



# DiscoveryGate

One place for the answers you need

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Title: Product Sales Manager, Life Science

Date: 1 Sep 2005

## 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



*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 3<sup>rd</sup> 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 & Logistics

### 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 stereoselection; 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.

# 3<sup>rd</sup> 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

Sorted based on Rule of Five

All other records

Sorted based on Rule of Five



# DiscoveryGate 2.0

SCREEN SHOTS

DiscoveryGate WHAT'S NEW IN DISCOVERYGATE!

Welcome to DiscoveryGate Home | Support | Logout dtan

Quick Start Guide

### How Do I?

View step-by-step procedures showing you how to use DiscoveryGate to locate compounds and their properties, and to discover and compare results that you need

[Click here...](#)

### What Is New?

[Linking from Scopus to DiscoveryGate now available.](#)

[What's New in DiscoveryGate?](#)

[LinkFinderPlus Replaces LitLink for Citation Retrieval](#)

[Looking for training? Review MDL's Web-based training courses](#)

[MDL offers DiscoveryGate research platform to academia](#)

[xPharm<sup>SM</sup> offers researchers on-demand pharmacology expertise](#)

### Applications

- Search individual databases**
- MDL® Database Browser**  
Query an individual database: synthesis, bioactivity, physical property, metabolism, toxicity or sourcing.
- Review synthetic methods**
- Integrated Major Reference Works**  
Review synthetic methods and learn about their scope and limitations.
- Link to literature**
- LinkFinderPlus**  
Link to over 20,000 journal titles and patent archives.
- Browse pharmacology articles**
- xPharm**  
Query and browse therapeutic agents, targets, disorders and principles in the xPharm pharmacological reference database

[Remove descriptive text](#)

### FDC Reports - The Pink Sheet

The Pink Sheet

Search publication:

**Other links...**

[NDA Pipeline](#)

[Pharmaceuticals Approvals Monthly](#)

### My Company Links

[google](#)

[EMBASE](#)

[Dept. Quimica i Fisica](#)

### My Company Alerts

[Internet Explorer 6.0 SP1 Now Supported](#)

### My Intranet Search

The search will be executed against an Intranet application setup by your administrator

Double-click.

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

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queries results reports

start search import save clear form help logout MDL® Compound Index

**Database:**

- MDL® Compound Index
- CrossFire Beilstein
- CrossFire Gmelin
- MDL® Compound Index**
- Bioactivity Information
- MDL® Comprehensive Medicinal Chemi
- MDL® Drug Data Report
- National Cancer Institute Database
- MDL® Metabolite Database
- MDL® Toxicity Database
- Chemical Sourcing and Logistics Inform
- MDL® Available Chemicals Directory
- MDL® Screening Compounds Direct
- Patent Information
- MDL® Patent Chemistry Database
- Synthetic Methodology Information
- ChemInform Reaction Library
- Current Synthetic Methodology
- Derwent Journal of Synthetic Metho
- ORGSYN Database
- MDL® Reference Library of Synthetic
- MDL® Solid-Phase Organic Reactions

**molstructure**

Select Search Type:  
Automatic

Double-click in this box to edit structure

An automatically executed series of searches (Current structure, Include isomers, Include tautomers, Include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.

Query Highlighting.

AND Molecular Formula Contains

AND Molecular Weight =

start search

show brackets save form

Reset  
Delete  
Duplicate  
Info

Delete  
Duplicate  
Info

Delete  
Duplicate  
Info

Drop down pick list for changing database to search

Applet WebClientApplet started

Internet

# Database browser – query form

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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
- cdbrigno
- molstructure
- Pharmacological
- Physical Chemical
- Preparation
- Safety
- Analytical
- Structure based
- Toxicity

Molecular Weight

Contains the calculated molecular weight of the compound.

molstructure

Select Search Type:

- Automatic
- Exact
- Substructure
- Similarity
- Include Isomers

Reset Delete Duplicate Info

Double-click in this box to edit structure

MDL Draw for Database Browser

File Edit Chemistry Help

Done Clear All Undo Redo

Home A-Z Print

Tooltips and Hints

Quick Start

Key differences from CrossFire and MDL ISIS/Draw

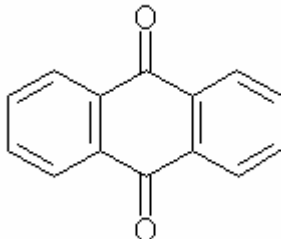
- Use the **Properties tool** to add **query features** for more effective searching.
- Use the **All-Purpose Drawing tool** to draw an entire structure with **one tool**.

Chemical-Drawing Conventions

Preferences and Menus

To **adjust** Help, drag the bar. For **help** on any tool, **click it**.

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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

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	=	<input type="text"/>	Delete Duplicate Info
AND	Molecular Formula	Contains	<input type="text"/>	Delete Duplicate Info
AND	cdbregno	=	<input type="text"/>	Delete Duplicate Info

start search

show brackets save form

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

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Internet

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queries results reports

copy to report export page setup print save refine query lists help logout MDL® Compound Index

Database: MDL® Compound Index ?

Find in History:  Next

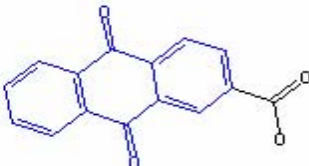
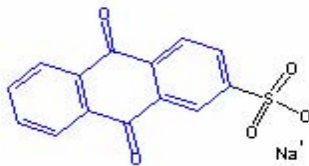
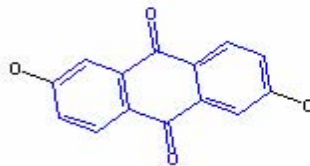
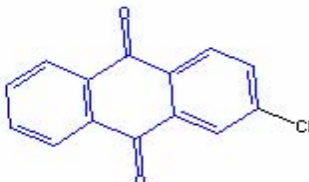
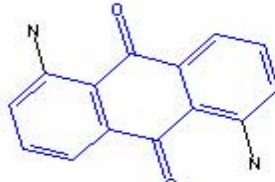
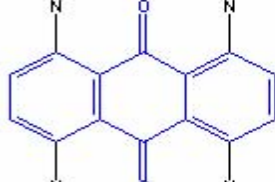
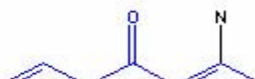
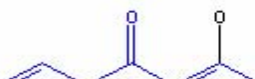
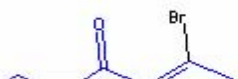
Field Index History

- 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](#)

 <a href="#">Details</a> <input type="checkbox"/> Record#1	 <a href="#">Details</a> <input type="checkbox"/> Record#2	 <a href="#">Details</a> <input type="checkbox"/> Record#3
 <a href="#">Details</a> <input type="checkbox"/> Record#4	 <a href="#">Details</a> <input type="checkbox"/> Record#5	 <a href="#">Details</a> <input type="checkbox"/> Record#6
		

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Database: MDL® Compound Index ?

Find in History:  Next

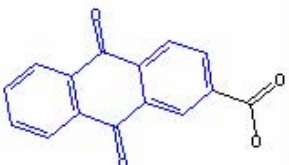
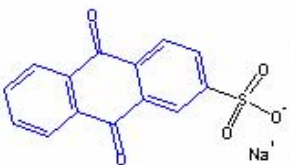
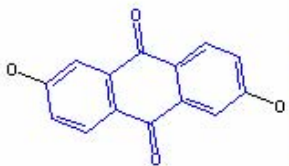
Field Index History

- 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	 <p><input type="checkbox"/> Record#1</p>	<a href="#">ACD</a> <a href="#">CIRX</a> <a href="#">NCI</a> <a href="#">SCD</a>	<a href="#">CCR</a> <a href="#">DWPI</a> <a href="#">Patent Chemistry</a>
2	 <p><input type="checkbox"/> Record#2</p>	<a href="#">ACD</a> <a href="#">DWPI</a> <a href="#">OHS MSDS</a> <a href="#">SCD</a>	<a href="#">CCR</a> <a href="#">NCI</a> <a href="#">Patent Chemistry</a> <a href="#">Toxicity</a>
3		<a href="#">ACD</a> <a href="#">Metabolite</a> <a href="#">OHS MSDS</a> <a href="#">SCD</a>	<a href="#">DWPI</a> <a href="#">NCI</a> <a href="#">Patent Chemistry</a> <a href="#">Toxicity</a>

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# Results 3 – Properties View

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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	 <input type="checkbox"/> Record#1	<a href="#">3d Configuration</a> <a href="#">Analytical</a> <a href="#">Commercially Available</a> <a href="#">Name</a> <a href="#">Physical Chemical</a>	<a href="#">Agrochemical</a> <a href="#">Chemical</a> <a href="#">Literature Reference</a> <a href="#">Pharmacological</a> <a href="#">Preparation</a>
2	 <input type="checkbox"/> Record#2	<a href="#">3d Configuration</a> <a href="#">Analytical</a> <a href="#">Commercially Available</a> <a href="#">Name</a> <a href="#">Preparation</a> <a href="#">Toxicity</a>	<a href="#">Agrochemical</a> <a href="#">Chemical</a> <a href="#">Literature Reference</a> <a href="#">Pharmacological</a> <a href="#">Safety</a>
3	 <input type="checkbox"/> Record#3	<a href="#">3d Configuration</a> <a href="#">Chemical</a> <a href="#">Literature Reference</a> <a href="#">Name</a> <a href="#">Preparation</a>	<a href="#">ADME</a> <a href="#">Commercially Available</a> <a href="#">Metabolism</a> <a href="#">Pharmacological</a> <a href="#">Safety</a>

View summary by clicking on hyperlink

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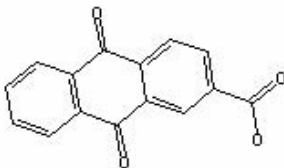
Database: MDL® Compound Index ?

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Record # 1 → Total Records: 15

## MDL® Available Chemicals Directory



**Available Data**

*Click on a link to add the information to this page*

Set current view as default

[Substance](#) (1)      [Suppliers](#) (9)

[Prices](#) (9)      [Model](#) (1)

**Substance** [\(hide\)](#)

ACD Registry Number	1191
MDL Number	MFC00001231
CAS Registry Number	117-78-2
<b>Chemical Name and Synonyms :</b>	
<ul style="list-style-type: none"> <li>9,10-DIHYDRO-9,10-DIOXO-2-ANTHRACENECARBOXYLIC ACID</li> <li>9,10-DIOXO-9,10-DIHYDRO-ANTHRACENE-2-CARBOXYLIC ACID</li> <li>ANTHRAQUINONE-2-CARBOXYLIC ACID</li> </ul>	
Molecular Formula	C15 H8 O4
Molecular Weight	252.224
Rule of Five	0
Computed partition coefficient	

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Internet

Indexed databases linked based on common structures

# 'Jumping' DBs: CI to CCR

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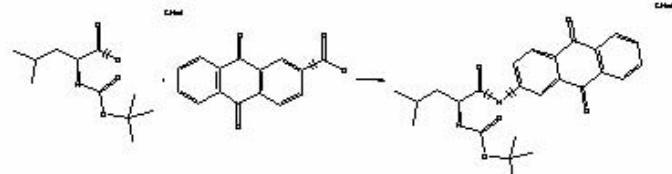
Database: MDL® Compound Index ?

[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	

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Commercial availability

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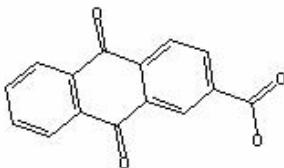
Database: MDL® Compound Index ?

[Return to MDL® Compound Index](#)

[CCR](#) [CIRX](#) [DWPI](#) [NCI](#) [Patent Chemistry](#) [SCD](#)

Record # 1 → Total Records: 15

## MDL® Available Chemicals Directory



**Available Data**

*Click on a link to add the information to this page*

Set current view as default

[Substance](#) (1)      [Suppliers](#) (9)

[Prices](#) (9)      [Model](#) (1)

**Prices** [\(hide\)](#)

<a href="#">ALDRICH</a> (1 of 9)				
Catalog Number	Package Size	Package Price	Purity	Other Info
25,272-7	250 MG	USD 20.80	98%	117-78-2 ANTHRAQUINONE-2-CARBOXYLIC ACID
25,272-7	1 G	USD 38.40	98%	
25,272-7	5 G	USD 127.00	98%	
25,272-7		USD POA	98%	

<a href="#">APOLLO-CHEM</a> (2 of 9)				
Catalog Number	Package Size	Package Price	Purity	Other Info
OR7750		UKL POA		117-78-2 ANTHRAQUINONE-2-CARBOXYLIC ACID

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Internet

View Supplier data for reaction components with a single click!

Return to reaction Db with another click!

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queries results reports

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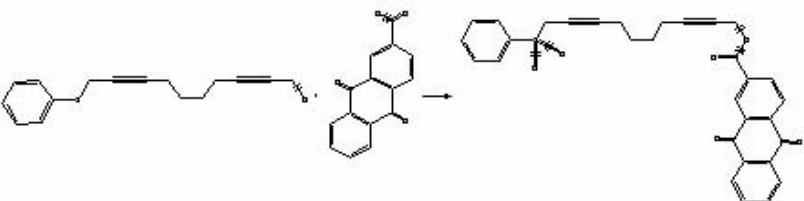
Database: MDL® Compound Index ?

[Return to MDL® Compound Index](#) [Find Similar Reactions](#)

[ACD](#) [CCR](#) [DWPI](#) [NCI](#) [Patent Chemistry](#) [SCD](#)

← Record # 8 → Total Records: 15

## ChemInform Reaction Library



**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 [\(hide\)](#)

RXC190510473 Reaction Variation 1 of 1

Product no.	% Yield	Grade	%cs	%ds	%de	%ee	Reactant no.	Reactant Grade
1	47 - 69		100				1	
							2	

Applet WebClientApplet started

Internet

“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

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 Version

Database:

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

molstructure

Select Search Type:

Automatic

Double-click in this box to edit structure

An automatically executed series of searches (Current structure, include isomers, include tautomers, include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.

Query Highlighting.

Reset Delete Duplicate Info

start search

show brackets save form

Applet WebClientApplet started



# Draw your query form

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 Chemical Sourcing and Logistics Information Version

Database: Chemical Sourcing and Logistics ... ?

Find in Field Index: [ ] Next

Field Index History

- Molecule
  - Structure
  - ACD Registry Number
  - CAS Registry Number
  - Catalog Number
  - Chemical Name and Synonyms
  - Computed partition coefficient (CL)
  - MDL Number
  - Molecular Formula
  - Molecular Weight
  - Molecular weight of largest fragment
  - New Chemical
  - Number of proton acceptors
  - Number of proton donors
  - Number of rotatable bonds (TDF)
  - Rule of 5
  - Supplier Name

**Molecule**

Structure

Select Search Type: Automatic

Double-click in this box to edit structure

An automatically executed series of searches (Current structure, Include isomers, Include tautomers, Include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database.

Query Highlighting.

AND Catalog Number Contains [ ]

AND Chemical Name and Synonyms Contains polypropylene

AND CAS Registry Number Ends with

AND MDL Number Exists

AND Supplier Name Contains [ ]

start search

Applet WebClientApplet started

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 Chemical Sourcing and Logistics Information Version

Database: Chemical Sourcing and Lo... ?

Find in History: [ ] Next

Field Index History

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

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 (4) Prices (4) Model (1)

Prices [\(hide\)](#)

**ALDRICH (1 of 4)**

Catalog Number	Package Size	Package Price	Purity	Other Info
41,911-7	250 G	USD 24.80		25266-02-8 POLY(MALEIC ANHYDRIDE-ALT-1-OCTADECENE)
41,911-7	1 KG	USD 68.20		1. AVERAGE MN 30,000-50,000
41,911-7		USD POA		2. FREE FLOWING POWDER 3. IRRITANT

**DOW-CHEMICAL (2 of 4)**

Catalog Number	Package Size	Package Price	Purity	Other Info
(000914)		POA		POLYPROPYLENE

**POLYSCI (3 of 4)**

Applet WebClientApplet started

Internet



# DiscoveryGate 2.0

LINKING FROM SCOPUS  
TO CROSSFIRE COMMANDER

# LINKING FROM SCOPUS TO CROSSFIRE COMMANDER

## CROSSFIRE COMMANDER

- It is 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

**SCOPUS** Register or Login:  username Password:   [Athens Login](#)

[Scopus Labs](#) [Help](#)

Quick Search   [Search Tips](#) Brought to you by [Scopus Team](#) [Library catalogue](#)

[results list](#) [previous](#) 9 of 17 [next](#)

[Tetrahedron Letters](#)  
Volume 35, Issue 14, 1994, Pages 2113-2116

DOI: 10.1016/S0040-4039(00)76773-6

Document Type: Article

**Mono-N-alkylation of anthranilamides via quinazolinones. An efficient synthesis of G5598, a benzodiazepine dione gpIIbIIIa antagonist**

[Webb II, R.R.](#), [Barker, P.L.](#), [Baier, M.](#), [Reynolds, M.E.](#), [Robarge, K.D.](#), [Blackburn, B.K.](#), [tischler, M.H.](#), [Weese, K.J.](#)

Genentech, Inc., 460 Pt. San Bruno Blvd., South San Francisco, CA 94080, United States

**Abstract**

The mono-N-**akylation** of an anthranilamide derivative via the reductive ring opening of a quinazoline precursor, enables the synthesis of benzodiazepine dione derivative G5598, a potent inhibitor of the in vitro binding of GPIIbIIIa to fibrinogen.

Information from the Beilstein Database

[View Compounds](#) [View Reactions](#)

**Cited By**

This article has been cited **17** times in Scopus:  
(Showing the 3 most recent)

- [Lakhrissi, B., Massoui, M.](#) **Synthesis of N',N'-diglucosylated benzimidazol-2-one via an unexpected rearrangement of benzodiazepine derivative** (2005) *Heterocyclic Communications*
- [Van Berkom, L.W.A., De Gelder, R.](#) **6-Spiro-1,4-diazepane-2,5-diones by head-to-tail N1/C2 amide bond formation** (2005) *European Journal of Organic Chemistry*
- [Lakhrissi, B., Massoui, M.](#) **The unexpected rearrangement of 1,5-benzodiazepin-2,4-dione to a benzimidazol-2-one**

Links to CrossFire Beilstein database via CrossFire Commander

# From Scopus to CrossFire Commander: Compound Summary Page

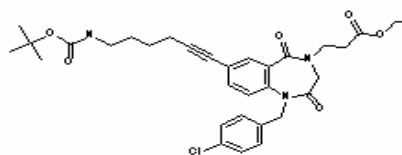
http://scopus-ls.mdli.com - Scopus - Chemical Compounds - Microsoft Internet Explorer

The following information is from the

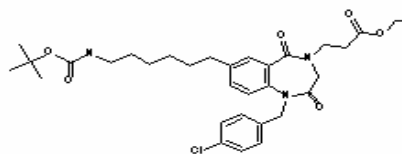
Webb, Robert R., II; Barker, Peter L.  
**Mono-N-Alkylation of Anthranyla**  
**Benzodiazepine Dione GpIIBIIIa**  
 1994, *Tetrahedron Lett.*, **35** (14), p

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

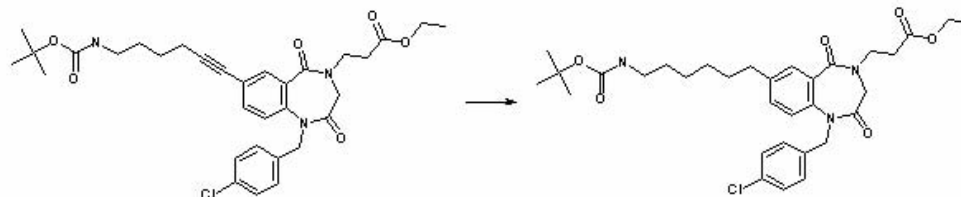
[Help](#) [close](#)

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

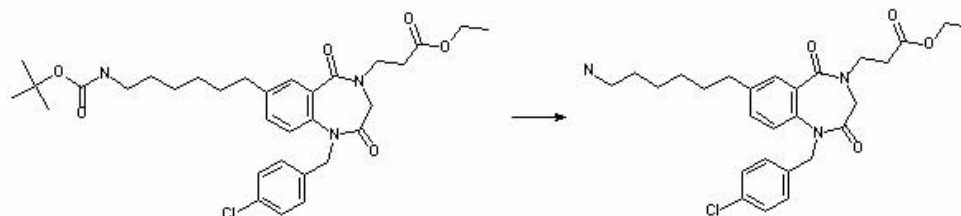
1.



Reaction number	Reaction conditions
3689284	H2 PtO2 ethanol

For more information access the Beilstein Database via:  
[CrossFire Commander](#)

2.





LIVE DEMONSTRATION

[WWW.DISCOVERYGATE.COM/20](http://WWW.DISCOVERYGATE.COM/20)



DiscoveryGate

WHAT'S **NEW** IN DISCOVERYGATE!

DiscoveryGate

Welcome to DiscoveryGate

[Home](#) | [Support](#) | [Logout](#) | [Login as different user](#)

## DOWNLOAD DISCOVERYGATE 2.0

**Note :** You must have administrative privileges or be authorized by your system administrator to install DiscoveryGate software.

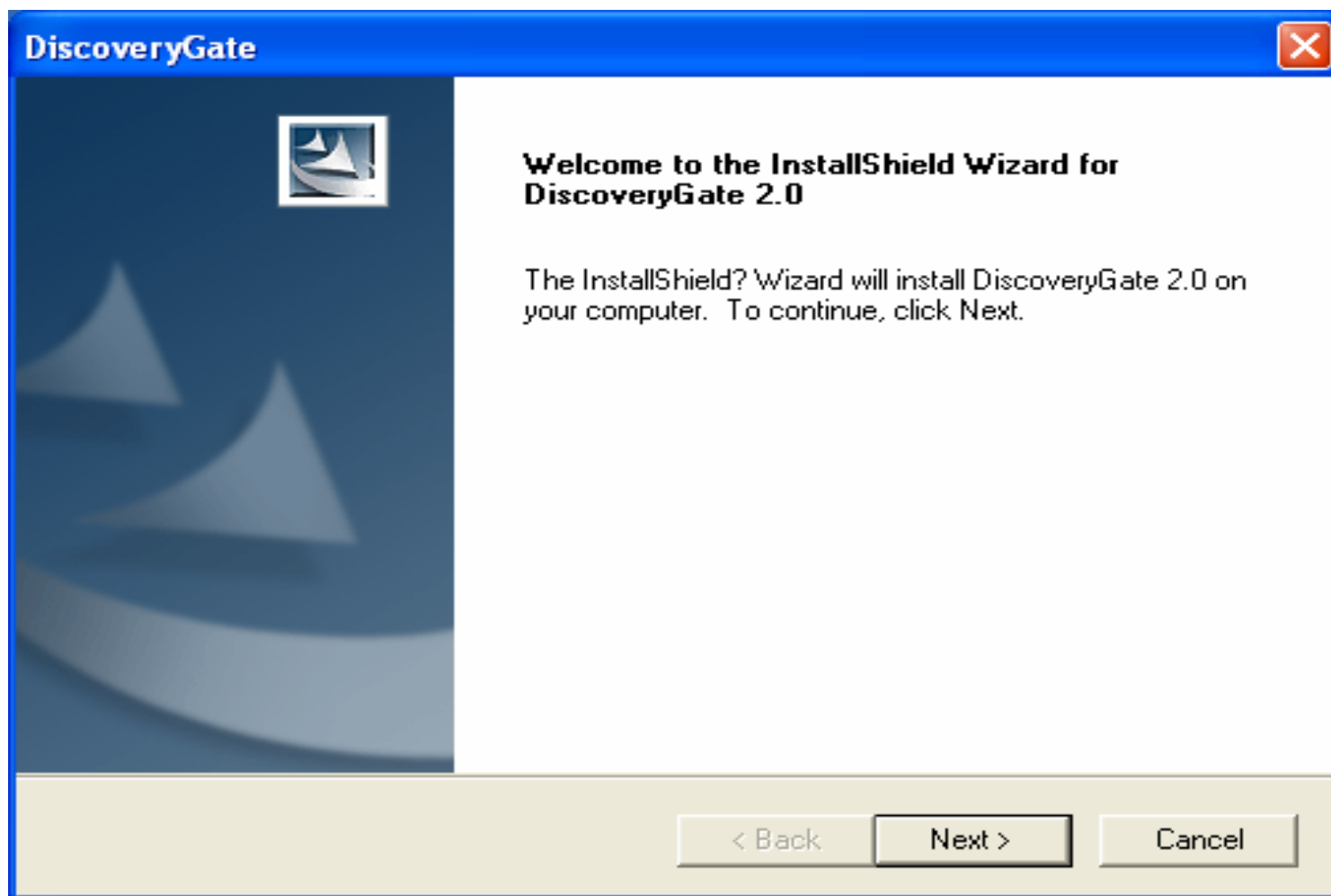
1. **Save the installer to your Desktop**  
Installer Size: +/- 37.7MB  
File Name:DiscoveryGate20.exe
2. **Save the DiscoveryGate Installation Guide (PDF)** (optional)  
Last Updated:May 2005
3. **Close all Internet Explorer Browser windows (and any IE processes running in the Task Manager) and then run the DiscoveryGate Installer.**

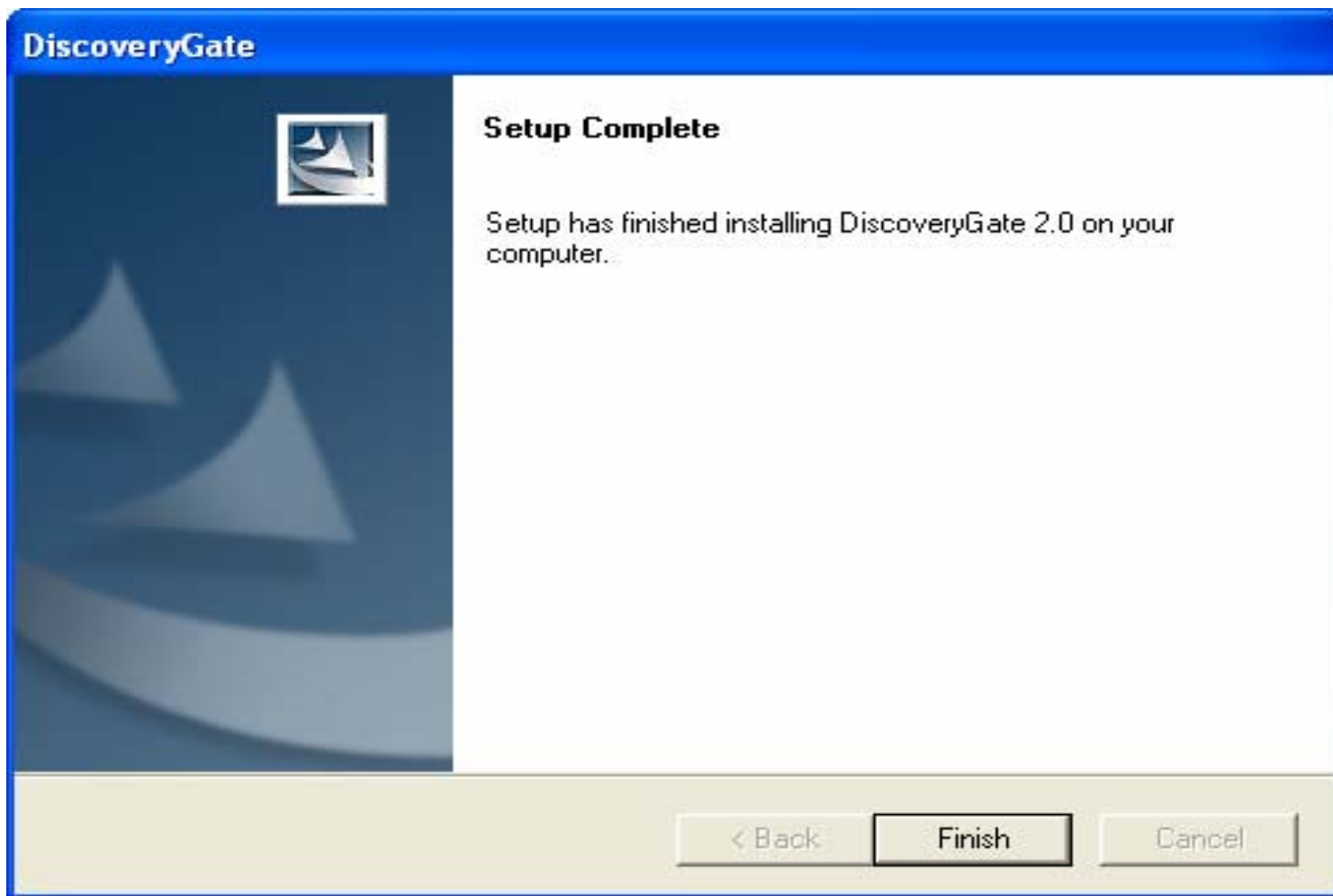
[Click Here](#) to continue if no installation is needed:

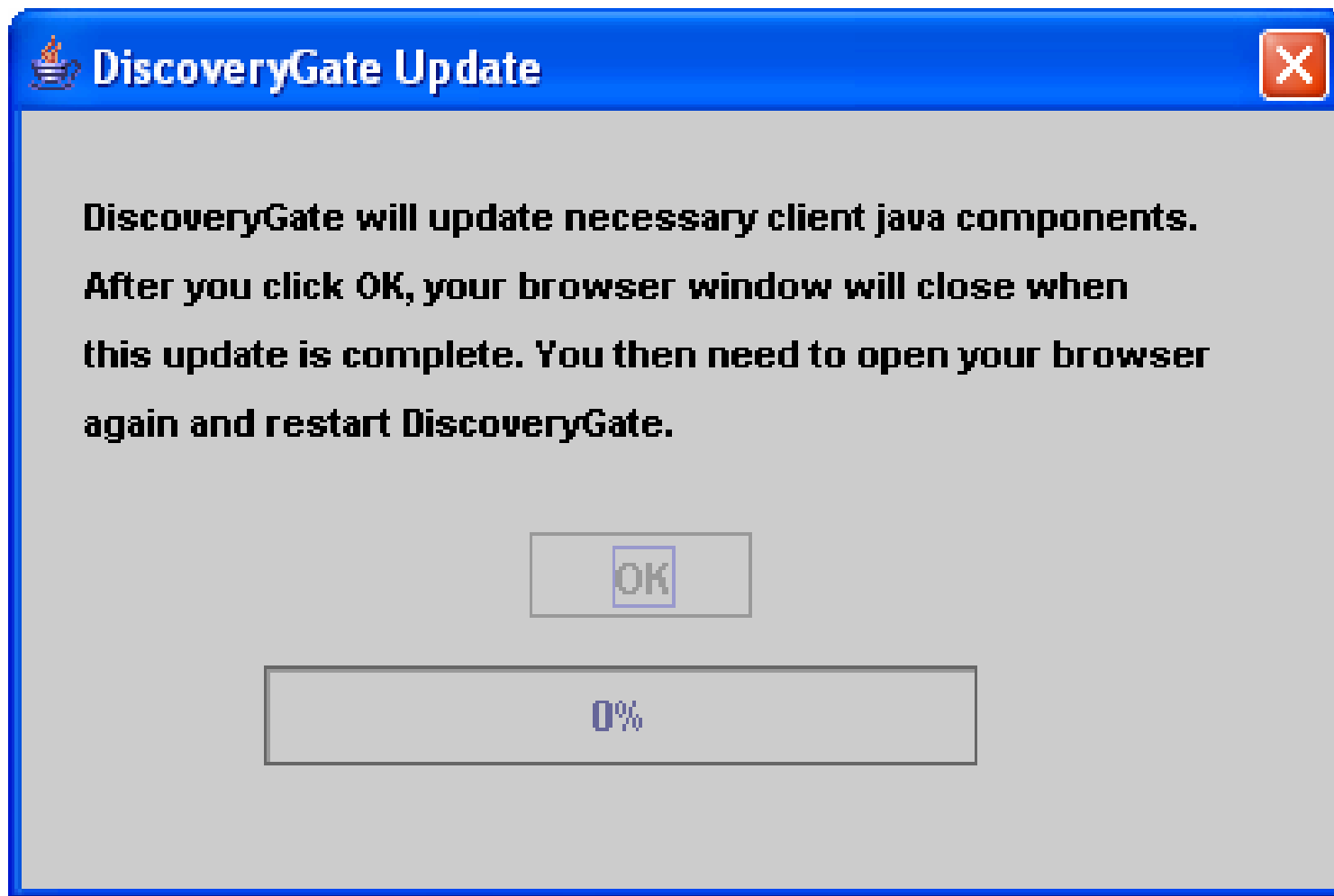
- A) XPharm-Only Users
- B) LinkFinderPlus-Only Users

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











# 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 Properties**

Property	Calculated Value	Experimental Value
H donors	1	
H acceptors	2	
Molecular Weight	204.26	
logP	4.312±0.350	
logD	4.31	pH 1
logD	3.97	pH 4
logD	1.27	pH 7
logD	0.52	pH 8
logD	0.22	pH 10
pKa	3.92±0.20	Most A
Molar Solubility	Sparingly Soluble	pH 1
Molar Solubility	Sparingly Soluble	pH 4
Molar Solubility	Slightly Soluble	pH 7
Molar Solubility	Soluble	pH 8
Molar Solubility	Soluble	pH 10
Melting Point	88.5-92.8 °C	Solv: h (110-54)

**DiscoveryGate Search Criteria**

AND	clogP (Syracuse Research Cen	<	5.5	Delete Duplicate Info
AND	Proton Acceptors (O+N)	>	1	Delete Duplicate Info
AND	Proton Donors	>	2	Delete Duplicate Info
AND	Torsional degree of freedom	>	4	Delete Duplicate Info

**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



- 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 RDFFile, 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](mailto:D.Tan@elsevier.com)
- For further information, visit [www.discoverygate.com](http://www.discoverygate.com) or [www.mdl.com/products/knowledge/index.jsp](http://www.mdl.com/products/knowledge/index.jsp)
- Personal 14-day trial coming soon



# PRICING MODEL

FOR ACADEMICS & GOVERNMENT  
INSTITUTIONS

# PRICING MODEL & FEATURES

<i>Population Band*</i>		<i>2005 Subscription US\$</i>		
<i>Lower limit</i>	<i>Upper limit</i>	<i>DiscoveryGate</i>	<i>xPharm</i>	<i>Patent Chemistry Database</i>
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.