

HOW TO

使用新功能



SciFinder®

Fall 2010

SciFinder推出的新功能包括：使用SMILES和InChi字串输入结构,改善了反应结果的显示，添加了实验过程的信息，添加了反应关联度的排列，并且标准化了物质信息的菜单。

查看结果集

实验过程

1. 来自特定期刊的反应结果集现在包含了完整的实验步骤信息。这一详细资料将有助于快速确定反应或合成策略是否适用。
2. “实验过程”既是反应结果集的一种排序选项又是一种分析选项。

The screenshot displays the SciFinder interface for a reaction. At the top, there are tabs for 'Reactions', 'Get References', and 'Combine Answer Sets'. Below this, a search bar shows '61 Reactions' and options to 'Select All' or 'Deselect All'. A dropdown menu is open, showing sorting options: 'Relevance (New)', 'Accession Number', 'Experimental Procedure', 'Number of Steps', 'Product Yield', and 'Publication Year'. The 'Experimental Procedure' option is highlighted. Below the search bar, a chemical reaction is shown, involving a complex polycyclic aromatic hydrocarbon derivative. The reaction is labeled '1. View Reaction' and 'Single Step'. Below the reaction, there is a section for 'Experimental Procedure' with a 'Show More' button. The procedure text is as follows: (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); [α]_D²⁴ -1990 (c 0.10, acetone); LRMS (EI, 70 eV) m/z 336 (M⁺, 100), 304 (M⁺ - 2NH₂, 38); HRMS m/z calcd for C₂₂H₁₄N₄ 336.1375, found 336.1383; UV-vis (CHCl₃, 0.01 mM) λ (ε) 258 nm (3.3 × 10⁴), 280 nm (2.4 × 10⁴), 318 nm (3.3 × 10⁴), 357 nm (2.3 × 10⁴), 435 nm (4.4 × 10⁴), 461 nm (6.2 × 10⁴); IR (KBr) 3500-3200, 2224 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 1.53 (6H, s), 4.15 (4H, s), 7.26 (2H, d, J = 8.6 Hz), 7.97 (2H, s), 8.13 (2H, d, J = 8.6 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 17.2, 109.8, 116.9, 117.8, 118.5, 124.0, 124.6, 128.3, 128.4, 130.2, 132.5, 145.0. Anal. (C₂₂H₁₄N₄) Calcd: C, 78.55; H, 4.79; N, 16.66. Found: C, 78.13; H, 5.09; N, 16.19.

依据关联度排列反应结果集

1. 关联度排行是反应结果集的新默认排序选项。关联度最高的答案将显示在最先位置。这能加快查看结果集的速度。
2. 关联度是由Tanimoto相似性确定的。

Reactions interface showing a dropdown menu for sorting options. The 'Relevance' option is highlighted. Below the menu, a chemical reaction is shown: a nitro-substituted naphthalene derivative is reduced to an amino-substituted naphthalene derivative with an 87% yield. The interface includes buttons for 'Get References', 'Find Additional Reactions', and 'Combine Answer Sets'. A 'Sort by:' dropdown menu is open, listing options: Relevance, Accession Number, Experimental Procedure, Number of Steps, Product Yield, and Publication Year. The 'Relevance' option is selected and highlighted with a pink box. Below the reaction, there is an 'Overview' section with 'Steps/Stages' and 'Notes'.

结果显示

改善了反应结果的显示

1. 简洁、流线型的反应显示改善了反应结果集的可读性、允许更快地查看结果，帮助您更快的做决策。
2. 将显示设置为图解和概览或仅图解。
3. 可以查看特定期刊中的实验过程。

Reactions interface showing a chemical reaction. The reaction shows a complex polycyclic aromatic hydrocarbon with multiple nitro and cyano groups being reduced to its corresponding diamine derivative with a 97% yield. The interface includes buttons for 'View Reaction Detail', 'Link', and 'Similar Reactions'. A 'Display:' dropdown menu is open, showing options for 'Overview', 'Steps/Stages', and 'Experimental Procedure'. The 'Experimental Procedure' option is highlighted with a pink box. Below the reaction, there is an 'Overview' section with 'Steps/Stages' and 'Notes'.

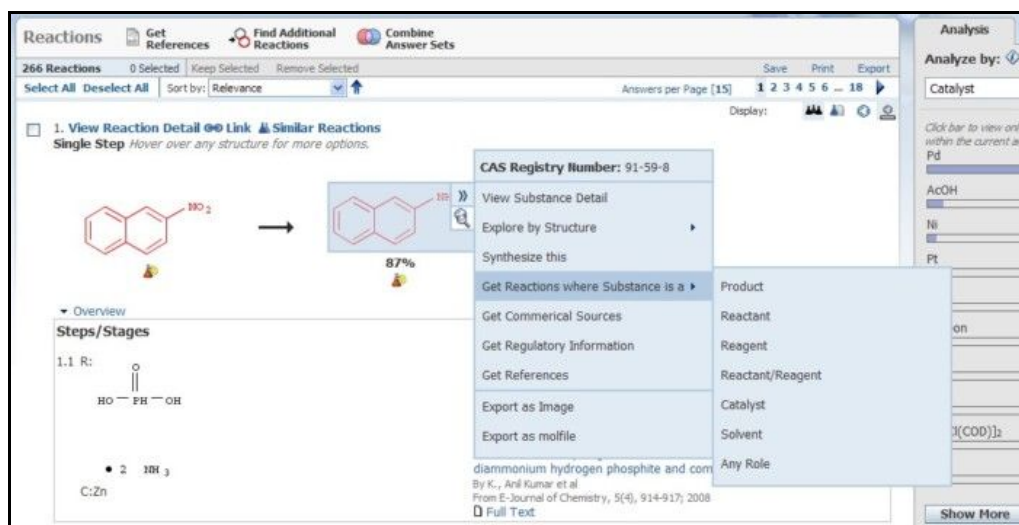
标准化了物质信息菜单

增强和标准化了物质信息菜单，提供对相关信息的一键式访问。

在反应和物质结果集中，都可以使用新的物质标准化菜单。

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)是新的选项。Synthesize this 等同于获取该物质为产物的反应。

放大镜是缩放选项。



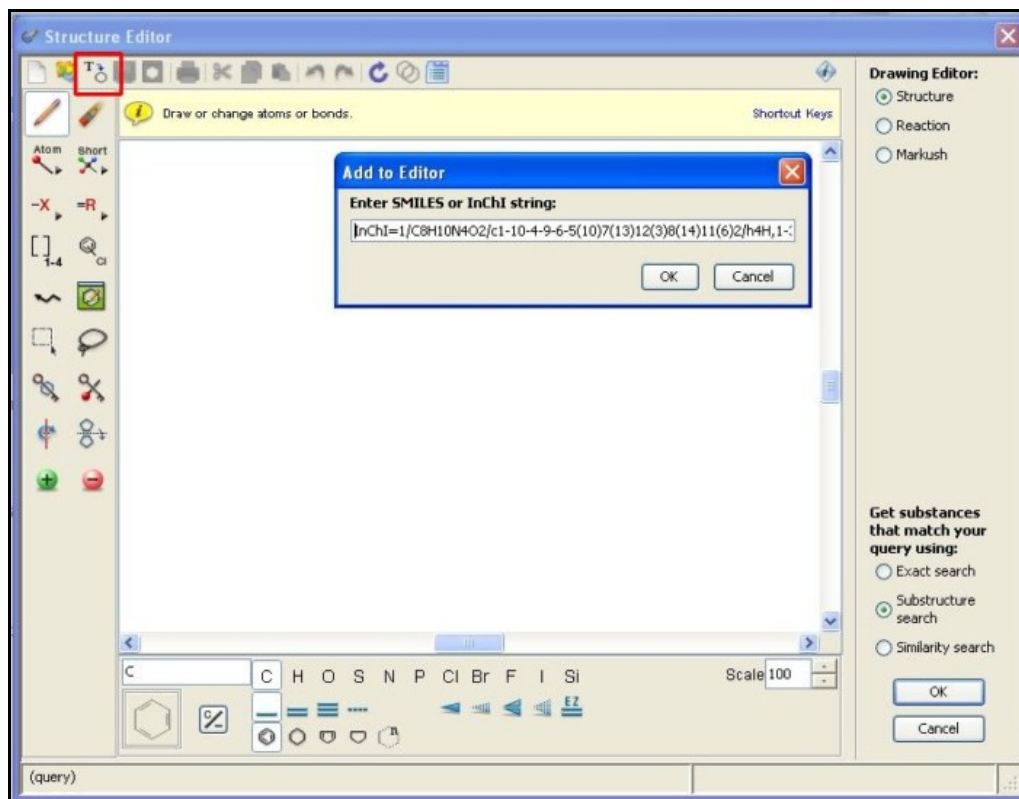
The screenshot shows the 'Reactions' window in a software application. It displays a chemical reaction where a naphthalene derivative with a nitro group reacts to form a naphthalene derivative with a nitro group and a methyl group, with a yield of 87%. A context menu is open over the product, listing 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' menu is further expanded to show roles: 'Product', 'Reactant', 'Reagent', 'Reactant/Reagent', 'Catalyst', 'Solvent', and 'Any Role'. The interface also includes a search bar, a list of reactions, and a sidebar with analysis options.

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 (简化分子线性输入规范)或 InChI (国际化学识别符)字符串输入到结构绘图编辑器中。

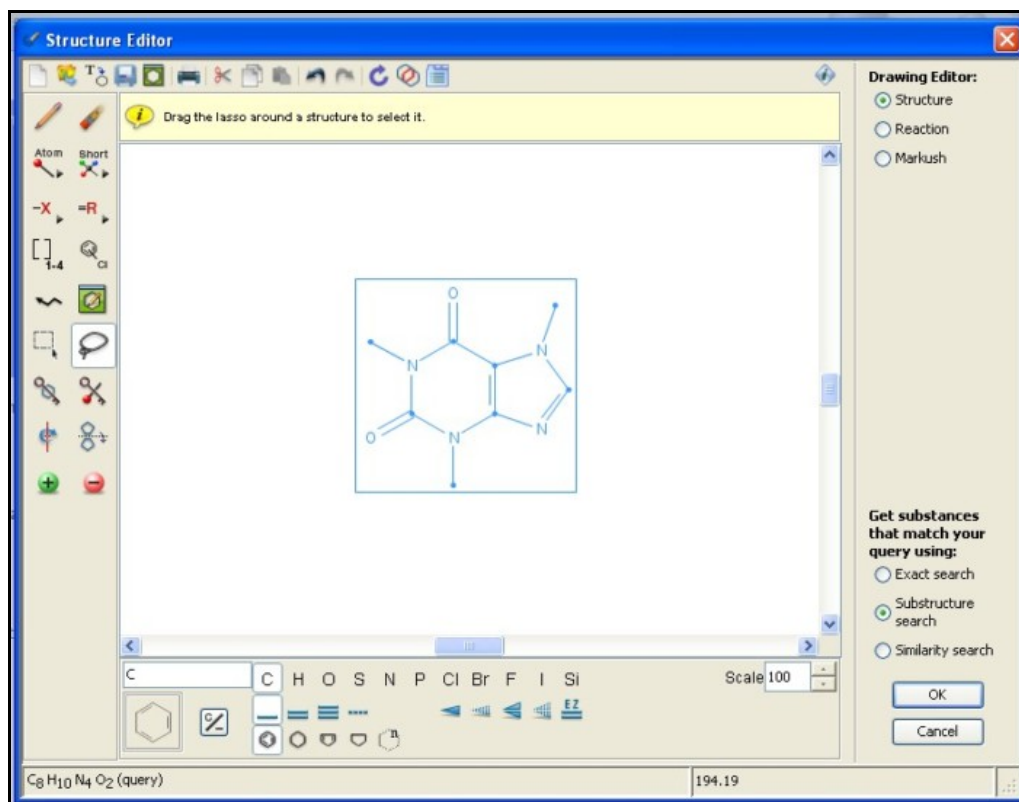
2. 如果SMILES或InChI是用户掌握的唯一信息，现在就可以在SciFinder中进行检索



The screenshot shows the 'Structure Editor' window. A dialog box titled 'Add to Editor' is open, prompting the user to 'Enter SMILES or InChI string:'. The input field contains the InChI string: InChI=1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-. The dialog has 'OK' and 'Cancel' buttons. The background shows the structure editor interface with various drawing tools and a drawing editor panel on the right.

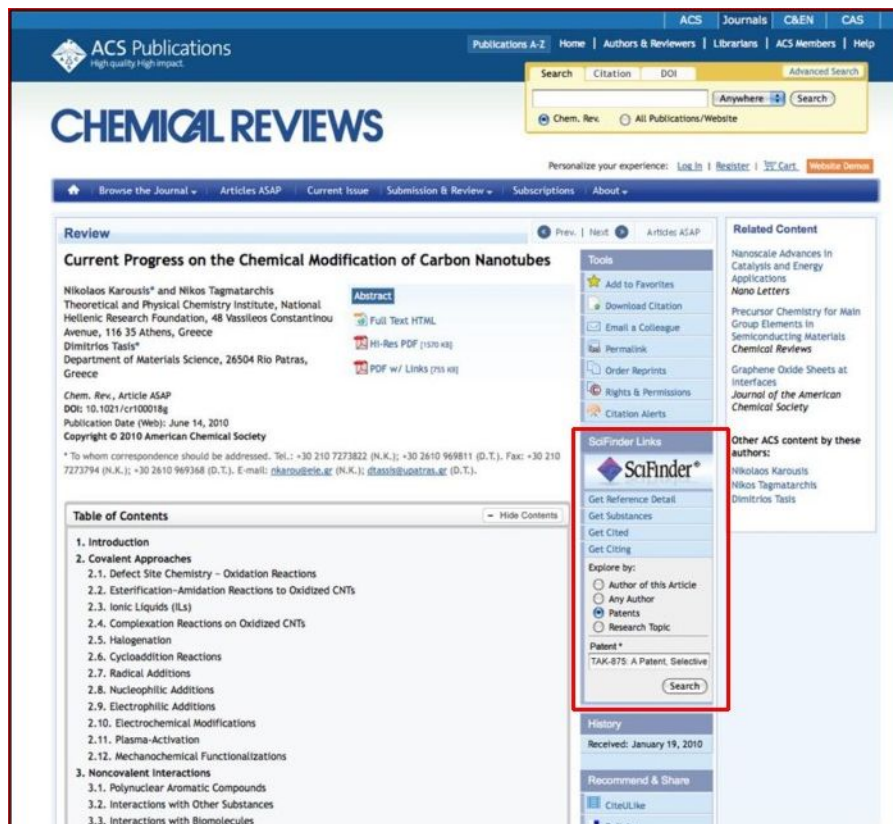
通过输入SMILES和InChI字符串检索结构---续

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



从ACS全文，可直接链接到SciFinder中相关的专利

ACS期刊的订阅者可在一篇文章中使用新的Explore by Patents (按专利搜索)选项查找其他或相关专利信息。(不可在预览时使用)



如有疑问，通过下列联系方式可获取更为详细的信息

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