

HOW TO

使用新功能



SciFinder®

2010 年秋季

SciFinder® 的增强功能包括一个通过 SMILES 和 InChI™ 字符串检索结构的新选项、改善了反应答案集(结果集)显示、添加了实验步骤信息、反应答案集(结果集)的关联度排行以及标准化的物质上下文菜单。

使用答案集(结果集)

实验步骤

1. 来自精选（特定）期刊的反应答案集(结果集)现在包含了完整的实验步骤信息。这一（些）详细资料将有助于快速确定反应或合成策略（方案）是否适用。
2. “实验步骤”既是 **Sort**（排序）选项又是 **Analyze**（分析）选项，都包含反应答案集(结果集)。

The screenshot displays the SciFinder interface for a reaction. At the top, there are options for 'Reactions', 'Get References', and 'Combine Answer Sets'. Below this, a table lists reaction details with columns for 'Sort by:' (set to 'Relevance (New)'), 'Accession Number', 'Experimental Procedure', 'Number of Steps', 'Product Yield', and 'Publication Year'. A chemical reaction is shown with a 97% yield. On the right, the 'Analyze by:' dropdown is set to 'Experimental Procedure', and a 'Show More' button is visible. At the bottom, the 'Experimental Procedure' section is expanded, showing a detailed text description of the reaction conditions and analytical data.

Experimental Procedure

(M)-2,11-Diamino-1,12-dimethylbenzo[*c*]phenanthrene-5,8-dicarbonitrile, (M)-8-A solution of (M)-7[1 g, 2.53 mmol] in ethanol (40 mL) and tetrahydrofuran (40 mL) was heated to 90 °C, to which was added concentrated hydrochloric acid (1.2 mL) and reduced iron (24 g, 43 mmol). After being stirred at 90 °C for 1 h, the reaction mixture was filtered through Celite pad, and the pad was washed three times with ethyl acetate. The organic layers were washed with saturated aqueous sodium hydrogen carbonate, brine, and dried over sodium sulfate. The solvents were evaporated under reduced pressure, and recrystallization from hexane-acetone gave (M)-8(823 mg, 2.45 mmol, 97%) mp > 300 °C (hexaneacetone); $[\alpha]_D^{24}$ 0 - 1990 (c 0.10, acetone); LRMS (EI, 70 eV) m/z 336 (M^+ , 100), 304 ($M^+ - 2NH_2$, 38); HRMS m/z calcd for $C_{22}H_{16}N_4$ 336.1375, found 336.1383; UV-vis ($CHCl_3$, 0.01 mM) λ (e) 258 nm (3.3×10^4), 280 nm (2.4×10^4), 318 nm (3.3×10^4), 357 nm (2.3×10^4), 435 nm (4.4×10^3), 461 nm (6.2×10^3); IR (KBr) 3500-3200, 2224 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 17.2 (s), 116.9, 117.8, 118.5, 124.0, 124.6, 128.3, 128.4, 130.2, 132.5, 145.0. Anal. ($C_{22}H_{16}N_4$) Calcd: C, 78.55; H, 4.79; N, 16.66. Found: C, 78.13; H, 5.09; N, 16.19.

反应答案集(结果集)的关联度(相似度)排行

1. **关联度(相似度)**排行是反应答案集(结果集)的新默认 **Sort(排序)** 选项。**关联度(相似度)**最高的答案将显示在最先位置。这能加快查看答案集(结果集)的速度。
2. **关联度(相似度)**是由 Tanimoto 相似性确定的。

266 Reactions 0 Selected | Knows Collected | Previous Collected

Sort by: Relevance

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

1. View Reaction Detail [Link](#) [Similar Reactions](#)

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

87%

Overview

Steps/Stages

1.1 R:

HO-C(=O)-OH

• 2 H₂

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

检索结果显示

增强的反应显示

1. 更简洁、流线型反应显示改善了可读性、允许(便捷您)更快地查看答案,并加快决策速度(提升您的决策能力)。
2. 看将显示设置为 Schema(图解)和 Overview(概览)或 Schema Only(仅图解)。
3. 可使用精选期刊中的 Experimental Procedure(实验步骤)。

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:H₂O, 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 Sugiyama, Hiroki et al

From Journal of Organic Chemistry, 70(14), 5698-5708; 2005

Full Text

Experimental Procedure **NEW**

一致（标准）的物质上下文菜单

物质上下文菜单已得到增强和标准化，提供对相关信息的直接一键式访问。

在物质和反应答案集(结果集)中都可使用新的物质上下文菜单。

CAS Registry Number[®] 包含在菜单中。**Export as Image**（导出为图像）和 **Export as molfile**（导出为 molfile）是新选项。**Synthesize this**（合成此物质）相当于 **Get Reactions where Substance is a Product**（获取反应，其中物质是一种产品）。

放大镜是缩放选项。

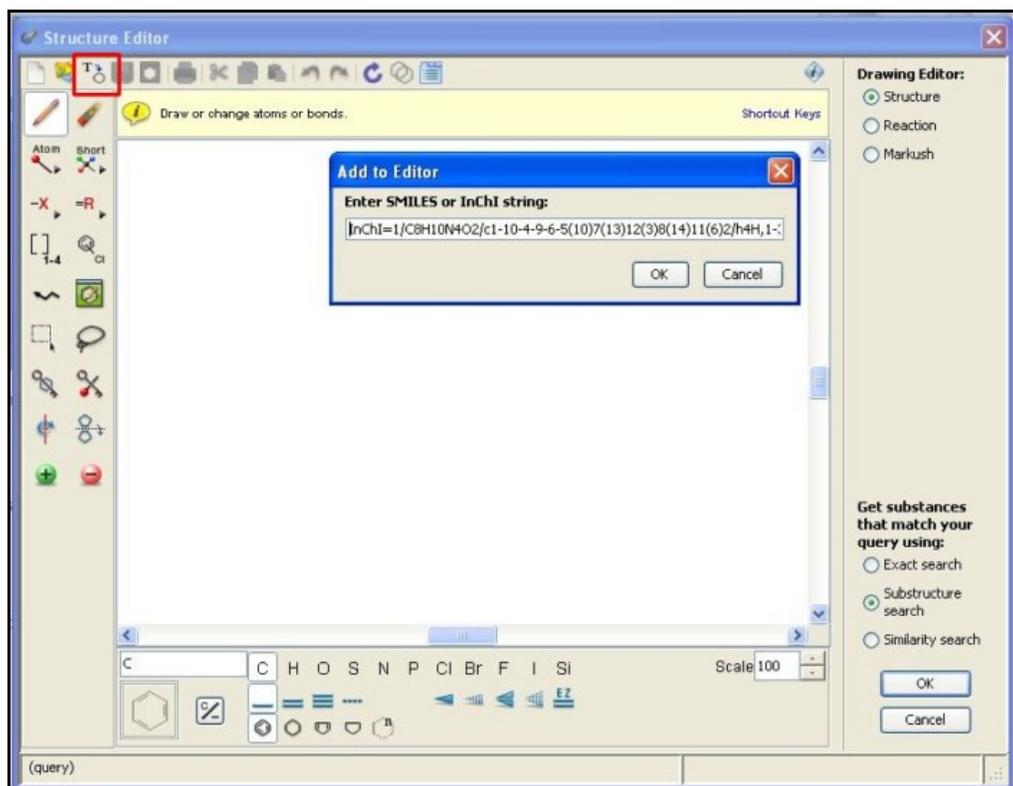


The screenshot shows the 'Reactions' interface. At the top, there are tabs for 'Get References', 'Find Additional Reactions', and 'Combine Answer Sets'. Below the tabs, there are options for 'Select All', 'Deselect All', and 'Sort by: Relevance'. The main area displays a chemical reaction: a naphthalene ring with a hydroxyl group and a bromine atom reacting to form a naphthalene ring with a bromine atom and a hydroxyl group, with a yield of 87%. A context menu is open over the product, listing options such as 'View Substance Detail', 'Explore by Structure', 'Synthesize this', 'Get Reactions where Substance is a Product', 'Get Commercial Sources', 'Get Regulatory Information', 'Get References', 'Export as Image', and 'Export as molfile'. The 'Synthesize this' option is highlighted. On the right side, there is an 'Analyze by:' section with a dropdown menu for 'Catalyst' and a list of catalysts including Pd, AcOH, Ni, and Pt. Below the list, there is a 'Show More' button.

查找信息

通过输入 SMILES 和 InChI 字符串检索结构

1. 该功能允许用户将 SMILES（Simplified Molecular Input Line Entry Specification，简化分子线性输入规范）或 InChI（International Chemical Identifier，国际化学识别符）字符串输入到结构绘图编辑器中。
2. 如果 SMILES 或 InChI 是用户掌握的唯一信息，则其仅可用于 Explore in SciFinder（在 SciFinder 中检索）。



The screenshot shows the 'Structure Editor' interface. At the top, there is a toolbar with various icons, including a 'T' icon for text entry. Below the toolbar, there is a yellow banner that says 'Draw or change atoms or bonds.' and 'Shortcut Keys'. The main area is a large white space for drawing the structure. A dialog box titled 'Add to Editor' is open in the center, with the text 'Enter SMILES or InChI string:' and a text input field containing the InChI string: InChI=1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-. Below the input field are 'OK' and 'Cancel' buttons. On the right side, there is a 'Drawing Editor:' section with three radio buttons: 'Structure' (selected), 'Reaction', and 'Markush'. Below this, there is a section titled 'Get substances that match your query using:' with three radio buttons: 'Exact search', 'Substructure search' (selected), and 'Similarity search'. At the bottom right, there are 'OK' and 'Cancel' buttons. At the bottom left, there is a '(query)' label.

通过输入 SMILES 和 InChI 字符串检索结构 – 续

3. SciFinder 将字符串重新转换为一个二维结构，随后可被用于检索结构和相关信息，或充当新（子）结构搜索的基础。

