

Crossfire Beilstein/Gmelin 使用方法介绍

陈湘萍

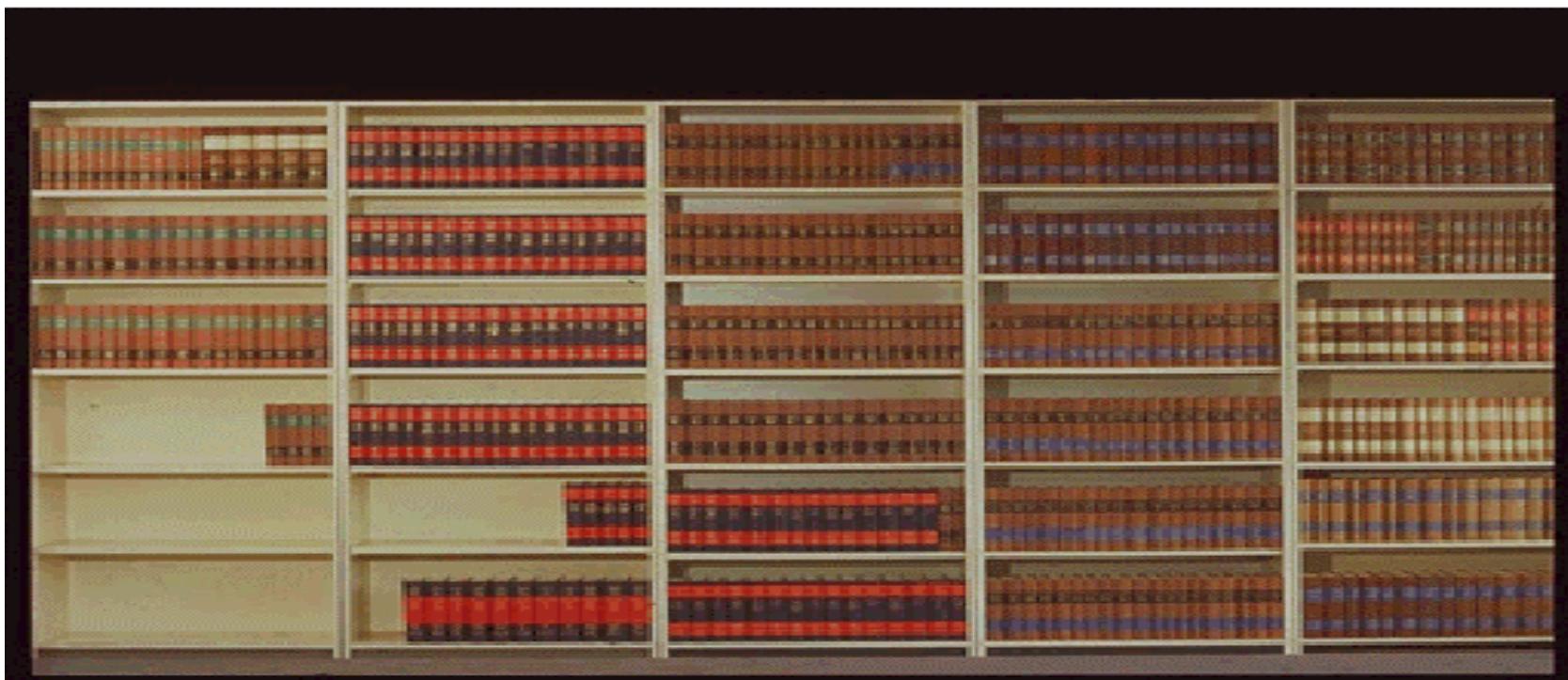
创腾科技有限公司

www.neotrident.com

Beilstein – 世界最全的有机化学数值和事实库

- 简单易用

- ✓ 界面友好，操作简单，任何有化学或相关背景的人都可以轻易上手
- ✓ 电子版本，检索方便，结果便于复制、保存和打印



印刷版的Beilstein

• 数据准确，可靠，全面

- ✓ 时间跨度从1771年至今
- ✓ 精选180种权威杂志
- ✓ 化学结构相关的化学、物理等方面的性质
- ✓ 化学反应相关的各种数据
- ✓ 详细的药理学，环境病毒学，生态学等最全面的信息资源



•功能强大

✓强大的搜寻引擎：

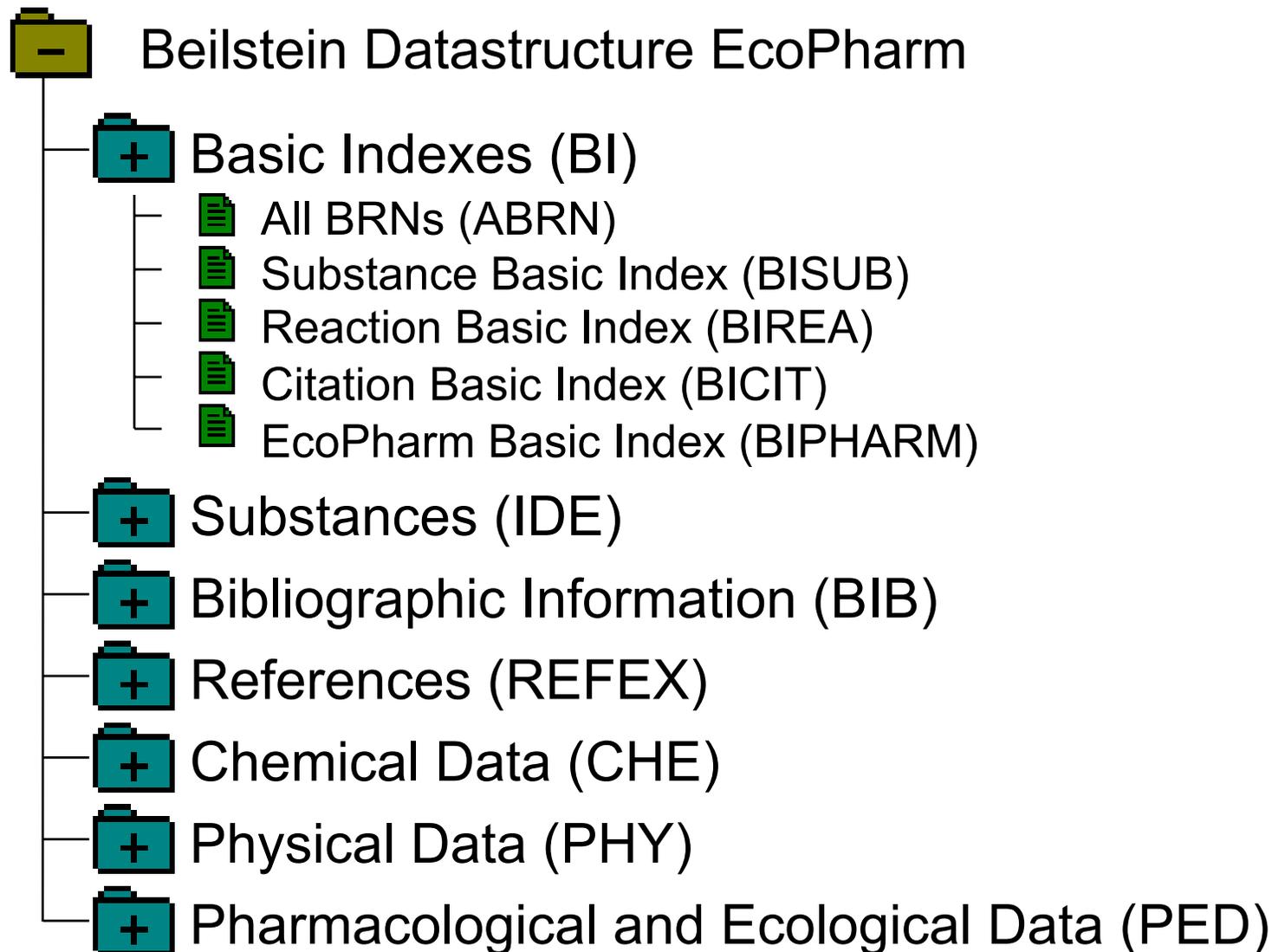
近百种高级查询方式：可以通过包括结构，子结构，反应，物化数据，制备条件以及关键字在内的近百种高级查询来方便灵活得到您需要的信息。

超过5000万个超级链接：在不同的数据类型间进行全面的搜索。

✓能够全面了解已有化合物的各方面信息：生物活性、代谢、吸收、分布和毒理信息，以及它们的红外、紫外、质谱、核磁等仪器分析信息，以快速确定所合成化合物的结构和成分。

✓能够了解最新最全的合成和反应信息：为反应和合成路线设计提供最全面的信息帮助。

☐ 全方位的搜索引擎



Gmelin – 全面的无机化学数值和事实库

- ✓ 从1772年至今，3个月更新一次
- ✓ 涵盖无机和金属有机化合物
- ✓ 相关的理化性质、结构数据
- ✓ 制备过程以及相关反应
- ✓ 详细的地质学，矿物学，冶金学等方面的信息资源。
 - 超过**2百万**的化合物
 - 超过110万篇文献
 - 超过15万篇摘要
 - 超过160万个可查询反应

Commander 7.0的使用界面

The screenshot shows the MDL CrossFire Commander 7.0 interface. The main window is titled "MDL CrossFire Commander - [Query for Server default]". The menu bar includes File, Edit, Task, View, Options, Query, and Help. The toolbar contains buttons for Query, Results, Reports, Alerts, and AutoNom. Below the toolbar is a navigation bar with buttons for Query History, Open Query, Save Query, Print Query, Clear Query, Select Database, Draw Structure, Modify Alert, Create Alert, and Start Search.

The interface is divided into several sections:

- Left Panel:** A tree view showing "Predefined Search Forms" and "Hitsets". Under "Hitsets", there is a folder "Beilstein(2004/02)" containing sub-items: "Basic Indexes", "Bibliographic Information", "Substance Identification", "Chemical Properties", "Physical Properties", and "Pharmacological and Ecological".
- Query Builder:** A large central area for building queries. It contains the text: "Structure/Reaction Search", "Double click to enter the Structure/Reaction editor.", and "Right click to copy or paste the structure." To the right of this area are several options: "Free Sites:" (hetero atom, all atom), "Stereo:" (off), "Search:" (as structure, as reactant, as product, as reagent, as, as), and "Allow:" (salts, addl. rings, isotopes, charges, radicals, mixtures, relat. Markus). There are also "Clear Structure" and "Extended Options" buttons.
- Search All Text:** A search bar with a dropdown menu set to "and", the text "antibiotic", and buttons for "Truncate..." and "Clear Text".
- Search Fields:** A table for defining search criteria. It has columns for "Operator", "Field name", "Relation", and "Field content". The table contains three rows: Row 1: Operator "and", Field name "", Relation "is", Field content ""; Row 2: Operator "and", Field name "", Relation "is", Field content ""; Row 3: Operator "and", Field name "", Relation "is", Field content ". Buttons for "Enlarge...", "Advanced Search", and "Clear Table" are present.
- Bottom:** A "Search" button, a dropdown menu set to "Substances", and a "Start Search" button.

Red annotations highlight specific features:

- A red box around the left panel is labeled "快速数据检索" (Fast Data Retrieval).
- A red box around the Query Builder area is labeled "结构检索" (Structure Retrieval).
- A red box around the Search All Text bar is labeled "关键字检索" (Keyword Retrieval).
- A red box around the Search Fields table is labeled "快速数据检索" (Fast Data Retrieval).

数据库选择

MDL CrossFire Commander - [Query for Server default]

File Edit Task View Options Query Help

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Query History | Open Query | Save Query | Print Query | Clear Query | **Select Database** | Draw Structure | Modify Alert | Create Alert | Start Search

Search Field Name in ?

Predefined Search Forms

Hitsets

Beilstein (2004/02)

- Basic I
- Bibliog
- Substan
- Chemica
- Physica
- Pharmac

Free Sites:
 hetero atom ?
 all atom

Stereo: off ?

Search: ?

Allow:
 salts
 addl. rings
 isotopes
 charges
 radicals
 mixtures
 relat. Markus

Extended Options

Select databases to be searched

Please check one or more databases:

- Smelin (2004/02)
- Beilstein (2004/02)

Click on a database to see information

Please note:
If you have selected multiple databases, the tree "All Search Fields" offers only fields common to all databases. Fields available in one database only are hidden.

Cancel Help... OK

and Search Fields ?

Enlarge... Advanced Search Clear Table

	Operator	(Field name	Relation	Field content	List)
1				is			
2	and			is			
3	and			is			

Search Substances Start Search

For Help, press F1

idle

关键字检索

The screenshot displays the MDL CrossFire Commander interface. The main window title is "MDL CrossFire Commander - [Query for Server default]". The menu bar includes File, Edit, Task, View, Options, Query, and Help. The toolbar contains buttons for Query, Results, Reports, Alerts, and AutoNom. Below the toolbar, there are buttons for Query History, Open Query, Save Query, Print Query, Clear Query, Select Database, Draw Structure, Modify Alert, Create Alert, and Start Search.

The interface is divided into several sections:

- Search Field Name in:** A dropdown menu with a "Find" button.
- Predefined Search Forms:** A list of search forms including Hitsets, Beilstein(2004/02), Basic Indexes, Bibliographic Information, Substance Identification, Chemical Properties, Physical Properties, and Pharmacological and Eco.
- Query Builder:** A large central area for building queries. It contains the text: "Structure/Reaction Search. Double click to enter the Structure/Reaction editor. Right click to copy or paste the structure."
- Free Sites:** Checkboxes for "hetero atom" and "all atom".
- Stereo:** A dropdown menu set to "off".
- Search:** Radio buttons for "as structure", "as reactant", "as product", and "as reagent".
- Allow:** Checkboxes for "salts", "addl. rings", "isotopes", "charges", "radicals", "mixtures", and "relat. Markus".
- Buttons:** "Clear Structure" and "Extended Options".

A red box highlights the search input area at the bottom of the interface:

- Search All Text:** A dropdown menu set to "and" and a text input field containing "antibiotic".
- Search Fields:** A dropdown menu set to "and" and a table for defining search criteria.
- Buttons:** "Enlarge...", "Advanced Search", and "Clear Table".
- Table:** A table with columns for Operator, Field name, Relation, Field content, List, and a right arrow. It contains three rows, all with "and" in the Operator column and "is" in the Relation column.
- Search:** A dropdown menu set to "Substances" and a "Start Search" button.

At the bottom of the window, there is a status bar with the text "For Help, press F1" and "idle".

检索环境的选择

Text Search

Preview
The following bars indicate the estimated frequency of a word in the selected databases. Please select the contexts in which you want to search your words.

Search Word in Context...	SUBSTANCES Substance Properties BISUB	REACTIONS Reaction Data BIREA	CITATIONS [AU, TI, AB, ...] BICIT
<input checked="" type="checkbox"/> antibiotic*			
Select Context:	<input checked="" type="checkbox"/> Substances	<input type="checkbox"/> Reactions	<input type="checkbox"/> Citations

■ Beilstein(2004/02)

Please note:

- Different contexts may give different hits. Search more than 1 context to be comprehensive! Results from different databases and contexts are displayed in different windows.
- Words from bibliographic data (Author, Patent Assignee, Journal Name, Patent Number, ...) are NOT searchable in SUBSTANCES or REACTIONS. Please uncheck words in the left column and use DATA SEARCH for these words to get records.
- Substance property data and reaction data are not searchable in Citation Context.

Search Plan
The following searches will be conducted in database(s) Beilstein (2004/02) (1 search(es)):

Beilstein(2004/02) (Substances)	antibiotic*
------------------------------------	-------------

Hitsets will be given in separate windows!

Cancel Help Start Search

定义查询的索引以及查询结果的显示方式。

检索结果的Grid方式显示

红色标记表示有生物活性的化合物

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Substances: hit 8 of 3803

History | Print Hits | View all | Show | Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to report

[-] Gmelin(2004/03)
[-] Beilstein(2004/03)
[-] Saved Hitsets/Alert Hitsets
[-] Session Hitsets
[-] Q: Q01 [3803 Substan...

Hit 1 BRN=15789 C ₆ H ₁₂ S ₄ ;Bio(4)	Hit 2 BRN=2012 C ₈ H ₉ N ₃ ;Bio(255)	Hit 3 BRN=3132 C ₆₆ H ₇₅ Cl ₂ N ₉ O ₂₄ ;Bio(188..)
Hit 4 BRN=5113 C ₁₀ H ₁₁ NO	Hit 5 BRN=9394 C ₉ H ₄ O ₅ ;Bio(78)	Hit 6 BRN=11744 C ₇ H ₁₅ Cl ₂ N ₂ O ₂ P;Bio(655)
Hit 7 BRN=15789 C ₁₅ H ₁₀ O ₃ ;Bio(40)	Hit 8 BRN=17705 C ₈ H ₁₀ N	
Hit 10 BRN=22135 C ₁₇ H ₂₅ N ₃ O ₃	Hit 11 BRN=23917 C ₂₁ H ₃₀ O ₂ ;Bio(167)	Hit 12 BRN=26714 C ₁₂ H ₂₆ N ₄ O ₆ ;Bio(27)

For Help, press F1

idle GRID Substances

双击某条记录，即可查看详细内容。

检索结果的List方式显示

可将化合物或反应用单独的窗口显示

MDL CrossFire Commander

Query Results Reports Alerts

History | Print Hits | View all | Show Grid List | Get | Sort Hits | Copy | Export Hits | Copy to Report

Substance Identification

Beilstein Registry Number	17705
Beilstein Preferred RN	58-08-2
CAS Registry Number	58-08-2
Chemical Name	1,3,7-trimethyl-3,7-dihydro-purine-2,6-dione 1,3,7-Trimethyl-3,7-dihydro-purin-2,6-dion, Kaffein caffeine 3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione
Autoname	1,3,7-trimethyl-3,7-dihydro-purine-2,6-dione
Molecular Formula	C ₈ H ₁₀ N ₄ O ₂
Molecular Weight	194.19
Lawson Number	30517, 2817
Type of Substance	heterocyclic
Constitution ID	12360
Tautomer ID	4946
Beilstein Reference	0-26-00-00461, 1-26-00-00136, 2-26-00-00266, 4-26-00-02338, 5-26-13-00558, 6-26

Field Availability List 1-10 of 69

Code	Field Name	Occ.
PHARM	Bioactivity: Pharmacological Data	584
ECT	Ecological Data: Ecotoxicology	57
ECA	Ecological Data: Exposure Assessment	1
ECC	Ecological Data: Concentration in the Environment	11
ECTD	Ecological Data: Transport and Distribution	2
BIOD	Ecological Data: Biodegradation	1
ECDH	Ecological Data: Abiotic Degradation, Hydrolysis	1
ECDP	Ecological Data: Abiotic Degradation, Photolysis	1
RX	Reaction	97
RSTR	Related Structure	11

Q01: Hit 8

CN1C=NC2=C1C(=O)N(C)C(=O)N2C

可访问数据内容总列表 (共69条)

超链接, 可以通过点击链接到相关的数据内容

相关数据的数量

对所链接的数据内容的描述

通过超链接访问药理学方面的数据和事实

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Substances: hit 8 of 3803

History Print Hits View all Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Gmelin(2004/03)
Beilstein(2004/03)
Saved Hitsets/Alert Hitsets
Session Hitsets
Q: Q01 (3803 Substances)

Pharmacological Data 1 of 584

Effect	cell migration; inhibition of
Species or Test-System	Wistar rat neurospheres
Concentration	10 - 50 mg/l
Method	migration assay; primary neurospheres plated on poly(D-lysine)-coated six-well plates; 10 ng/ml EGF used as reference comp.
Note 1	No effect
Ref. 1	6437113, LitLink ; Journal; Chen, Chia-Nan; Lian, Jen-Kun; JAFCAU; J.Agric.Food Chem.; EN; 51; 25; 2003; 7495 - 7503.

Pharmacological Data 2 of 584

Effect	cell adhesion; inhibition of
Species or Test-System	Wistar rat neurospheres
Concentration	10 - 50 mg/l
Method	neural stem cell adhesion assay; primary neurospheres plated on poly(D-lysine)-coated six-well plates; serum-free B27-supplemented neurobasal medium; humidified 5 percent CO2/95 percent air atmosphere; 37 deg C; incubated for 24 h to evaluate adhesion
Further Details	10 ng/ml EGF used as reference comp.
Note 1	No effect
Ref. 1	6437113, LitLink ; Journal; Chen, Chia-Nan; Lian, Jen-Kun; JAFCAU; J.Agric.Food Chem.; EN; 51; 25; 2003; 7495 - 7503.

Pharmacological Data 3 of 584

Effect	drug interaction
Species or Test-System	man
Sex	male
Route of Application	peroral
Concentration	100 mg
Kind of Dosing	each subject received a total of 7 regimens with a minimum 1-week washout period in between
Method	14 healthy volunt. (mean 21.6 y, 72.1 kg; nonsmok.; no caffeine, alcohol or medication); fasted ON; random. crossover study; title comp. alone or in comb. with 100 mg dapsone, 10 mg debrisoquin, 100 mg mephenytoin; W/O 250 mg chlorzoxazone; HPLC anal.
Further Details	poor metabolizers of CYP2D6 were excluded from the study; HPLC analysis of plasma samples (before, 4 and 8 h after title comp.) and collec. urine (0-8 h after title comp.); ON: over night; W/O: with or without

For Help, press F1

idle ALL: Substance as Product Substances

亦可通过超链接
访问文献记录

每条记录都有对测试条件,
方法, 以及结果等方面的
详细数据。

文献记录的显示

MDL CrossFire Commander

Query Results Reports Alerts AutoHom

Substances: hit 1 of 462

History | Print Hits | View all | Show Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report

Smelin(2004/03)
Beilstein(2004/03)
Saved Hitsets/Alert Hitsets
Session Hitsets
Q: Q01 (3803 Substances)
Q: Q02 (462 Substances)
L: 6437113 (1 Citations)

Citation Number [LitLink](#)
Citation Number **6437113**

Field Availability List 1-3

Code	Field Name	Occ.
CIT	Citation	1
AB	Abstract	1
IDE	Substance Identification	3

Citation

Document Type: Journal
Authors: Chen, Chia-Nan; Liang, Chia-Min; Lai, Jueng-Rong; Tsai, Yao-Jen; Tsay, Jyh-Shyan; Lin, Jen-Kun
CODEN: JAFCAU
Journal Title: J.Agric.Food Chem.
Language Code: EN
(Series) Volume: 51
Number: 25
Publication Year: 2003
Page: 7495 - 7503

Abstract

Title: Capillary Electrophoretic Determination of Theanine, Caffeine, and Catechins in Fresh Tea Leaves and Oolong Tea and Their Effects on Rat Neurosphere Adhesion and Migration

Abstract: Theanine, caffeine, and catechins in fresh tea leaves and oolong tea were determined by using capillary electrophoresis (CE). CE separated these tea polyphenols from three other tea ingredients, namely, caffeine, theophylline, and theanine, within 8 min. The young leaves (apical bud and the two youngest leaves) were found to be richer in caffeine, (-)-epigallocatechin gallate (EGCg), and (-)-epicatechin gallate (ECg) than old leaves (from 5th to 7th leaves). On the other hand, the old leaves (from 8th to 10th leaves) contained higher levels of theanine, (-)-epigallocatechin (EGC), and (-)-epicatechin (EC). Results from a comparison of fresh young tea and oolong tea compositions indicated oolong tea contained more theanine and catechins than fresh young tea. Furthermore, it was found that the levels of theanine, EGC, and EGCg in young leaves rose markedly with the withering process. Caffeine did not markedly change. However, fully or partially fermented teas (oolong tea or pauchong tea) have a common initial step in the withering process. Fresh tea leaves or oolong tea extract (0.1 percent, w/w) markedly inhibited neurosphere adhesion, cell migration, and neurite outgrowth in rat neurospheres. Theanine (348 µg/mL)

For Help, press F1 | idle | ALL | Citations

文献记录提供文献的引用情况和重新整理过的摘要。

File Edit Task **View** Options Window Help

MDL Cross

History | Print Hits |

- Grid View / List View F4
- Open Hitset in Grid View
- All Fields
 - Identification Data only
 - Hit only
 - Select User View
 - Define User View...
- Highlight Hit Terms
 - Selected Hits only
 - Goto Hit
- Structures included** F2
 - Structure in separate window
 - All Reactions
 - Substance as Reactant only
 - Substance as Product only
- Update Dates included
- Field Availability included
 - Field Availability in separate window... F5
- Show Hitset History... F6
- Show Tree View F3
- Show Status Bar

Query Results Reports Alerts AutoNom Substances: hit 8 of 3803

Grid List Get Sort Hits Copy Export Hits Copy to Report

17705

58-08-2

58-08-2

1,3,7-trimethyl-3,7-dihydro-purine-2,6-dione

1,3,7-Trimethyl-3,7-dihydro-purin-2,6-dion, Kaffein

caffeine

3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione

1,3,7-trimethyl-3,7-dihydro-purine-2,6-dione

C8H10N4O2

94.19

0517, 2817

aromatic

2360

946

0-26-00-00461, 1-26-00-00136, 2-26-00-00266, 4-26-00-02338, 5-26-13-00558, 6-26

-10 of 69

	Occ.
Ecotoxicology	584
Ecotoxicology	57
ECA Ecological Data: Exposure Assessment	1
ECC Ecological Data: Concentration in the Environment	11
ECTD Ecological Data: Transport and Distribution	2
BIOD Ecological Data: Biodegradation	1
ECDH Ecological Data: Abiotic Degradation, Hydrolysis	1
ECDP Ecological Data: Abiotic Degradation, Photolysis	1
RX Reaction	97
RSTR Related Structure	11

For Help, press F1

idle ALL: Substance as Product Substances

对记录中的化合物结构和反应显示方法的定义

MDL CrossFire Commander

Substances: hit 8 of 3803

View all Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Define...

Identification

- All Fields
- Hit only

Compound All Data All_AE8.udf

Compound all IDE Compound_all_ID_AE8.udf

Compound IDE Compound_ID_AE8.udf

ID+References ID+References_AE8.udf

ne-2,6-dione

in-2,6-dion, Kaffein

purine-2,6-dione

ne-2,6-dione

Autoname

Molecular

Molecular

Lawson Number 30517, 2817

Type of Substance heterocyclic

Constitution ID 12360

Tautomer ID 4946

Beilstein Reference 0-26-00-00461, 1-26-00-00136, 2-26-00-00266, 4-26-00-02338, 5-26-13-00558, 6-26

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RSTR	Related Structure	11

对记录中显示的数据内容进行定义

idle ALL: Substance as Product Substances

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Substances: hit 8 of 3803

History | Print Hits | View all | Show Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report

Gmelin(2004/03)
 Beilstein(2004/03)
 Saved Hitsets/Alert Hitsets
 Session Hitsets
 Q: Q01 [3803 Substan

Beilstein Registry Number 17705
 Beilstein Preferred RN 58-08-2
 CAS Registry Number 58-08-2
 Chemical Name 1,3,7-trimethyl-3,7-dihydro-1H-pyrazolo[4,3-c]pyridine
 Autname 1,3,7-trimethyl-3,7-dihydro-1H-pyrazolo[4,3-c]pyridine
 Molecular Formula C₈H₁₀N₄O₂
 Molecular Weight 194.19
 Lawson Number 30517, 2817
 Type of Substance heterocyclic
 Constitution ID 12360
 Tautomer ID 4946
 Beilstein Reference 0-26-00-00461, 1-26-00-00136, 2-26-00-00266, 4-26-00-02338, 5-26-13-00558, 6-26

Get
 Get All Related Substances...
 Get All Related Reactions...
 Get All Related Citations...
 Get Substances by RegNo
 Get Reactions by RegNo
 Get Citations by RegNo

通过菜单选项可直接查询相关记录，而不用重新进行提问。

Field Availability List 1-10 of 69

Code	Field Name	Occ.
PHARM	Bioactivity: Pharmacological Data	584
ECT	Ecological Data: Ecotoxicology	57
ECA	Ecological Data: Exposure Assessment	1
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ECDH	Ecological Data: Abiotic Degradation, Hydrolysis	1
ECDP	Ecological Data: Abiotic Degradation, Photolysis	1
RX	Reaction	97
RSTR	Related Structure	11

For Help, press F1

idle

ALL: Substance as Product

Substances

快速数据检索

The screenshot displays the MDL CrossFire Commander interface. The main window is titled "MDL CrossFire Commander - [Query for Server default]". The menu bar includes File, Edit, Task, View, Options, Query, and Help. The toolbar contains buttons for Query, Results, Reports, Alerts, and AutoNom. Below the toolbar is a navigation bar with options like Query History, Open Query, Save Query, Print Query, Clear Query, Select Database, Draw Structure, Modify Alert, Create Alert, and Start Search.

The interface is divided into several sections:

- Search Field Name in:** A dropdown menu with a "Find" button.
- Predefined Search Forms:** A list of search forms including Hitsets, Beilstein(2004/02), Basic Indexes, Bibliographic Information, Substance Identification, Chemical Properties, Physical Properties, and Pharmacological and Ecological.
- Query Builder:** A central area for building queries, currently showing "Search in: Beilstein(2004/02)". It includes instructions for Structure/Reaction Search and options for Free Sites, Stereo, Search, and Allow.
- Search All Text:** A section with a dropdown menu set to "and" and a search box containing "antibiotic".
- Search Fields:** A section with a dropdown menu set to "and" and a table for defining search conditions.
- Buttons:** Buttons for "Truncate...", "Clear Text", "Enlarge...", "Advanced Search", "Clear Table", "Clear Structure", and "Extended Options".

Two red boxes highlight specific areas:

- A red box on the left side of the "Predefined Search Forms" list is labeled "数据索引区" (Data Index Area).
- A red box around the "Search Fields" table is labeled "查询条件填充区" (Query Condition Filling Area).

	Operator	(Field name	Relation	Field content	List)	▲
1				is				
2	and			is				
3	and			is				

At the bottom of the interface, there are checkboxes for "Show Help for Search Fields" and "For Help, press F1", a status bar showing "idle", and a "Start Search" button.

预定义的检索表格



Beilstein
预定义
表格

预定义表格可以简化检索条件的
填充过程。



Gmelin
预定义
表格

预定义表格：反应查询

The image shows a software window titled "Query Form" with a standard Windows-style title bar. At the top, there are four buttons: "Cancel", "Clear", "Help", and "OK". The main content area is divided into two sections. The first section, "Reaction Data", contains a sub-section "Find all reactions where" with four rows of search criteria. Each row has a label, a dropdown menu, a text input field, and a "list" link. The second section, "Search in Reaction Basic Index", contains a text input field with a "starts with" dropdown menu and a "list" link. A vertical scrollbar is on the right side of the main content area.

Query Form

Cancel Clear Help OK

Reaction Data

Find all reactions where

Reactant name	starts with	<input type="text"/>	list
Product name	starts with	<input type="text"/>	list
Reagent/Catalyst/Solvent	starts with	<input type="text"/>	list
Yield	=	<input type="text"/>	list

Search in Reaction Basic Index

Search any keyword in all fields related to reactions or chemical data which

	starts with	<input type="text"/>	list
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预定义表格：药理学数据查询

The image shows a software window titled "Query Form" with a standard Windows-style title bar (minimize, maximize, close buttons). The window contains several sections for defining a search query:

- Buttons:** "Cancel", "Clear", "Help", and "OK" are located at the top of the window.
- Section 1:** A box labeled "Pharmacological Data".
- Section 2:** A checkbox labeled "Find Compounds with Pharmacological Data", which is currently unchecked.
- Section 3:** A heading "Find all compounds having Pharmacological Data where" followed by five rows of search criteria:
 - Effect: starts with [dropdown] [text input] [list](#)
 - Species: starts with [dropdown] [text input] [list](#)
 - Route of Application: starts with [dropdown] [text input] [list](#)
 - Type of Effect: starts with [dropdown] [text input] [list](#)
 - Results: starts with [dropdown] [text input] [list](#)
- Section 4:** A heading "Search in EcoPharm Basic Index" followed by a search box:
 - Search any keyword in all Bioactivity related data fields which starts with [dropdown] [text input] [list](#)

预定义表格：物理数据查询

The image shows a software window titled "Query Form" with a standard Windows-style title bar (blue background, close button on the right). The window contains several controls for searching physical data:

- Buttons:** "Cancel", "Clear", "Help", and "OK" are located at the top of the window.
- Physical Data:** A section header "Physical Data" is followed by a scrollable area containing search options.
- Find all compounds with:** A group box containing four checkboxes: "Melting Point", "Boiling Point", "Density", and "Refractive Index".
- Or search for detailed values:** A group box containing search criteria for four properties:
 - Melting Point:** "value or range" followed by a dropdown menu with "=", a text input field, a blue "list" link, the text "from solvent", another text input field, and another blue "list" link.
 - Boiling Point:** "value or range" followed by a dropdown menu with "=", a text input field, a blue "list" link, the text "at pressure", a dropdown menu with "=", a text input field, and a blue "list" link.
 - Density:** "value or range" followed by a dropdown menu with "=", a text input field, and a blue "list" link.
 - Refractive Index:** "value or range" followed by a dropdown menu with "=", a text input field, and a blue "list" link.

例： 寻找一种溶剂，要求它在760毫米汞柱下的沸点小于120°C ，不能含氯元素，而且需要了解它的密度和黏度方面的数据。

- 用自定义表格来进行查询

Query Builder: Data Search



	Operator	(Field name	Relation	Field content	List)	▲
1			Boiling Point(BP)	<	120	▼		
2	proximity	▼	Pressure(BP.P)	is	760	▼		
3	and	▼	Dynamic Viscosity(DV)	exists		▼		
4	and	▼	Density of the Liquid(DEN)	exists		▼		
5	not	▼	Element Counts(ELC)	is	cl*	▼		
6	and	▼		is		▼		
7	and	▼		is		▼		
8	and	▼		is		▼		
9	and	▼		is		▼		
10	and	▼		is		▼		
11	and	▼		is		▼		
12	and	▼		is		▼		
13	and	▼		is		▼		
14	and	▼		is		▼		
15	and	▼		is		▼		
16	and	▼		is		▼		
17	and	▼		is		▼		
18	and	▼		is		▼		

填充完毕的表格

Cancel

OK

快速数据查询结果显示

MDL CrossFire Commander - [Beilstein(2004/02):Q02 Substance 1 of 386]

File Edit Task View Options Window Help

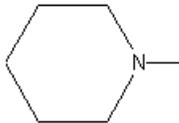
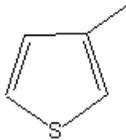
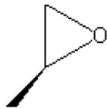
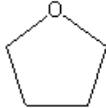
MDL CrossFire Commander

Query Results Reports Alerts AutoHom

Substances: hit 1 of 5777

History | Print Hits | View **all** | Show Grid List Get Sort Hits | Copy Export Hits Copy to Report

- [-] Gmelin (2004/02)
- [-] Beilstein (2004/02)
 - [-] Saved Hitsets/Alert Hitsets
 - [-] Session Hitsets
 - [-] Q: Q01 (5777 Substances)
 - [-] **Q: Q02 (386 Substances)**

Hit 1 BRN=1073 C ₆ H ₁₃ N ;Bio(1)	Hit 2 BRN=1300 C ₅ H ₆ S ;Bio(4)
	
Hit 3 BRN=79766 C ₃ H ₆ O	Hit 4 BRN=102378 C ₂ H ₄ O ;Bio(42)
 racemate	
Hit 5 BRN=102383 C ₃ H ₆ S	Hit 6 BRN=102391 C ₄ H ₈ O ;Bio(27)
	

For Help, press F1

idle GRID Substances

仅显示与查询条件相匹配的数据项。

MDL CrossFire Commander - [Beilstein(2004/02): Q02 Substance 1 of 386]

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Substances: hit 1 of 386

View Hit

Substance Identification

Beilstein Registry Number **1073**

Beilstein Preferred RN 626-67-5

CAS Registry Number 626-67-5

Chemical Name 1-methyl-piperidine
N-Methyl-piperidin

Autoname 1-methyl-piperidine

Molecular Formula C₆H₁₃N

Molecular Weight 99.18

Lawson Number 24081, 2817

Type of Substance heterocyclic

Constitution ID 1378

Tautomer ID 1210

Beilstein Reference 0-20-00-00016, 1-20-00-00007, 2-20-00-00012, 4-20-00-00305, 5-20-02-00021, 6-20

Boiling Point 11-20 of 23

VALUE (BP) C	Pressure (.P) Torr	Entry Date	Note	Ref.
107 - 110				1
145				2
105	760			3
105.7	760			4,4
105.9	760		1	5
106 - 107	760			6
107	760			7
107	760		2	8
106 - 107	757.6		3	9
107	748		4	10-11

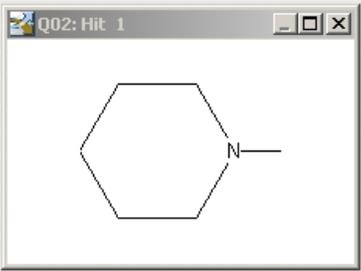
Note 1 Handbook

Note 2 Handbook

Note 3 Handbook

Note 4 Handbook

Ref. 1 [236649, LitLink](#); Journal; Nametkin, N.S. et al.; BACCAT; Bull. Acad. Sci. USSR Div. Chem. Sci. (Engl. Transl.); EN; 22; 1973; 836-840; IASKA6; Izv. Akad. Nauk SSSR Ser. Khim.; RU: 22; 1973; 865-870.



Q02: Hit 1

Matched items are highlighted in yellow background.

For Help, press F1

idle HITONLY Substances

匹配项以高亮的背景颜色显示。

MDL CrossFire Commander - [Beilstein(2004/02):Q02 Substance 1 of 386]

File Edit Task View Options Window Help

MDL CrossFire Commander Query Results Reports Alerts AutoHom Substances: hit 1 of 386

History Print Hits View Hit Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Gmelin(2004/01)
 Beilstein(2004/02)
 Saved Hits/Alert Hits
 Session Hits
 Q: Q01 (3603 Substances)
 L: 6401099 (1 Citations)
 Q: Q02 (386 Substances)

Ref. 6 [2829277, Lit.link](#) ; Journal; Lanum; Morris; JCEAAX; J. Chem. Eng. Data; 14; 1969; 93,97.

Ref. 7 [236649, Lit.link](#) ; Journal; Nametkin, N.S. et al.; BACCAT: Bull. Acad. Sci. USSR Div. Chem. Sci. (Engl. Transl.); EN; 22; 1973; 836-840; IASKA6; Izv. Akad. Nauk SSSR Ser. Khim. **Q02: Hit 1** 1895; 214;

Ref. 8 [1217546, Lit.link](#) ; Journal; Bruehl; ZEPCAC; Z. Phys. CHBEAM; Chem. Ber.; 26; 1893; 2515.

Ref. 9 [976049, Lit.link](#) ; Journal; Magnusson; Schierz; Univ. W

Density of the Liquid 11-16 of 16

VALUE (DEN)	Ref. Temp. (.RT) C	Meas. Temp. (.MT) C	Entry Date	Note	Ref
0.8133	4	21.7		1	1
0.8108		24.9		2	2
0.87076	4	25			3
0.87202	4	25			3
0.87335	4	25			3
0.84687		30		3	4

Note 1 Handbook

Note 2 g/cm**3

Note 3 g/cm**3

Ref. 1 [976125, Lit.link](#) ; Journal; Lukes; Grossmann; CCCCAK; Collect. Czech. Chem. Commun.; 7; 1935; 344, 351.

Ref. 2 [6119919, Lit.link](#) ; Journal; Lydzba, B. I.; Wrzeszcz, W.; Hawranek, J. P.; JMOSB4; J. Mol. Struct.; EN; 450; 1-3; 1998; 171-178.

Ref. 3 [5871714, Lit.link](#) ; Journal; Hegyes, P.; Foeldeak, S.; Hencsei, P.; Zsombok, G.; Nagy, J.; JORCAI; J. Organomet. Chem.; EN; 251; 3; 1983; 289-294.

Ref. 4 [5848373, Lit.link](#) ; Journal; Prabhavathi, C. L.; Rambabu, K.; Venkateswarlu, P.; Raman, C. K.; JICSAH; J. Indian Chem. Soc.; EN; 69; 12; 1992; 810-812.

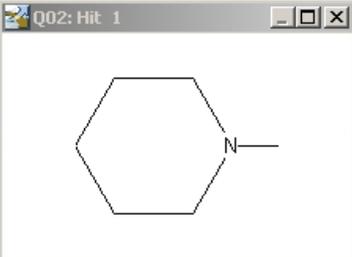
Dynamic Viscosity

VALUE (DV) g cm-1 s-1	Temperature (.T) C	Entry Date	Note	Ref.
1.2167	303.2			1

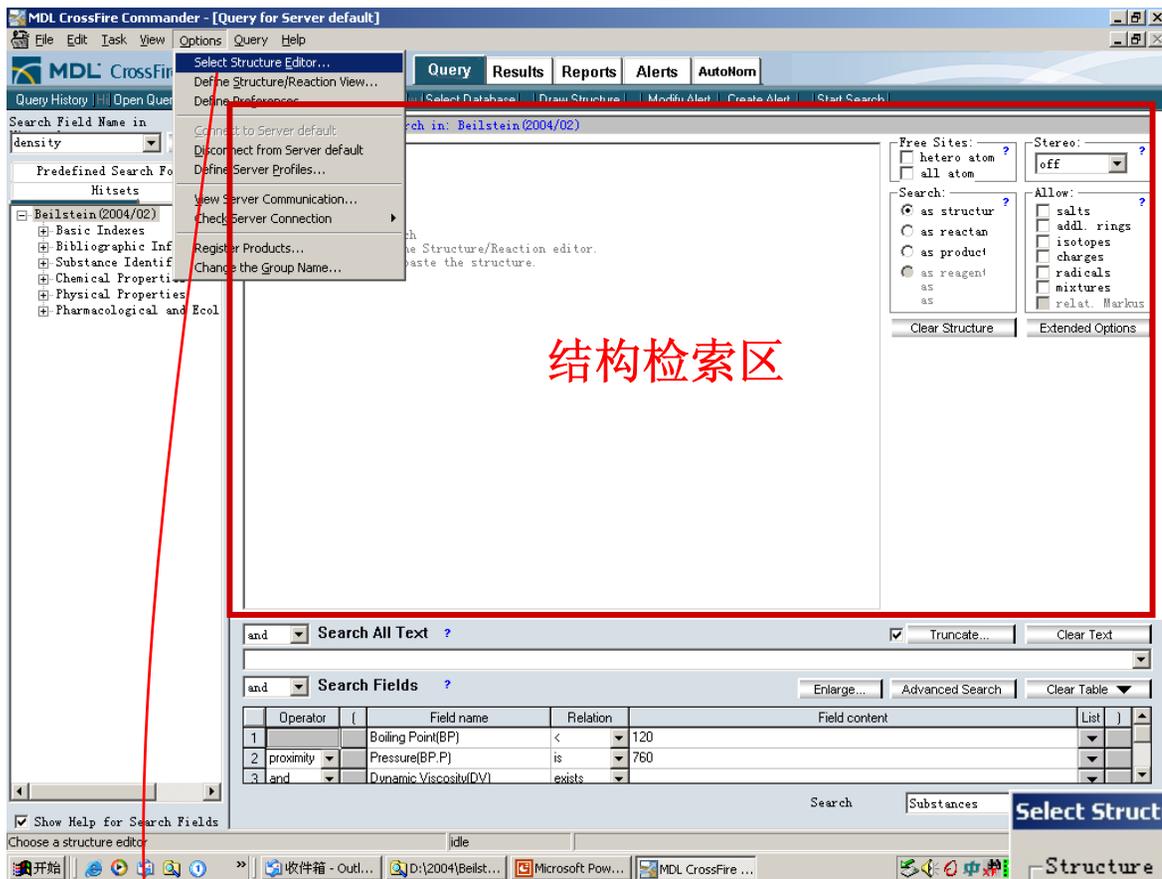
Ref. 1 [5848373, Lit.link](#) ; Journal; Prabhavathi, C. L.; Rambabu, K.; Venkateswarlu, P.; Raman, C. K.; JICSAH; J. Indian Chem. Soc.; EN; 69; 12; 1992; 810-812.

idle HITONLY Substances

For Help, press F1



结构检索

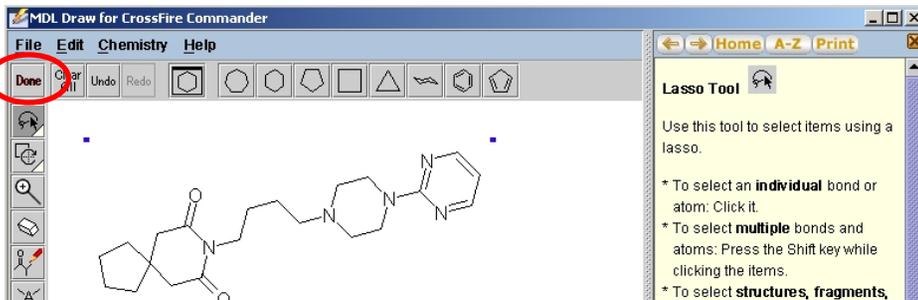


结构检索区

画图工具的选择：
**Options->Select
Structure Editor。**



精确结构检索



点击“Done”按钮即可将画好的结构返回 Commander 结构检索区。

MDL CrossFire Commander - [Query for Server default]

File Edit Task View Options Query Help

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Query History | Open Query | Save Query | Print Query | Clear Query | Select Database | Draw Structure | Modify Alert | Create Alert | Start Search

Search Field Name in ? Find

Predefined Search Forms

Hitsets

- Beilstein(2004/02)
- Basic Indexes
- Bibliographic Information
- Substance Identification
- Chemical Properties
- Physical Properties
- Pharmacological and Ecol

Query Builder ? Search in: Beilstein(2004/02)

total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST

在此区域内双击即可弹出画图工具。

O=C1CC2(CCCN2C1)C3CCCC3

Free Sites: hetero atom all atom Stereo: off

Search: as structure as reactan as product as reagent as as

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markus

Clear Structure Extended Options

and Search All Text ? Truncate... Clear Text

and Search Fields ? Advanced Search Clear Table

<< Select (and edit) Search Form, Search Field, Query, or Hitset from left box and append to query

Search Substances Start Search

Show Help for Search Fields For Help, press F1

结构检索选项区

The screenshot shows the MDL CrossFire Commander Query Builder interface. The main window displays a chemical structure of a complex organic molecule. The interface includes a menu bar (File, Edit, Task, View, Options, Query, Help), a toolbar with various search actions, and a central query builder area. The query builder area contains several sections: 'Free Sites' with checkboxes for 'hetero atom' and 'all atom'; 'Stereo' with a dropdown menu set to 'off'; 'Search' with radio buttons for 'as structure', 'as reactan', 'as product', and 'as reagent'; and 'Allow' with checkboxes for 'salts', 'addl. rings', 'isotopes', 'charges', 'radicals', 'mixtures', and 'relat. Markus'. A large green arrow points from the 'Stereo' dropdown to a callout box. Red arrows point from the 'Free Sites' and 'Search' sections to their respective callout boxes. The 'Clear Structure' and 'Extended Options' buttons are visible at the bottom.

MDL CrossFire Commander - [Query for Server default]

Query Results Reports Alerts AutoHom

Query Builder Search in: Beilstein(2004/02)

total charge = 0, radicals = 0, components = 1, no impl. ring closures, no isotopes, no IST

Free Sites: hetero atom all atom

Stereo: off

Search: as structure as reactan as product as reagent

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markus

Clear Structure Extended Options

立体化学检索条件定义

是否允许有取代基（有则为子结构检索）以及取代基位置的要求

结构检索

半反应检索

其他检索条件的定义

精确结构检索结果显示

MDL CrossFire Commander - [Beilstein(2004/02):Q01 Substance 1 of 1]

File Edit Task View Options Window Help

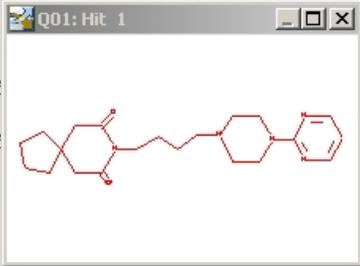
MDL CrossFire Commander Query Results Reports Alerts AutoNom Substances: hit 1 of 1

History | Print Hits | View a11 | Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Gmelin (2004/01)
Beilstein (2004/02)
Saved Hitsets/Alert Hitsets
Session Hitsets
Q: Q01 (1 Substance)

Substance Identification

Beilstein Registry Number **964904**
Beilstein Preferred RN 36505-84-7
CAS Registry Number 36505-84-7
Chemical Name 8-[4-(4-pyrimidin-2-yl-piperazin-1-yl)-butyl]-8-aza-spiro[4.5]undecane
Autoname 8-[4-(4-pyrimidin-2-yl-piperazin-1-yl)-butyl]-8-aza-spiro[4.5]undecane
Molecular Formula C₂₁H₃₁N₅O₂
Molecular Weight 385.51
Lawson Number 29553, 28000, 25729, 3036
Type of Substance heterocyclic
Constitution ID 933653
Tautomer ID 943148
Beilstein Reference 5-25-10-00059, 6-25



Q01: Hit 1

Field Availability List 1-10 of 13

Code	Field Name	Occ.
PHARM	Bioactivity: Pharmacological Data	128
RX	Reaction	8
CDER	Derivative	5
CNF	Conformation	1
EBC	Energy Barriers	2
MP	Melting Point	2
BP	Boiling Point	1
NMR	NMR Spectroscopy	3
IR	IR Spectroscopy	3
RAMAN	Raman Spectroscopy	1

Field Availability List 11-13 of 13

Code	Field Name	Occ.
MS	Mass Spectrometry	2
LLSM	Liquid/Liquid Systems (MCS)	1

For Help, press F1 idle ALL Substances

子结构检索

MDL CrossFireCommander

Query Results Reports Alerts AutoNom

Query History | Open Query | Save Query | Print Query | Clear Query | Select Database | Draw Structure | Modify Alert | Create Alert | Start Search

Search Field Name in Hierarchy: ?

Predefined Search Forms Hitsets

Search Fields Queries

Beilstein(2004/03)

- Basic Indexes
- Bibliographic Information
- Substance Identification
- Chemical Properties
- Physical Properties
- Pharmacological and Ecologic.

Query Builder ? Search in: Beilstein(2004/03)

Free Sites: hetero atoms ? all atoms

Stereo: off ?

Search: as structure as reactant as product as reagent/ as catalyst/ as solvent

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markush

Clear Structure Extended Options

and Search All Text ? Truncate... Clear Text

and Search Fields ? Advanced Search Clear Table

<- Select (and edit) Search Form, Search Field, Query, or Hitset from left box and append to query

Show Help for Search Fields

Search Context Substances Start Search

For Help, press F1

idle

Beilstein定义的广义基团，代表非环烷基。

代表这个C原子上可以有任意的取代基。

子结构检索结果显示

MDL CrossFire Commander

Query Results Reports Alerts AutoHom

Substances: hit 1 of 462

History | Print Hits | View all | Show | Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report

- Gmelin(2004/03)
- Beilstein(2004/03)
 - Saved Hitsets/Alert Hitsets
 - Session Hitsets
 - Q: Q01 (3803 Substances)
 - Q: Q02 (462 Substances)

Hit 1 BRN=1110 C₅H₁₁NO

Hit 2 BRN=3027 C₁₀H₂₀N₂O₂

Hit 3 BRN=80230 C₉H₁₉NO

Hit 4 BRN=102747 C₅H₁₁NO

Hit 5 BRN=102780 C₅H₁₁NO

Hit 6 BRN=102842 C₆H₁₃NO

02850 C₆H₁₃NO

Hit 8 BRN=103542 C₇H₁₅NO

Hit 9 BRN=103551 C₇H₁₅NO

Hit 10 BRN=103742 C₈H₁₇NO

Hit 11 BRN=104131 C₈H₁₇NO

Hit 12 BRN=104134 C₈H₁₇NO

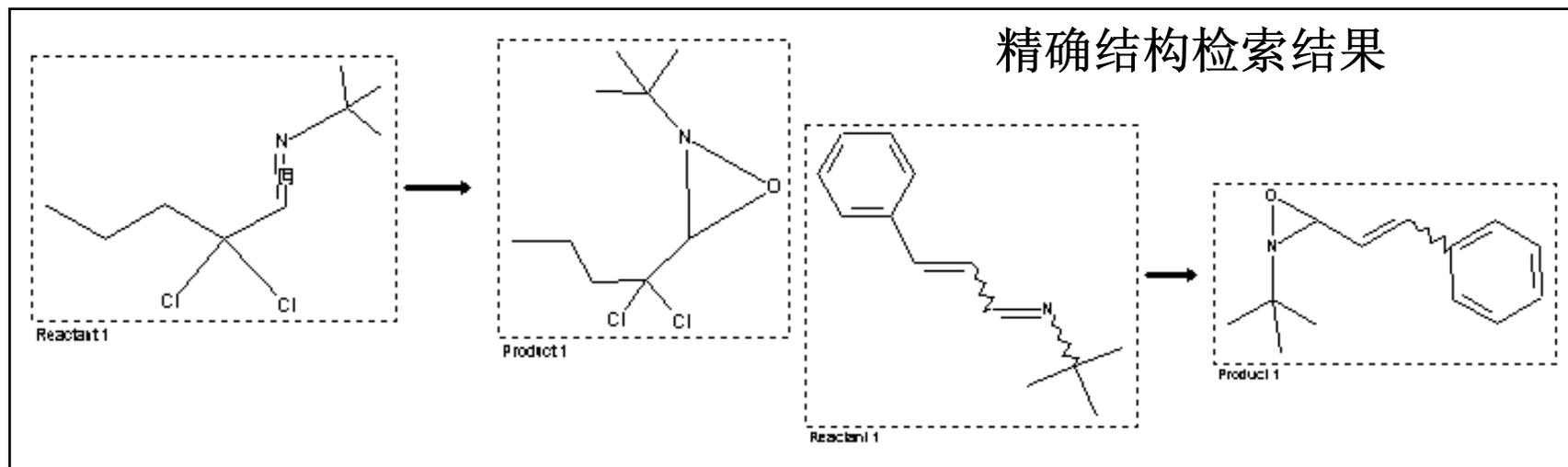
For Help, press F1

idle GRID Substances

红色标记处为结构中
与提问子结构
匹配的部分。

反应检索—原子匹配

例： 查询从亚胺生成唑烷的反应途径，通过原子匹配来得到合适的反应，再通过限定反应产率来进一步查找合适的反应路径。



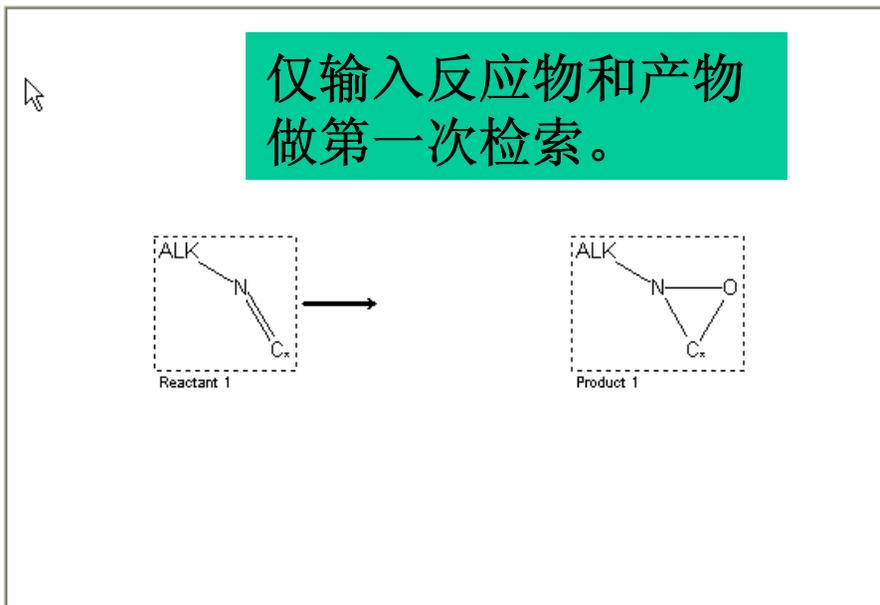
Search Field Name in Hierarchy: ?

Find

Predefined Search Forms | Hitsets
Search Fields | Queries

- [-] Beilstein(2004/03)
 - [+] Basic Indexes
 - [+] Bibliographic Information
 - [+] Substance Identification
 - [+] Chemical Properties
 - [+] Physical Properties
 - [+] Pharmacological and Ecologic.

Query Builder ? Search in: Beilstein(2004/03)



Free Sites: <input type="checkbox"/> hetero atoms ? <input type="checkbox"/> all atoms	Stereo: off
Search: <input checked="" type="radio"/> as reaction ? <input type="radio"/> as reactant <input type="radio"/> as product <input type="radio"/> as reagent/ as catalyst/ as solvent	Allow: <input checked="" type="checkbox"/> salts ? <input checked="" type="checkbox"/> addl. rings <input checked="" type="checkbox"/> isotopes <input checked="" type="checkbox"/> charges <input checked="" type="checkbox"/> radicals <input checked="" type="checkbox"/> mixtures <input type="checkbox"/> relat. Markush
Clear Structure	Extended Options

and Search All Text ? Truncate... Clear Text

and Search Fields ? Clear Table

<- Select (and edit) Search Form, Search Field, Query, or Hitset from left box and append to query

Show Help for Search Fields

Search Context

第一次检索结果，有242条记录。

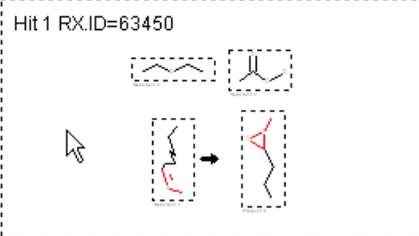
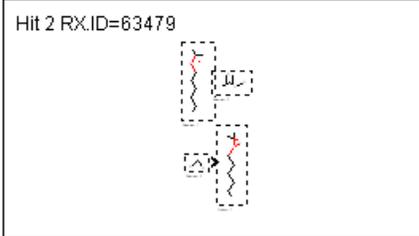
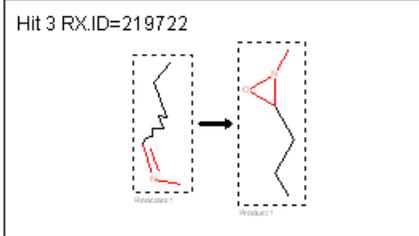
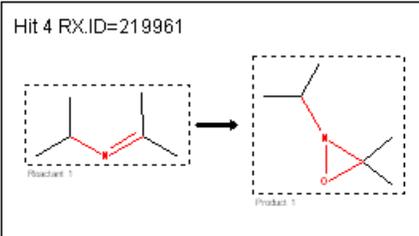
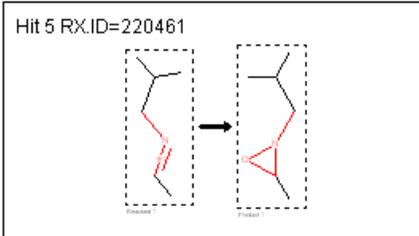
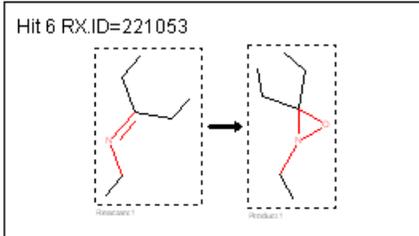
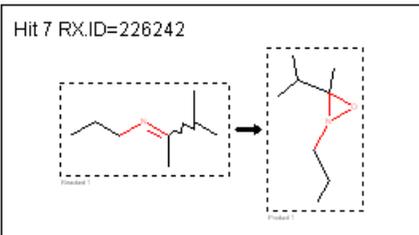
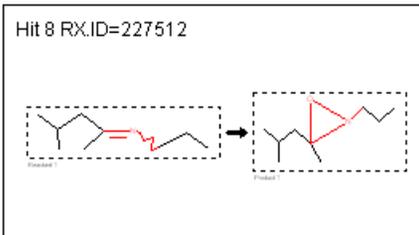
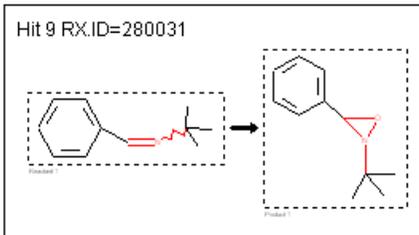
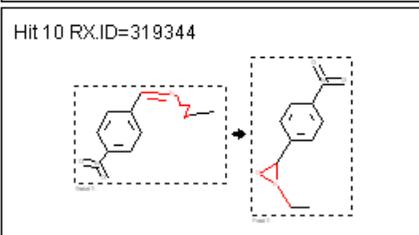
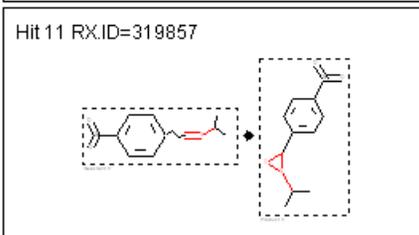
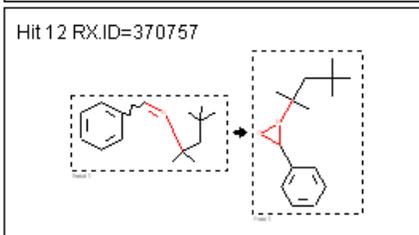
MDL CrossFire Commander

Query Results Reports Alerts AutoHom

Substances: hit 1 of 462

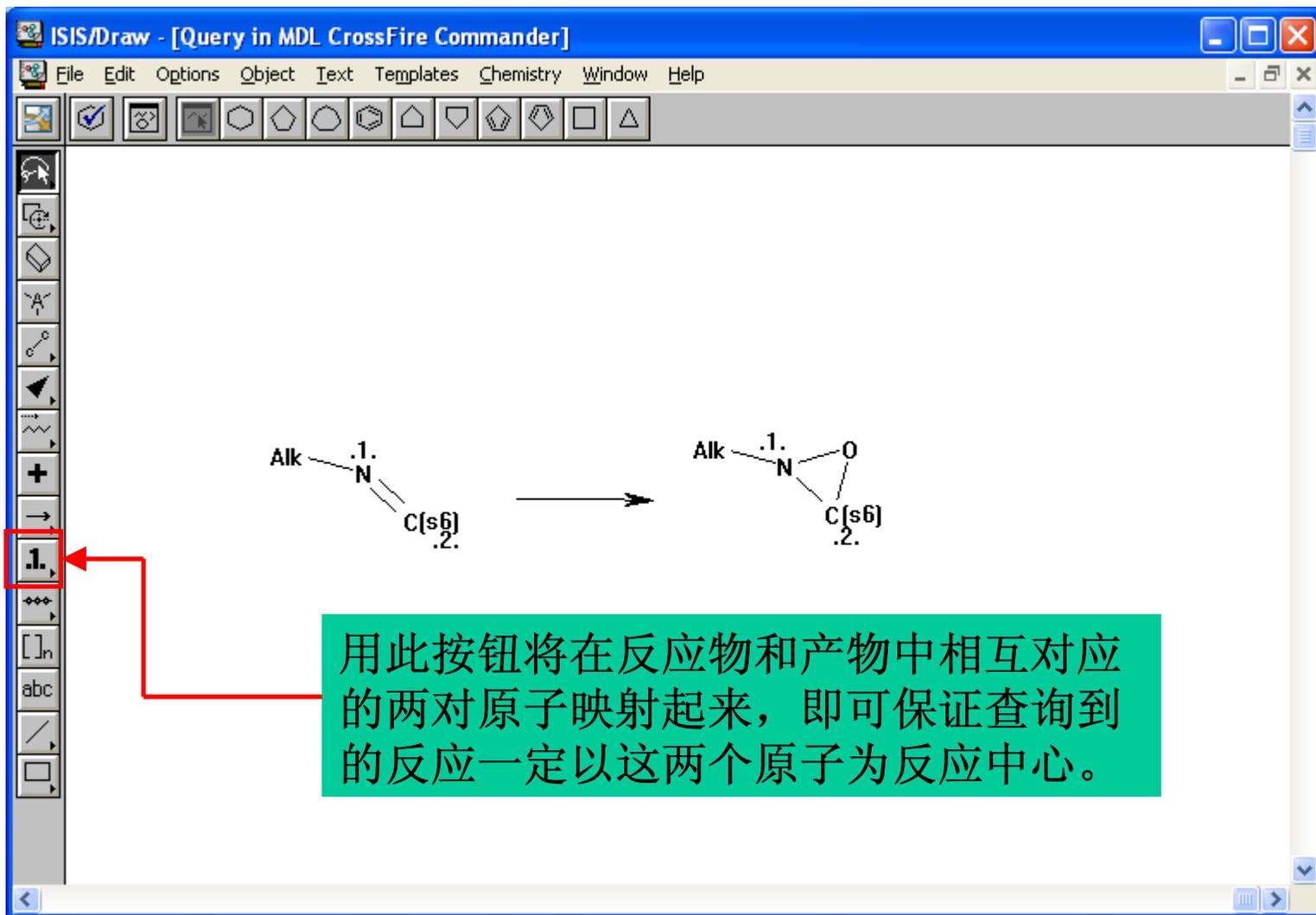
History | Print Hits | View all | Show | Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report

Gmelin(2004/03)
Beilstein(2004/03)
+ Saved Hitsets/Alert Hitsets
- Session Hitsets
+ Q: Q01 (3803 Substances)
+ Q: Q02 (462 Substances)
+ L: 6437113 (1 Citations)
+ **Q: Q06 (242 Reactions)**

Hit 1 RX.ID=63450 	Hit 2 RX.ID=63479 	Hit 3 RX.ID=219722 
Hit 4 RX.ID=219961 	Hit 5 RX.ID=220461 	Hit 6 RX.ID=221053 
Hit 7 RX.ID=226242 	Hit 8 RX.ID=227512 	Hit 9 RX.ID=280031 
Hit 10 RX.ID=319344 	Hit 11 RX.ID=319857 	Hit 12 RX.ID=370757 

For Help, press F1

idle GRID Reactions



第二次检索结果，有187条记录。

MDL CrossFire Commander

Query Results Reports Alerts AutoHom

Substances: hit 1 of 462

History | Print Hits | View all | Show Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report

Smelin(2004/03)
Beilstein(2004/03)
+ Saved Hitsets/Alert Hitsets
- Session Hitsets
+ Q: Q01 (3803 Substances)
+ Q: Q02 (462 Substances)
+ L: 6437113 (1 Citations)
+ Q: Q06 (242 Reactions)
+ **Q: Q07 (187 Reactions)**

Hit 1 RX.ID=63479

Hit 2 RX.ID=219722

Hit 3 RX.ID=219961

Hit 4 RX.ID=220461

Hit 5 RX.ID=221053

Hit 6 RX.ID=226242

Hit 7 RX.ID=227512

Hit 8 RX.ID=280031

Hit 9 RX.ID=319344

Hit 10 RX.ID=319857

Hit 11 RX.ID=370757

Hit 12 RX.ID=374108

idle GRID Reactions

For Help, press F1

Cancel Clear Help OK

Reaction Data

Find all reactions where

Reactant name starts with [list](#)

Product name starts with [list](#)

Reagent/Catalyst/Solvent starts with [list](#)

Yield >= [list](#)

Search in Reaction Basic Index

Search any keyword in all fields related to reactions or chemical data which starts with [list](#)

通过反应查询的预定义表格，
输入对反应产率的要求。

Alerts AutoHom

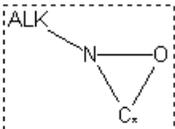
Modify Alert Create Alert Start Search

Free Sites: hetero atoms all atoms Stereo: off

Search: as reaction as reactant as product as reagent/
as catalyst/
as solvent

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markush

Clear Structure Extended Options



Product 1

and Search All Text Truncate... Clear Text

and Search Fields Enlarge... Advanced Search Clear Table

	Operator	(Field name	Relation	Field content	List)	▲
1			Yield (numerical)(RX.NYD)	>=	85			
2	and			is				
3	and			is				

Sort Entries above by Default

Search Context Substances **Start Search**

idle

第三次检索结果，有26条记录。

MDL CrossFire Commander

Query Results Reports Alerts AutoHom

Substances: hit 1 of 462

History | Print Hits | View all | Show Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report

Gmelin(2004/03)
Beilstein(2004/03)
+ Saved Hitsets/Alert Hitsets
- Session Hitsets
+ Q: Q01 (3803 Substances)
+ Q: Q02 (462 Substances)
+ L: 6437113 (1 Citations)
+ Q: Q06 (242 Reactions)
+ Q: Q07 (187 Reactions)
+ **Q: Q08 (26 Reactions)**

Hit 1 RX.ID=280031

Hit 2 RX.ID=319857

Hit 3 RX.ID=1073714

Hit 4 RX.ID=1082861

Hit 5 RX.ID=1982952

Hit 6 RX.ID=2017732

Hit 7 RX.ID=2017738

Hit 8 RX.ID=2113677

Hit 9 RX.ID=2117781

Hit 10 RX.ID=2119356

Hit 11 RX.ID=2119752

Hit 12 RX.ID=2130394

For Help, press F1

idle GRID Reactions

各种检索方式的比较

检索方式	命中结果的数目
反应检索	242条
进行原子匹配的反应检索	187条
反应与数据的联合检索	26条

采用原子匹配和联合检索等方式
可以更有效进行针对性的查询

二次检索

MDL CrossFire Commander - [Query for Server default]

File Edit Task View Options Query Help

MDL CrossFire Commander

Query Results Reports Alerts AutoHom

Query History | Open Query | Save Query | Print Query | Clear Query | Select Database | Draw Structure | Modify Alert | Create Alert | Start Search

Text in the Hitsets: Find

Search Fields Queries

Predefined Search Forms **Hitsets**

- Beilstein (inactive)
- Beilstein(2004/03)
 - CROMACLIN (14 Substances)
 - Q01 (242 Reactions)
 - Q02 (187 Reactions)

在此选择AND, OR, NOT 来对命中集进行组合。

	Operator	(Field name	Relation	Field content	List)
1			Q01 (242 Reactions)[.Q01]	exists			
2	not		Q02 (187 Reactions)[.Q02]	exists			
3	and			is			
4	and			is			
5	and			is			
6	and						
7	and						
8	and						
9	and						
10	and						
11	and			is			
12	and			is			
13	and			is			
14	and			is			
15	and			is			
16	and			is			
17	and			is			
18	and			is			
19	and			is			
20	and			is			

Cancel OK

and Search Fields ?

	Operator	(Field name	Relation	Field content	List)
1			Q01 (242 Reactions)[.Q01]	exists			
2	not		Q02 (187 Reactions)[.Q02]	exists			
3	and			is			

Enlarge... Advanced Search Clear Table

Search Context Reactions **Start Search**

For Help, press F1 idle

start Microsoft PowerPoint ... MDL CrossFire Comm... 10:25

二次检索结果显示

MDL CrossFire Commander

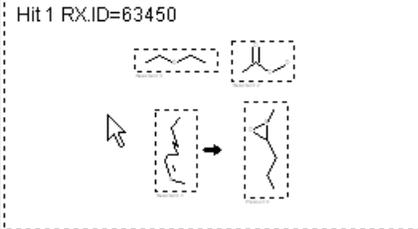
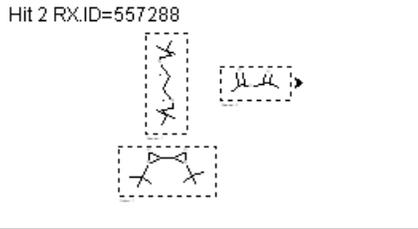
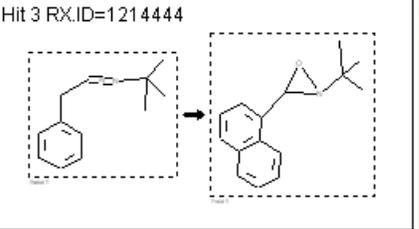
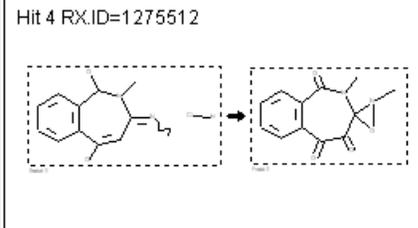
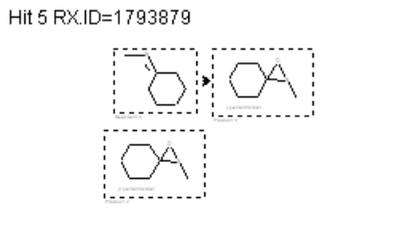
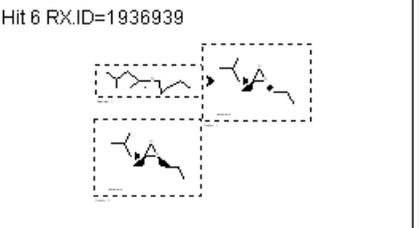
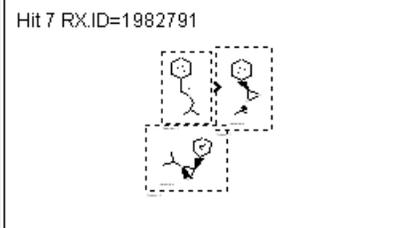
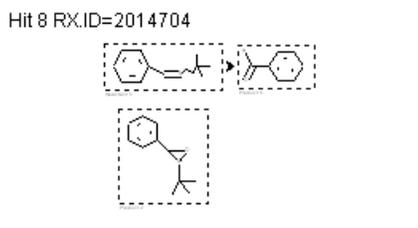
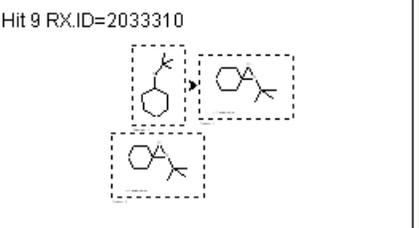
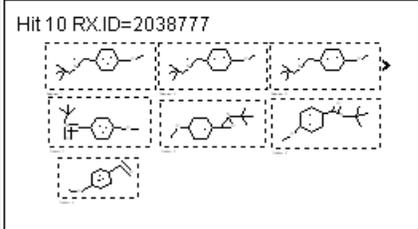
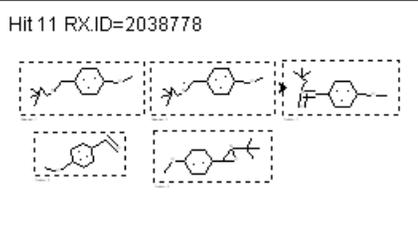
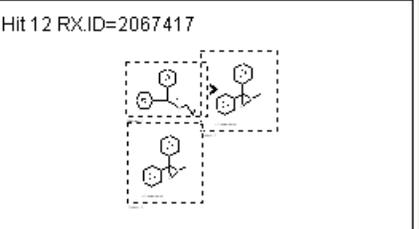
Query Results Reports Alerts AutoHom

Substances: hit 1 of 462

History | Print Hits | View all | Show | Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report

Smelin(2004/03)
Beilstein(2004/03)

- Saved Hitsets/Alert Hitsets
- Session Hitsets
 - Q: Q01 (3803 Substances)
 - Q: Q02 (462 Substances)
 - L: 6437113 (1 Citations)
 - Q: Q06 (242 Reactions)
 - Q: Q07 (187 Reactions)
 - Q: Q08 (26 Reactions)
 - Q: Q09 (55 Reactions)**

Hit 1 RX.ID=63450 	Hit 2 RX.ID=557288 	Hit 3 RX.ID=1214444 
Hit 4 RX.ID=1275512 	Hit 5 RX.ID=1793879 	Hit 6 RX.ID=1936939 
Hit 7 RX.ID=1982791 	Hit 8 RX.ID=2014704 	Hit 9 RX.ID=2033310 
Hit 10 RX.ID=2038777 	Hit 11 RX.ID=2038778 	Hit 12 RX.ID=2067417 

For Help, press F1

idle GRID Reactions

例： 检索吸入时有平喘疗效的化合物的合成方法

- 查询有这种药效的化合物
- 从这些化合物的结构中提出公共的母体结构
- 对母体结构进行修饰
- 进行子结构反应检索

Query Form

Cancel Clear Help OK

Pharmacological Data

Find Compounds with Pharmacological Data

Find all compounds having Pharmacological Data where

Effect starts with antiasthma list

Species starts with list

Route of Application starts with inhalation list

Type of Effect starts with list

Results starts with list

Search in EcoPharm Basic Index

Search any keyword in all Bioactivity related data fields which starts with list

通过预定义的药理学数据查询表格进行化合物查询。

Query Results Reports Alerts AutoHom

ect Database | Draw Structure | Modify Alert | Create Alert | Start Search

Beilstein(2004/02)

Free Sites: hetero atom all atom Stereo: off

Search: as structure as reactan as product as reagent as

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markus

Clear Structure Extended Options

Structure/Reaction editor. the structure.

and Search All Text Truncate... Clear Text

and Search Fields Enlarge... Advanced Search Clear Table

	Operator	(Field name	Relation	Field content	List)	▲
1			Effect(PHARM.E)	starts with	antiasthma			
2	proximity		Route of Application(PHARM.RA)	starts with	inhalation			
3	and			is				

Sort Entries ab by Default

Search Substances Start Search

idle

For Help, press F1

数据查询结果显示

MDL CrossFire Commander - [Beilstein(2004/02):Q04 Substance 1 of 14]

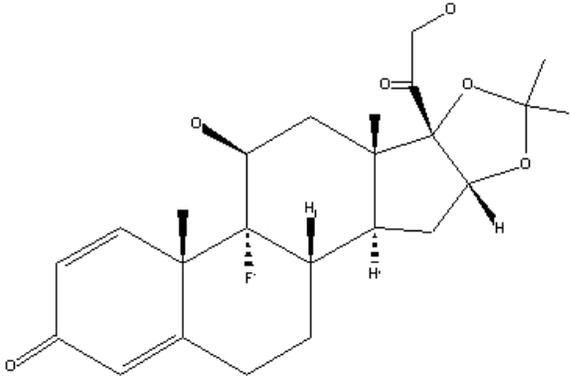
File Edit Task View Options Window Help

MDL CrossFire Commander Query Results Reports Alerts AutoNom Substances: hit 1 of 14

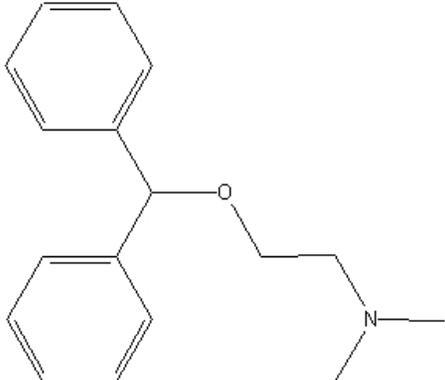
History Print Hits View 11 Show Grid List Get Sort Hits Copy Export Hits Copy to Report

[-] Gmelin(2004/01)
[-] Beilstein(2004/02)
 [-] Saved Hitsets/Alert Hitsets
 [-] Session Hitsets
 [-] Q: Q04 (14 Substances)

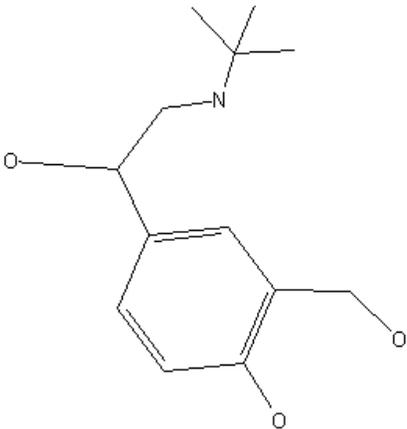
Hit 1 BRN=60069 C₂₄H₃₁FO₆ ;Bio(52)



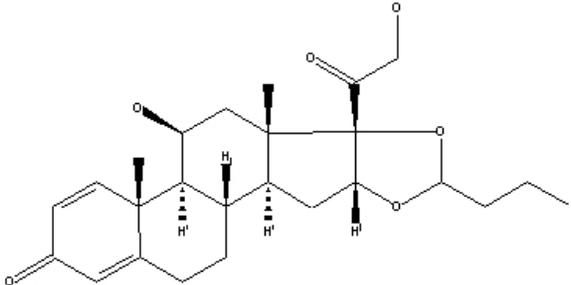
Hit 2 BRN=1914136 C₁₇H₂₁NO ;Bio(130)



Hit 3 BRN=2213614 C₁₃H₂₁NO₃ ;Bio(196)



Hit 4 BRN=3633996 C₂₅H₃₄O₆ ;Bio(79)



For Help, press F1 idle GRID Substances

选择性的显示所需要的记录

MDL CrossFire Commander - [Beilstein(2004/03):Q01 Substance 1 of 14 selected (1) EN English (United States) ?

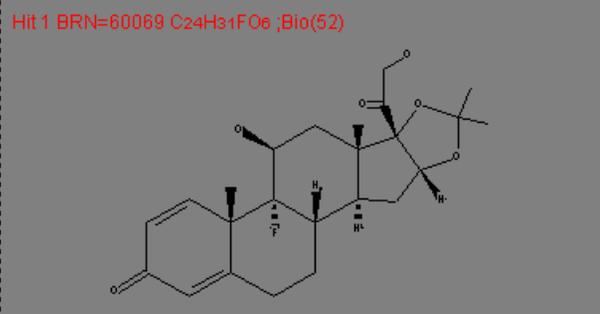
File Edit Task View Options Window Help

MDL CrossFire Commander Query Results Reports Alerts AutoHom Substances: hit 1 of 14 selected (1 of 6)

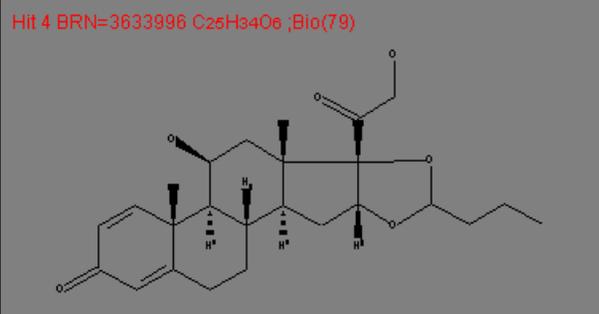
History Print Hits View all Show Grid List Get Sort Hits Copy Export Hits Copy to Report

[-] Gmelin(2004/02)
[-] Beilstein(2004/03)
 [-] Saved Hitsets/Alert Hitsets
 [-] Session Hitsets
 + Q: Q01 (14 Substances)

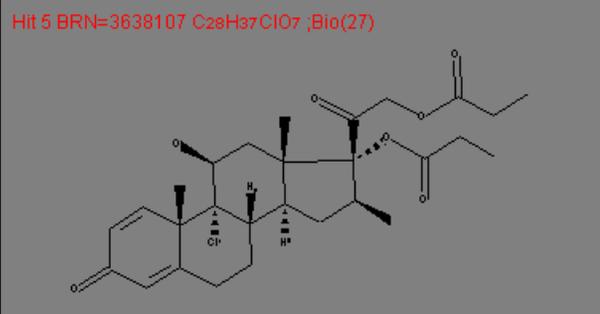
Hit 1 BRN=60089 C₂₄H₃₁FO₆ ;Bio(52)



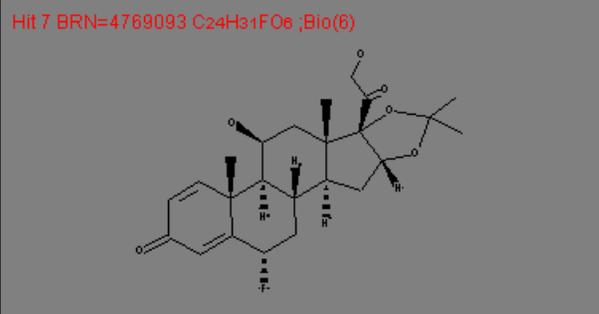
Hit 4 BRN=3633996 C₂₅H₃₄O₆ ;Bio(79)



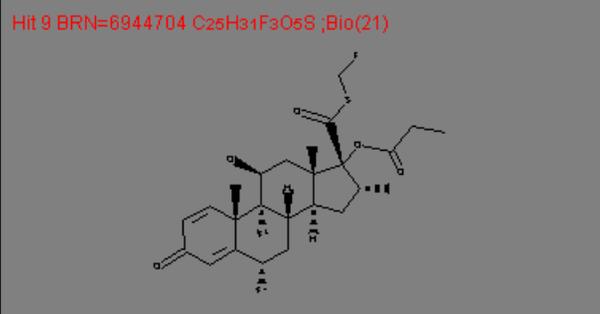
Hit 5 BRN=3638107 C₂₈H₃₇ClO₇ ;Bio(27)



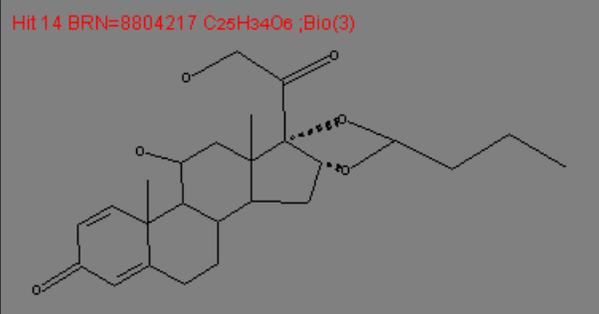
Hit 7 BRN=4769093 C₂₄H₃₁FO₆ ;Bio(6)



Hit 9 BRN=6944704 C₂₅H₃₁F₃O₅S ;Bio(21)



Hit 14 BRN=8804217 C₂₅H₃₄O₆ ;Bio(3)



For Help, press F1 idle GRID: SelectedHitsOnly Substances

提取的公共母体结构

MDL CrossFire Commander - [Query for Server default]

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Query History | Open Query | Save Query | Print Query | Clear Query | Select Database | Draw Structure | Modify Alert | Create Alert | Start Search

Text in the Forms: ?

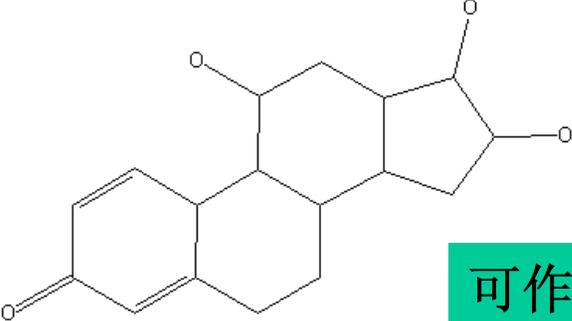
Search Fields | Queries

Hitsets

- Bibliographic Data
- Substance Identification Data
- Molecular Formula Search
- Reaction Data
- Physical Data
- Spectroscopic Data
- Pharmacological Data
- Ecotoxicological Data
- Solubility Data

Query Builder ? Search in: Beilstein(2004/02)

components = 1, impl. free sites, no IST



Free Sites: hetero atom ? all atom

Stereo: off ?

Search: as structure ? as reactant as product as reagent as

Allow: salts addl. rings isotopes charges radicals mixtures relat. Markus

Clear Structure Extended Options

and Search All Text ?

and Search Fields ?

<-- Select (and edit) Search Form, Search Field, Query, or Hitset from left box and append to query

Sort Entries ab by Default

Search Substances Start Search

For Help, press F1

idle GRID: SelectedHitsOnly Substances

可作为子结构进行查询，得到一系列具有相同分子骨架的分子结构，用来进行构效关系的分析和分子设计。

例： 检索1991年在Journal of Medicinal Chemistry (J.Med.Chem.) 上发表的关于Cromakalim 化合物(结构已知)的文章。并查询此化合物的合成方法。

- 进行结构和数据的联合检索
- 查询此化合物的合成方法

检索条件的填充

The screenshot displays the MDL CrossFire Commander interface. The main window is titled "MDL CrossFire Commander - [Query for Server default]". The menu bar includes File, Edit, Task, View, Options, Query, and Help. The toolbar contains buttons for Query, Results, Reports, Alerts, and AutoNom. Below the toolbar, there are buttons for Query History, Open Query, Save Query, Print Query, Clear Query, Select Database, Draw Structure, Modify Alert, Create Alert, and Start Search.

The "Query Builder" window is active, showing a search query: "Search in: Beilstein(2004/02)". The main display area shows a chemical structure of a complex molecule with a nitrile group, a benzene ring, and a fused ring system. The structure is rendered in a 3D perspective view.

The "Query Form" dialog box is open, showing the "Bibliographic Data" section. It includes fields for Author, Patent Assignee, Journal Title, CODEN, Article Title, and Publication Year. The "Find all citations where" section is expanded, showing the following search criteria:

- Author: starts with [] list
- Patent Assignee: starts with [] list
- Journal Title: starts with j. med. chem. list
- CODEN: starts with [] list
- Article Title: starts with [] list
- Publication Year: = 1991 list

The "Search in Citation Basic Index" section is also visible, with a search keyword field and a "list" button.

The "Search Fields" table is shown at the bottom of the interface:

Operator	(Field name	Relation	Field content	List)
		Journal Title(JT)	starts with	j. med. chem.		
proximity		Publication Year(PY)	is	1991		
and			is			

The "Search" button is highlighted, and the "Substances" dropdown menu is visible. The "Start Search" button is also present.

Bibliographic entry

联合检索结果显示

MDL CrossFire Commander - [Beilstein(2004/03):Q07 Substance 1 of 2] EN English (United States)

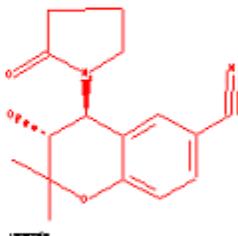
File Edit Task View Options Window Help

MDL CrossFire Commander Query Results Reports Alerts AutoNom Substances: hit 1 of 2

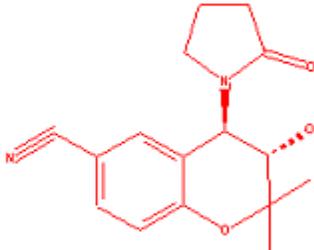
History | Print Hits | View all | Show Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report

- Gmelin(2004/02)
- Beilstein(2004/03)
 - Saved Hitsets/Alert Hitsets
 - Session Hitsets
 - Q: Q05 (7 Substances)
 - Q: Q06 (14 Substances)
 - Q: Q07 (2 Substances)**

Hit 1 BRN=3560683 C₁₆H₁₈N₂O₃;Bio(90)



Hit 2 BRN=3622889 C₁₆H₁₈N₂O₃;Bio(172)



MDL CrossFire Commander - [Beilstein(2004/03):Q07 Substance 2 of 2] EN English (United States)

File Edit Task View Options Window Help

MDL CrossFire Commander Query Results Reports Alerts AutoHom Substances: hit 2 of 2

History Print Hits View all Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Gmelin(2004/02)
 Beilstein(2004/03)
 Saved Hitsets/Alert Hitsets
 Session Hitsets
 Q: Q05 (7 Substances)
 Q: Q06 (14 Substances)
Q: Q07 (2 Substances)
 Q: Q08 (2 Substances)

Substance Identification

Beilstein Registry Number [3622889](#)
 Beilstein Preferred RN 94535-50-9
 CAS Registry Number 86776-67-2, 94470-67-4, 94535-50-9, 94535-51-0, 99095-58-6, 103774-92-1, 148811-93-2, 148811-94-3, 150871-62-8
 Chemical Name cromakalim
 Autname 3-hydroxy-2,2-dimethyl-4-(2-oxo-pyrrolidin-1-yl)-chroman-6-carbonitrile
 Molecular Formula C₁₆H₁₈N₂O₃
 Molecular Weight 286.33
 InChI Number 25310, 20691
 Stereo Keyword Stereo compound
 Type of Substance heterocyclic
 Beilstein ID 3157885
 CAS ID 3499010
 Beilstein Reference 6-21

Availability List 1-7

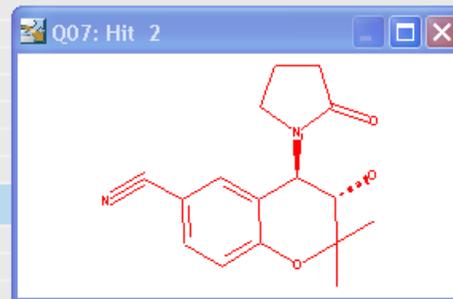
Code	Field Name	Occ.
PHARM	Bioactivity: Pharmacological Data	172
RX	Reaction	2
CNF	Conformation	2
EBC	Energy Barriers	1
ORP	Optical Rotatory Power	1
NMR	NMR Spectroscopy	10
CNR	Reference	95

Reaction 1 of 2

Reaction ID [1522022](#)
 Reactant BRN [4841731](#) (3S,4S)-6-cyano-2,2-dimethyl-3,4-epoxychroman
[105241](#) pyrrolidin-2-one
 Product BRN [3622889](#) cromakalim
 No. of Reaction Details 1
 Reaction Classification Preparation

For Help, press F1 idle ALL Substances

选中菜单中View->
substance as product
选项。



此化合物合成反应的
超链接，点击即可访
问相应的反应。

MDL CrossFire Commander - [Beilstein(2004/03):1522022 Reaction 1 of 1] EN English (United States)

File Edit Task View Options Window Help

MDL CrossFire Commander Query Results Reports Alerts AutoHom Substances: hit 6 of 14

History Print Hits View all Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Gmelin(2004/02)
Beilstein(2004/03)
 Saved Hitssets/Alert Hitssets
 Session Hitssets
 Q: Q05 (7 Substances)
 Q: Q06 (14 Substances)
 Q: Q07 (2 Substances)
 Q: Q08 (2 Substances)
 L: 1522022 (1 Reactions)

Reaction

Reaction ID [1522022](#)
Reactant BRN [4841731](#) (3S,4S)-6-cyano-2,2-dimethyl-3,4-epoxychroman
Product BRN [105241](#) pyrrolidin-2-one
No. of Reaction Details 1
Find similar reactions [click here](#)

Field Availability List

Code	Field Name	Occ.
RX	Reaction Details	1

Reaction Details

Reaction Classification Preparation
Yield 56 percent (BRN=3622889)
Reagent NaH
Solvent dimethylsulfoxide

Ref. 1 [5592529](#), [Lit link](#); Journal; Lee, Nam Ho; Muci, Alexander R.; Jacobsen, Eric N.; TELEAY; Tetrahedron Lett.; EN; 32; 38; 1991; 5055-5058.

1522022 Hit 1

Reaction scheme showing the conversion of the reactant to the product.

For Help, press F1 idle ALL Reactions

反应物的超链接，可以访问相应的化合物信息。

MDL CrossFire Commander - [Beilstein(2004/03):4841731 Substance 1 of 1] EN English (United States)

File Edit Task View Options Window Help

MDL CrossFire Commander Query Results Reports Alerts AutoNom Substances: hit 1 of 1

History Print Hits View all Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Find similar reactions [click here](#)

Ref. 1 [5592529, LitLink](#); Journ...; Tetrahedron

Reaction 2 of 34

Reaction ID [1771003](#)

Reactant BRN [1367827](#) 2,2-dimethyl-2H-ch...
Product BRN [4841731](#) (3S,4S)-6-cyano-2...
No. of Reaction Details 6
Reaction Classification Preparation
Yield 99 percent (BRN=4841731)
Reagent pyridine N-oxide
chiral Mn(III) Schiff base complex
NaOCl
Solvent CH₂Cl₂
Temperature 0 C
Find similar reactions [click here](#)

Ref. 1 [6375902, LitLink](#); Journal; Kureshy, Rukhs...; mil T...
lyer, Parameswar K.; Subramanian, P. S.; Jasra, Raksh V.; JCTLA5; J. Catal.; EN; 209; 1; 2002; 99 - 104.

Reaction 3 of 34

Reaction ID [3762491](#)

Reactant BRN [4841731](#) (3S,4S)-6-cyano-2,2-dimethyl-3,4-epoxychroman
[742548](#) 6-hydroxy-2-methyl-2H-pyridazin-3-one
Product BRN [4822349](#) 3-hydroxy-2,2-dimethyl-4-(1-methyl-6-oxo-1,6-dihydro-pyridazin-3-yloxy)-chroman-6-carbonitrile
No. of Reaction Details 1
Reaction Classification Preparation
Yield 85 percent (BRN=4822349)
Reagent pyridine
Find similar reactions [click here](#)

Ref. 1 [5592529, LitLink](#); Journal; Lee, Nam Ho; Muci, Alexander R.; Jacobsen, Eric N.; TELEAY; Tetrahedron
Lett.; EN; 32; 38; 1991; 5055-5058.

Reaction 4 of 34

4841731: Hit 1

For Help, press F1 idle ALL Substances

此化合物合成反应的超链接，点击即可访问相应的反应。

MDL CrossFire Commander - [Beilstein(2004/03):1771003 Reaction 1 of 1] EN English (United States)

File Edit Task View Options Window Help

MDL CrossFire Commander Query Results Reports Alerts AutoNom Reactions: hit 1 of 1

History Print Hits View all Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Reaction

Reaction ID [1774003](#)

Reactant BRN [1367827](#) 2,2-dimethyl-2H-chromene-6-carbonitrile

Product BRN [4841731](#) (3S,4S)-6-cyano-2,2-dimethyl-3,4-epoxychroman

No. of Reaction Details 6

Find similar reactions [click here](#)

Field Availability List

Code	Field Name	Occ.
RX	Reaction Details	6

Reaction Details 1 of 6

Reaction Classification Preparation

Yield 99 percent (BRN=4841731)

Reagent pyridine N-oxide
chiral Mn(III) Schiff base complex
NaOCl

Solvent CH₂Cl₂

Temperature 0 C

Ref. 1 [6375902](#) [LitLink](#) ; Journal; Kureshy, Rukhsana I.; Khan, Noor-ul H.; Abdi, Sayed H. R.; Patel, Sunil T.; Iyer, Parameswar K.; Subramanian, P. S.; Jasra, Raksh V.; JCTLA5; J. Catal.; EN; 209; 1; 2002; 99 - 104.

Reaction Details 2 of 6

Reaction Classification Preparation

Yield

Reagent

Ca

Sol

Time 0 hour(s)

Temperature 0 C

Ref. 1 [6342279](#) [LitLink](#) ; Journal; Kureshw. Rukhsana I.; Khan. Noor-ul H.; Abdi. Sayed H. R.; Patel. Sunil T.

For Help, press F1 idle ALL Reactions

反应物的超链接，可以访问相应的化合物信息.....

MDL CrossFire Commander - [Beilstein(2004/03):241 3025 Reaction 1 of 1] EN English (United States)

File Edit Task View Options Window Help

Grid View / List View F4
Open Hitset in Grid View

History | Print Hits |

- All Fields
- Identification Data only
- Hit only
- Select User View
- Define User View...
- Highlight Hit Terms
- Selected Hits only
- Goto Hit
- Structures included
- Structure in separate window F2
- All Reactions
- Substance as Reactant only
- Substance as Product only
- Update Dates included
- Field Availability included
- Field Availability in separate window... F5
- Show Hitset History... F6
- Show tree view F3
- Show Status Bar

Query Results Reports Alerts AutoNom

Grid List Get Sort Hits Copy Export Hits Copy to Report

Reactions: hit 1 of 1

2413025
386130 4-hydroxy-benzonitrile
1236349 3-chloro-3-methyl-but-1-yne
1367559 3-(4-cyanophenoxy)-3-methylbut-1-yne

Click here

Reaction Details

Name	Occ.
Reaction Details	2

Reactions 1 of 2

Reaction	Preparation
Reaction	78 percent (BRN=1367559) 0.1 mole percent CuCl ₂ * 2 H ₂ O, 1,8-dia... acetonitrile 5 hour(s) 0 C

Ref. 1 [5903652, LitLink](#); Journal; Godfrey, Jollie D.; Mueller, Richard H.; Sedergran, Thomas C.; Soundarajan, Nachimuthu; Colandrea, Vincent J.; TELEAY; Tetrahedron Lett.; EN; 35; 35; 1994; 6405-6408.

Reaction Details 2 of 2

Reaction Classification	Preparation
Reaction Classification	96 percent (BRN=1367559) K ₂ CO ₃ , CuI, KI dimethylformamide 65 C

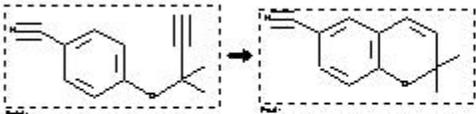
Ref. 2 [5968029, LitLink](#); Journal; Bell, David; Davies, Mark R.; Geen, Graham R.; Mann, Inderjit S.; SYNTBF; Synthesis; EN; 6; 1995; 707-712.

idle ALL Reactions

start Microsoft PowerPoint ... untitled - Paint MDL CrossFire Comm... ISIS/Draw 18:24

追溯到起始反应物以后，
可通过View->Show
Hitset History选项来查
看历史记录。

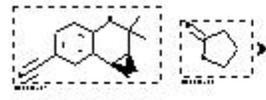
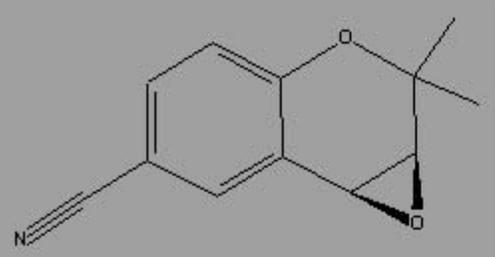
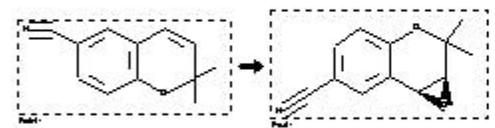
Hitset History



- Beilstein(2004/03):Q01(Substances)
- Beilstein(2004/03):Q02(Substances)
- Beilstein(2004/03):Q06(Substances)
- Beilstein(2004/03):Q07(Substances)
 - Reaction(1522022) from hit 2, fact Reaction
 - Substance(4841731) from field Reaction:Reactant

Go To Go Back

Hitset History

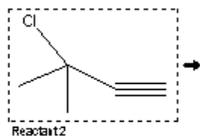
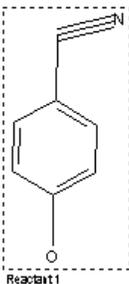
- Beilstein(2004/03):Q01(Substances)
- Beilstein(2004/03):Q02(Substances)
- Beilstein(2004/03):Q06(Substances)
- Beilstein(2004/03):Q07(Substances)
 - Reaction(1522022) from hit 2, fact Reaction
 - Substance(4841731) from field Reaction:Reactant
 - Reaction(1771003) from fact Reaction
 - Substance(1367827) from field Reaction:Reactant
 - Reaction(1770878) from fact Reaction
 - Substance(1367559) from field Reaction:Reactant
 - Reaction(2413025) from fact Reaction

Go To Go Back to Clipboard Help Close

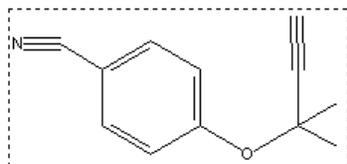
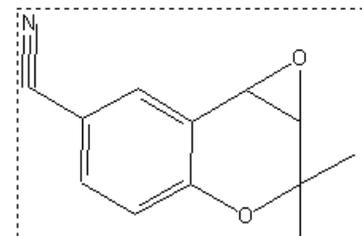
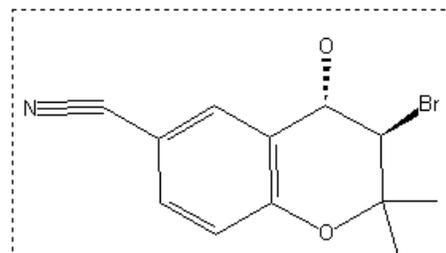
记录编号与化学结构
或反应相对应。

利用超链接追溯反合成路径

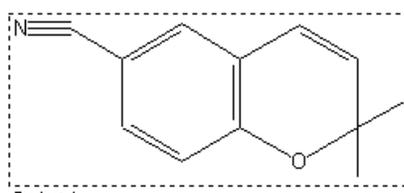
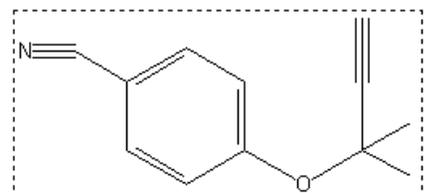
Step 1



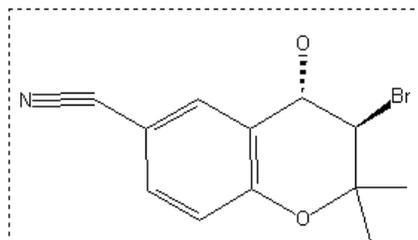
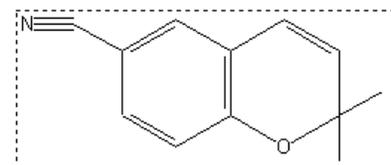
Step 4



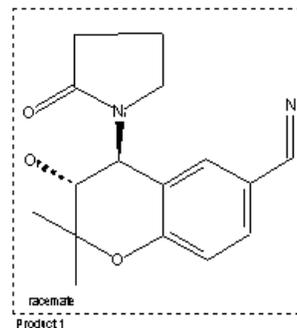
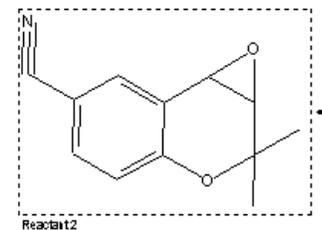
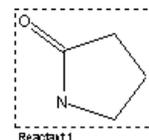
Step 2



Step 3



Step 5



检索结果的导出和报告的生成

The screenshot displays the MDL CrossFire Commander interface. The main window shows search results for reaction 2413025. The 'Export Hits' menu is open, listing various export options. A red box highlights the menu, and a red arrow points to a green text box at the bottom right.

Reaction

Reaction ID	2413025
Reactant BRN	386130 4-hydroxy-benzonitrile
	1236349 3-chloro-3-methyl-but-1-yne
Product BRN	1367559 3-(4-cyanophenoxy)-3-methylbut-1-
No. of Reaction Details	2
Find similar reactions	click here

Field Availability List

Code	Field Name	Occ.
RX	Reaction Details	2

Reaction Details 1 of 2

Reaction Classification	Preparation
Yield	78 percent (BRN=1367559)
Reagent	0.1 mole percent CuCl ₂ * 2 H ₂ O, 1,8-diazabi
Solvent	acetonitrile
Time	5 hour(s)
Temperature	0 C

Ref. 1 [5903652, LitLink](#) ; Journal; Godfrey, Jollie D.; Mueller, Richard H.; Sedergran, Thomas C.; Soundarajan, Nachimuthu; Colandrea, Vincent J.; TELEAY; Tetrahedron Lett.; EN; 35; 35; 1994; 6405-6408

Reaction Details 2 of 2

Reaction Classification	Preparation
Yield	96 percent (BRN=1367559)
Reagent	K ₂ CO ₃ , Cul, KI
Solvent	dimethylformamide
Temperature	65 C

Ref. 1 [5968029, LitLink](#) ; Journal; Bell, David; Davies

EN; 6; 1995; 707-712.

Settings...

- Compounds and ALL Data to HTML as Report
- Compound ID to Excel as Table
- Compound ID to Word as Table
- Compound List to Excel
- Compound List to HTML
- Compound List to Word
- Compound ID to HTML as Report
- Compound ID to RD-File
- Compound ID to SD-File
- Hits and Compound Report to HTML
- Hit References to HTML
- References of all to HTML as Table
- References of Hits to HTML as Table
- References of Hits to HTML as Report

For Help, press F1

idle ALL Reactions

可以选择不同的格式
将记录或记录集导出。

MDL CrossFire Commander - [Beilstein(2004/02):2413025 Reaction 1 of 1]

File Edit Task View Options Window Help

MDL CrossFire Commander Query Results Reports Alerts AutoNom Reactions: hit 1 of 1

History Print Hits View a11 Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Session Hitsets

- Q: Q04 (25 Substances)
- L: 5588964 (1 Citations)
- L: Q05 (58 Substances)
- L: 1521966 (1 Reactions)
- L: 3543598 (1 Substances)
- L: 2792138 (1 Reactions)
- L: 4865558 (1 Substances)
- L: 1771004 (1 Reactions)
- L: 1367827 (1 Substances)
- L: 1770878 (1 Reactions)
- L: 1367559 (1 Substances)
- L: 2413025 (1 Reactions)

Reaction

Reaction ID: **2413025**

Reactant BRN: **386130** 4-hydroxy-benzonitrile

Product BRN: **1236349** 3-chloro-3-methyl-but-1-yne

Product BRN: **1367559** 3-(4-cyanophenoxy)-3-methylbut-1-yne

No. of Reaction Details: 2

Find similar reactions: [click here](#)

Field Availability List

Code	Field Name	Occ.
RX	Reaction Details	2

2413025: Hit 1

Selected Facts to Report report2.html

Open the Report

Define Report File...

Set Report Title...

Clear Report File

Copy Fact to Clipboard

Selected Facts to Word

Options

Select all the Facts: Reaction

Select all Facts

Unselect all Facts

Reaction Details 1 of 2

Reaction Classification: Preparation

Yield: 78 percent (BRN=1367559)

Reagent: 0.1 mole percent CuCl₂ * 2 H₂O, 1,8-diazabicyclo<5.4.0>undec-7-ene

Solvent: acetonitrile

Time: 5 hour(s)

Temperature: 0 C

Ref. 1: [5903652](#), [Lit link](#); Journal; Godfrey, Jollie D.; Mueller, Richard H.; Sedergran, Thomas C.; Sundarajan, Nachimuthu; Colandrea, Vincent J.; TELEAY; Tetrahedron Lett.; EN; 35; 35; 1994; 6405-6408.

Reaction Details 2 of 2

Reaction Classification: Preparation

Yield: 96 percent (BRN=1367559)

Reagent: K₂CO₃, CuI, KI

Solvent: dimethylformamide

Temperature: 65 C

Ref. 1: [5968029](#), [Lit link](#); Journal; Bell, David; Davies, Mark R.; Geen, Graham R.; Mann, Inderjit S.; SYNTBF; Synthesis; EN; 6; 1995; 707-712.

For Help, press F1

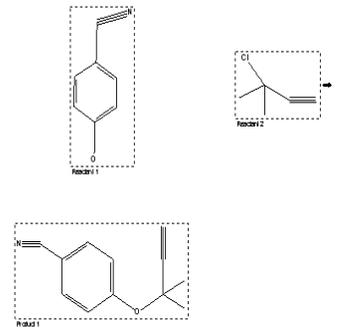
idle ALL Reactions

可用不同的格式将记录中所选择的部分内容导出。

记录导出后生成的报告示例

Microsoft Word window showing a table with reaction details and chemical structures.

Product BRN	1236349 3-chloro-3-methyl-but-1-yne
No. of Reaction Details	2
Find similar reactions	click here



Reaction scheme showing the conversion of Reactant 1 and Reactant 2 into Product 1.

MDL CrossFire Commander window showing a report for Reaction ID 2413025.

MDL CrossFire Commander - [Reports - report2.html]

Query Results Reports Alerts AutoNom

Open Document Print Refresh

Find in Report/Export File: report2.html

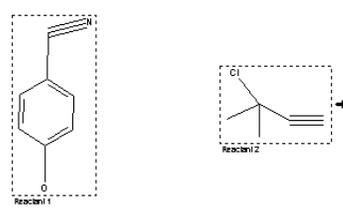
Report: Report

Beilstein Data: Copyright (c) 1988-2004, Beilstein Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH. All rights reserved.

Reaction (Beilstein(2004/02):Reactions:2413025 hit 1, RX.ID [2413025](#))

Reaction ID	2413025
Reactant BRN	386130 4-hydroxy-benzotrifluoride
	1236349 3-chloro-3-methyl-but-1-yne
Product BRN	1367559 3-(4-cyanophenoxy)-3-methylbut-1-yne
No. of Reaction Details	2
Find similar reactions	click here

RX.ID=2413025:



Reaction scheme showing the conversion of Reactant 1 and Reactant 2 into Product 1.

跟踪服务的建立

MDL CrossFire Commander - [Query for Server default]

Query Results Reports Alerts **Alerts** AutoHom

Query History | Open Query | Save Query | Print Query | Clear Query | Select Database | Draw Structure | Modify Alert | **Create Alert** | Start Search

Text in the Forms: ? **Query Builder** ? Search in: Beilstein(2004/02)

Search Fields | Queries

Hitsets

Bibliographic Data
Substance Identification Data
Molecular Formula Search
Reaction Data
Physical Data
Spectroscopic Data
Pharmacological Data
Ecotoxicological Data
Solubility Data

Free Sites:
 hetero atom
 all atom

Stereo: off

Search:
 as structure
 as reactant
 as product
 as reagent
as
as

Allow:
 salts
 addl. rings
 isotopes
 charges
 radicals
 mixtures
 relat. Markus

Clear Structure | Extended Options

and Search All Text ?

and Search Fields ?

	Operator	(Field name	Relation	
1			Journal Title(JT)	starts with	j med. chem.
2	proximity		Publication Year(PY)	is	1991
3	and			is	

Sort Entries ab by Default

For Help, press F1

idle

建立检索条件后点击此按钮，

MDL CrossFire Commander - [Alerts on Server default]

Query Results Reports **Alerts** AutoHom

Show all Profiles | Print Profile | Export Profile | Import Profile | Delete Profile | Deactivate Profile | Edit / Modify Query | Clear | Save Profile

Find Alert (Search in Profile ?) **Alert Profile:** titled - enter name [at most 14 letters, digits, underscores] (Alert hitsets see)

Find

Alert Profiles

To create a new query:

- Choose QUERY tab to enter the Query Builder
- Define your structure/reaction/text query as usual
- Test your query
- Choose "Create Alert" from the Query Builder.

To modify an existing alert profile:

- Click an entry in the Alert Profiles tree (left box).

Database: Today Last Frequency: After each update Hits [last] Show

Send results: Enter your own E-mail address [You are the owner of the alert]

Send a copy: Enter further E-mail addresses [and/or existing alert E-mail lists] separated by semicolons

Comment: Save Profile

Sort Entries ab by Name

For Help, press F1

idle

在此对话框中填入相关信息即可。

化学结构的自动命名

MDL CrossFire Commander - [AutoNom]

File Edit Task View Options Help

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Print Page

Find AutoNom Name: Find

m Namings
2004/07/23
2004/08/03
1: 3-Hydroxy-2,2-dimethyl-4-(2-

AutoNom

Messages:

Generate Name

Structure Show Locants Clear

impl. free sites

3-Hydroxy-2,2-dimethyl-4-(2-oxo-pyrrolidin-1-yl)-chroman-6-carbonitrile

AutoNom Name: Options

Ring Names: Beilstein

For Help, press F1

idle

输入化学结构后点击“Generate Name”按钮，化合物命名便会出现于右下角的文本框内。

可选择命名时所参考的环系。

Gmelin数据库检索示例1

例： 查询锌含量在**5—30%**（重量百分比）之间的铜合金，并要求查到的结果含有热力学方面的数据。

- 使用表格查询方式查询合金
- 利用二次查询筛选含有热力学数据的记录

Query Builder: Data Search

	Operator	(Field name	Relation	Field content	List)	▲
1			Alloy Search Field(ALLOY)	is	cu,Zn(5-30) (W%)	▼		
2	and	▼		is				
3	and			is				

任何时候都可以
靠下拉箭头得到
帮助和提示。

百分比类型:

- A - 原子
- W - 重量
- V - 体积
- X - 摩尔

Component Formula:
(e.g. Fe or Fe2O3)

Percentage:
(Number or range: 20 or 20-40)

Cu	
Zn	5-30

Percentage Type: A
W
V
X

OK Cancel Help

表格查询结果显示

MDL CrossFire Commander - [Gmelin(2004/02):Q01 Substance 198 of 377]

File Edit Task View Options Window Help

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

History Print Hits View hit Show Grid List Get Sort Hits Copy Export Hits Copy to Report

Gmelin (2004/02)
... Saved Hitsets/Alert Hitsets
... Session Hitsets
 + Q: Q01 (377 Substances)
Beilstein (2004/02)

Substance Identification

GMELIN Registry Number **502930**
Linear Structure Formula Cu(73.4),Al(7.54),Zn(19.06) (W%)
Type of Substance Alloy

Composition 1-3

Formula	Comp. GRN	%	Type of %	Role	Modification
Al	16248	7.54	weight%		
Cu	16269	73.4	weight%		
Zn	16321	19.06	weight%		

与检索条件匹配的数据内容以高亮背景颜色标记。

	Operator	(Field name	Relation	Field content	List)	▲
1			Alloy Search Field(ALLOY)	is	cuZn(5-30) (w%)	▼		
2	and	▼	Thermodynamic Data(TDD)	exists		▼		
3	and	▼		is		▼		
4	and	▼		is		▼		
5	and	▼		is		▼		
6	and	▼		is		▼		
7	and	▼		is		▼		
8	and	▼		is		▼		
9	and	▼		is		▼		
10	and	▼		is		▼		

从索引中查找热力学数据域的名称，填入“Field Name”，“Relation”列选择“exists”。

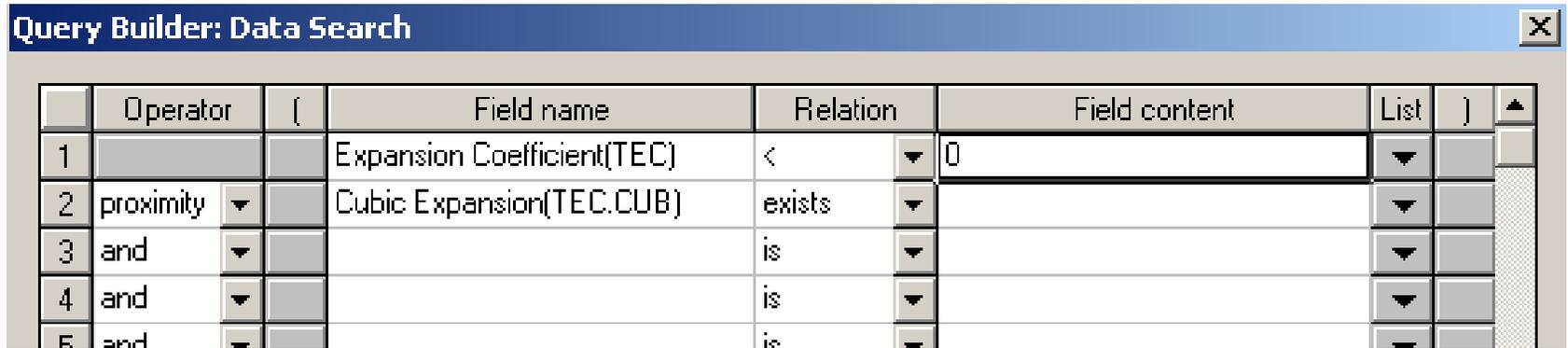
-  Thermodynamic Data (TDD)
 -  Specific Heat at Constant Pressure (CP)
 -  Cp (Further Information) (CPFI)
 -  Specific Heat at Constant Volume (CV)
 -  Cv (Further Information) (CVFI)
 -  Enthalpy of Formation (HFOR)
 -  Enthalpy of Formation (Further Information) (HFFI)
 -  Gibbs Energy of Formation (GFOR)
 -  Gibbs Energy of Formation (Further Information) (GFFI)
 -  Entropy of Formation (SFOR)
 -  Entropy of Formation (Further Information) (SFFI)
 -  Equation of State (EQST)
 -  Acentric Factor (ACEN)

表格查询结果显示

<p>Hit 1:70093 Al(8),Cu(75.9),Zn(16.1) (W%) type = alloy</p> <p>Al(8),Cu(75.9),Zn(16.1) (W%)</p>	<p>Hit 2:462627 Al(8),Cu(75.9),Zn(16.1) (W%) type = alloy</p> <p>Al(8),Cu(75.9),Zn(16.1) (W%) Modification: .beta.1'</p>	<p>Hit 3:463238 Al(8),Cu(75.9),Zn(16.1) (W%) type = alloy</p> <p>Al(8),Cu(75.9),Zn(16.1) (W%) Modification: .beta.1</p>	<p>Hit 4:806394 Cu(83.714),Zn(16.286) (W%) type = alloy</p> <p>Cu(83.714),Zn(16.286) (W%)</p>
<p>Hit 5:827534 Al(90.366),Cu(1.608),Mg(2... type = alloy</p> <p>Al(90.366),Cu(1.608),Mg(2.484),Zn(5.542) (W%)</p>	<p>Hit 6:1234171 Cu(60.889),Ni(18.745),Zn(.. type = alloy</p> <p>Cu(60.889),Ni(18.745),Zn(20.366) (W%)</p>	<p>Hit 7:1236514 Cu(51.026),Ni(21.837),Zn(.. type = alloy</p> <p>Cu(51.026),Ni(21.837),Zn(27.137) (W%)</p>	<p>Hit 8:1258695 B(0.173),Cu(59.161),Mn(0... type = alloy</p> <p>B(0.173),Cu(59.161),Mn(0.264),Ni(17.181),Zn (23.221) (W%)</p>
<p>Hit 9:1258697 B(0.086),Cu(58.789),Mn(0... type = alloy</p> <p>B(0.086),Cu(58.789),Mn(0.262),Ni(16.915),Zn (23.948) (W%)</p>	<p>Hit 10:1279346 Cu(58.759),Mn(0.261),Ni(.. type = alloy</p> <p>Cu(58.759),Mn(0.261),Ni(17.127),Zn(23.853) (W%)</p>	<p>Hit 11:1281914 Cu(70.619),Ni(14.142),Z.. type = alloy</p> <p>Cu(70.619),Ni(14.142),Zn(15.239) (W%)</p>	<p>Hit 12:1283900 Cu(60.253),Ni(12.408),Z.. type = alloy</p> <p>Cu(60.253),Ni(12.408),Zn(27.339) (W%)</p>
<p>Hit 13:1492510 Al(44.5),Cu(45.9),Zn(9.5) .. type = alloy</p> <p>Al(44.5),Cu(45.9),Zn(9.5) (A%) Modification : .tau.'</p>			

Gmelin数据库检索示例2

例： 查找膨胀系数小于零的化合物，然后修改查询条件来查找含有立体膨胀系数的记录。



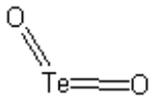
The screenshot shows a window titled "Query Builder: Data Search" with a close button in the top right corner. The main area contains a table with the following columns: Operator, Field name, Relation, Field content, and List. The table is currently empty, with only the header row visible.

	Operator	(Field name	Relation	Field content	List)	▲
1			Expansion Coefficient(TEC)	<	0	▼		
2	proximity	▼	Cubic Expansion(TEC.CUB)	exists		▼		
3	and	▼		is		▼		
4	and	▼		is		▼		
5	and	▼		is		▼		

表格查询结果显示

Identification	
GMELIN Registry Number	1411
Linearized Structure Formula	TeO ₂
Molecular Formula	O ₂ Te
Molecular Weight	159.599
Chemical Name	tellurium dioxide tellurium oxide tellurous dioxide tellurium(IV) oxide paratellurite tellurium(IV) dioxide Tellurdioxid
Entry Date	1995/12/11
Update Date	2003/06/18

Q04: Hit 2



Thermal Expansion 85 of 126	
Expansion Coefficient	-8*10 ⁻⁹ K ⁻¹
Cubic Expansion	yes
Temperature	-270 Deg C
Forms of State	Unspecified

与检索条件匹配的数据内容以高亮背景颜色标记。

Ref. 1	556323 , LitLink ; White, G. K.; Collocott, S. J.; Collins, J. G.; JCOMEL; J. Phys. Condens. Matter; Vol. 2; (1990) 7715-7718; English.
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Thermal Expansion 87 of 126	
Expansion Coefficient	-2*10 ⁻⁹ K ⁻¹
Cubic Expansion	yes
Temperature	-271 Deg C
Forms of State	Unspecified

Ref. 1	556323 , LitLink ; White, G. K.; Collocott, S. J.; Collins, J. G.; JCOMEL; J. Phys. Condens. Matter; Vol. 2; (1990) 7715-7718; English.
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Gmelin数据库检索示例3

例： Ziegler/Natta络合物是聚合物工业中的重要催化剂。查询这类化合物的合成信息，并利用超链接访问相关的催化作用数据合文献信息。

- 采用半反应查询方式
- 利用超链接访问催化作用数据和文献信息

检索条件的建立

MDL CrossFire Commander - [Query for Server default]

File Edit Task View Options Query Help

MDL CrossFire Commander

Query Results Reports Alerts AutoNom

Query History Open Query Save Query Print Query Clear Query Select Database Draw Structure Modify Alert Create Alert Start Search

Search Field Name in ?

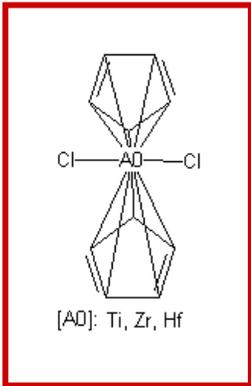
tdd Find

Predefined Search Forms

Hitsets

Gmelin(2004/02)

Query Builder ? Search in: Gmelin(2004/02)



[AD]: Ti, Zr, Hf

Free Sites: ?

hetero atom ?

all atom ?

Stereo: ?

off

Search: ?

as structure ?

as reagent

as product

as

as

Allow: ?

salts

addl. rings

isotopes

charges

radicals

mixtures

relat. Markus

Clear Structure Extended Options

and Search All Text ?

Truncate... Clear Text

and Search Fields ?

Advanced Search Clear Table

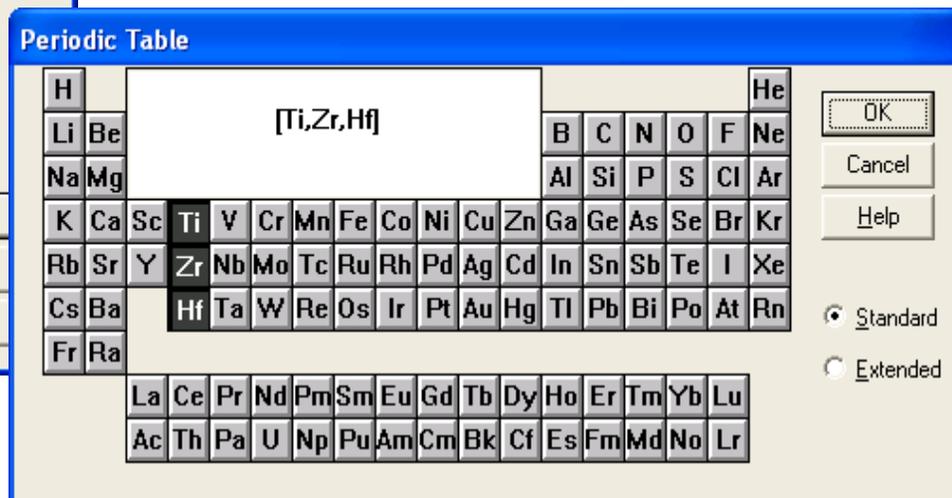
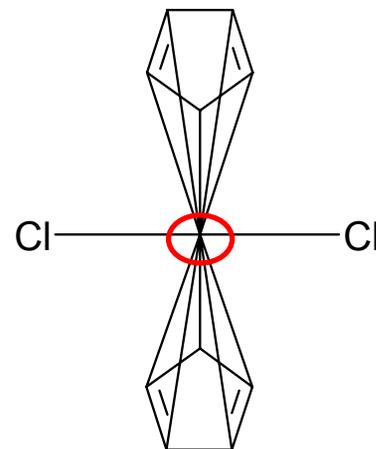
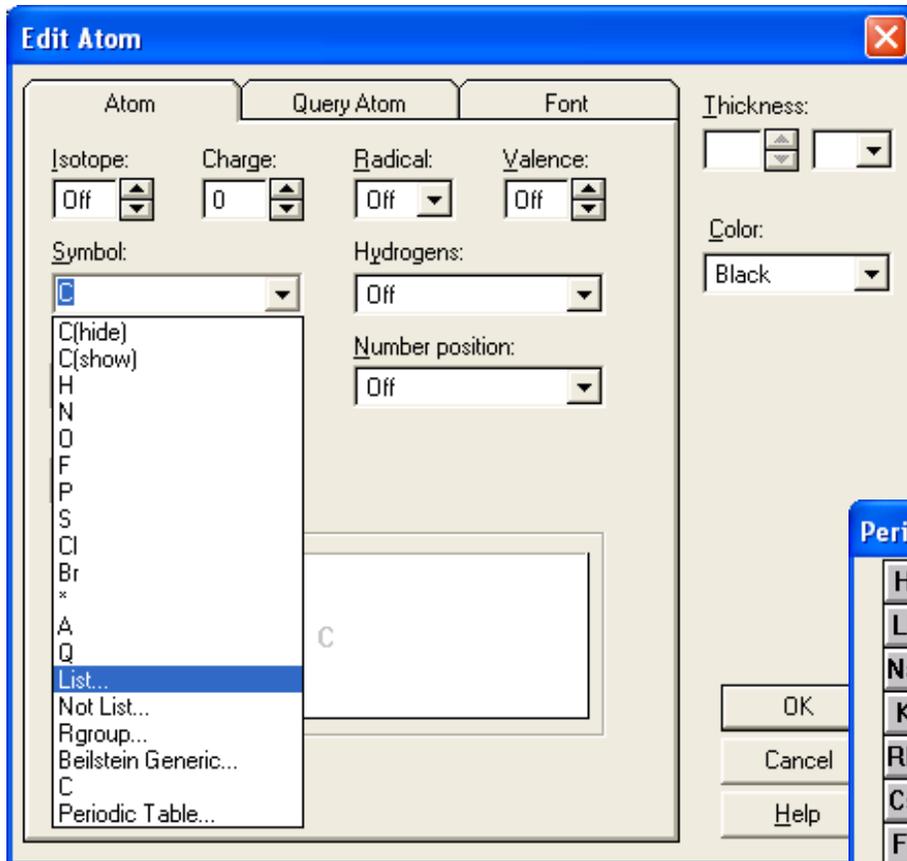
<- Select (and edit) Search Form, Search Field, Query, or Hitset from left box and append to query

Search Substances Start Search

Show Help for Search Fields

For Help, press F1

idle



在ISIS/Draw中用“选择”工具双击络合物的中心原子，弹出“Edit Atom”对话框，在“Symble”下拉菜单中选择“List”，然后在弹出的元素周期表中选择所有可能的中心原子的符号，点击“OK”，即可将中心原子定义为多种可能的原子类型。

查询结果显示

链接到化合物信息的超链接

Reaction

Reaction ID	21107
Reactant(s) (GRN)	101338 C ₅ H ₅ MgBr cyclopentadienyl magnesium bromide
	2469 ZrCl ₄ zirconium tetrachloride
Product(s) (GRN)	4056 C ₅ H ₅) ₂ ZrCl ₂ Cp ₂ ZrCl ₂

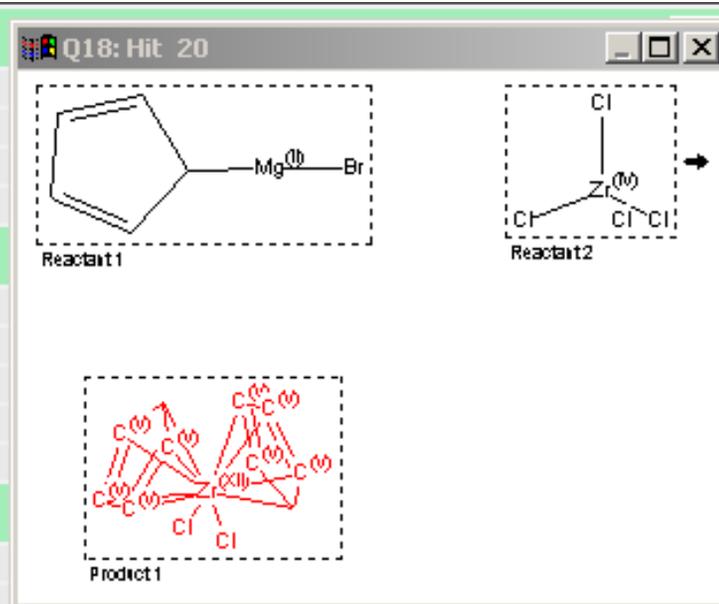
Field Availability List

Code	Field Name	Occ.
RX	Reaction Details	1

Reaction Details

Solvent	ether
General Conditions	ZrCl ₄ /C ₅ H ₅ MgBr (molar ratio: 1:2); dry ether;
Update Date	2001/12/19

Ref. 1	554921 , LitLink ; Vol. Zr: Org. Verb.; Pages 26 - 33.
Ref. 2	554926 , LitLink ; anonymous; (1954) 1957; Ethyl Corporation; Brit.; 768083.
Ref. 3	554933 , LitLink ; anonymous; (1955) 1958; National Lead Co.; Brit.; 793354.



Identification

GMELIN Registry Number	4056
Linearized Structure Formula	(C ₅ H ₅) ₂ ZrCl ₂
Molecular Formula	C ₁₀ H ₁₀ Cl ₂ Zr
Ligand Molecular Formula	Zr{(5)L}2{X}2
Ligand Formulas	(5)L
Ligand Formula Count	(5)L:2
Ligand Formulas	X
Ligand Formula Count	X:2
Molecular Weight	292.319
CAS Registry Number	001291-32-3
Chemical Name	Cp ₂ ZrCl ₂

Scroll down and click the Behavior as Catalyst (BCAT) hyperlink.

催化数据超链接

Field Availability List 31-38 of 38

Code	Field Name	Occ.
BCAT	Behavior as Catalyst	84
POLY	Polymerisation	2
CRT	Crystal Structure	1
DEN	Density	1
POT	Electrochemical Reaction	19
SLB	Solubility	4
MPRO	Magnetic Properties	1
CNR	Reference	820

Behavior as Catalyst 1 of 84

Ref. 1 [1210957, Lit.Link](#) ; Lipshutz, Bruce H.; Mollard, Paul; Pfeiffer, Steven S.; Chrisman, Will; JACSAT; J. Am. Chem. Soc.; Vol. 124; (2002) 14282 - 14283; English.

Behavior as Catalyst 2 of 84

Ref. 1 [1199015, Lit.Link](#) ; Huang, Jiling; Feng, Zuofeng; Wang, Hong; Qian, Yanlong; Sun, Junquan; et al.; JMCCF2; J. Mol. Catal. A Chem.; Vol. 189; (2002) 187 - 194; English.

Behavior as Catalyst 3 of 84

Ref. 1 [1192709, Lit.Link](#) ; Ignat'ev, R. A.; Maslennikov, S. V.; Spirina, I. V.; Artemov, A. N.; Maslennikov, V. P.; Lineva, A. N.; ZOKHA4; Zh. Obshch. Khim.; Vol. 72; (2002) 944 - 947; Russian; RJGCEK; Russ. J. Gen. Chem. (Engl. Transl.); Vol. 72; (2002) 882 - 885; English.

Behavior as Catalyst 4 of 84

Ref. 1 [1186933, Lit.Link](#) ; Zi, Guofu; Li, Hung-Wing; Xie, Zuowei; ORGND7; Organometallics; Vol. 21; (2002) 3850 - 3855; English.

Behavior as Catalyst 5 of 84

Ref. 1 [1175037, Lit.Link](#) ; Grimmer, Neil E.; Coville, Neil J.; Koning, Charles B. de; JMCCF2; J. Mol. Catal. A Chem.; Vol. 188; (2002) 105 - 114; English.



Ref. 1 **1175037** [LitLink](#) ; Grimmer, Neil E.; Coville, Neil J.; Koning, Charles B. de; JMCCF2; J. Mol. Catal. A Chem.; Vol. 188; (2002) 105 - 114; English.

Reference [LitLink](#)

Citation Number **1175037**

Field Availability List 1-3 of 3

Code	Field Name	Occ.
CIT	Citation	1
AB	Abstract	1
IDE	Identification	7

Citation

Author Grimmer, Neil E.
 Coville, Neil J.
 Koning, Charles B. de
 CODEN JMCCF2
 Journal Title J. Mol. Catal. A Chem.
 Volume 188
 Publication Year 2002
 Page 105 - 114
 Language English

Abstract

Title Zirconium bis-cyclopentadienyl compounds. An investigation into polymerisation behaviour of (CpR)₂ZrCl₂/MAO catalysts

Abstract The ethylene polymerization behavior of several mono-substituted (CpR)₂ZrCl₂/MAO catalysts (R = Me, Et, iPr, tBu, SiMe₃, CMe₂Ph) was studied. The catalytic activity was influenced by the steric and electronic effects. The highest activity was exhibited by the catalysts stabilized by small substituents on the cyclopentadienyl rings that do not undergo catalyst disproportionation.

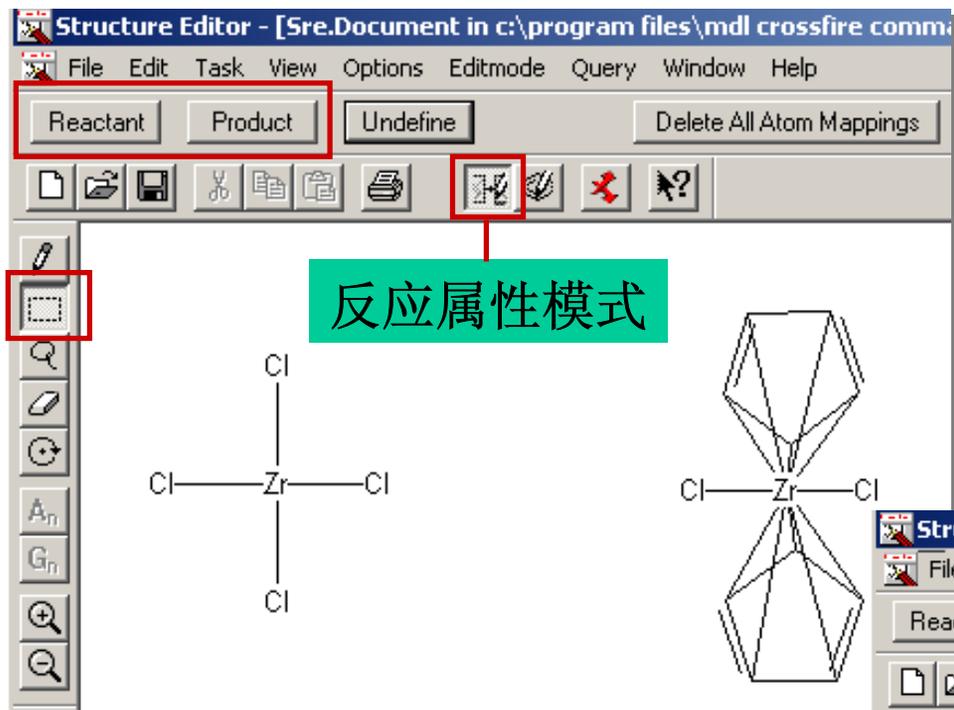
Language English

重新编写过的摘要: Zirconium bis-cyclopentadienyl compounds. An investigation into the influence of substituent effects on the ethene polymerisation behaviour of (CpR)₂ZrCl₂/MAO catalysts.

Gmelin数据库检索示例4

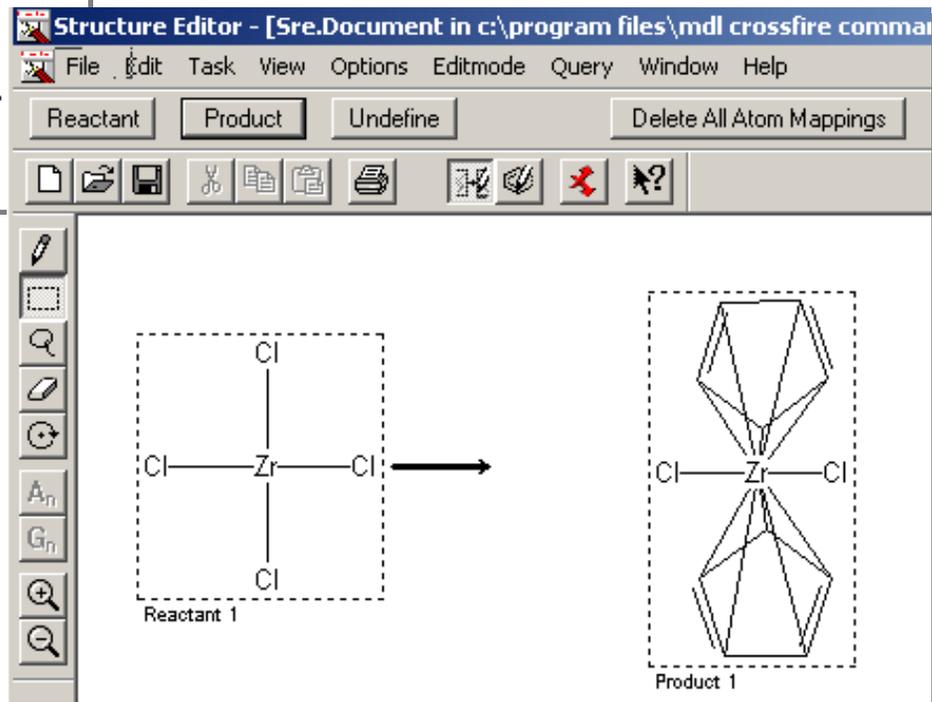
例： 查询催化剂 Cp_2ZrCl_2 的合成方法。反应物为 ZrCl_4 。

- 建立全反应检索条件



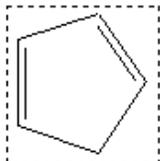
在反应模式下：

- 选中ZrCl₄整个分子结构后点击“Reactant”按钮。
- 选中CpZrCl₂整个分子结构后点击“Product”按钮。

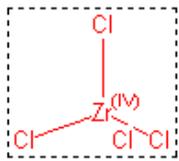


查询结果显示

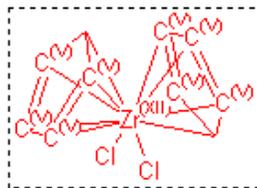
Hit 9:318641



Reactant 1

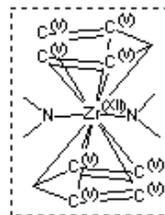


Reactant 2

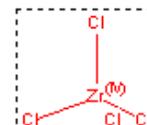


Product 1

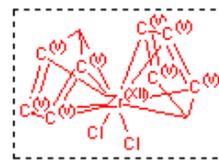
Hit 10:472960



Reactant 1

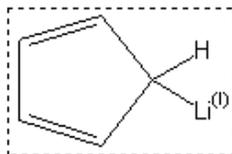


Reactant2

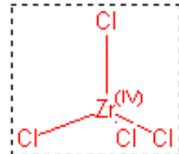


Product1

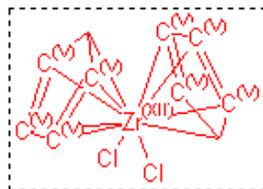
Hit 11:845351



Reactant 1

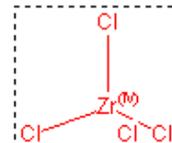


Reactant 2

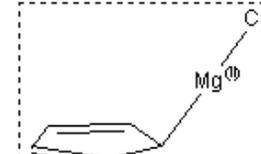


Product 1

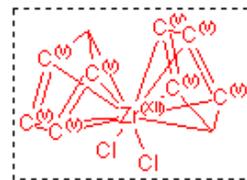
Hit 12:940016



Reactant1



Reactant2



Product1

总结

- **信息量：** Crossfire Beilsten/Gmelin数据库含有丰富数据量，涵盖了有机化学，无机和金属有机化学最主要的、最新的研究内容。
- **检索功能：** Commander提供了各种先进高效的检索方法，可以帮助用户快速从海量的数据中找出所需要的信息。
- **界面：** 十分友好，易于操作，浏览方便。
- **检索结果的处理：** 得到了很大程度的简化，可以十分方便的导出数据并生成报告。