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- To encourage the increase and diffusion of chemical knowledge for the benefit of industry and education



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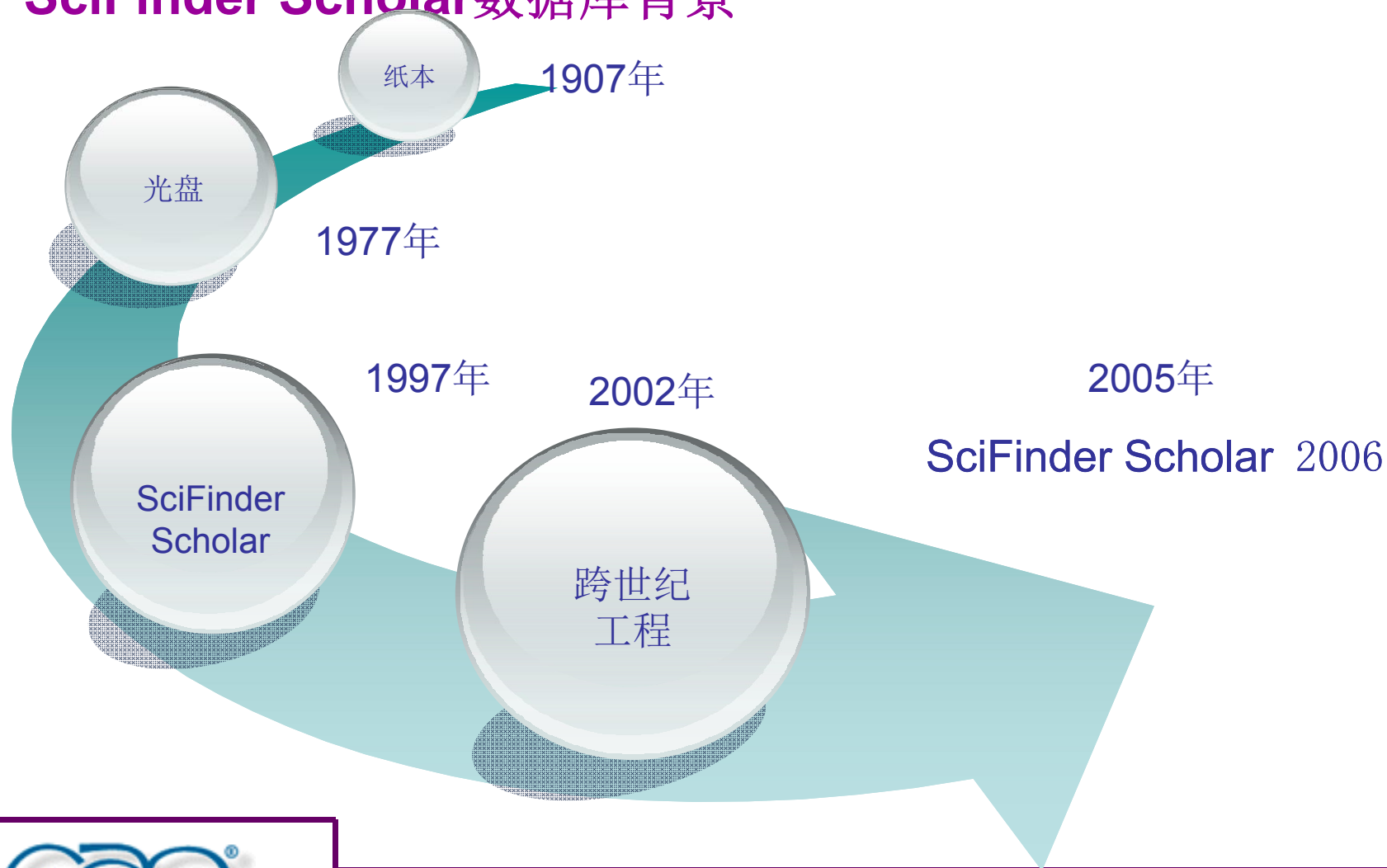
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- 全球最大的学协会组织
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SciFinder Scholar数据库背景



SciFinder Scholar数据库与CACD/Print区别

	CA print	CA on CD	SciFinder
包含文献起始日期	1907	1977	1907（上万条记录回溯到1900年以前）
得到最新信息的延迟	几个月	一个多月	一天
主题检索	√	√	√
普通物质名称检索	×	×	√
分子式检索	√	√	√
结构式检索	×	×	√
亚结构式检索	×	×	√
相似结构式检索	×	×	√
反应式检索	×	×	√
类反应式检索	×	×	√
分析与二次检索	×	×	√
检索效率	低	不高	高效
检索速度	慢	尚可	快捷



SciFinder Scholar: 内容

CAplus: 大于**2600**万条文章记录；包含**CA**纸本的所有内容，同时还收录**1907**年以前的上万条记录

Medline: 大于**1600**万条文章记录；

Registry: **3000**多万个有机无机物质，**5800**多万生物序列，
世界上最大的物质数据库

Chemcats: **1100**万条化合物商品信息
世界上最大的化学品商业数据库

Chemlist: 近**24**万条管制品信息

CASReact: **1100**多万条单步多步反应
世界上最大的反应数据库



SciFinder Scholar: 覆盖范围

- 生物化学、遗传学、免疫学、药理学、毒理学、发酵
- 有机化学
- 材料化学（高分子）— 聚合物、塑料、纺织、橡胶粘合剂等
- 应用化学和化学工程— 加工、工业化学、金属/合金、陶瓷、环境科学等
- 物理化学、无机化学和分析化学



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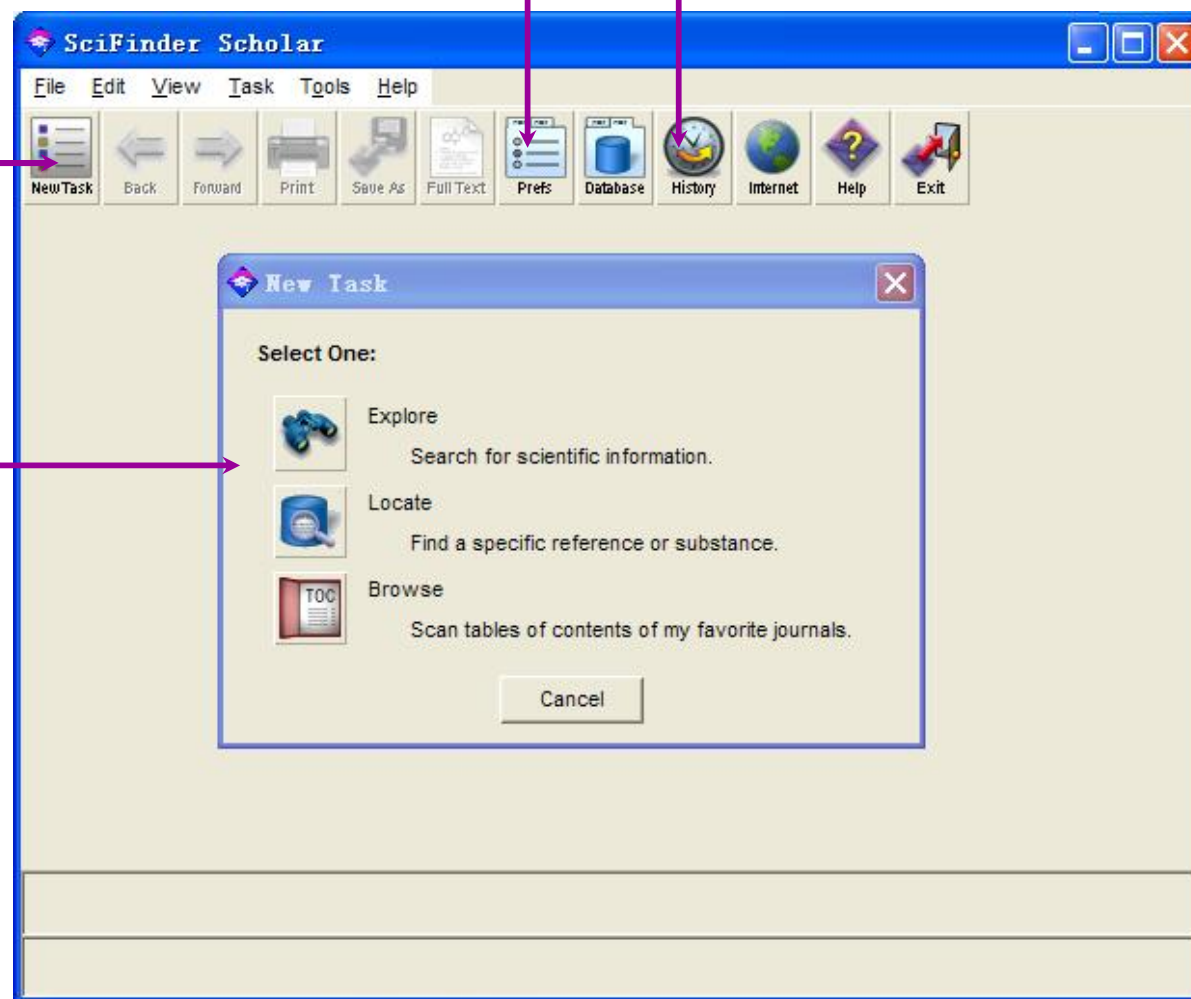
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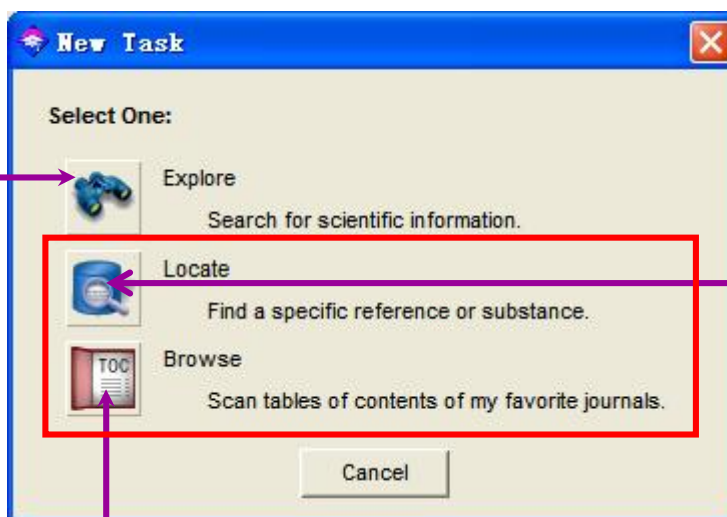
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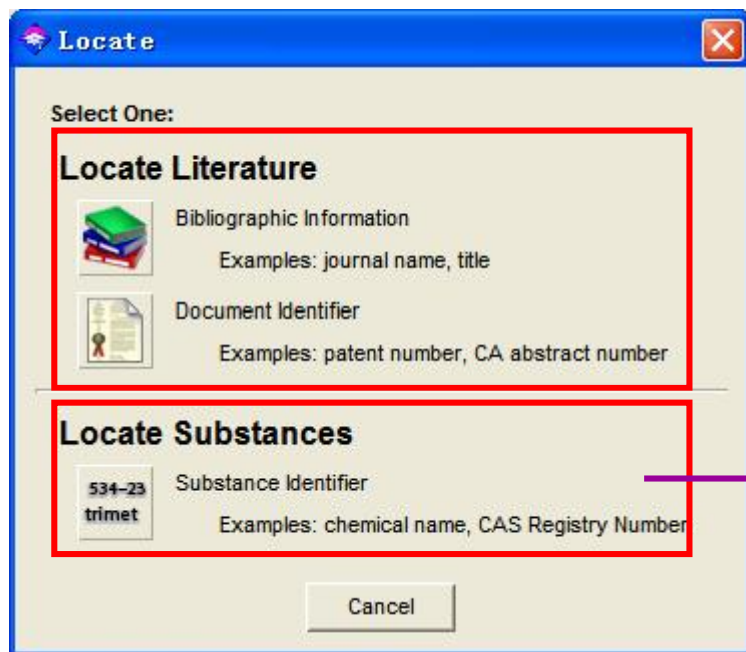
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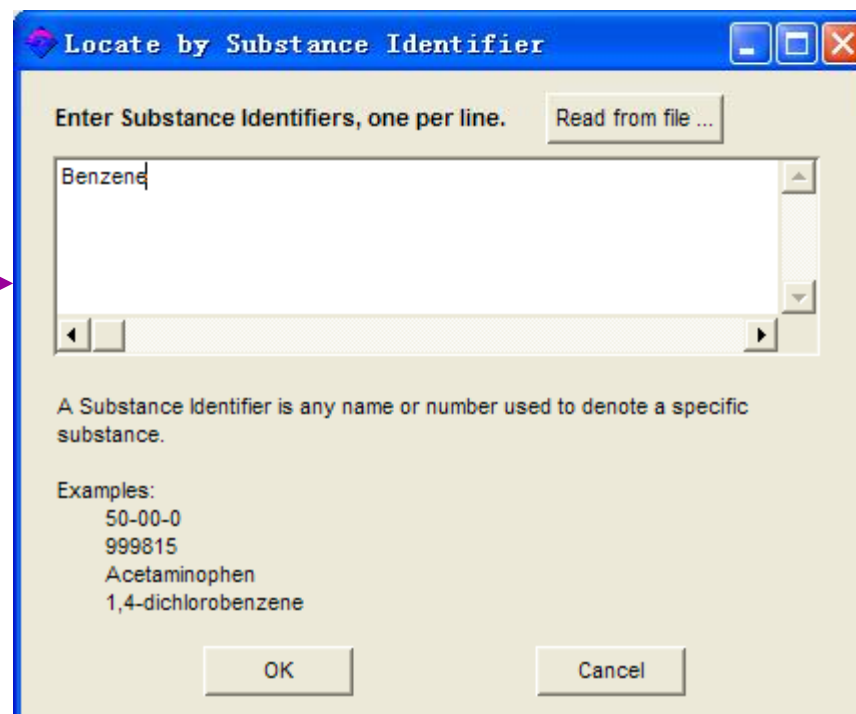
对于确定信息的检索，我们一般用**Locate**检索

浏览，可以让科研工作者，浏览核心期刊的内容

Locate检索



输入苯的名称benzene



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File Edit View Task Tools

NewTask Back Forward Print Save

71-43-2

~120151 References
REGISTRY

Detail of Substance 1

File Edit Help

Registry Number: 71-43-2

Formula: C₆H₆

CA Index Name: Benzene (8CI,9CI)

Other Names: 1,3,5-Cyclohexatriene; Coal naphthalene; 67315; Phenyl; Pyrobenzol;

Class Identifier: Ring Parent

Experimental Properties

Calculated Properties

-- Resources

References: ~120151

STN Files: CAPLUS, ANABSTR, BIOSIS, BIOBASE, CAOLD, CASC, CHEMCATS, CHEMLIST.

Experimental Properties for 71-43-2

File Edit Help

Boiling Point	75-109	See full text	1 of 6
Boiling Point	75-95	See full text	
Boiling Point	75-80	See full text	
Boiling Point	70-190	See full text	
Bond Angle	See full text		
Bond Length	See full text		
Carbon-13 NMR Spectrum	See spectrum		
Carbon-13 NMR Spectrum	See spectrum		
Carbon-13 NMR Spectrum	See spectrum		
Carbon-13 NMR Spectrum	See spectrum		
Carbon-13 NMR Spectrum	See spectrum		
Gibbs Free Energy	See full text		1 of 3
Heat Capacity	See full text		1 of 3
Interfacial Tension	See full text		
Ionization Potential	See full text		1 of 3
IR Absorption Spectrum	See spectrum		
IR Absorption Spectrum	See full text		1 of 25
IR Spectrum	See full text		1 of 5
LC50	See full text		1 of 4
LD50	See full text		1 of 3
Light Scattering	See full text		
logP	See full text		1 of 11
Magnetic Susceptibility	See full text		
Mass Spectrum	See spectrum		
Mass Spectrum	See spectrum		
Mass Spectrum	See spectrum		
Mass Spectrum	See full text		1 of 33
Median Lethal Dose (LD50)	26500 mg/kg		Organism: mouse Route: subcutaneous

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CAS Registry Number: 71-43-2
Formula: C₆H₆
CA Index Name: Benzene (8CI,9CI)

¹³C NMR Spectrum

arbitrary units

130 127.5 125 122.5 120 ppm

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CAS Registry Number: 71-43-2
Formula: C₆H₆
CA Index Name: Benzene (8CI,9CI)

IR Absorption Spectrum

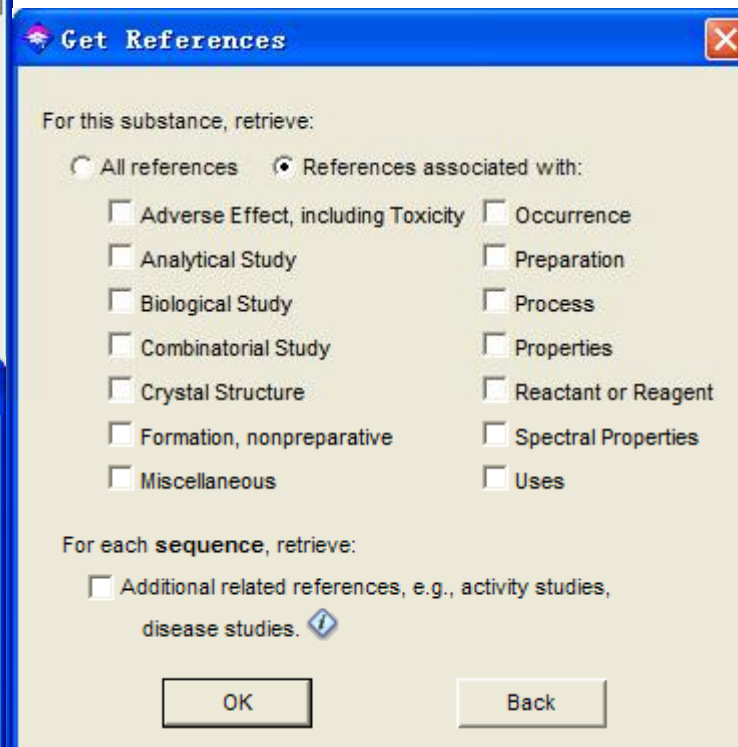
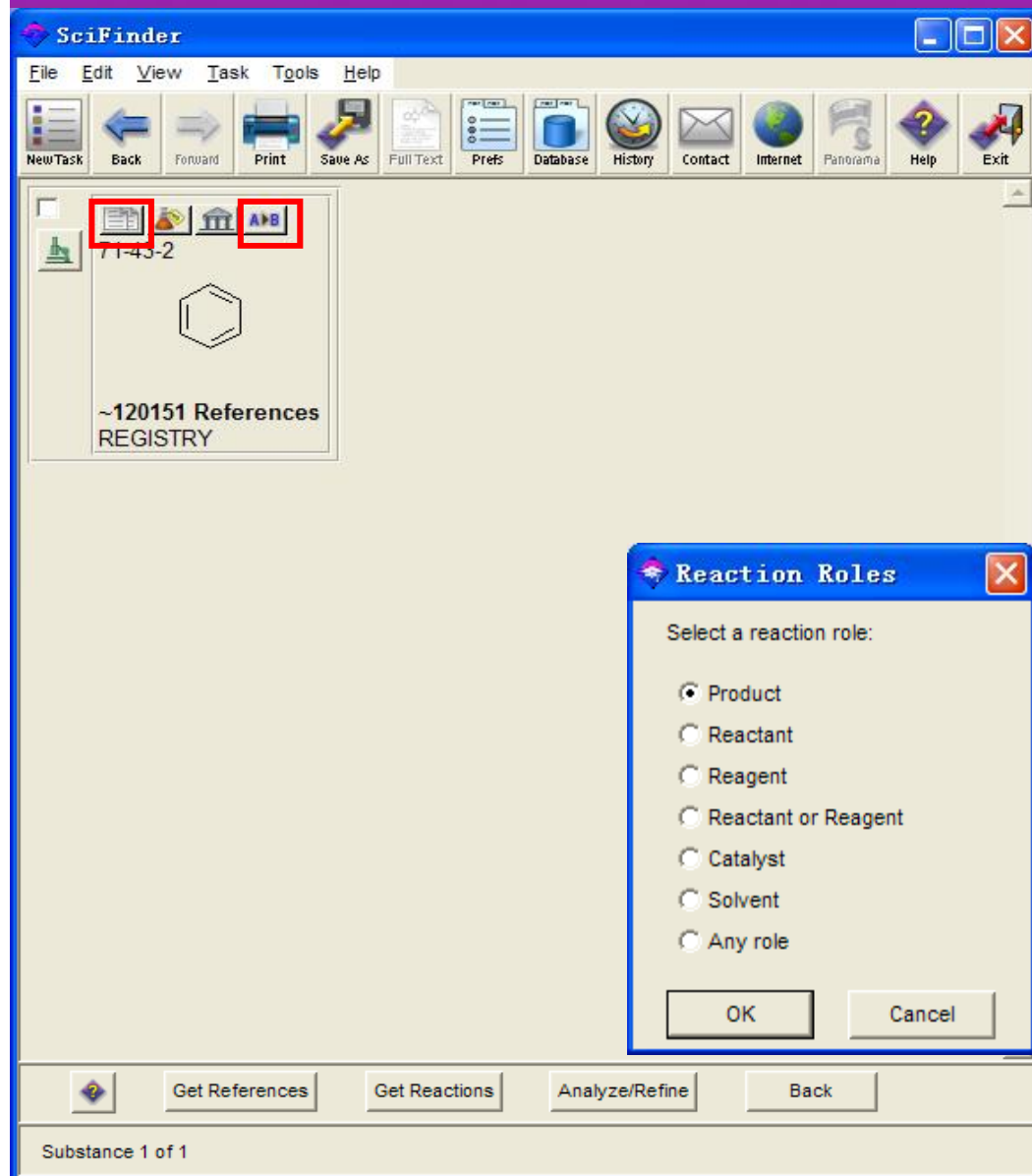
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Substance 1 of 1



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- Journal of Nutritional Biochemistry
- Journal of Nutritional Science and Vitaminology
- Journal of Ocular Pharmacology
- Journal of Ocular Pharmacology and Therapeutics
- Journal of Oleo Science
- Journal of Organic Chemistry**
- Journal of Organometallic Chemistry
- Journal of Peptide Research
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View

Journals 1102-1115 of 1939

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Journal of Organic Chemistry
Volume: 71 Issue: 17 2006

- Enzymatic Resolution, Desymmetrization, and Dynamic Kinetic Asymmetric Transformation of 1,3-Cycloalkanediols. Fra... Ann-Britt L.; Xu, Yongmei; Lejondahl, Karin; Baekvall, Jan-E. Journal CAPLUS
- Total carbo-Mer of Benzene, Its carbo-Trannulene Form, and the Zigzag Nanotube Thereof. Lepetit, Christine; Zou, Chunh... Chauvin, Remi. Journal CAPLUS
- Electronic and Hydrogen Bonding Effects on the Chain-Breaking Activity of Sulfur-Containing Phenolic Antioxidants. Amo... Riccardo, Fumo, Maria Grazia; Menichetti, Stefano; Mugnani, Veronica; Pedulli, Gian Franco. Journal CAPLUS
- Investigations of Metal-Coordinated Peptides as Supramolecular Synthons. Gerhardt, Warren W.; Weck, Marcus. Journa... CAPLUS
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- Generation and Reactivity of the Phenyl Cation in Cryogenic Argon Matrices: Monitoring the Reactions with Nitrogen and... Monoxide Directly by IR Spectroscopy. Winkler, Michael; Sander, Wolfram. Journal CAPLUS
- Functionalization of N-[(Silyl)methyl]- β -lactam Carbanions with Carbon Electrophiles. Palomo, Claudio; Aizpurua, Jesus M... Ana; Cuervo, Lourdes; Fratila, Raluca M.; Miranda, Jose I.; Linden, Anthony. Journal CAPLUS
- Electrochemically Induced Cascade Reaction for the Assembly of Libraries of Biologically Relevant 1,4-Benzoxazine Derivatives. Xu, Daiwang; Chiaroni, Angele; Fleury, Maurice-Bernard; Largeron, Martine. Journal CAPLUS
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Available Journal Issues

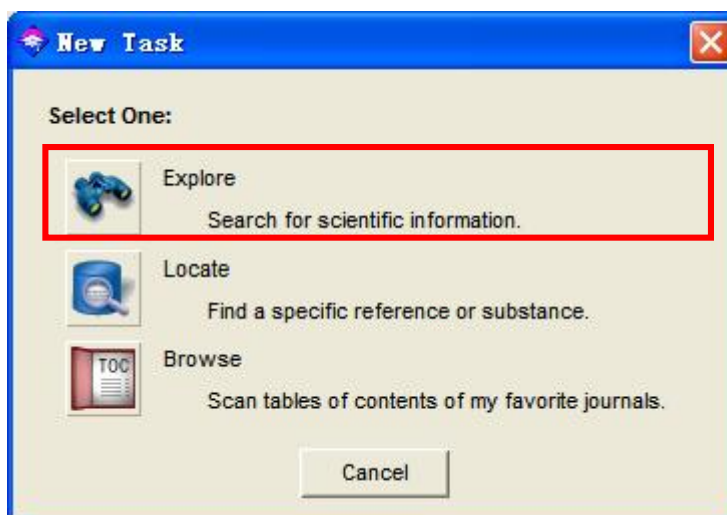
Journal of Organic Chemistry

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- Volume: 71 Issue: 11 2006
- Volume: 71 Issue: 10 2006
- Volume: 71 Issue: 9 2006
- Volume: 71 Issue: 8 2006
- Volume: 71 Issue: 7 2006
- Volume: 71 Issue: 6 2006
- Volume: 71 Issue: 5 2006
- Volume: 71 Issue: 4 2006
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- Volume: 71 Issue: 2 2006
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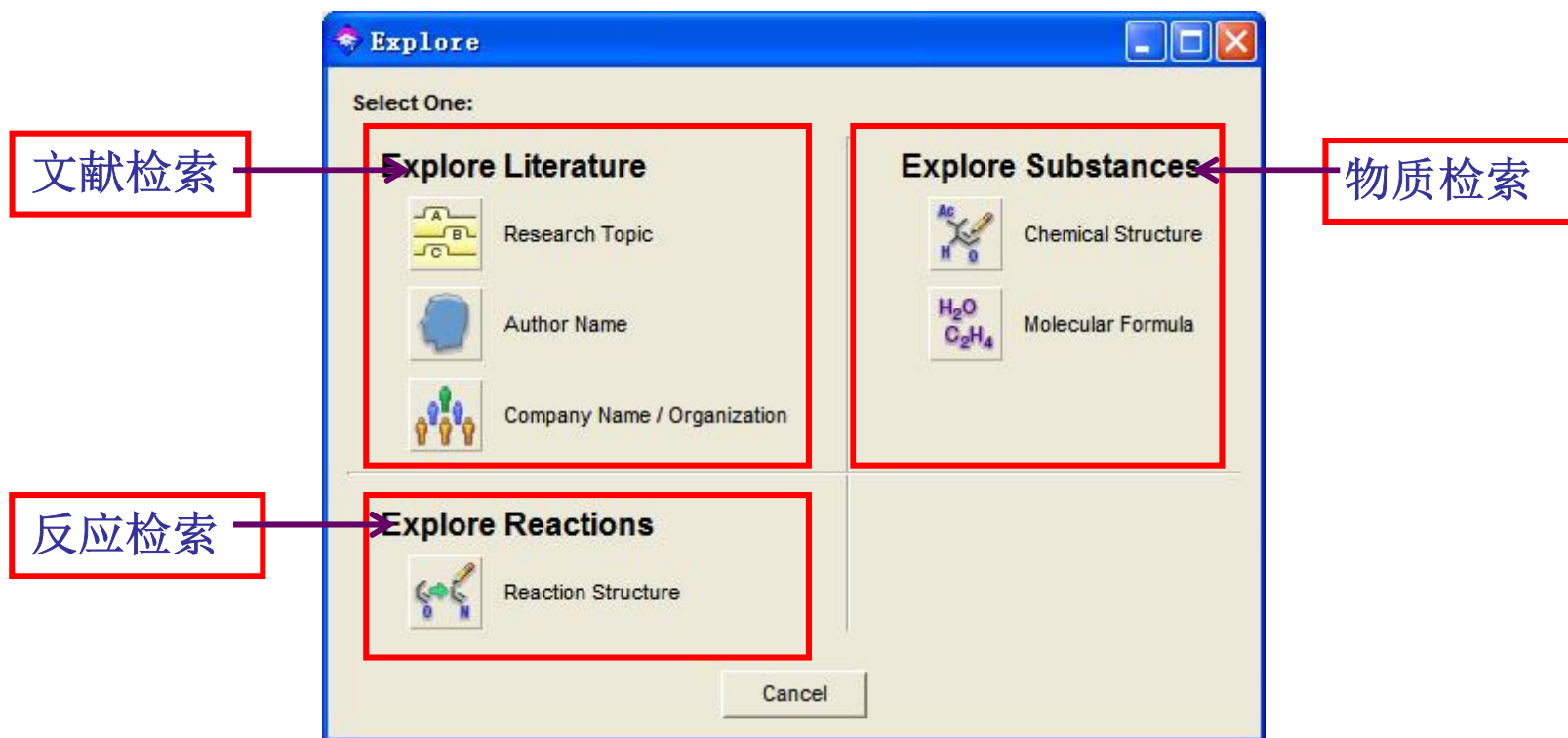
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Issues 1 to 19 of 307

主检索界面



Explore检索



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提出问题

获得关于有机发光物质的参考文献

存在问题:

有机发光物质存在什么方面的应用研究

如果我对金属有机化合物感兴趣, 那么什么金属元素最为广泛

我能否获得结构上面的信息



我们用Luminescent substances with organic来做初次的检索

Explore by Research Topic

Describe your topic using a phrase.

I am interested in:

Luminescent substances with organic

Examples:
The effect of
Photocyanatic
Hydrocarbon

Filters ▶

Topic Candidates

File Edit Task Tools Help

Select Candidates of interest:

- ☐ 1 reference was found containing "Luminescent substances with organic" as entered.
- ☒ 5504 references were found containing the two concepts "Luminescent substances" and "organic" closely associated with one another.
- ☐ 9728 references were found where the two concepts "Luminescent substances" and "organic" were present anywhere in the reference.
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- ☐ Astakhov, M. V.; Belanov, G. S.; Vasil'chenko, V. G.; Rodin, A. O.; Samoilenko, V. D.; Solov'ev, A. S. **Properties of composite scintillators based on severely deformed powder fillers.** Instruments and Experimental Techniques (2006), 49(5), 645-650. CODEN: INETAK ISSN:0020-4412. AN 2006:1027053 CAPLUS
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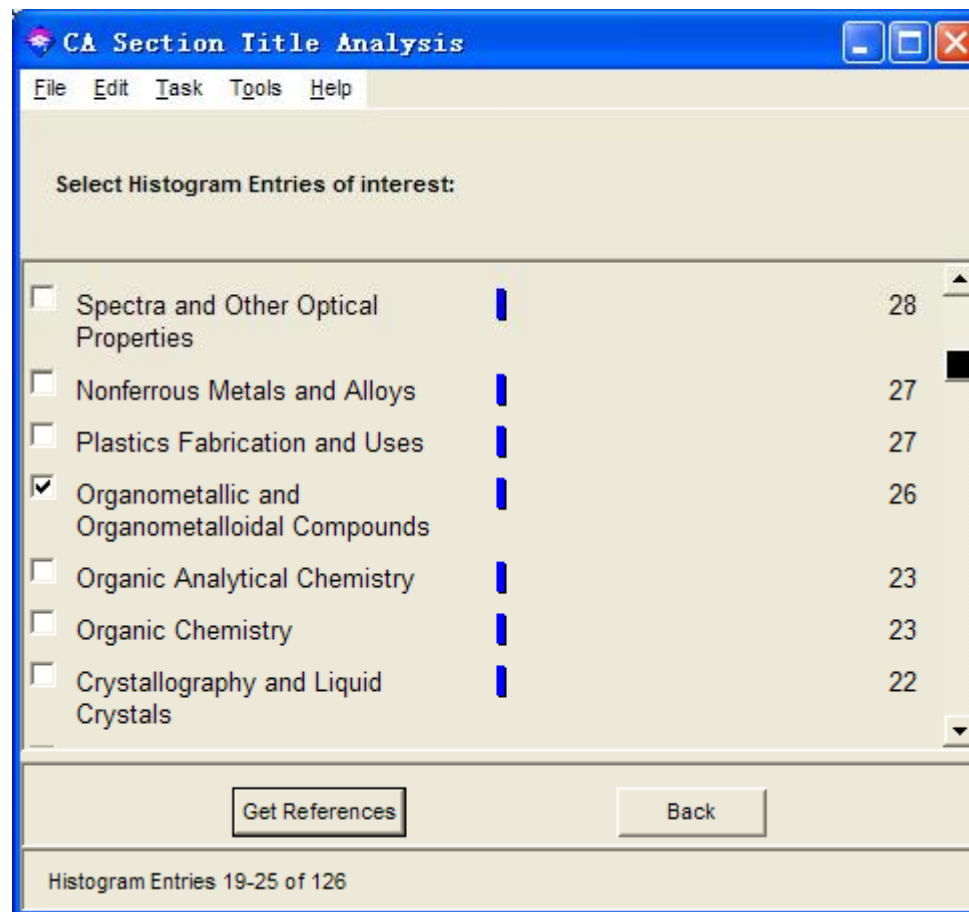
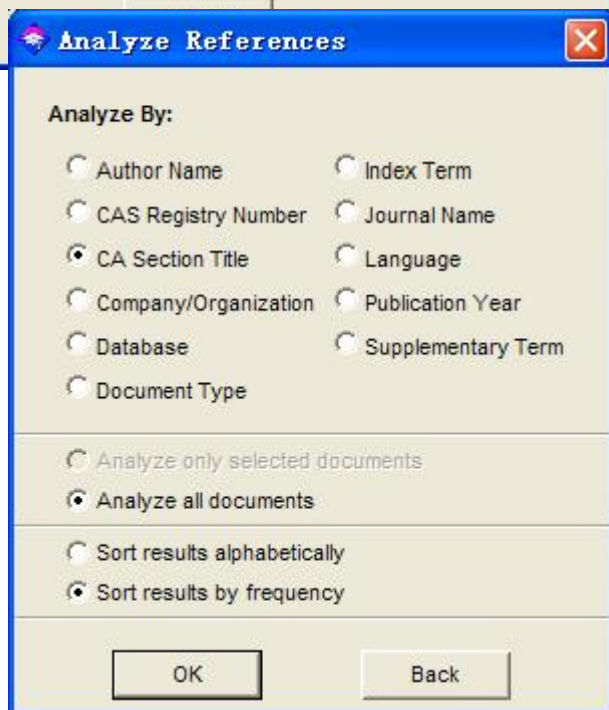
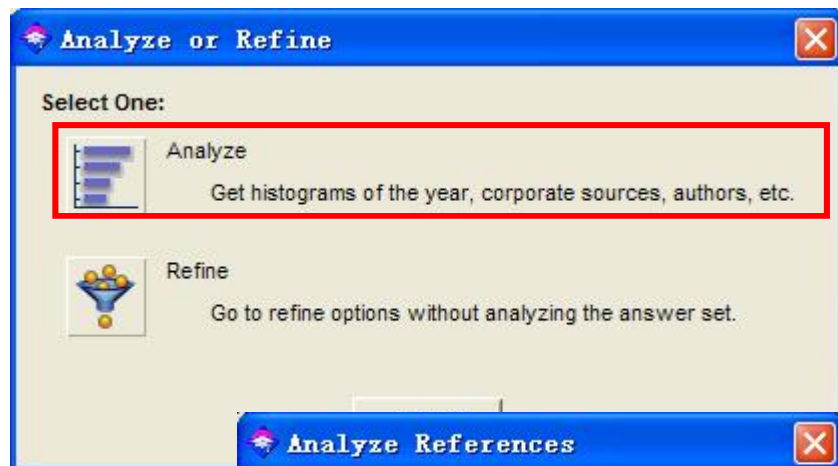
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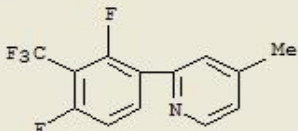
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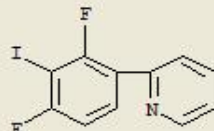
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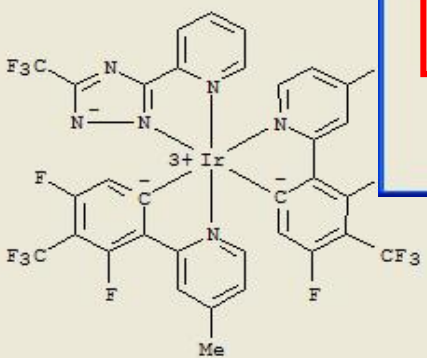
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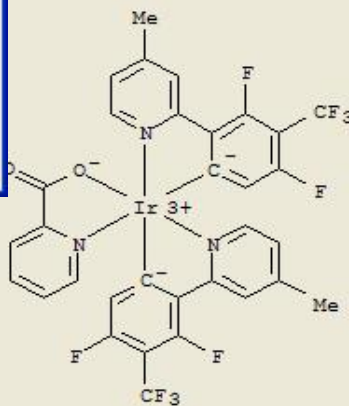
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Select One:

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Display histograms by Precision, Ring Skeletons, etc.

Refine
Narrow your answer set by Structure, Availability, or Property Data.

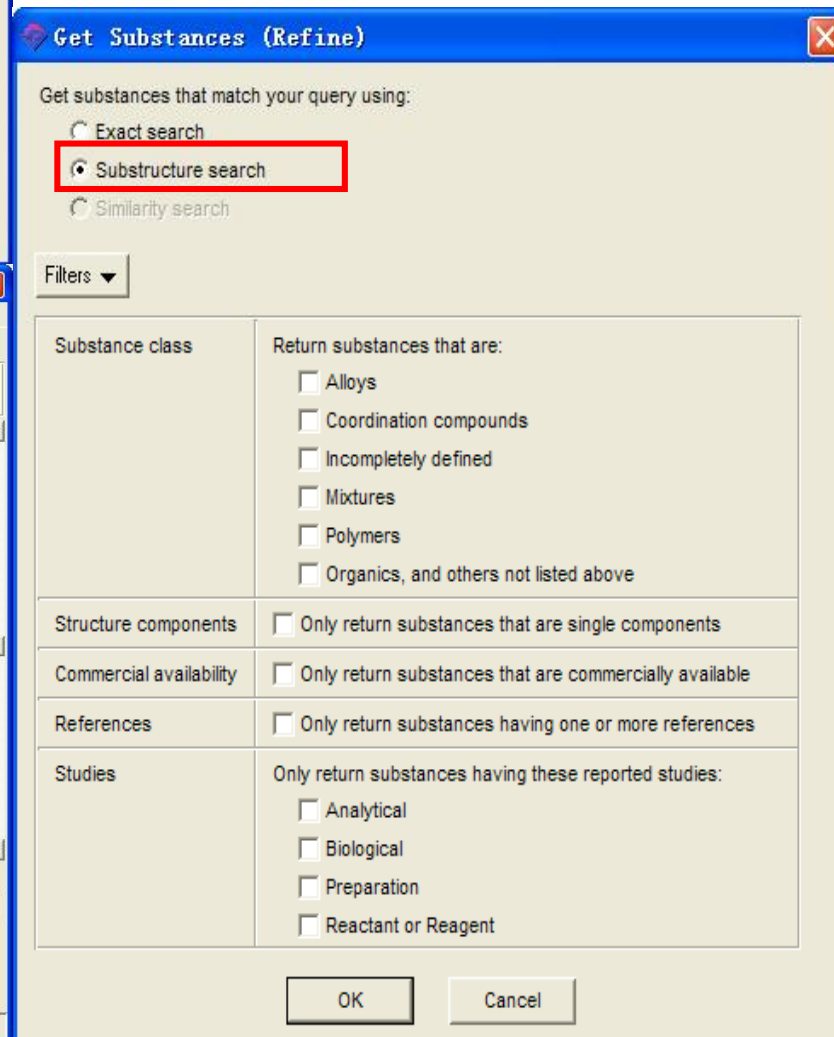
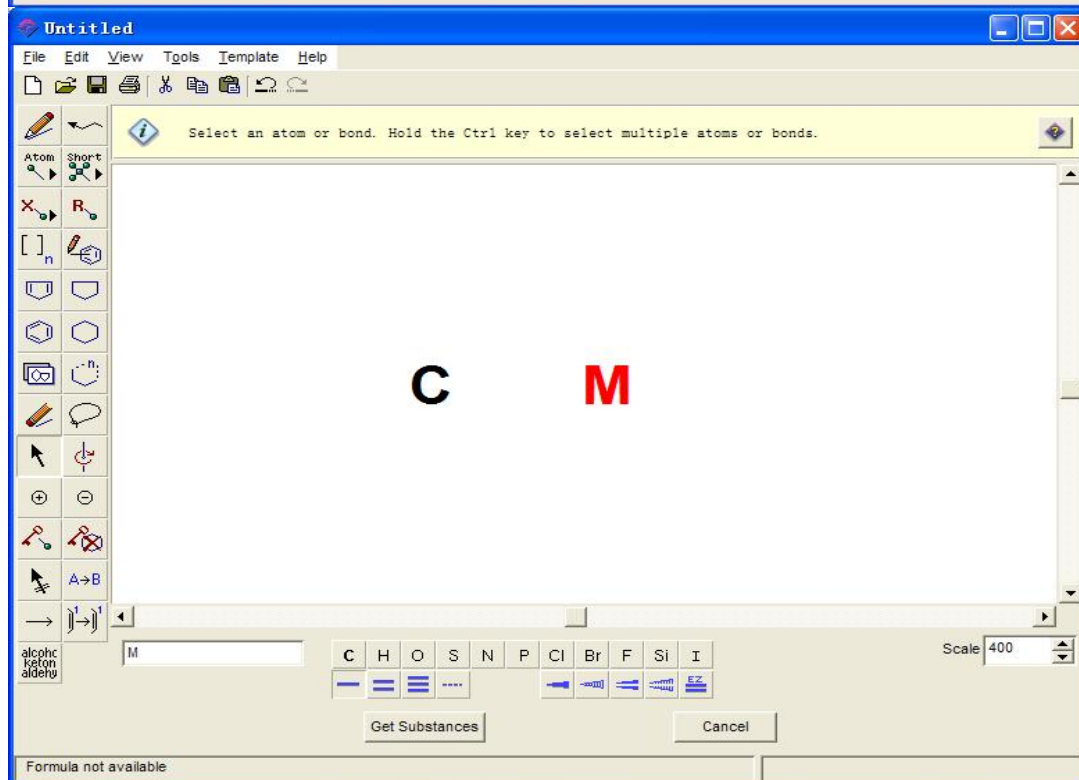
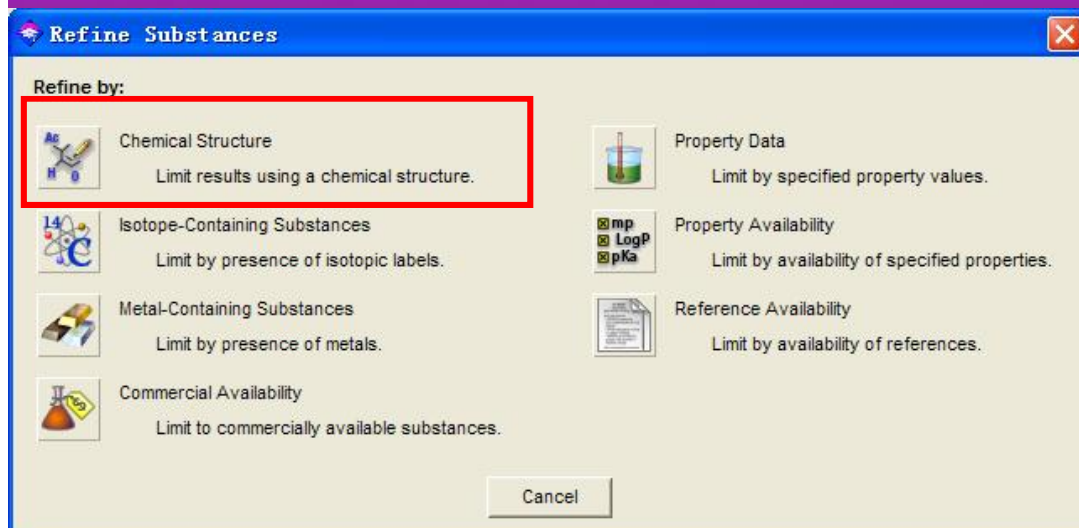
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Substances 1-6 of 598

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909905-21-1

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7-5

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Substances 1-6 of 207

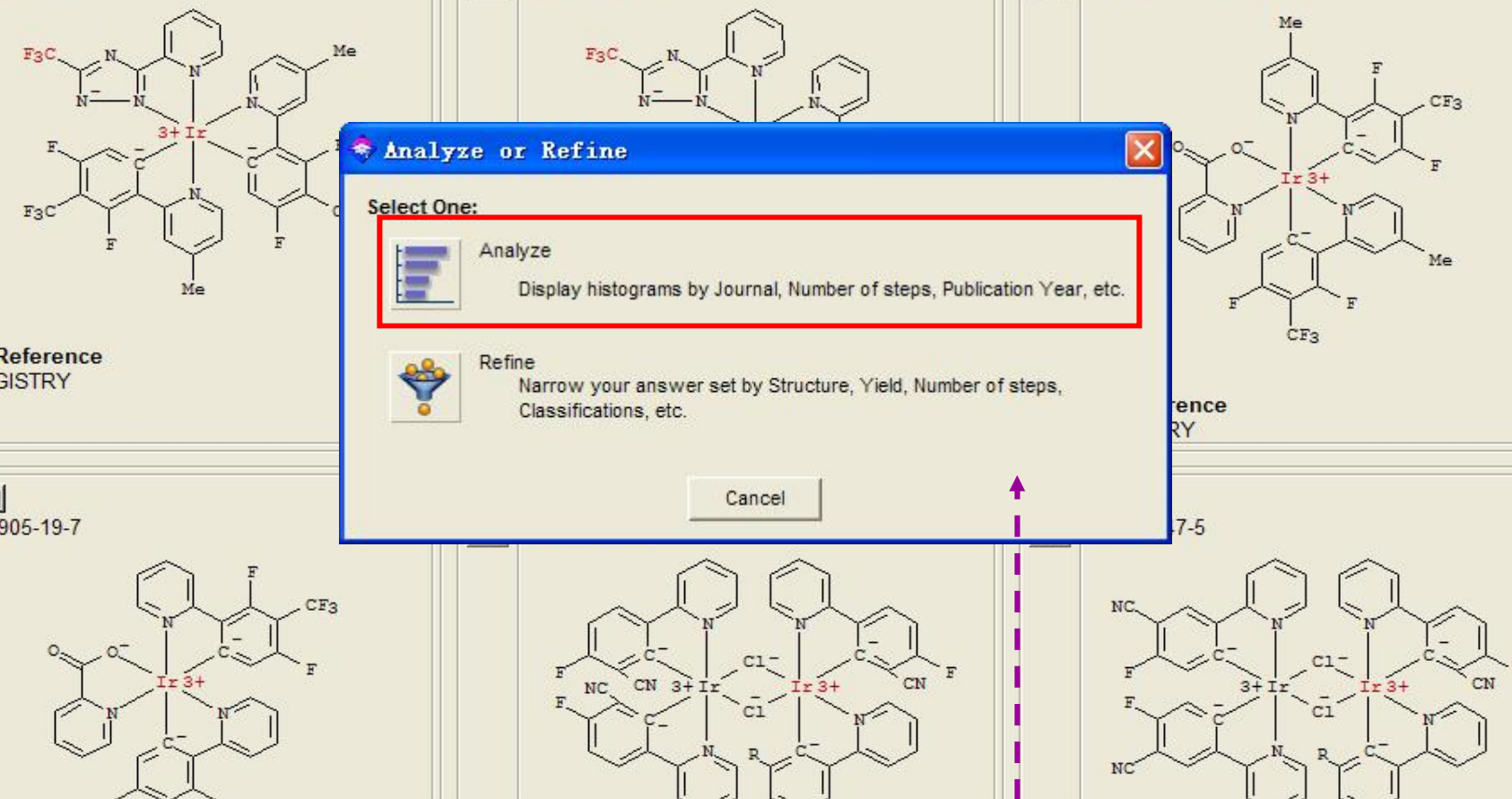
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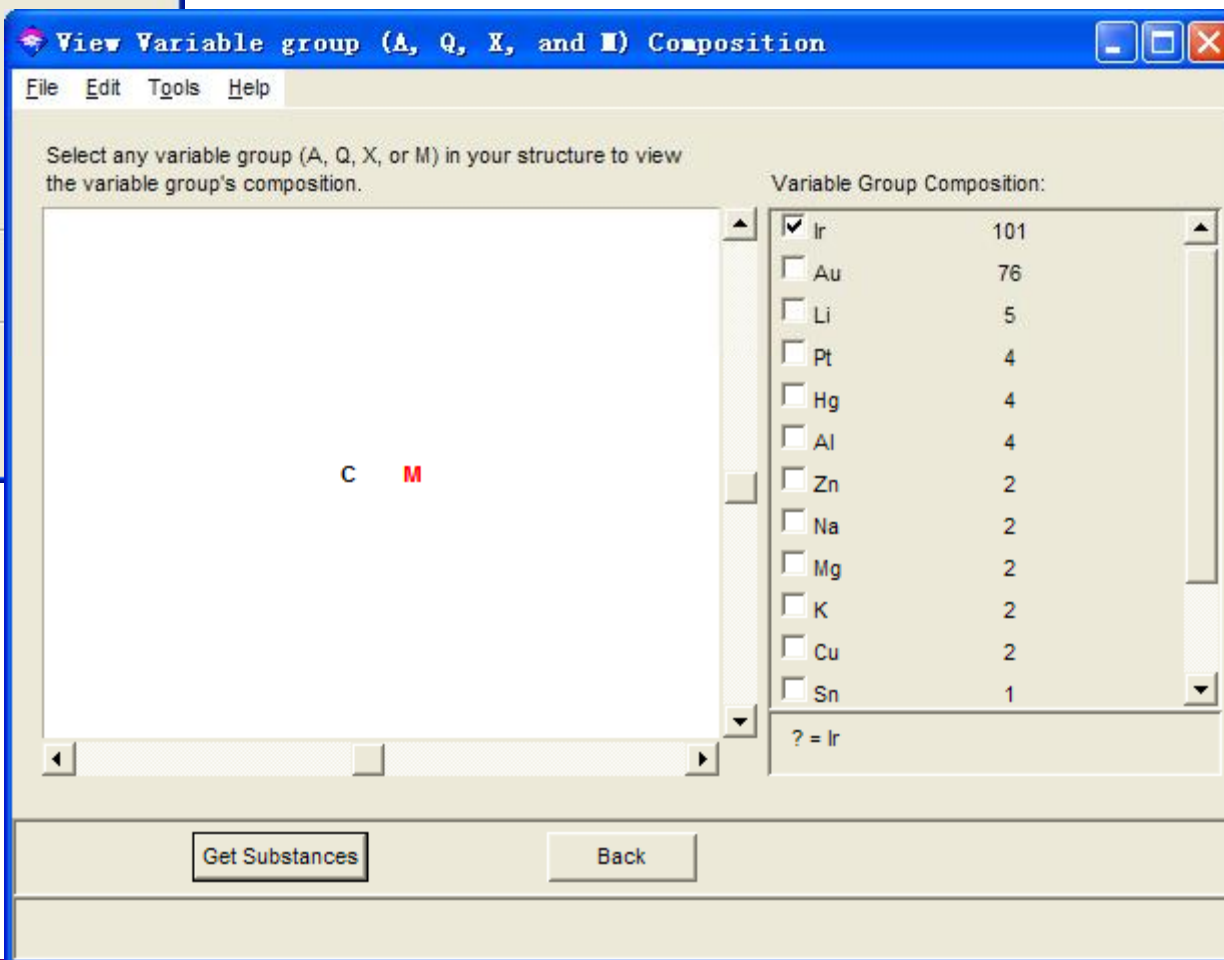
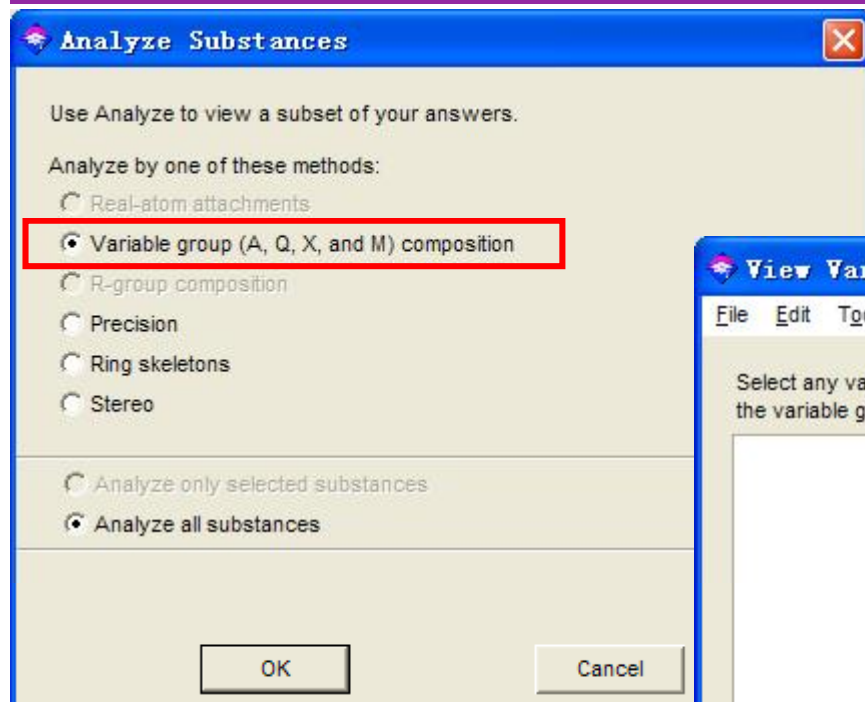
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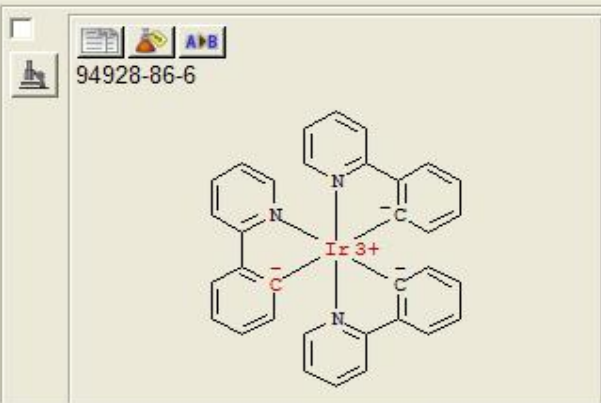
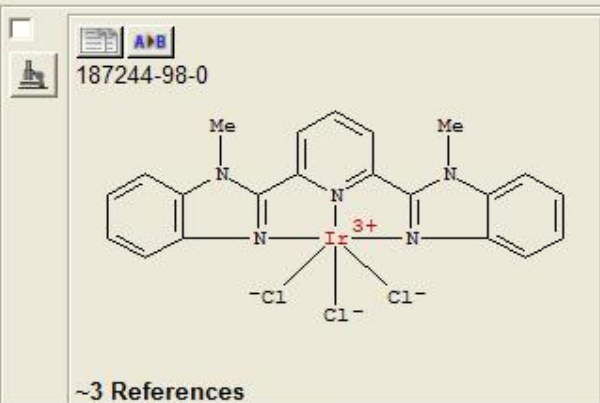
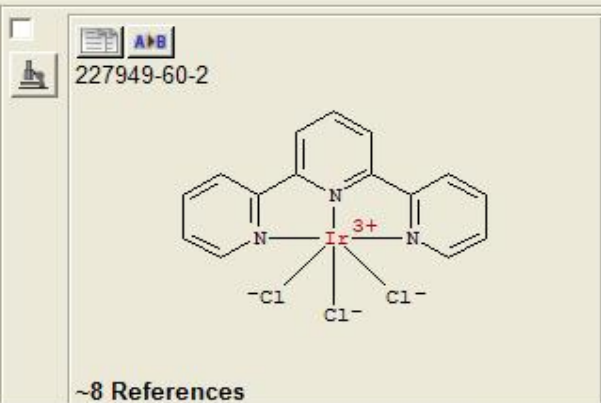
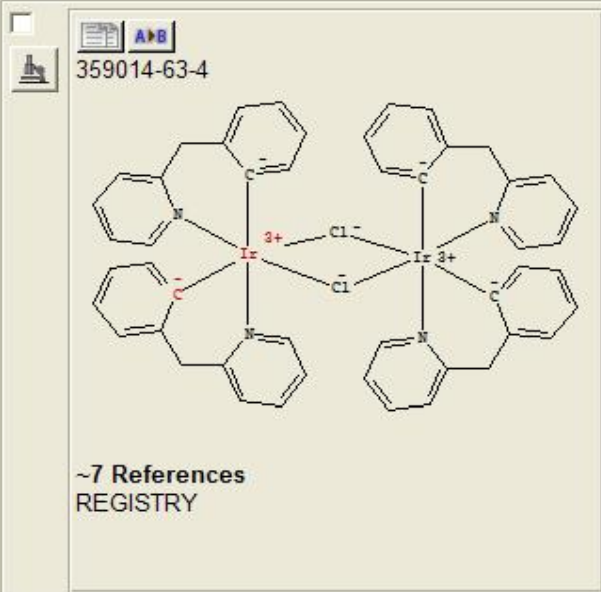
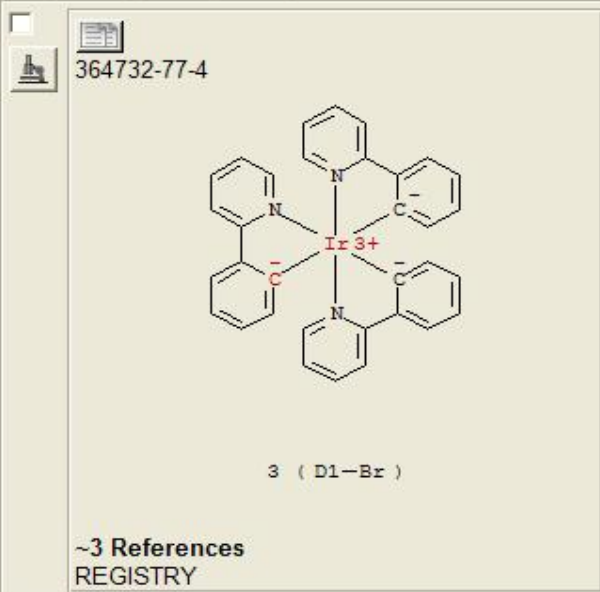
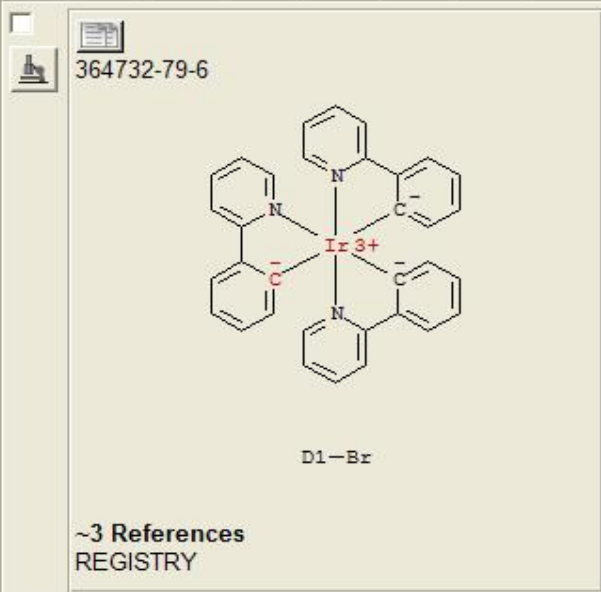


The background of the interface displays six chemical structures of Ir(III) complexes. Each structure is a tris(bipyridine) type complex where the central Ir(III) ion is coordinated by three bipyridine ligands. The ligands are substituted with various groups including trifluoromethyl (CF3), methyl (Me), and cyano (CN) groups. The structures are arranged in a 2x3 grid, with the top row showing three different complexes and the bottom row showing three more. The central complex in the bottom row is highlighted with a red box around its 'Analyze/Refine' button.

SciFinder[®]



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Get References

Get Reactions

Analyze/Refine

Back

检索思路回顾

- 尝试进行有机发光物质的主题检索
- 对检索结果进行分析，获得感兴趣领域的参考文献
- 从文献获得物质
- 对物质进行结构分析
- 获得含有特定金属的有机发光物质

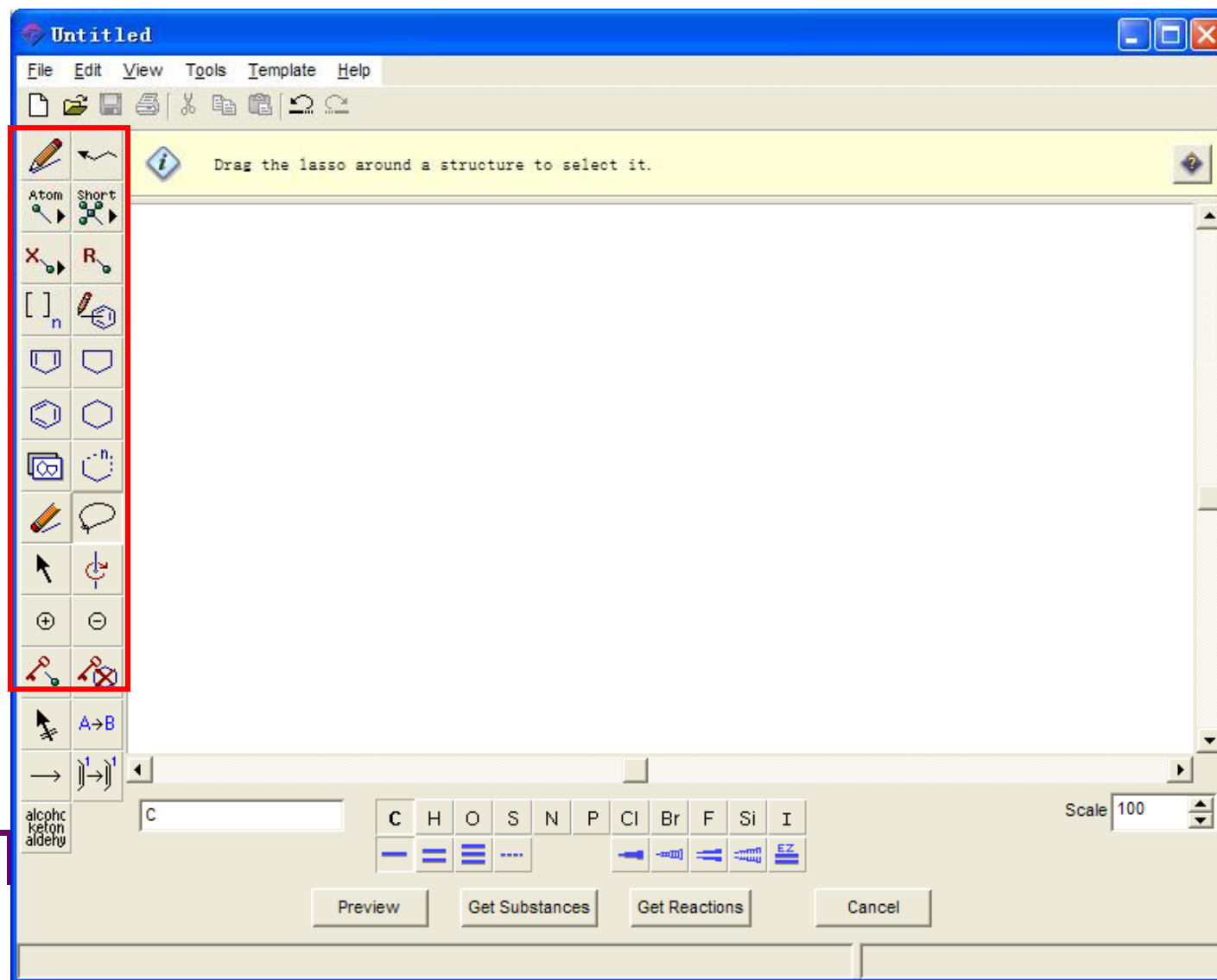
SciFinder Scholar文献检索小结

- 向**SciFinder Scholar**提一个最为广泛的问题
- 可以通过**SciFinder Scholar**的**Analyze/Refine**功能来不断的修正我们的检索思路
- 可以通过**SciFinder Scholar**的**Analyze/Refine**功能来缩小检索的范围
- 可以通过**SciFinder Scholar**的**Analyze/Refine**功能来获取新的知识点和灵感
- 尝试将不同的**Analyze/Refine**功能组合起来用，会有更多的收益
- 通过**Get Related**来获得更多的信息



SciFinder Scholar查询举例----物质信息的查询

结构工具



SciFinder Scholar 查询举例----物质信息的查询

The image shows the SciFinder Scholar chemical structure editor interface. The window is titled "Untitled" and has a menu bar with "File", "Edit", "View", "Tools", "Template", and "Help". Below the menu bar is a toolbar with various icons. The main workspace is a large white area with a yellow status bar at the top that says "Draw the bond around a structure to select it." The bottom of the window features a chemical element palette with buttons for "C", "H", "O", "S", "N", "P", "Cl", "Br", "F", "Si", "I", and a "Scale" dropdown set to "100". At the very bottom are buttons for "Preview", "Get Substances", "Get Reactions", and "Cancel".

Red boxes and lines point to specific tools in the interface, labeled with Chinese text:

- 铅笔 (Pencil)
- 元素周期表 (Periodic Table)
- 可变基团 (Variable Group)
- 重复基团工具 (Repeat Group Tool)
- 结构模版 (Structure Template)
- 橡皮 (Eraser)
- 选择工具 (Selection Tool)
- 正电子 (Positron)
- 原子锁定工具 (Atom Locking Tool)
- 碳链工具 (Carbon Chain Tool)
- 常用基团 (Common Group)
- R基团定义工具 (R-Group Definition Tool)
- 可变位置连接工具 (Variable Position Connection Tool)
- 多元环工具 (Polycyclic Ring Tool)
- 索套选择工具 (Lasso Selection Tool)
- 旋转工具 (Rotation Tool)
- 负电子 (Negatron)
- 环锁定工具 (Ring Locking Tool)

The CAS logo is visible in the bottom left corner.

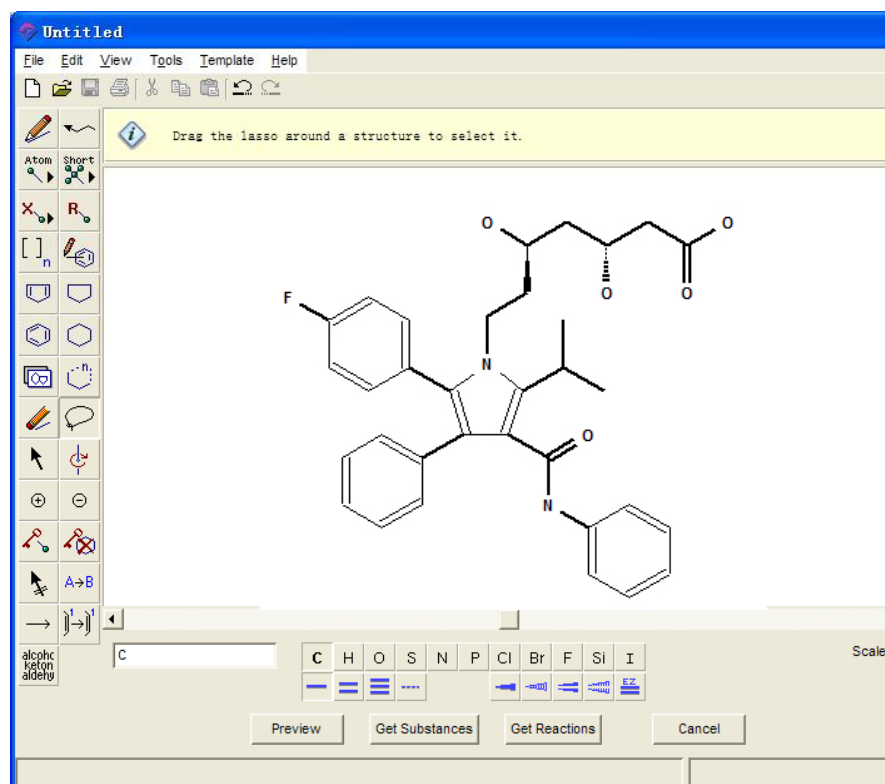
SciFinder Scholar查询举例----物质信息的查询

问题：我们到底需要什么样的物质？

1. 是否可以得到物质的盐，或者其他的混合物，聚合物
2. 是否可以通过修饰结构，来获得更多的应用
3. 是否存在类似的，但是我不知道的结构
4. 是否物质的相似结构，可以有更多的应用



精确结构检索



Get Substances

Get substances that match your query using:

☒ Exact search

☐ Substructure search

☐ Similarity search

Filters ▼

Substance class	Return substances that are:
	☐ Alloys ☐ Coordination compounds ☐ Incompletely defined ☐ Mixtures ☐ Polymers ☐ Organics, and others not listed above
Structure components	☐ Only return substances that are single components
Commercial availability	☐ Only return substances that are commercially available
References	☐ Only return substances having one or more references
Studies	Only return substances having these reported studies:
	☐ Analytical ☐ Biological ☐ Preparation ☐ Reactant or Reagent

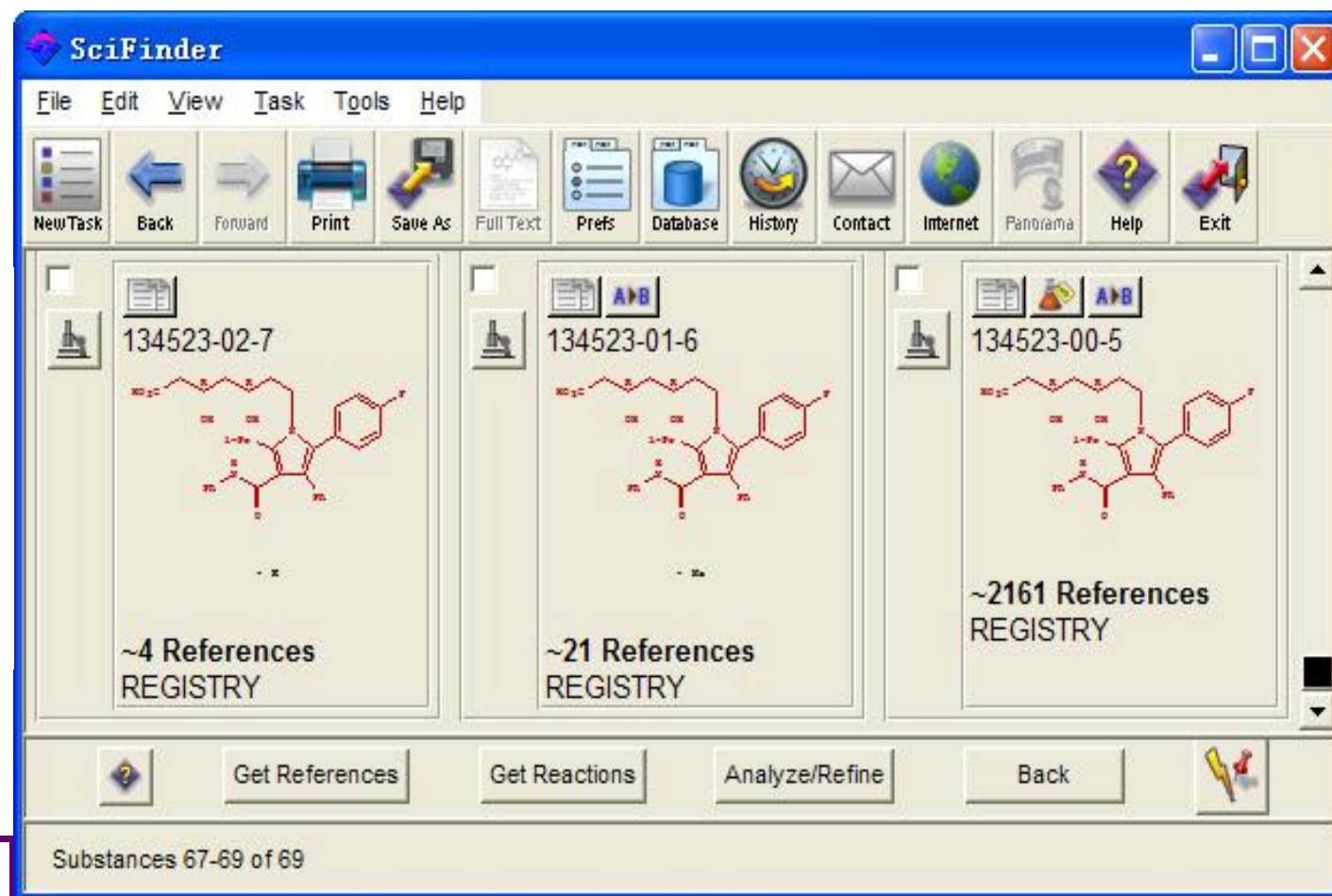
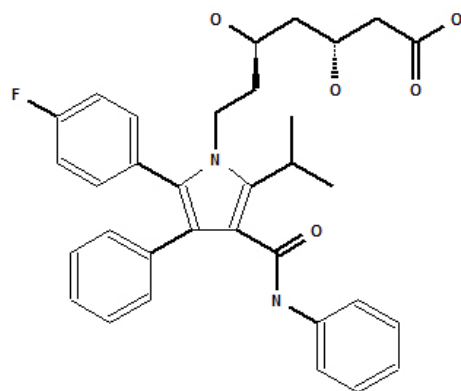
?

OK

Cancel

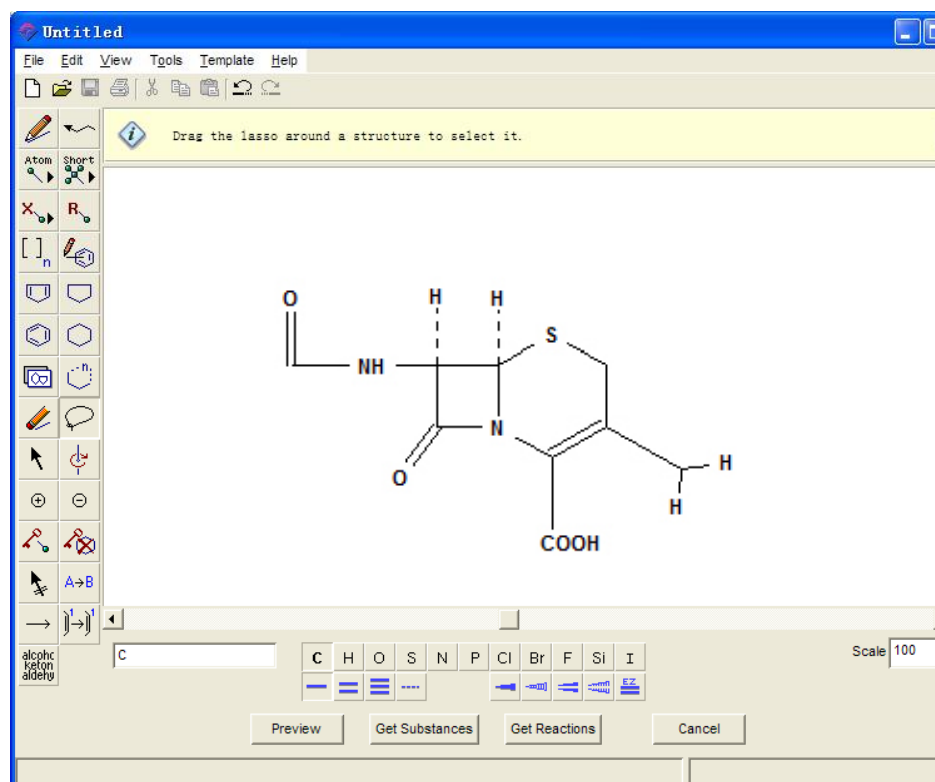
SciFinder[®]

得到物质的盐，或者其他的混合物



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亚结构检索



Get Substances

Get substances that match your query using:

☐ Exact search
☒ Substructure search
☐ Similarity search

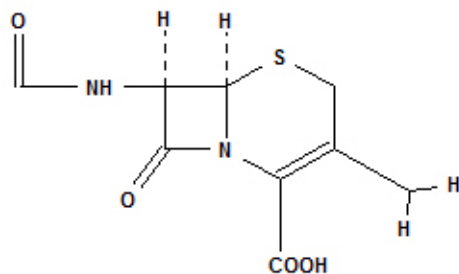
Filters ▼

Substance class	Return substances that are:
	☐ Alloys ☐ Coordination compounds ☐ Incompletely defined ☐ Mixtures ☐ Polymers ☐ Organics, and others not listed above
Structure components	☐ Only return substances that are single components
Commercial availability	☐ Only return substances that are commercially available
References	☐ Only return substances having one or more references
Studies	Only return substances having these reported studies:
	☐ Analytical ☐ Biological ☐ Preparation ☐ Reactant or Reagent

OK Cancel

SciFinder[®]

得到物质的修饰信息



33246种修饰信息

The screenshot displays the SciFinder software interface. The top menu bar includes File, Edit, View, Task, Tools, and Help. Below the menu is a toolbar with icons for NewTask, Back, Forward, Print, Save As, Full Text, Prefs, Database, History, Contact, Internet, Panorama, Help, and Exit. The main window is divided into three panels, each showing a chemical structure and associated reference information:

- Panel 1 (Left):** ID 875251-64-2. Shows a chemical structure of a thiazolidine derivative. Below the structure, it indicates "~2 References" and "REGISTRY".
- Panel 2 (Middle):** ID 875221-87-7. Shows a chemical structure of a thiazolidine derivative. Below the structure, it indicates "~4 References".
- Panel 3 (Right):** ID 875220-63-6. Shows a chemical structure of a thiazolidine derivative. Below the structure, it indicates "~3 References" and "REGISTRY".

At the bottom of the interface, there are buttons for "Get References", "Get Reactions", "Analyze/Refine", and "Back". A status bar at the very bottom indicates "Substances 121-123 of 33246".



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强大的后处理功能

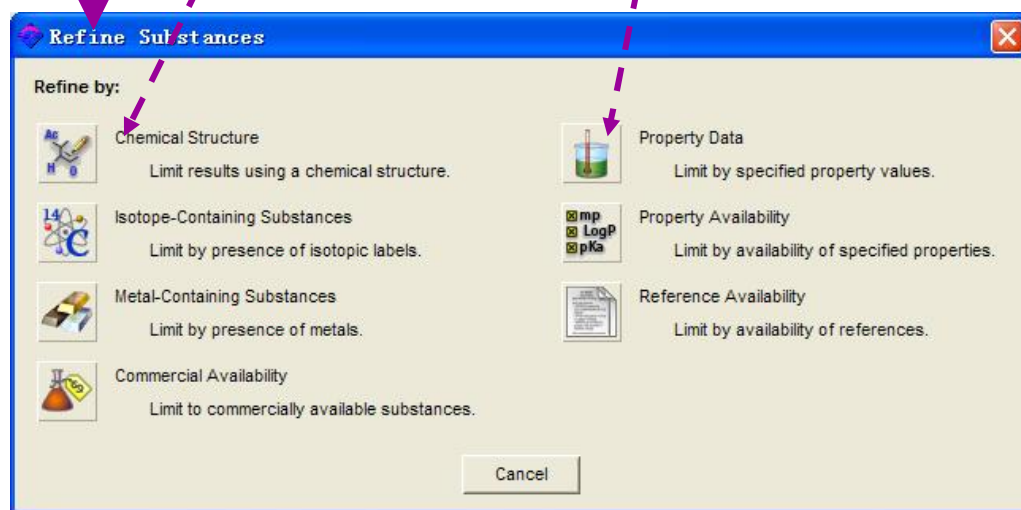
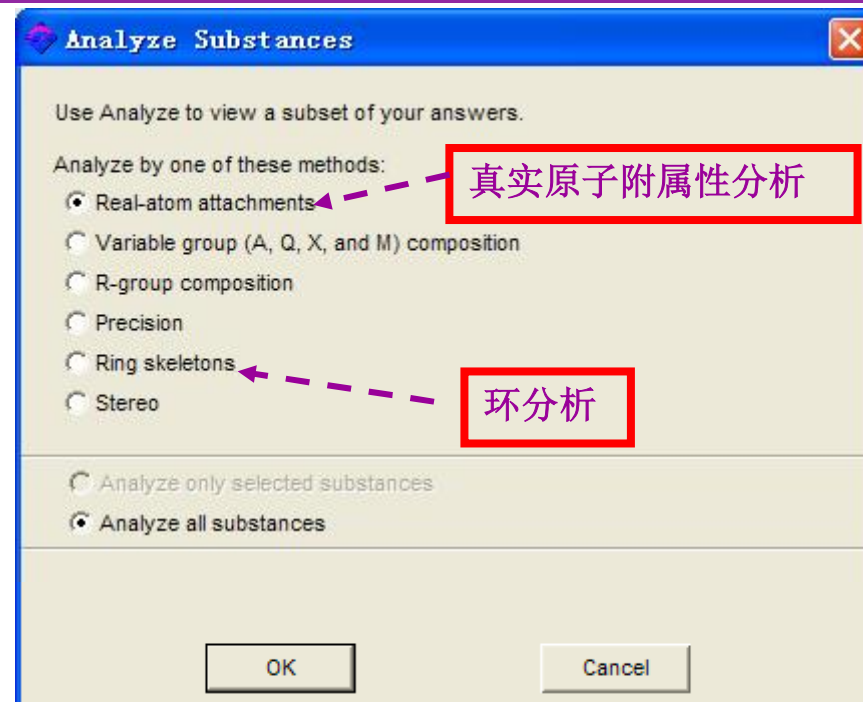
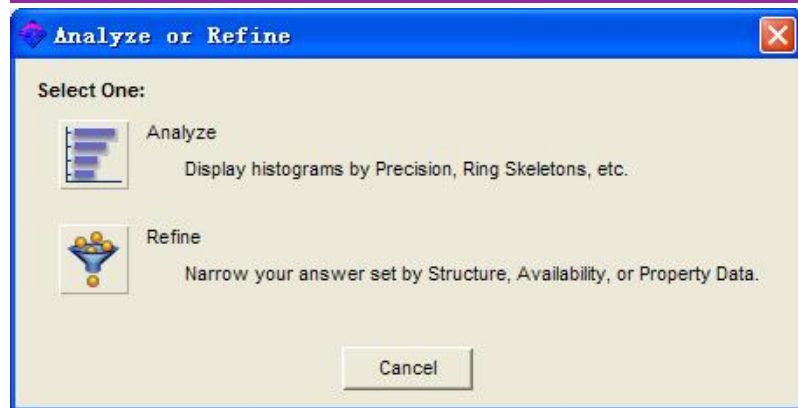
我们做科研

往往是希望得到我们不知道的信息

那么对于这**33246**种物质，我们如何去分析来获得我们需要的信息呢？

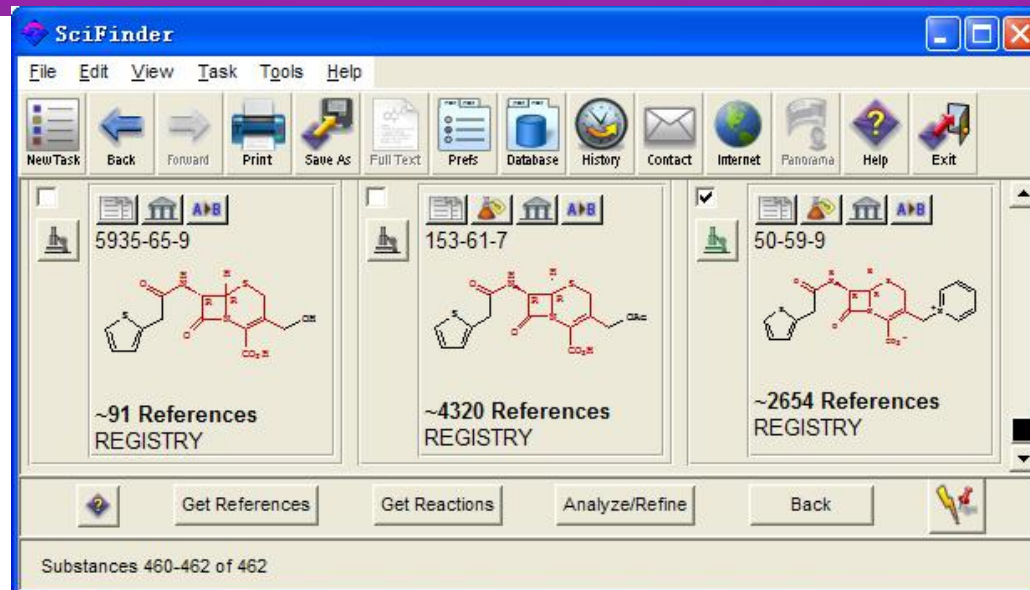
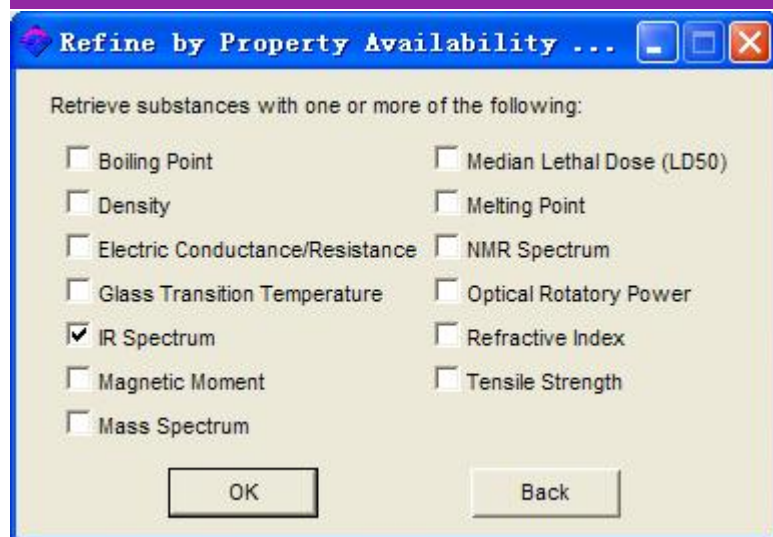


SciFinder[®]



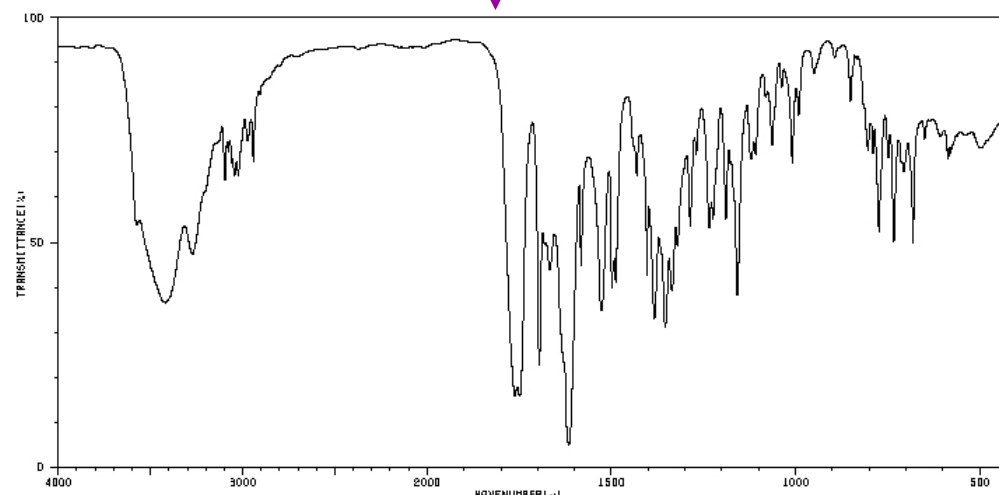
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SciFinder[®]



如果:

我只关心具有红外光谱信息的物质



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实际上

我们有的时候，更多关注的是结构上面的信息

修饰信息？

修饰上某一特定原子后该原子的修饰信息？

.....



SciFinder[®]

Analyze Substances

Use Analyze to view a subset of your answers.

Analyze by one of these methods:

- ☒ Real-atom attachments
- ☐ Variable group (A, Q, X, and M) composition
- ☐ R-group composition
- ☐ Precision
- ☐ Ring skeletons
- ☐ Stereo

☐ Analyze only selected substances

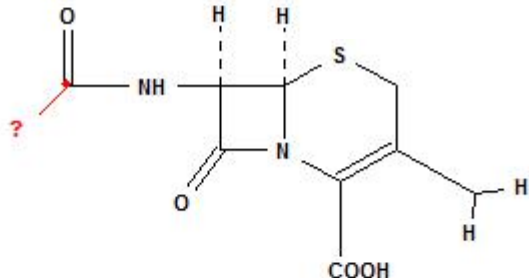
☒ Analyze all substances

OK Cancel

View Real-atom Attachments

File Edit Tools Help

Select any real atom in your structure to view the atom's attachments.



Atom attachments:

☐ H or None	65
☐ C	32803
☐ N	154
☐ O	111
☐ S	5
☐ Cl	1
☐ Other	107
☐ A - Any (not H)	33074
☐ Hy - Heterocycle	426
☐ Q - Any (not C, H)	271
☐ Cb - Carbocycle	247
☐ Ak - Alkyl chain	12

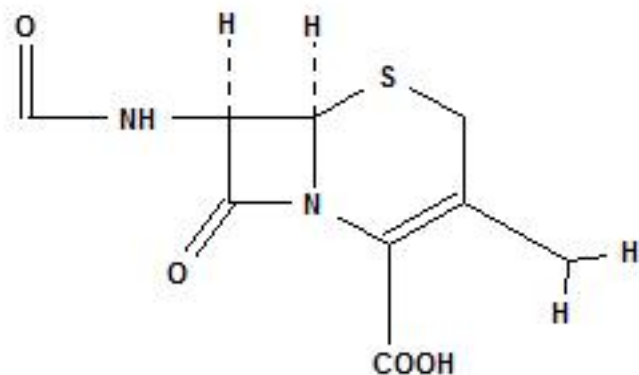
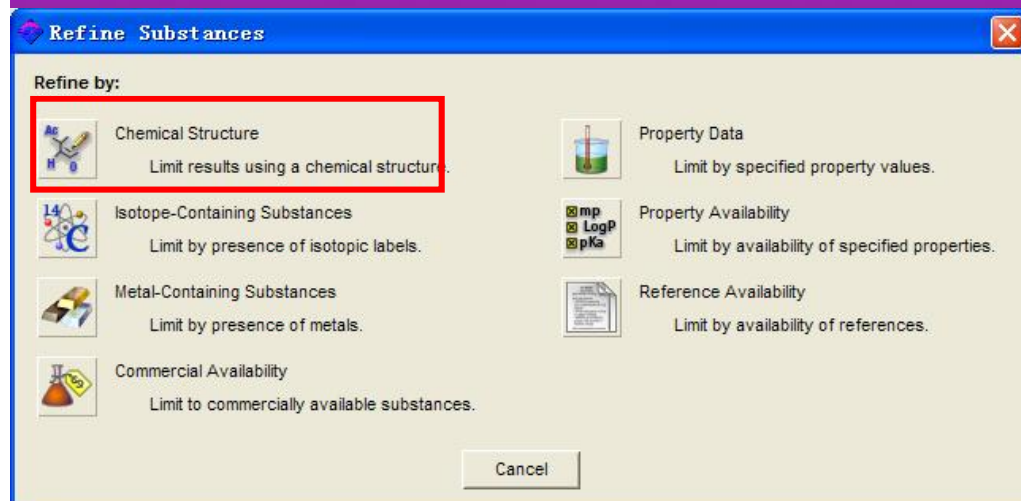
? =

Get Substances Back

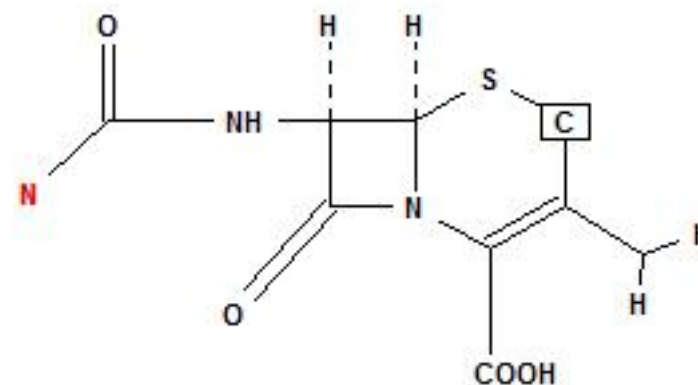


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SciFinder[®]



修正结构



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SciFinder

File Edit View Task Tools Help

New Task Back Forward Print Save As Full Text Prefs Database History Contact Internet Panorama Help Exit

51647-20-2
~4 References
REGISTRY

51647-19-9
~1 Reference
REGISTRY

51647-18-8
~4 Re
REGIS

Get References Get Reactions Analyze/Refine Ba

Substances 61-63 of 154

View Real-atom Attachments

File Edit Tools Help

Select any real atom in your structure to view the atom's attachments.

Atom attachments:

☐ H or None	7
☐ C	142
☒ O	5
☐ A - Any (not H)	147
☐ Ak - Alkyl chain	130
☐ Cb - Carbocycle	10
☐ Q - Any (not C, H)	5
☐ Hy - Heterocycle	2

? = 0

Get Substances Back



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有的时候，

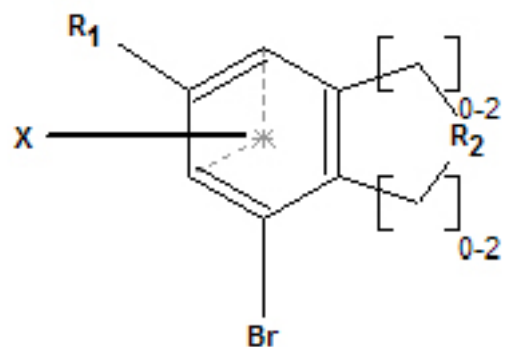
我们对我们的结构只有一定的了解，不确定的信息太多

我们来看我们所要找的结构：

- 结构中含有苯环，
- 苯环上有一个杂环，环结构不定，可以是**3**元环，**4**元环或者**5**元环
- 杂环上原子必须是**O**或者**S**，且杂原子位置不确定
- 苯环上与杂环相邻的位置接个**Br**
- 苯环上某**2**个处于间位的**C**必须有**1**个**C**接卤素，但是接什么卤素不确定
- 该**2**个位置之间的**C**必须接一个基团，该基团可以是**H**，**OH**，**X**



得到具备一定条件的结构信息



问题:

- 存在多少种环结构
- **X= F, Cl, Br, I** 分别有多少种物质
- **R1=H, OH, X** 分别有多少物质

R1= H, OH, X

R2= O, S

SciFinder[®]

Get Substances

Get substances that match your query using:

☐ Exact search

☒ Substructure search

☐ Similarity search

Filters ▾

Substance class	Return substances that are:
	☐ Alloys
	☐ Coordination compounds
	☐ Incompletely defined
	☐ Mixtures
	☐ Polymers
	☐ Organics, and others not listed
Structure components	☒ Only return substances that are similar
Commercial availability	☐ Only return substances that are commercially available
References	☐ Only return substances having one or more references
Studies	Only return substances having these studies:
	☐ Analytical
	☐ Biological
	☐ Preparation
	☐ Reactant or Reagent

OK Cancel

SciFinder Scholar

File Edit View Task Tools Help

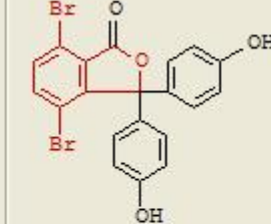
New Task Back Forward Print Save As Full Text Prefs Database History Internet Help Exit

3029-16-1



~16 References
REGISTRY

2391-57-3



~3 References
REGISTRY

632-79-1



~614 References
REGISTRY

Get References Get Reactions Analyze/Refine Back

Substances 370-376 of 376



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SciFinder[®]

Analyze Substances

Use Analyze to view a subset of your answers.

Analyze by one of these methods:

- ☐ Real-atom attachments
- ☐ Variable group (A, Q, X, and M) composition
- ☐ R-group composition
- ☐ Precision
- ☒ Ring skeletons
- ☐ Stereo

☐ Analyze only selected substances

☒ Analyze all substances

OK Cancel

环骨架分析



A

Ring Skeleton/Atom/Bond Analysis

File Edit Task Tools Help

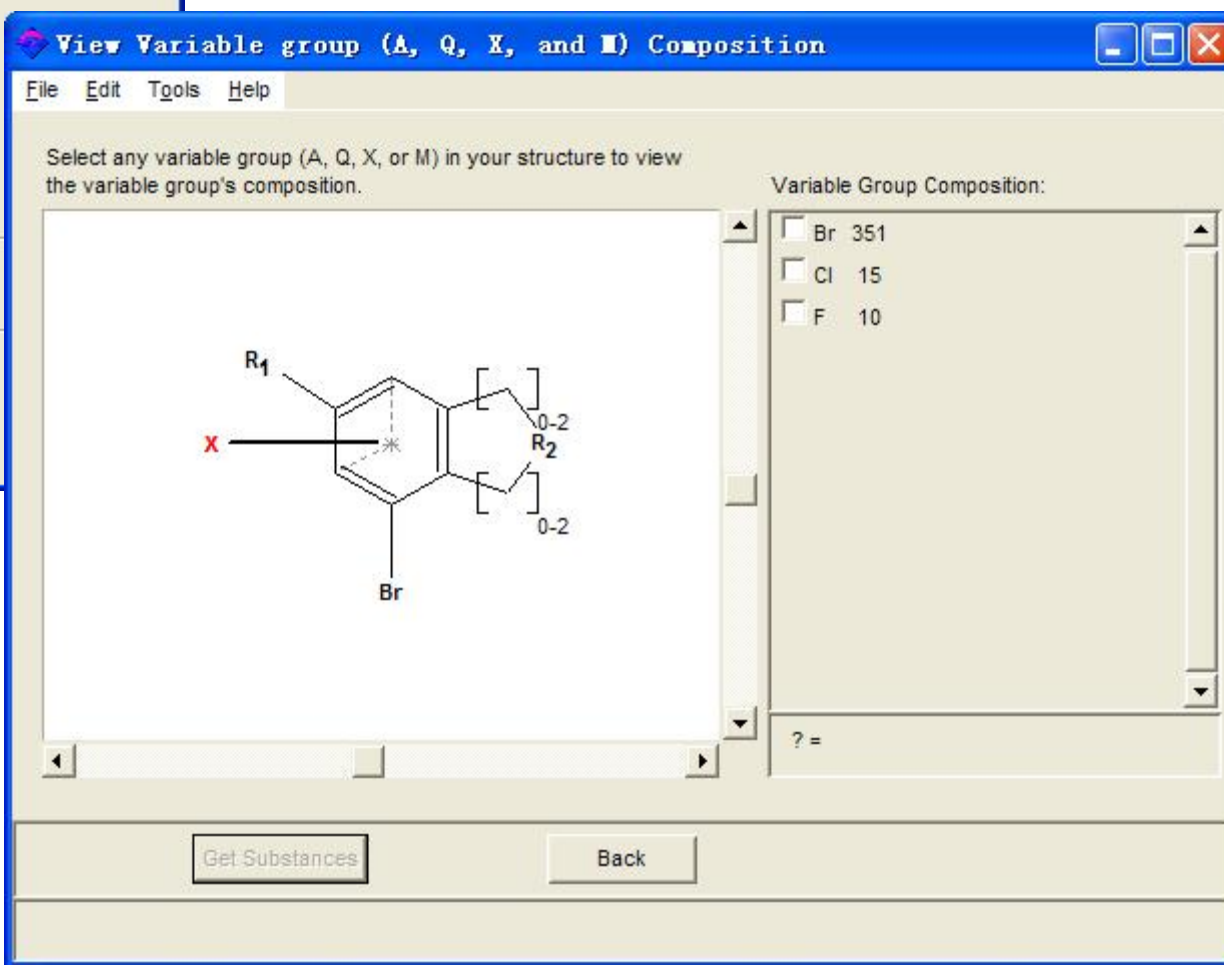
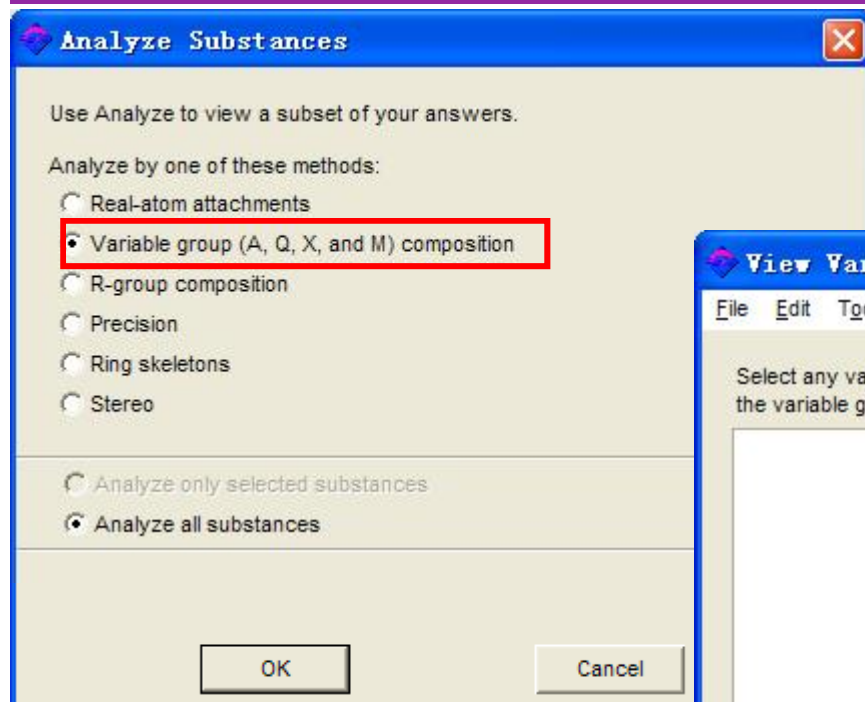
Select groups of interest

☐ 194 Substances containing: 	☐ 115 Substances containing: 	☐ 13 Substances containing:
☐ 10 Substances containing: 	☐ 8 Substances containing: 	☐ 8 Substances containing:
☐ 6 Substances containing: 	☐ 4 Substances containing: 	☐ 2 Substances containing:

Get Substances Back

Ring Analyzes 1-9 of 20

SciFinder[®]

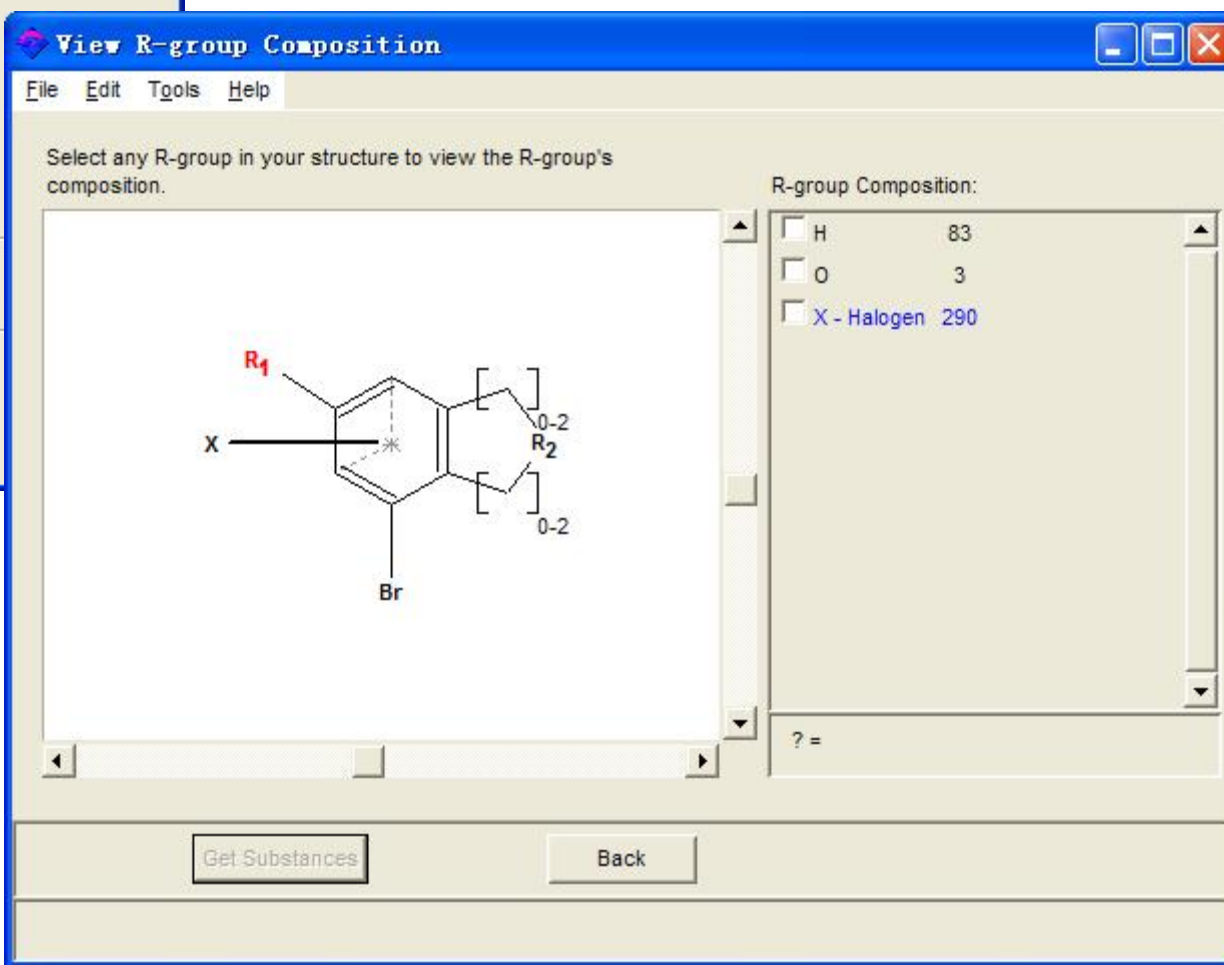
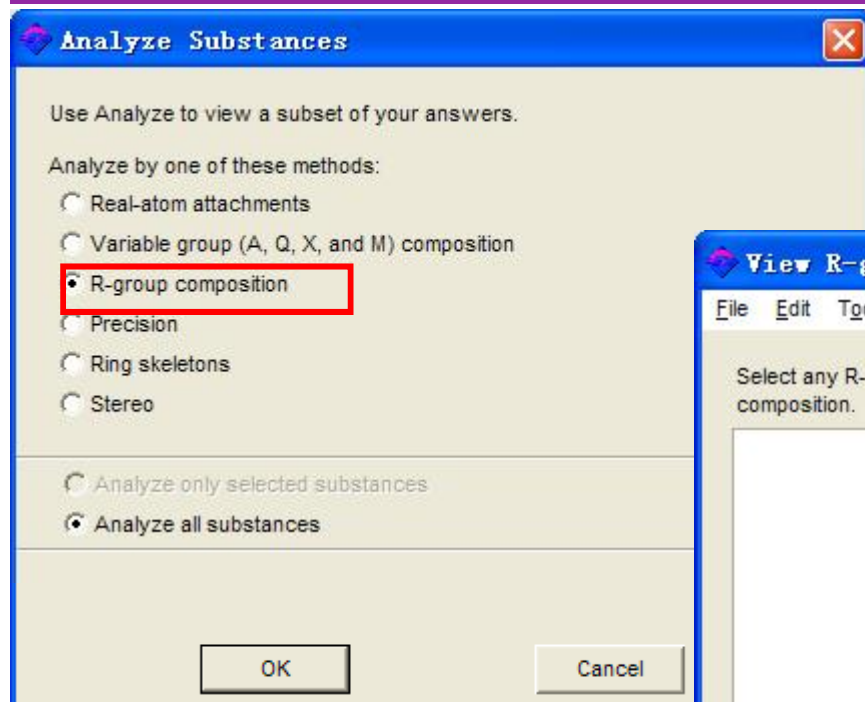


可变基团分析



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SciFinder[®]

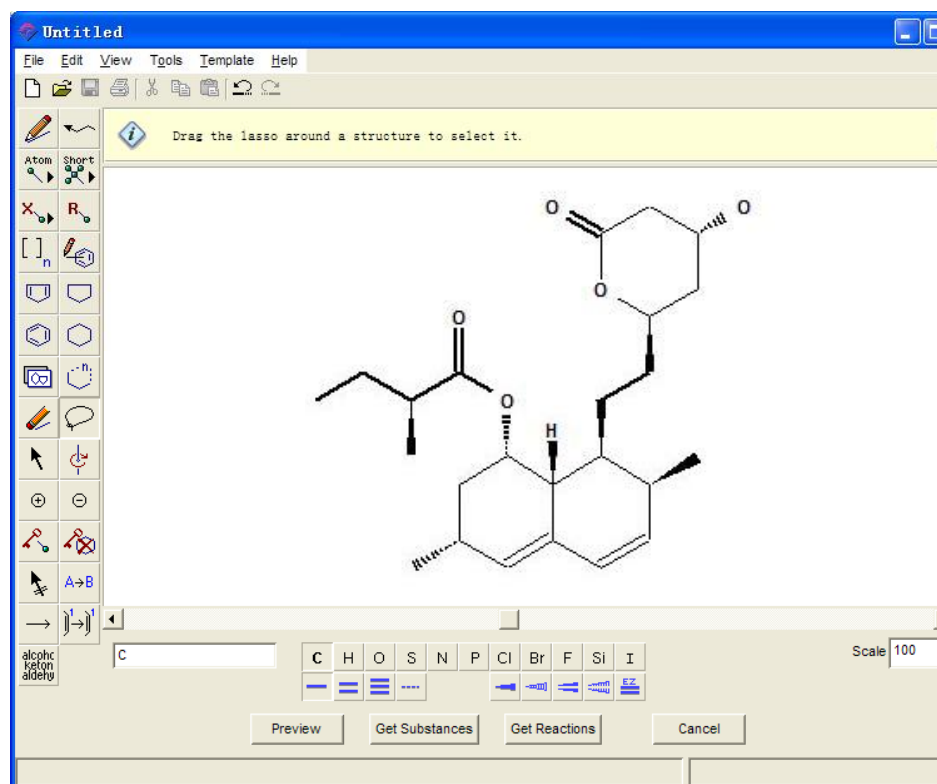


R基团分析



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相似结构检索



Get Substances

Get substances that match your query using:

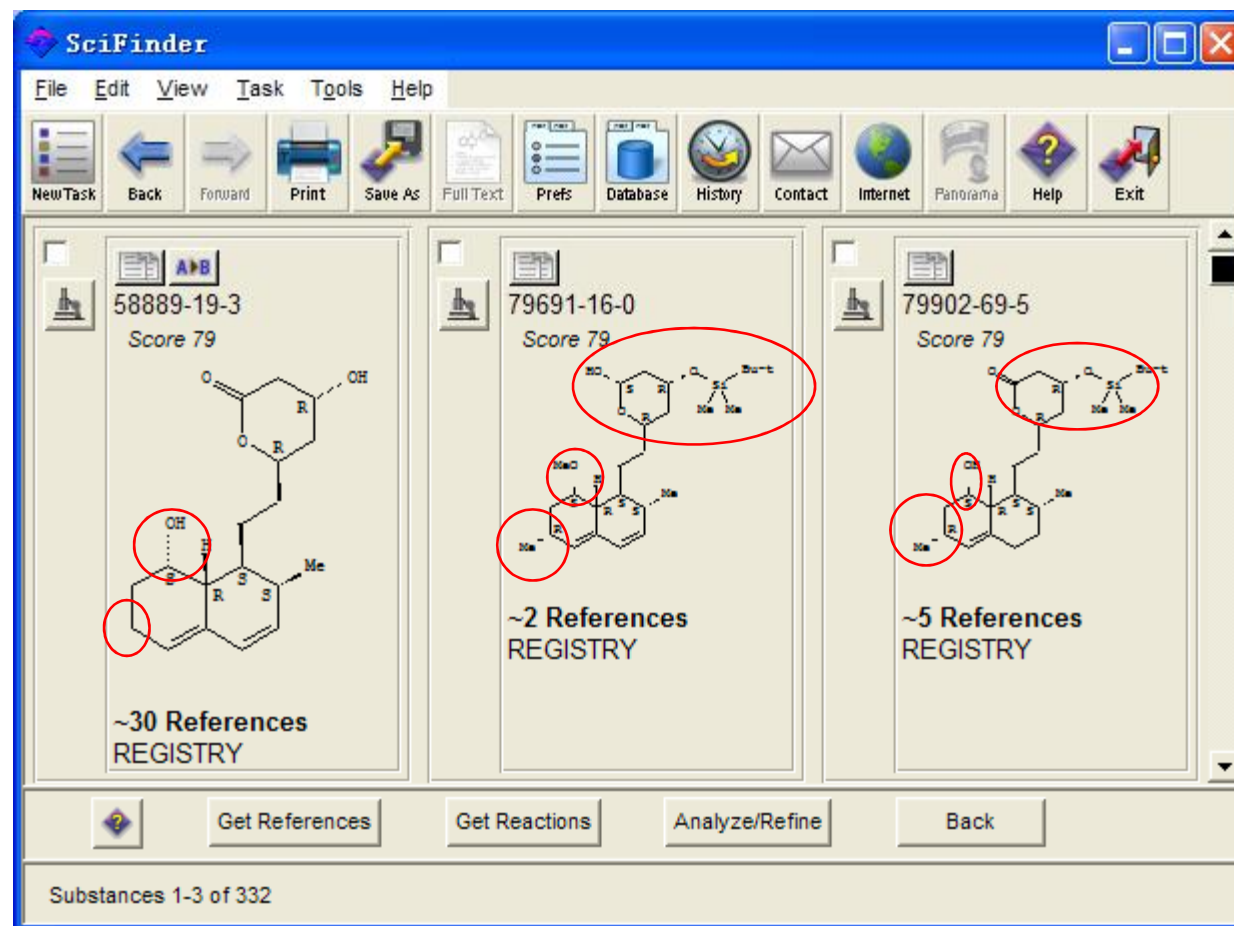
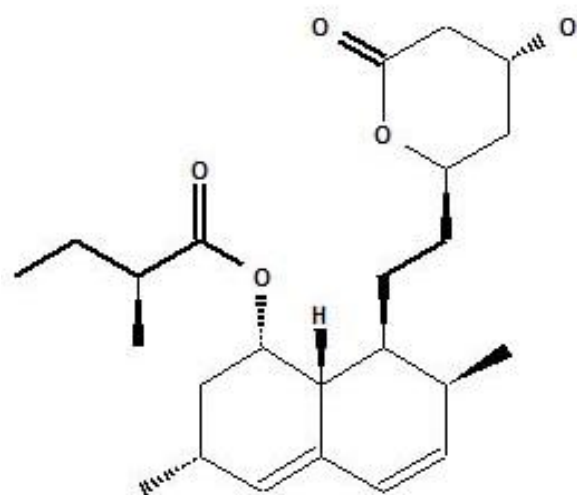
☐ Exact search
☐ Substructure search
☒ Similarity search

Filters ▼

Substance class	Return substances that are:
	☐ Alloys ☐ Coordination compounds ☐ Incompletely defined ☐ Mixtures ☐ Polymers ☐ Organics, and others not listed above
Structure components	☐ Only return substances that are single components
Commercial availability	☐ Only return substances that are commercially available
References	☐ Only return substances having one or more references
Studies	Only return substances having these reported studies:
	☐ Analytical ☐ Biological ☐ Preparation ☐ Reactant or Reagent

SciFinder[®]

得到相似结构信息



The screenshot displays the SciFinder software interface. The top menu bar includes File, Edit, View, Task, Tools, and Help. Below the menu is a toolbar with icons for New Task, Back, Forward, Print, Save As, Full Text, Prefs, Database, History, Contact, Internet, Panorama, Help, and Exit. The main area shows three search results panels, each displaying a chemical structure and its associated references. The first panel (58889-19-3, Score 79) shows a structure with a hydroxyl group and a side chain, with a score of 79 and approximately 30 references. The second panel (79691-16-0, Score 79) shows a structure with a hydroxyl group and a side chain, with a score of 79 and approximately 2 references. The third panel (79902-69-5, Score 79) shows a structure with a hydroxyl group and a side chain, with a score of 79 and approximately 5 references. The bottom of the interface includes buttons for Get References, Get Reactions, Analyze/Refine, and Back, along with a status bar indicating 'Substances 1-3 of 332'.



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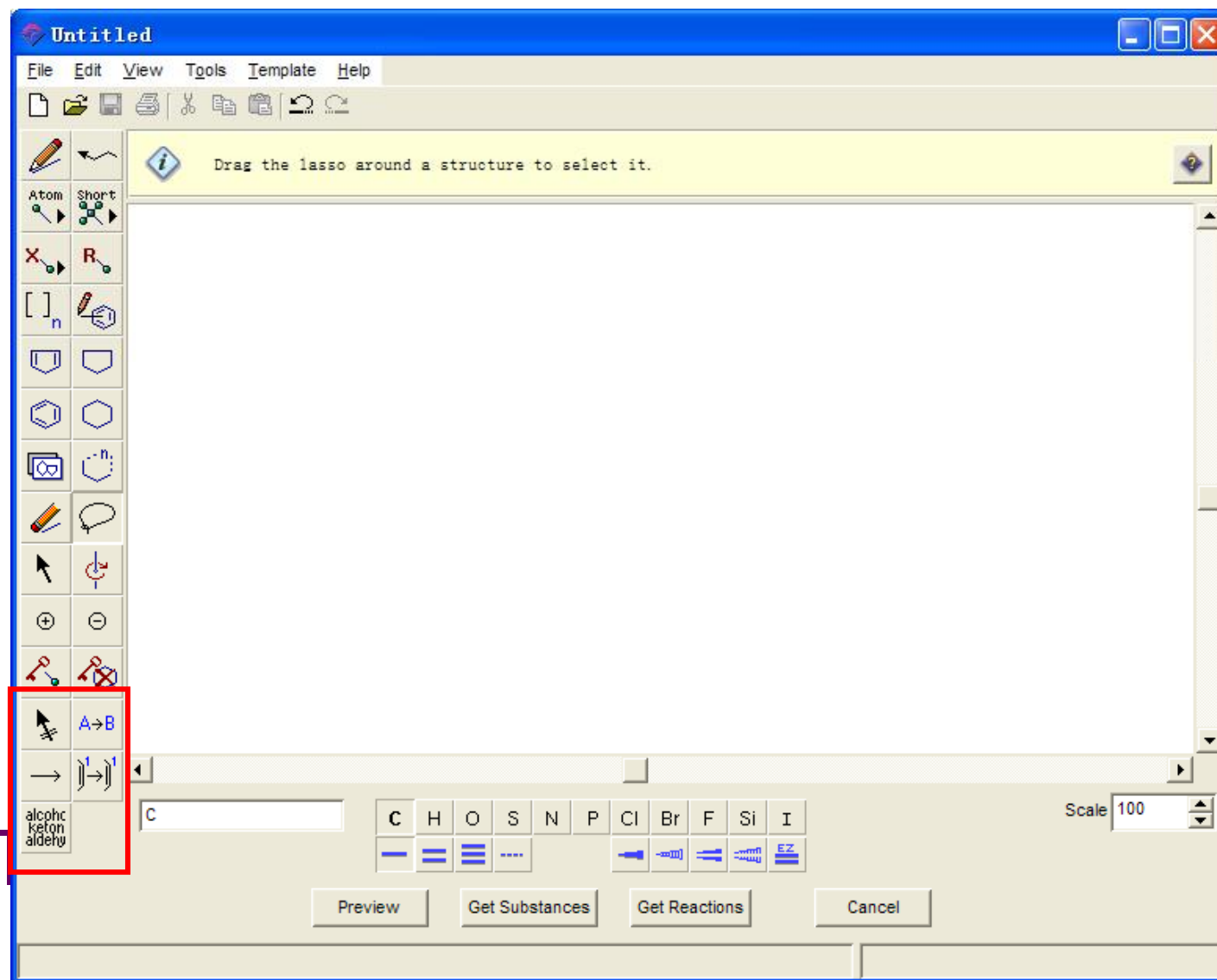
SciFinder Scholar物质检索小结

问题：我们到底需要什么样的物质？

- | | |
|----------------------------|--------|
| 1. 是否可以得到物质的盐，或者其他的混合物，聚合物 | 精确结构检索 |
| 2. 是否可以通过修饰结构，来获得更多的应用 | 亚结构检索 |
| 3. 是否存在类似的，但是我不知道的结构 | 亚结构检索 |
| 4. 是否物质的相似结构，可以有更多的应用 | 相似结构检索 |

SciFinder Scholar查询举例----反应信息的查询

反应查询工具



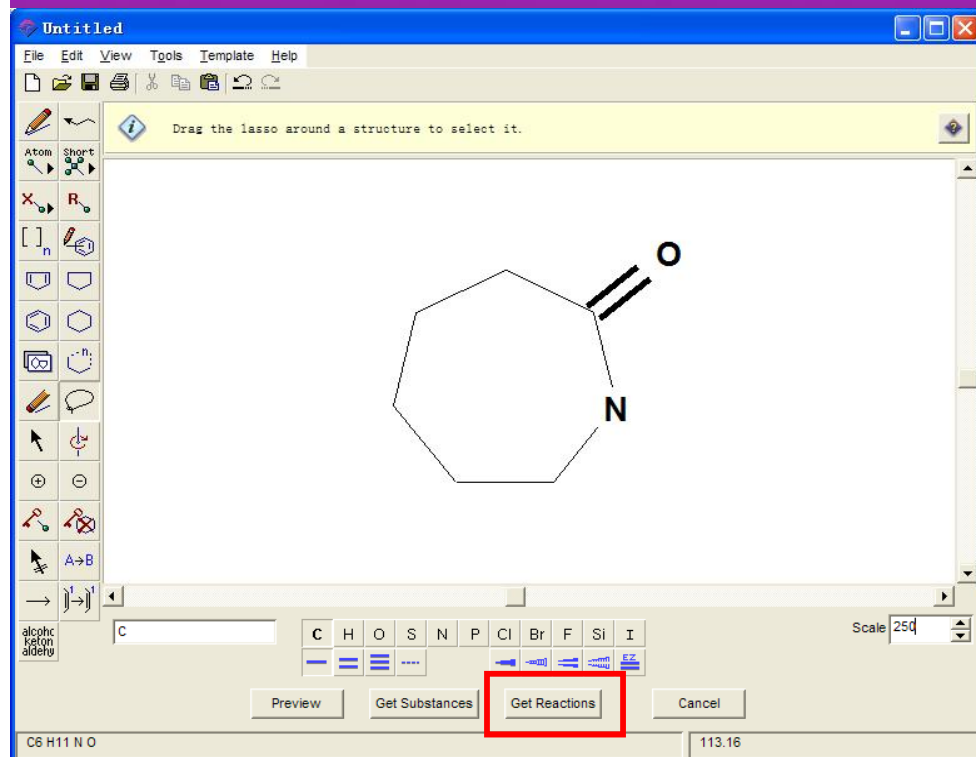
SciFinder Scholar查询举例----反应信息的查询

The screenshot shows the SciFinder Scholar interface with the following components and labels:

- Reaction Location Marking Tool (反应位置标记工具):** Points to the mouse cursor icon in the left toolbar.
- Reaction Arrow (反应箭头):** Points to the reaction arrow icon in the left toolbar.
- Reaction Functional Group List (反应官能团列表):** Points to the list of functional groups (alcohol, ketone, aldehyde) at the bottom left.
- Reaction Role Tool (反应角色工具):** Points to the 'A' and 'B' atom marking icons in the left toolbar.
- Reaction Atom Marking Tool (反应原子标记工具):** Points to the 'A' and 'B' atom marking icons in the left toolbar.

The interface includes a menu bar (File, Edit, View, Tools, Template, Help), a toolbar with various drawing and editing tools, a central workspace with a yellow instruction bar that says "Drag the lasso around a structure to select it.", and a bottom panel with a search input field (containing 'C'), a list of elements (C, H, O, S, N, P, Cl, Br, F, Si, I), and buttons for "Preview", "Get Substances", "Get Reactions", and "Cancel". A scale control is set to 100.

SciFinder[®]



Get Reactions

Get reactions where the structure(s) are:

- ☒ variable only at the specified positions
- ☐ substructures of more complex structures

Filters ▼

Reaction steps	Only return reactions having this number or range of steps:
Reaction classification	Only return reactions of the following type(s): ☐ Biotransformation ☐ Catalyzed ☐ Chemoselective ☐ Combinatorial ☐ Electrochemical ☐ Gas-phase ☐ Non-catalyzed ☐ Photochemical ☐ Radiochemical ☐ Regioselective ☐ Stereoselective
Patents	Only return reactions from these sources: ☐ Patents ☐ Sources other than patents
Publication year	Only return reactions published in this year or range of years:

OK Cancel

Get Reactions - Role...

Get Reactions where this structure is:

- ☒ a Product
- ☐ a Reactant
- ☐ a Reagent
- ☐ a Reactant or a Reagent
- ☐ Anywhere in the reaction

OK Cancel



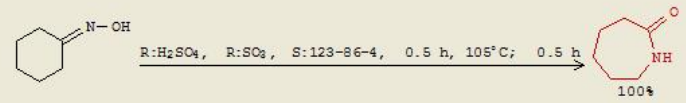
A division of the American Chemical Society

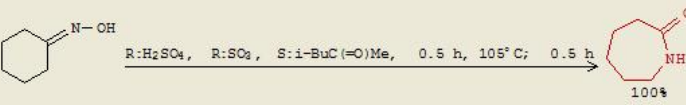
SciFinder[®]

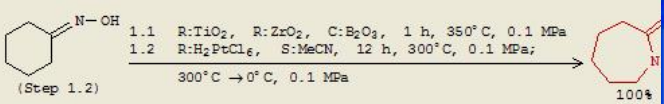
SciFinder Scholar

File Edit View Task Tools Help

NewTask Back Forward Print Save As Full Text Prefs Database History Internet Help Exit


NOTE: Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1
[Faming Zhuanli Shengqing Gongkai Shuomingshu, 1508128, 30 Jun 2004](#)
CASREACT


NOTE: Reactants: 1, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1
[Faming Zhuanli Shengqing Gongkai Shuomingshu, 1508128, 30 Jun 2004](#)
CASREACT


(Step 1.2)
NOTE: yield depends on reaction conditions, fixed-bed reactor, N2 used phase, Beckmann rearrangement,
[Get References](#) [Analyze/Refine](#)

Reactions 39-41 of 304

Analyze or Refine

Select One:

 Analyze
Display histograms by Journal, Number of steps, Publication Year, etc.

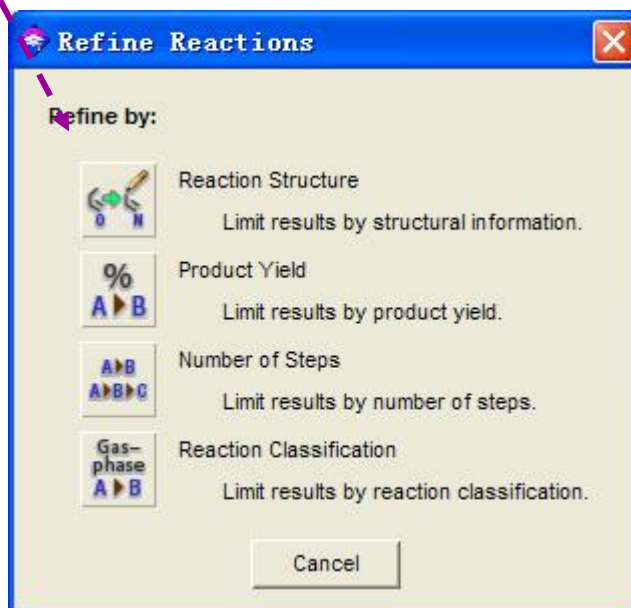
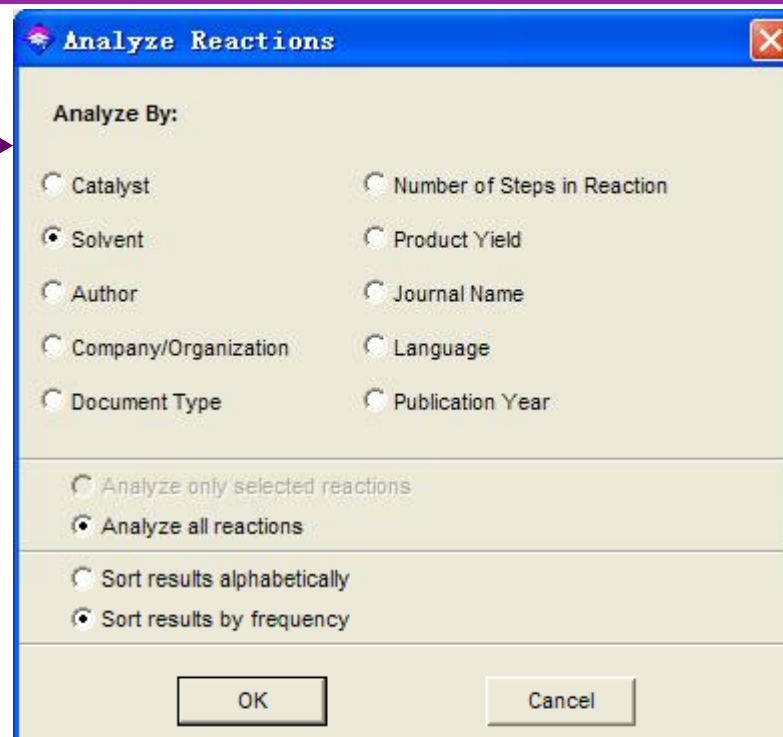
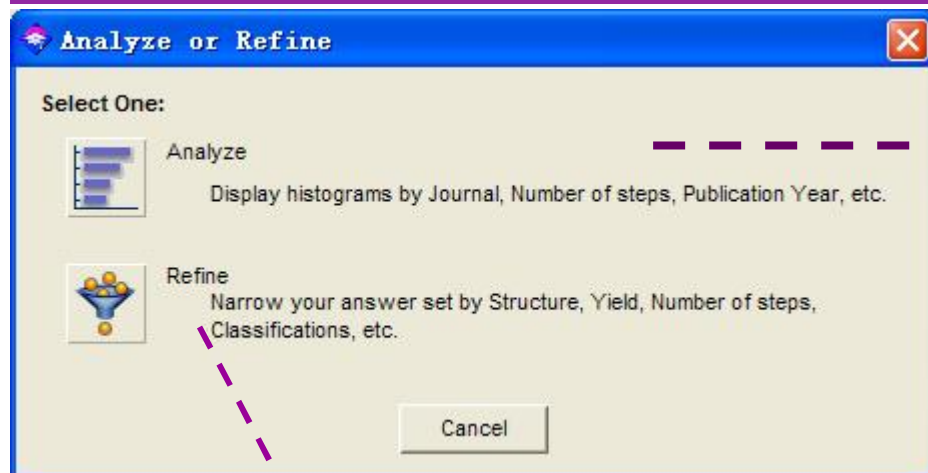
 Refine
Narrow your answer set by Structure, Yield, Number of steps, Classifications, etc.

[Cancel](#)



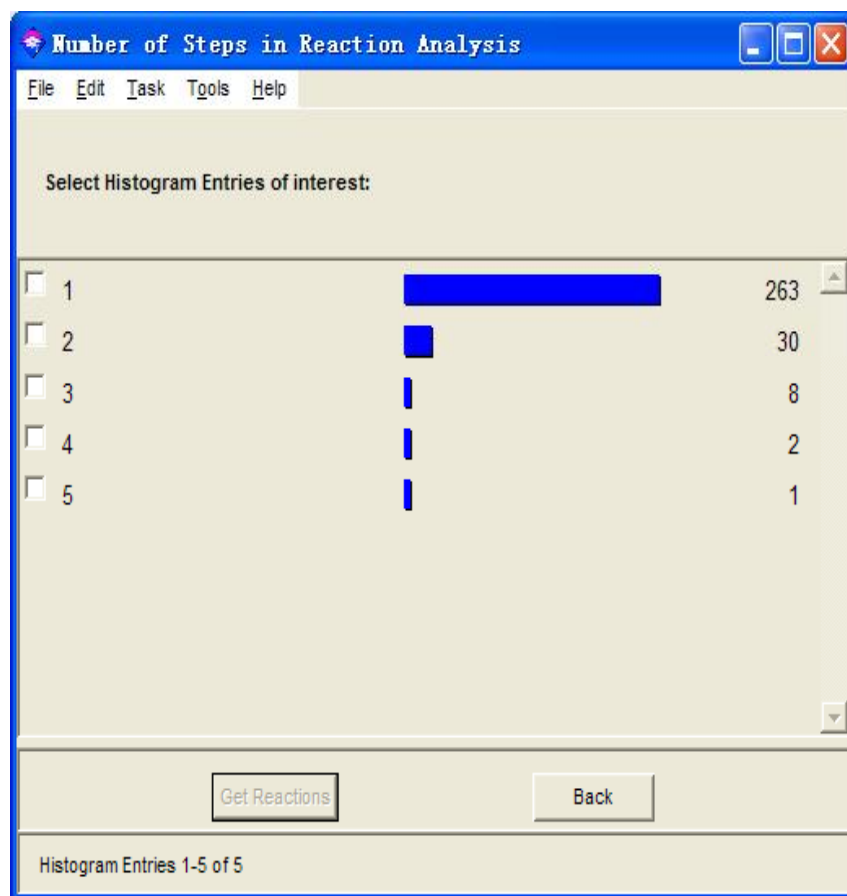
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SciFinder[®]

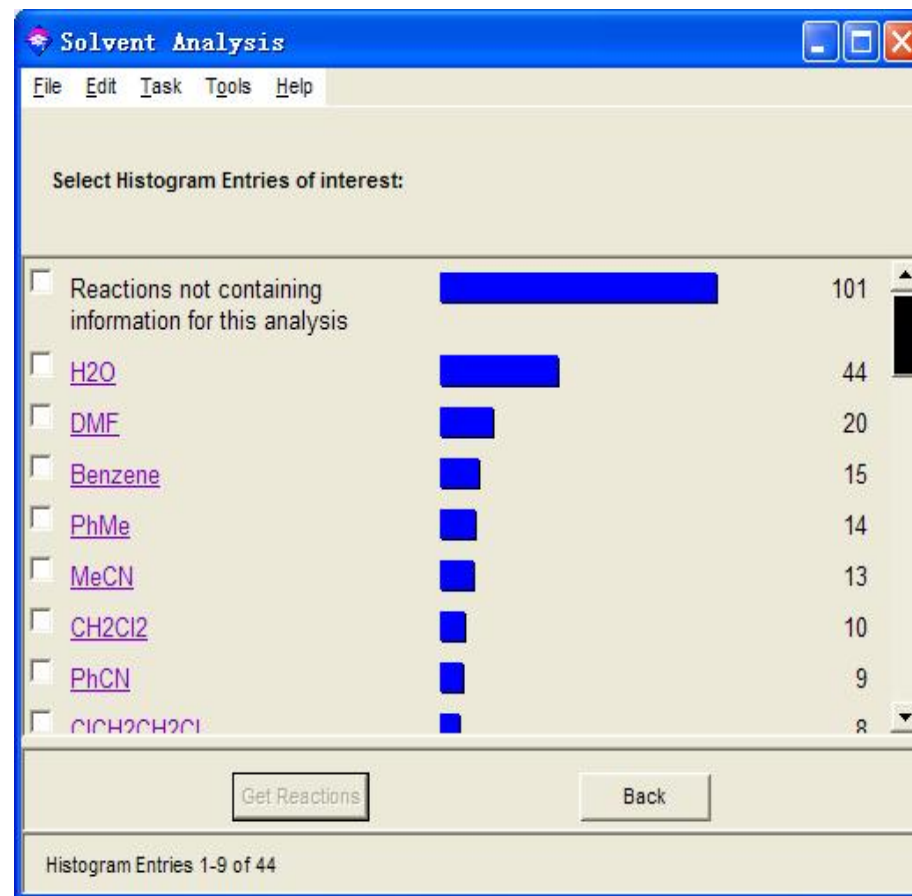


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反应步数分析



溶剂分析



拓展思路的反应检索

通常

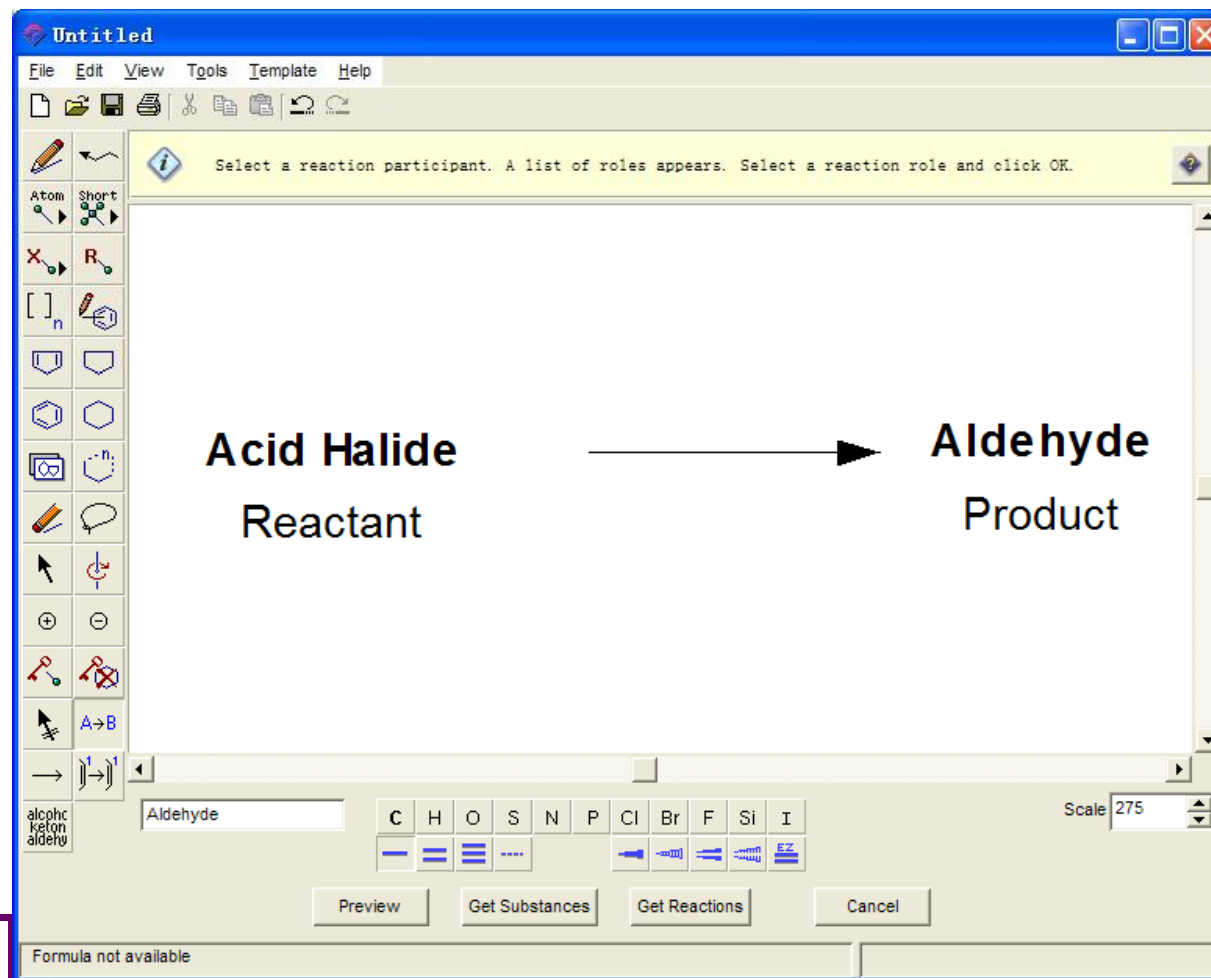
我们需要一些对我们科研有参考意义的反应

官能团之间的反应

亚结构反应检索



官能团之间的反应



SciFinder[®]

Get Reactions

You may limit your search by any of the following:

Reaction steps	Only return reactions having this number or range of steps: 1
Reaction classification	Only return reactions of the following type(s): ☐ Biotransformation ☐ Non-catalyzed ☐ Catalyzed ☐ Photochemical ☐ Chemoselective ☐ Radiochemical ☐ Combinatorial ☐ Regioselective ☐ Electrochemical ☐ Stereoselective ☐ Gas-phase
Patents	Only return reactions from these sources: ☐ Patents ☐ Sources other than patents
Publication year	Only return reactions published in this year or range of years:

OK Cancel

假如我们只想得到一步反应

SciFinder

File Edit View Task Tools Help

New Task Back Forward Print Save As Full Text Pref Database History Contact Internet Panorama Help Exit

Reaction 1:

PhC(=O)Cl + CC1=C(C)C(=N)C=C1 $\xrightarrow{\text{S:DMF, rt} \rightarrow 0^\circ\text{C}; < 0^\circ\text{C}; 15 \text{ min, } 0^\circ\text{C} \rightarrow \text{rt}}$ CC1=C(C)C(=N)C=C1C(=O)C 75%

NOTE: Reactants: 2, Solvents: 1, Steps: 1, Stages: 1

[Tetrahedron, 61\(49\), 11577-11600, 2005](#)
CASREACT

Reaction 2:

PhC(=O)Cl + CC1=C(C)C(=N)C=C1 $\xrightarrow{\text{S:DMF, rt} \rightarrow 0^\circ\text{C}; < 0^\circ\text{C}; 15 \text{ min, } 0^\circ\text{C} \rightarrow \text{rt}}$ CC1=C(C)C(=N)C=C1C(=O)C 75%

NOTE: Reactants: 2, Solvents: 1, Steps: 1, Stages: 1

[Tetrahedron, 61\(49\), 11577-11600, 2005](#)
CASREACT

Reaction 3:

t-BuOCH (Step 1.2) + CC(=O)Cl $\xrightarrow{\begin{matrix} 1.1 \text{ C:Ph}_2\text{-pentadienone Pd, C:Tri-2-furylphosphine, S:THF, 15 min, rt} \\ 1.2 \text{ R:Bu}_4\text{SnF, R: (CH}_3\text{OSi)n, C:Bu}_4\text{N}^+\text{F}^-, \text{ S:THF, 2 h, rt} \\ 1.3 \text{ 6 h, 65}^\circ\text{C} \end{matrix}}$ CC(=O)Cl

Reactions 1-3 of 647

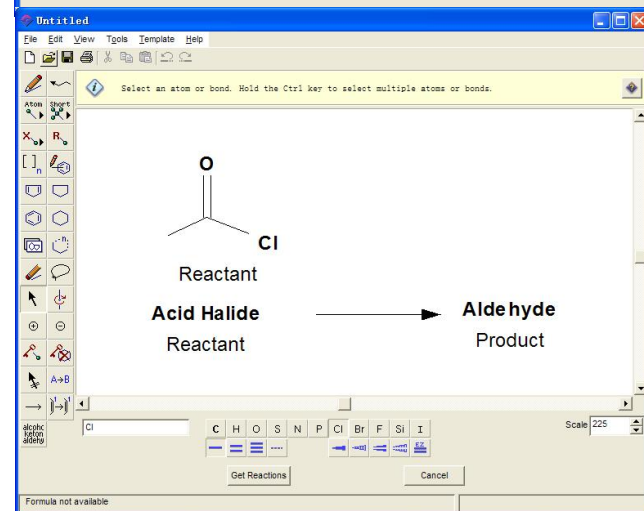
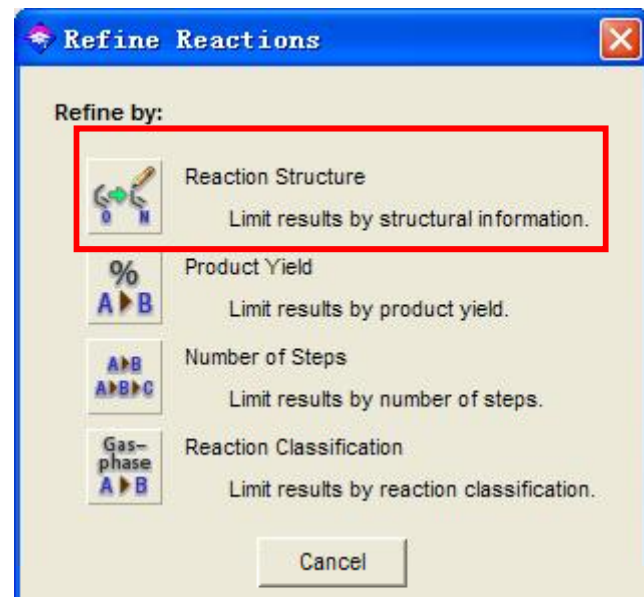
Get References Analyze/Refine Back



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假如我们规定反应物必须是乙酰氯



SciFinder

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Reaction 1:

$$\text{Cl}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_3 \xrightarrow{\text{R:Bu}_3\text{SnH, C: Pd(PPh}_3)_4} \text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{H}$$

NOTE: Reactants: 1, Reagents: 1, Catalysts: 1, Steps: 1, Stages: 1

Journal of the American Chemical Society, 127(23), 8424-8432, 2005
CASREACT

Reaction 2:

$$\text{Cl}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_3 \xrightarrow{\text{R:Bu}_3\text{SnH, C: Pd(PPh}_3)_4} \text{H}_3\text{C}-\overset{\text{O}}{\parallel}{\text{C}}-\text{H}$$

NOTE: Reactants: 1, Reagents: 1, Catalysts: 1, Steps: 1, Stages: 1

Journal of the American Chemical Society, 127(23), 8424-8432, 2005
CASREACT

Reaction 3:

$$\text{Cl}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_3 + \text{Fluorene derivative} \xrightarrow{\begin{matrix} 1.1 \text{ R: AlCl}_3, \text{ S: CS}_2 \\ 1.2 \text{ R: Br}_2, \text{ R: NaCH}_3, \text{ S: THF} \\ 1.3 \text{ R: Red-Al, S: PhMe} \\ 1.4 \text{ R: CrO}_3, \text{ S: C}_6\text{H}_5\text{N} \end{matrix}} \text{Fluorene derivative with CHO groups}$$

NOTE: literature prepn., regioselective in first stage, Reactants: 2, Reagents: 5, Solvents: 4, Steps: 1, Stages: 4

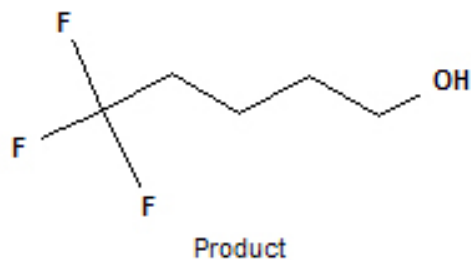
Reactions 1-3 of 16

Get References Analyze/Refine Back



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亚结构反应检索



想获得1步合成
该物质的反应

Get Reactions

Get reactions where the structure(s) are:

☒ variable only at the specified positions

☐ substructures of more complex structures

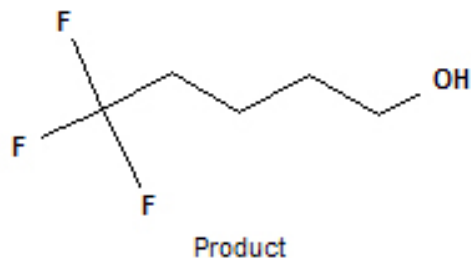
Filters ▼

Reaction steps	Only return reactions having this number or range of steps: 1
Reaction classification	Only return reactions of the following type(s): ☐ Biotransformation ☐ Non-catalyzed ☐ Catalyzed ☐ Photochemical ☐ Chemoselective ☐ Radiochemical ☐ Combinatorial ☐ Regioselective ☐ Electrochemical ☐ Gas-phase
Patents	Only return reactions from: ☐ Patents ☐ Sources other than
Publication year	Only return reactions published:

OK Cancel



亚结构反应检索



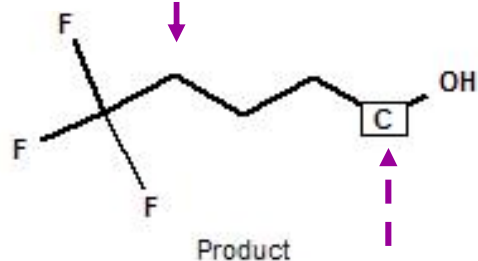
必须的条件:

- 羟基接的**C**必须是**CH₂**
- 整个**C**链不允许是某个环结构的部分结构
- 其余的**3**个**C**原子链接什么基团对反应没有影响

据此，我们修改我们的检索方式

亚结构反应检索

用环锁定功能，锁定**C**链，
保证其不成为环结构的一部分



用原子锁定功能，锁定**C**原子，保证**C**原子上两个**H**不被取代

Get Reactions

Get reactions where the structure(s) are:

☐ variable only at the specified positions

☒ substructures of more complex structures

Filters ▼

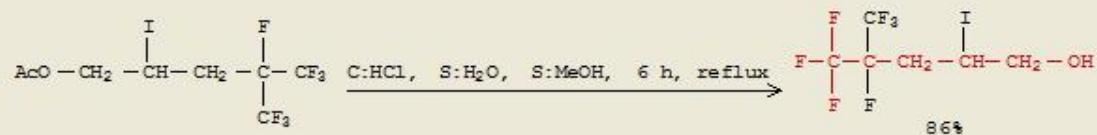
Reaction steps	Only return reactions having this number or range of steps: 1
Reaction classification	Only return reactions of the following type(s): ☐ Biotransformation ☐ Non-catalyzed ☐ Catalyzed ☐ Photochemical ☐ Chemoselective ☐ Radiochemical ☐ Combinatorial ☐ Regioselective ☐ Electrochemical ☐ Stereoselective ☐ Gas-phase
Patents	Only return reactions from these sources: ☐ Patents ☐ Sources other than patents
Publication year	Only return reactions published in this year or range of years:

OK Cancel

SciFinder[®]

SciFinder

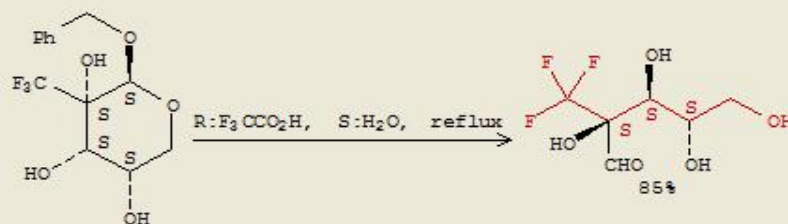
File Edit View Task Tools Help



NOTE: Reactants: 1, Catalysts: 1, Solvents: 2,
Steps: 1, Stages: 1

[Journal of Fluorine Chemistry, 121\(1\), 101-104: 2003](#)

CASREACT



NOTE: stereoselective,
Reactants: 1, Reagents: 1, Solvents: 1,
Steps: 1, Stages: 1

[Journal of Heterocyclic Chemistry, 40\(2\), 329-335: 2003](#)

CASREACT



Get References

Analyze/Refine

Back

SciFinder 反应检索小结

- 多用**Analyze/Refine**，来获得催化剂，溶剂，产率等信息
- 如果反应只涉及基团之间的变化，用官能团反应可以获得更多的参考信息
- 当无法找到具体反应，或者检索结果并不满意，尝试用亚结构反应查询，可以获得更多的参考信息



SciFinder Scholar检索Tips

- Explore by Research Topic
- Explore by Document Identifier
- Explore by Substance Identifier
- Explore by Molecular Formula



Explore by Research Topic ----Tips

- 一般最佳在**2—3个Concepts**（关键词），最多不超过**5个**
- 最好使用介词而不用**Boolean**运算符，如**AND**、**OR**、**NOT**；介词能被识别；
- 识别常用缩写、单复数、过去式等；
- 支持同意词，近义词检索；
- 不能用！或*（删减字符或通配符）
- 可用括号，括号内为前词的同义词；
- 修饰语不能自行分配，需各自写明；



Explore by Document Identifier----Tips

Number↴	Examples↴
CA Accession Number↴	120:15297↓ 1994:15297↴
Patent number↴	CA 2107100↴
Patent application number↴	JP 1992-502228↴
Priority application number↴	IT 1998-BO661↴
PubMed ID↓ (National Library of Medicine)↴	2004123↴

Explore by Substance Identifier----Tips

- 最多输入**25**条；
- **Read File**必须是 **.txt**文件；
- 每个条目输入**<200**字符；
- 可以有空格，不区分大小写；
- 如果检索结果不理想，也可在主题检索中再检；
- 支持俗名，商品名检索



Explore by Molecular Formula----Tips

- 区分大小写;
- 输入必须规范, 否则会自动要求重输;
- 输入时不同元素之间可用空格隔开, 系统也会自动分割;
- 输入盐类, 可分为酸碱组分以 . 相连;
如: **H3 O4 P . 3 Na**; **H3 O4 P . 2 Na**; **H3 O4 P . Na**
分别代表不同的物质
- 聚合物则输入单体组成以括号加X, 如**(C4H6)X**;
- 对于复杂的有机物质, 可以通过分子式查询, 并通过亚结构限定获得

SciFinder Scholar的程序安装

- SciFinder Scholar 客户端程序:

SciFinder Scholar2006.exe

安装过程中, 提示:

Do you have a disk labeled Custom Site Files? (选择 No)

- **site.prf (site)** 文件

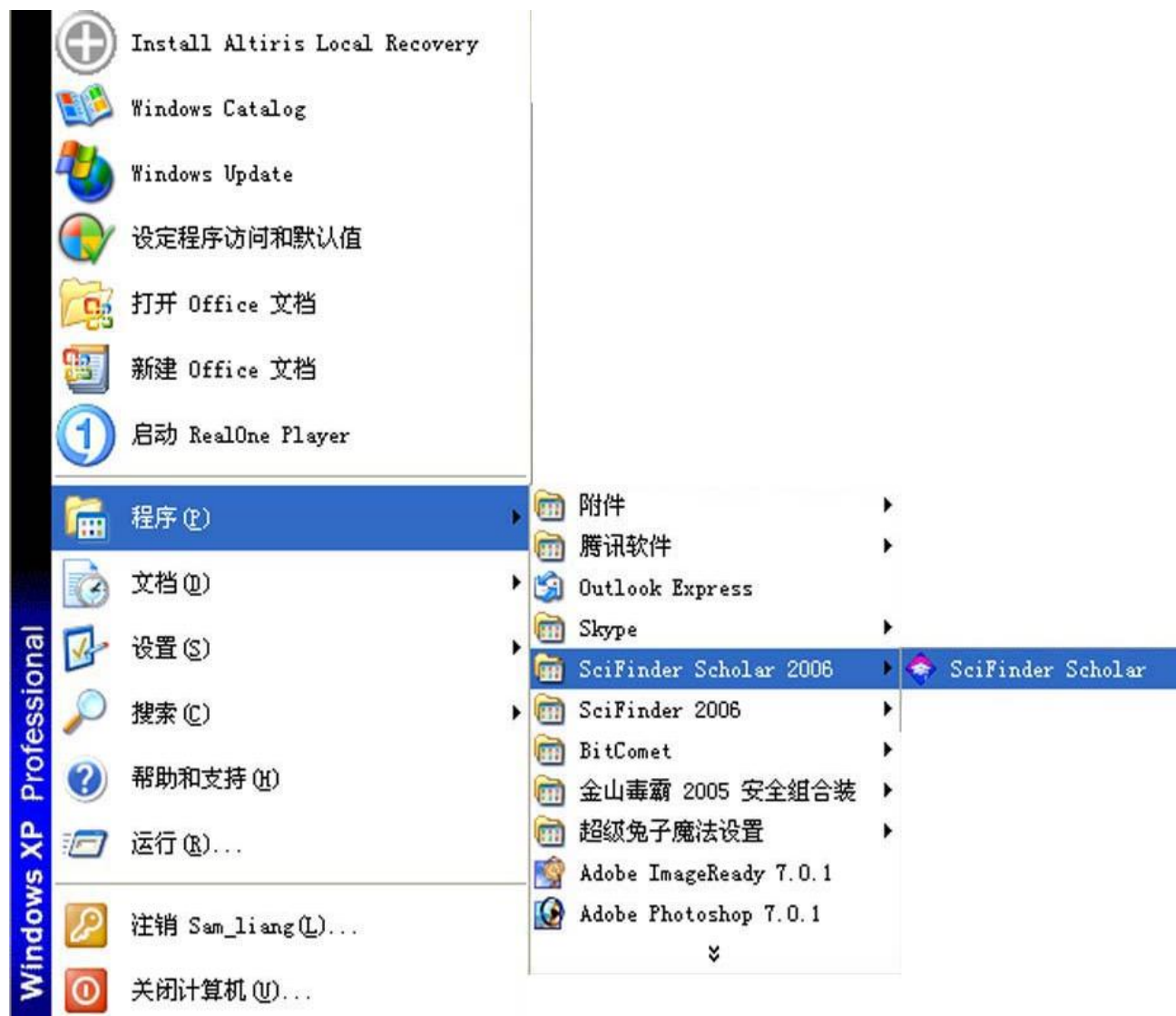
只需将 **site.prf** 文件复制粘贴到

X:\ScholarCHLR目录下

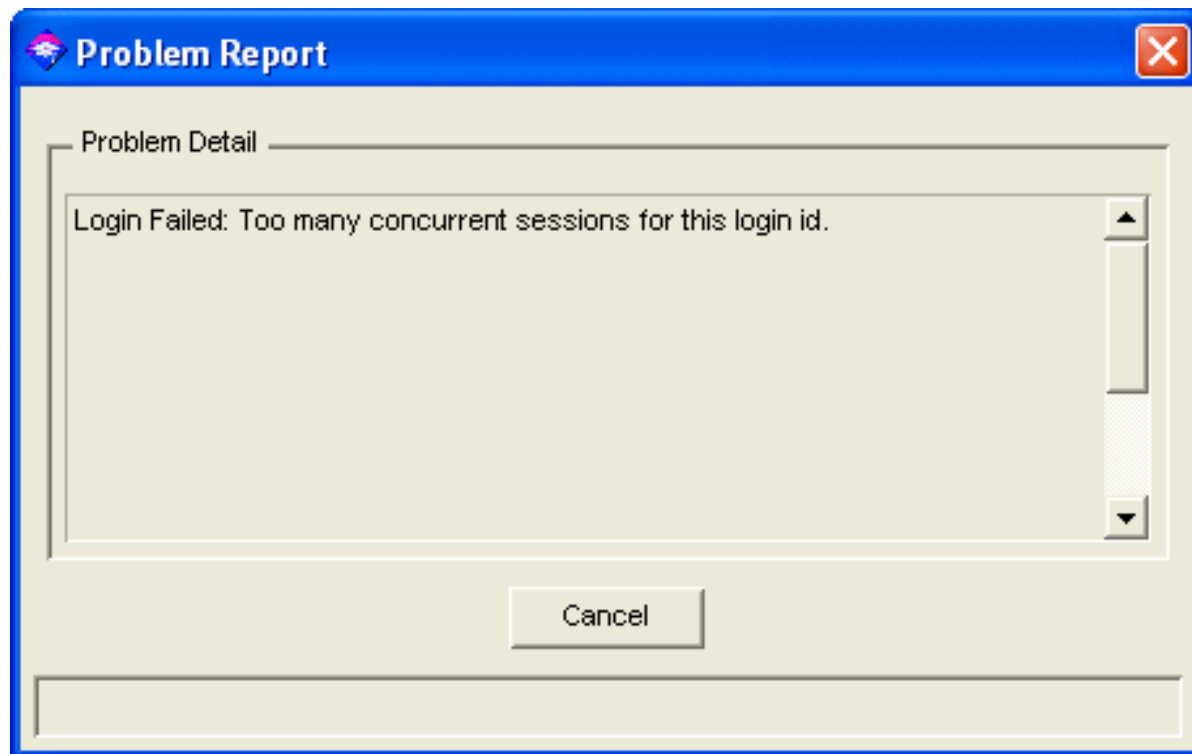
- 还可安装 **ViewerLite**用于查看**3D**结构



运行SciFinder Scholar

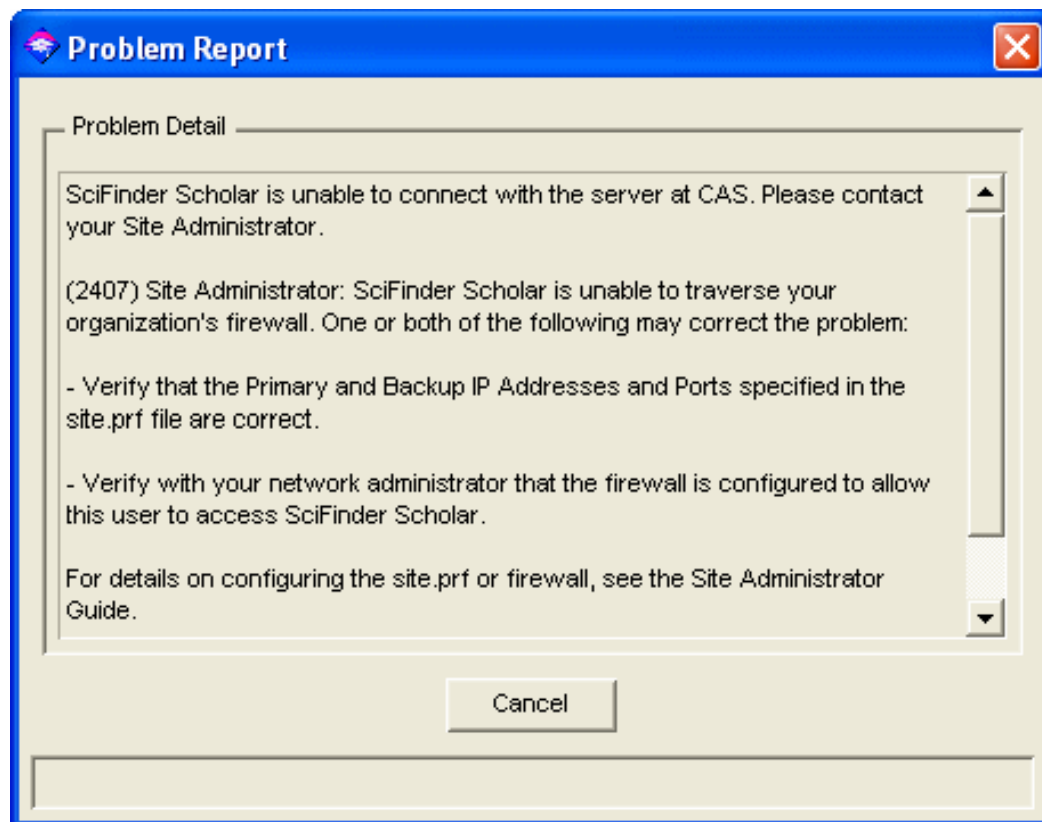


可能1：（并发用户数限制）



解决方法：请耐心等待 ！

可能2：（网络故障）



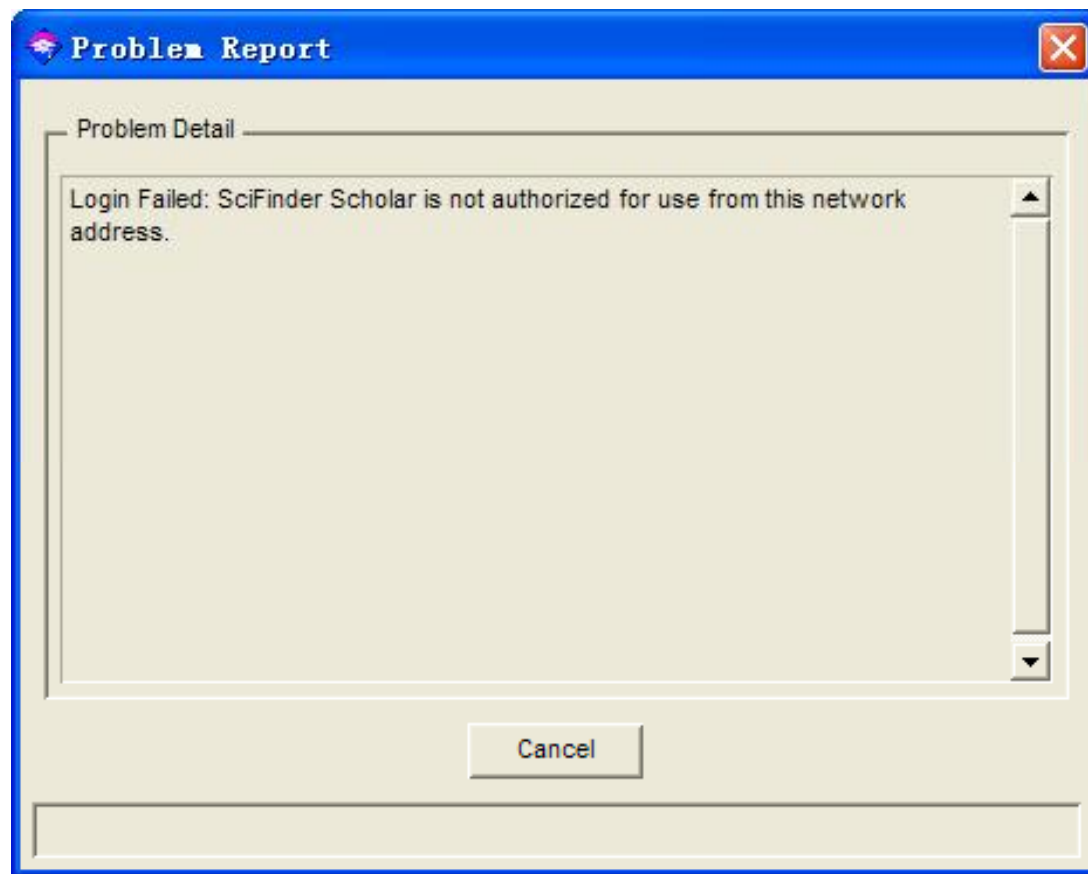
解决方法：检查网络

可能3：网络故障



解决方法：点击**OK**，再次运行SciFinder/Scholar

可能4: IP地址未被授权



解决方法：确认IP地址是否在校内， 并与图书馆管理员联系。

合理使用

CAS会监控与每个授权**IP**地址相关联的日常的检索和下载活动，目的是

- (1) 确定授权**IP**地址之间的平均使用标准；
- (2) 关注个别授权**IP**地址上使用状况的显著变化。

CAS可能会要求主要联系人和相关的授权用户对**CAS**提出质疑的使用状况进行讨论，如果有必要，与**CAS**一起针对已发现的问题找出解决办法。此类使用问题包括但不限于：

用作商业目的，非授权用户的使用，超出限定，大量的下载和储存数据。**CAS**会积极和获许可人以及成员单位配合解决任何过量或非正常使用的问题。如果这样的过量或非正常使用的状况继续发生，**CAS**会要求成员单位禁止滥用者使用**SciFinder/Scholar**。如果滥用的情形仍旧继续，在经过所有的努力和解决方法都尝试无效时，**CAS**将禁止该成员使用**SciFinder/Scholar**。



请合理使用SciFinder Scholar!!!

- 千万不要过量下载!
- 只下载自己要看 的记录（缩小范围）
- 不要用工具下载
- 不使用请关闭客户端程序
- 其他注意事项（参看使用协议）





谢谢

THANKS FOR YOUR ATTENTION