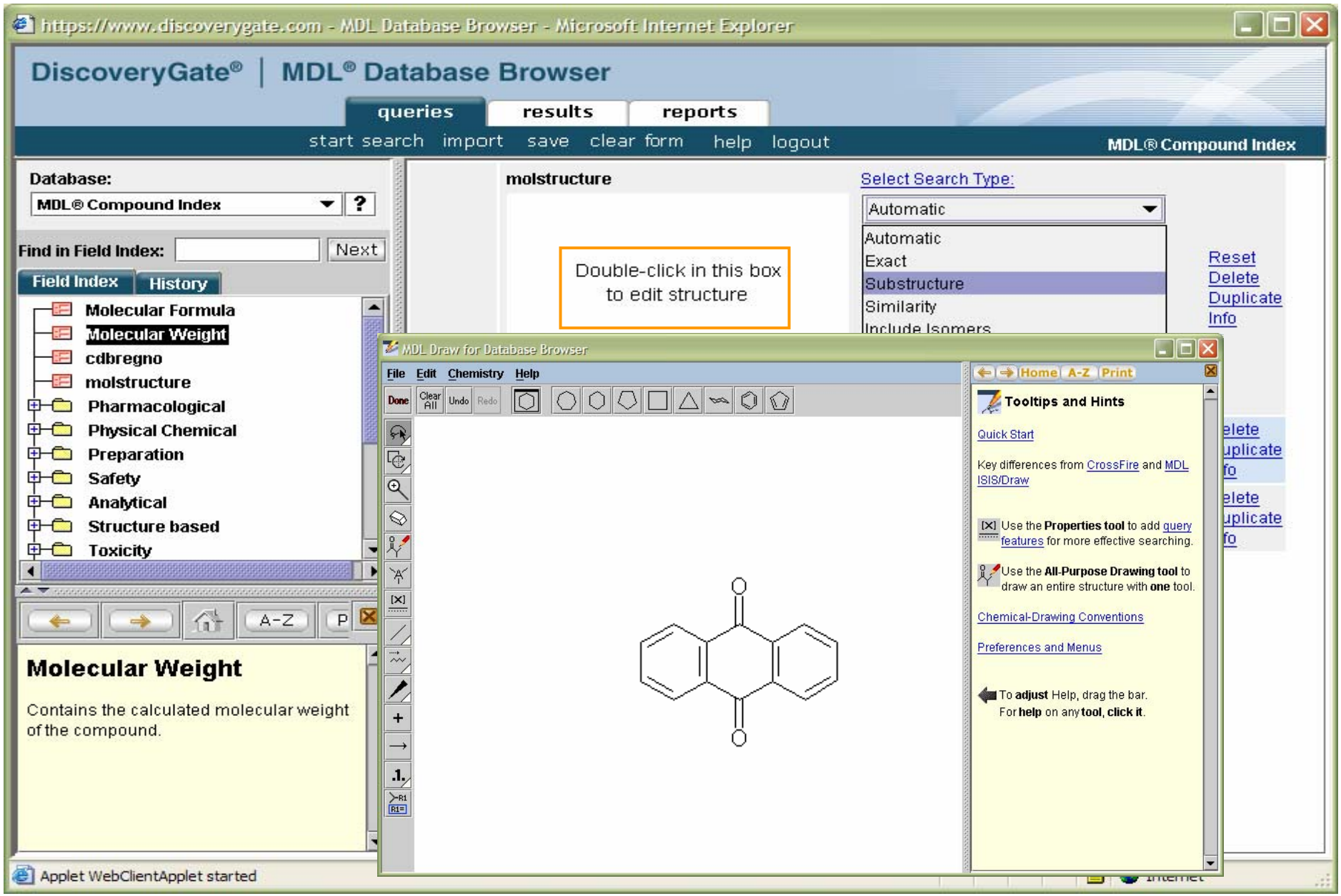
www.discoverygate.com/20



Database Browser – Selecting DB



Database browser – query form



Searching in Compound Index

https://www.discoverygate.com - MDL Database Browser - Microsoft Internet Explorer

DiscoveryGate® | MDL® Database Browser

queries | results | reports

start search | import | save | clear form | help | logout

MDL® Compound Index

Database: MDL® Compound Index ?

Find in Field Index: Next

Field Index | History

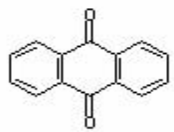
- Molecular Formula
- Molecular Weight
- cdbregno
- molstructure
- Pharmacological
- Physical Chemical
- Preparation
- Safety
- Analytical
- Structure based
- Toxicity

A-Z P

Double-click a search to retrieve the associated query. Optionally, you can modify the query (click here for more information on how to refine your query for better search results). Click **Start Search** to see the results.

We encourage you to **save the queries of all searches to which you might want to refer later**. Click the **Save** button in the

MolStructure



Select Search Type: Substructure

A Molecule Substructure search finds molecule records that contain your query as a substructure wholly within a larger structure.

☑ Query Highlighting.

Reset Delete Duplicate Info

AND	Molecular Weight	=		Delete Duplicate Info
AND	Molecular Formula	Contains		Delete Duplicate Info
AND	cdbregno	=		Delete Duplicate Info

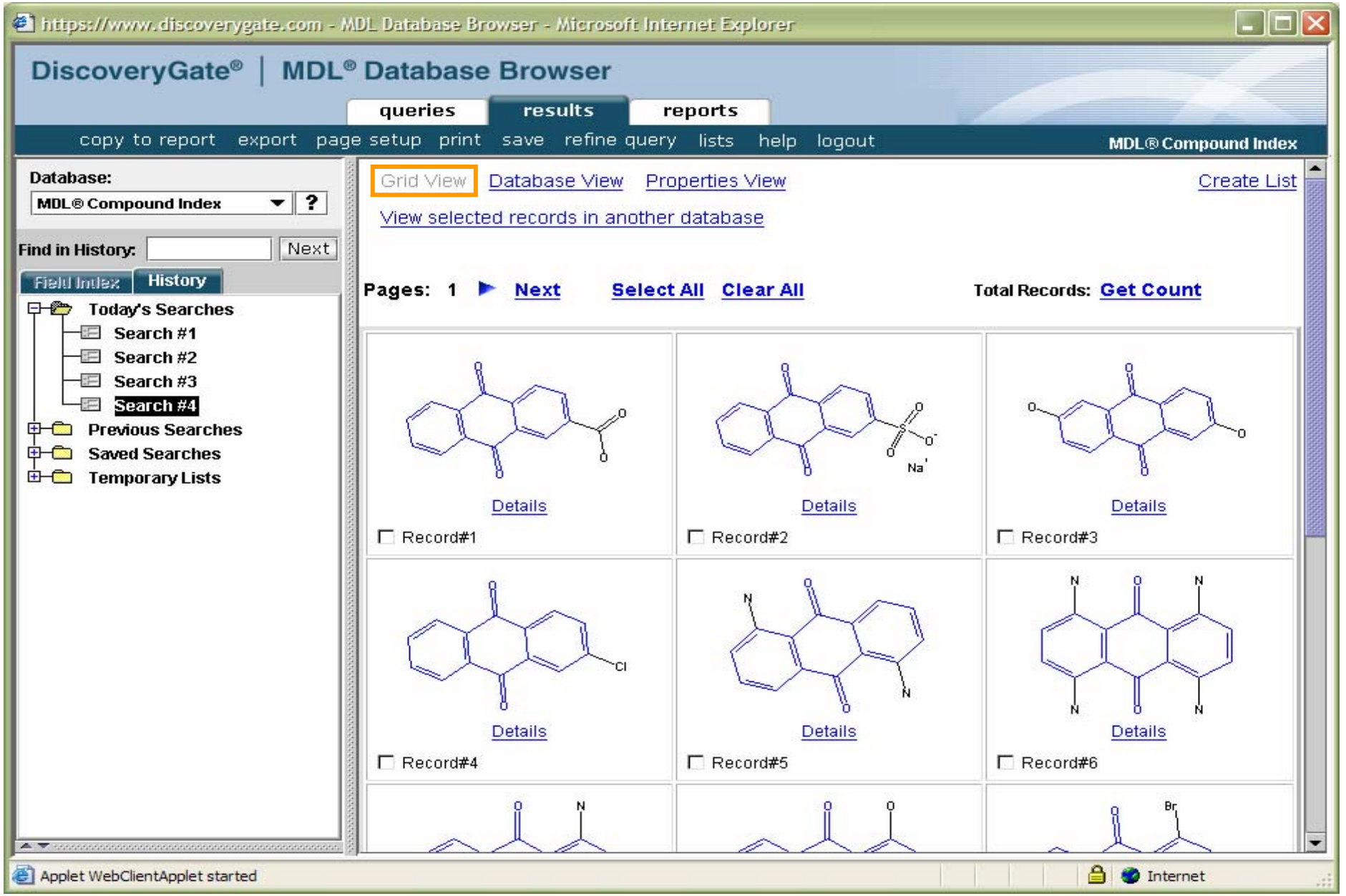
start search

show brackets | save form

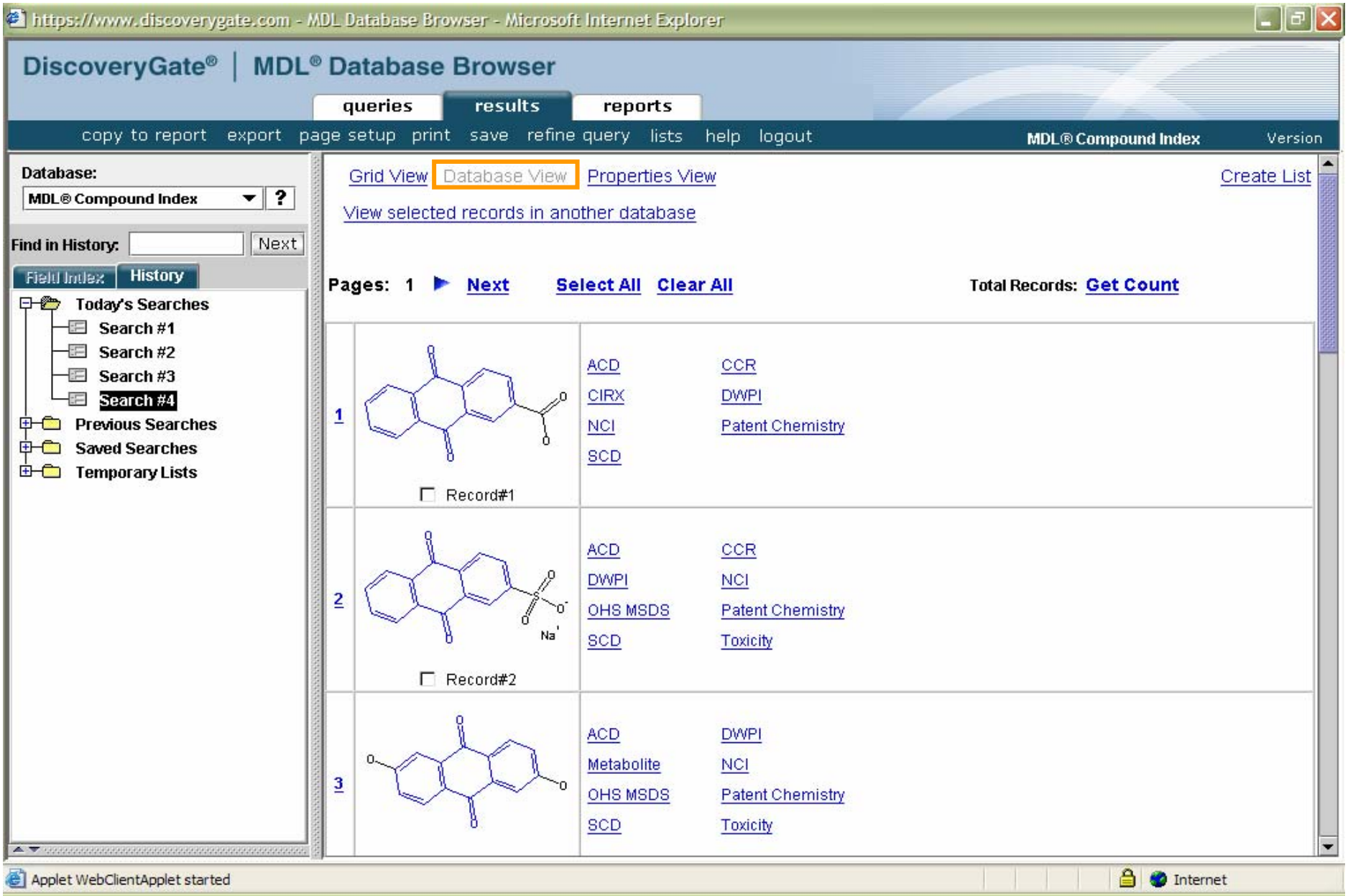
Applet WebClientApplet started

Internet

Results 1 – Grid View



Results 2 – Database View



Results 3 – Properties View

https://www.discoverygate.com - MDL Database Browser - Microsoft Internet Explorer

DiscoveryGate® | MDL® Database Browser

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

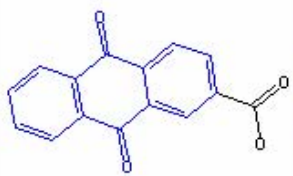
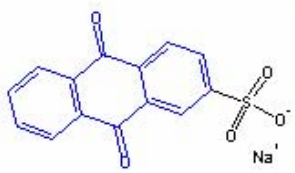
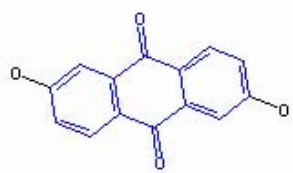
Field Index | History

- Today's Searches
  - Search #1
  - Search #2
  - Search #3
  - Search #4
- Previous Searches
- Saved Searches
- Temporary Lists

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

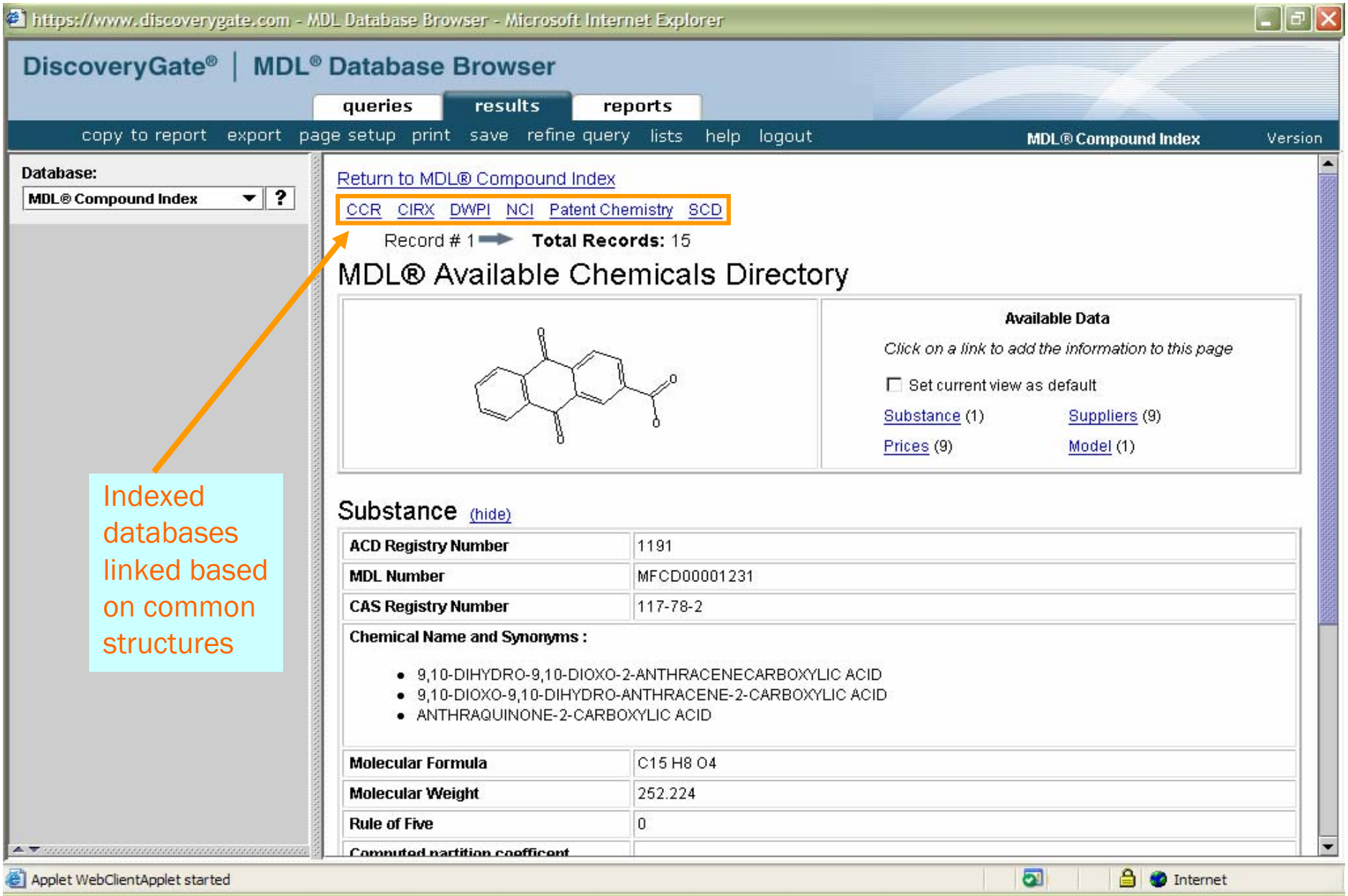
1	 Record#1	3d Configuration Analytical Commercially Available Name Physical Chemical	Agrochemical Chemical Literature Reference Pharmacological Preparation
2	 Record#2	3d Configuration Analytical Commercially Available Name Preparation Toxicity	Agrochemical Chemical Literature Reference Pharmacological Safety
3		3d Configuration Chemical Literature Reference Name Preparation	ADME Commercially Available Metabolism Pharmacological Safety

View summary by clicking on hyperlink

Applet WebClientApplet started

Internet

View compound summary



Indexed databases linked based on common structures

‘Jumping’ DBs: CI to CCR

https://www.discoverygate.com - MDL Database Browser - Microsoft Internet Explorer

DiscoveryGate® | MDL® Database Browser

queries | results | reports

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

MDL® Compound Index Version

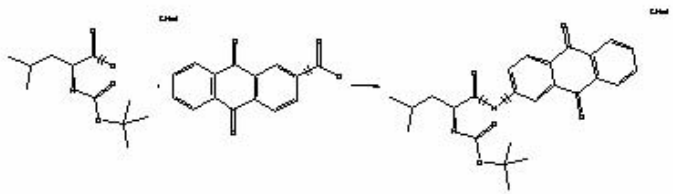
Database: MDL® Compound Index ?

Return to MDL® Compound Index | Find Similar Reactions

ACD | CIRX | DWPI | NCI | Patent Chemistry | SCD

Record # 2 **Total Records:** 15

Current Chemical Reactions (CCR) Database®



MDL Reaction Number: RCCR04145104

Document Reference in CCR	
41451	NEW METHODS AND REAGENTS IN ORGANIC-SYNTHESIS .69. A NEW SYNTHESIS OF ALPHA-AMINO-ACID AND PEPTIDE AMIDES OF AROMATIC-AMINES USING A MODIFIED CURTIUS REACTION WITH DIPHENYL PHOSPHORAZIDATE.

Reagent(s)	DPPA Et3N ClCH2CH2Cl

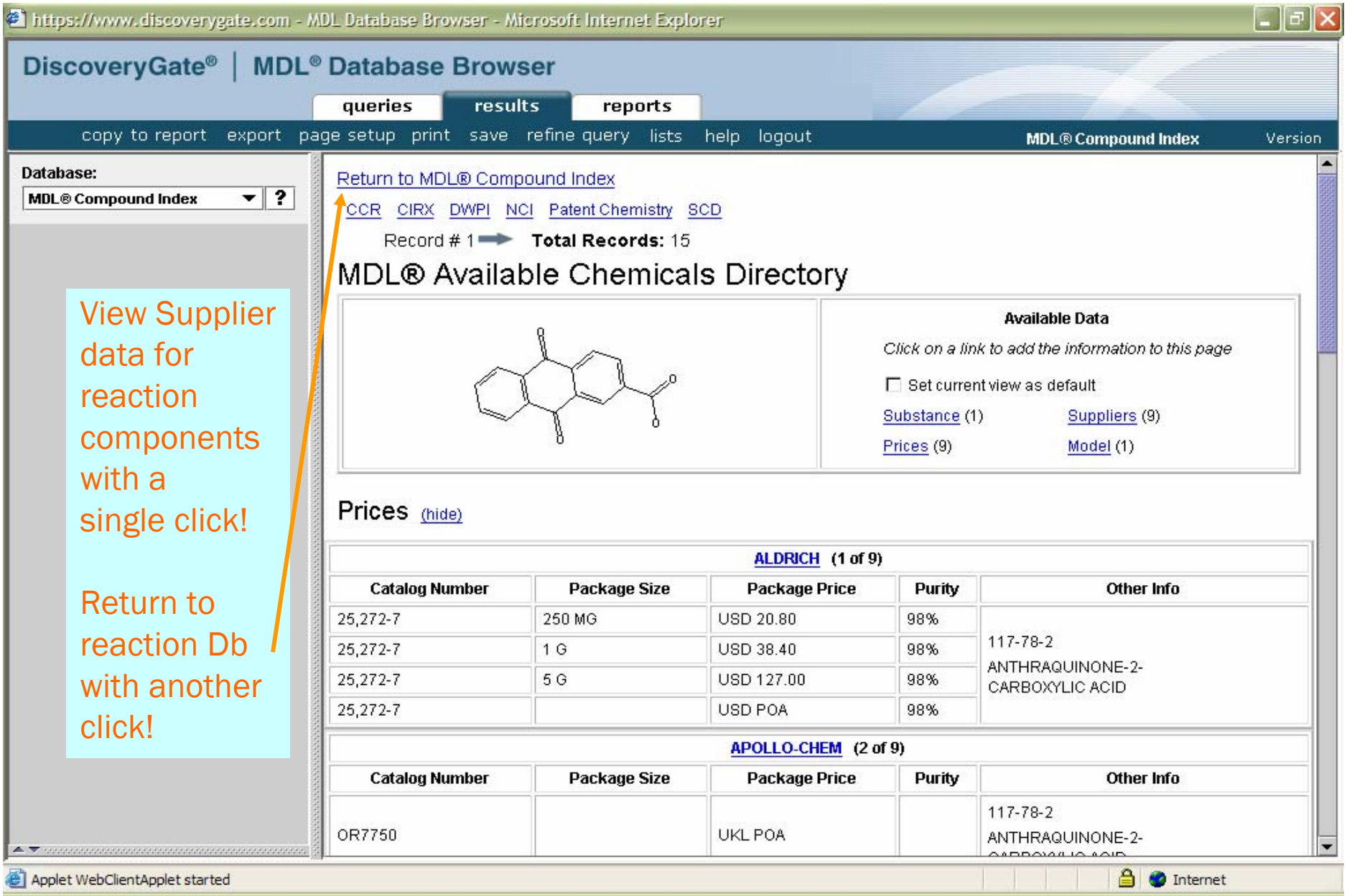
Product Number	Yield	Grade
1	92	

Applet WebClientApplet started

Internet

Commercial availability

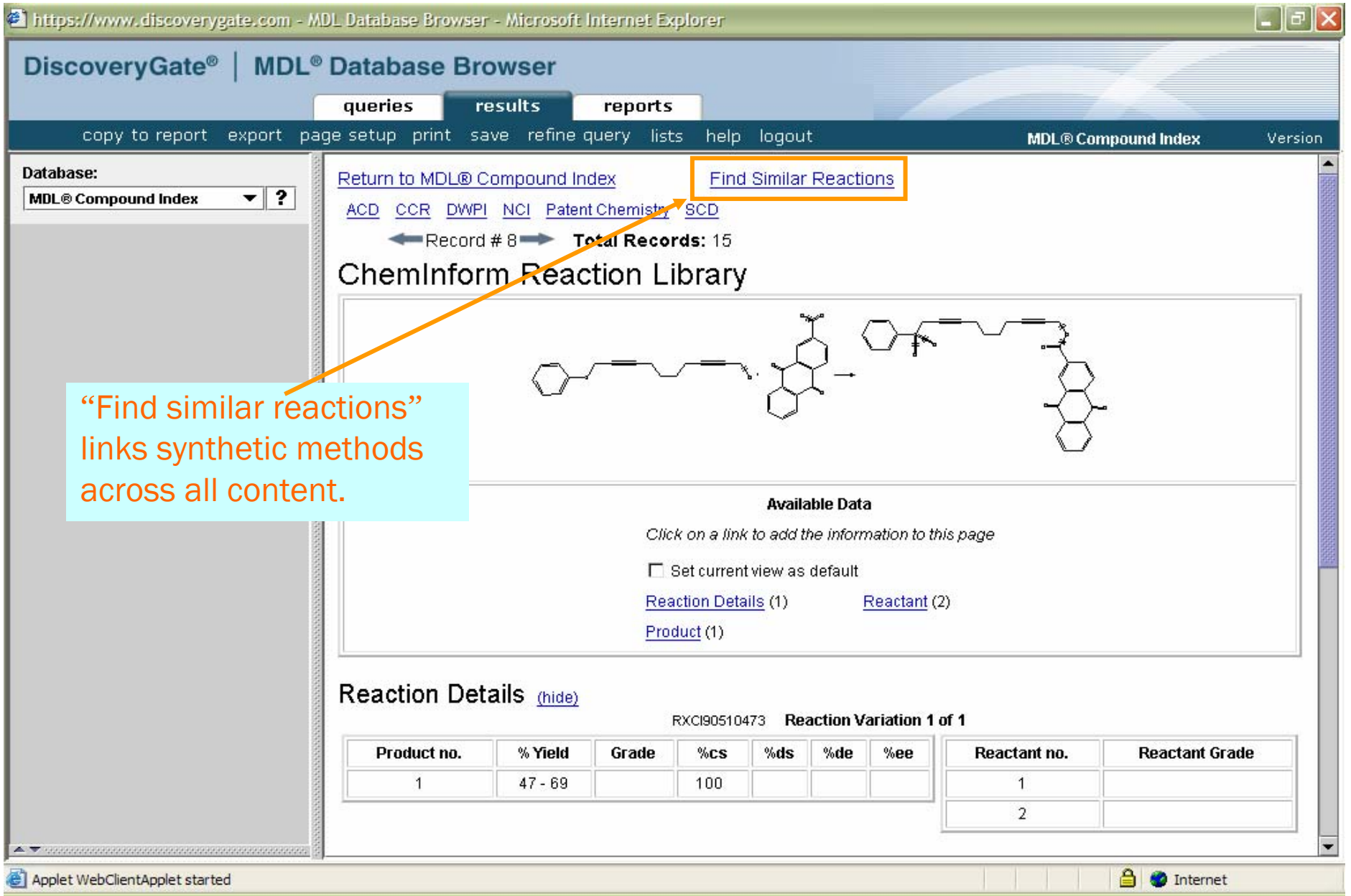
Chemical Sourcing Logistics



View Supplier data for reaction components with a single click!

Return to reaction Db with another click!

Finding Similar Reactions



"Find similar reactions" links synthetic methods across all content.

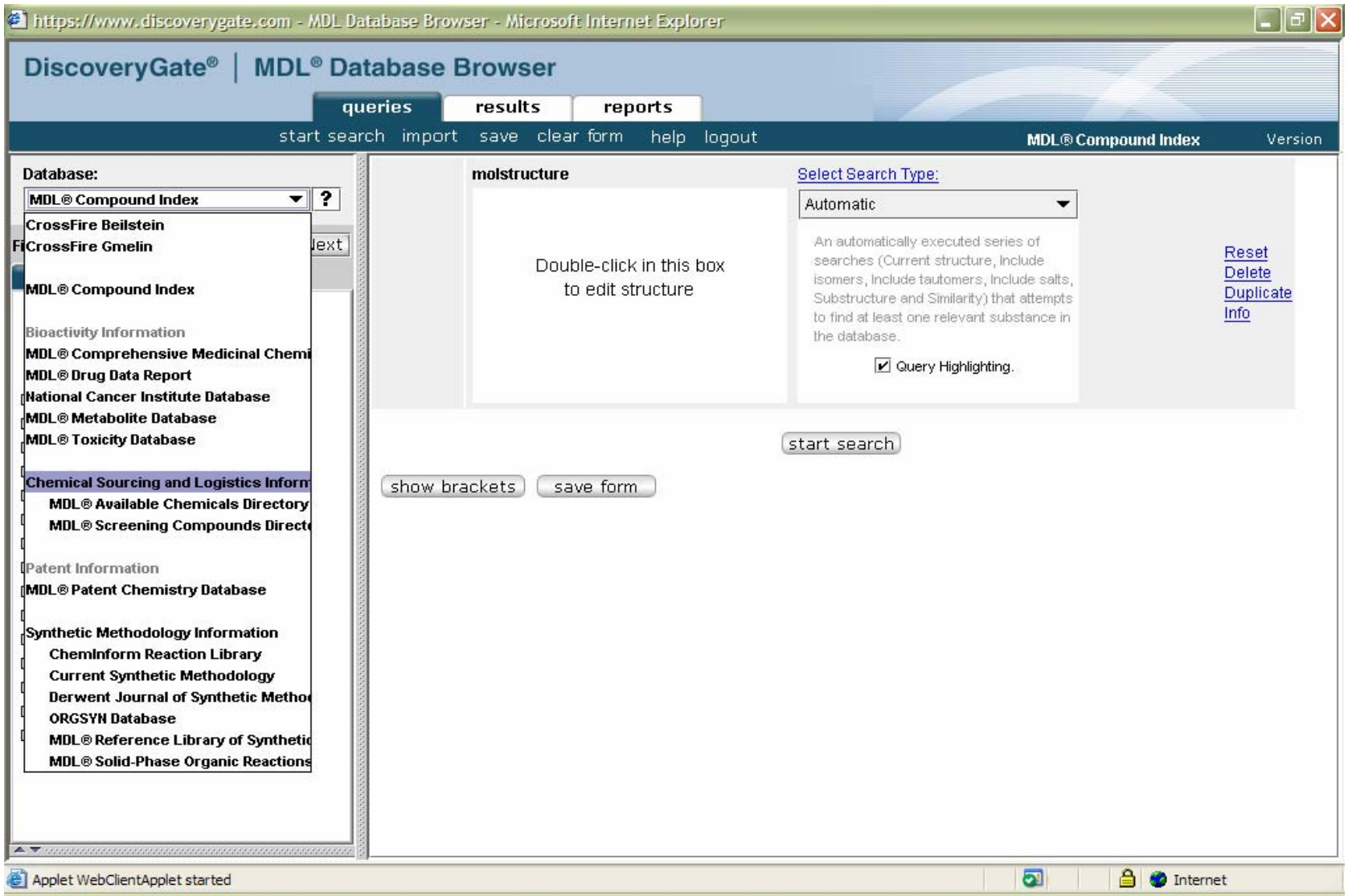
DiscoveryGate

SEARCH EXAMPLES

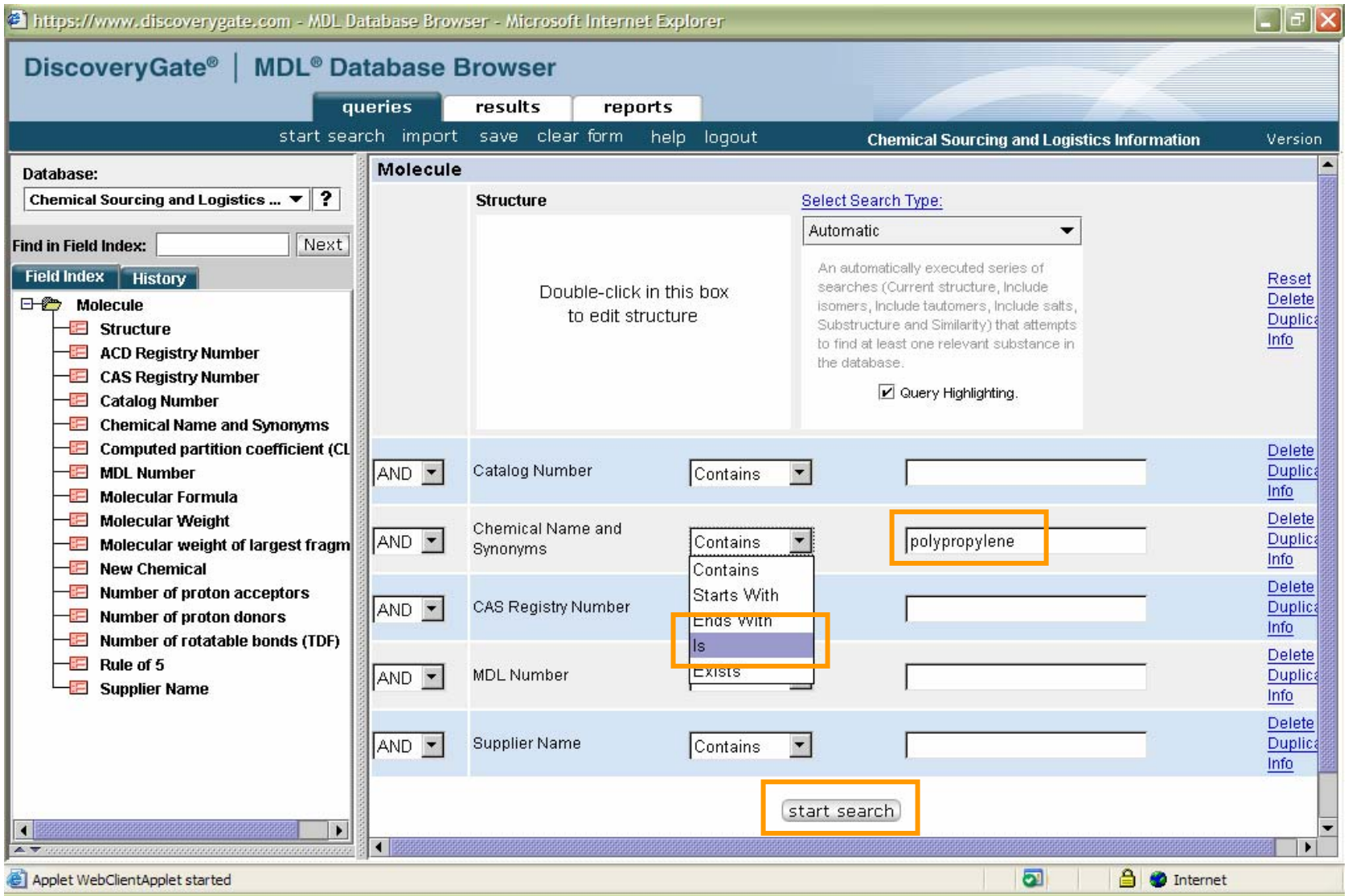
Search scenario 1

You are a post-doc student tasked to source for commercial availability of a form of crude oil. You only know the name as polypropylene, and have no idea what the molecule structure is like. Where do you start?

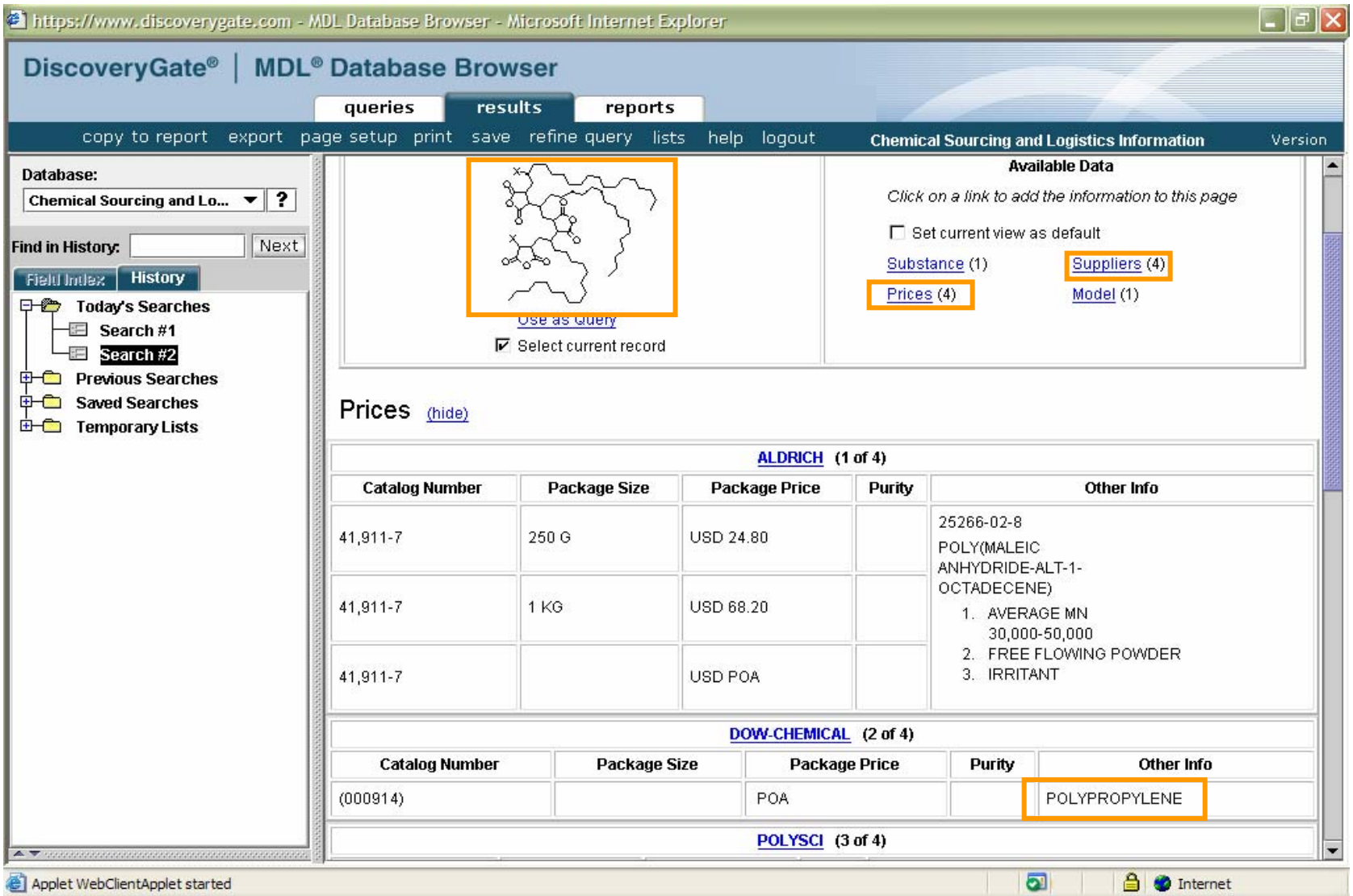
Start with Chemical Sourcing



Draw your query form



Viola! Search Results



DiscoveryGate 2.0

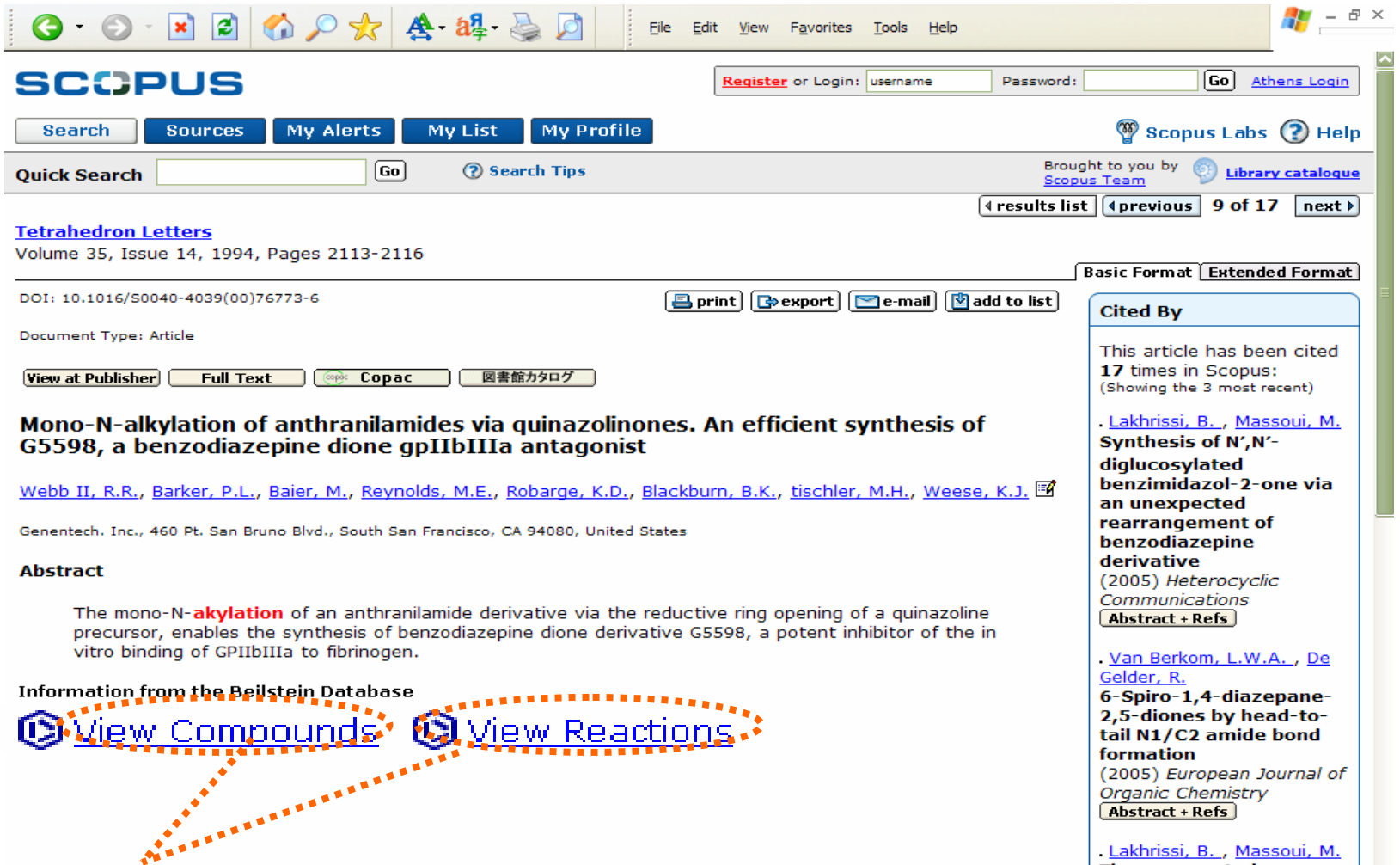
LINKING FROM SCOPUS TO CROSSFIRE COMMANDER

LINKING FROM SCOPUS TO CROSSFIRE COMMANDER

CROSSFIRE COMMANDER

- It an integrated client/server application for searching CrossFire Beilstein, Crossfire Gmelin, and MDL Patent Chemistry Database.
- Allows scientists to quickly search the databases and hyperlink to relevant related data (e.g. chemical structures, bioactivity data, synthesis preparation, etc).
- Subscribers of DiscoveryGate will receive CrossFire Commander.

Linking from Scopus to Crossfire Commander



Links to CrossFire Beilstein database via CrossFire Commander

From Scopus to CrossFire Commander:
Compound Summary Page

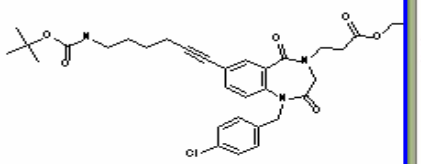
http://scopus-ls.mdli.com - Scopus - Chemical Compounds - Microsoft Internet Explorer

The following information is from th

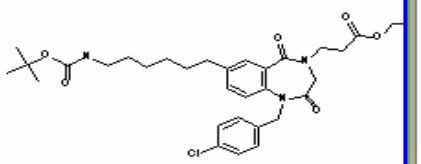
Webb, Robert R., II; Barker, Peter L
Mono-N-Alkylation of Anthranyla
Benzodiazepine Dione GpIIbIIIa A
1994, *Tetrahedron Lett.*, **35** (14), p

49 Chemical Compounds View re

1.



2.



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

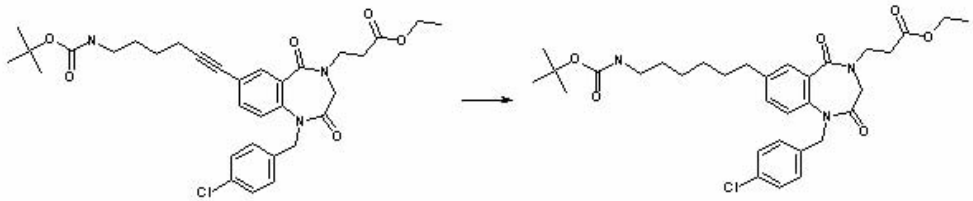
The following information is from the Beilstein Database ©

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

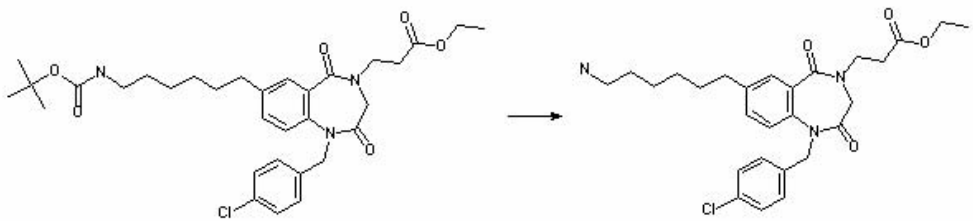
1.



Reaction number	Reaction conditions
3689284	H2 PtO2 ethanol

For more information access the Beilstein Database via:
CrossFire Commander

2.

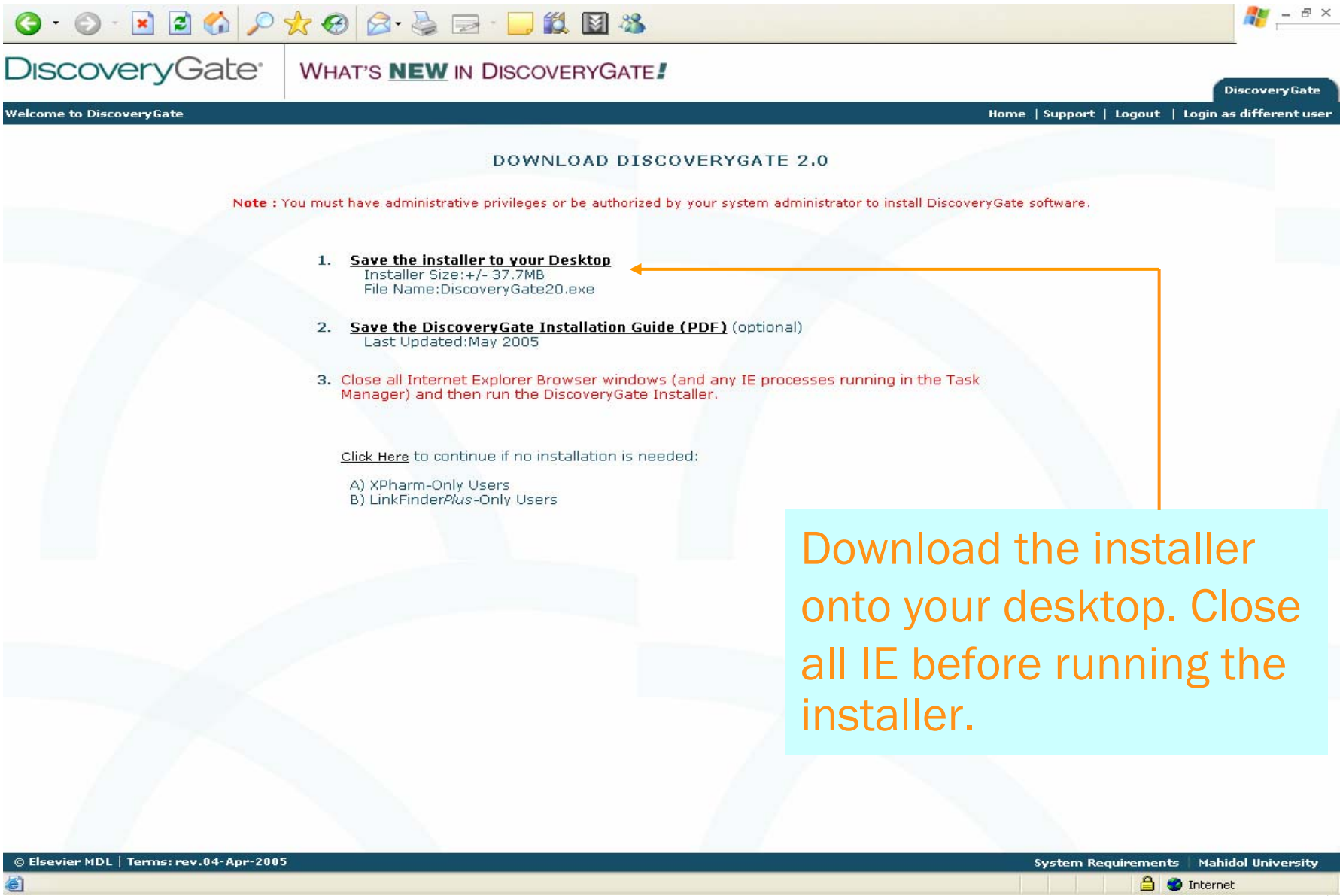


Done Internet

LIVE DEMONSTRATION

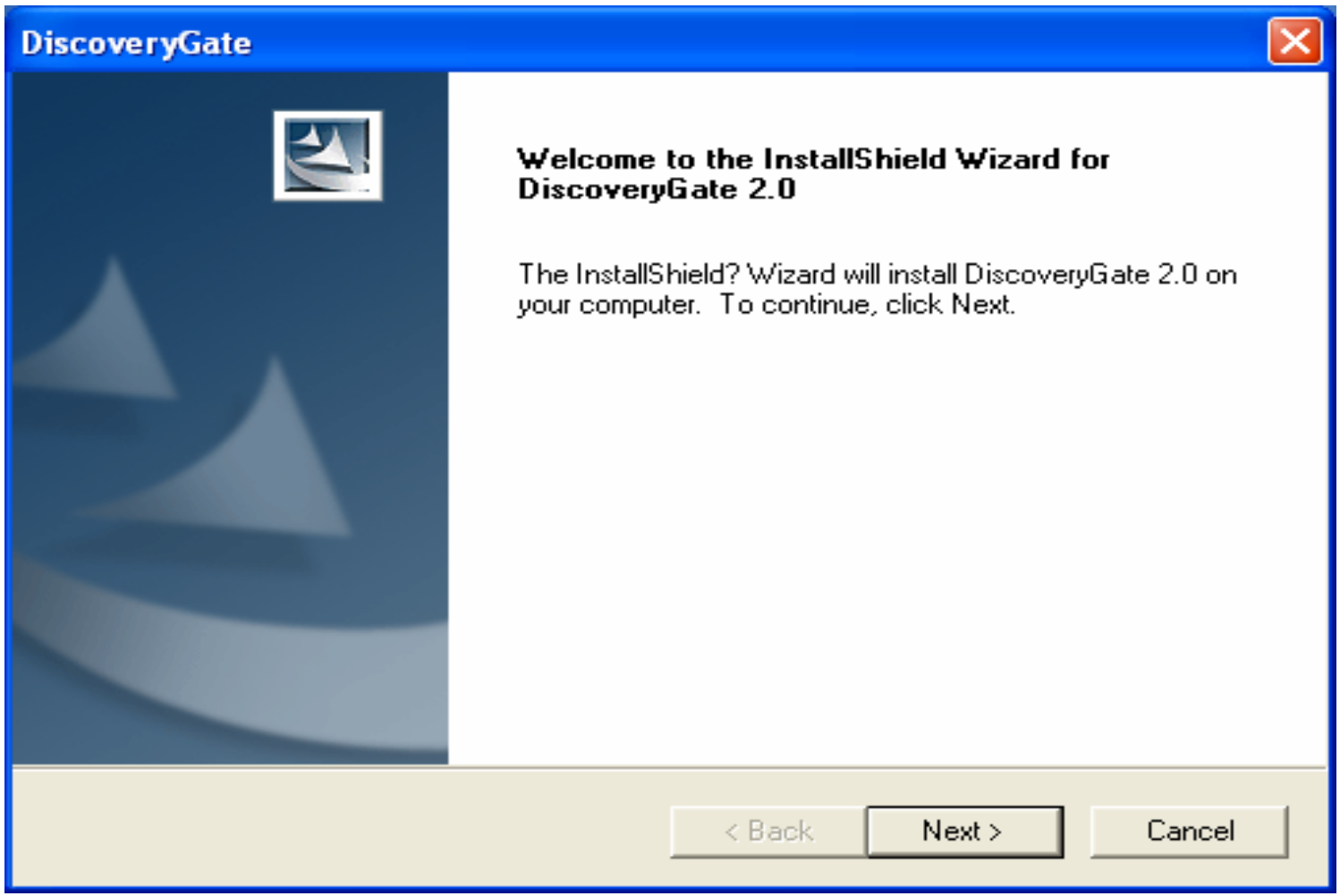
WWW.DISCOVERYGATE.COM/20

GETTING STARTED

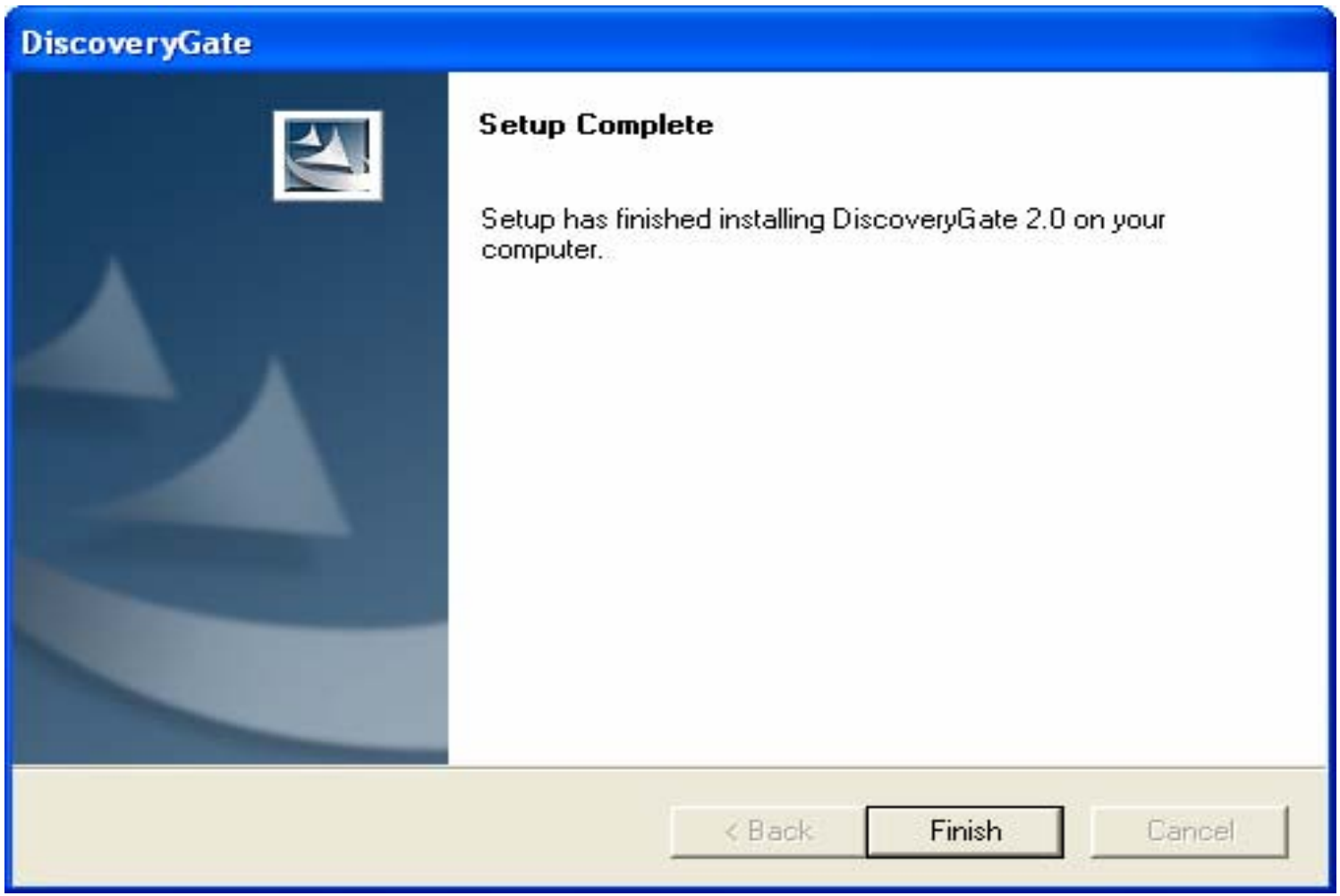


Download the installer onto your desktop. Close all IE before running the installer.

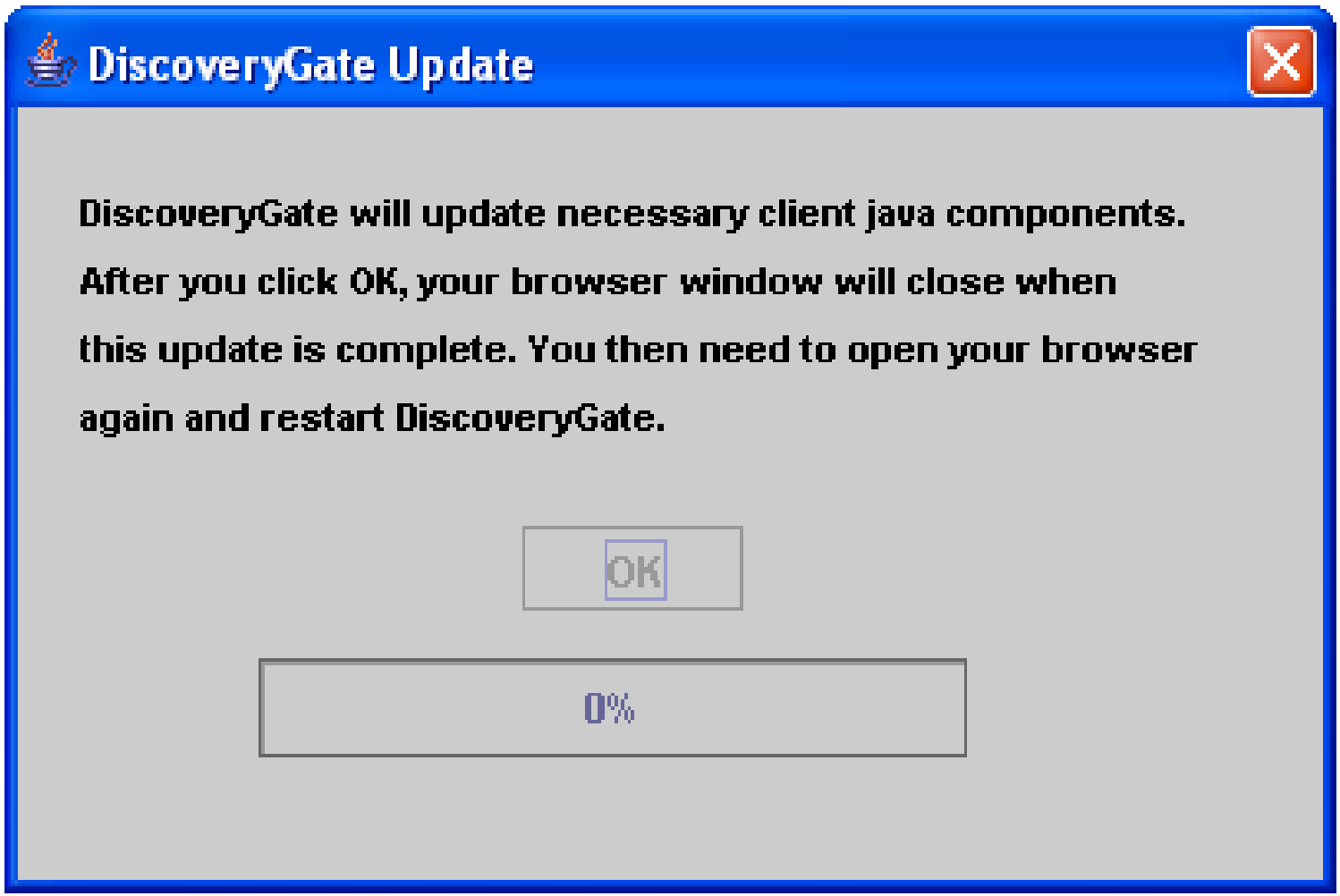
RUNNING THE INSTALLER



RUNNING THE INSTALLER 2



UPDATING JAVA COMPONENTS



DiscoveryGate 2.0

BENEFITS IN SUMMARY

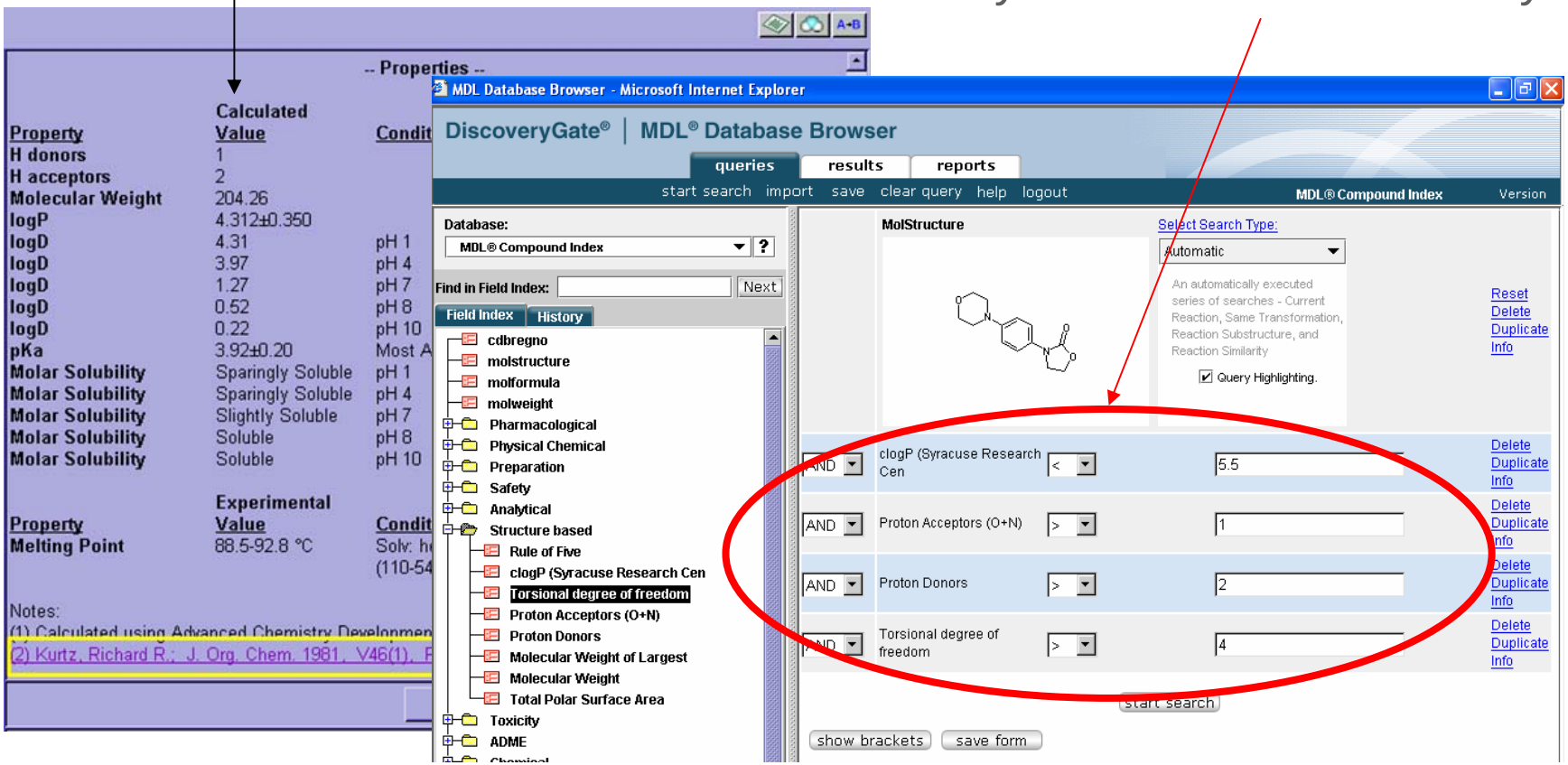
Benefits for the Information Specialist

- Factual data is searchable in DiscoveryGate
  - Properties are not static
- More than 150,000,000 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 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 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, & clicks, easier & more intuitive
- Database pick list as pull down menu in DB Browser
- Easy administration – Centralised authentication

Better Usability

- Exploit Indexed content with “Also Found In” links
- Link common records from different sources
- 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

Thank you!

- Questions?
- Product Sales Manager: Doreen Tan
- D.Tan@elsevier.com
- For further information, visit www.discoverygate.com or www.mdl.com/products/knowledge/index.jsp
- Personal 14-day trial coming soon

PRICING MODEL

FOR ACADEMICS & GOVERNMENT INSTITUTIONS

PRICING MODEL & FEATURES

*Population Band**		*2005 Subscription US$*		
Lower limit	*Upper limit*	*DiscoveryGate*	*xPharm*	*Patent Chemistry Database*
1	50	27,657	8,018	8,627
51	250	34,213	10,023	10,783
251	500	39,961	12,528	13,479

- ✓ UNLIMITED ACCESS CAMPUS-WIDE; NO MORE BLOCKED-OUTS.
- ✓ IP ACCESS; NO NEED TO REMEMBER USERNAME AND PASSWORDS.
- ✓ SUPPORTED ON MACINTOSH OS X (DiscoveryGate v2.1, rel Sep 05)

* For Academics, population band refers to the number of faculty members + post-doc students in the relevant life science disciplines. E.g.. Pharmacy dept for xPharm.