

# SciFinder 即将添加的新功能

## 对结果集的处理

### 实验步骤

1. 某些期刊的反应结果集包含了反应步骤的描述信息。这些细节可以帮助您快速判断这个反应或合成策略是否可行。
2. 实验步骤同时还是反应结果集的分类和分析工具。

The screenshot displays the SciFinder 'Reactions' interface. At the top, there are options for 'Get References' and 'Combine Answer Sets'. Below this, a list of 61 reactions is shown, with a 'Sort by' dropdown menu set to 'Relevance (New)'. A 'Detail' button is visible next to the selected reaction. The main area shows a chemical reaction scheme for the synthesis of (M)-7, with a yield of 97%. Below the reaction, there is an 'Overview' section and an 'Experimental Procedures' section. The 'Experimental Procedures' section contains detailed text describing the reaction conditions, reagents, and analytical data. On the right side, there is an 'Analysis' panel with a dropdown menu for 'Analyze by:' set to 'Experimental Procedure' and a 'Show More' button.

### 反应结果集的相关性排序

1. 相关性排序是反应结果集最新的默认分类工具。最相关的结果会显示在最前面。这样可以加快对结果集的浏览速度。
2. 相关性是由Tanimoto相似程度决定的。

Reactions Get References Find Additional Reactions Combine Answer Sets

266 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: Relevance Answers per Page [15] 1 2 3 4 5 6 ... 18 Display:

1. View Reaction Detail **Single Step** *Hover over any structure for more options.*

Relevance  
Accession Number  
Experimental Procedure  
Number of Steps  
Product Yield  
Publication Year

87%

Overview

**Steps/Stages**

1.1 R:

• 2 H<sub>2</sub>

C:Zn

**Notes**

exothermic reaction, green chemistry-process simplification, catalyst recyclable, Reactants: 1, Reagents: 1, Catalyst: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

Chemoselective hydrogenation of aromatic nitro compounds using diammonium hydrogen phosphite and commercial zinc dust  
By K., Anil Kumar et al  
From E-Journal of Chemistry, 5(4), 914-917; 2008  
[Full Text](#)

## 结果的显示

### 增强的反应结果显示

1. 更简洁明了的反应显示方式增强了可读性，方便对结果集的快速浏览，加快了判别的速度。
2. 显示方式可以设置为Schema和Overview，或者仅仅显示Schema。
3. 加入了一些期刊中的实验步骤信息。

Display:

1. View Reaction Detail Link Similar Reactions

**Single Step** *Hover over any structure for more options.*

97%

Overview

**Steps/Stages**

1.1 R:HCl, R:Fe, S:H<sub>2</sub>O, S:EtOH, S:THF, 1 h, 90°C

**Notes**

Reactants: 1, Reagents: 2, Solvents: 3, Steps: 1, Stages: 1, Most stages in any one step: 1

**References**

Functionalized [3+3] Cycloalkynes: Substituent Effect on Self-Aggregation by Nonplanar n-n Interactions  
By Sugiura, Hiroki et al  
From Journal of Organic Chemistry, 70(14), 5698-5708; 2005  
[Full Text](#)

[Experimental Procedure](#) **NEW**

## 物质链接的快捷菜单

物质的快捷菜单功能被加强和标准化，提供了相关信息的一键链接途径。

新的物质快捷菜单在物质结果集和反应结果集都是可以应用的。

菜单中也包含了物质的CAS号。**Export as Image**和**Export as molfile**是新的选项。**Synthesize this**等同于**Get Reactions where Substance is a Product**。

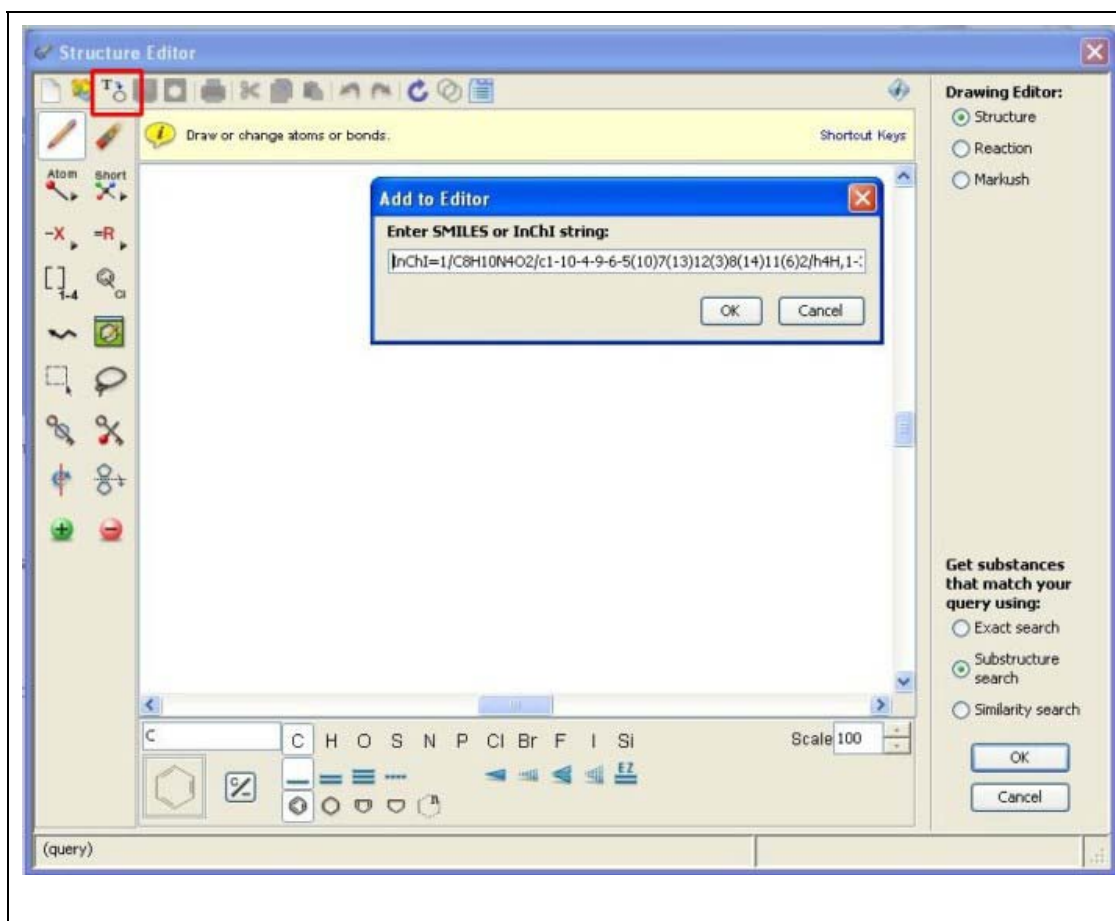
放大镜图标是一个可以选择的结构放大工具。

The screenshot shows a web-based chemical reaction interface. At the top, there are navigation buttons: 'Reactions', 'Get References', 'Find Additional Reactions', and 'Combine Answer Sets'. Below this, a status bar indicates '266 Reactions' and '0 Selected'. A search bar is present with 'Sort by: Relevance'. The main content area displays a reaction scheme for the reduction of 1-nitro-2-naphthol to 1-amino-2-naphthol. The product molecule is highlighted with a magnifying glass icon. A context menu is open over the product, listing various actions: 'View Substance Detail', 'Explore by Structure', 'Synthesize this', 'Get Reactions where Substance is a', 'Get Commercial Sources', 'Get Regulatory Information', 'Get References', 'Export as Image', and 'Export as molfile'. The 'Get Reactions where Substance is a' option is expanded to show roles: 'Product', 'Reactant', 'Reagent', 'Reactant/Reagent', 'Catalyst', 'Solvent', and 'Any Role'. The CAS Registry Number for the product is 91-59-8. The reaction conditions are listed as '1.1 R: HO-C(=O)-OH' and '2. IR3, C:Zn'. The yield is 87%. The interface also includes an 'Analysis' sidebar on the right with 'Analyze by:' and 'Catalyst' options.

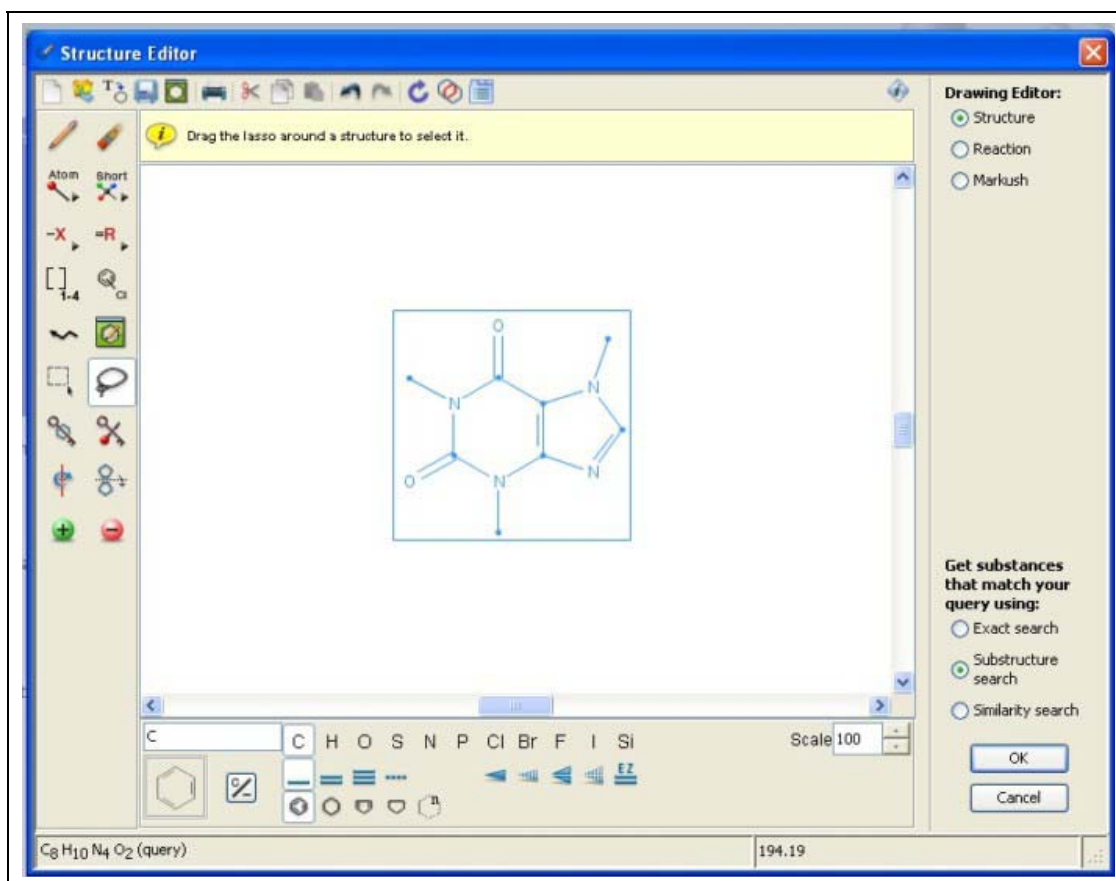
## 信息的检索

### 通过输入SMILES和InChI Strings检索物质

1. 用户可以在结构编辑界面输入SMILES (Simplified Molecular Input Line Entry Specification)或者InChI (International Chemical Identifier) strings。
2. 如果SMILES或者InChI string是用户仅有的信息，如今可以直接在SciFinder中进行检索。



3. SciFinder将这种字符串转化成2D结构式，可以直接用于结构及相关信息的检索，或者作为母核结构进行新的结构或亚结构检索。



### 从ACS的出版物中直接链接SciFinder的附加专利信息

ACS期刊的订阅者可以直接在SciFinder中点击新增的**Explore by Patents**，检索附加的或相关的专利信息。(预览版本不支持)

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## Review

### Current Progress on the Chemical Modification of Carbon Nanotubes

Nikolaos Karousis\* and Nikos Tagmatarchis  
Theoretical and Physical Chemistry Institute, National  
Hellenic Research Foundation, 48 Vassileos Constantinou  
Avenue, 116 35 Athens, Greece  
Dimitrios Tasis\*  
Department of Materials Science, 26504 Rio Patras,  
Greece

#### Abstracts

- Full Text HTML
- Hi-Res PDF (1570 kb)
- PDF w/ Links (753 kb)

Chem. Rev., Article ASAP

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\* To whom correspondence should be addressed. Tel.: +30 210 7273822 (N.K.); +30 2610 969811 (D.T.); Fax: +30 210 7273794 (N.K.); +30 2610 969368 (D.T.). E-mail: [nkarouside@tcm.ac.gr](mailto:nkarouside@tcm.ac.gr) (N.K.); [dtasis@upatras.gr](mailto:dtasis@upatras.gr) (D.T.).

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TAK-875: A Patent, Selective

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#### History

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Nikolaos Karousis  
Nikos Tagmatarchis  
Dimitrios Tasis