Crossfire Beilstein/Gmelin
使用方法介绍

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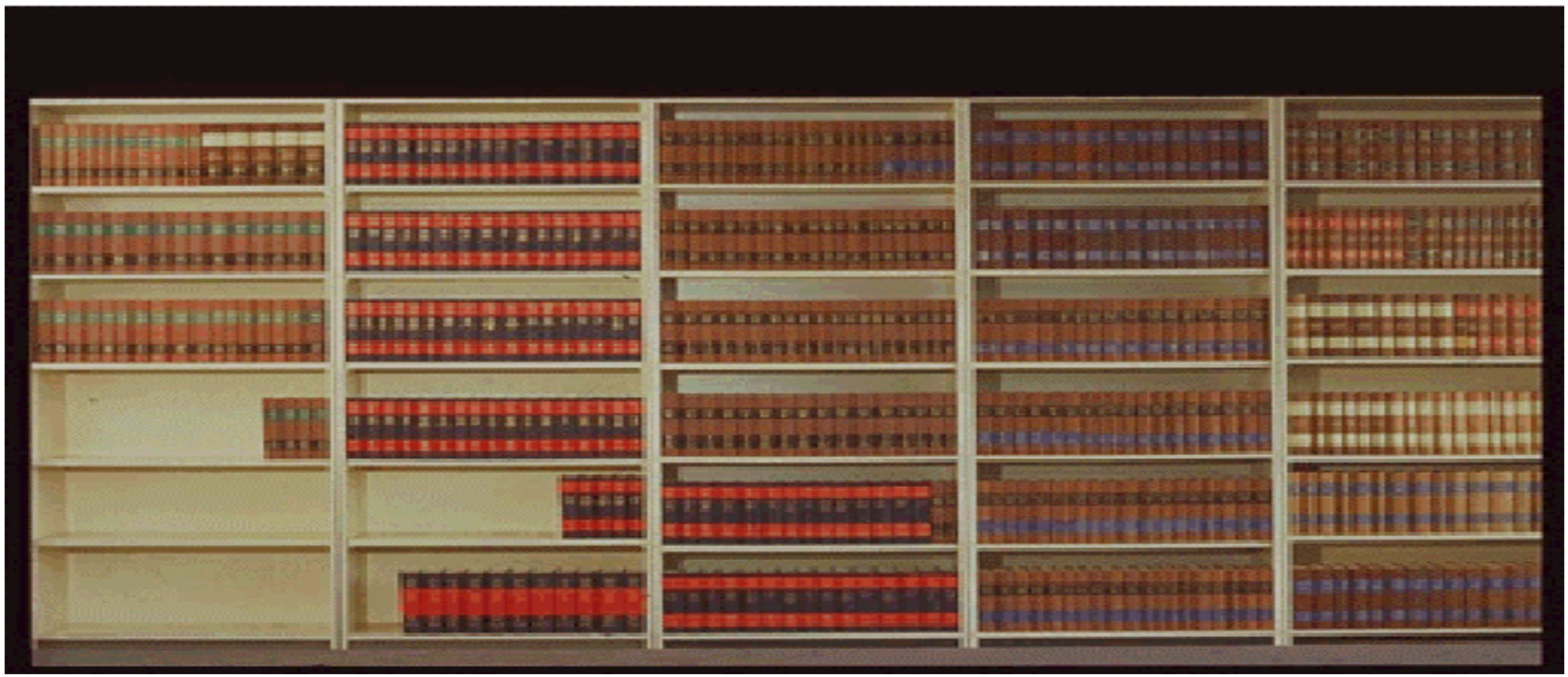
www.neotrident.com

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

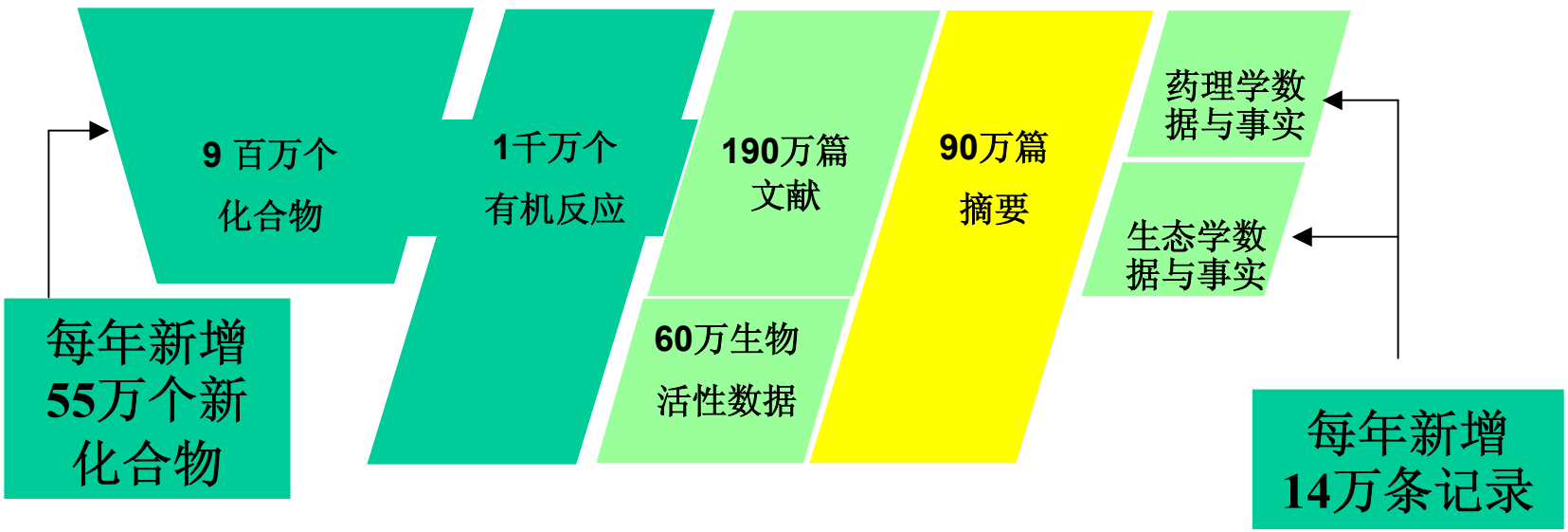
✓ 电子版本，检索方便，结果便于复制、保存和打印



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：

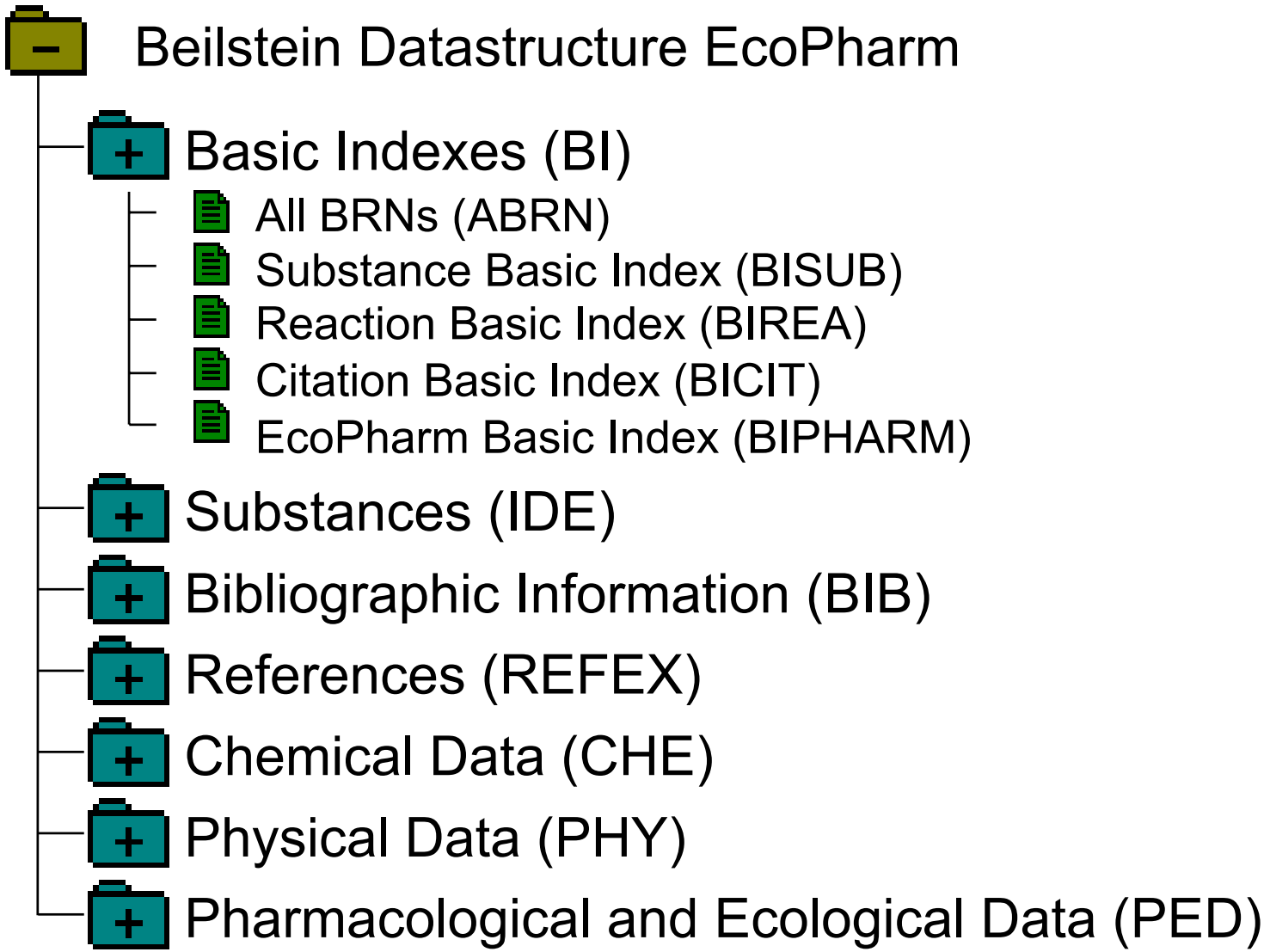
近百种高级查询方式：可以通过包括结构，子结构，反应，物化数据，制备条件以及关键字在内的近百种高级查询来方便灵活得到您需要的信息。

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


Beilstein Datastructure EcoPharm
Basic Indexes (BI)
All BRNs (ABRN)
Substance Basic Index (BISUB)
Reaction Basic Index (BIREA)
Citation Basic Index (BICIT)
EcoPharm Basic Index (BIPHARM)
Substances (IDE)
Bibliographic Information (BIB)
References (REFEX)
Chemical Data (CHE)
Physical Data (PHY)
Pharmacological and Ecological Data (PED)

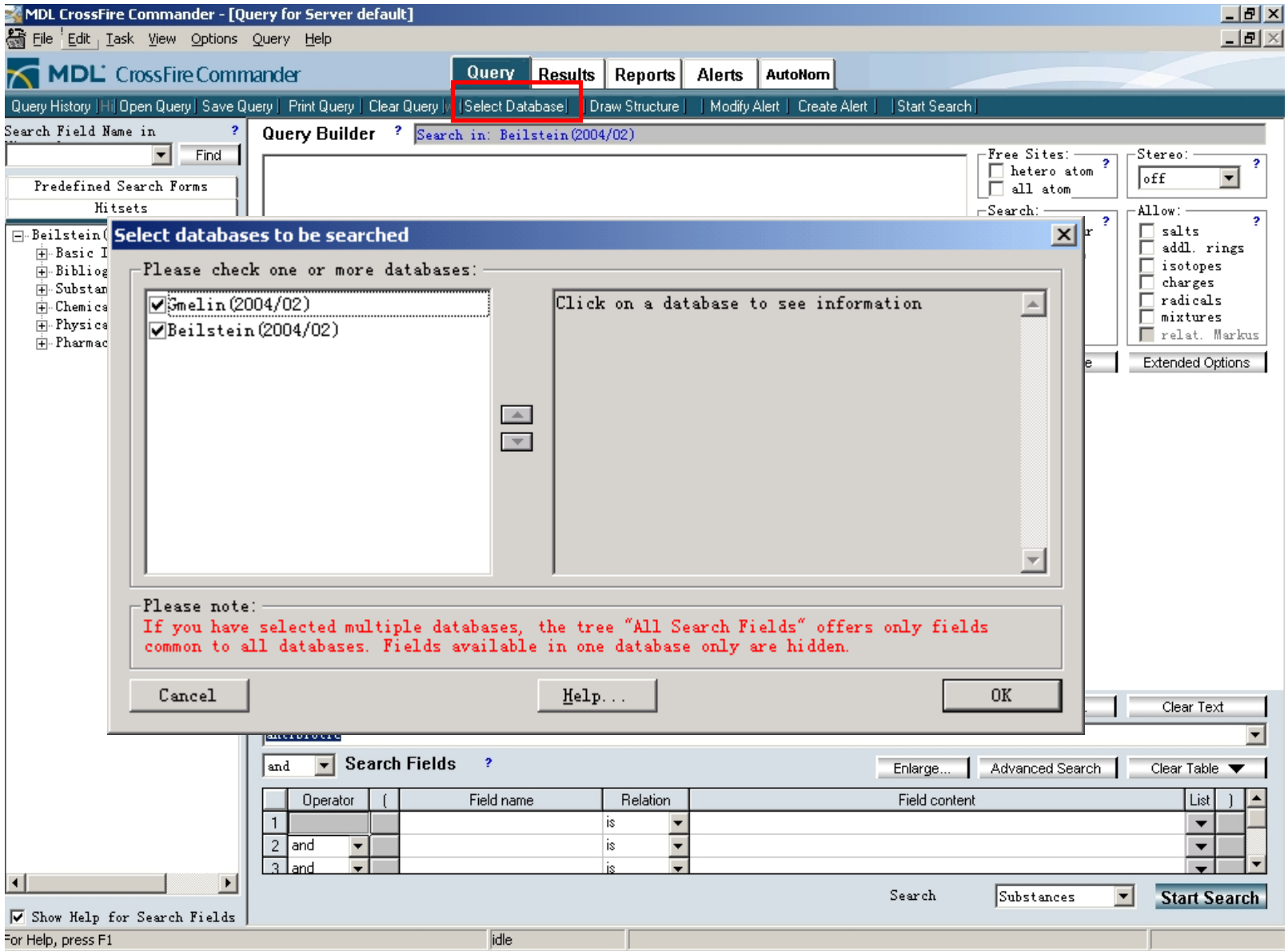
Gmelin – 全面的无机化学数值和事实库

- ✓ 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。

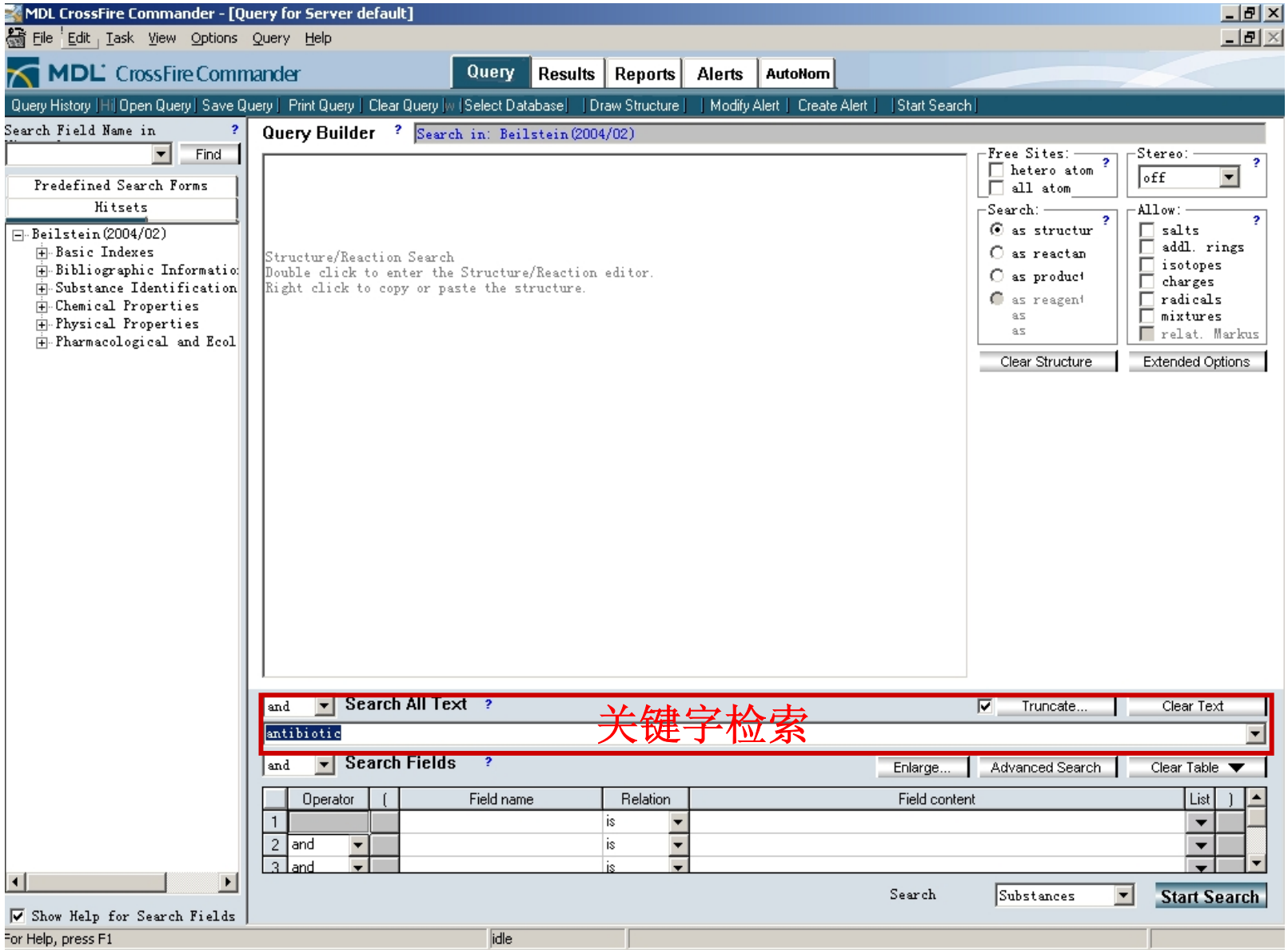
  - 超过2百万的化合物
  - 超过110万篇文献
  - 超过15万篇摘要
  - 超过160万个可查询反应

Commander 7.0的使用界面

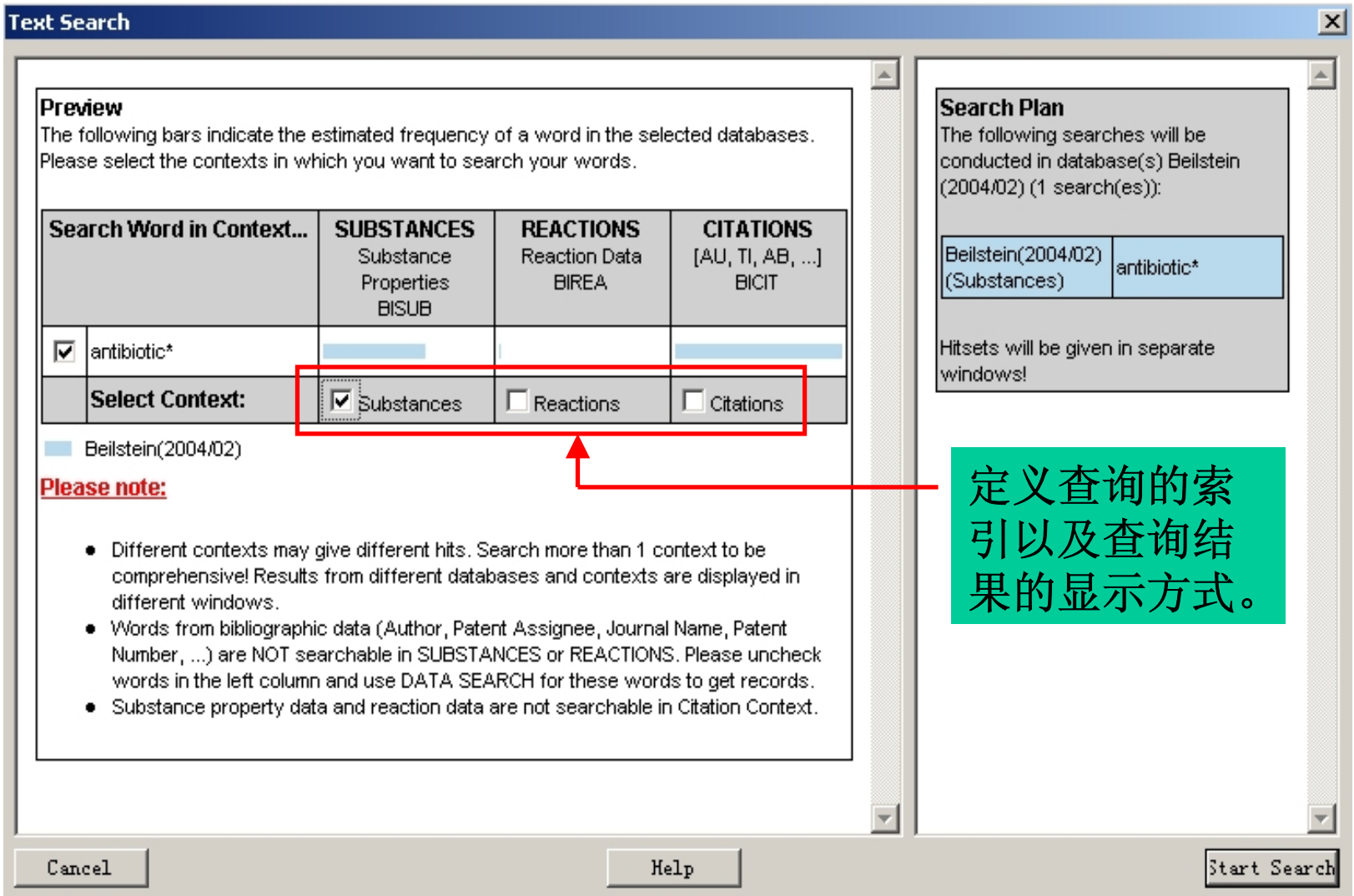
数据库选择


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
Find
Predefined Search Forms
Hitsets
Query Builder
Search in: Beilstein(2004/02)
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:
Gmelin(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
Clear Text
and
Search Fields
Enlarge...
Advanced Search
Clear Table
Operator
(
Field name
Relation
Field content
List
)
1
2 and
3 and
is
Search
Substances
Start Search
Show Help for Search Fields
For Help, press F1
idle

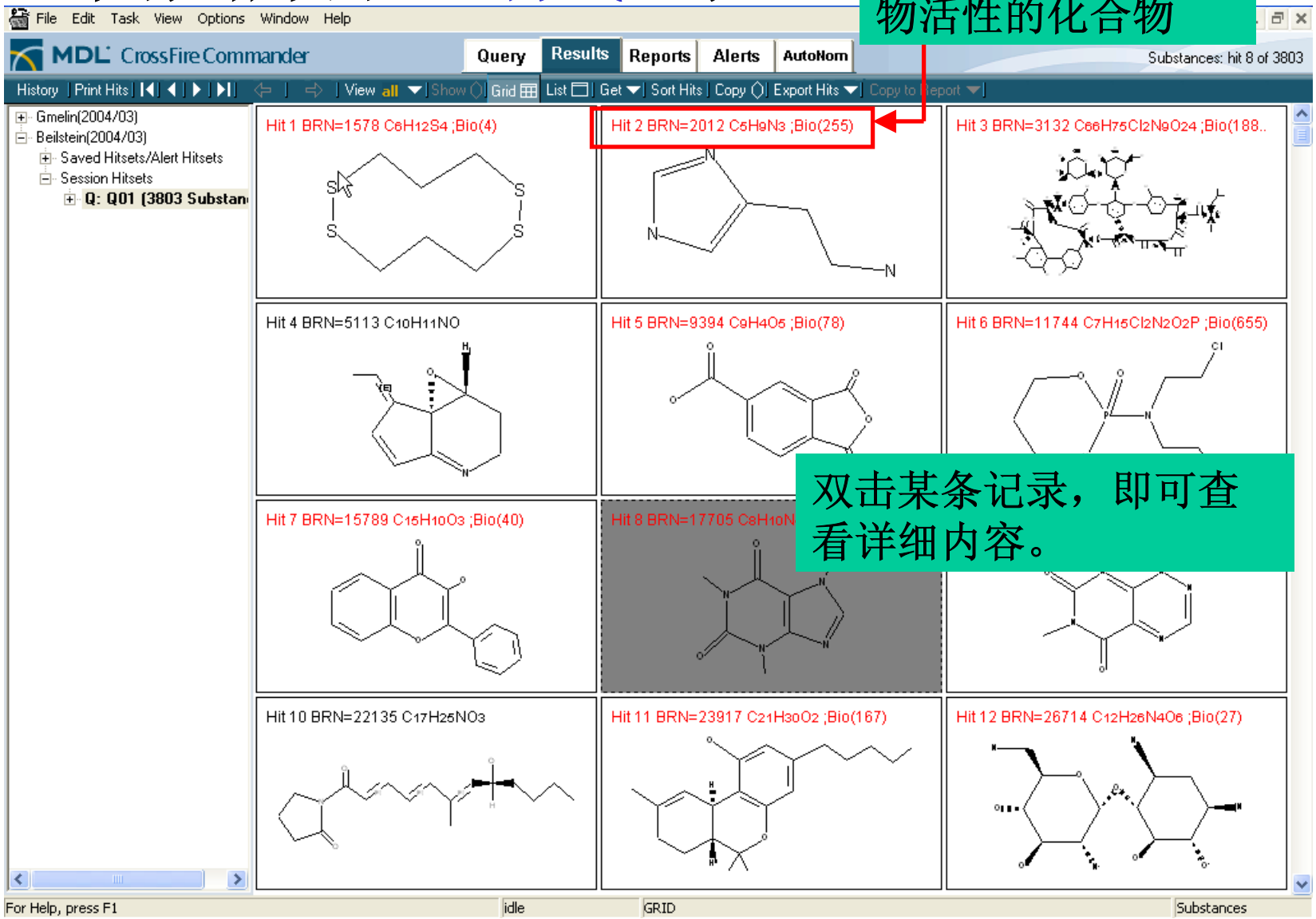
关键字检索


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 Informatio
Substance Identification
Chemical Properties
Physical Properties
Pharmacological and Ecol
Show Help for Search Fields
Query Builder
Search in: Beilstein(2004/02)
Structure/Reaction Search
Double click to enter the Structure/Reaction editor.
Right click to copy or paste the structure.
Free Sites:
hetero atom
all atom
Stereo:
off
Search:
as structur
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
antibiotic
关键字检索
and
Search Fields
Enlarge...
Advanced Search
Clear Table
Operator
(
Field name
Relation
Field content
List
)
1
2 and
3 and
is
Search
Substances
Start Search
For Help, press F1
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
antibiotic*
Select Context:
Substances
Reactions
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!
定义查询的索引以及查询结果的显示方式。
Cancel
Help
Start Search

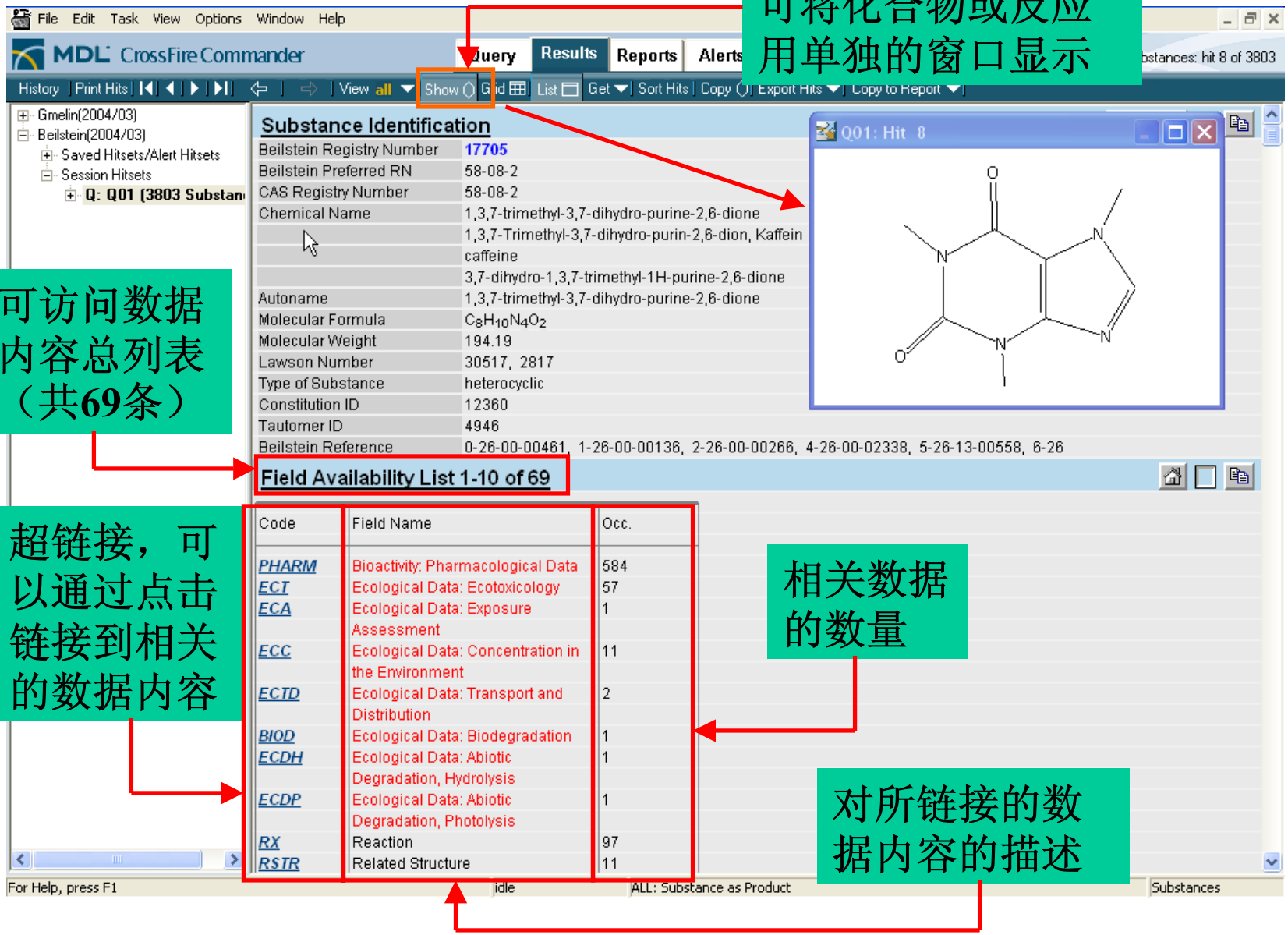
检索结果的Grid方式显示



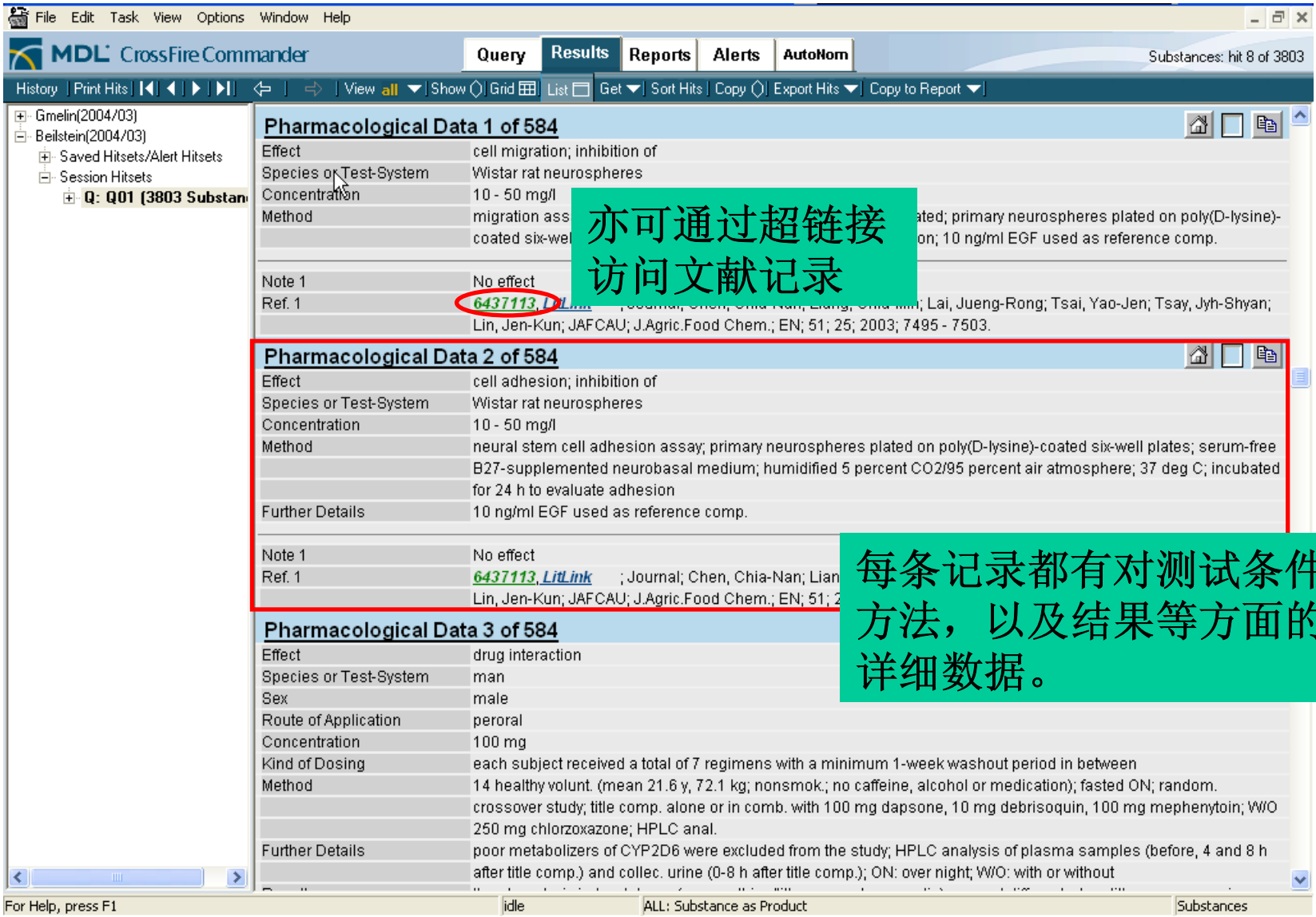
红色标记表示有生物活性的化合物

双击某条记录，即可查看详细内容。

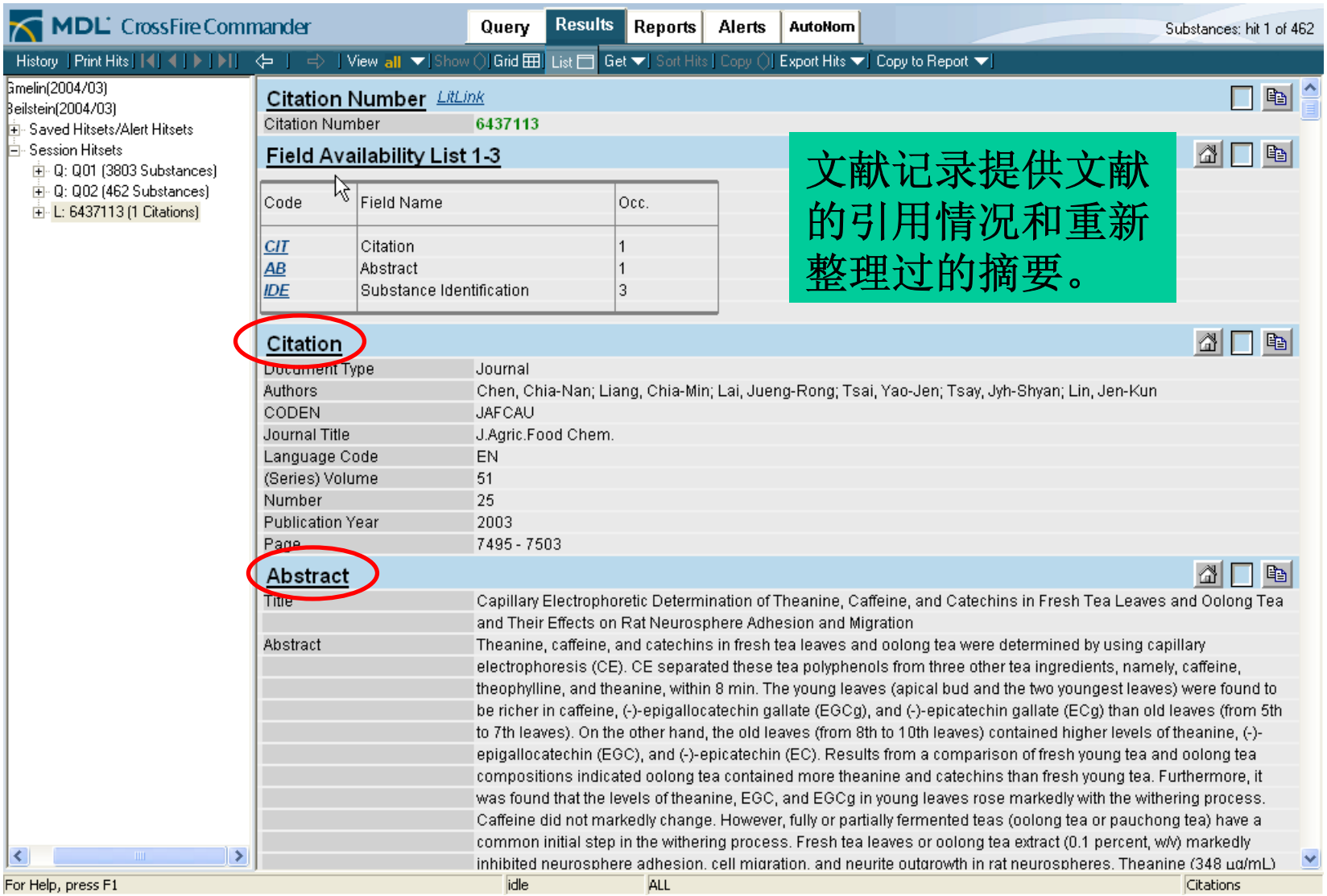
检索结果的List方式显示

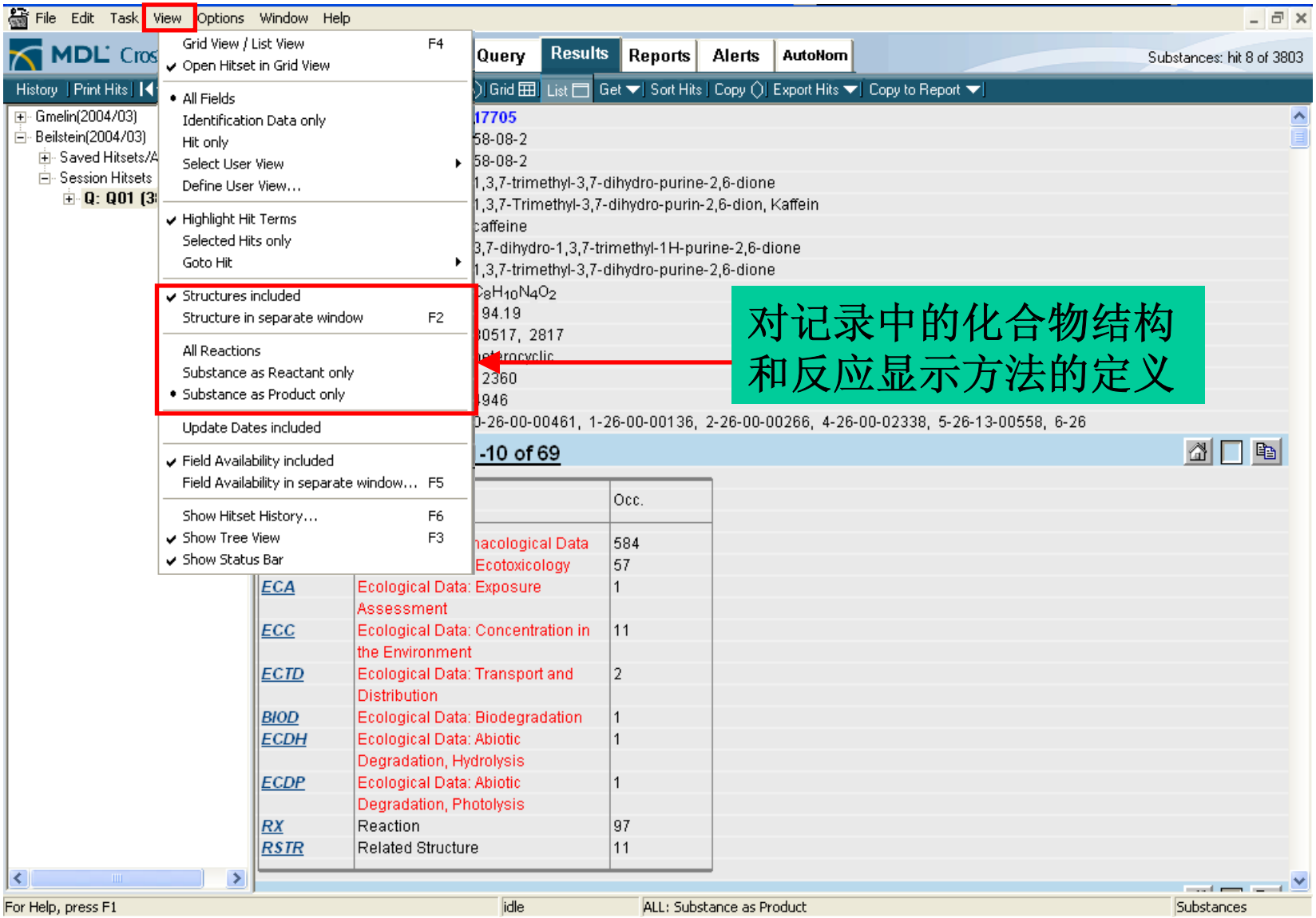


通过超链接访问药理学方面的数据和事实



文献记录的显示

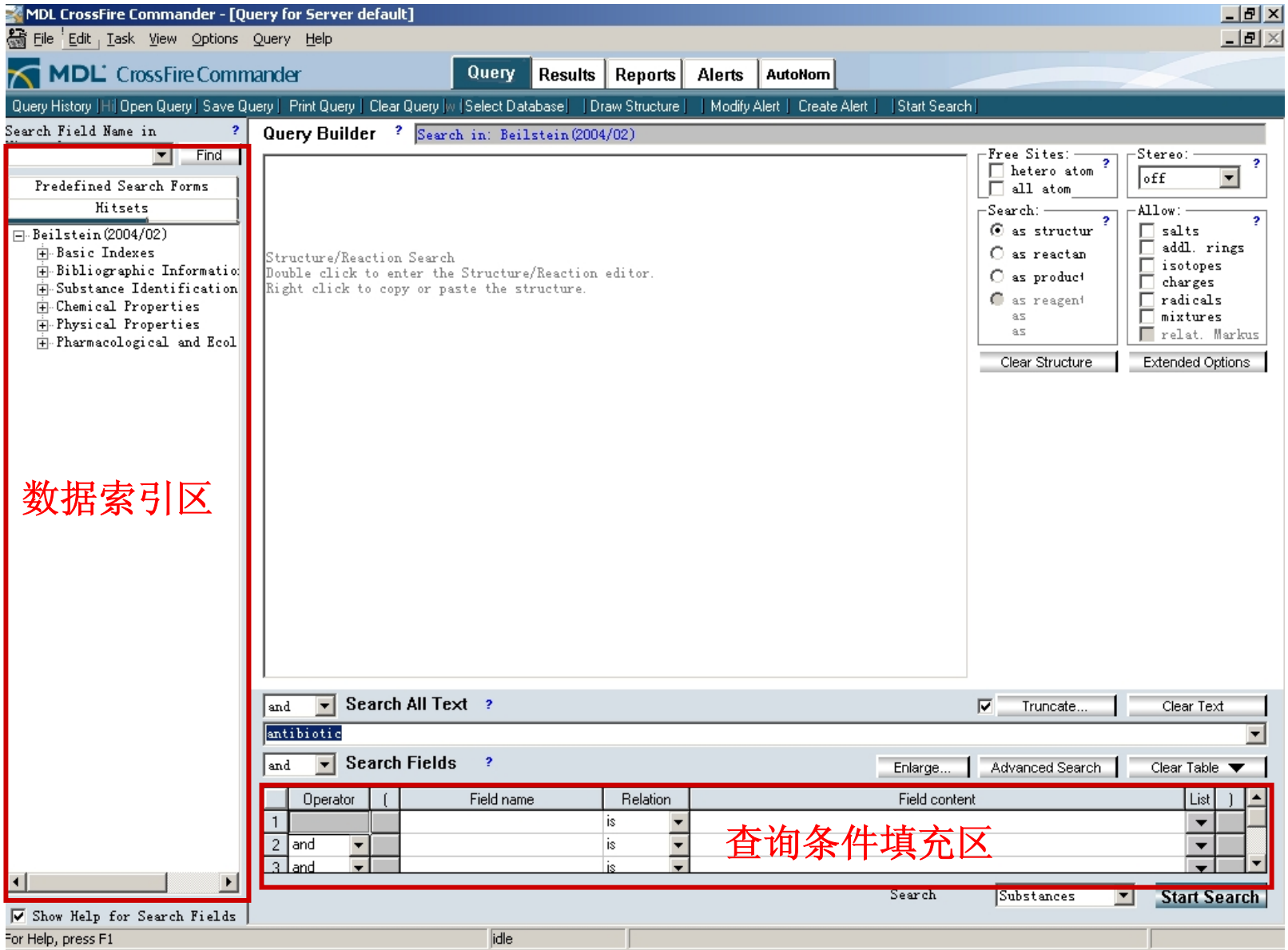

MDL CrossFire Commander
Query
Results
Reports
Alerts
AutoNom
Substances: hit 1 of 462
History | Print Hits | View all | Show | Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report
Gmelin(2004/03)
Beilstein(2004/03)
Saved Hitsets/Alert Hitsets
Session Hitsets
Q: Q01 (3803 Substances)
Q: Q02 (462 Substances)
L: 6437113 (1 Citations)
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
文献记录提供文献的引用情况和重新整理过的摘要。
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/v) markedly inhibited neurosphere adhesion, cell migration, and neurite outgrowth in rat neurospheres. Theanine (348 uq/mL)
For Help, press F1
idle
ALL
Citations


File Edit Task View Options Window Help
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
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
Substances: hit 8 of 3803
History Print Hits
Grid List Get Sort Hits Copy Export Hits Copy to Report
Gmelin(2004/03)
Beilstein(2004/03)
Saved Hitsets/A
Session Hitsets
Q: Q01 (3
对记录中的化合物结构
和反应显示方法的定义
-10 of 69
Occ.
ECA Ecological Data: Exposure Assessment
ECC Ecological Data: Concentration in the Environment
ECTD Ecological Data: Transport and Distribution
BIOD Ecological Data: Biodegradation
ECDH Ecological Data: Abiotic Degradation, Hydrolysis
ECDP Ecological Data: Abiotic Degradation, Photolysis
RX Reaction
RSTR Related Structure
For Help, press F1
idle
ALL: Substance as Product
Substances


File Edit Task View Options Window Help
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
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
对记录中显示的数据内容进行定义
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
For Help, press F1
idle
ALL: Substance as Product
Substances


File Edit Task View Options Window Help
MDL CrossFire Commander
Query Results Reports Alerts AutoNom
Substances: hit 8 of 3803
History Print Hits View all Show Grid List Get Copy Export Hits Copy to Report
Gmelin(2004/03)
Beilstein(2004/03)
Saved Hitsets/Alert Hitsets
Session Hitsets
Q: Q01 (3803 Substan
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。
Beilstein Registry Number 17705
Beilstein Preferred RN 58-08-2
CAS Registry Number 58-08-2
Chemical Name 1,3,7-trimethyl-3,
1,3,7-Trimethyl-3
caffeine
3,7-dihydro-1,3,7
Autoname 1,3,7-trimethyl-3,
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
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
For Help, press F1
idle
ALL: Substance as Product
Substances

快速数据检索


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 Informatio
Substance Identification
Chemical Properties
Physical Properties
Pharmacological and Ecol
数据索引区
Show Help for Search Fields
Query Builder
Search in: Beilstein(2004/02)
Structure/Reaction Search
Double click to enter the Structure/Reaction editor.
Right click to copy or paste the structure.
Free Sites:
hetero atom
all atom
Stereo:
off
Search:
as structur
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
antibiotic
and
Search Fields
Enlarge...
Advanced Search
Clear Table
Operator
(
Field name
Relation
Field content
List
)
1
2 and
3 and
is
查询条件填充区
Search
Substances
Start Search
For Help, press F1
Idle

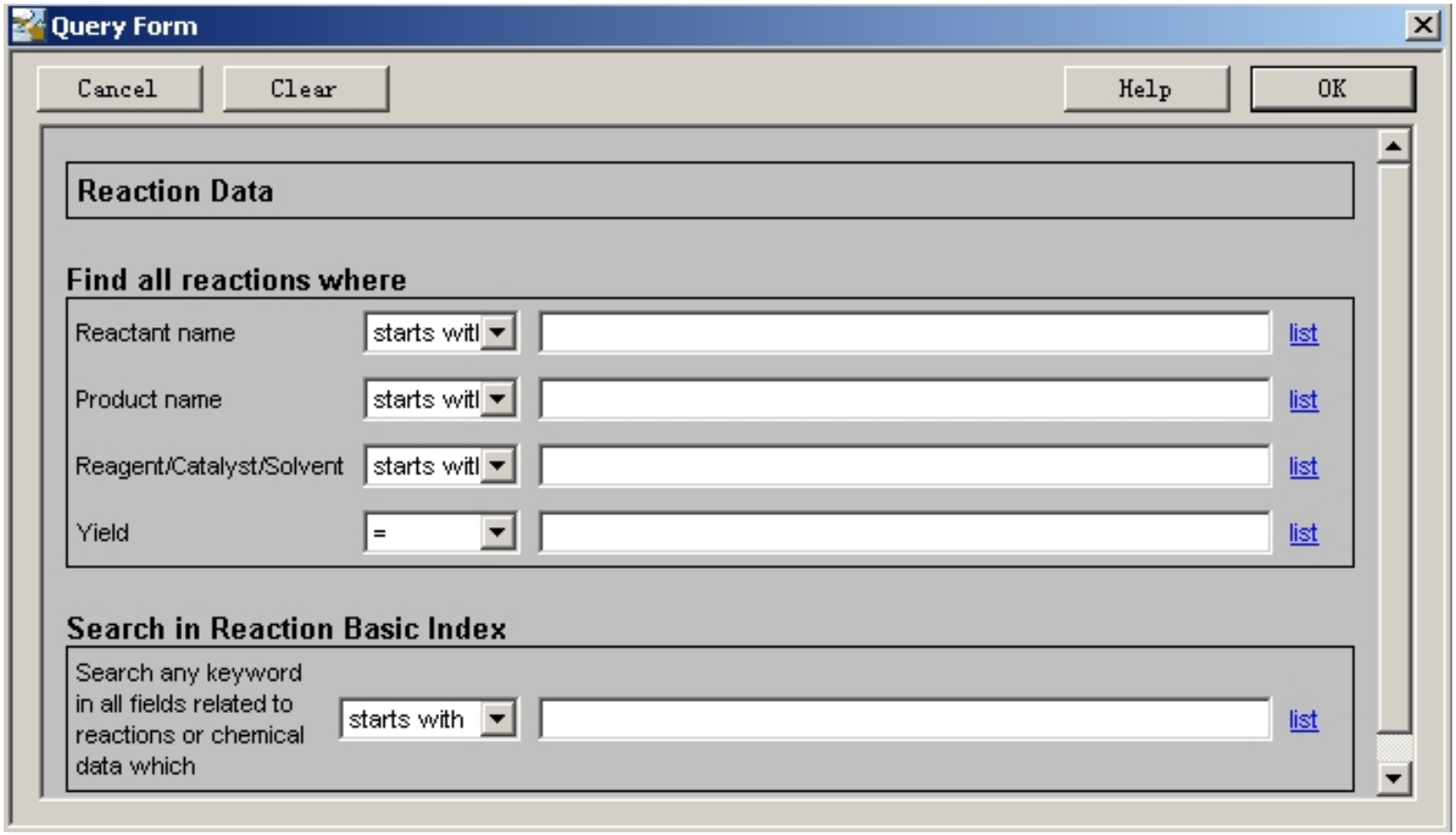
预定义的检索表格

Beilstein
预定义
表格

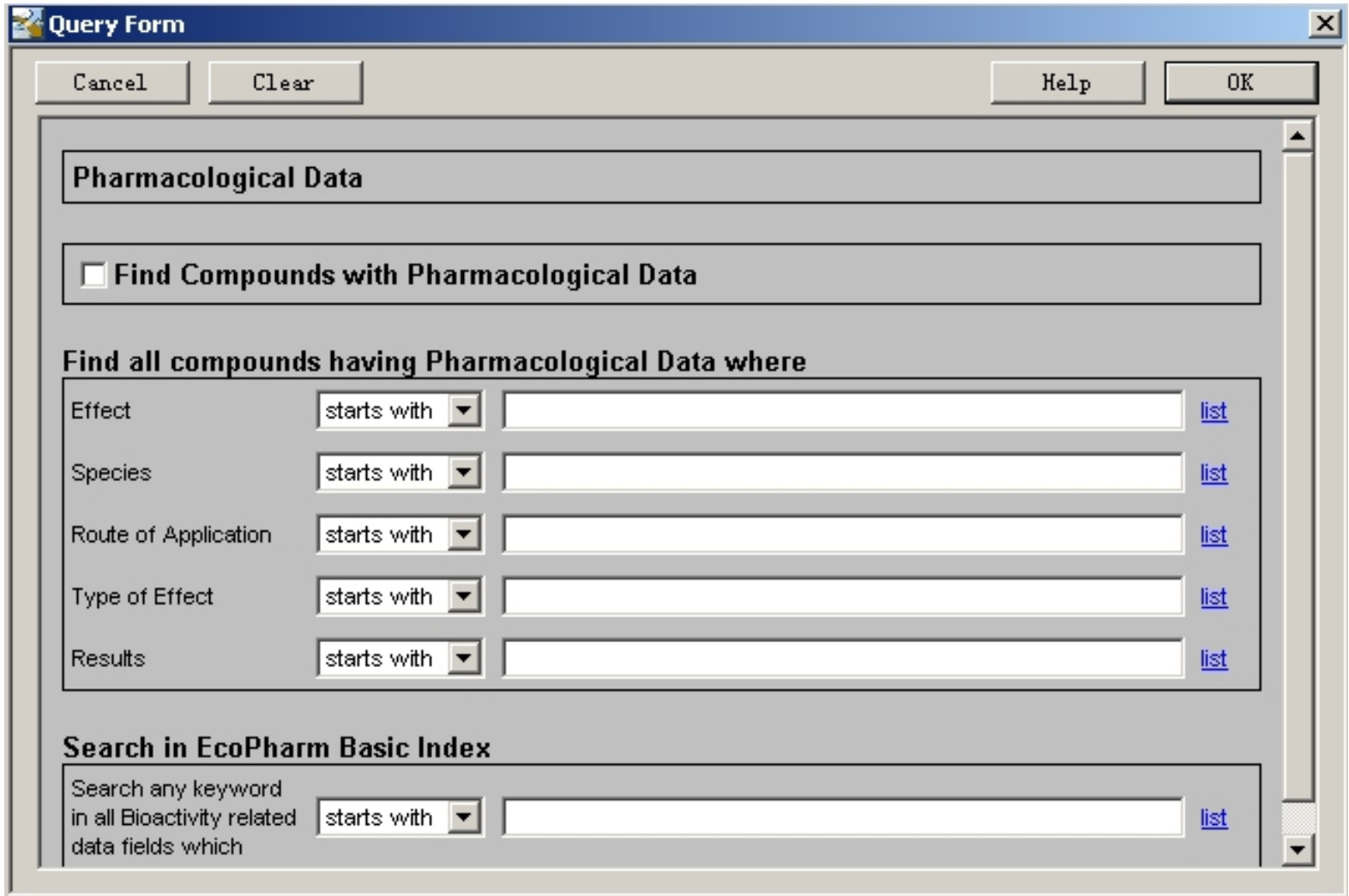
Gmelin
预定义
表格

预定义表格可以简化检索条件的填充过程。

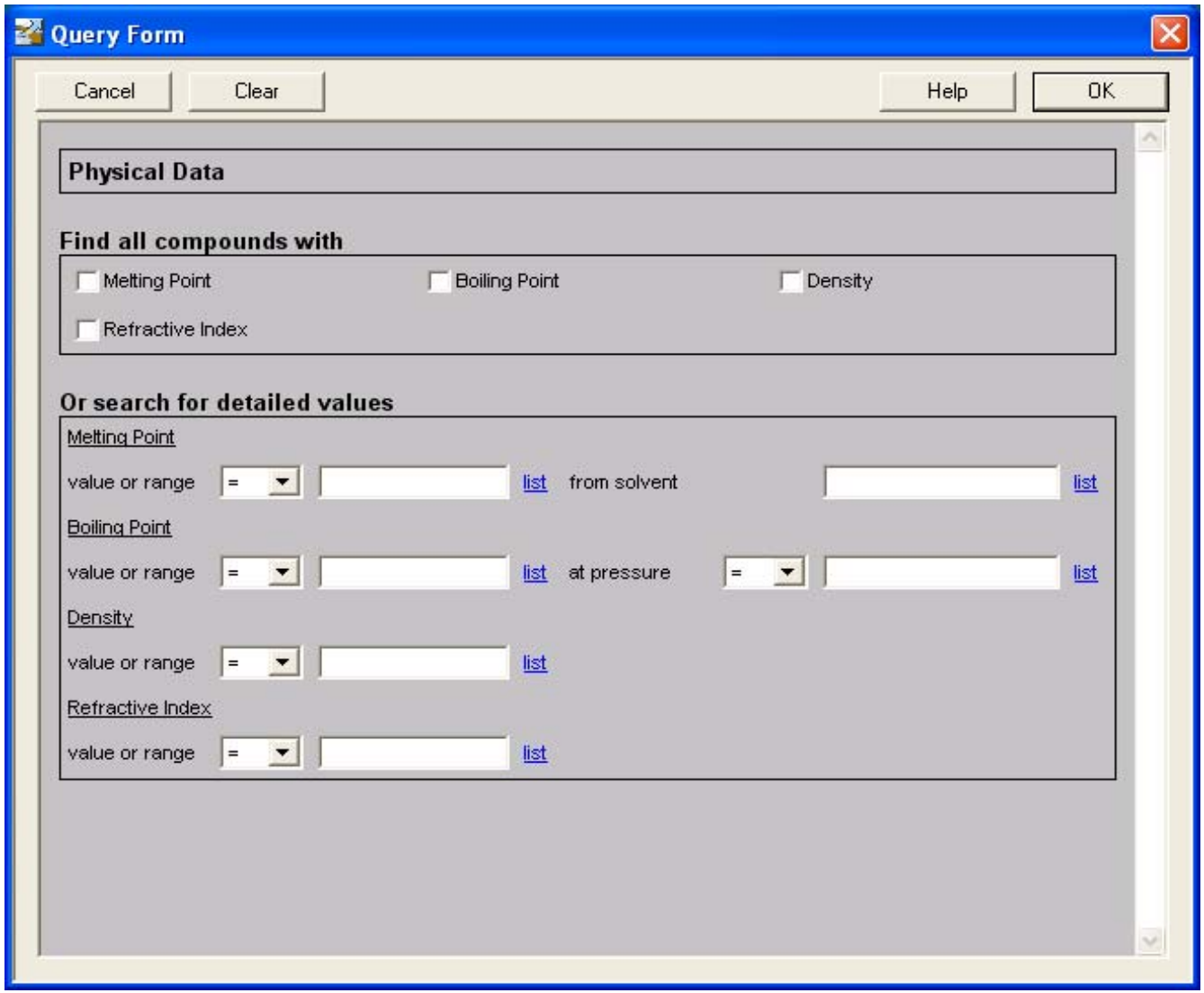
预定义表格：反应查询


Query Form
Cancel
Clear
Help
OK
Reaction Data
Find all reactions where
Reactant name
starts witl
list
Product name
starts witl
list
Reagent/Catalyst/Solvent
starts witl
list
Yield
=
list
Search in Reaction Basic Index
Search any keyword in all fields related to reactions or chemical data which
starts with
list

预定义表格：药理学数据查询



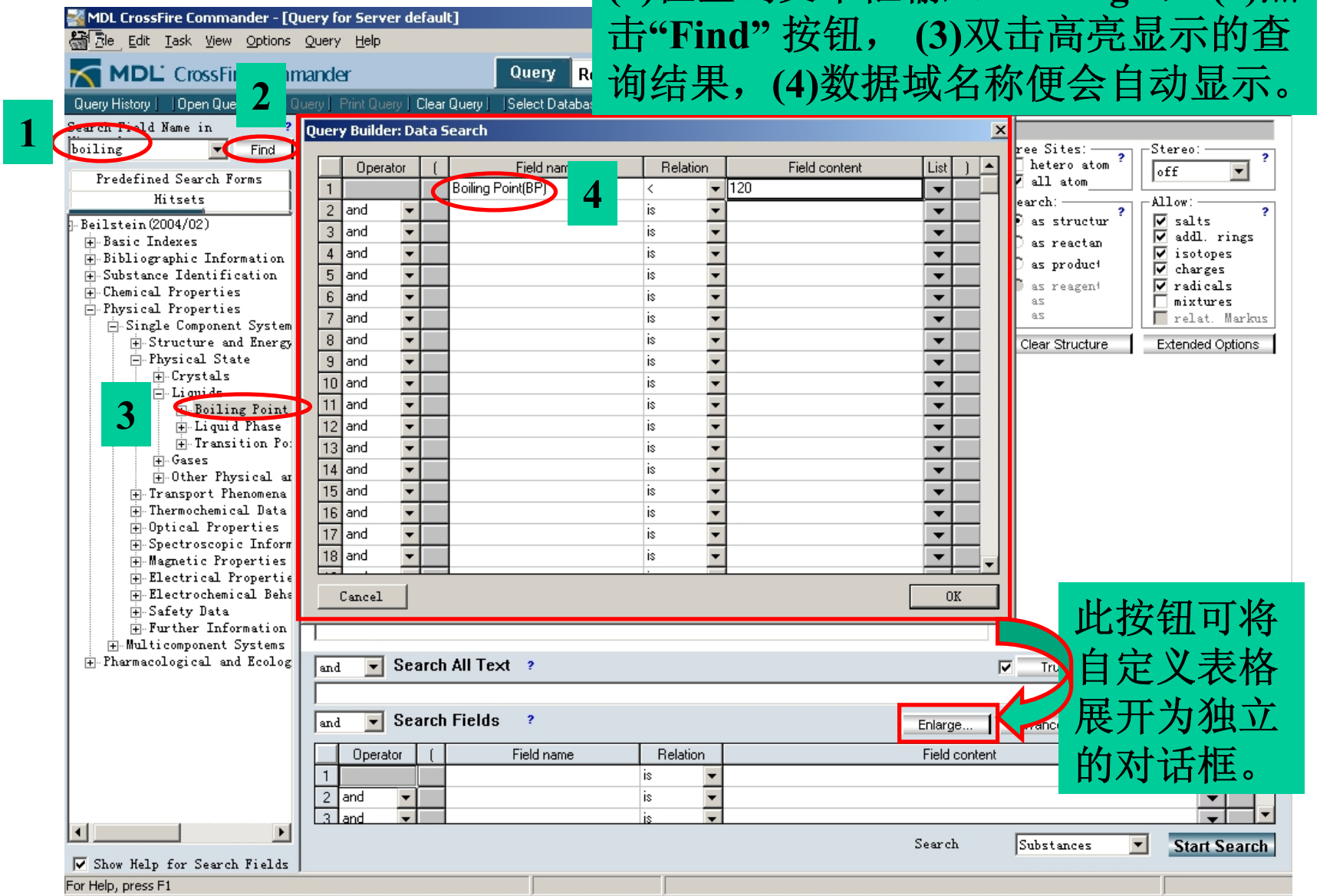
预定义表格：物理数据查询



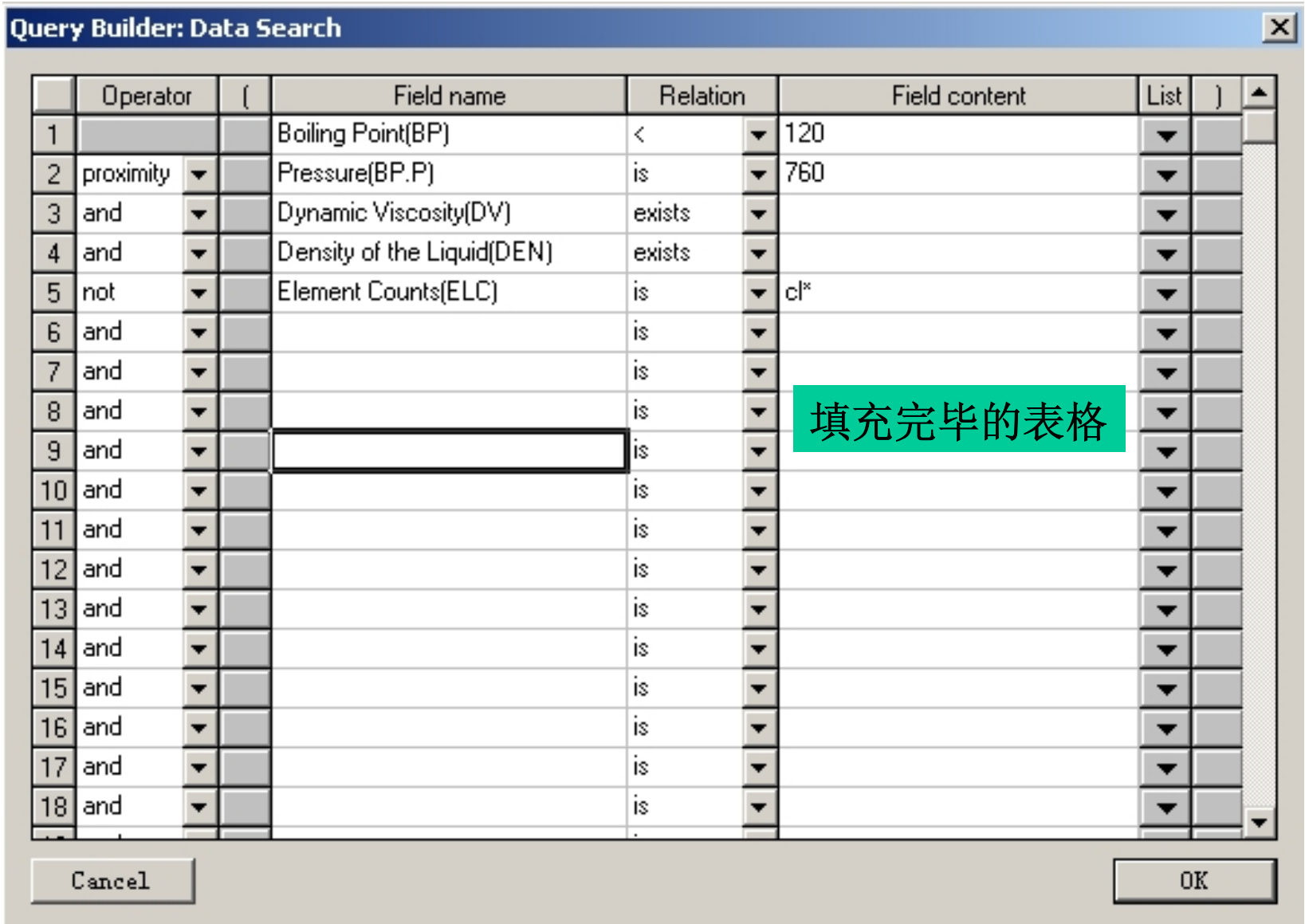
例：　寻找一种溶剂，要求它在760毫米汞柱下的沸点小于120°C ，不能含氯元素，而且需要了解它的密度和黏度方面的数据。

- 用自定义表格来进行查询

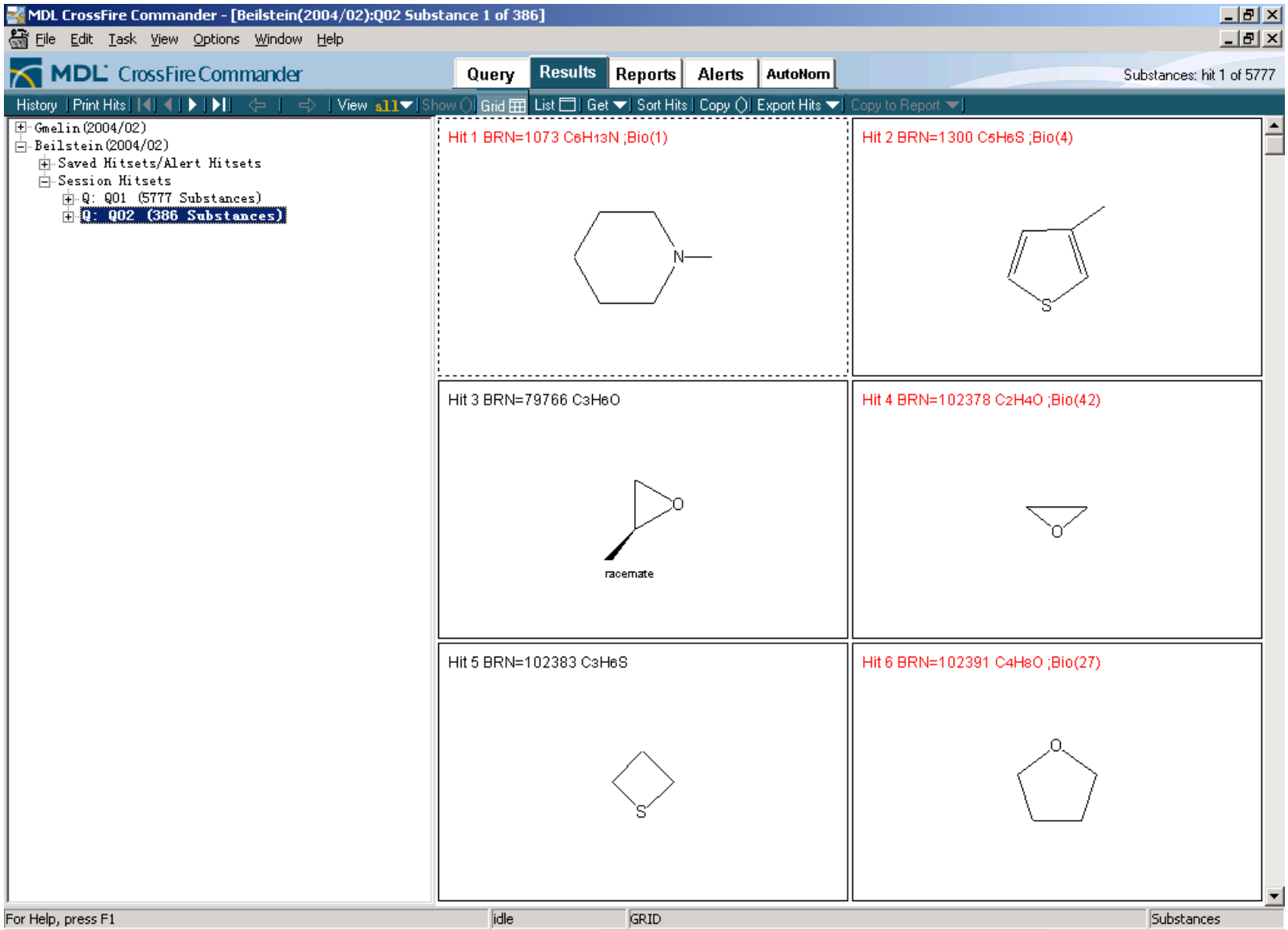
数据域名称的查询方法(以沸点为例)：(1)在查询文本框输入“Boiling”， (2)点击“Find” 按钮， (3)双击高亮显示的查询结果，(4)数据域名称便会自动显示。



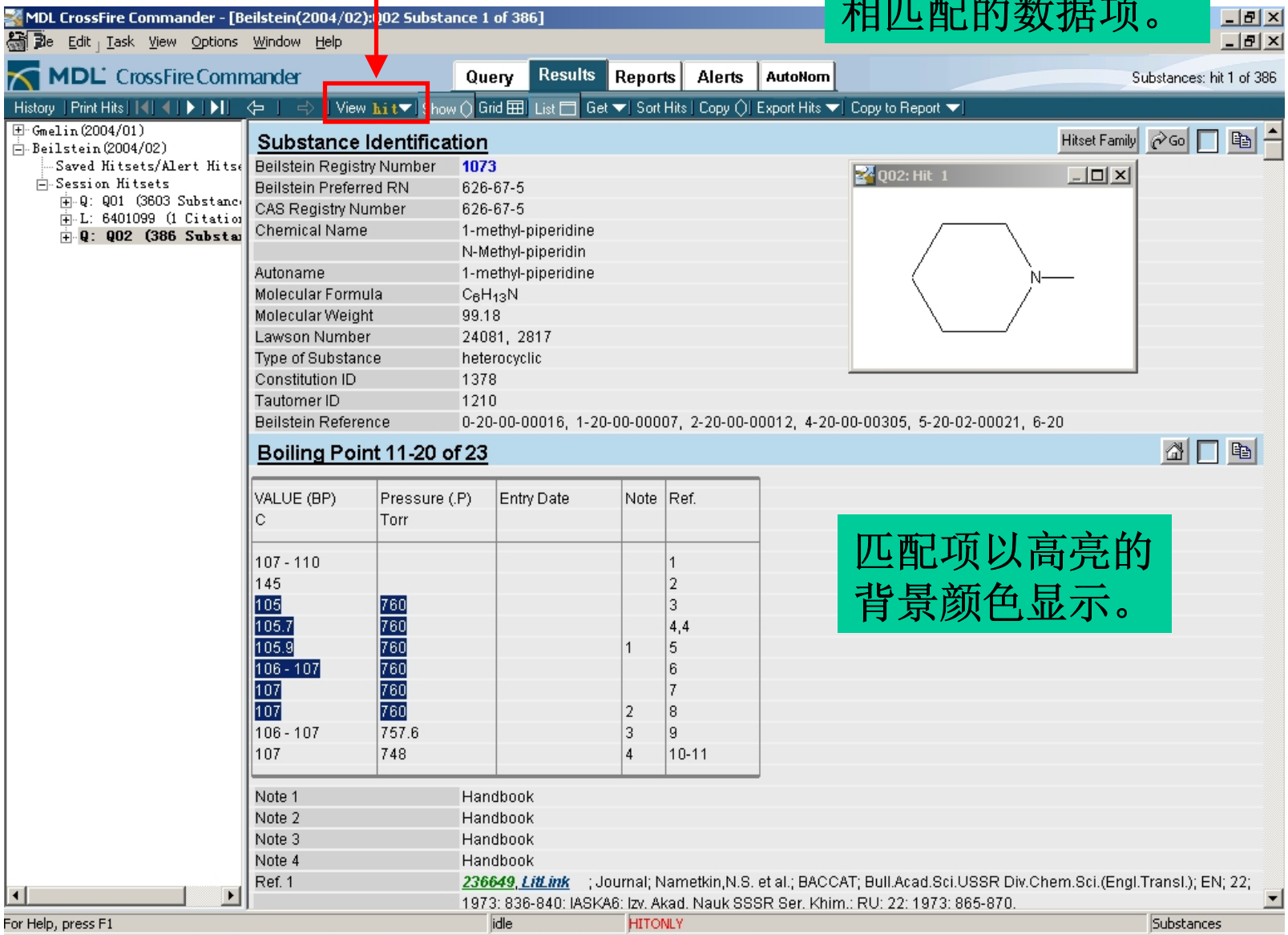
此按钮可将自定义表格展开为独立的对话框。


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

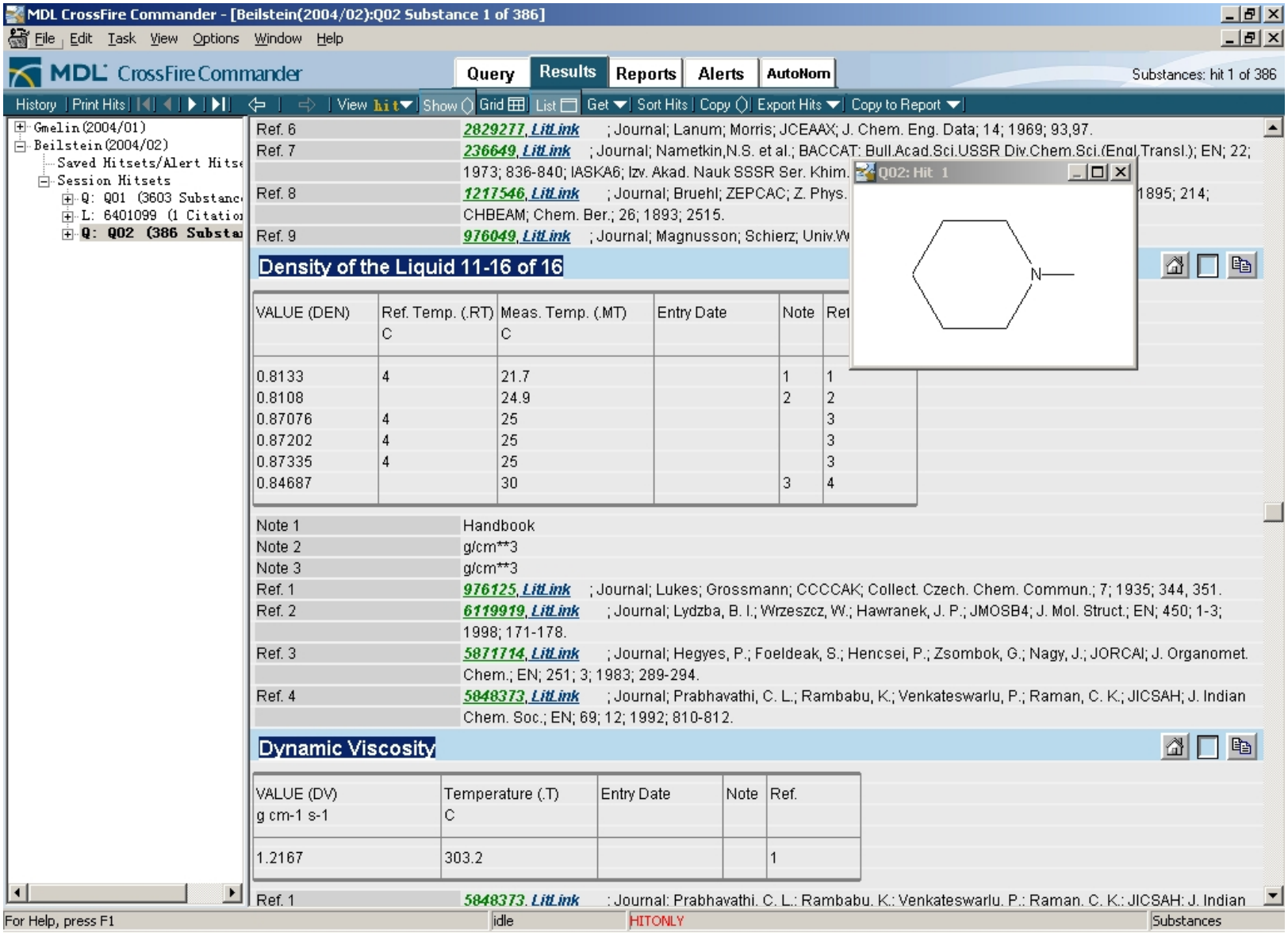
快速数据查询结果显示


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 AutoNom
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 C6H13N ;Bio(1)
Hit 2 BRN=1300 C5H6S ;Bio(4)
Hit 3 BRN=79766 C3H6O
racemate
Hit 4 BRN=102378 C2H4O ;Bio(42)
Hit 5 BRN=102383 C3H6S
Hit 6 BRN=102391 C4H8O ;Bio(27)
For Help, press F1
idle
GRID
Substances

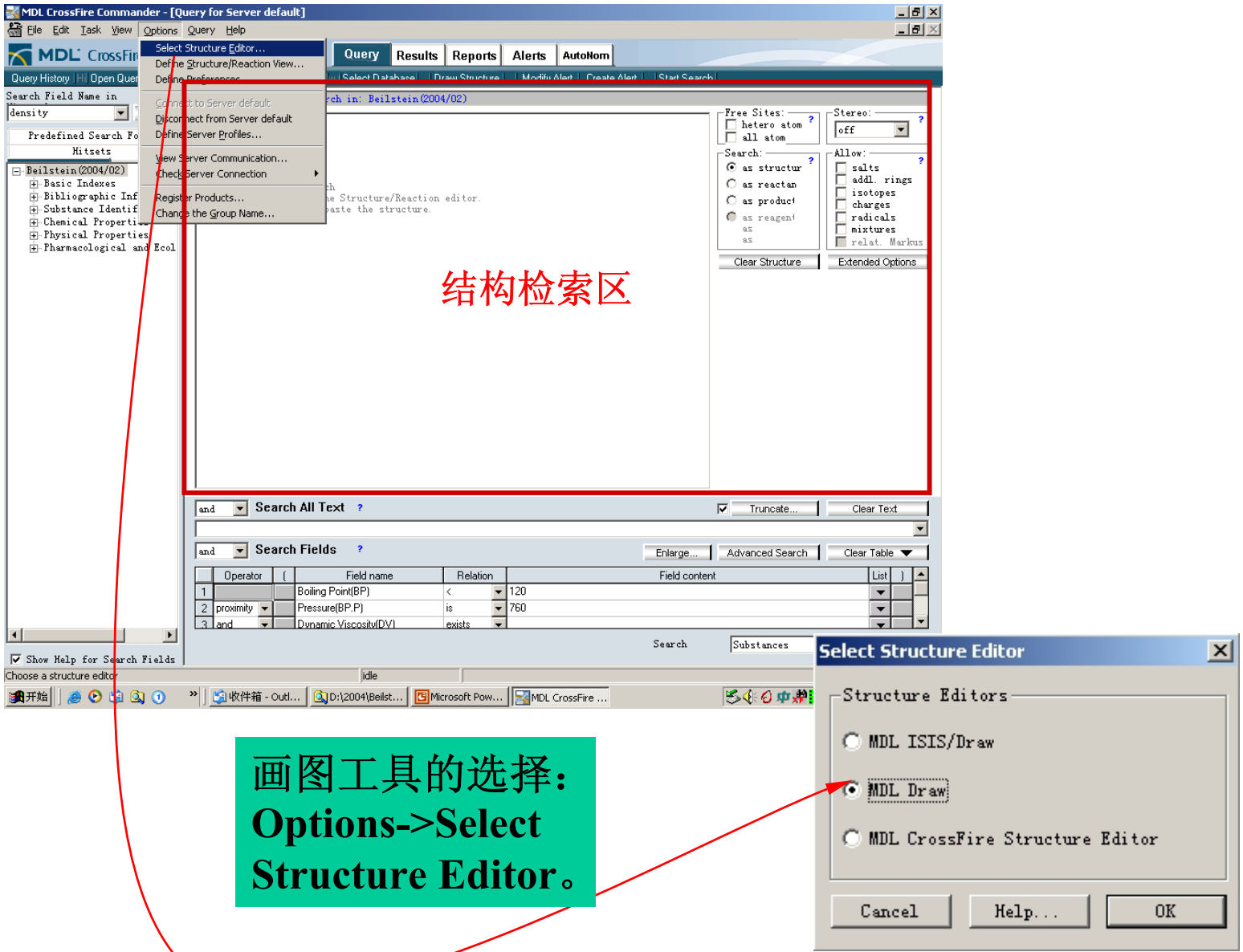
仅显示与查询条件相匹配的数据项。



匹配项以高亮的背景颜色显示。

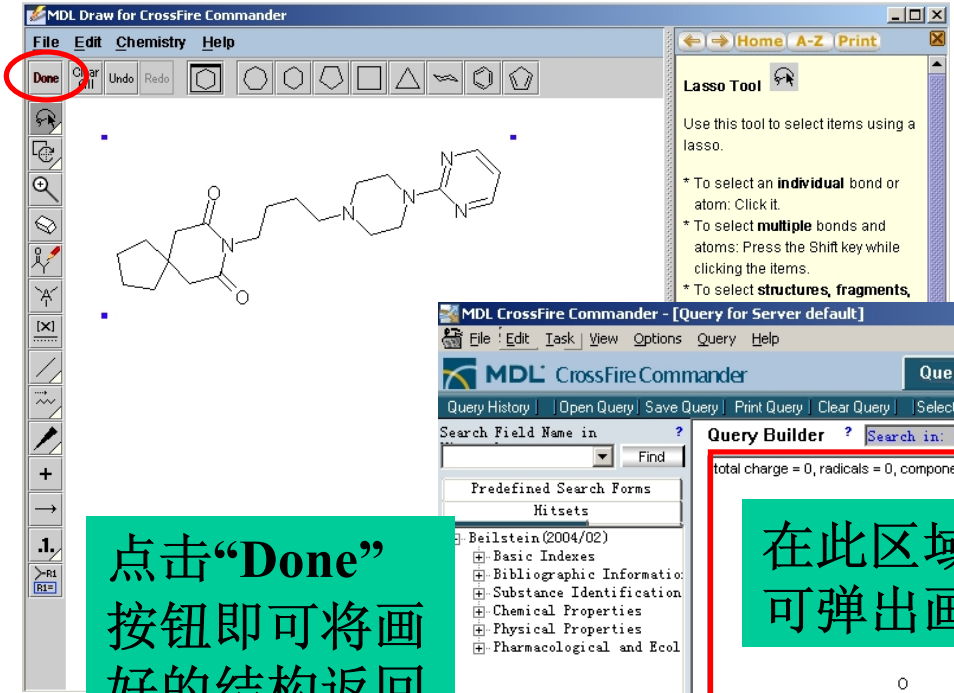

MDL CrossFire Commander - [Beilstein(2004/02):Q02 Substance 1 of 386]
File Edit Task View Options Window Help
MDL CrossFire Commander
Query Results Reports Alerts AutoNom
Substances: hit 1 of 386
History | Print Hits | View hit | Show | Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report
Gmelin(2004/01)
Beilstein(2004/02)
Saved Hitsets/Alert Hits
Session Hitsets
Q: Q01 (3603 Substanc
L: 6401099 (1 Citatio
Q: Q02 (386 Substa
Ref. 6 2829277, LitLink ; Journal; Lanum; Morris; JCEAAX; J. Chem. Eng. Data; 14; 1969; 93,97.
Ref. 7 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.
Ref. 8 1217546, LitLink ; Journal; Bruehl; ZEPCAC; Z. Phys. 1895; 214; CHBEAM; Chem. Ber.; 26; 1893; 2515.
Ref. 9 976049, LitLink ; Journal; Magnusson; Schierz; Univ.W
Q02: Hit 1
N
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, LitLink ; Journal; Lukes; Grossmann; CCCCAK; Collect. Czech. Chem. Commun.; 7; 1935; 344, 351.
Ref. 2 6119919, LitLink ; Journal; Lydzba, B. I.; Wrzeszcz, W.; Hawranek, J. P.; JMOSB4; J. Mol. Struct.; EN; 450; 1-3; 1998; 171-178.
Ref. 3 5871714, LitLink ; Journal; Hegyes, P.; Foeldeak, S.; Hencsei, P.; Zsombok, G.; Nagy, J.; JORCAI; J. Organomet. Chem.; EN; 251; 3; 1983; 289-294.
Ref. 4 5848373, LitLink ; 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, LitLink ; Journal; Prabhavathi, C. L.; Rambabu, K.; Venkateswarlu, P.; Raman, C. K.; JICSAH; J. Indian
For Help, press F1
idle
HITONLY
Substances

结构检索



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

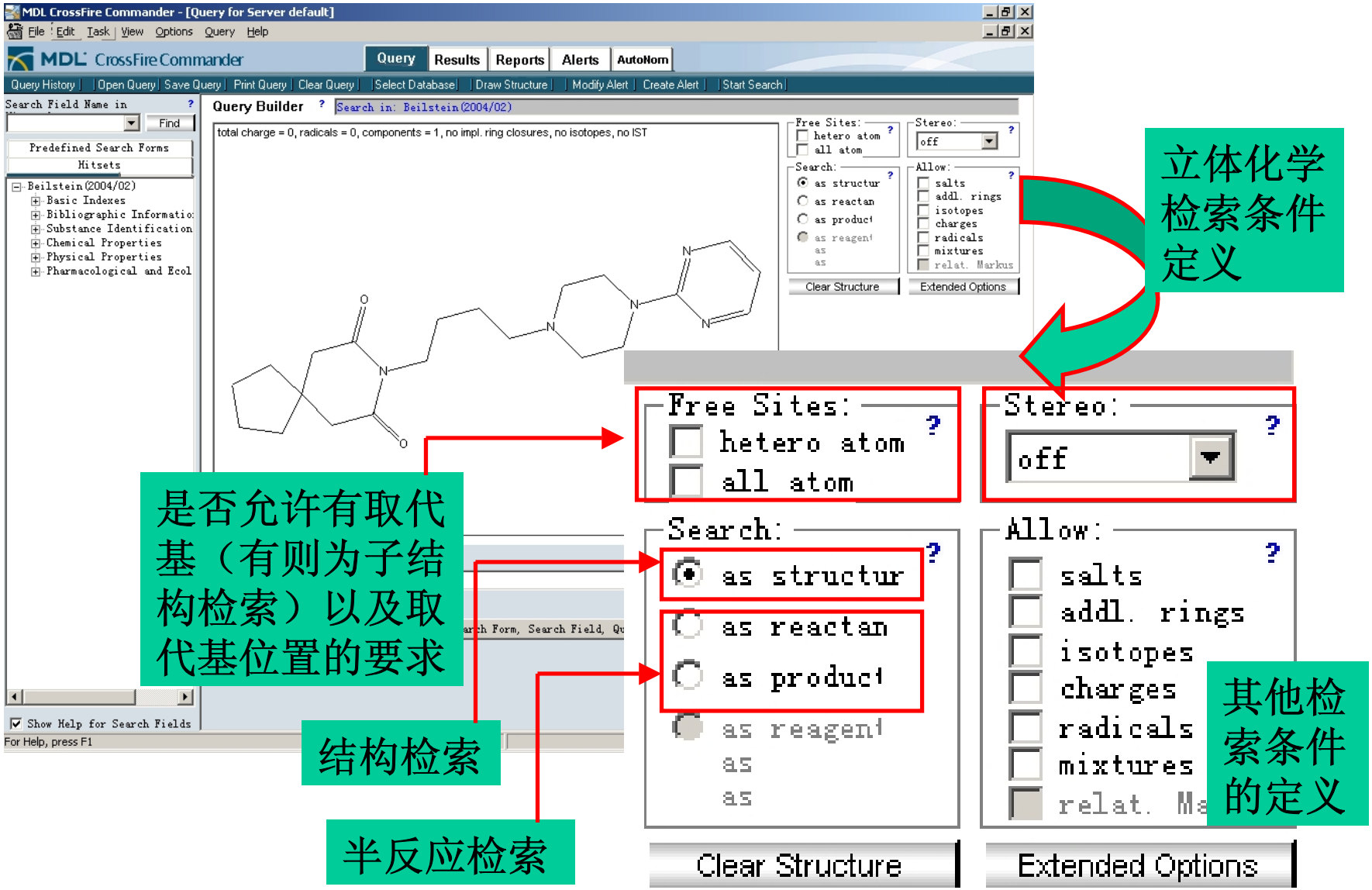
精确结构检索



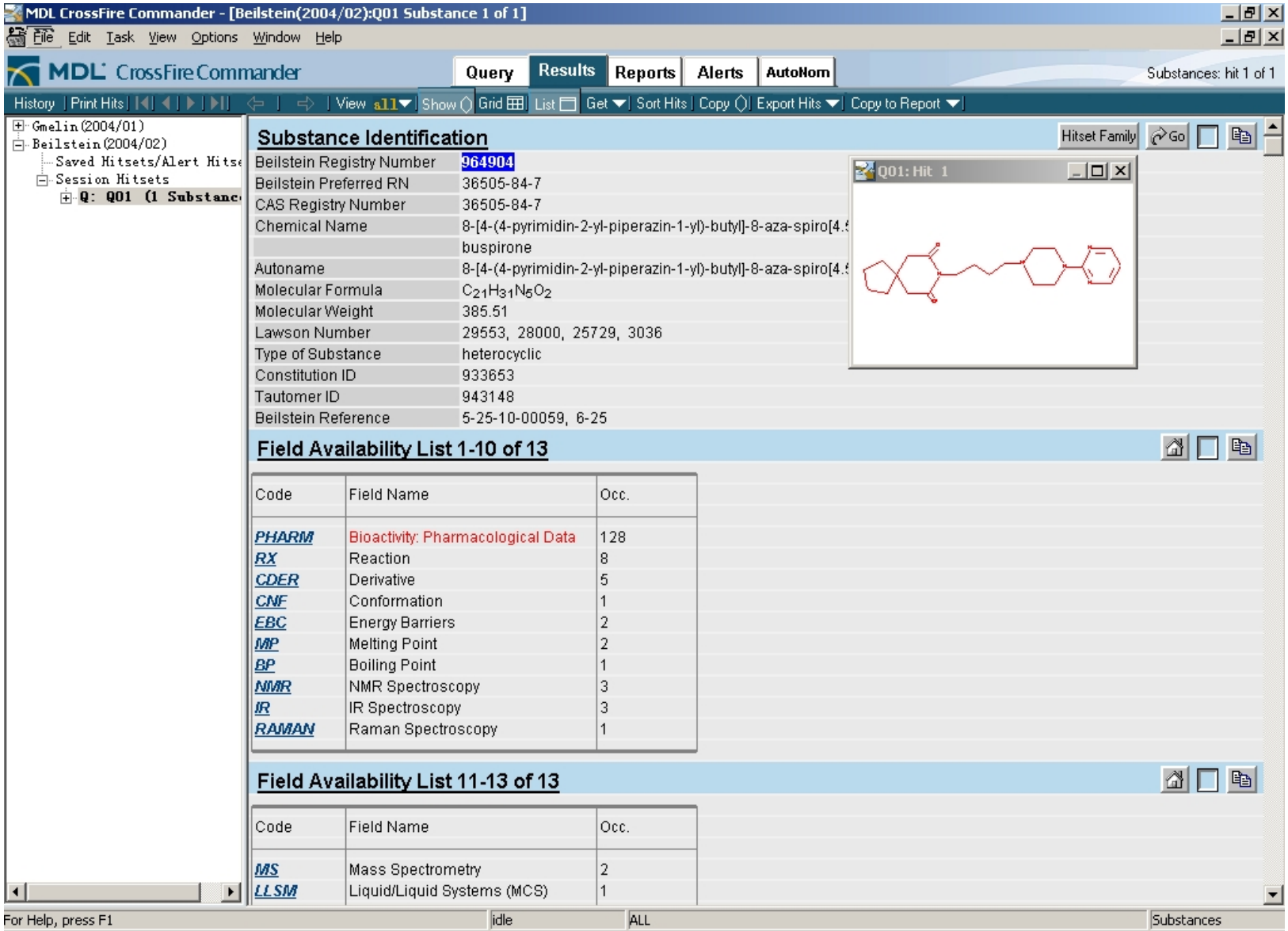
点击“Done”按钮即可将画好的结构返回Commander结构检索区。

在此区域内双击即可弹出画图工具。

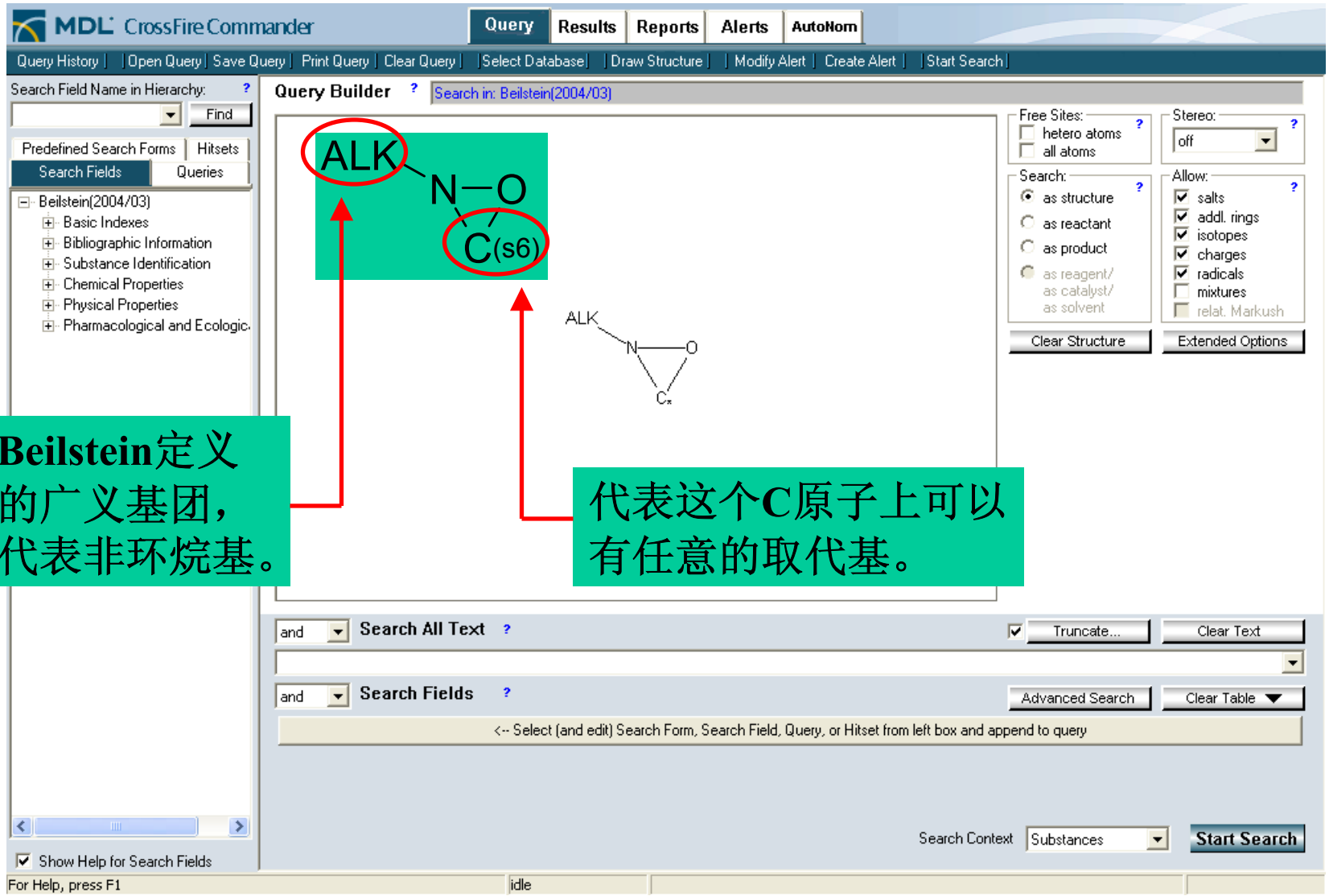
结构检索选项区


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 Informatio
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
Free Sites:
hetero atom
all atom
Stereo:
off
Search:
as structur
as reactan
as product
as reagent
Allow:
salts
addl. rings
isotopes
charges
radicals
mixtures
relat. Markus
Clear Structure
Extended Options
Show Help for Search Fields
For Help, press F1
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
Free Sites:
hetero atom
all atom
Stereo:
off
Search:
as structur
as reactan
as product
as reagent
Allow:
salts
addl. rings
isotopes
charges
radicals
mixtures
Clear Structure
Extended Options

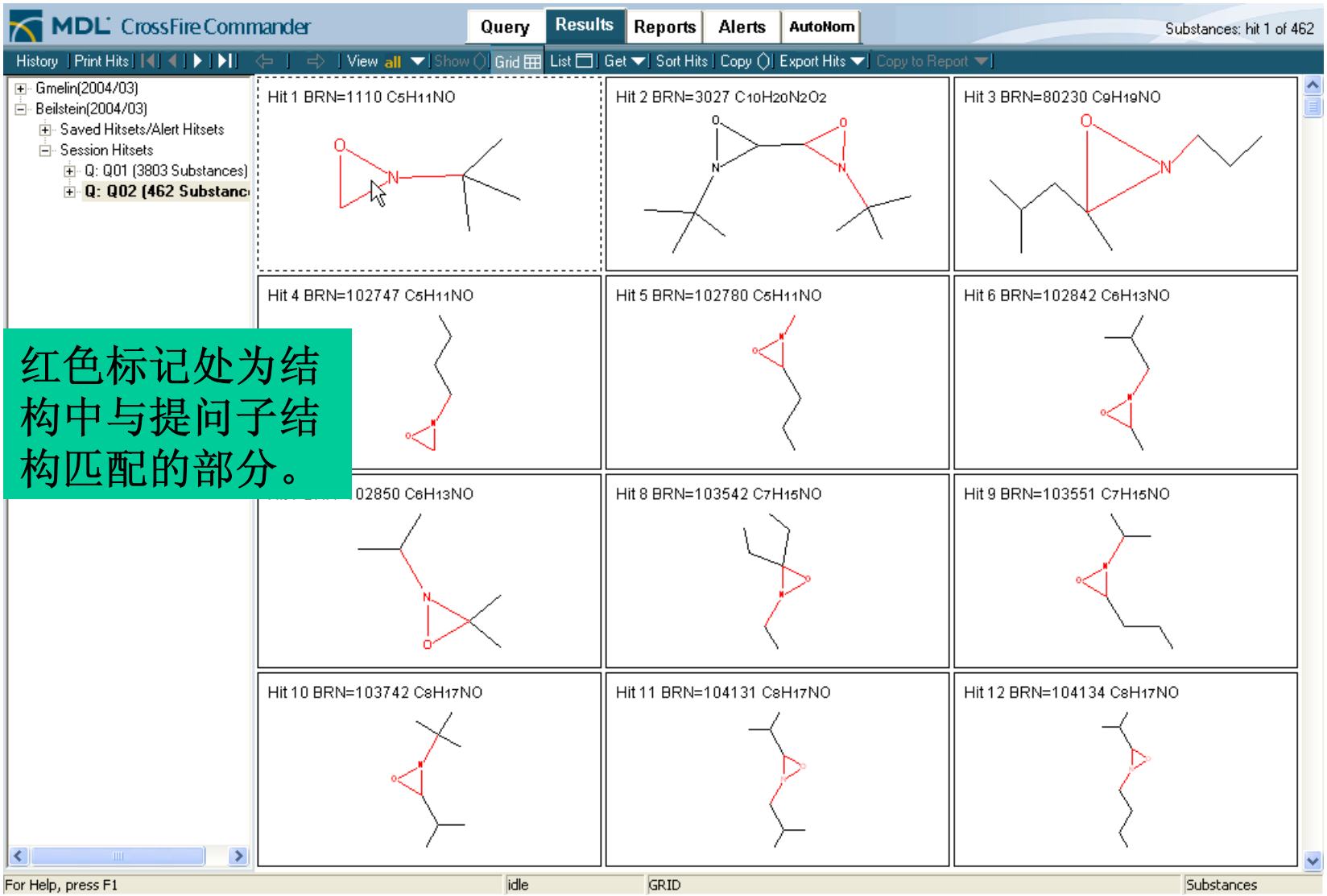
精确结构检索结果显示


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 all Show Grid List Get Sort Hits Copy Export Hits Copy to Report
Gmelin (2004/01)
Beilstein (2004/02)
Saved Hitsets/Alert Hits
Session Hitsets
Q: Q01 (1 Substanc
Substance Identification
Hitset Family
Go
Q01: Hit 1
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
buspirone
Autoname 8-[4-(4-pyrimidin-2-yl-piperazin-1-yl)-butyl]-8-aza-spiro[4.5
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
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 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 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)
ALK
N—O
C(s6)
ALK
N
O
C
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
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。
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 Context
Substances
Start Search
Show Help for Search Fields
For Help, press F1
idle

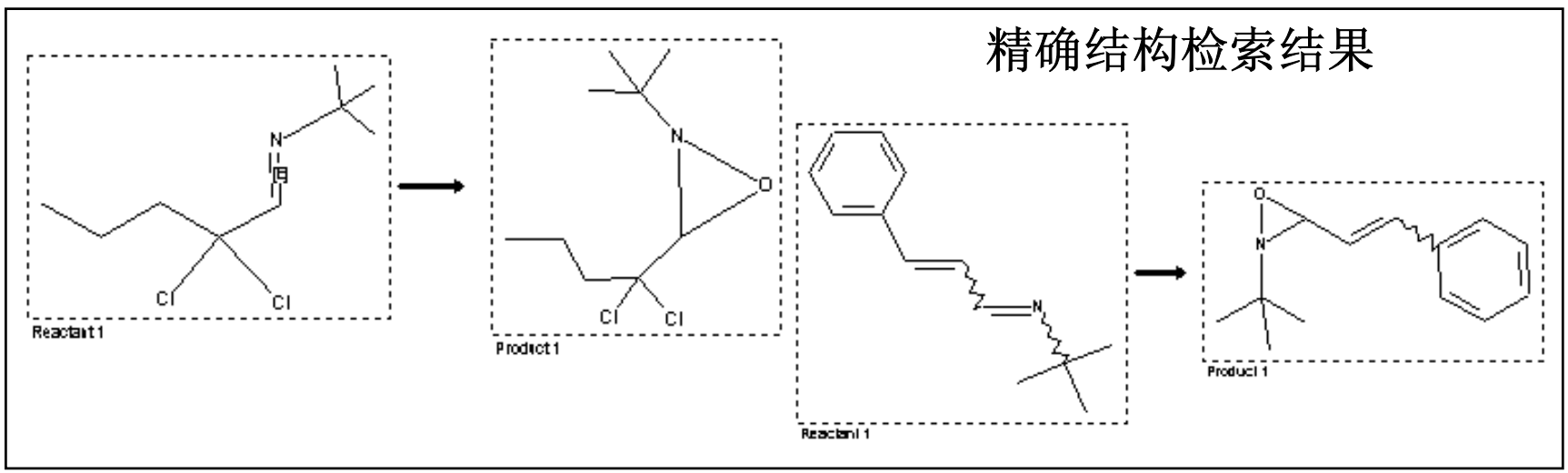
子结构检索结果显示

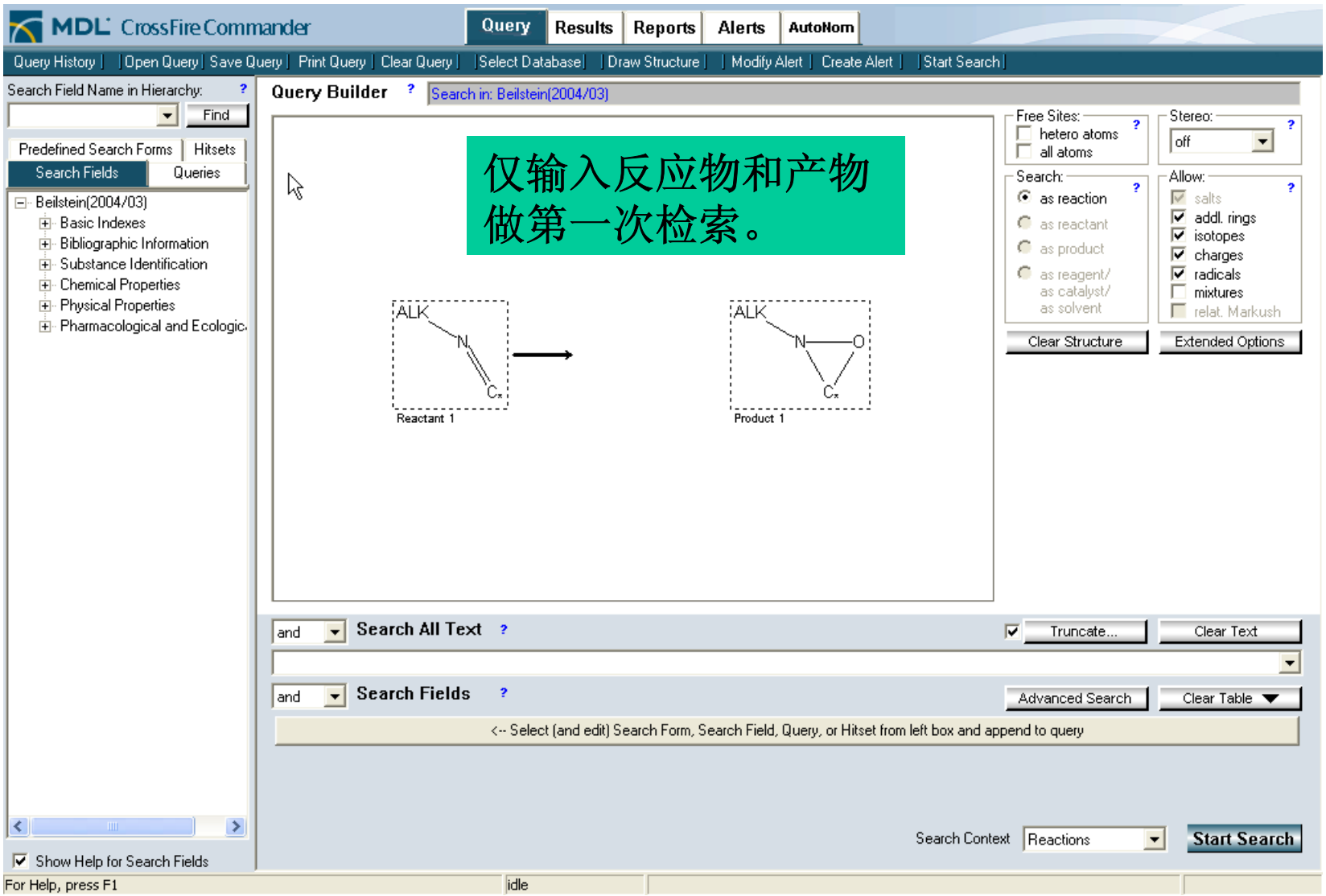


红色标记处为结构中与提问子结构匹配的部分。

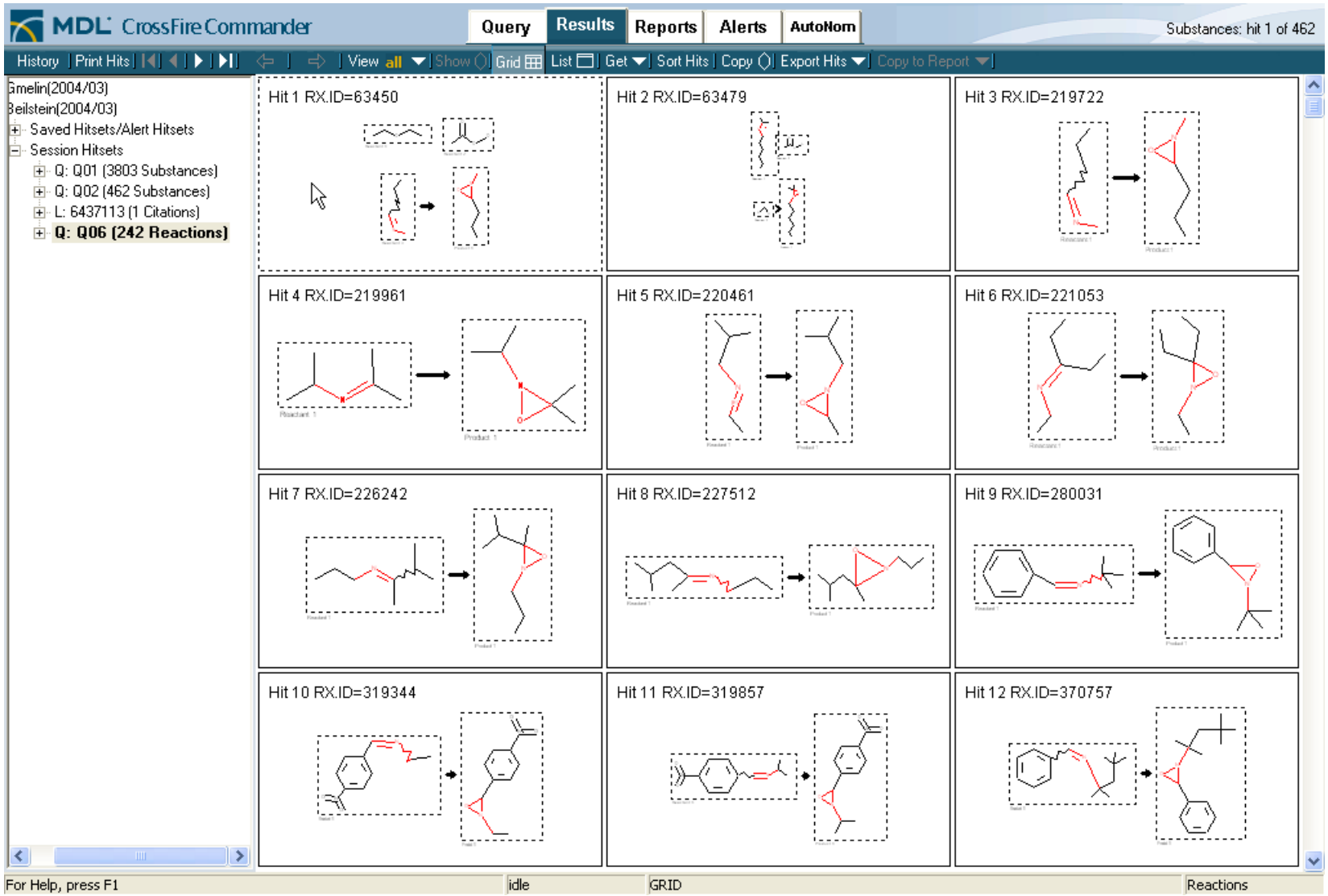
反应检索－原子匹配

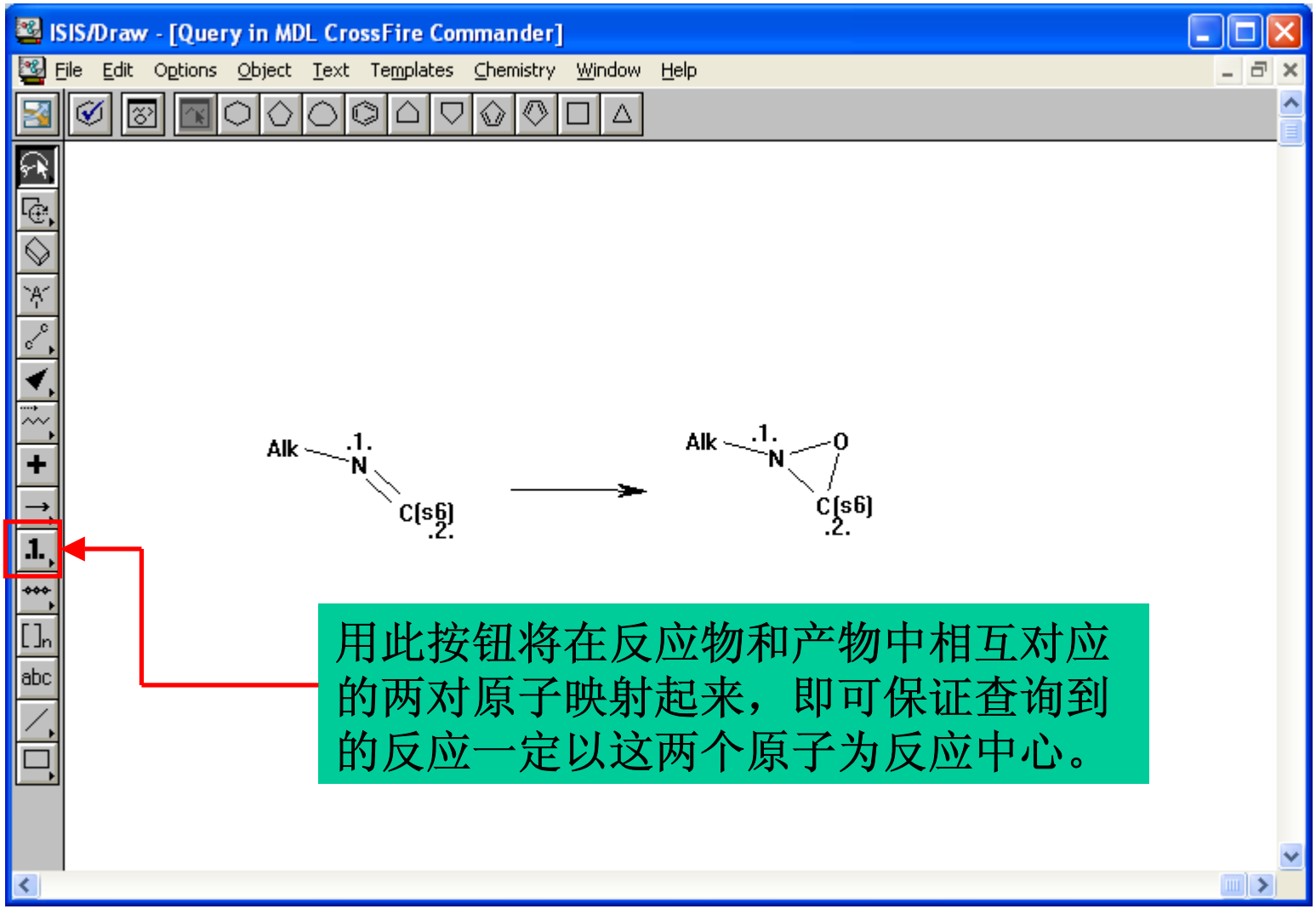
例：　查询从亚胺生成唑烷的反应途径，通过原子匹配来得到合适的反应，再通过限定反应产率来进一步查找合适的反应路径。



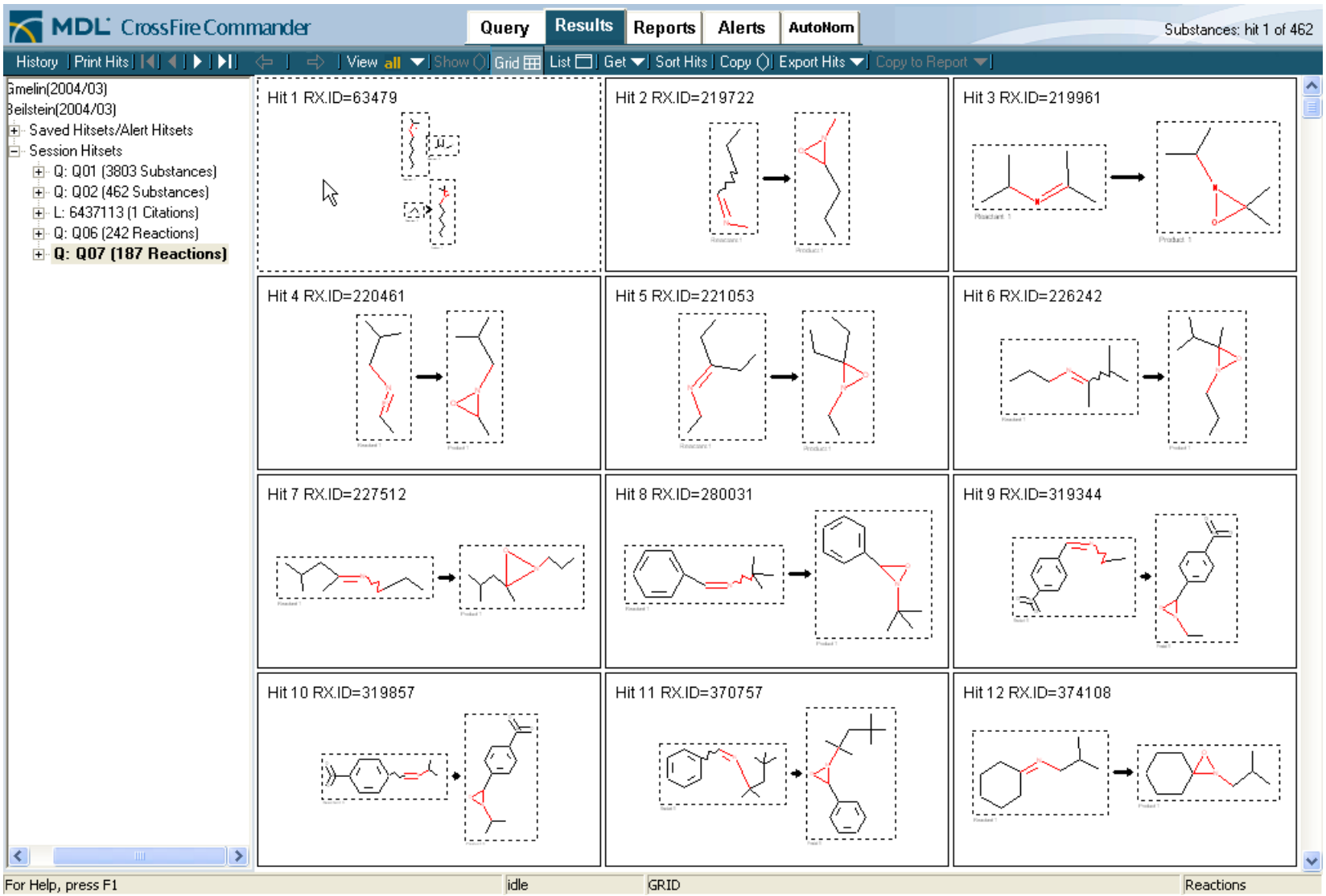

MDL CrossFire Commander
Query
Results
Reports
Alerts
AutoNom
Query History | Open Query | Save Query | Print Query | Clear Query | Select Database | Draw Structure | Modify Alert | Create Alert | Start Search
Search Field Name in Hierarchy:
Find
Predefined Search Forms
Hitsets
Search Fields
Queries
Beilstein(2004/03)
Basic Indexes
Bibliographic Information
Substance Identification
Chemical Properties
Physical Properties
Pharmacological and Ecologic
Show Help for Search Fields
Query Builder
Search in: Beilstein(2004/03)
仅输入反应物和产物
做第一次检索。
ALK
N
Cx
Reactant 1
ALK
N
O
Cx
Product 1
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
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 Context
Reactions
Start Search
For Help, press F1
idle

第一次检索结果，有242条记录。

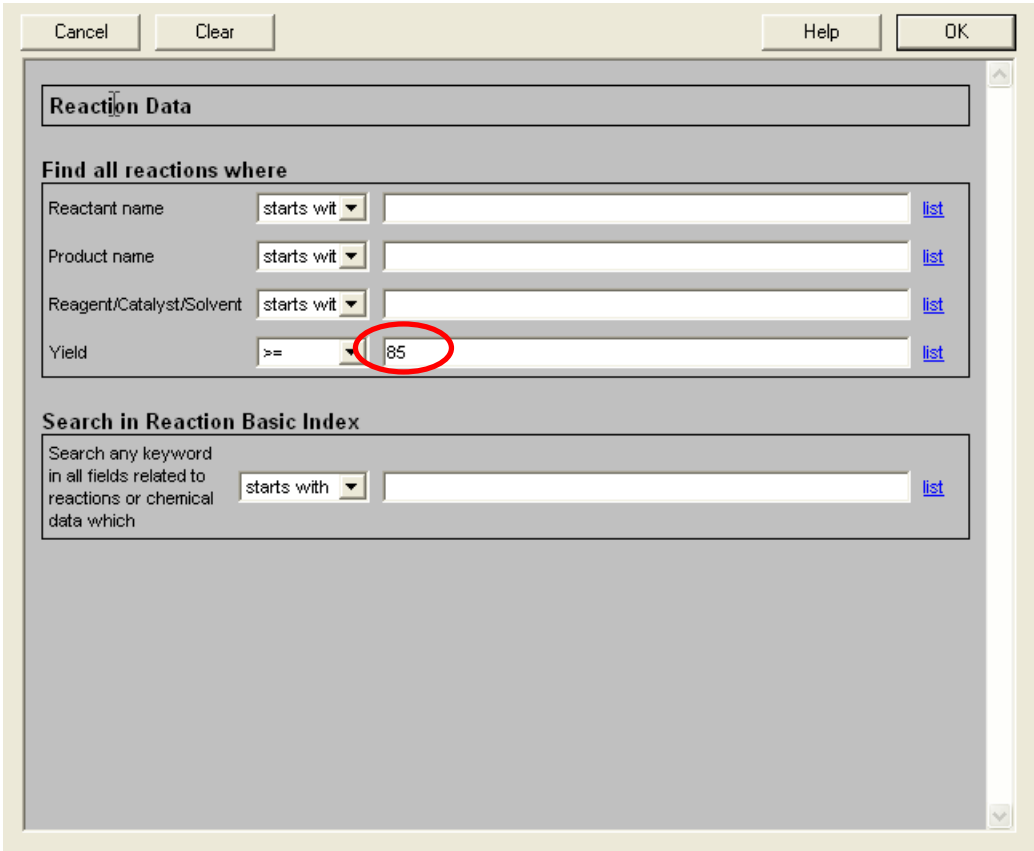



ISIS/Draw - [Query in MDL CrossFire Commander]
File Edit Options Object Text Templates Chemistry Window Help
Alk .1. N C[s6] .2.
Alk .1. N O C[s6] .2.
abc
用此按钮将在反应物和产物中相互对应的两对原子映射起来，即可保证查询到的反应一定以这两个原子为反应中心。

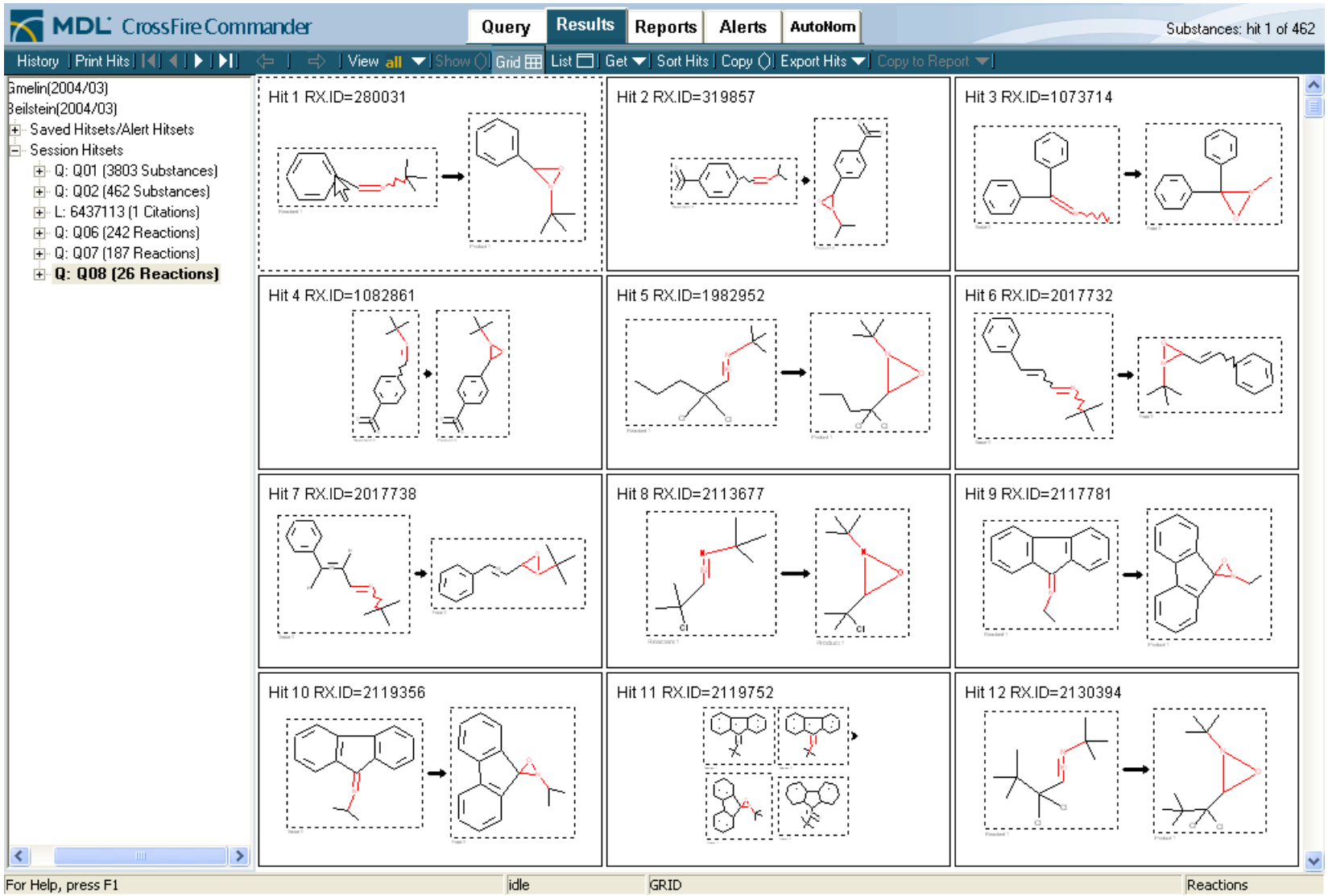
第二次检索结果，有187条记录。



通过反应查询的预定义表格，输入对反应产率的要求。



第三次检索结果，有26条记录。

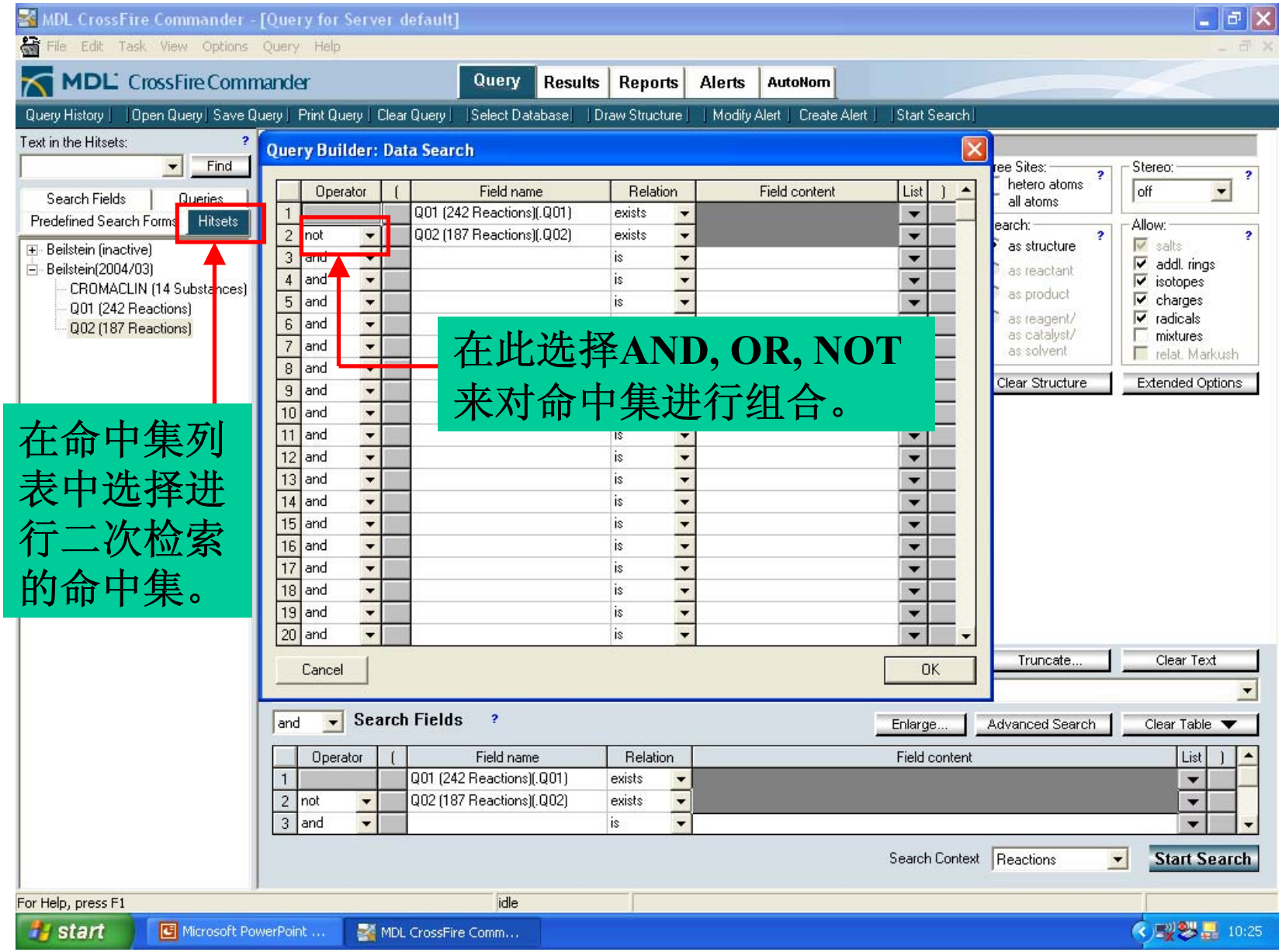


各种检索方式的比较

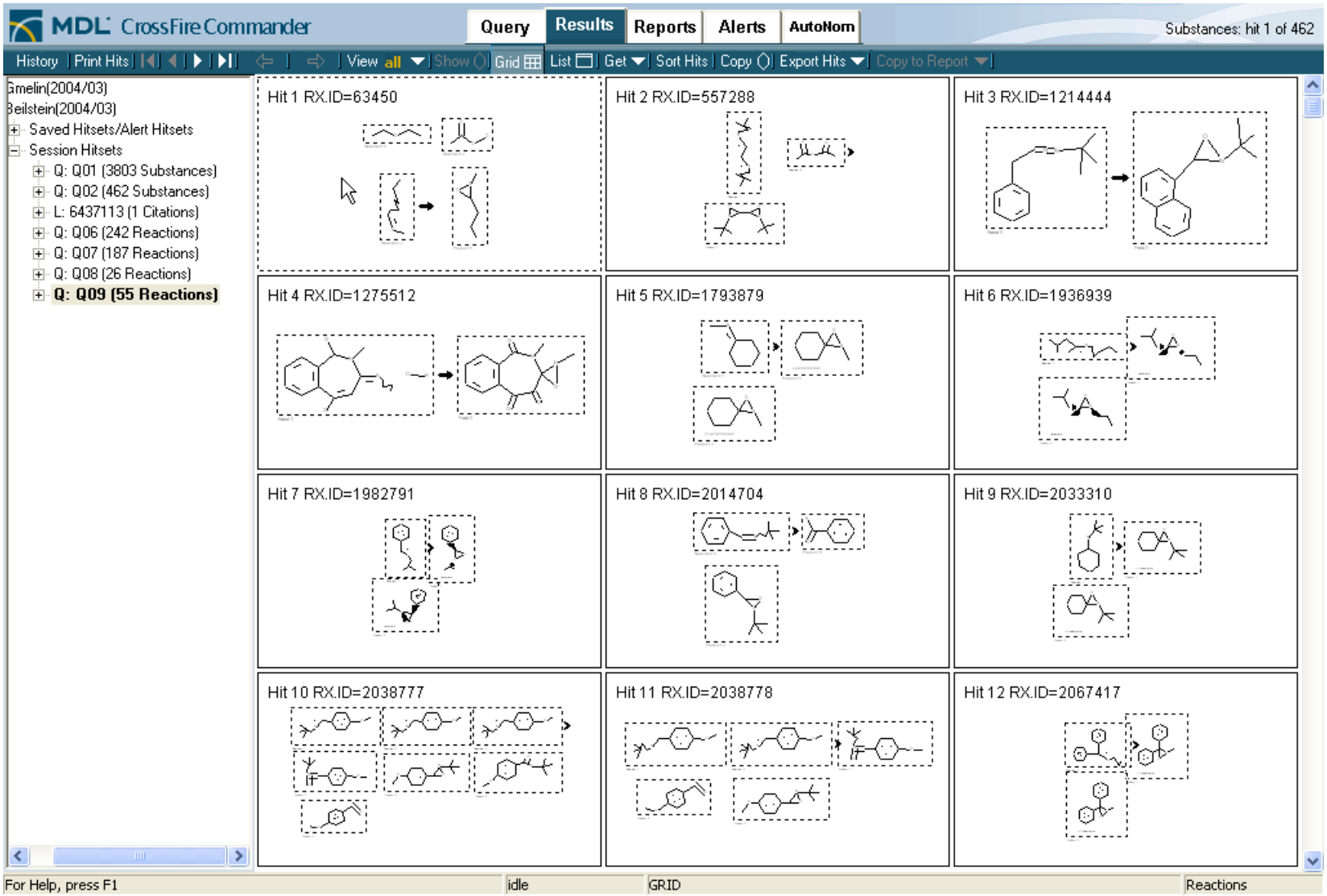
检索方式	命中结果的数目
反应检索	242条
进行原子匹配的反应检索	187条
反应与数据的联合检索	26条

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 AutoNom
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)
在命中集列表中选择进行二次检索的命中集。
Query Builder: Data Search
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
在此选择AND, OR, NOT来对命中集进行组合。
Cancel
OK
Stereo:
off
Allow:
salts
addl. rings
isotopes
charges
radicals
mixtures
relat. Markush
as structure
as reactant
as product
as reagent/
as catalyst/
as solvent
Clear Structure
Extended Options
Truncate...
Clear Text
and
Search Fields
Enlarge...
Advanced Search
Clear Table
Search Context
Reactions
Start Search
For Help, press F1
idle
start
Microsoft PowerPoint ...
MDL CrossFire Comm...
10:25

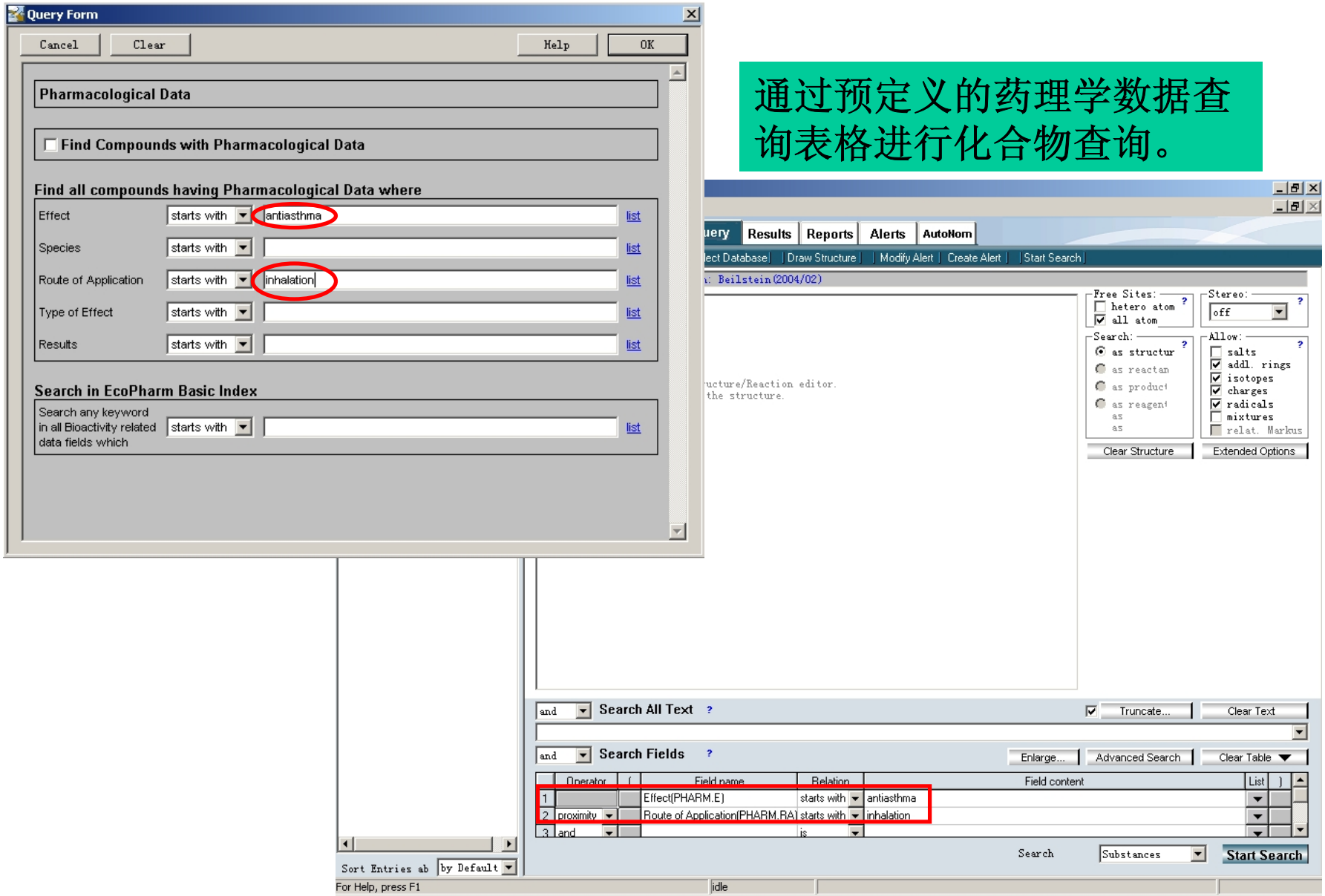
二次检索结果显示


MDL CrossFire Commander
Query
Results
Reports
Alerts
AutoNom
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)
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

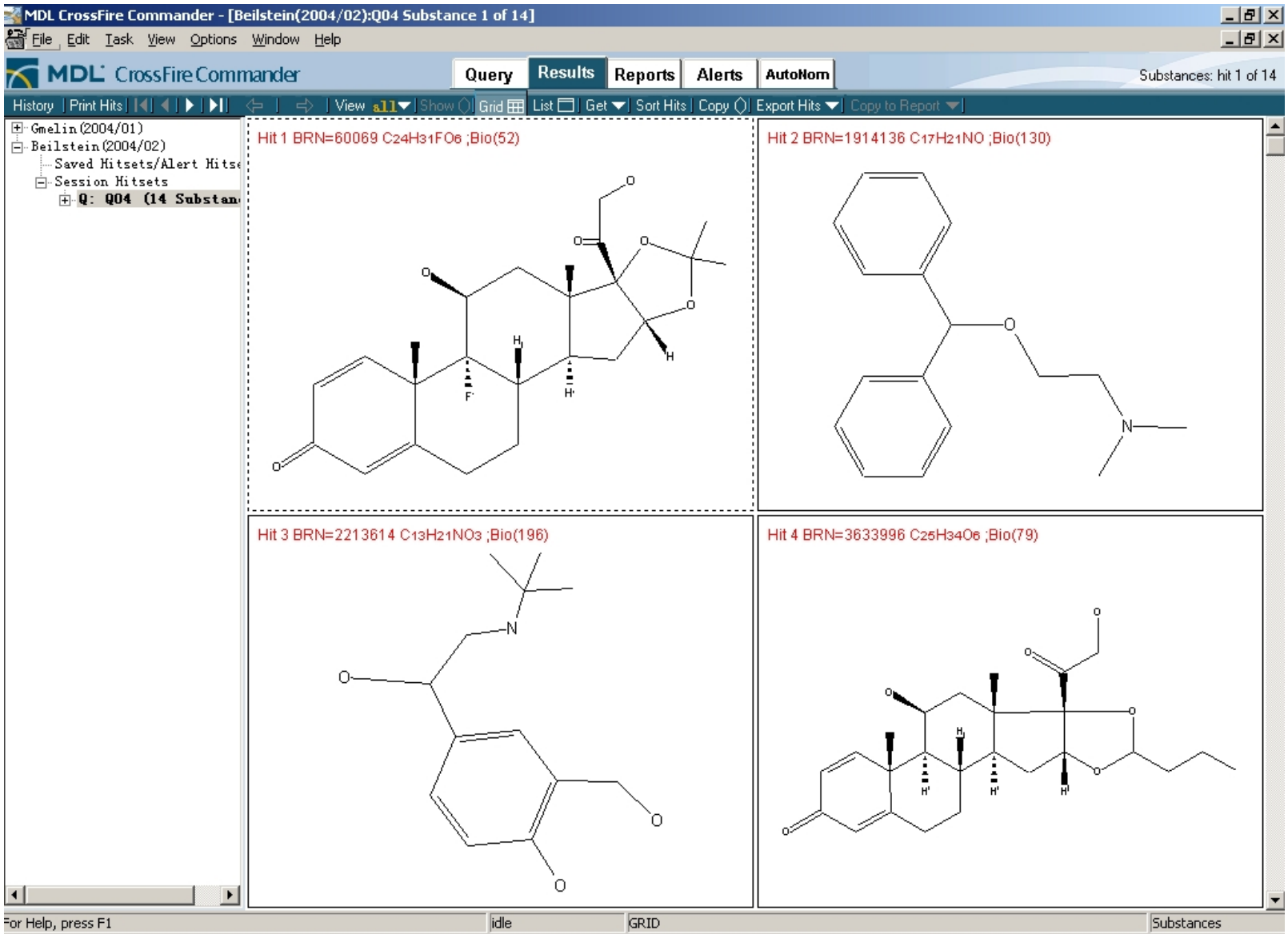
例：　检索吸入时有平喘疗效的化合物的合成方法

- 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

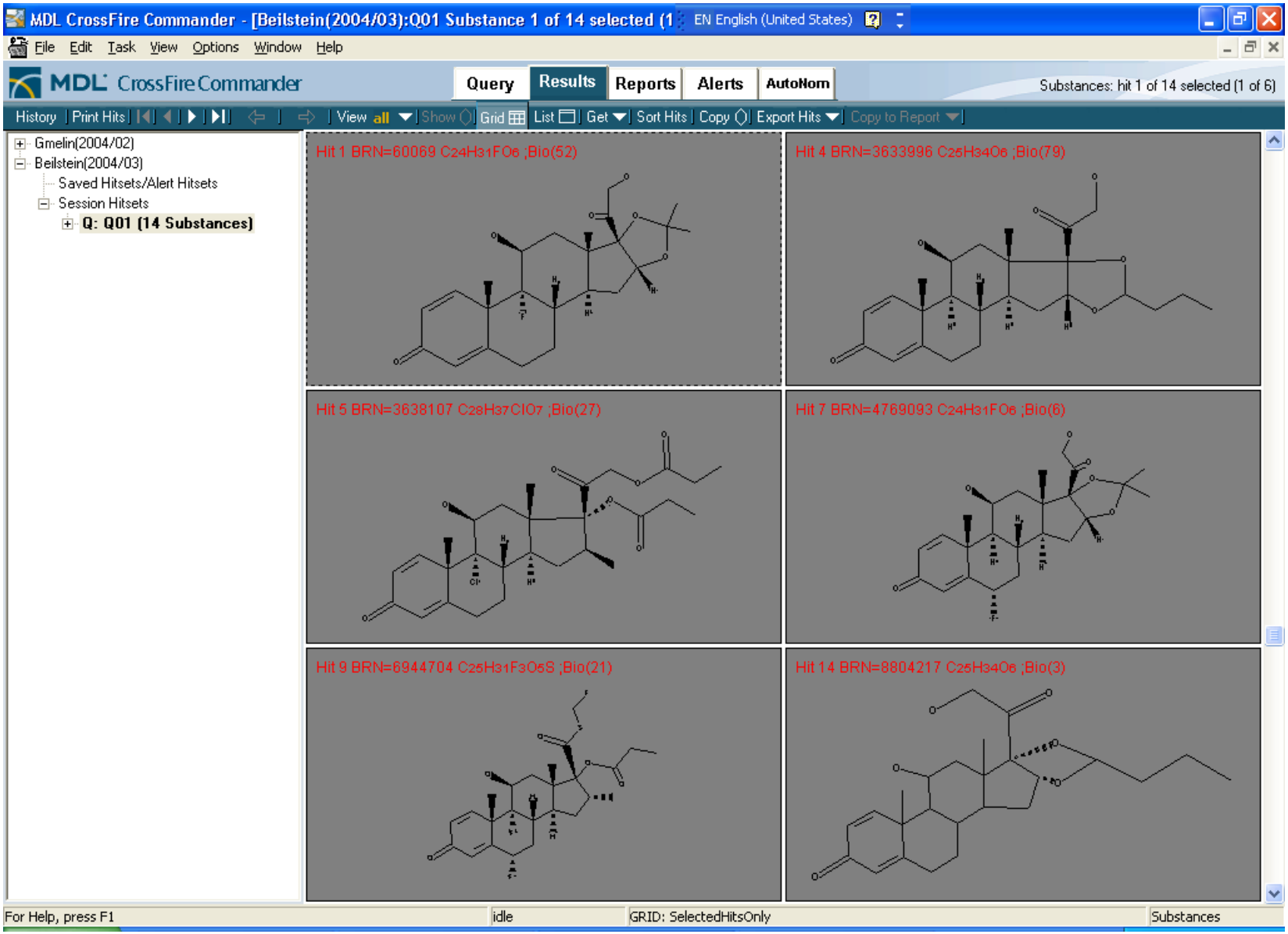
通过预定义的药理学数据查询表格进行化合物查询。



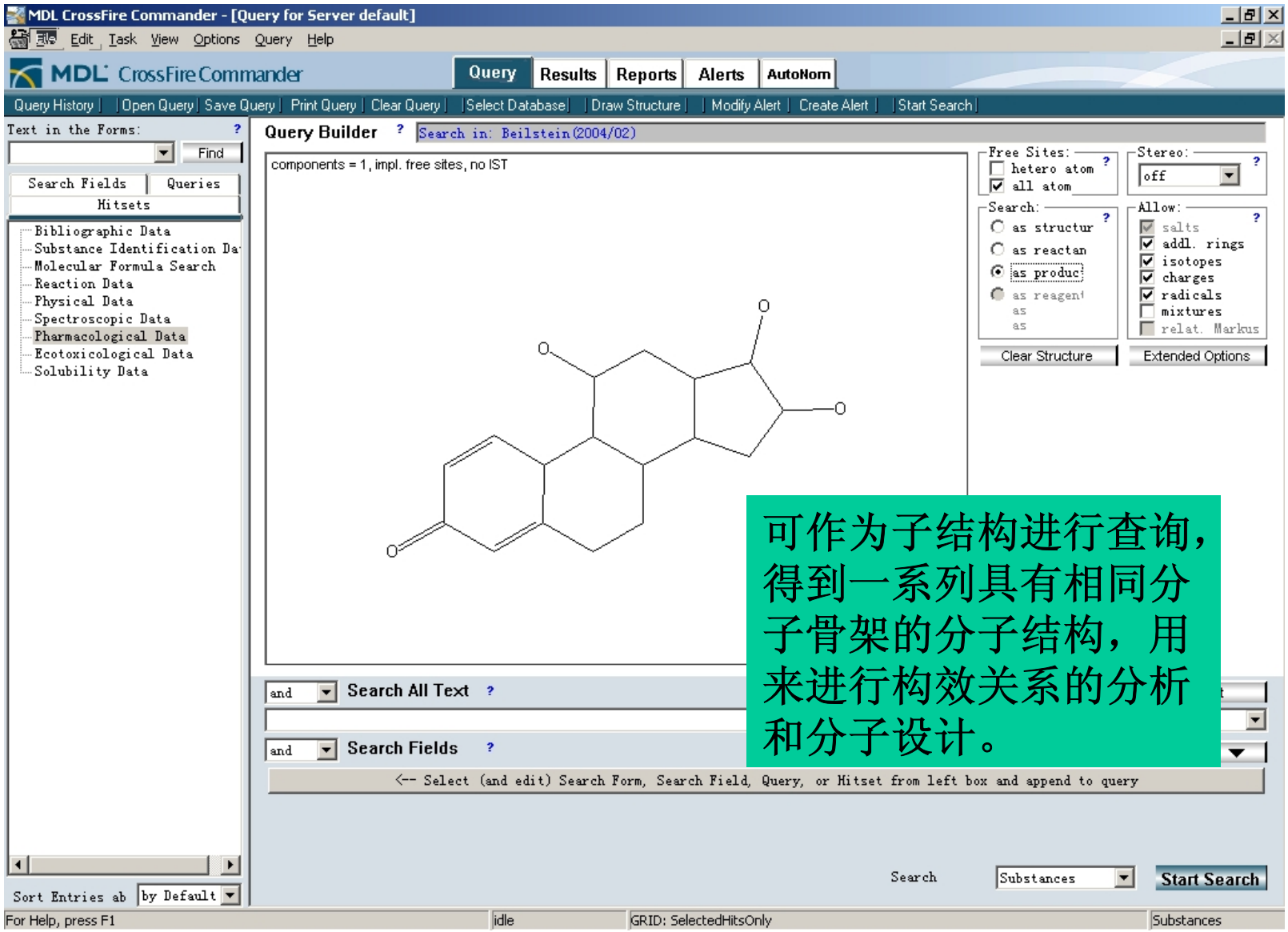
数据查询结果显示


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 all | Show | Grid | List | Get | Sort Hits | Copy | Export Hits | Copy to Report
Gmelin(2004/01)
Beilstein(2004/02)
Saved Hitsets/Alert Hits
Session Hitsets
Q: Q04 (14 Substan
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



提取的公共母体结构

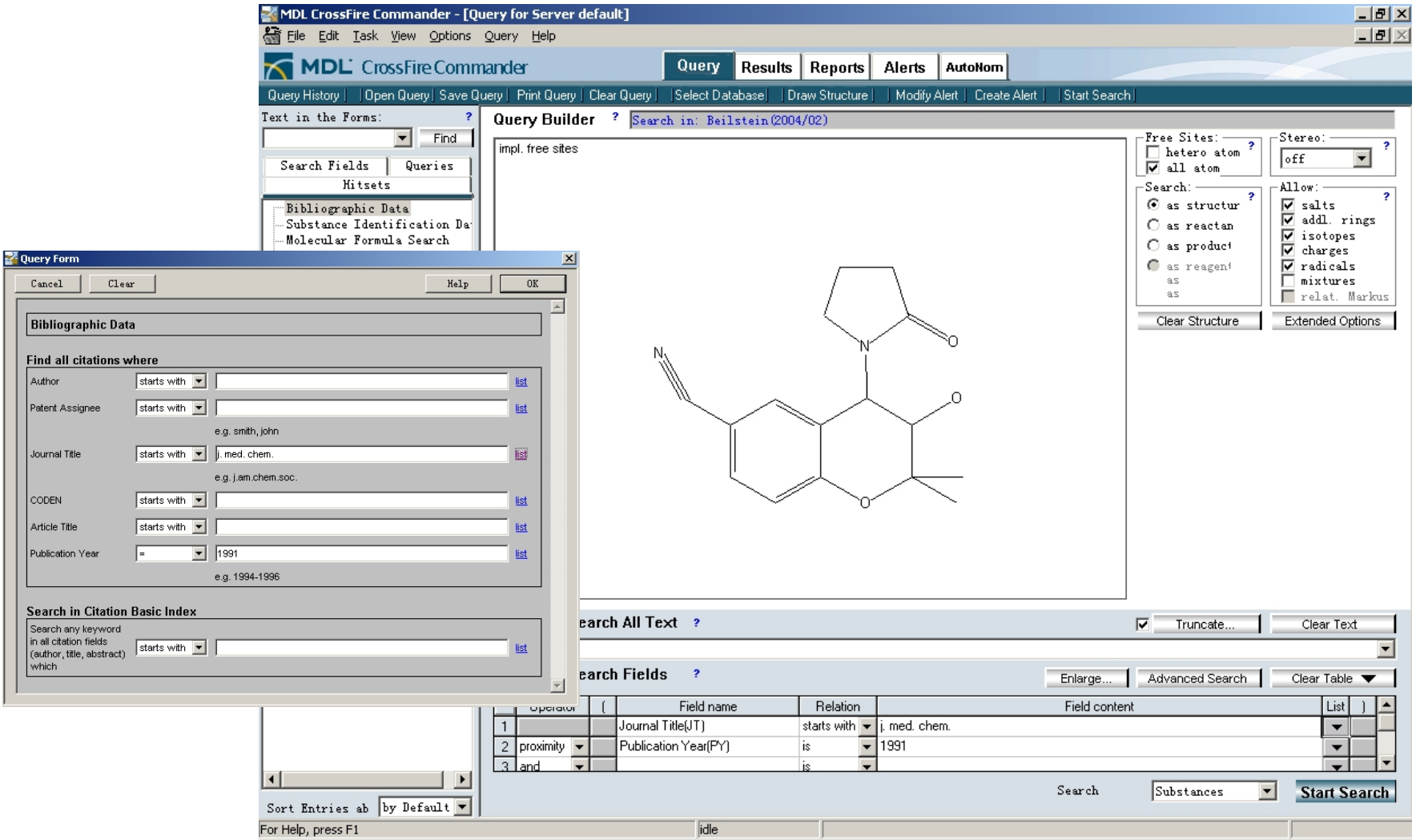


可作为子结构进行查询，得到一系列具有相同分子骨架的分子结构，用来进行构效关系的分析和分子设计。

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。

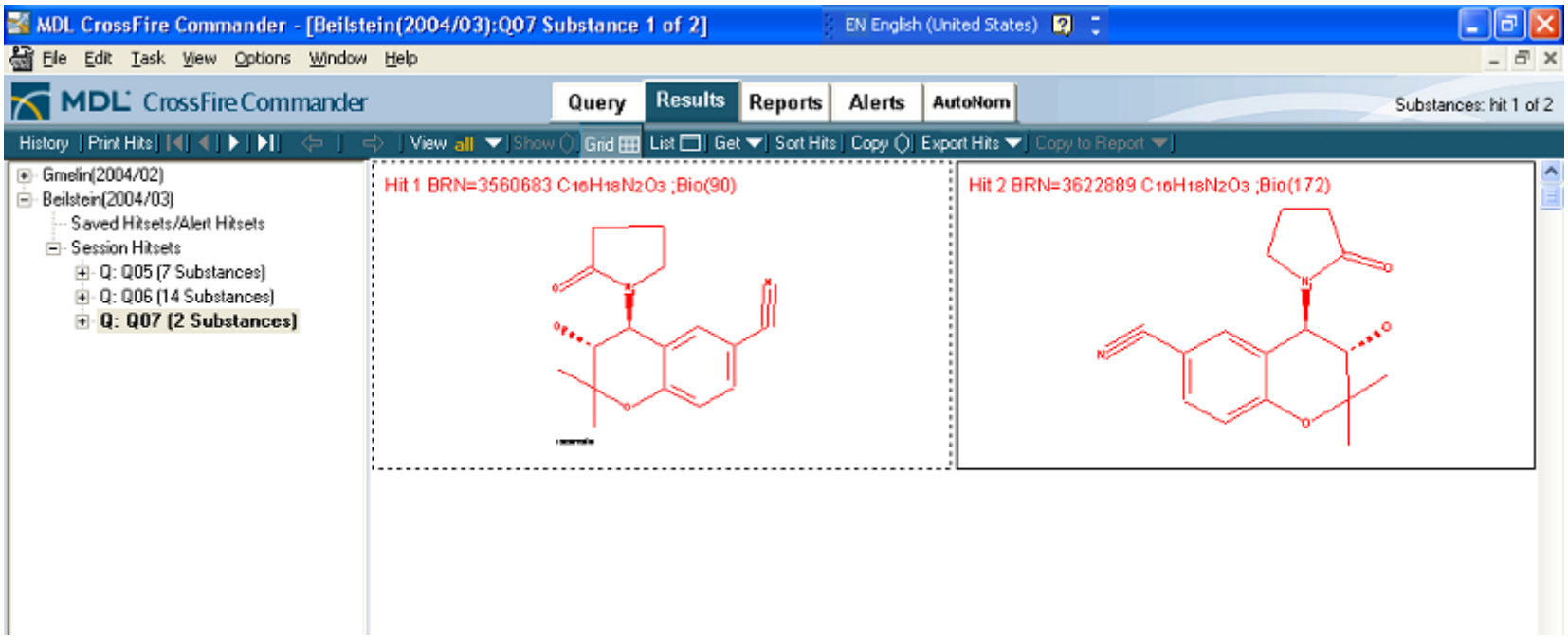
- 进行结构和数据的联合检索
- 查询此化合物的合成方法

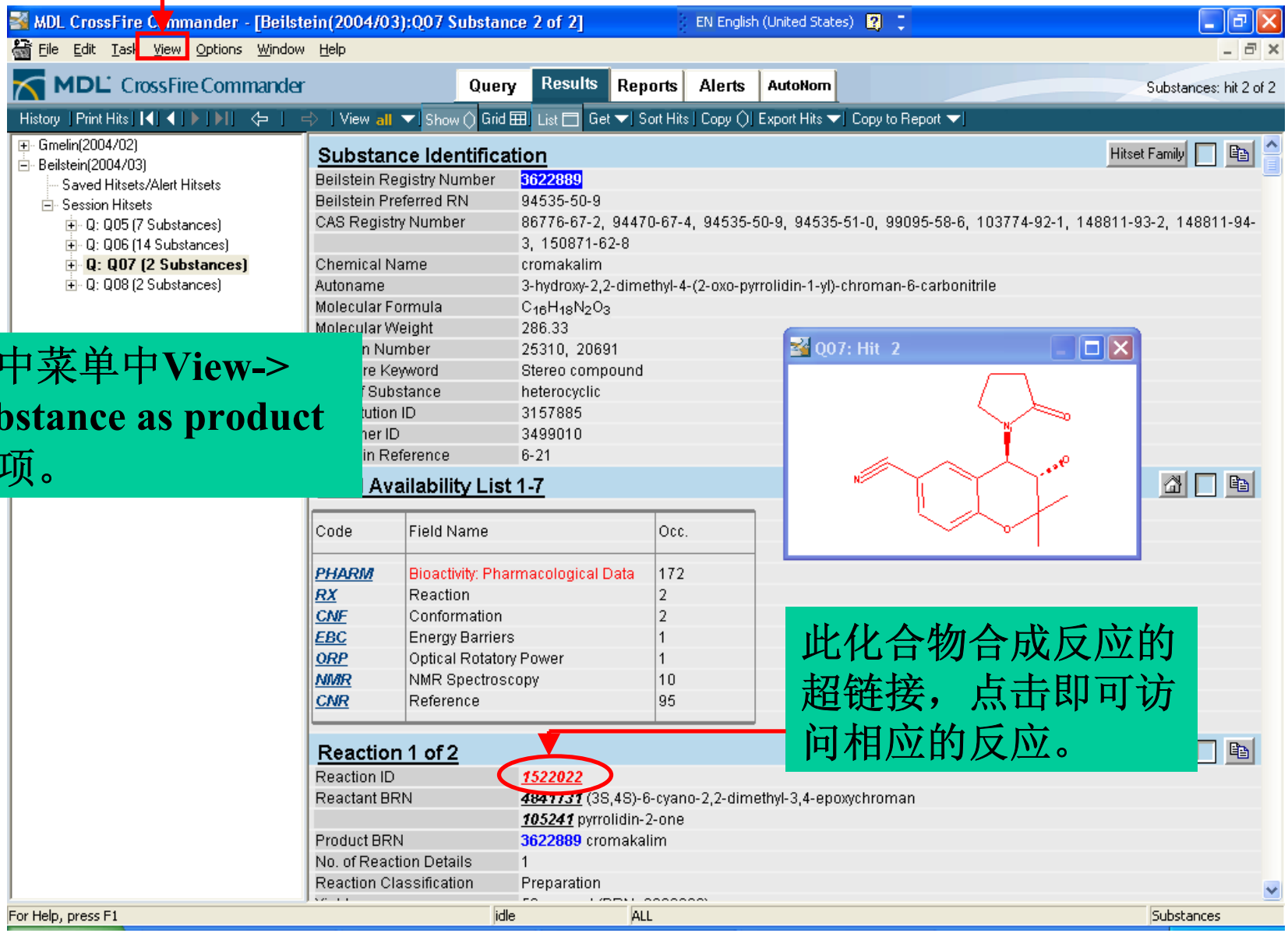
检索条件的填充



Bibliographic entry

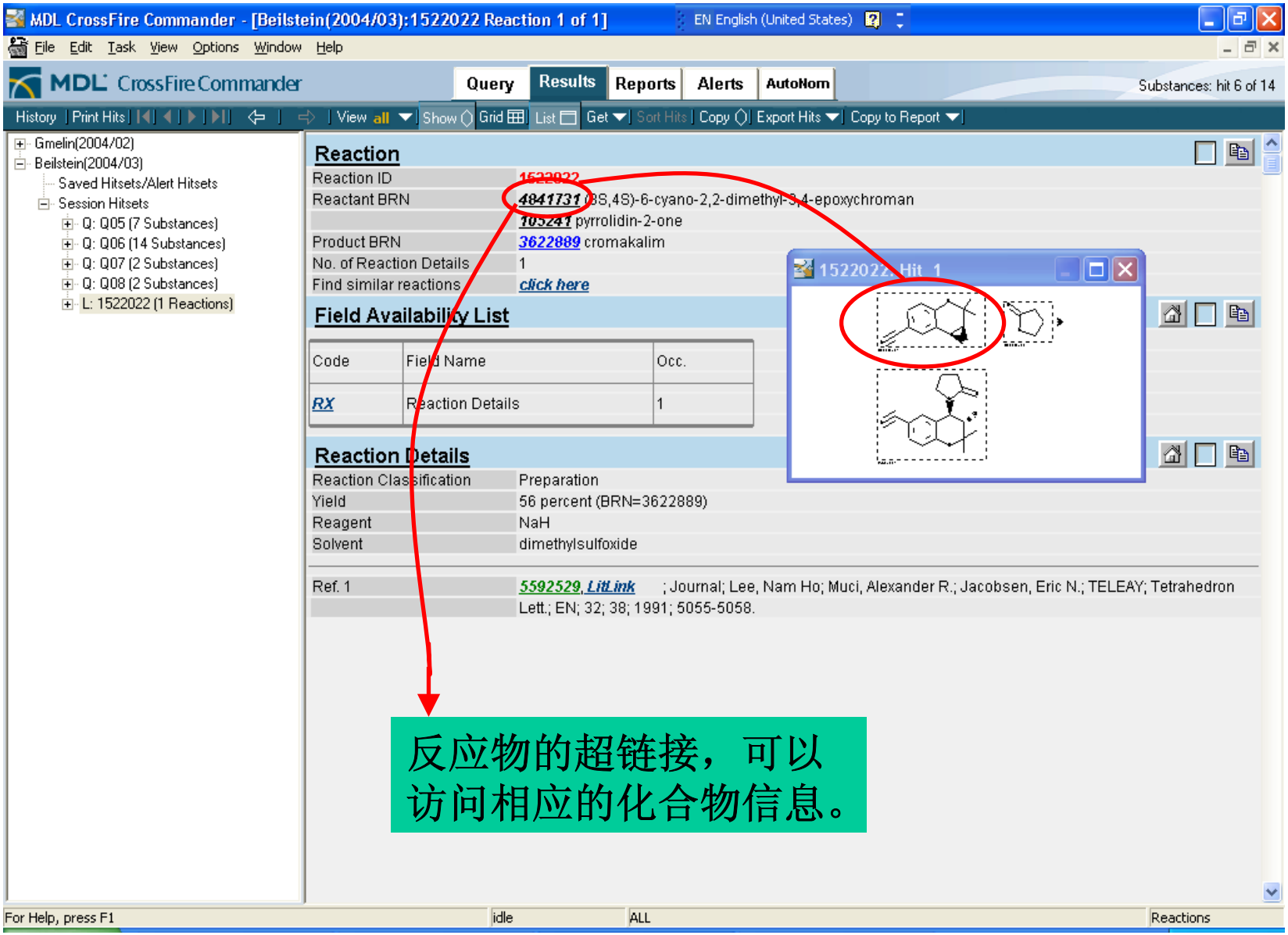
联合检索结果显示


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)



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。



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

- 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)
    - L: 1522022 (1 Reactions)
    - L: 4841731 (1 Substances)

Find similar reactions	click here

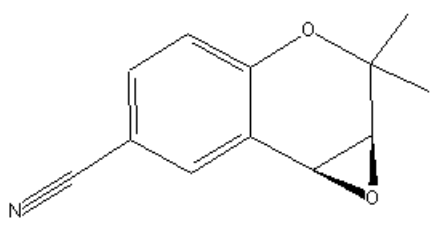
Ref. 1	5592529, LitLink ; Journ ...AY; Tetrahedron
	Lett.; EN; 32; 38; 1991; 5055

此化合物合成反应的超链接，点击即可访问相应的反应。

Reaction 2 of 34

Reaction ID	1771003
Reactant BRN	1367827 2,2-dimethyl-2*H*-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	CH_2Cl_2
Temperature	0 C
Find similar reactions	click here

4841731: Hit 1



Ref. 1	6375902, LitLink ; Journal; Kureshy, Rukhs ...hil T.;
	Iyer, Parameswar K.; Subramanian, P. S.; Jasra, Raksh V.; JCTLA5; J. Catal.; EN; 209; 1; 2002; 99 - 104.

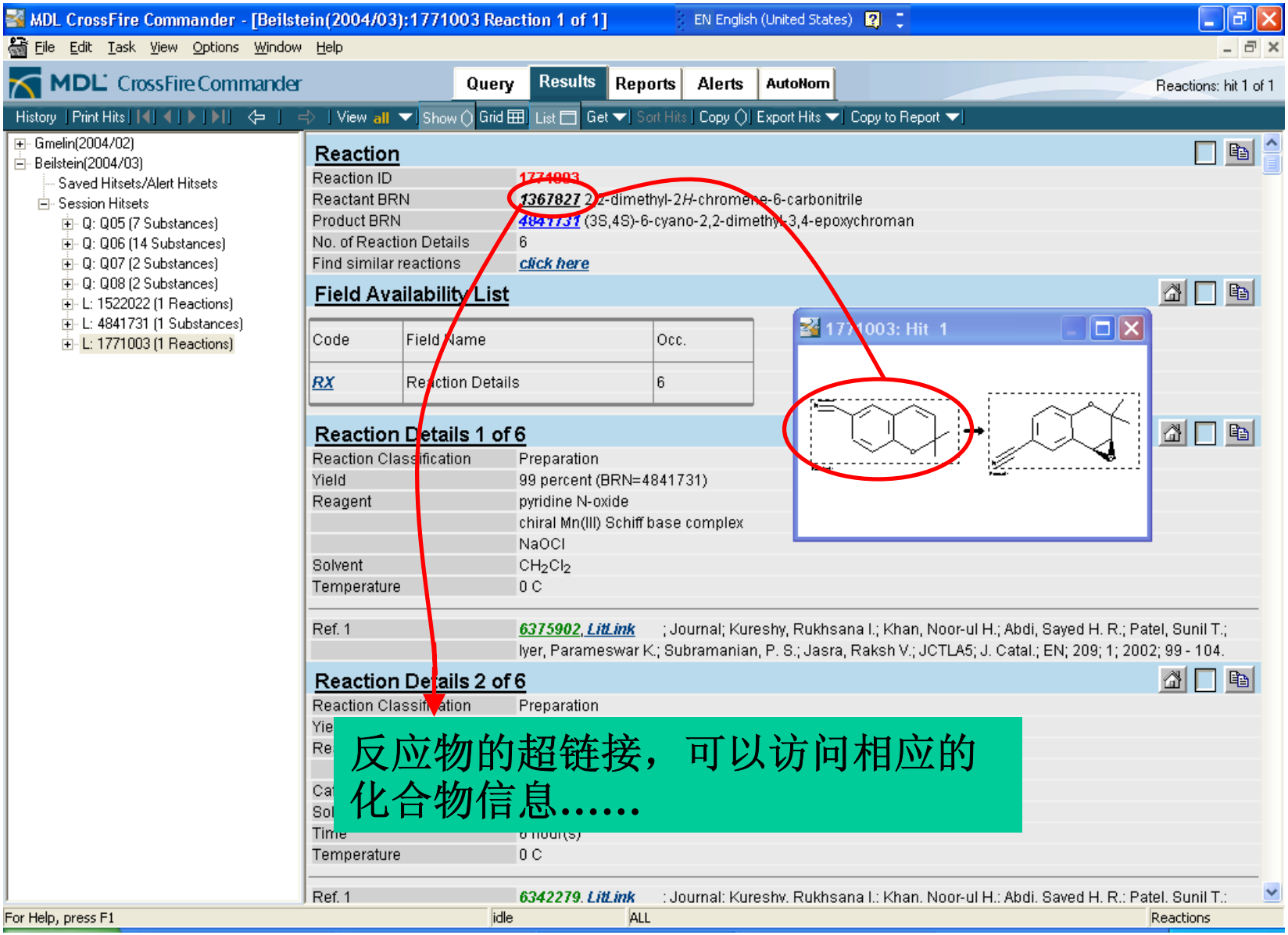
Reaction 3 of 34

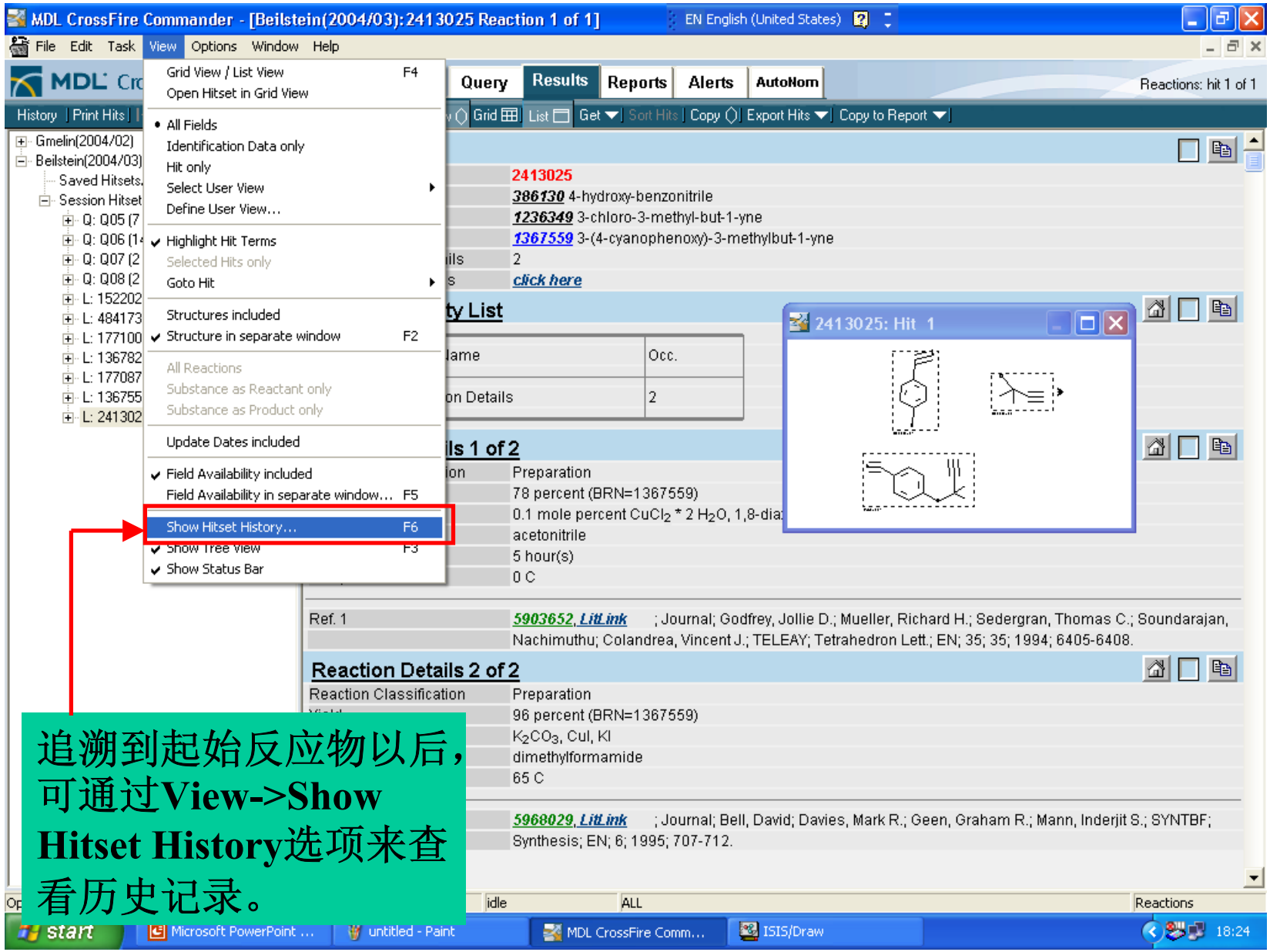
Reaction ID	3762491
Reactant BRN	4841731 (3S,4S)-6-cyano-2,2-dimethyl-3,4-epoxychroman
	742548 6-hydroxy-2-methyl-2*H*-pyridazin-3-one
Product BRN	4822349 3-hydroxy-2,2-dimethyl-4-(1-methyl-6-oxo-1,6-dihydro-pyridazin-3-yloxy)-chroman-6-carbonitrile
No. of Reaction Details	1
Reaction Classification	Preparation
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.

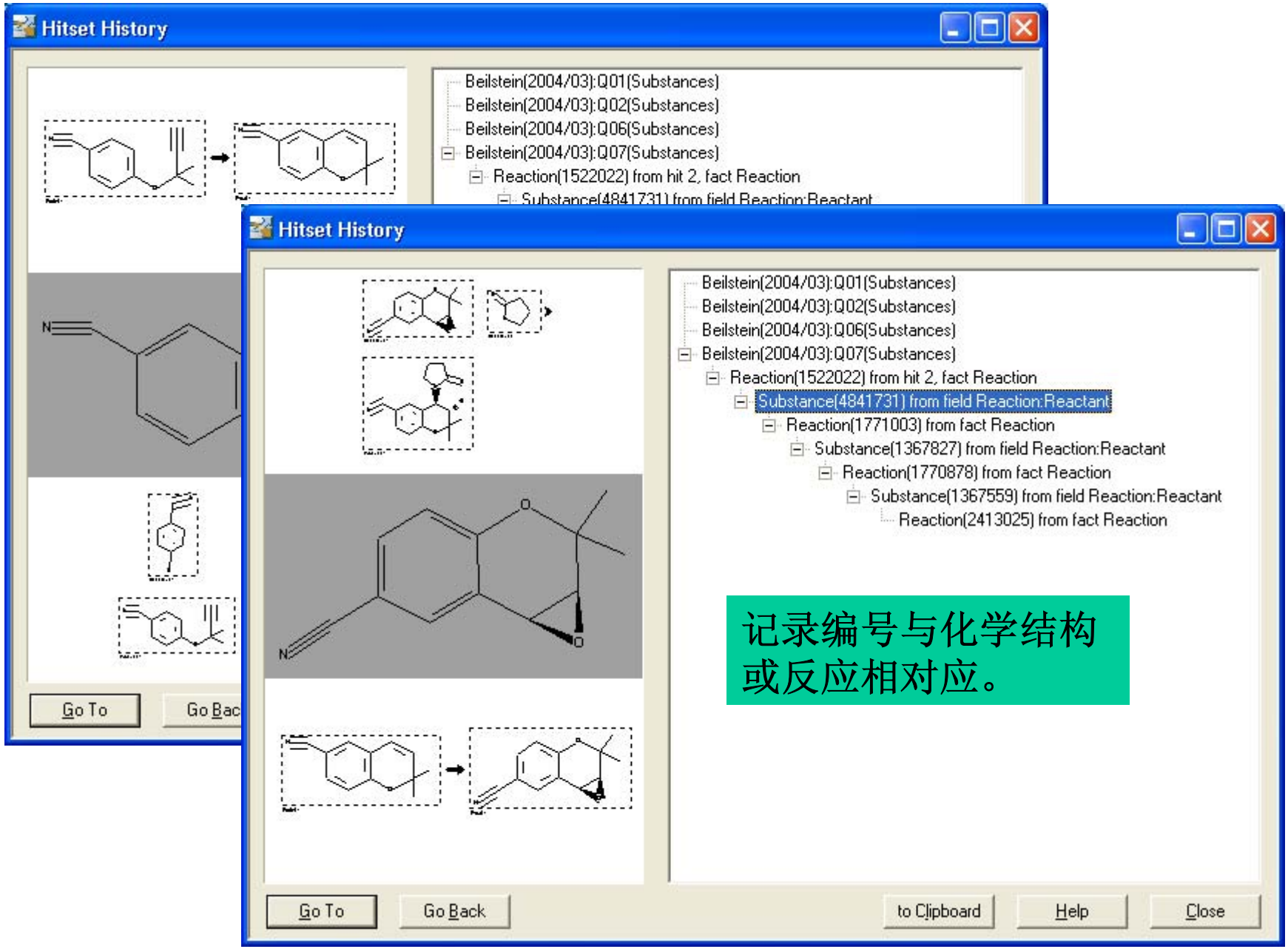
Reaction 4 of 34

For Help, press F1 | idle | ALL | Substances


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
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)
L: 1522022 (1 Reactions)
L: 4841731 (1 Substances)
L: 1771003 (1 Reactions)
Reaction
Reaction ID 1771003
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
1771003: Hit 1
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
Temperature 0 C
Ref. 1 6342279, LitLink ; Journal; Kureshy, Rukhsana I.; Khan, Noor-ul H.; Abdi, Sayed H. R.; Patel, Sunil T.;
反应物的超链接，可以访问相应的化合物信息.....
For Help, press F1
idle
ALL
Reactions

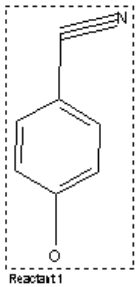


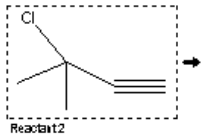
追溯到起始反应物以后，可通过**View->Show Hitset History**选项来查看历史记录。

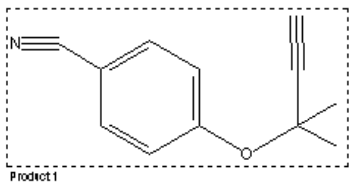

Hitset History
Beilstein(2004/03):Q01(Substances)
Beilstein(2004/03):Q02(Substances)
Beilstein(2004/03):Q06(Substances)
Beilstein(2004/03):Q07(Substances)
Reaction(1522022) from hit 2, fact Reaction
Substance(4841731) from field Reaction:Reactant
Reaction(1771003) from fact Reaction
Substance(1367827)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

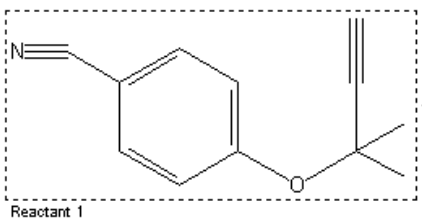
Step 1

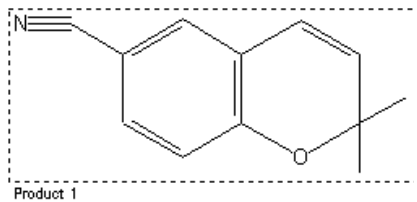




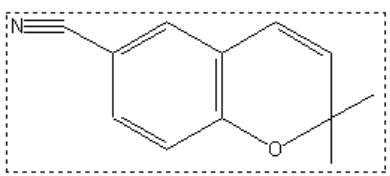


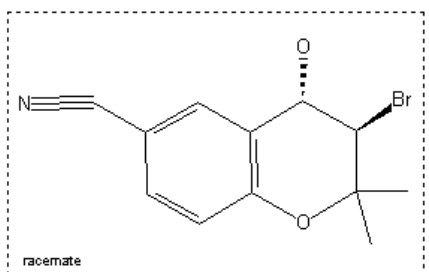
Step 2



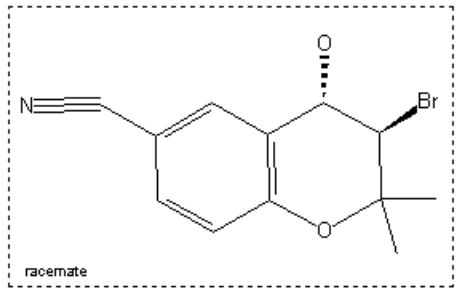


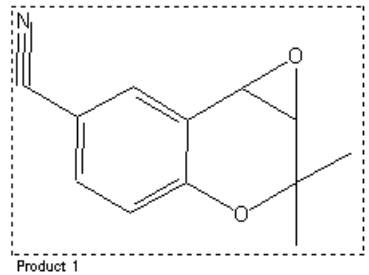
Step 3



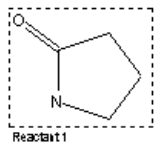


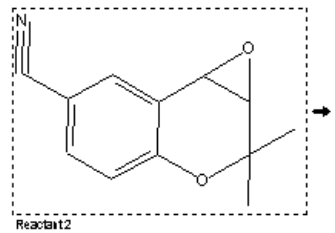
Step 4

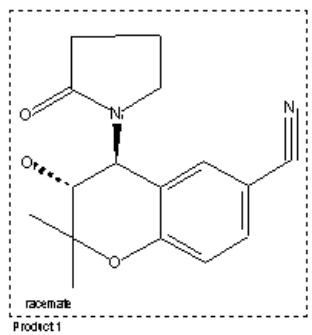




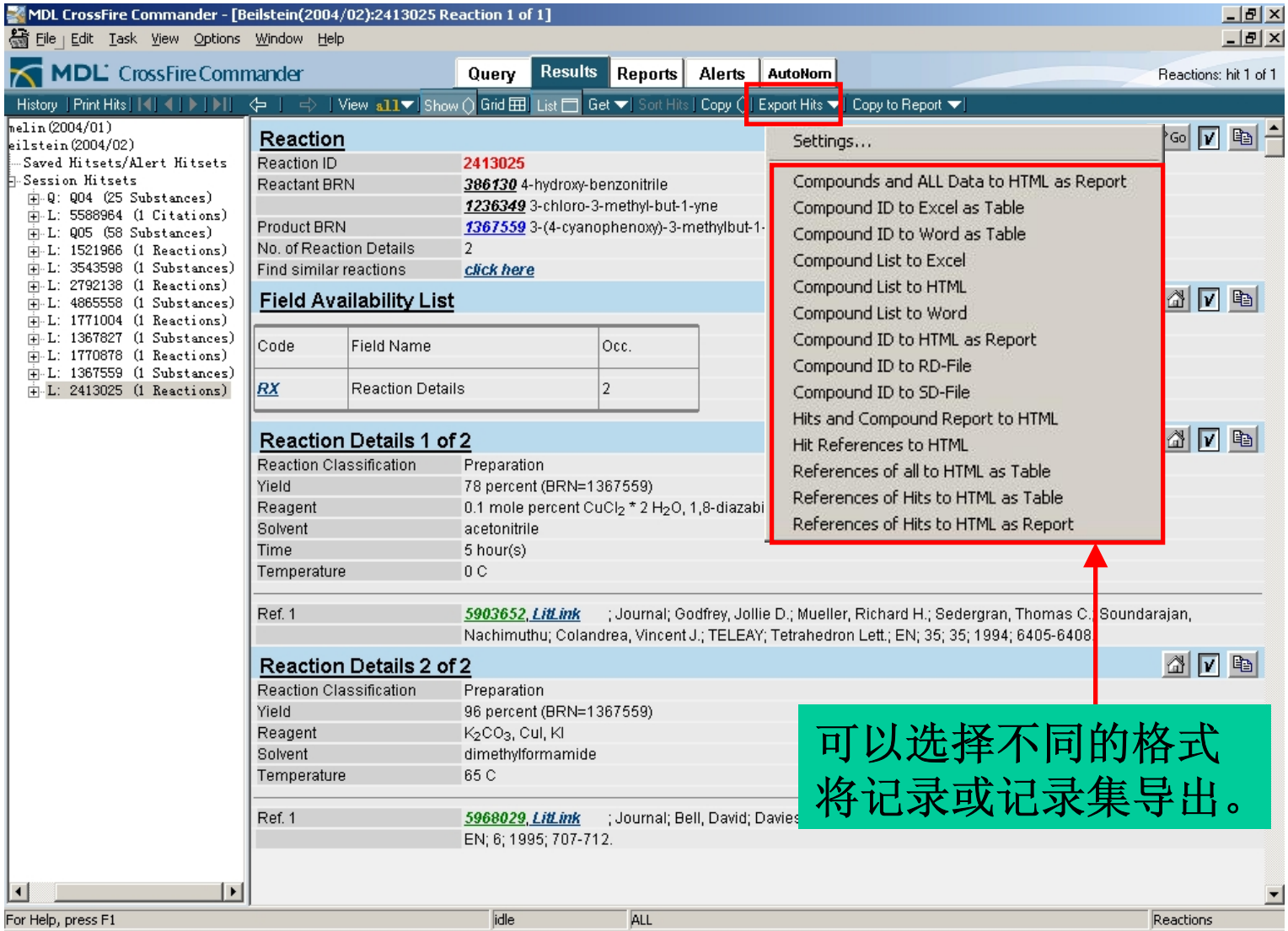
Step 5

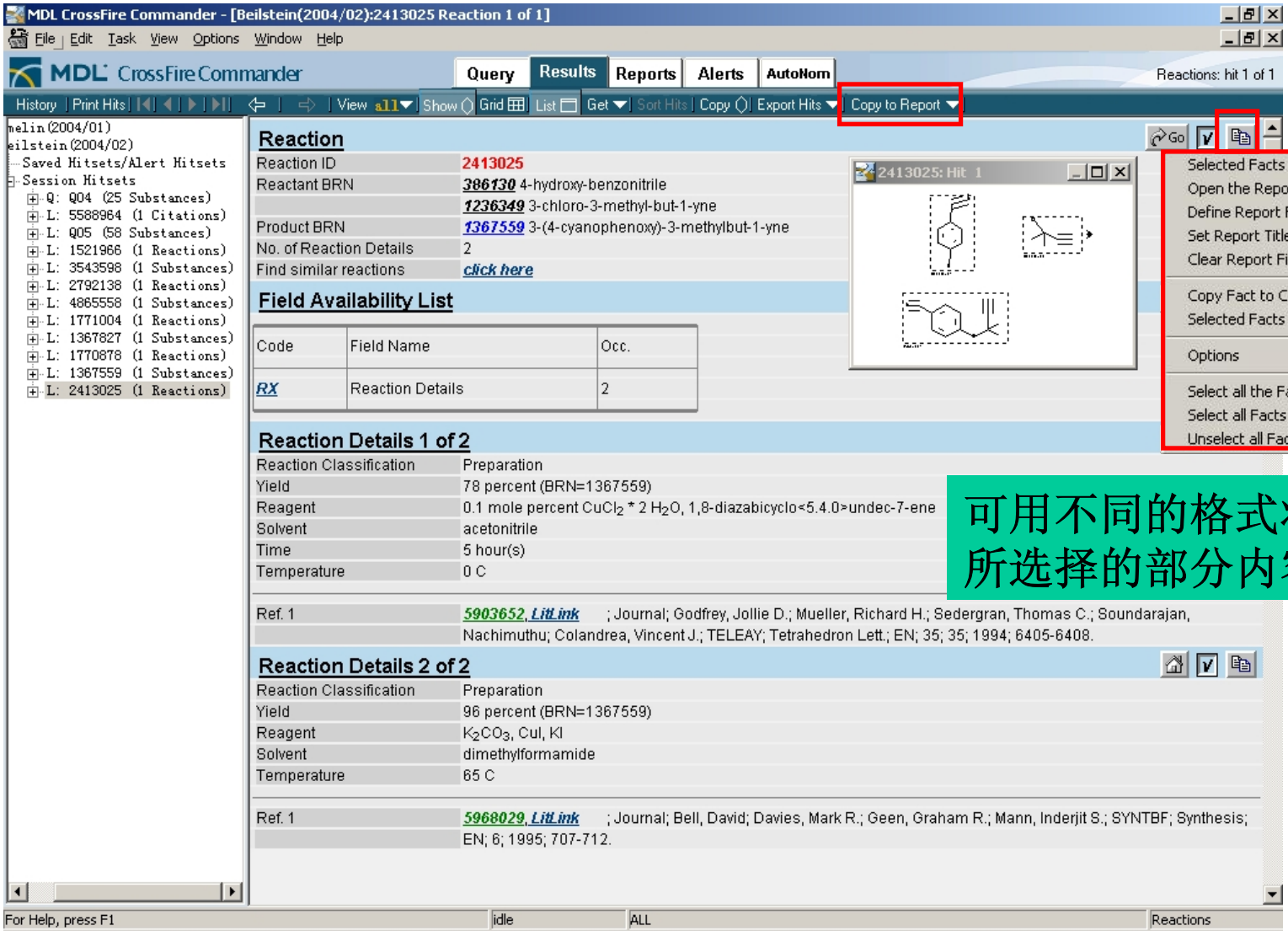






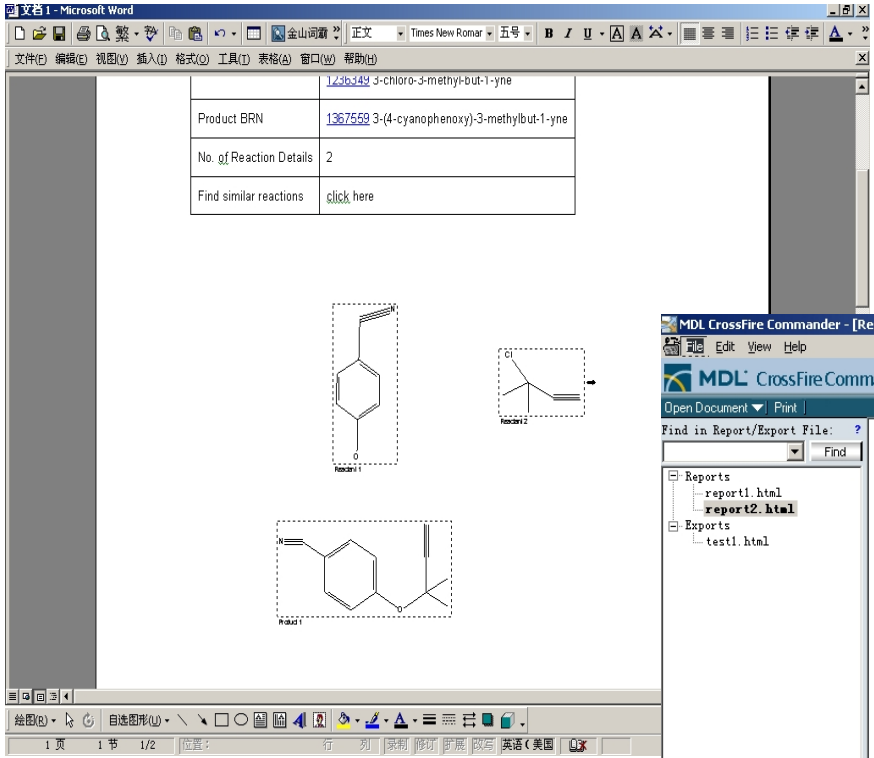
检索结果的导出和报告的生成

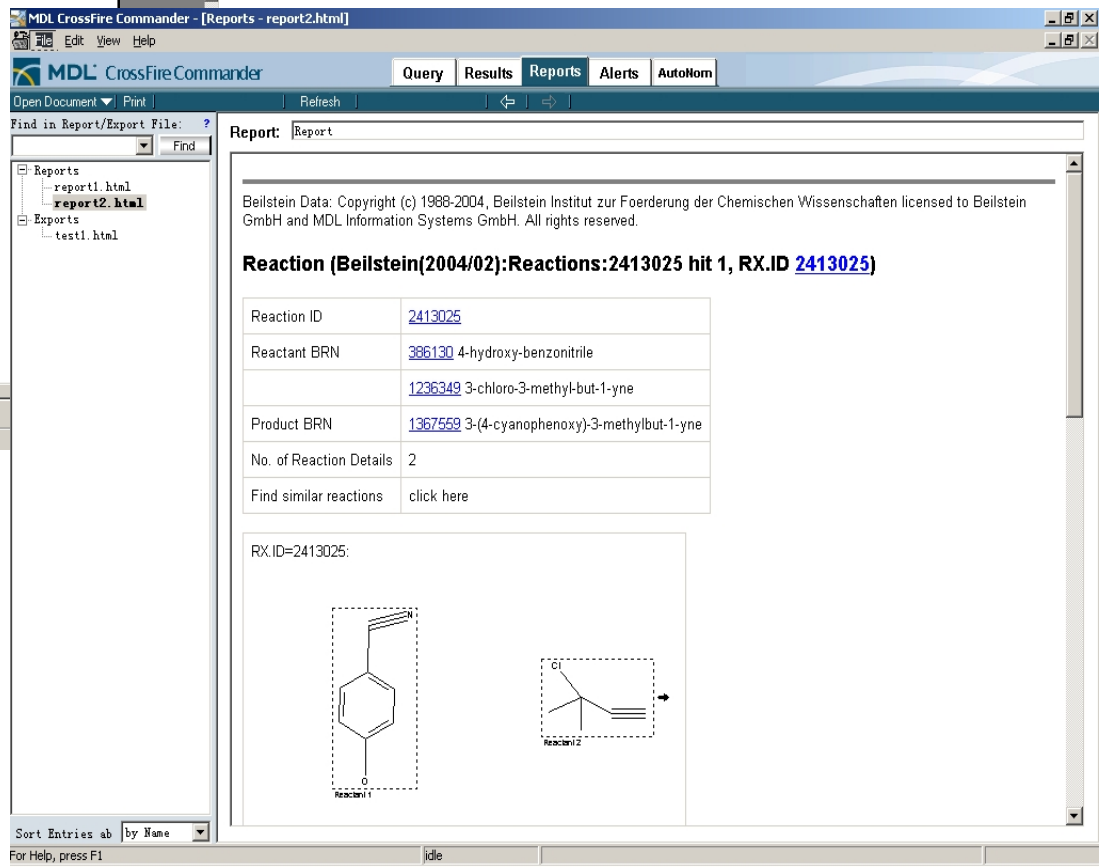




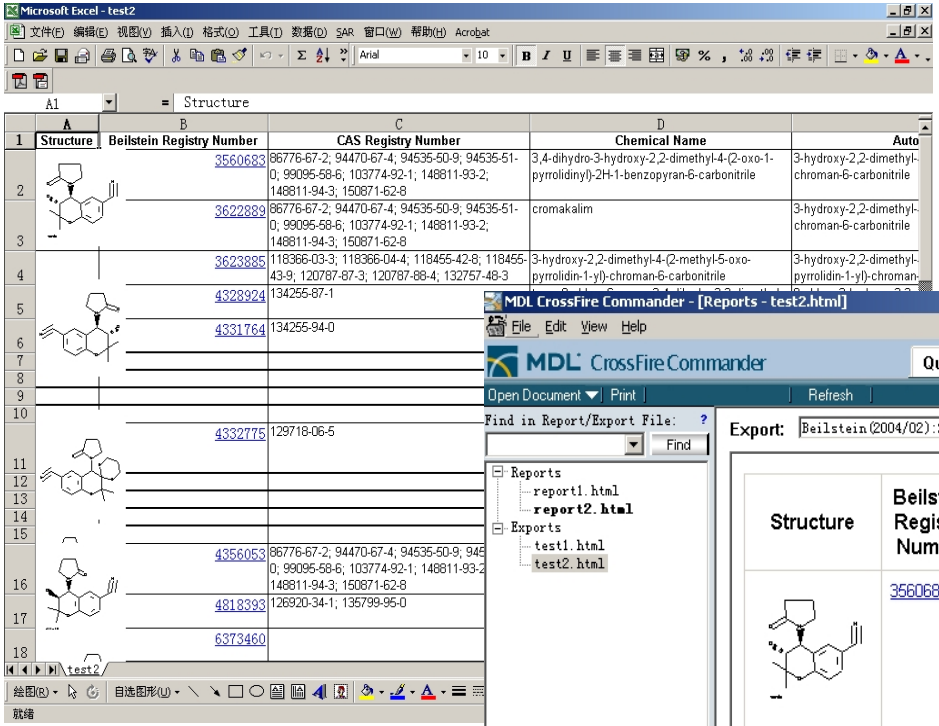
可用不同的格式将记录中所选择的部分内容导出。

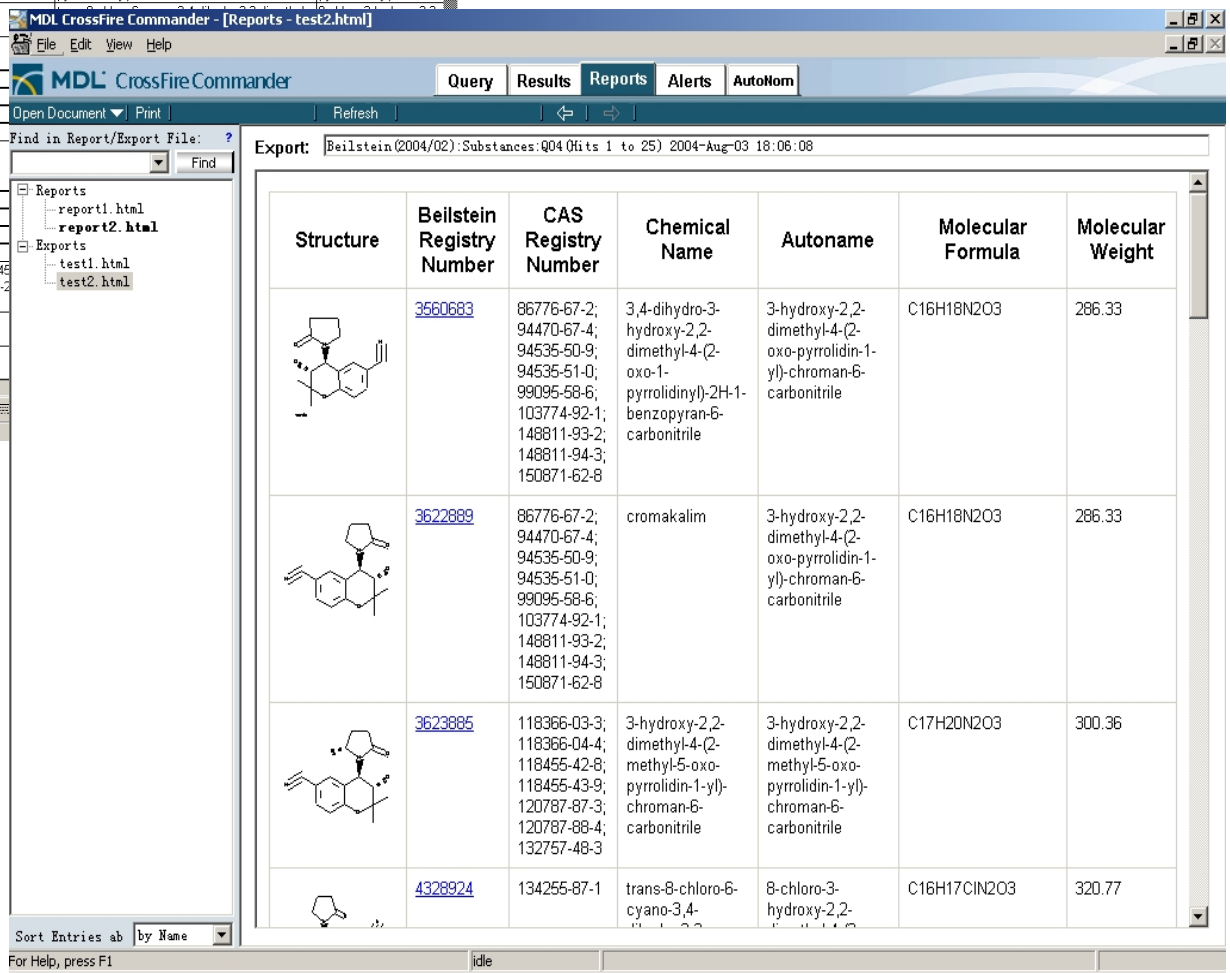
记录导出后生成的报告示例



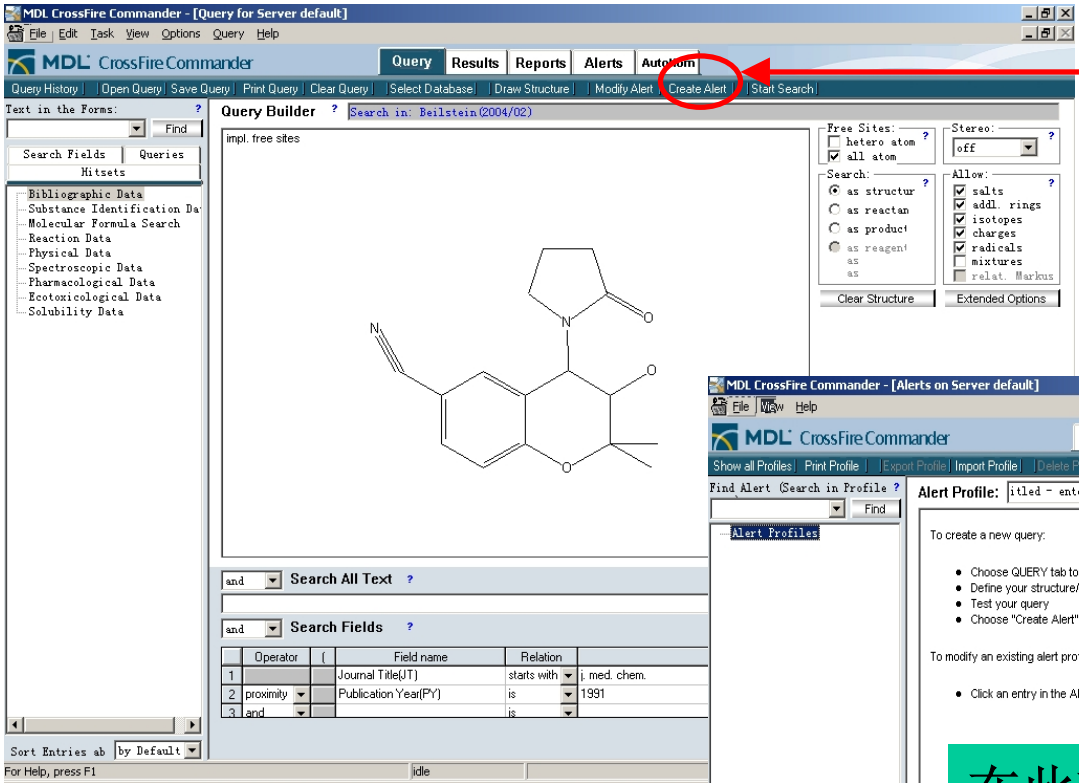


记录导出后生成的表格示例

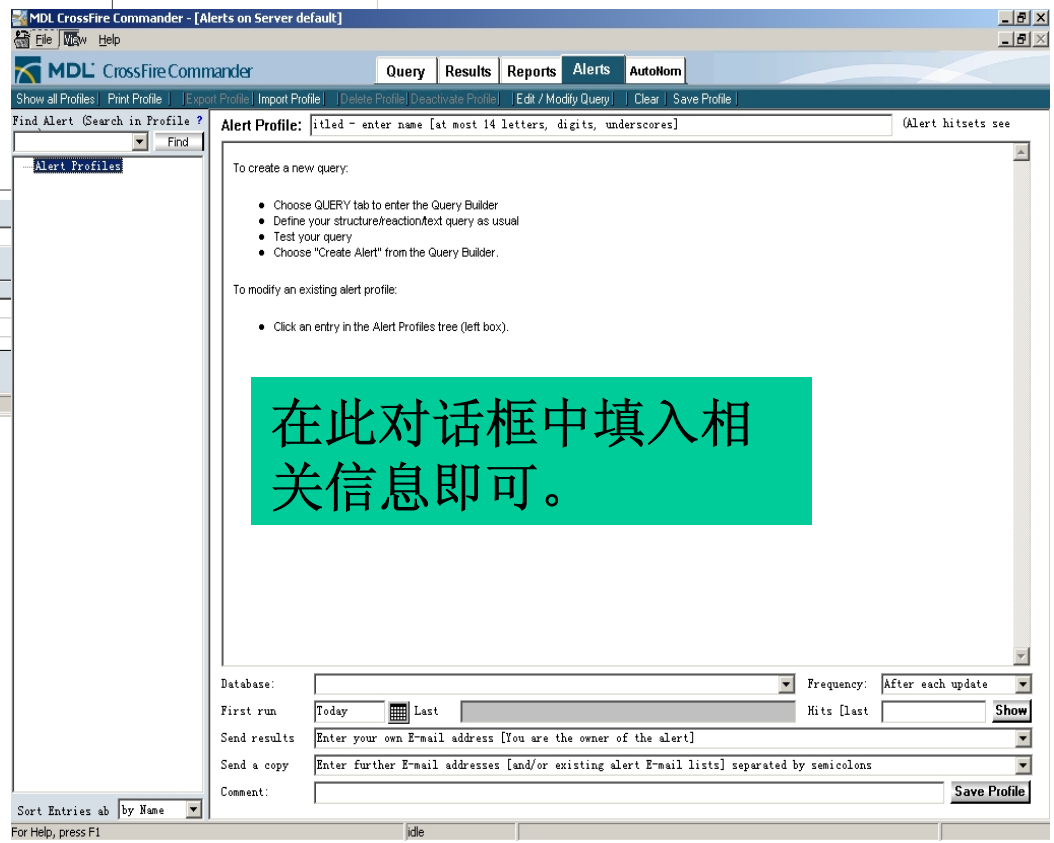




跟踪服务的建立

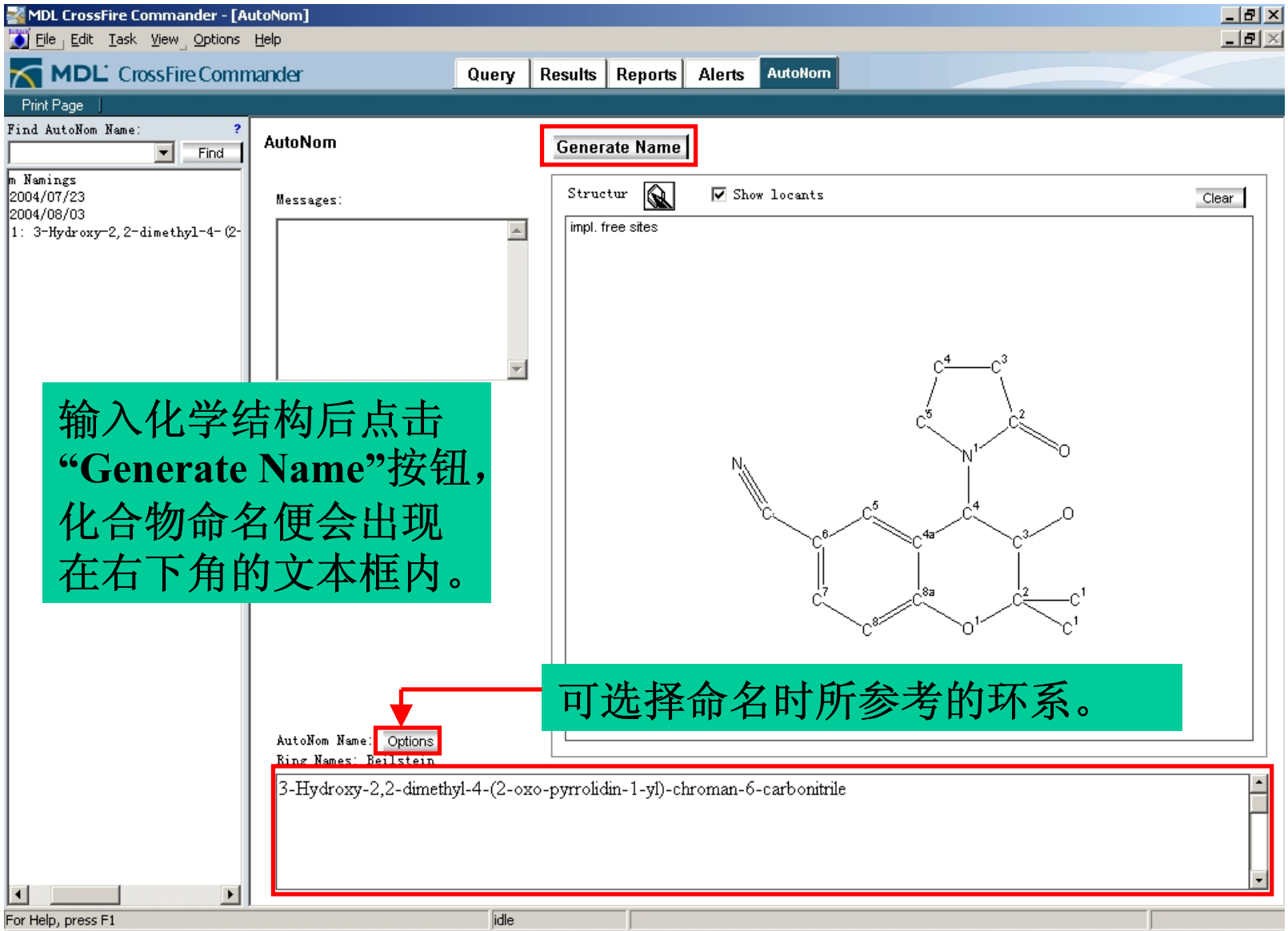


建立检索条件后点击此按钮，



在此对话框中填入相关信息即可。

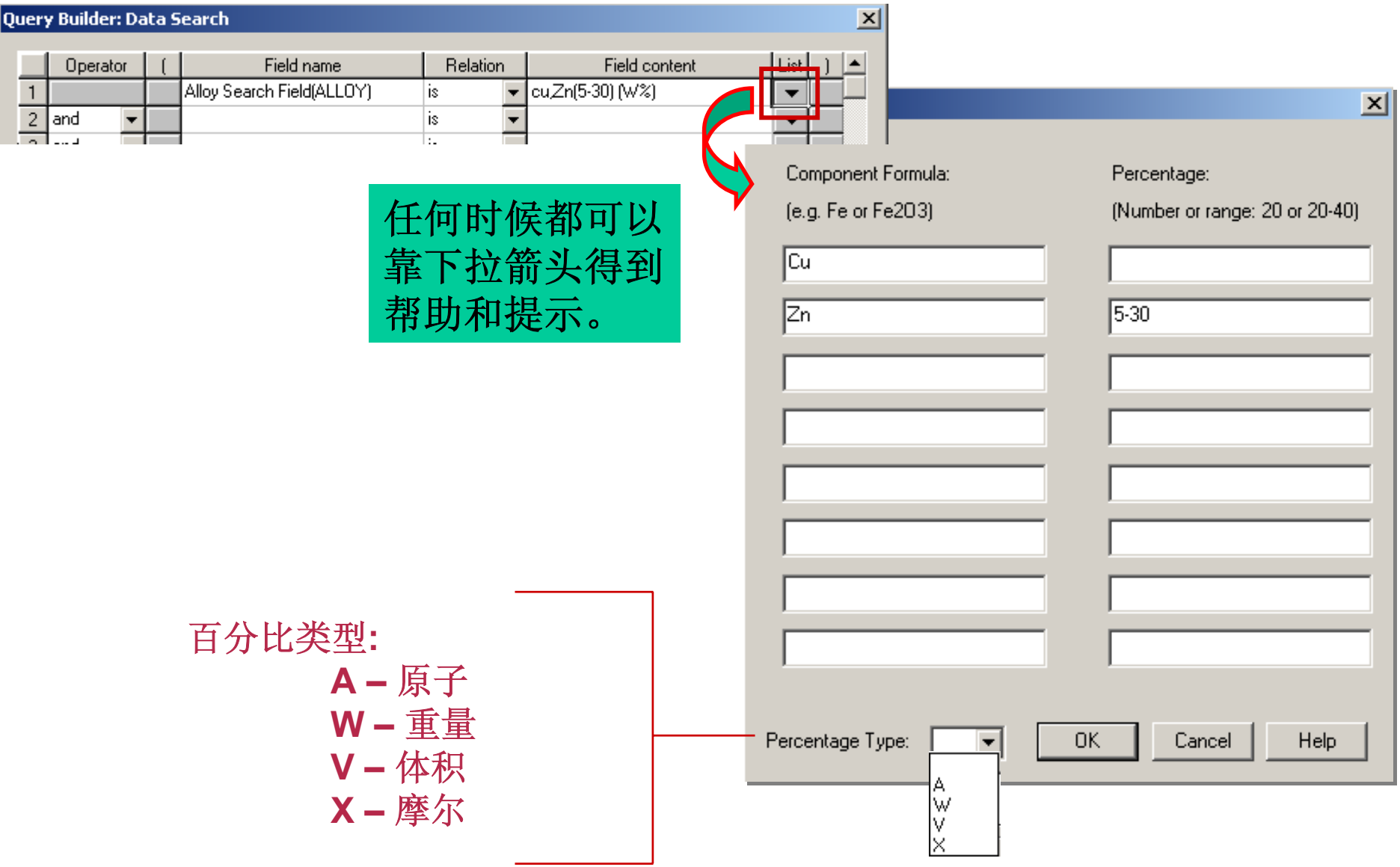
化学结构的自动命名


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
Generate Name
Messages:
Structur
Show locants
Clear
impl. free sites
输入化学结构后点击“Generate Name”按钮，化合物命名便会出现在右下角的文本框内。
可选择命名时所参考的环系。
AutoNom Name:
Options
Ring Names: Beilstein
3-Hydroxy-2,2-dimethyl-4-(2-oxo-pyrrolidin-1-yl)-chroman-6-carbonitrile
For Help, press F1
idle

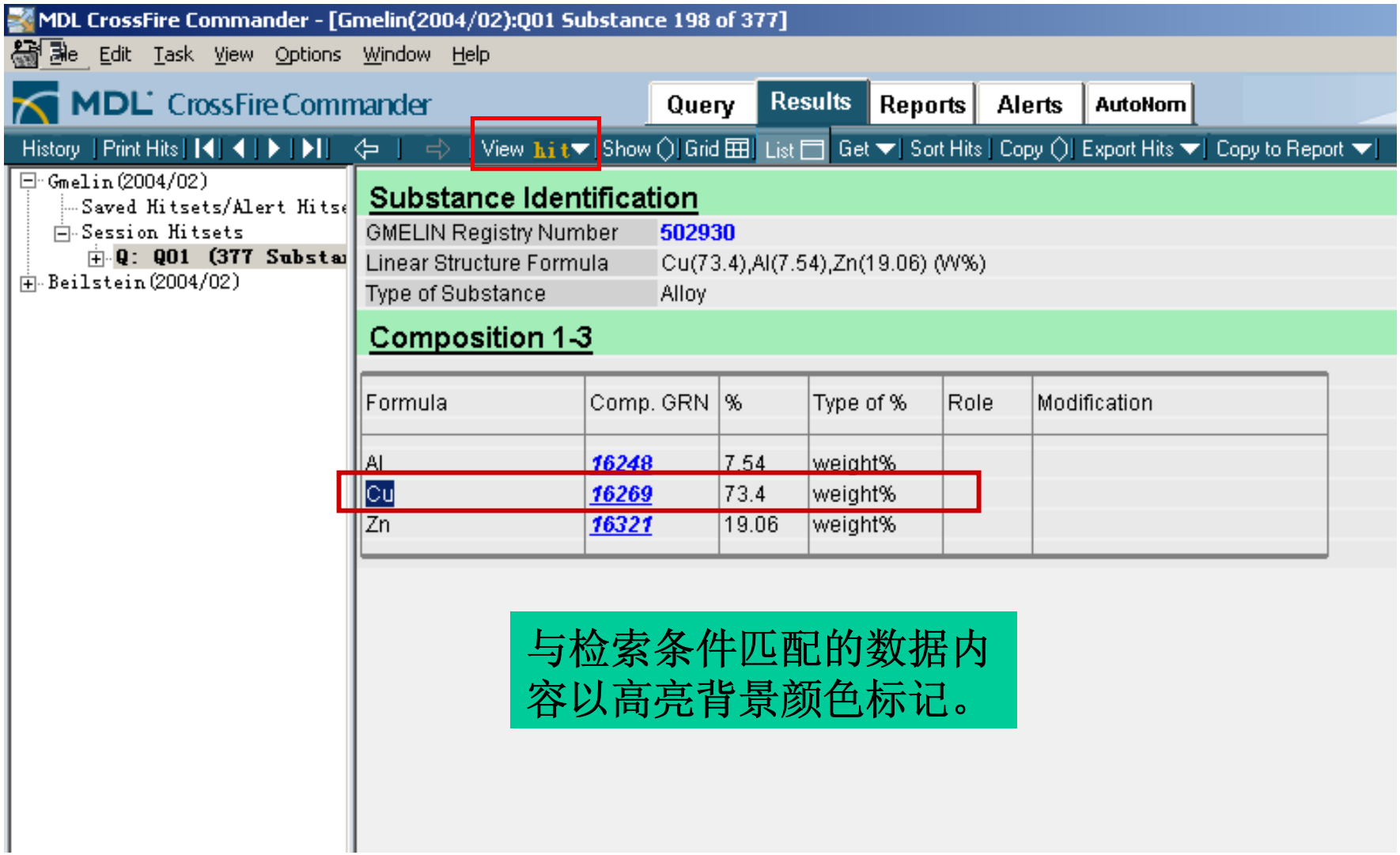
Gmelin数据库检索示例1

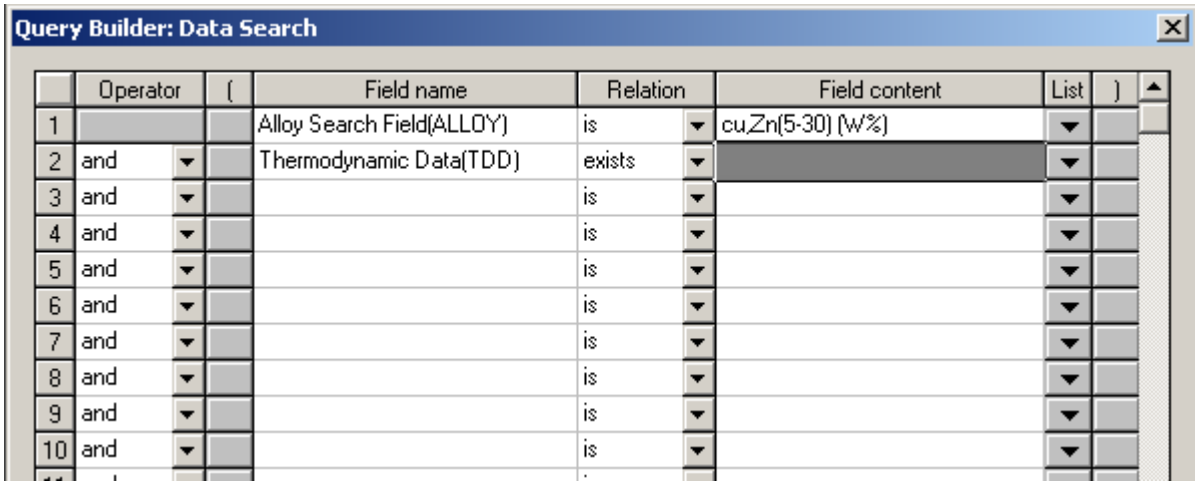
例：　查询锌含量在5－30%（重量百分比）之间的铜合金，并要求查到的结果含有热力学方面的数据。

- 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

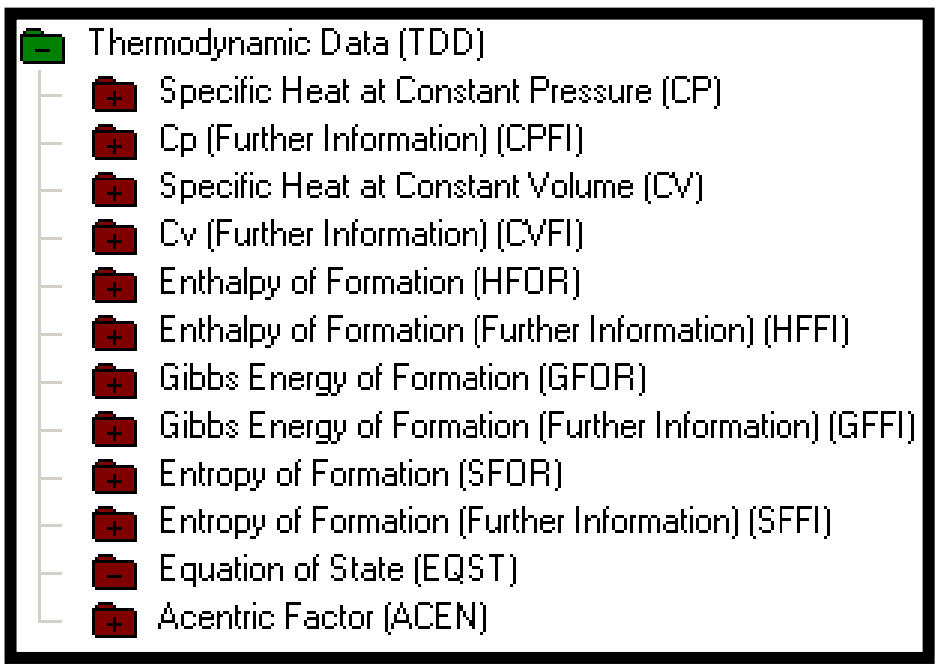

Query Builder: Data Search
Operator
(
Field name
Relation
Field content
List
)
1
Alloy Search Field(ALLOY)
is
cu,Zn(5-30) (W%)
2
and
is
任何时候都可以靠下拉箭头得到帮助和提示。
Component Formula:
(e.g. Fe or Fe2O3)
Percentage:
(Number or range: 20 or 20-40)
Cu
Zn
5-30
Percentage Type:
OK
Cancel
Help
A
W
V
X
百分比类型:
A – 原子
W – 重量
V – 体积
X – 摩尔

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 Hitse
Session Hitsets
Q: Q01 (377 Substa
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。



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

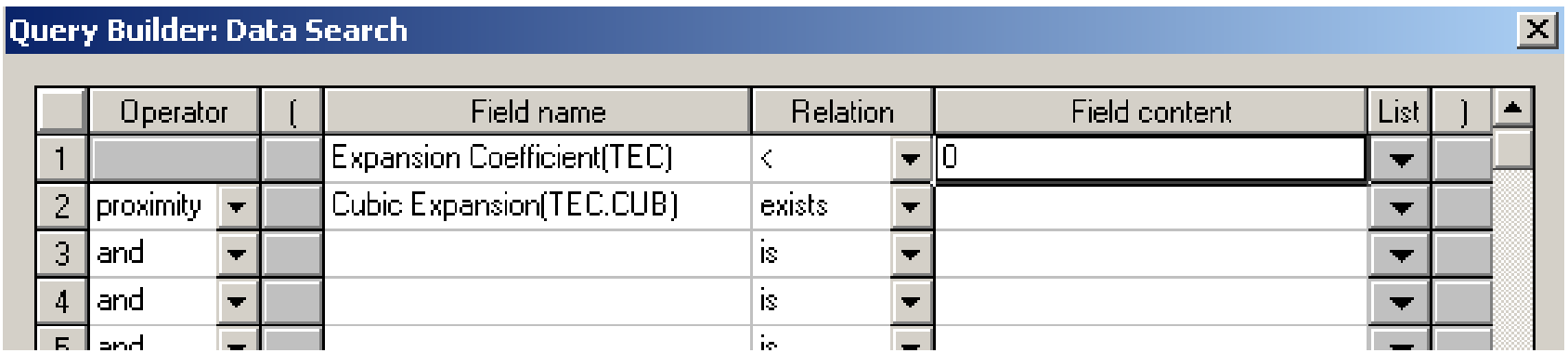


表格查询结果显示

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

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。

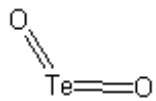


表格查询结果显示

Identification

GMELIN Registry Number	1411
Linearized Structure Formula	TeO_2
Molecular Formula	O_2Te
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.

Thermal Expansion 87 of 126

Expansion Coefficient	-2*10-9 K**-1
Cubic Expansion	yes
Temperature	-271 Deg C
Forms of State	Unspecified

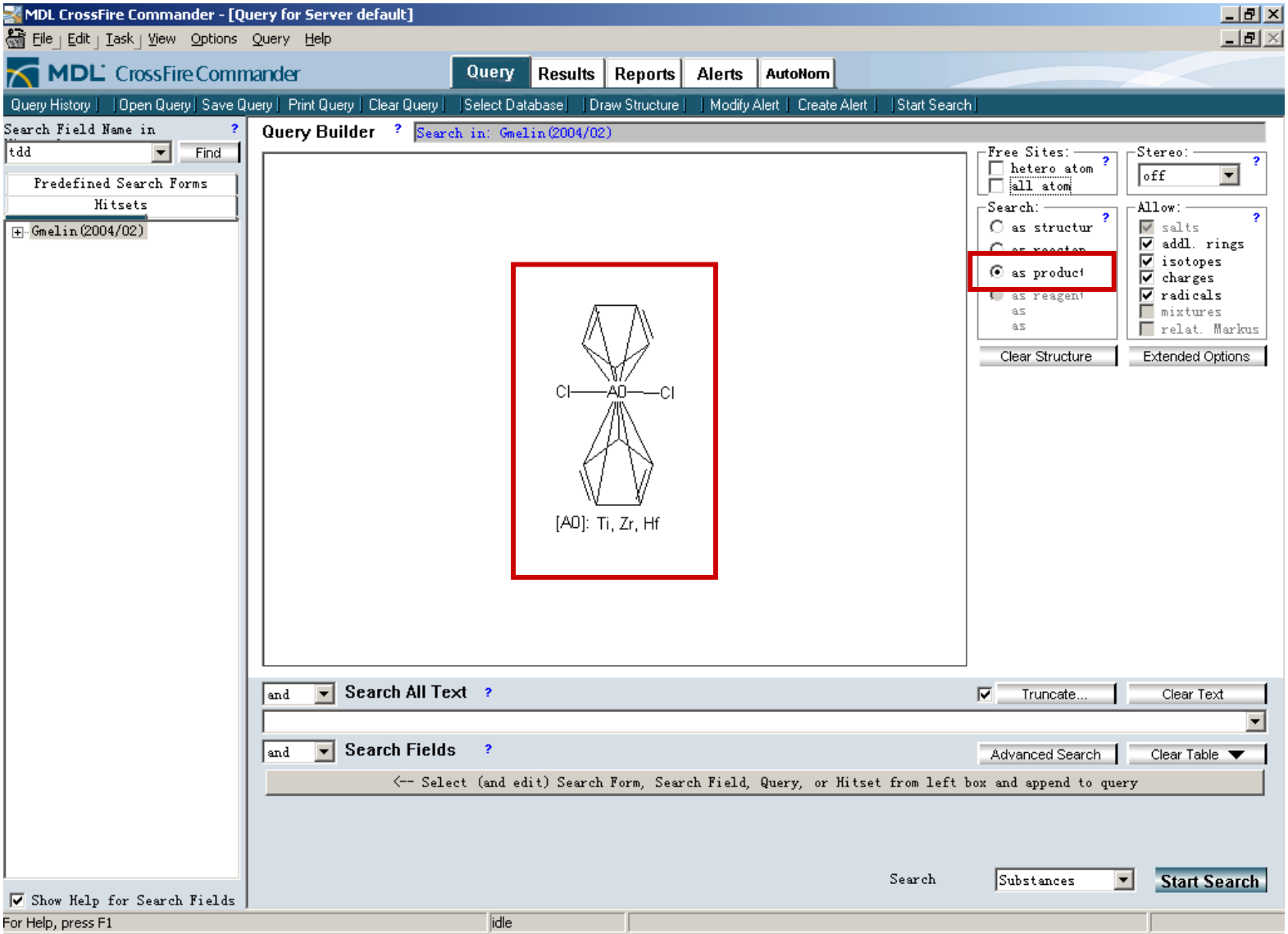
Ref. 1	556323, LitLink ; White, G. K.; Collocott, S. J.; Collins, J. G.; JCOMEL; J. Phys. Condens. Matter; Vol. 2; (1990) 7715 - 7718; English.

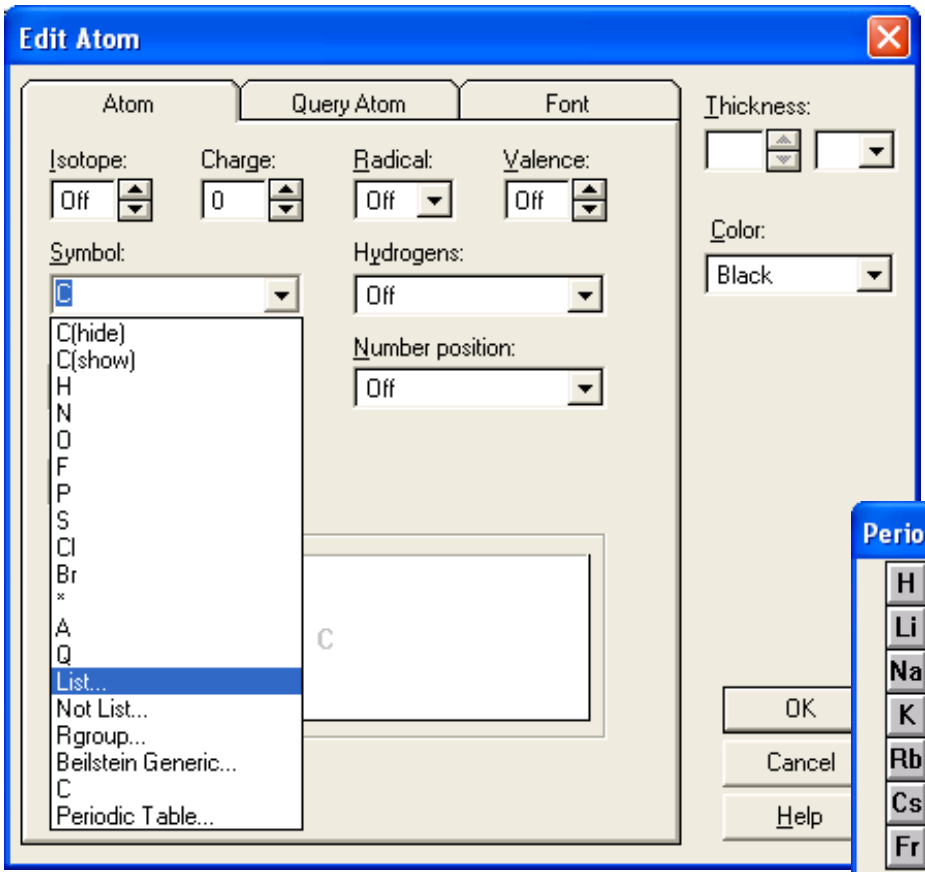
Gmelin数据库检索示例3

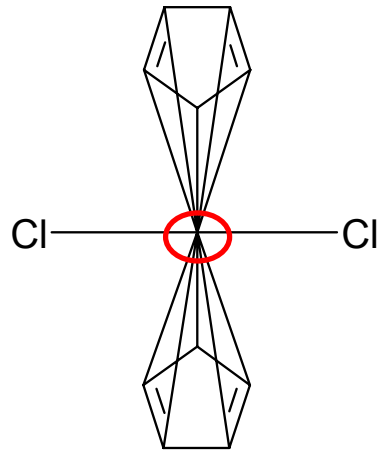
例：　Ziegler/Natta络合物是聚合物工业中的重要的催化剂。查询这类化合物的合成信息，并利用超链接访问相关的催化作用数据合文献信息。

- 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)
Free Sites:
hetero atom
all atom
Stereo:
off
Search:
as structur
as product
as reagent
Allow:
salts
addl. rings
isotopes
charges
radicals
mixtures
relat. Markus
Cl
A0
Cl
[A0]: Ti, Zr, Hf
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





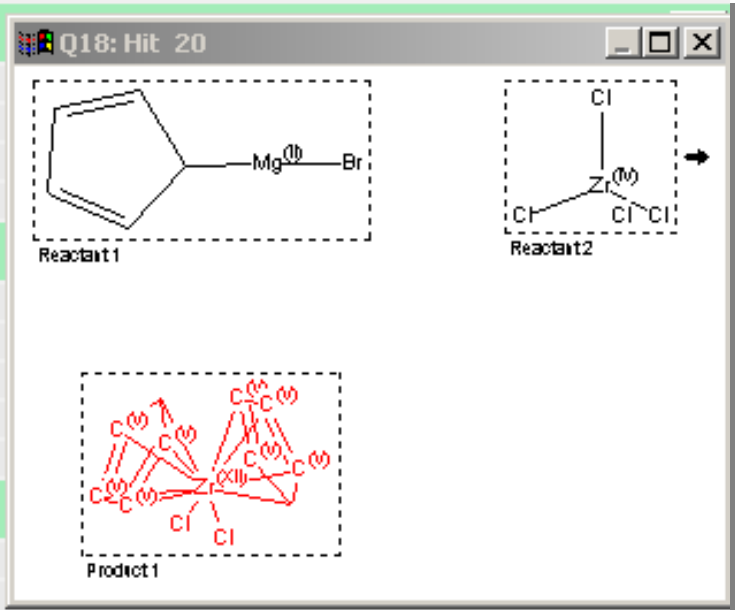
在ISIS/Draw中用“选择”工具双击络合物的中心原子，弹出“Edit Atom”对话框，在“Symble”下拉菜单中选择“List”，然后在弹出的元素周期表中选择所有可能的中心原子的符号，点击“OK”，即可将中心原子定义为多种可能的原子类型。

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_5H_5MgBr cyclopentadienyl magnesium bromide
	2469 $ZrCl_4$ zirconium tetrachloride
Product(s) (GRN)	***4056*** $(C_5H_5)_2ZrCl_2$ Cp_2ZrCl_2



Field Availability List

Code	Field Name	Occ.
RX	Reaction Details	1

Reaction Details

Solvent	ether
General Conditions	ZrCl4/C5H5MgBr (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	$(C_5H_5)_2ZrCl_2$
Molecular Formula	$C_{10}H_{10}Cl_2Zr$
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	Cp2ZrCl2

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, LitLink ; 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, LitLink ; 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, LitLink ; 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, LitLink ; Zi, Guofu; Li, Hung-Wing; Xie, Zuowei; ORGND7; Organometallics; Vol. 21; (2002) 3850 - 3855; English.

Behavior as Catalyst 5 of 84

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.

文献记录超链接

Behavior as Catalyst 5 of 84

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

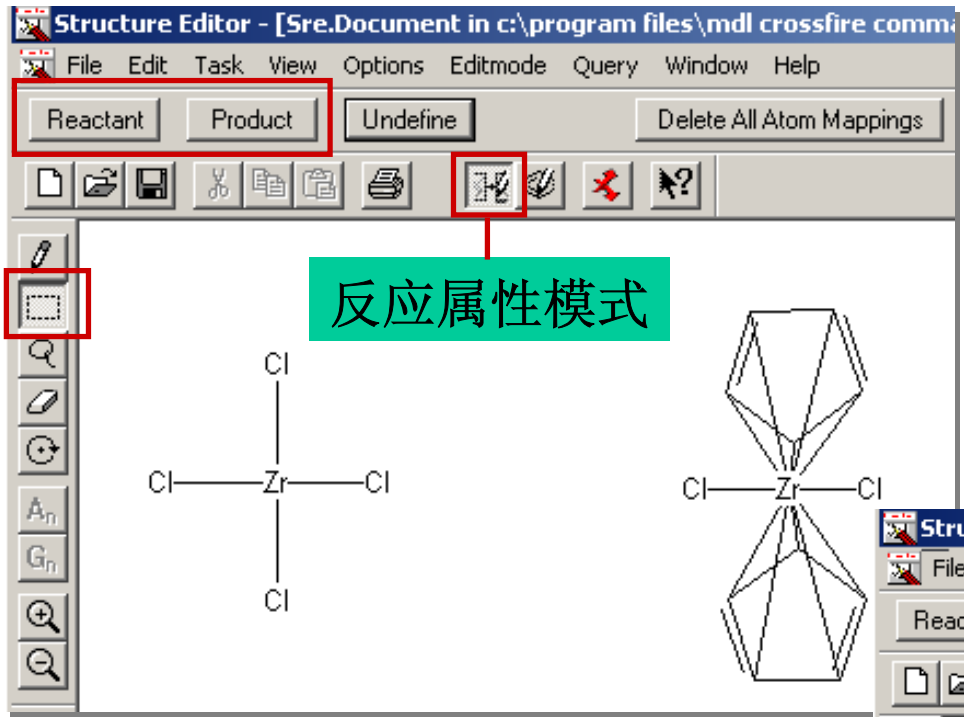
Title	Zirconium bis-cyclopentadienyl compounds. An investigation into
	polymerisation behaviour of $(CpR)_2ZrCl_2$/MAO catalysts
Abstract	The ethylene polymerization behavior of several mono-substitute
	Me, Et, ^{i}Pr, ^{t}Bu, $SiMe_3$, CMe_2Ph) was studied. The catalytic activity
	electronic effects. The highest activity was exhibited by the catalys
	stabilized by small substituents on the cyclopentadienyl rings tha
	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 $(CpR)_2ZrCl_2$/MAO catalysts.**

Gmelin数据库检索示例4

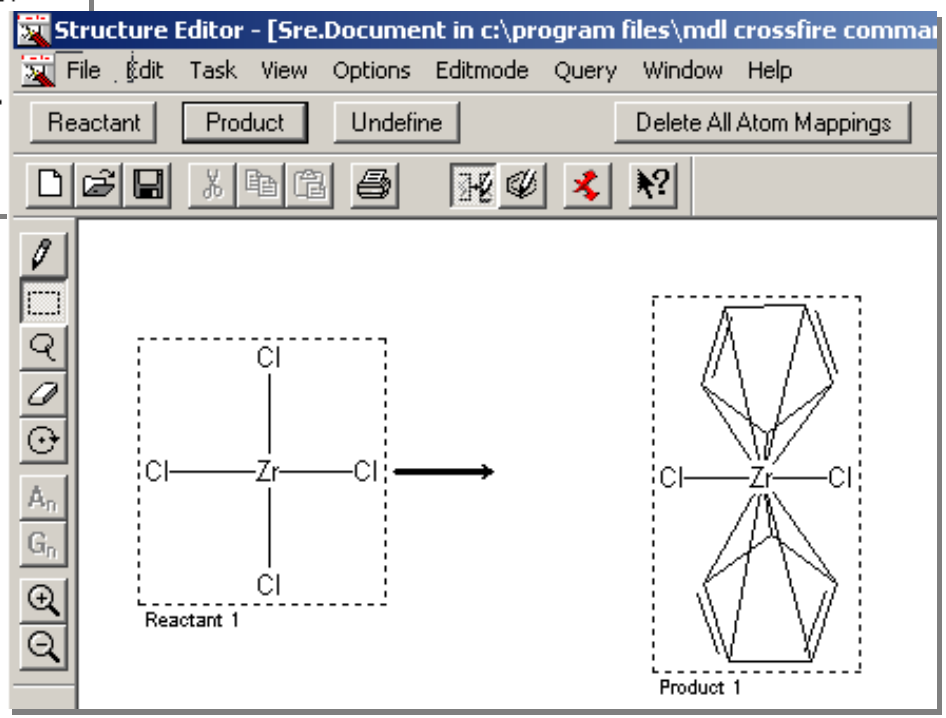
例：　查询催化剂Cp_2ZrCl_2的合成方法。反应物为$ZrCl_4$。

- 建立全反应检索条件



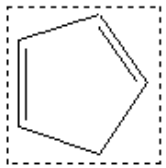
在反应模式下：

- 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。

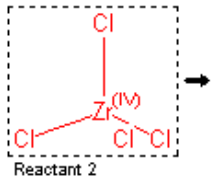


查询结果显示

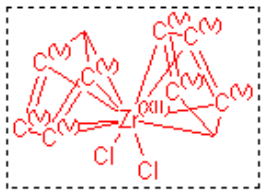
Hit 9:318641



Reactant 1

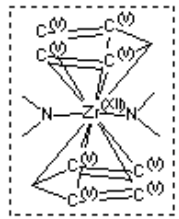


Reactant 2



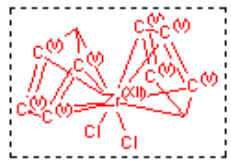
Product 1

Hit 10:472960



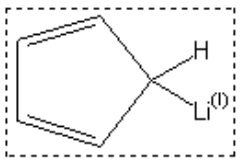
Reactant1

Reactant2

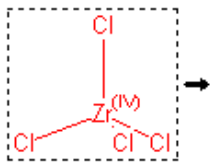


Product1

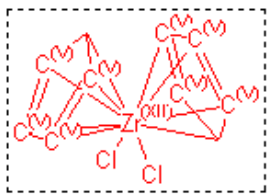
Hit 11:845351



Reactant 1

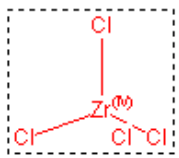


Reactant 2

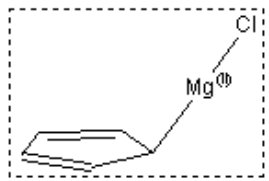


Product 1

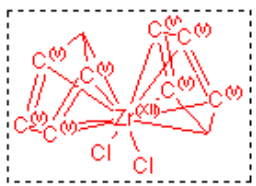
Hit 12:940016



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。