

SciFinderⁿ 使用技巧手冊

2024 年 12 月 19 日

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SciFinderⁿ 使用技巧 | 專利資訊的獲取—— PatentPak 的使用

References ▾ pcsk9 inhibitors

Document Type

- Journal (2M)
- Patent (271K)**
- Review (234K)
- Biography (79)
- Book (684)

Substance Role

- Adverse Effect (19)
- Analytical Study (123)
- Biological Study (621)
- Combinatorial Study (2)
- Occurrence (2)

Language

- English (125K)
- Chinese (53K)

Treating autosomal dominant hypercholesterolemia associated with PCSK9 gain-of-function mutations using a PCSK9 inhibitor, such as anti-PCSK9 antibody

By: Swergold, Gary; Mellis, Scott; Sasiela, William J.
World Intellectual Property Organization, WO2014194111 A1 2014-12-04 | Language: English, Database: Cplus
View Reference Detail

Abstract: The present invention provides methods for treating autosomal dominant hypercholesterolemia (ADH). According to certain embodiments, the ADH is caused by or associated with a gain-of-function mutation (GOFm) in a gene encoding PCSK9. The GOFm encodes a PCSK9 variant protein comprising an amino acid substitution of V4I, E32K, D35Y, E48K, P71L, R96C, L108R, S127R, D129N, R215H, F216L, R218S, R357H, D374H, D374Y, S465L or R496W. The present invention therefore includes methods comprising selecting a patient who carries a GOFm in one or both alleles of the PCSK9 gene, and administering to the patient a pharmaceutical composition comprising a PCSK9 inhibitor. In certain embodiments, the PCSK9 inhibitor is an anti-PCSK9 antibody such as the exemplary antibody referred to herein as mAb316P (Alirocumab).

PATENTPAK Text Substances (22) Reactions (0) Cited By (7) Citation Map

Patent	Language	Kind Code	PDF	PDF+	Viewer
WO2014194111	English	A1	PDF	PDF+	Viewer
US20140356370	English	A1	PDF		
AU2014274077	English	A1	PDF		
CN105263963	Chinese	A	PDF		
KR2016013046	Korean	A	PDF		
JP2016522211	Japanese	T	PDF		
JP6423868	Japanese	B2	PDF		

kexin 9 (PCSK9) inhibitors for treating complications associated therewith

13-11-21 | Language: English, Database: Cplus

an inflammatory response to infection and complications
tein convertase subtilisin kexin 9 (PCSK9) inhibitor to a subject,
monoclonal antibody or antigen-binding fragment thereof. The
AR236553/REGN727 (Alirocumab); RN-316; LGT209; or RG7652.

The PCSK9 inhibitor may be a peptide mimetic. The PCSK9 inhibitor may be an EGFA domain mimic, EGF-A peptide, a fibronectin-based scaffold domain proteins, or a neutralizing PCSK9 variant. The PCSK9 inhibitor

1. 在文獻結果集中選擇文獻類型為Patent
2. 點擊 PatentPak 旁的小箭頭，查看專利族列表
3. PDF: 獲取專利PDF 全文
4. PDF+: 獲取附有物質標記資訊的專利 PDF 全文
5. Viewer: PatentPak 流覽器，線上快速閱讀專利全文

PatentPak 流覽器

Key Substances in Patent

CAS RN
1297530-29-0

Analyst Markup Locations (1)
Page 76

CAS RN
1297530-36-9

Analyst Markup Locations (1)
Page 76

CAS RN
1297530-33-6

Analyst Markup Locations (1)
Page 76

CAS RN
1297530-49-4

PAGE: 76 / 86

ZOOM: - +

DOWNLOAD: PDF PDF+

4

5 oxoethyl)-1,3-dioxane-2-carboxamide;
2-methyl-5-*l*-((5-methyl-2-phenyloxazol-4-yl)methyl)-N-(2-morpholino-2-oxoethyl)-1,3-dioxane-2-carboxamide;

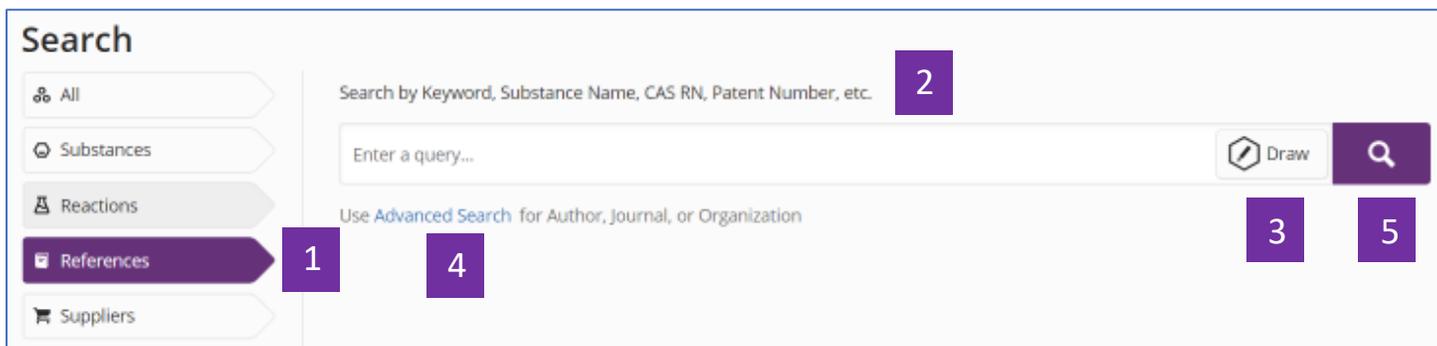
10 2-methyl-5-*c*-((5-methyl-2-phenyloxazol-4-yl)methyl)-N-(2-(4-methylpiperazin-1-yl)-2-oxoethyl)-1,3-dioxane-2-carboxamide;
2-methyl-5-*c*-((5-methyl-2-phenyloxazol-4-yl)methyl)-N-(2-oxo-2-(piperidin-1-yl)methyl)-1,3-dioxane-2-carboxamide;

15 2-methyl-5-*c*-((5-methyl-2-phenyloxazol-4-yl)methyl)-N-(2-oxo-2-(1,1-dioxidothiomorpholino)-2-oxoethyl)-2-methyl-5-*c*-((5-methyl-2-phenyloxazol-4-yl)methyl)-1,3-dioxane-2-carboxamide;

20 2-methyl-5-*c*-((5-methyl-2-phenyloxazol-4-yl)methyl)-N-(2-oxo-2-(((tetrahydro-2H-pyran-4-yl)methyl)amino)ethyl)-1,3-dioxane-2-carboxamide;
2-methyl-5-*c*-((5-methyl-2-phenyloxazol-4-yl)methyl)-N-(3-morpholino-3-oxopropyl)-1,3-dioxane-2-carboxamide;
2-methyl-5-*c*-((5-methyl-2-phenyloxazol-4-yl)methyl)-N-(3-oxo-3-(((tetrahydro-2H-pyran-4-yl)methyl)amino)propyl)-1,3-dioxane-2-carboxamide;
2-methyl-5-*c*-((5-methyl-2-phenyloxazol-4-yl)methyl)-N-(3-oxo-3-thiomorpholinopropyl)-1,3-dioxane-2-carboxamide;

1. 物質位置資訊：點擊頁碼定位符號，右側PDF 全文快速跳轉至該物質出現的頁碼處，同時對應物質的位置符號由藍色變為紫色。
2. PDF 全文中對應的物質位置符號
3. 點擊 CAS 登記號，獲取物質詳情
4. 下載專利全文：PDF: 獲取專利 PDF 全文；PDF+: 獲取附有物質標記資訊的專利 PDF 全文。

SciFinderⁿ 使用技巧 | 文獻資訊的獲取



1. 選擇 **References**，進行文獻檢索
2. 輸入檢索資訊：關鍵字、物質名稱、**CAS** 登記號和專利號等
3. 點擊 **Draw**，繪製檢索。並在2所示的文字方塊中輸入相應文本，獲取相關文獻，所得文獻結果包含輸入文本及繪製的物質（反應）結構
4. 點擊 **Advanced Search**，進行作者、期刊名或組織機構名檢索
5. 點擊放大鏡，開始檢索

The screenshot shows a search results page for 'References' (664). The interface includes a left sidebar with filters for Relevance (Best, Good, Fair), Document Type (Journal, Patent, Review, Book, Clinical Trial), and Language (English, German, Chinese, Spanish, Russian). The main content area displays two search results. The first result is 'Synthesis, Surface and Thermodynamic Properties of Substituted Polytriethanolamine Nonionic Surfactants' with an abstract describing the synthesis and properties of surfactants. The second result is 'Novel method for preparing polyols by transesterification and thiolation' with an abstract describing a method for preparing polyols. Numbered callouts (1-13) point to specific UI elements: 1 (Sort dropdown), 2 (View dropdown), 3 (Filter by dropdown), 4 (PDF icon), 5 (Email icon), 6 (Save icon), 7 (Abstract text), 8 (Full Text dropdown), 9 (Substances icon), 10 (Reactions icon), 11 (Cited By icon), 12 (Reaction Map icon), and 13 (Return to Home link).

1. 點擊 **Sort** 右側小箭頭，對結果按照引用次數，公開年份等重新進行排序
2. 點擊 **View** 右側小箭頭，選擇結果展示的詳略
3. 全面的文獻結果篩選選項
4. 通過PDF, rtf, ris, txt等格式下載檢索結果
5. 通過電子郵件分享檢索結果
6. 保存檢索結果，並可同時設定資訊更新提醒
7. 查看文獻詳情
8. 獲取全文連結
9. 獲取文獻中的物質
10. 獲取文獻中的反應
11. 獲取被引用文獻

12. 引文地圖，獲取引用及被引用文獻

13. 回到首頁介面

The screenshot shows a reference detail page for the article "Synthesis, Surface and Thermodynamic Properties of Substituted Polytriethanolamine Nonionic Surfactants". The page is annotated with purple boxes containing numbers 1 through 8, corresponding to the numbered list below. Callout 1 points to the "Return to Results" link. Callout 2 points to the "Journal" section. Callout 3 points to the "Citation Map" button. Callout 4 points to the "Prev" and "Next" navigation arrows. Callout 5 points to the "Full Text" button. Callout 6 points to the "Concepts" dropdown menu. Callout 7 points to the "Company/Organization" section. Callout 8 points to the "Citations" section.

1. Return to Results

2. Journal

3. Citation Map

4. Prev Next

5. Full Text

6. Concepts

7. Company/Organization

8. Citations

1. 返回至文獻結果集介面

2. 文獻書目資訊

3. 文獻相關資訊：物質、反應、引文

4. 點擊左右箭頭，查看上一篇或下一篇文章詳情

5. 全文連結

6. 概念詞語

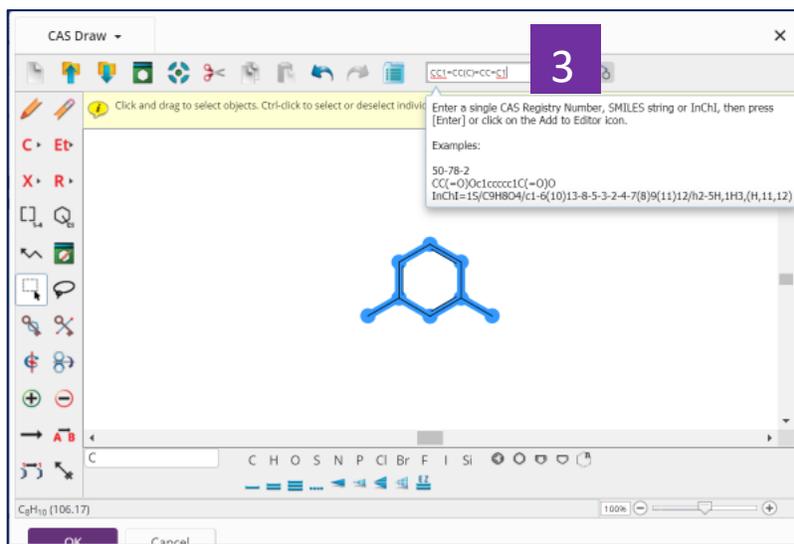
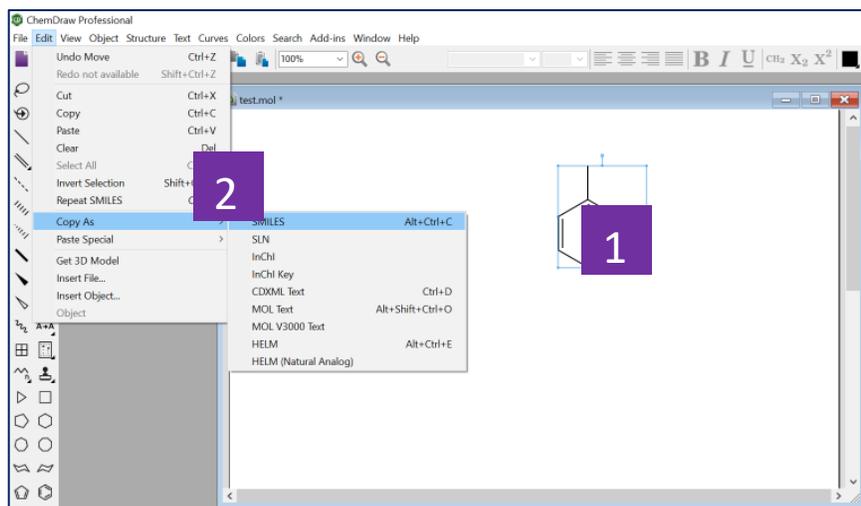
7. 文獻中報導的物質

8. 引文信息

SciFinderⁿ 使用技巧 | 與 ChemDraw 聯用

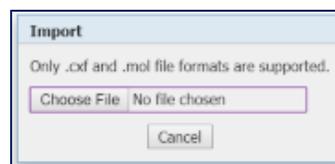
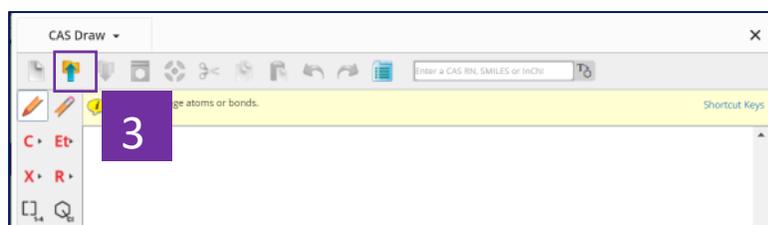
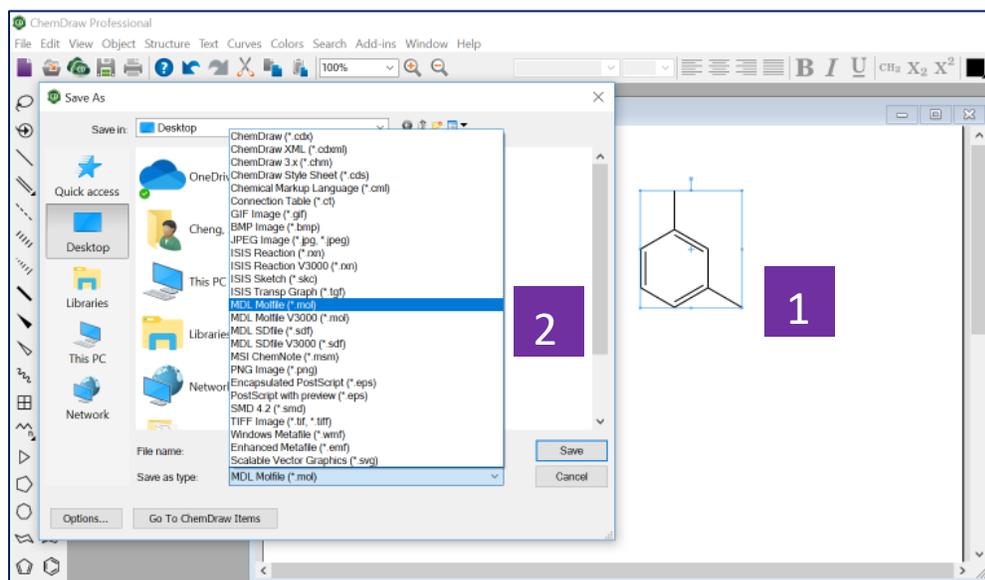
可通過以下三種方式利用 ChemDraw 所繪製的結構在 SciFinderⁿ 中進行檢索。

一. 利用在 ChemDraw 中獲得的物質 SMILES、InChI，將結構導入到 SciFinderⁿ 的結構編輯器中



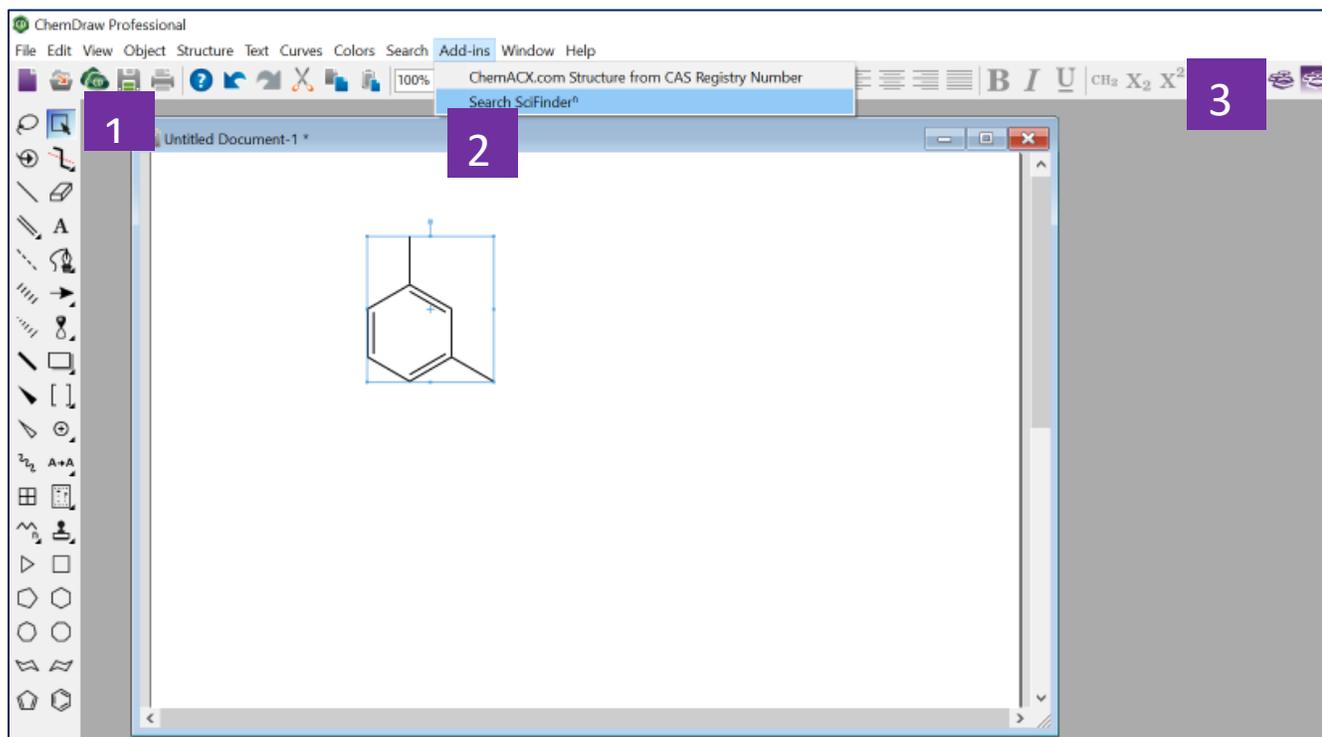
1. 在 ChemDraw 中繪製好結構，並選中
2. 點擊上方功能表 Edit，選擇 Copy As，然後再選擇 SMILES 或 InChI
3. 在此粘貼在 ChemDraw 中獲得的 SMILES 或 InChI，將結構導入到 SciFinderⁿ 的結構編輯器中。

二. 將 ChemDraw 中繪製的結構保存為 .mol 格式檔，然後再導入到 SciFinderⁿ 的結構編輯器中



1. 在 ChemDraw 中繪製好結構，並選中
2. 點擊上方功能表 File，選擇 Save As, 將其保存為 MDL Molfile (*.mol) 格式的檔
3. 導入結構
4. 根據保存的路徑，導入 .mol 格式的檔

三. 直接在 ChemDraw 18.2 以上版本中，點擊 Search SciFinder[®] 或點擊右上角的 SciFinder[®] 標識圖示在 SciFinder[®] 中進行檢索



1. 在 ChemDraw18.2 以上的版本中繪製結構，並選中該結構
2. 點擊上方功能表中的 Add-ins，並選中 Search SciFinder[®]，開始在 SciFinder[®] 中進行檢索
3. 也可以直接點擊右上角 SciFinder[®] 的標識圖，開始在 SciFinder[®] 中進行檢索

SciFinderⁿ 使用技巧 | 逆合成路線的獲取——Retrosynthesis 的使用

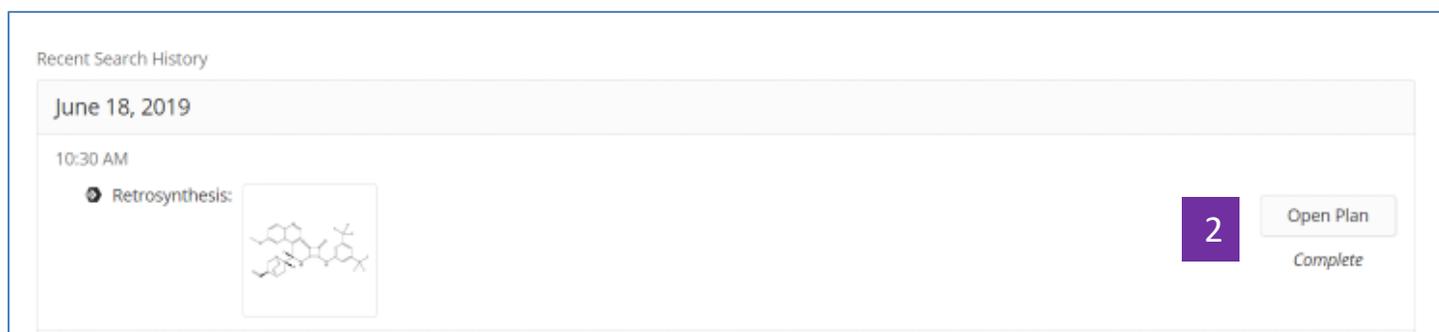
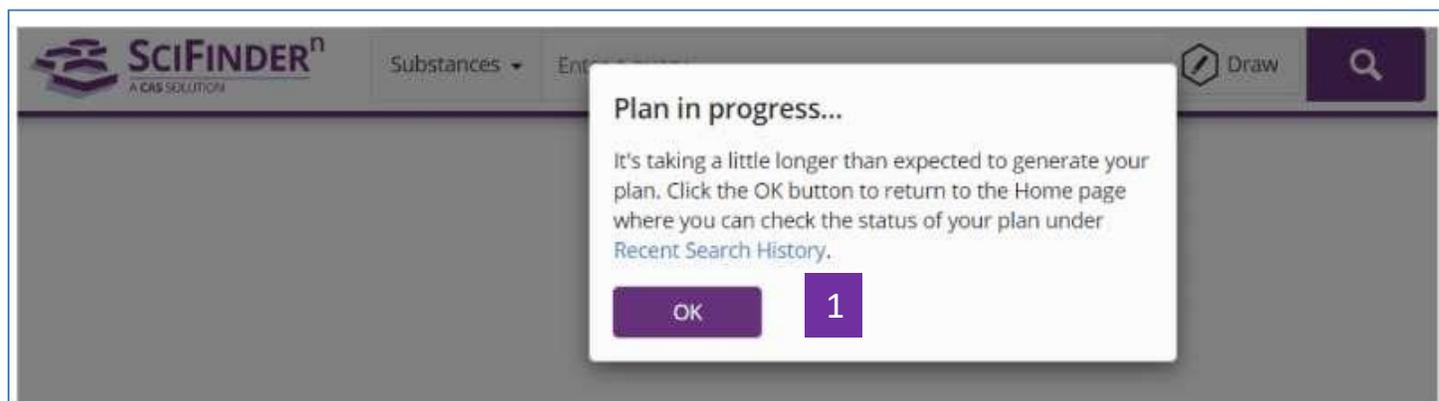
The screenshot displays the SciFinder interface for the substance Sofosbuvir (CAS RN 1190307-88-0). On the left, the 'Substances (1)' panel shows the chemical structure and a purple box with the number '1' next to it. Below the structure, the molecular formula $C_{22}H_{29}FN_3O_9P$ and the name 'Sofosbuvir' are listed, along with statistics: 2,644 References, 567 Reactions, and 75 Suppliers. On the right, the 'CAS Detail' panel shows the CAS RN and Name, and a list of actions: Substance Detail, Reactions (567), Synthesize (498), **Create Retrosynthesis Plan** (with a purple box and number '2'), References (2,644), and Suppliers (75). To the right of the panels is a larger view of the chemical structure with absolute stereochemistry shown, and buttons for 'Edit Structure', 'Reset', and a download icon.

1. 在SciFinderⁿ中找到所需合成物質後，點擊物質結構
2. 在快顯視窗中點擊：**Create Retrosynthesis Plan**

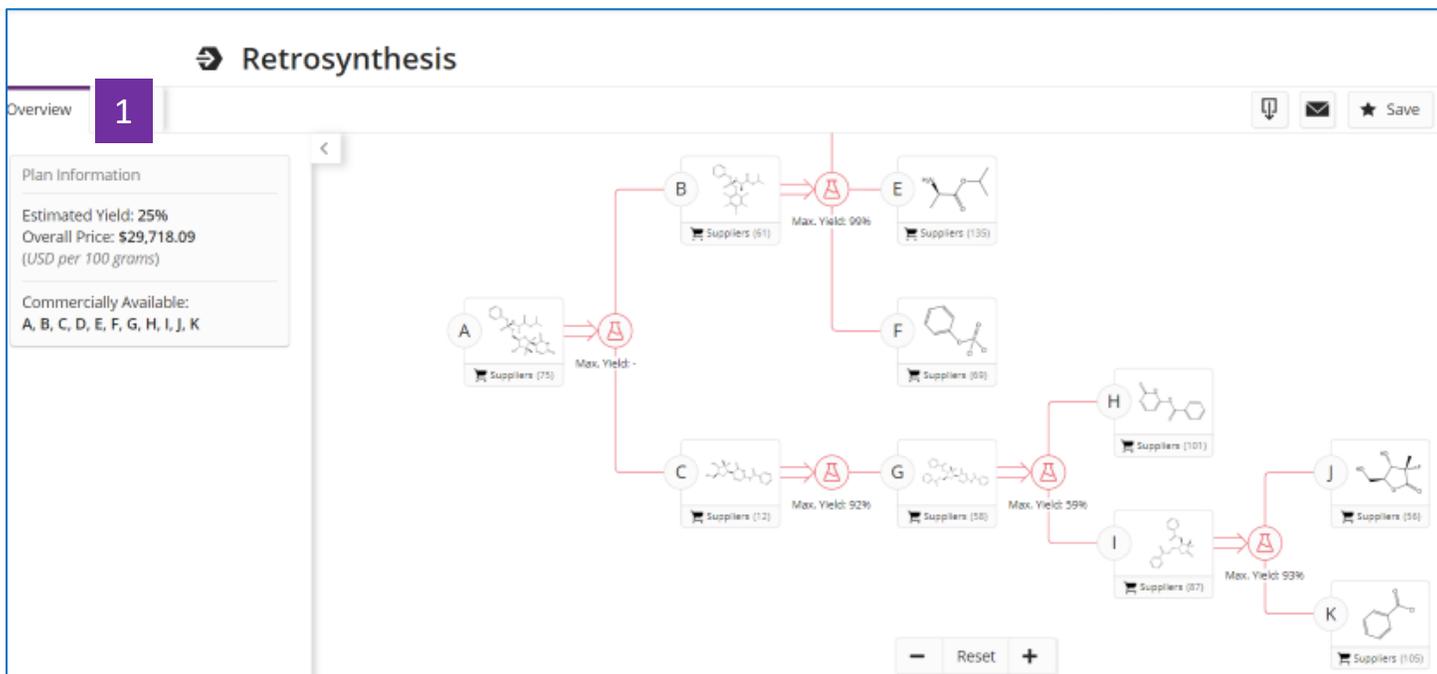
The screenshot shows the 'CAS Draw' editor window on the left, where the chemical structure of Sofosbuvir is being drawn. A purple box with the number '1' is placed over the structure. The editor includes a toolbar with various drawing tools and a search bar. On the right, a pop-up menu is visible, containing an 'Edit' button, a search icon, a thumbnail of the structure with a retrosynthesis arrow, and buttons for 'Edit Drawing', 'Remove', and **Create Retrosynthesis Plan** (with a purple box and number '2').

3. 在結構編輯器中繪製所需合成結構

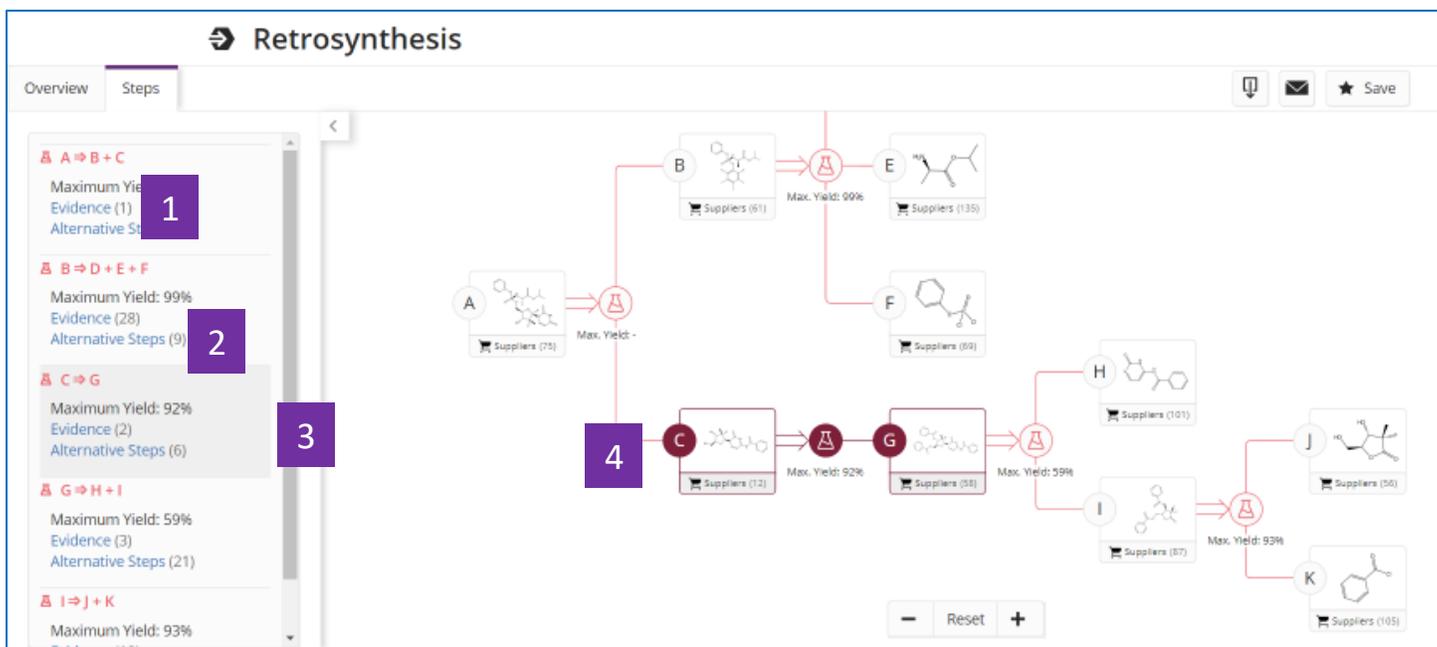
4. 點擊: Create Retrosynthesis Plan



1. 如果出現這種提示，點擊OK
2. 稍後點擊Recent Search History中的Open Plan



1. Overview顯示完整逆合成路線，預估產率和成本



1. 精確匹配反應物和產物結構的反應，點擊即獲得反應資訊詳情
2. 可替代步驟

- 當滑鼠移到某一步驟時
- 右側路線圖中該反應的反應物和產物標識轉為反亮

The screenshot displays a web interface for chemical reactions. On the left, a sidebar lists several reaction types: **A → B + C** (Maximum Yield: Evidence (1), Alternative Steps), **B → D + E + F** (Maximum Yield: 99%, Evidence (28), Alternative Steps (9)), **C → G** (Maximum Yield: 92%, Evidence (2), Alternative Steps (6)), and **G → H + I** (Maximum Yield: 59%, Evidence (3), Alternative Steps (21)). A purple box with the number '1' highlights the 'Evidence (1)' link for the first reaction.

The main area is titled 'Reactions (1)' and features a purple box with the number '2' above the reaction scheme. The reaction scheme shows the synthesis of Sofosbuvir from cytidine. Below the scheme, there are buttons for 'Suppliers (61)', 'Suppliers (12)', and 'Suppliers (75)'. A 'Reaction Summary' table is visible, listing reagents (Water), catalysts (-), and solvents (Tetrahydrofuran). On the right, there is a 'Process for synthesizing Sofosbuvir from cytidine' section with a 'View Reference Detail' link, author information (By: Liu, Ke), and a patent reference (China, CN105646626 A 2016-06-08). Buttons for 'PATENTPAK' and 'Full Text' are also present.

- 點擊Evidence
- 查看反應資訊詳情

Overview Steps

A ⇒ B + C
 Maximum Yield: -
 Evidence (1)
 Alternative Steps (51) **1**

B ⇒ D + E + F
 Maximum Yield: 99%
 Evidence (28)
 Alternative Steps (9)

C ⇒ G
 Maximum Yield: 92%
 Evidence (2)
 Alternative Steps (6)

G ⇒ H + I
 Maximum Yield: 59%
 Evidence (3)
 Alternative Steps (21)

Alternative Steps (51)

2 Select Evidence (2) Maximum Yield: -

3 of 51

Select Evidence (8) Maximum Yield: **88%**

Retrosynthesis

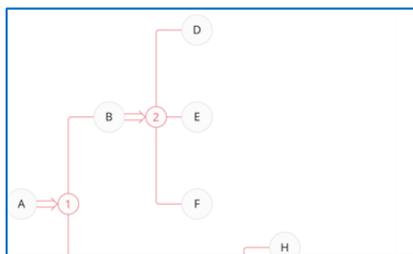
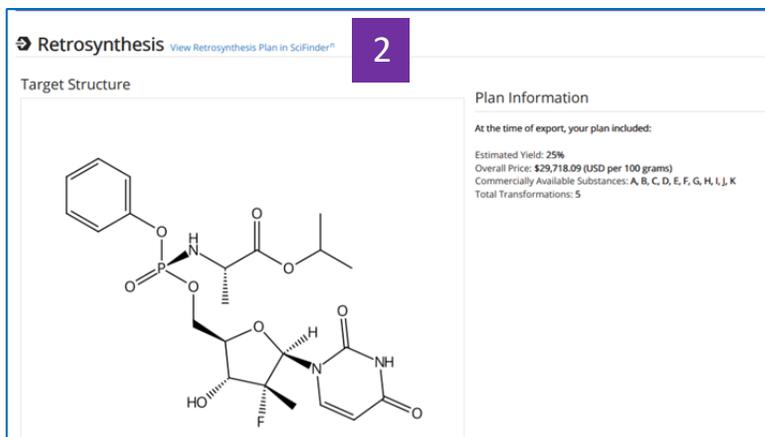
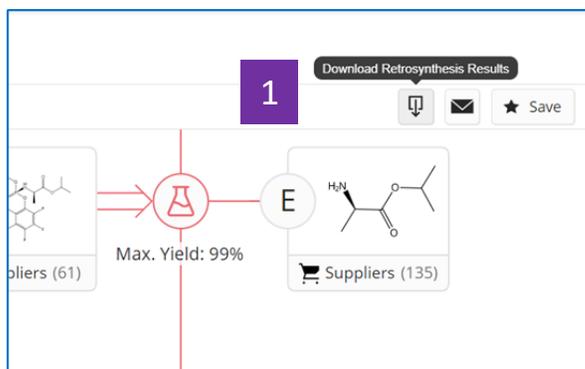
Overview Steps

Plan Information

Estimated Yield: **38%**
 Overall Price: **\$19,855.91**
 (USD per 100 grams) **3**

Commercially Available:
 A, B, C, D, E, F, G, H, I, J, K

1. 點擊Alternative Steps,查看其他可能的路線
2. 點擊Select, 結果將更換成新路線
3. 自動生成新路線



Steps

#	Step	Yield	Evidence	Alternative Steps	Commercially Available
1	A ⇒ B + C	Max.: -	1	51	A, B, C
2	B ⇒ D + E + F	Max.: 99%	28	9	B, D, E, F
3	C ⇒ G	Max.: 92%	2	6	C, G
4	G ⇒ H + I	Max.: 59%	3	21	G, H, I
5	I ⇒ J + K	Max.: 93%	19	13	I, J, K

1. 將路線結果匯出為pdf格式檔，查看反應路線及反應資訊
2. 點擊: [View Retrosynthesis Plan in SciFinderⁿ](#) 線上查看路線詳情

SciFinderⁿ 使用技巧 | 合成實驗詳情的獲取

Structure Match

As Drawn (3)

Substructure (4,368)

Filter by

- Yield
- Number of Steps
- Experimental Protocols
 - MethodsNow: Synthesis (273)
 - Experimental Procedure (222)
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes
- Search Within Results

Reactions (273)

View Collapsed

References

Scheme 1 (1 Reaction) View

Steps: 1
Yield: 72%

Suppliers (7)

Suppliers (56)

Reaction Summary

Reagents:	Cesium carbonate	Steps: 1
Catalysts:	-	Yield: 72%
Solvents:	Acetonitrile Water	
Conditions:	rt; 10 h, 80 °C	

View Reaction Detail | Experimental Protocols

Full Text

TBHP as Methyl Source under Metal-Free Aerobic Conditions To Synthesize Quinazolin-4(3H)-ones and Quinazolines by Oxidative Amination of C(sp³)-H Bond

View Reference Detail

By: Mukhopadhyay, Sushobhan; et al

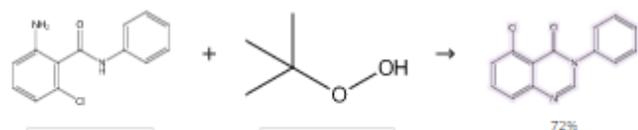
European Journal of Organic Chemistry (2018), 2018(22), 2784-2794

1. 在反應結果集中選擇 Experimental Protocols 中的 MethodsNow: Synthesis
2. 點擊 Experimental Protocols 獲取增值標引的實驗詳情

Reaction Detail (Scheme 1, Reaction 1 of 1)

7

← Prev Next →



Suppliers (7)

Suppliers (56)

Steps: 1

Yield: 72%

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Cesium carbonate	-	Acetonitrile Water	rt; 10 h, 80 °C

CAS Reaction Number: Not assigned

Experimental Protocols

MethodsNow™

3

Products 4(3H)-Quinazolinone, 5-chloro-3-phenyl-, Yield: 72%

Reactants *tert*-Butyl hydroperoxide
2-Amino-6-chloro-*N*-phenylbenzamide

Reagents Cesium carbonate

Solvents Acetonitrile
Water

Procedure

1. Add Cs₂CO₃ (0.74 mmol) and TBHP (70 % aqueous solution, 7.4 mmol) in a round-bottom flask that contained amide (0.2 g, 0.74 mmol) in MeCN (6 mL) at room temperature.
2. Heat the mixture at 80 °C for 10 h under air.
3. Monitor the reaction progress by TLC analysis and remove the solvent under vacuum.
4. Dilute the residue with H₂O (20 mL) and extract the resulting mixture with EtOAc (3 × 20 mL).
5. Dry the combine organic layers with anhydrous Na₂SO₄ and filter.
6. Evaporate the filtrate under reduced pressure to obtain the crude residue.
7. Purify the crude residue by column chromatography over silica gel (hexanes/EtOAc, 7:3 v/v) to obtain the product.

4

Scale gram

5

Characterization Data

4(3H)-Quinazolinone, 5-chloro-3-phenyl-

Proton NMR Spectrum (400 MHz, [D₆]DMSO): δ = 7.33–7.42 (m, 2 H), 7.60–7.64 (m, 2 H), 7.74–7.78 (m, 3 H), 7.86–7.89 (m, 1 H), 8.00 (s, 1 H) ppm.

Carbon-13 NMR (100 MHz, [D₆]DMSO): δ = 124.9, 127.0, 127.7, 128.4, 129.2, 129.3, 132.7, 134.5, 136.9, 145.9, 147.2, 160.4 ppm.

IR Absorption Spectrum (KBr): ν_{max} = 1680 (CO) cm⁻¹.

HRMS (ESI): calcd. for C₁₄H₉ClN₂O [M+H]⁺ 257.0482; found 257.0480.

Mass Spectrum MS (ESI+): = 257.1.

Melting Point 167–169 °C.

R_f 0.61.

State white solid

6

Reference

TBHP as Methyl Source under Metal-Free Aerobic Conditions To Synthesize Quinazolin-4(3H)-ones and Quinazolines by Oxidative Amination of C(sp²)-H Bond

View Reference Detail

By: Mukhopadhyay, Sushobhar; et al

View All ↓

European Journal of Organic Chemistry (2018), 2018(22), 2784-2794

Full Text ↓

Company/Organization

Medicinal and Process Chemistry Division
CSIR-Central Drug Research Institute
Lucknow 226031
India

3. 實驗中涉及的所有物質及其在反應中的角色
4. 實驗中涉及的所有實驗步驟
5. 產物的譜圖表徵資訊及屬性特徵
6. 產物的形態
7. 下載、分享或保存實驗詳情

SciFinderⁿ 使用技巧 | 作者名/期刊名/機構名檢索

The screenshot shows the SciFinderⁿ interface. At the top left is the SciFinderⁿ logo with the tagline "A CAS SOLUTION". Below the logo is a navigation bar with a link "Return to Home Page" and a purple square containing the number "1". To the left of the main content area is a sidebar with two buttons: "Substances" and "References". The "References" button is highlighted in purple. The main content area is titled "Advanced Reference Search" with a document icon. Below the title is a section for "Author" with a purple square containing the number "2". Under "Author" is the label "Author Name (Last, First Middle)" and a text input field containing "Nakamura, Eiichi". Below the input field is the text "Ex: Schubert, J A". Below the input field is a button labeled "Add Another Author" with a purple square containing the number "3". At the bottom of the section is a line with "— AND —" and a horizontal line.

1. 回到首頁介面
2. 在文字方塊輸入作者名，按照“姓，名（中間名）”的格式輸入，姓需要輸入完整，名可以簡寫為首字母。
3. 可以添加其他作者姓名

Advanced Reference Search

Author

Author Name (Last, First Middle)

Ex: Schubert, J A

— AND —

Journal

1

Journal Name

Volume

Issue

Starting Page

2

Title Word(s)

3

Ex: Antibiotic

— AND —

Organization

4

Organization Name

Ex: Bayer, Dupont



5

Clear All

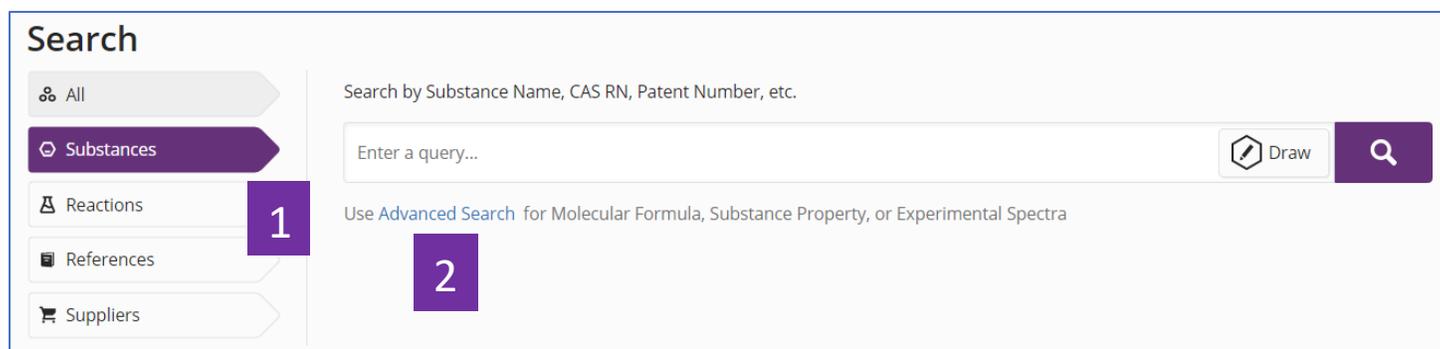
1. 在文字方塊中輸入期刊名稱，推薦輸入完整期刊名稱
2. 若有“卷”，“期”或者“起始頁”資訊，可以在文字方塊中輸入

3. 可以輸入希望在題名中出現的關鍵字
4. (選填) 可以輸入研究機構名稱與期刊名或作者名聯合檢索，也可以直接按照研究機構名稱進行文獻檢索
5. 點擊進行檢索

The screenshot shows a search results page for 'References' with 256 results. The page includes a left sidebar with filters for Document Type, Language, Publication Year (with a histogram from 1975 to 2019), Available at My Institution, Author (listing Nakamura, Eiichi, Matsuo, Yutaka, Nakamura, Masaharu, Ilies, Laurean, and Tsuji, Hayato), Organization, Publication Name (Journal of the American Chemical Society), Concept, Database, and Search Within Results. The main content area displays three reference entries, each with a title, authors, journal information, and an abstract. The first entry is 'Enantioselective synthesis of alpha-substituted ketones by asymmetric addition of chiral zinc enamides to 1-alkenes.' by Nakamura, Masaharu; Hatakeyama, Takuji; Hirai, Atsushi; Nakamura, Eiichi, published in the Journal of the American Chemical Society (2003), 125(11), 6362-3. The second entry is 'Synthesis, structure, and aromaticity of a hoop-shaped cyclic benzenoid [10]cyclophenacene.' by Nakamura, Eiichi; Tahara, Kazukuni; Matsuo, Yutaka; Sawamura, Masaya, published in the Journal of the American Chemical Society (2003), 125(10), 2834-5. The third entry is 'Reaction pathways of the Simmons-Smith reaction.' by Nakamura, Masaharu; Hirai, Atsushi; Nakamura, Eiichi, published in the Journal of the American Chemical Society (2003), 125(8), 2341-50. Each entry has a 'Full Text' button and buttons for 'Substances', 'Reactions', 'Cited By', and 'Citation Map'. A purple box with the number '1' is overlaid on the 'References (256)' header, and another purple box with the number '2' is overlaid on the author name 'Nakamura, Eiichi' in the first entry.

1. 查看文獻結果集
2. 輸入的資訊在結果中會被反亮顯示

SciFinderⁿ 使用技巧 | 通過核磁譜圖獲得物質



The screenshot shows the SciFinder search interface. On the left, there is a vertical menu with five options: 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The 'Substances' option is highlighted with a purple arrow and a purple box containing the number '1'. To the right of the menu, there is a search area with the text 'Search by Substance Name, CAS RN, Patent Number, etc.' and a search input field containing the placeholder text 'Enter a query...'. Below the input field, there is a link for 'Advanced Search' and a note: 'Use Advanced Search for Molecular Formula, Substance Property, or Experimental Spectra'. A purple box containing the number '2' is positioned over the 'Advanced Search' link. To the right of the input field, there is a 'Draw' button with a chemical structure icon and a search button with a magnifying glass icon.

1. 選擇 Substances
2. 點擊 Advanced Search

[← Return to Home Page](#)

Substances

References

Advanced Substance Search

Molecular Formula

Enter one Molecular Formula.

Ex: C₆H₆
(C₈H₈)_x
C₂₂H₂₆CuN₂O₅.C₂H₃N

Add Another Molecular Formula

— AND —

Substance Property

Select Property

- Select One -

Enter Value

Add Another Property

AND

Experimental Spectra

Select Spectrum

1

Carbon-13 NMR

Enter Value

155.02, 127.6 to 129.01

2

(Search includes allowance of ± 2 ppm)

Example: 152.3, 127.6, 133.1
155.02 to 207.59
187

Add Another Spectra

3



4

Clear All

1. 選擇具體的核磁譜類型
2. 輸入核磁譜峰值
3. 可繼續添加其他核磁譜值
4. 開始檢索

Filter by

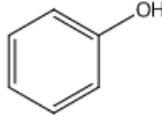
- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
 - Carbon-13 NMR (11K)
 - Proton NMR (3,196)
 - Mass (2,364)
 - IR Absorption (420)
 - Nitrogen-15 NMR (195)
 - Fluorine-19 NMR (156)
 - UV and Visible Absorption (112)
 - Raman (106)
 - Phosphorus-31 NMR (89)
 - Oxygen-17 NMR (61)
 - Silicon-29 NMR (18)
 - Boron-11 NMR (1)
- View Fewer
- Regulatory Information
- Bioactivity Indicator
- Target Indicator
- Search Within Results

1

Substances (11,384) Sort: Relevance View Partial

References Reactions Suppliers

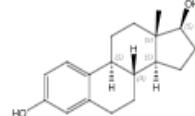
108-95-2
View Detail



C_6H_6O
Phenol

198K References 76K Reactions 199 Suppliers

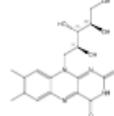
50-28-2 **2**
View Detail



$C_{18}H_{24}O_2$
Estradiol

178K References 828 Reactions 156 Suppliers

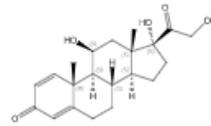
83-88-5
View Detail



$C_{17}H_{20}N_4O_6$
Riboflavin

51K References 440 Reactions 150 Suppliers

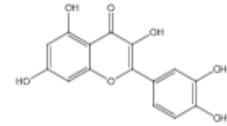
50-24-8
View Detail



$C_{21}H_{28}O_5$
Prednisolone

51K References 421 Reactions 113 Suppliers

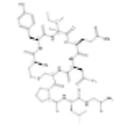
117-39-5
View Detail



$C_{15}H_{10}O_7$
Quercetin

50K References 871 Reactions 110 Suppliers

50-56-6
View Detail

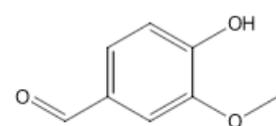


$C_{43}H_{66}N_{12}O_{12}S_2$
Oxytocin

Protein/Peptide Sequence
Sequence Length: 9

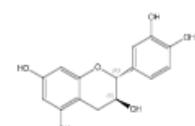
37K References 349 Reactions 76 Suppliers

121-33-5
View Detail



$C_8H_8O_3$
Vanillin

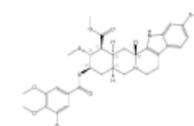
154-23-4
View Detail



$C_{15}H_{14}O_6$

Absolute stereochemistry shown, Rotation (+)

50-55-5
View Detail



$C_{33}H_{40}N_2O_9$

Absolute stereochemistry shown, Rotation (-)

1. 通過實驗譜圖聚類物質
2. 點擊物質 CAS 登記號查看物質詳情

Experimental Spectra **1**

¹ H NMR	¹³ C NMR	Hetero NMR	IR	Mass	UV and Visible	Additional Spectra
						Source
View Carbon-13 NMR Spectrum						(1) BIORAD
View Carbon-13 NMR Spectrum						(2) ACD-A
View Carbon-13 NMR Spectrum						(3) ACD
View Carbon-13 NMR Spectrum						(3) ACD
View Carbon-13 NMR Spectrum						(3) ACD
Carbon-13 NMR Spectrum - 4 Sources						(4-7) CAS

Sources **3**

(1) Copyright Bio-Rad Laboratories. All Rights Reserved.
 (2) Sigma-Aldrich (Spectral data were obtained from Advanced Chemistry Development, Inc.)
 (3) Spectral data were obtained from Advanced Chemistry Development, Inc.
 (4) Wang, Xingbin; Journal of Chemical Research, (2011), 35(5), 291-293, CAplus
 (5) Wang, Bijia; Organic Letters, (2010), 12(15), 3352-3355, CAplus
 (6) Commodari, Fernando; Magnetic Resonance in Chemistry, (2005), 43(6), 444-450, CAplus
 (7) Boovannahalli, Shanthaveerappa K.; Journal of Organic Chemistry, (2004), 69(10), 3340-3344, CAplus

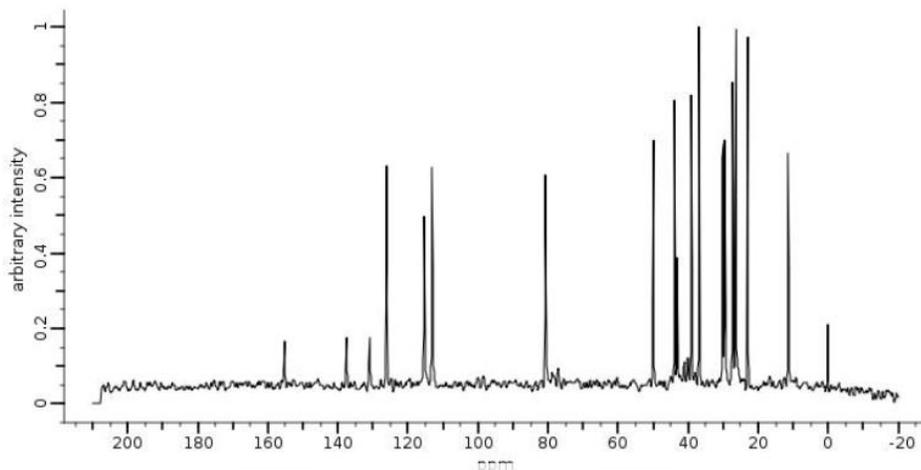
[Predicted Properties](#)
[Predicted Spectra](#)

1. 物質詳情中的實驗譜圖
2. 點擊超連結，查看核磁譜圖
3. 譜圖資訊的文獻來源

Carbon-13 NMR Spectrum Detail (1 of 5)

← Prev Next →

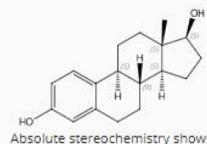
4



1



2



CAS Registry Number
50-28-2

$C_{18}H_{24}O_2$

CAS Name
Estradiol

Spectrum Summary

Spectrum ID NC_18679

Spectrometer VARIAN CFT-20

Source Copyright Bio-Rad Laboratories. All Rights Reserved.

Conditions

Standard Tetramethylsilane (75-76-3)

3

1. 縮放譜圖
2. 下載譜圖圖片
3. 譜圖概覽：測試儀器、條件、來源等
4. 下載譜圖詳情

SciFinderⁿ 使用技巧 | 通過生物活性、靶點篩選物質

The screenshot displays the SciFinder search results page. On the left, there is a sidebar with filters: 'Experimental Spectrum', 'Regulatory Information', 'Bioactivity Indicator' (1), 'Target Indicator' (2), and 'Search Within Results'. The 'Bioactivity Indicator' section is expanded, showing 'Anti-infective agents (13K)' selected, along with other categories like 'Pharmaceutical immune agents (6,787)', 'Antitumor agents (5,691)', 'Nervous system agents (4,700)', and 'Anti-inflammatory agents (3,963)'. The 'Target Indicator' section shows 'Enzymes (13K)' selected, along with 'Viral proteins (6,217)', 'Ligand-binding proteins (3,517)', 'Blood proteins (3,456)', and 'Metalloproteins (3,338)'. The main area contains six chemical compound cards. Each card includes a chemical structure, a CAS number, the name of the compound, and statistics for references, reactions, and suppliers. Card 3, representing Emtricitabine (CAS 143491-57-0), is highlighted with a purple box and the number 3. The other cards are: Rilpivirine (CAS 500287-72-9), Atazanavir (CAS 198904-31-3), and Daclatasvir (CAS 1009119-64-5). The bottom card, Tenofovir disoproxil fumarate (CAS 202138-50-9), shows its components and the fumarate salt.

1. 在物質結果集頁面，點擊 **Bioactivity Indicator**, 根據適應症篩選物質
2. 點擊 **Target Indicator**，根據靶點篩選物質
3. 點擊物質 **CAS** 登記號，獲取物質的生物活性及靶點詳情

Bioactivity Indicator X

By Count Alphanumeric 1

<input checked="" type="checkbox"/> Anti-infective agents (13K) <input type="checkbox"/> Pharmaceutical immune agents (6,787) <input checked="" type="checkbox"/> Antitumor agents (5,691) <input type="checkbox"/> Nervous system agents (4,700) <input checked="" type="checkbox"/> Anti-inflammatory agents (3,963) <input type="checkbox"/> Cytoprotective agents (3,455) <input type="checkbox"/> Enzyme inhibitors (3,315) <input type="checkbox"/> Cardiovascular agents (3,021) <input type="checkbox"/> Antidiabetic agents (3,004) <input type="checkbox"/> Gastrointestinal agents (2,876) <input type="checkbox"/> Hematologic agents (2,851) <input type="checkbox"/> Respiratory system agents (2,786) 2 <input type="checkbox"/> Renal agents (2,711)	<input type="checkbox"/> Peptide analogs (1,657) <input type="checkbox"/> Receptor antagonists (1,620) <input type="checkbox"/> Membrane transport modulators (1,237) <input type="checkbox"/> Receptor agonists (444) <input type="checkbox"/> Cytotoxic agents (386) <input type="checkbox"/> Pharmaceutical natural products (371) <input type="checkbox"/> Hormone antagonists (288) <input type="checkbox"/> Antiproliferative agents (278) <input type="checkbox"/> Lipid-regulating agents (229) <input type="checkbox"/> Pharmaceutical adjuvants (198) <input type="checkbox"/> Neuromuscular agents (142) <input type="checkbox"/> Antiulcer agents (103) <input type="checkbox"/> Antiosteoporotic agents (96)	<input type="checkbox"/> Biopharmaceuticals (66) <input type="checkbox"/> Radioprotectants (43) <input type="checkbox"/> Reproductive control agents (38) <input type="checkbox"/> Receptor modulators (33) <input type="checkbox"/> Peroxisome proliferators (25) <input type="checkbox"/> Pharmaceutical photosensitizers (24) <input type="checkbox"/> Hair growth stimulants (13) <input type="checkbox"/> Ion channel openers (7) <input type="checkbox"/> Antianemic agents (6) <input type="checkbox"/> Antigout agents (5) <input type="checkbox"/> Cell differentiation inducers (5) <input type="checkbox"/> Anabolic agents (3) <input type="checkbox"/> Antidotes (3)
--	---	---

Apply
Cancel

1. 在點擊 **View All** 獲得的所有適應症資訊後，可根據研究密集程度或適應症字母順序進行排序
2. 選擇感興趣的適應症，然後點擊 **Apply**，即可獲得針對某適應症的物質

^ Bioactivity Indicators

Anti-infective agents (56)

1

Anti-HIV agents (1498)

Antibacterial agents (76)

Antibiotics (87)

Antiviral agents (1050)

Fungicides (62)

Highly active antiretroviral therapy agents (161)

Integrase inhibitors (150)

Virus entry inhibitors (89)

Anti-inflammatory agents (96)

Antitumor agents (193)

Enzyme inhibitors

HIV protease inhibitors (289)

Integrase inhibitors (150)

Non-nucleoside reverse transcriptase inhibitors (485)

Nucleoside reverse transcriptase inhibitors (552)

Nucleotide reverse transcriptase inhibitors (120)

Reverse transcriptase inhibitors (221)

Pharmaceutical immune agents

Immunomodulators (80)

Immunosuppressants (50)

^ Target Indicators

Apoproteins

Apolipoprotein A-I (10)

2

Apoptosis-regulating proteins

Programmed cell death protein 1 (23)

Programmed death-ligand 1 (13)

1. 點擊物質的 **CAS** 登記號，即可獲得物質詳情，在物質詳情頁面，點擊藍色超連結的適應症，即可獲得相應的研究文獻
2. 在物質詳情頁面，點擊藍色超連結的靶點，獲得相應的研究文獻

SciFinderⁿ 使用技巧 | 馬庫什結構檢索

The screenshot shows the SciFinder search interface. On the left, there is a navigation menu with options: All, Substances (highlighted with a purple bar and callout 1), Reactions, References, and Suppliers. The main search area has a search bar with the text "Enter a query..." and a search button (callout 3). Above the search bar, there is a prompt "Search by Substance Name, CAS RN, Patent Number, etc." and a callout 2. Below the search bar, there is a link "Use Advanced Search for Molecular Formula, Substance Property, or Experimental Spectra". On the right, there is a drawing tool with a callout 4 for "Edit Drawing" and a callout 5 for "Remove". At the bottom right, there is a checkbox for "Search Patent Markush" with a callout 6. A chemical structure is shown in the drawing tool area.

1. 選擇 Substances，進行 Markush 結構檢索
2. 點擊 Draw，繪製檢索結構
3. 點擊放大鏡，開始檢索
4. 點擊 Edit Drawing，重新編輯結構
5. 點擊 Remove，去除結構
6. 勾選 Search Patent Markush 進行馬庫什檢索

The screenshot shows the Patent Markush Match results page. On the left, there is a filter menu with options: As Drawn (1) (highlighted with a purple bar and callout 1), Substructure (34), and Filter by Patent Office (Japan (1)). The main area shows a search result for "Patent Markush (1)" with a callout 2. The result is for patent JP2003261514, with a callout 3 for "Patent claim 1". There are dropdown menus for "PATENTPAK" (callout 4) and "Full Text" (callout 5). A chemical structure is shown with callouts 4 and 6. The text "There are no notes to display for this structure." is visible.

1. Markush 結構檢索的匹配程度：As Drawn，Substructure
2. 點擊專利號，獲取專利文獻詳情
3. 該馬庫什結構在專利中出現的位置

4. PatantPak：獲取專利全文、定位專利中的重要物質
5. 專利全文的連結
6. 馬庫什結構詳情

SciFinderⁿ 使用技巧 | 設置 Alert

在 SciFinderⁿ 中，可對以下幾種結果集設置 Alert：

1. Markush 結構檢索結果集
2. 文獻檢索結果集
3. 物質檢索結果集
4. 反應檢索結果集

1. 設置 Markush 結構檢索結果集的 Alert

The screenshot displays the 'Patent Markush' search results page. On the left, there are filters for 'Patent Office' (Japan) and 'Substructure' (34). The main area shows a search result for 'JP2003261514' with a chemical structure and a 'Patent claim 1' section. A 'Save Search' dialog box is overlaid on the right, with the following elements:

- 1. A 'Save' button in the top right corner of the main interface.
- 2. The 'Name' field containing 'Markush alert'.
- 3. The 'Weekly' alert frequency selected among 'No Alerts', 'Weekly', and 'Monthly'.
- 4. The 'Save' button in the dialog box.

1. 在Markush檢索結果集中點擊Save
2. 輸入保存檔的名稱
3. 點擊Weekly或者Monthly設置提醒頻率
4. 點擊Save完成設置

如果在保存結果集的過程中未設置Alert,則可以通過以下方法進行設置。

The screenshot shows the SciFinder interface with the following elements:

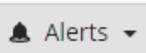
- Top Bar:** SciFinder logo, "Substances" dropdown, search bar "Enter a query...", "Edit" button, search icon, star icon (1), and user profile icon.
- Left Panel:** "Filter by" section with "Result Type" (Patent Markush (1), References (14), Retrosynthesis (5), Substances (1)), "Combine Saved Results" (Combine button), and "Migrate Alerts & Saved Results" (Migrate button).
- Main Content:** "★ Saved (12)" header, a "Markush alert" card for a chemical structure (September 6, 2019, 2:32 PM, Patent Markush, As Drawn). The card includes an "Alerts" dropdown (2) and an "Add Tags" dropdown. Below the card is a "Frequency" dropdown (3) with options "No Alerts", "Weekly", and "Daily".
- Buttons:** "Rerun Search" buttons are present on the right side of the alert card and below the frequency dropdown.

1. 點擊  , 查看保存結果集
2. 點擊  , 進行設置
3. 設置發送頻率

2. 設置文獻檢索結果集的Alert

The screenshot shows the SCIFINDER interface with the search term "Programmed cell death protein 1". The left sidebar contains filters for Relevance (Best, Good, Fair), Document Type (Journal, Patent, Review, Biography, Clinical Trial), and Language (English, Chinese, Japanese, Korean, Russian). The main area displays a list of references. The first reference is "Immunological reagents targeting programmed cell death 1 protein" by Pantaleo, Giuseppe; Ferwick, Craig. The second reference is "Methods for treatment of cancer with inhibitors of programmed cell death protein 1 (PD-1) pathway" by Cantwell, Mark J. Three numbered callouts are present: 1. A purple box with the number "1" is placed over the "Learn more about Relevance" link in the filter sidebar. 2. A purple box with the number "2" is placed over the "Save" button in the top right of the reference list. 3. A purple box with the number "3" is placed over the star icon in the top right of the reference list.

1. 根據需求，對文獻結果集進行篩選。
2. 點擊Save，保存文獻。
3. 點擊★，查看保存結果集。

1. 點擊  ，設置Alert
2. 選擇發送頻率
3. 設置物質檢索結果集的Alert

1. 在物質檢索結果集中點擊Save
2. 在快顯視窗中輸入保存名稱
3. 點擊Weekly或者Monthly設置提醒頻率

4. 點擊Save完成設置

如果保存過程中未設置Alert, 則可以打開已保存的結果集清單, 選擇需要設置的結果集, 再進行設置

★ Saved (23)

ORP = 1.15

September 6, 2019, 4:38 PM

Rerun Search

Substances **Advanced Search**
Property: Optical Rotatory Power (degrees): 1.15

Alerts **1** Add Tags

Frequency **2**
No Alerts **Weekly** Monthly

Rerun Search

1. 然後點擊  , 進行設置
2. 選擇發送頻率

4. 設置反應檢索結果集的Alert

The screenshot shows the SciFinder interface for the 'Reactions' section. On the left, there are filters for 'Structure Match' (As Drawn, Substructure, Similarity) and 'Filter by' (Yield, Number of Steps). The main area displays 'Scheme 1' with a chemical reaction involving a complex and a brominated benzene ring. A 'Save Search' dialog box is overlaid on the right, with the following fields and options:

- Name:** ArCN
- Frequency:** No Alerts, Weekly, Monthly
- Tags (optional):** No tags defined
- New Tag (optional):** (empty field)
- Buttons:** Save, Cancel

1. 在反應檢索結果集中點擊Save

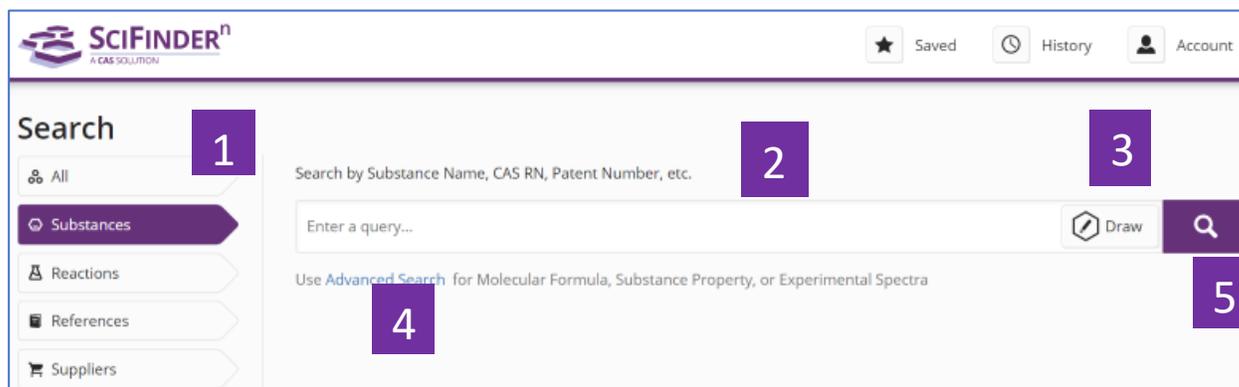
2. 在快顯視窗中輸入保存名稱
3. 點擊Weekly或者Monthly設置提醒頻率
4. 點擊Save完成設置

如果保存過程中未設置Alert, 則可以打開已保存的結果集清單，選擇需要設置的結果集，再進行設置

The screenshot displays a 'Saved' results list with 24 items. The first item is 'ArCN', dated September 6, 2019, 4:53 PM, with the label 'As Drawn'. It includes a 'Reactions' section showing a chemical reaction diagram. Below the diagram are controls for 'Alerts' (highlighted with a purple box labeled '1') and 'Add Tags'. A 'Frequency' dropdown menu is shown below, with options 'No Alerts', 'Weekly' (highlighted with a purple box labeled '2'), and 'Monthly'. A 'Rerun Search' button is located to the right of the reaction diagram and the frequency dropdown.

1. 點擊  Alerts ▾，進行設置
2. 設置發送頻率

SciFinderⁿ 使用技巧 | 獲取物質資訊



1. 選擇 **Substances**，進行物質檢索
2. 輸入檢索文本：物質名稱、**CAS** 登記號、專利號等
3. 點擊 **Draw**，繪製結構
4. 點擊 **Advanced Search**，進行分子式、物質屬性和實驗譜圖等檢索
5. 點擊搜索圖示，開始檢索

The screenshot displays the SciFinder search results for Morphine. The interface includes a search bar at the top, a left sidebar with filters, and a main results area. The results are organized into three rows, each showing a chemical structure, its name, and a table of key physical properties.

Key Physical Properties	Value	Condition
Molecular Weight	227.34	-
Melting Point (Experimental)	<25 °C	-
Boiling Point (Experimental)	115 °C	-
Density (Predicted)	1.09±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.11±0.20	Most Basic Temp: 25 °C

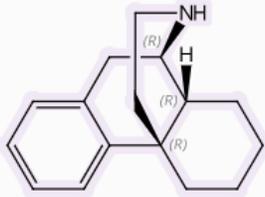
1. 結構匹配程度：As Drawn 精確結構，Substructure 衍生結構，Similarity 相似結構
2. 點擊 Analyze Structure Precision，對精確結構和衍生結構的檢索結果進行更細化的結構分類

3. 物質結果的聚類分析：商業上可獲得性、反應角色、文獻角色、立體化學、組份數、物質類型、同位素、金屬、分子量、實驗屬性、實驗譜圖、管控資訊、生物活性、靶點、二次篩選
4. 相關的文獻、反應和供應商
5. 重新排序
6. 選擇是否展示物質的物理屬性資訊
7. 下載、郵件、保存並設置提醒
8. 點擊 **CAS** 登記號，查看物質詳情
9. 此物質相關的文獻、反應和供應商
10. 此物質的物理屬性資訊

Substance Detail (1 of 30,974) 1 Prev Next →

References (397) Reactions (0) Suppliers (3) 2 ↓ ✉ ★ Save

CAS Registry Number
468-10-0 3



Absolute stereochemistry shown

$C_{16}H_{21}N$
Morphinan

Key Physical Properties	Value	Condition
Molecular Weight	227.34	-
Melting Point (Experimental)	<25 °C	-
Boiling Point (Experimental)	115 °C	-
Density (Predicted)	1.09±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	10.11±0.20	Most Basic Temp: 25 °C

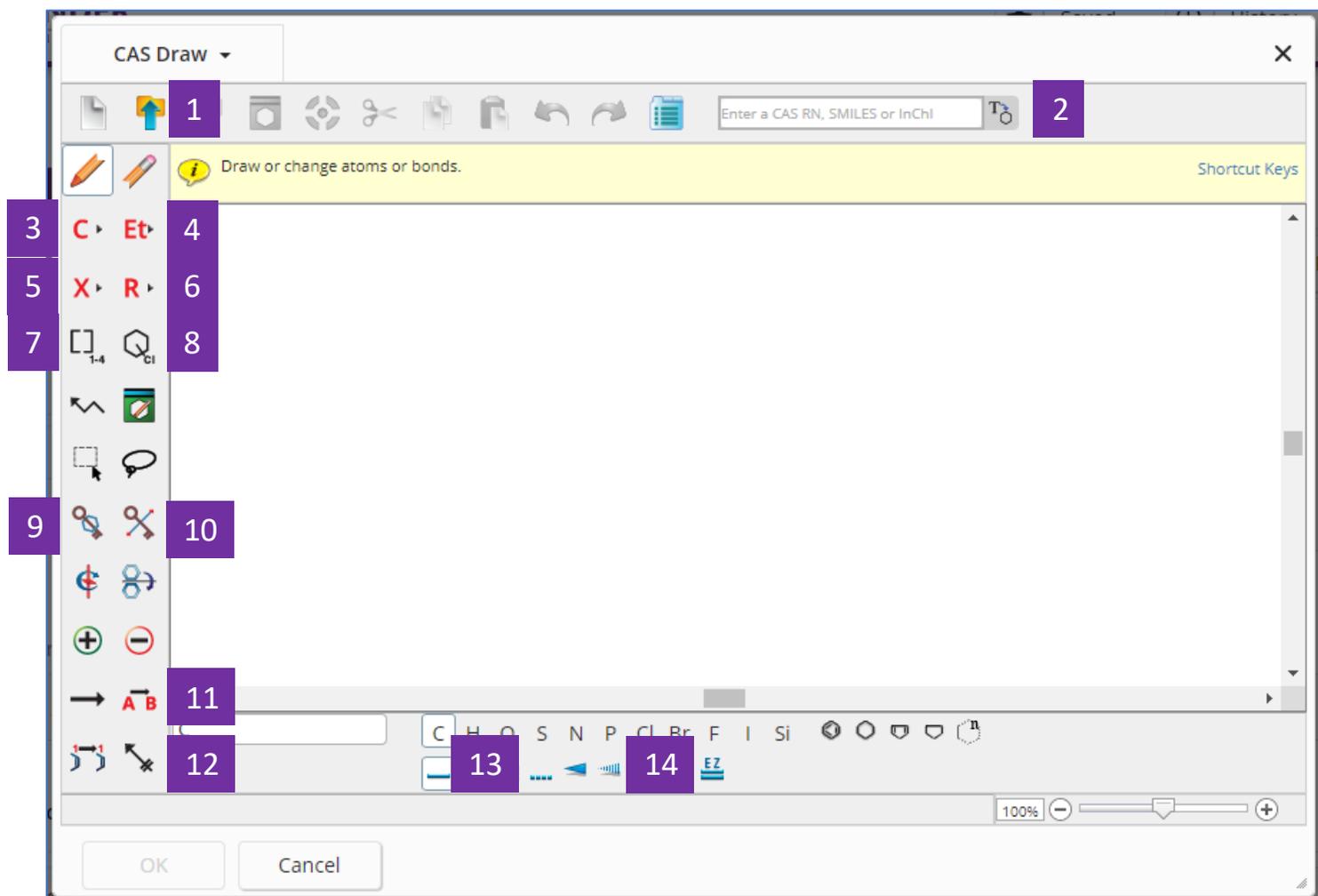
[Experimental Properties](#) | [Spectra](#)

[Expand All](#) | [Collapse All](#)

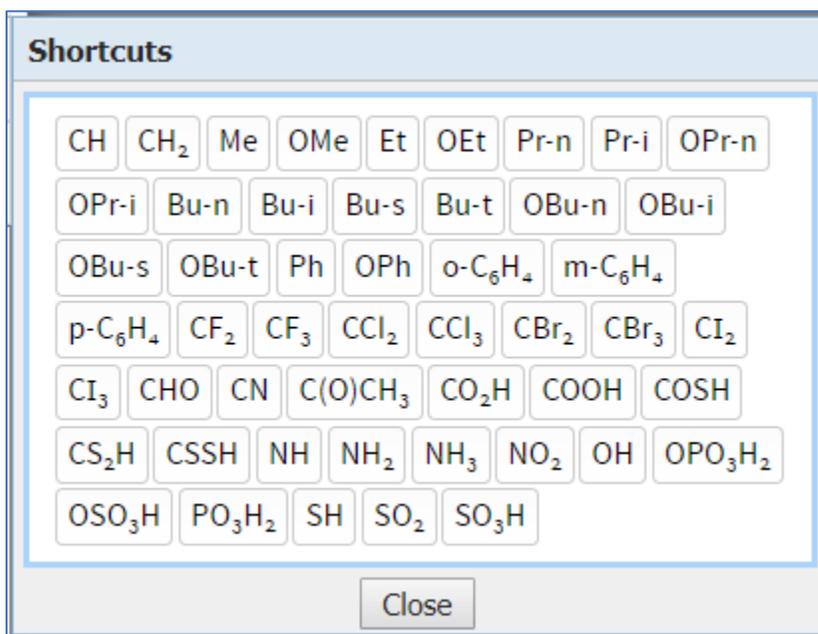
- ✓ Other Names 5
- ✓ Experimental Properties 5
- ✓ Experimental Spectra
- ✓ Predicted Properties
- ✓ Predicted Spectra
- ✓ Regulatory Information
- ✓ Additional Details

1. 點擊左右箭頭，查看前一個或後一個物質詳情
2. 此物質相關的文獻、反應和供應商
3. 下載、分享及保存物質詳情
4. 物質的物理屬性資訊
5. 物質名稱、實驗屬性、實驗譜圖、預測屬性、預測譜圖、管控資訊及其他補充細節

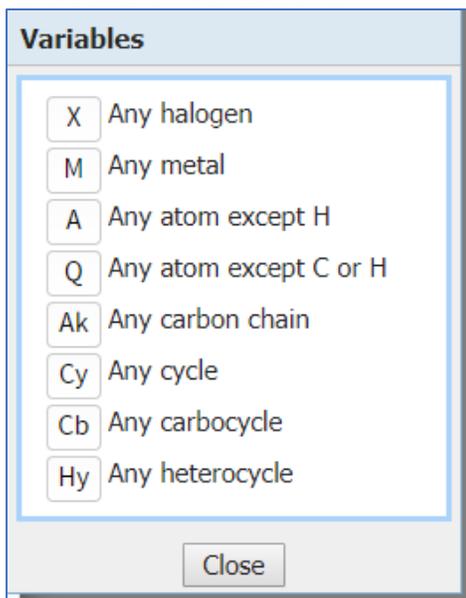
SciFinderⁿ 使用技巧 | 結構編輯器



1.  導入.cxf或者.mol格式檔。
2. , 可以直接輸入物質的CAS登記號、SMILES或者InChI 直接轉化為結構。
3.  為元素週期表。
4.  為常用官能團列表。



5. **X** 選擇可變基團，包括：**X**: 任意鹵素；**M**: 任意金屬；**A**: 除氫外的任意原子；**Q**: 除碳/氫外的任意原子；**Ak**: 任意碳鏈；**Cy**: 任意環；**Cb**: 任意碳環；**Hy**: 任意雜環。



6. **R** 定義R基團，可以設置R為 **C**，**Et** 或者 **X** 的任意組合。

R-group Definitions

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10

R1 =

▼ Atoms

H																			He
Li	Be										B	C	N	O	F				Ne
Na	Mg										Al	Si	P	S	Cl				Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br			Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I			Xe
Cs	Ba	·	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At			Rn
Fr	Ra	·																	

* Lanthanides

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
----	----	----	----	----	----	----	----	----	----	----	----	----	----	----

** Actinides

Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
----	----	----	---	----	----	----	----	----	----	----	----	----	----	----

► Variables

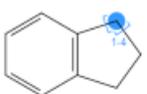
► Shortcuts

7.   重複原子或者基團。

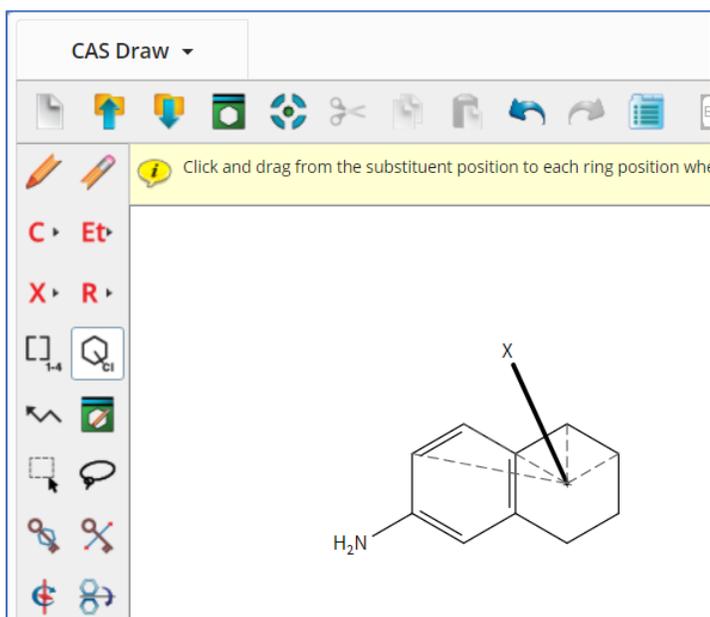
CAS Draw

Enter a CAS RN, SMILES or InChI

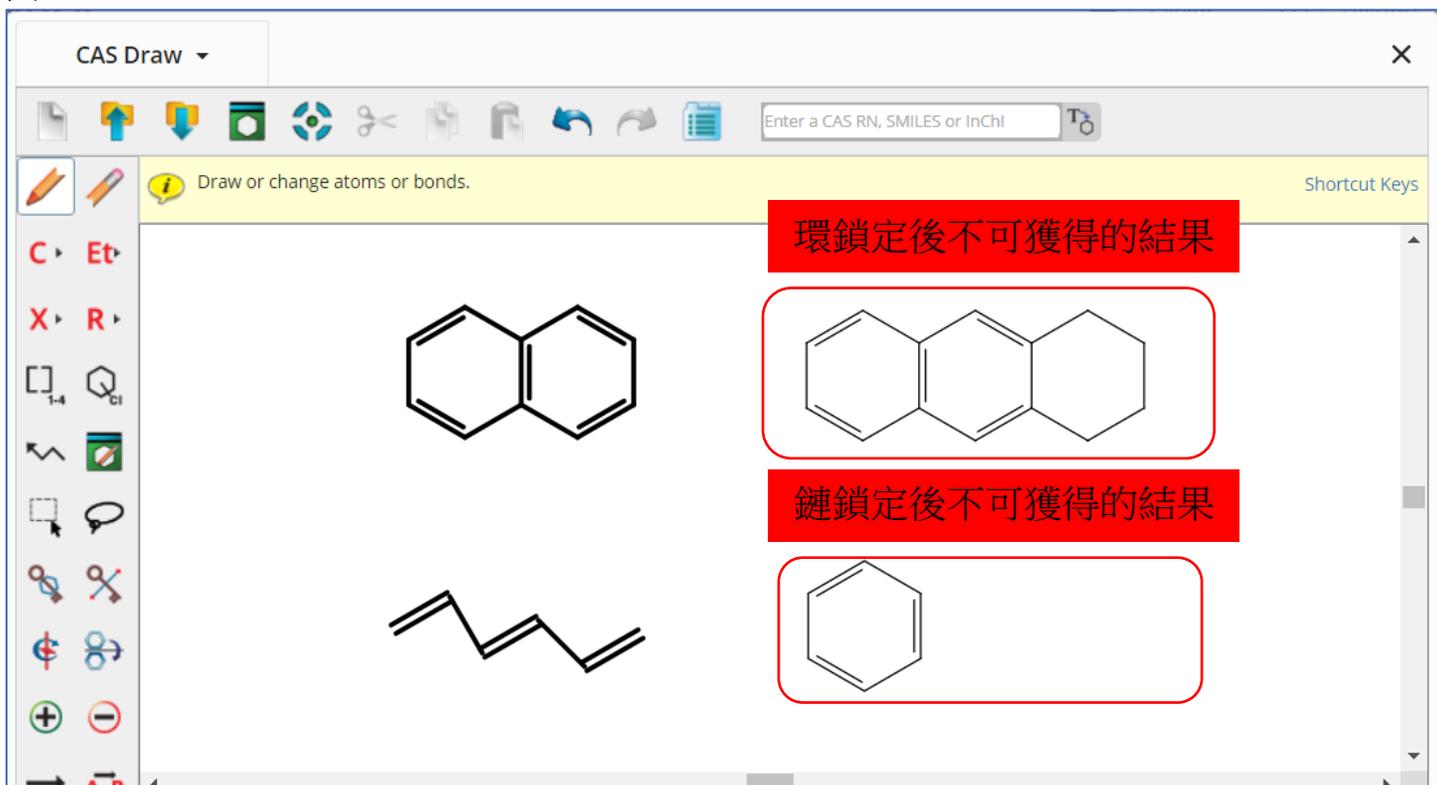
Click to select an atom to be repeated or drag to select a group to be repeated. Enter the number of repetitions. From 1 To 4 Apply



8.  環上的取代位點不固定。

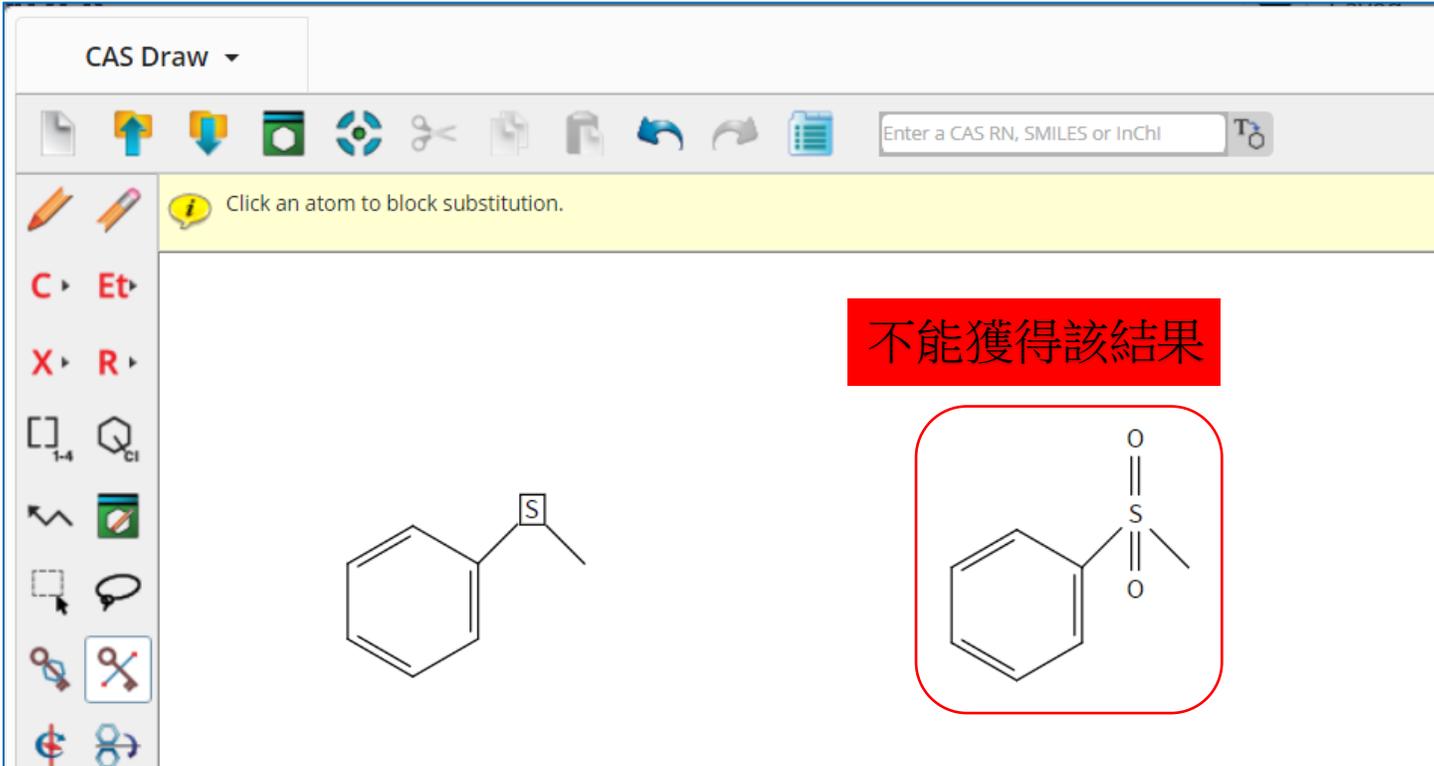


9.  環鎖定。當用該功能鎖定某個環（系），表示該環（系）不能成為更大環系的一部分；如果用該功能鎖定某個鏈，則表示該鏈不能成為某個環（系）的一部分。
例：



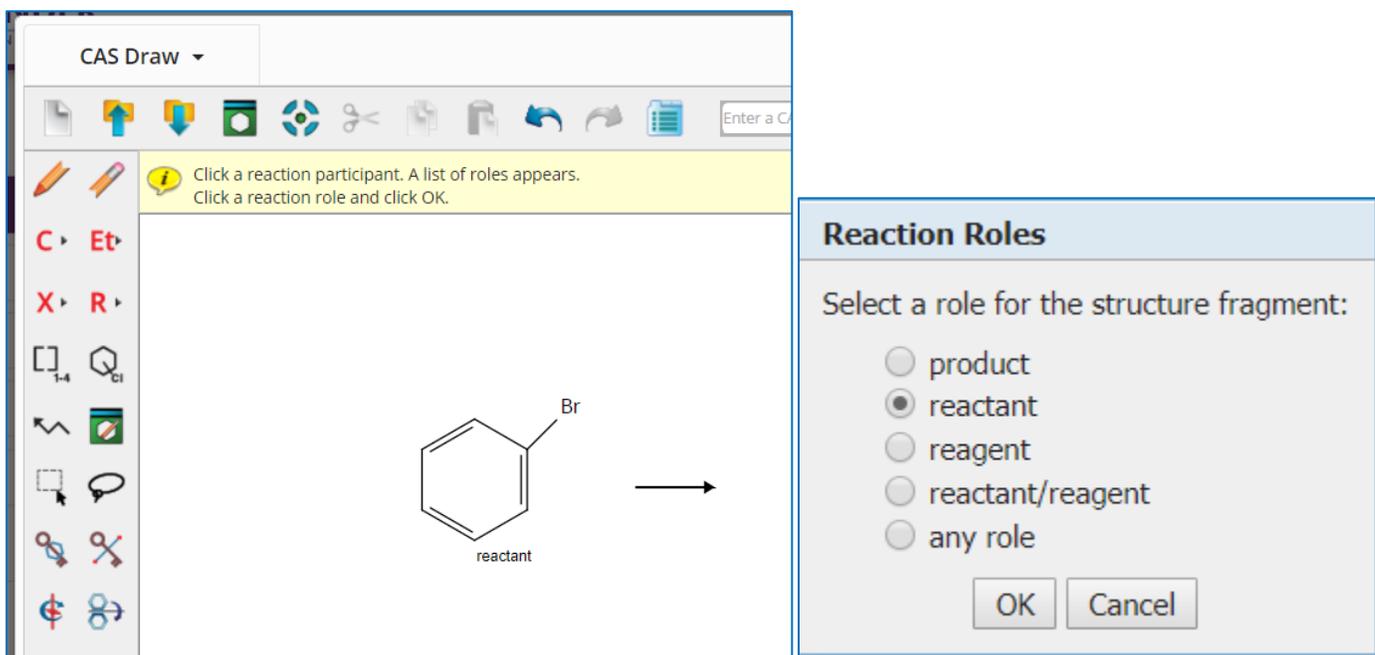
10.  鎖定原子。若某原子被鎖定，則表明該原子只能連接氫原子。

例：

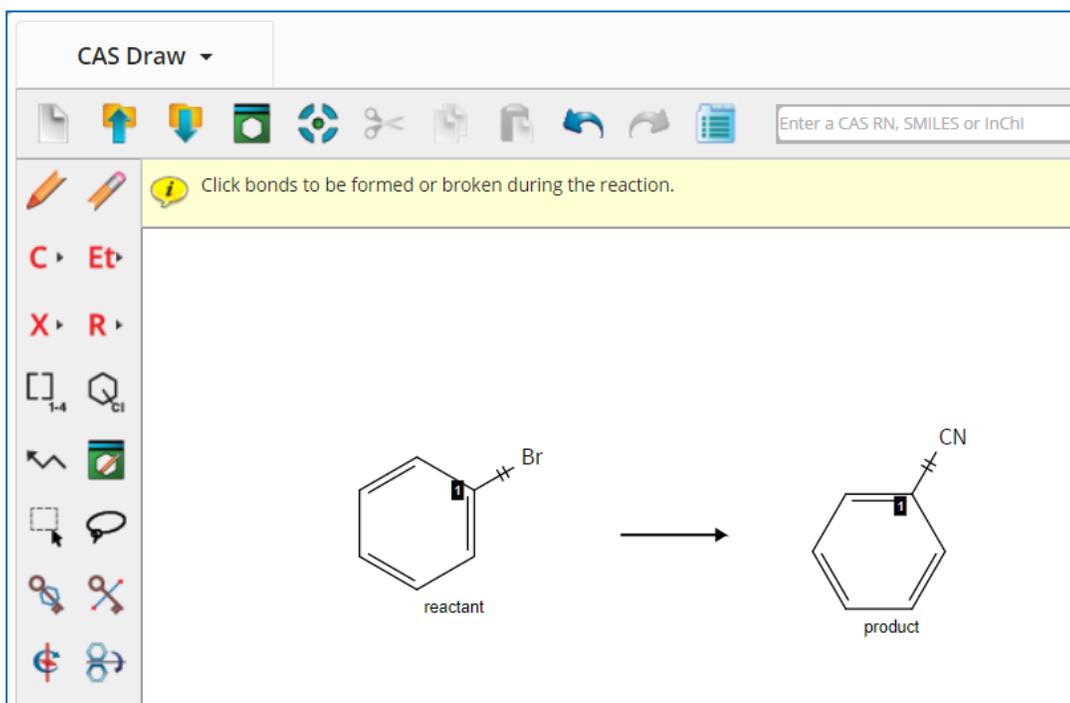


不能獲得該結果

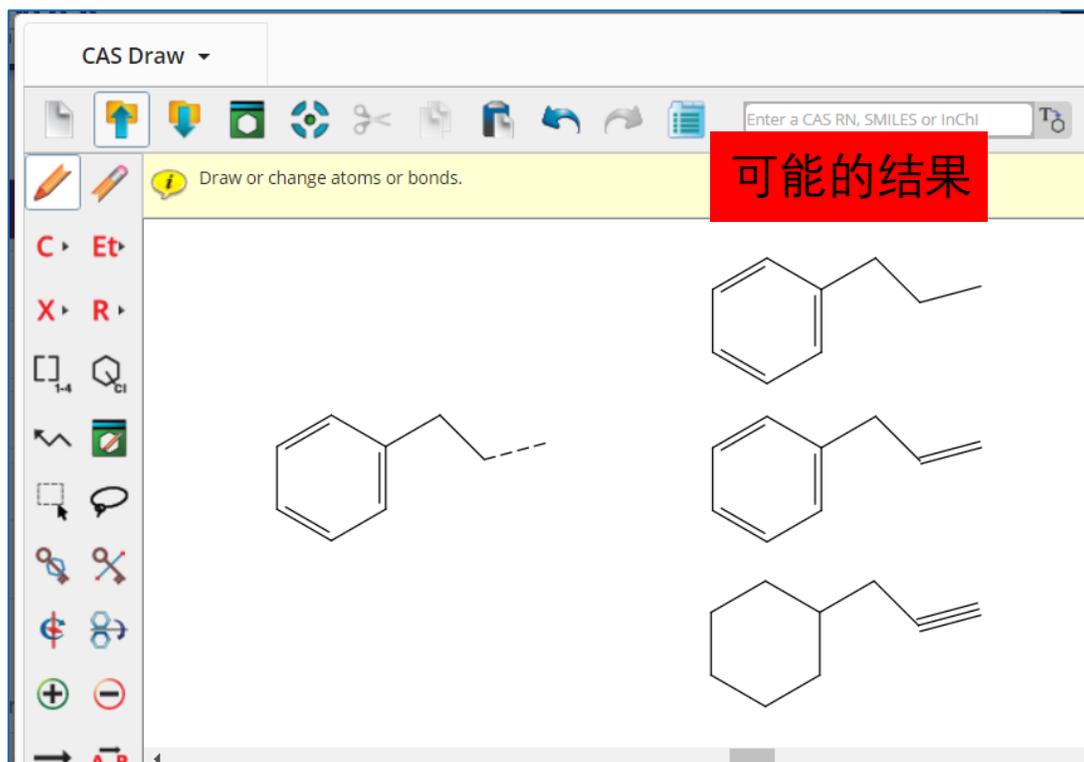
11.  反應箭頭。箭頭左邊的物質是起始物或者試劑，右邊為產物。 為反應角色定義工具，用於定義物質在反應中的角色。



12.  為反應原子標記工具。在原料和產物中以相同數位被標記的原子，表明其反應前後為同一原子。 為反應鍵標記工具，起始物的某鍵被標記，則表明此鍵在反應過程中發生斷開等變化；產物的某鍵被標記，則表明此鍵在反應過程中是新生成的鍵。



13.  為不確定鍵，可以指單鍵，雙鍵或者三鍵。



14.  用於鎖定雙鍵的立體構型，若繪製E構型烯烴，使用此鍵鎖定後，結果集只包含該雙鍵位置為E構型的烯烴，Z構型同理。

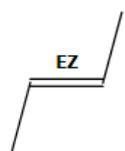
CAS Draw ▾



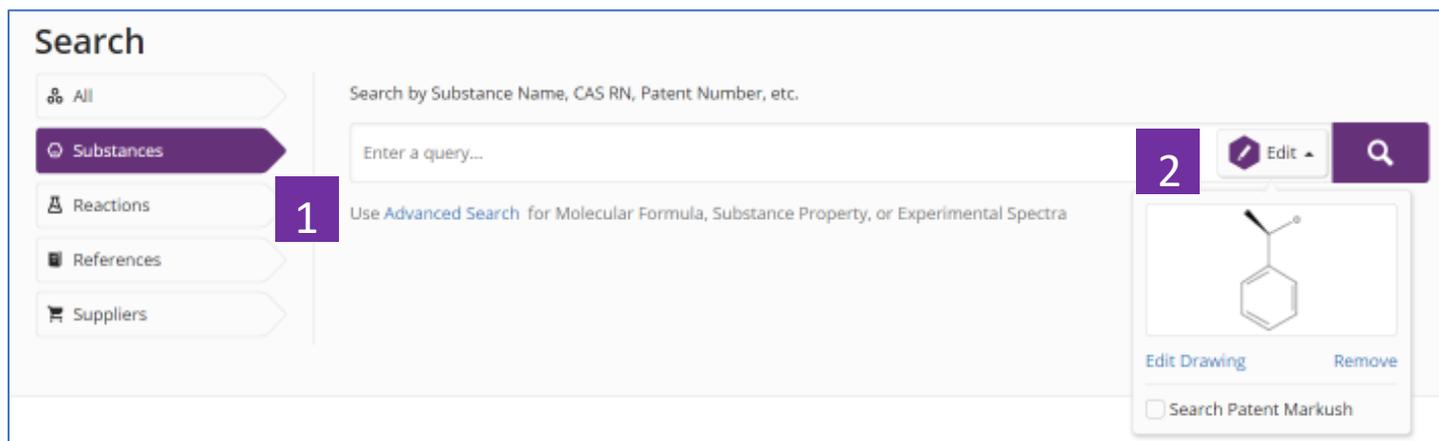
 Draw or change atoms or bonds.

C ▾ Et ▾

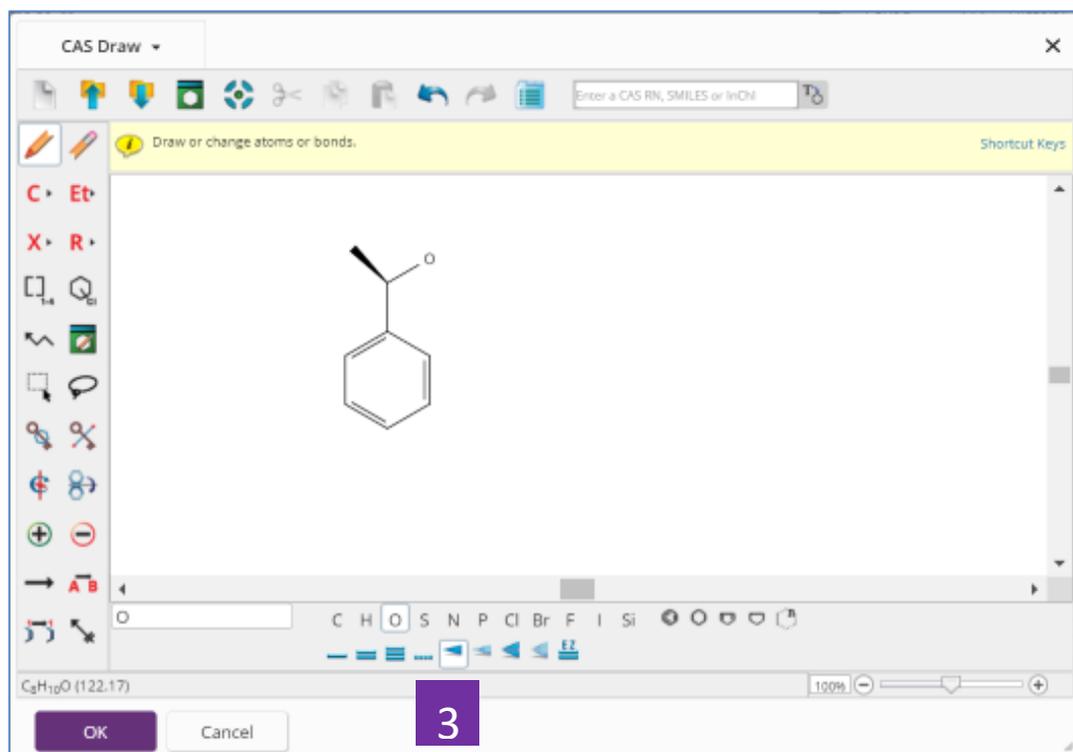
X ▾ R ▾



SciFinderⁿ 使用技巧 | 立體化合物的檢索



1. 選擇 **Substances**，進行物質檢索
2. 在結構編輯器中繪製出立體化合物的結構



3. 繪製結構時，使用立體異構鍵標注結構中的立體特徵

Structure Match

As Drawn (250)

Substructure (4.7M)

Similarity (15K)

Analyze Structure Precision

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
 - Absolute Stereo Match (56)
 - Absolute Stereo Mirror Image (53)
 - Stereo that Doesn't Match Query (29)
 - No Stereo in Answer Structure (112)
- Number of Components
- Substance Class

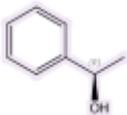
4

Substances (56)

Sort: Relevance View Partial

References Reactions Suppliers

1517-69-7
View Detail

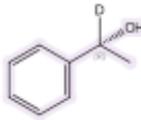


Absolute stereochemistry shown, Rotation (+)

$C_8H_{10}O$
(+)-1-Phenylethanol

3,701 References 9,271 Reactions 92 Suppliers

71886-65-2
View Detail

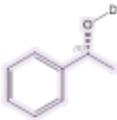


Absolute stereochemistry shown

C_8H_9DO
(αR)- α -Methylbenzenemethanol-*d*-ol

14 References 19 Reactions 1 Supplier

1246182-86-4
View Detail

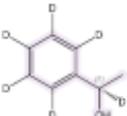


Absolute stereochemistry shown

C_8H_9DO
(αR)- α -Methylbenzenemethanol-*d*

6 References 13 Reactions 0 Suppliers

159146-97-1
View Detail



Absolute stereochemistry shown

$C_8H_4D_6O$
Benzene-*d*₅-methanol-*d*-ol, α -methyl-, (*R*)-

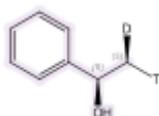
155797-94-7
View Detail



Absolute stereochemistry shown

$C_8H_{10}O$
Benzenemethanol-¹⁸O, α -methyl-, (*R*)-

101860-64-4
View Detail



Absolute stereochemistry shown

C_8H_8DOT
Benzenemethanol, α -(methyl-*d*-*t*), [*R*-(*R**,*S**)]-

4.在物質結果集中，通過左側 Stereochemistry 流覽並選擇需要的立體物質

SciFinderⁿ 使用技巧 | 同位素化合物的檢索

The screenshot shows the SciFinder search interface. On the left, there is a vertical menu with options: All, Substances, Reactions, References, and Suppliers. The 'Substances' option is highlighted with a purple arrow and a purple box containing the number '1'. The main search area has a header 'Search by Substance Name, CAS RN, Patent Number, etc.' and a search input field with the placeholder text 'Enter a query...'. Below the input field, there is a link for 'Advanced Search' with a purple box containing the number '2'. On the right side of the search area, there is a 'Draw' button with a chemical structure icon and a magnifying glass icon. The 'Draw' button is highlighted with a purple box containing the number '3', and the magnifying glass icon is highlighted with a purple box containing the number '4'.

1. 選擇 **Substances**，進行物質檢索
2. 點擊 **Advanced Search**，根據分子式、屬性或實驗譜圖來檢索物質
3. 點擊 **Draw**，進行結構檢索
4. 點擊放大鏡，開始物質檢索

Substances

References

Advanced Substance Search

1

Molecular Formula

Enter one Molecular Formula.

Ex: C6H6
(C8H8)_x
C22H26CuN2O5.C2H3N

Add Another Molecular Formula

— AND —

Substance Property

Select Property Enter Value

- Select One -

Add Another Property

— AND —

Experimental Spectra

Select Spectrum Enter Value

- Select One -

Add Another Sp **2**

Clear All

1. 可以通過分子式輸入 **H** 的同位素 (**D** 或 **T**)，進行同位素化合物檢索
2. 點擊放大鏡，開始檢索

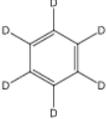
Substances (19) Sort: Relevance View Partial

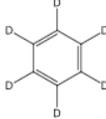
References Reactions Suppliers Save

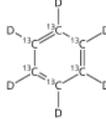
Filter by

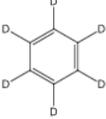
- Commercial Availability
 - Available (4)
 - Not Available (15)
- Reaction Role
- Reference Role
- Number of Components
- Substance Class
- Isotopes **1**
 - Containing Isotopes (19)
- Metals
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Search Within Results

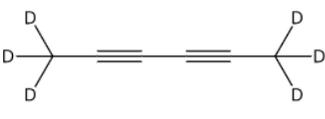
2

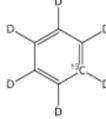
1076-43-3 View Detail

 C_6D_6
 Benzene- d_6
 2,823 References 27K Reactions 134 Suppliers

38091-14-4 View Detail

 C_6D_6
 Benzene- d_6 , radical ion(1+)
 45 References 0 Reactions 0 Suppliers

32602-97-4 View Detail

 C_6D_6
 Benzene-1,2,3,4,5,6- $^{13}C_6$ -1,2,3,4,5,6- d_6
 9 References 0 Reactions 4 Suppliers

34525-57-0 View Detail

 C_6D_6
 Benzene- d_6 , radical ion(1-)
 8 References 0 Reactions 0 Suppliers

73113-25-4 View Detail

 C_6D_6
 2,4-Hexadiyne-1,1,1,6,6,6- d_6 , radical ion(1+)
 7 References 0 Reactions 0 Suppliers

55153-53-2 View Detail

 C_6D_6
 Benzene- ^{13}C - d_6
 6 References 0 Reactions 1 Supplier

1. 獲得符合輸入分子式的同位素標記物質
2. 流覽並選擇需要獲取的物質結果

SCIFINDERⁿ
A CAS SOLUTION

Substances ▾ Enter a query... Edit 🔍 ⭐ ⌚ 👤

← Return to Home

Structure Match

As Drawn (11K)

Substructure (109.1M)

Similarity (7,034)

Analyze Structure Precision

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry
- Number of Components
- Substance Class
- Isotopes
 - Containing Isotopes (725)
 - Not Containing Isotopes (10K)
- Metals
- Experimental Property
- Experimental Spectrum

Substances (725)

References ▾ Reactions ▾ Suppliers ▾

1

1076-43-3
View Detail

C6D6
Benzene-*d*₆

2,823 References 27K Reactions 134 Suppliers

1120-89-4
View Detail

C6H5D
Benzene-*d*

377 References 144 Reactions 14 Suppliers

134-47-5
View Detail

C6H3D3
Benzene-1,3,5-*d*₃

176 References 11 Reactions 12 Suppliers

13657-09-5
View Detail

C6HD5
Benzene-1,2,3,4,5-*d*₅

130 References 29 Reactions 12 Suppliers

1684-46-4
View Detail

C6H4D2
Benzene-1,4-*d*₂

117 References 11 Reactions 6 Suppliers

32488-44-1
View Detail

C6H6
Benzene-1,2,3,4,5,6-¹³C₆

98 References 47 Reactions 20 Suppliers

2

Edit Drawing Remove

Search Patent Markush

1. 根據結構式來檢索物質
2. 在物質結果中，通過左側 Isotopes 選擇 containing isotopes，獲取含有同位素標記的物質結果

SciFinderⁿ 使用技巧 | 獲取製劑（配方）資訊

在 SciFinderⁿ 中可通過以下 2 種方式獲取製劑（配方）資訊：

直接在 **Reference** 檢索框中輸入檢索式，在得到的文獻結果頁面左側選擇 **Formulation Purpose**, 獲得感興趣的製劑（配方）資訊

從物質檢索開始，通過物質獲取文獻，然後在文獻結果頁面左側選擇

Formulation Purpose, 獲得感興趣的製劑（配方）資訊

方法 1、直接在 **Reference** 檢索框中輸入檢索式，在得到的文獻結果頁面左側選擇 **Formulation Purpose**, 獲得感興趣的製劑（配方）資訊（以獲取依託必利緩釋劑為例）：

SCIFINDERⁿ A CAS SOLUTION

References ▾ Itopride sustained release 1

Draw 🔍 ★ ⌚ 👤

← Return to Home

Filter by

- Relevance
- Document Type
- Substance Role
- Language
- Publication Year
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept
- CAS Solutions
 - Formulus (6,747) 2
 - MethodsNow: Analysis (263)
- Formulation Purpose
 - Drug delivery systems (961)
 - Drugs (658)
 - Antitumor agents (404)
 - Antidiabetic agents (243)
 - Anti-inflammatory agents (241) 3[View All](#)
- Database
- Search Within Results

References (60,082) Sort: Relevance ▾ View: Full Abstract ▾

Substances ▾ Reactions ▾ Cited By ▾ Save

Formulation & evaluation of itopride HCl sustained release pellets P

By: Rao, P. Sambha Siva; Babu, G. Raveendra; Praveen, T. Kala; Surekha, P. Sri Lakshmi; Shekhar, M. Chandra
International Journal of Pharmaceutical Sciences and Research (2014), 5(5), 2074-2083, 10 pp. | Language: English, Database: CAPlus
[View Reference Detail](#)

Abstract: The present work is aimed to formulate itopride HCl sustained release pellets using Et cellulose N50 such as hydrophobic polymer by employing the solution/suspension layer technique. The drug excipients compatibility study was carried out by Furor Transform IR spectroscopy (FTIR) which reveals no interaction between drug and excipients. Total 12 batches were formulated. Six formulations were prepared by using each natural polymer like Et cellulose N50. All the formulations were evaluated for micromeritic properties, phys. evaluation, which includes particle size anal., percentage yield, drug content, drug entrapment efficacy, percent moisture loss and swelling index, in vitro dissolution studies, SEM, and drug polymer interaction studies. The formulated pellets were evaluated for various pellet properties, like hardness, bulk d., tapped d., cars index and dissolution rate. Comparative evaluation of the above-mentioned parameters established the superiority of the pellets formulated with Et cellulose those formulated with different grades. The Optimized batch F3 was found to release the drug for 12 h (96.46%) and follows Higuchi Matrix model in dissolution studies, indicating the matrix-forming potential of natural polymer and diffusion controlled release mechanism.

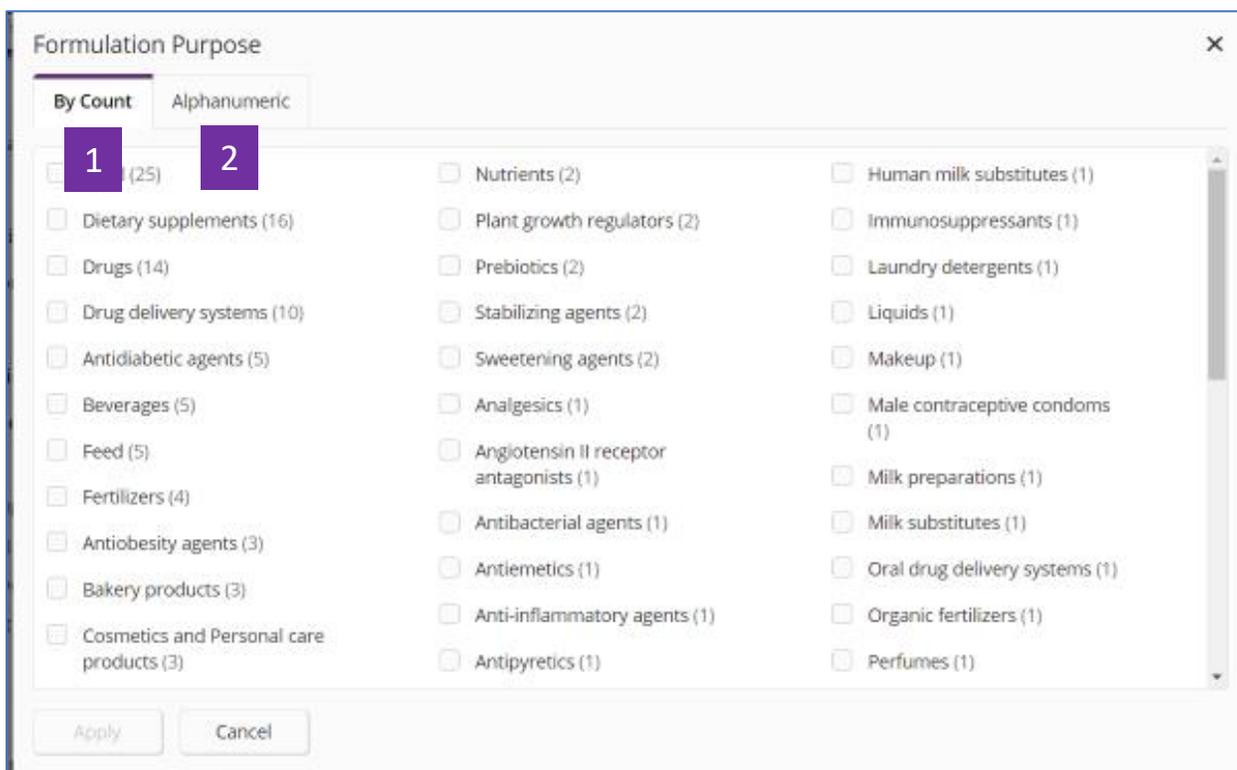
Full Text ▾ Substances (4) Reactions (0) Cited By (2) Citation Map

Sustained release Itopride hydrochloride matrix tablet

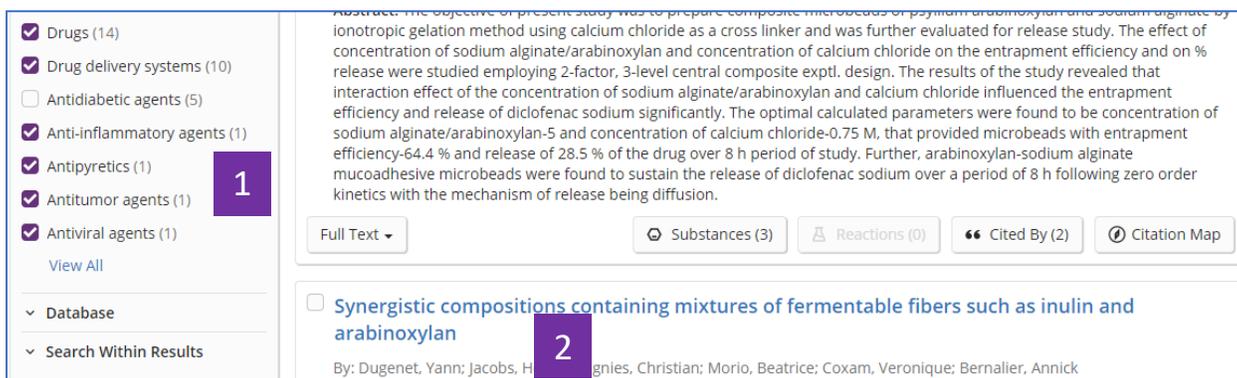
By: Prajapati, Bhupendra G.; Patel, Niklesh; Patel, Hitesh K.
Journal of Pharmaceutical Research and Health Care (2010), 2(1), 75-83 | Language: English, Database: CAPlus
[View Reference Detail](#)

Abstract: Oral route gets the highest priority for the delivery of the drug as well as better patient compliance in case of self delivery dosage formulation. The aim of present investigation was undertaken with the objective of formulating sustain release formulation of utopride hydrochloride for oral drug delivery. Itopride hydrochloride is highly water soluble prokinetic drug. Hydroxypropyl methylcellulose K4M (lower viscosity grade) and K100M (higher viscosity grade) were used as a matrix forming agents to control the release of drug. HPMC K4M and HPMC K100M were used individually as well as in combination with different proportion in the preparation of the Sustained release formulation. 3² Factorial designs were applied to the polymer concentration that affects the drug release profile. Reduced equation for drug release at 2hr, 6hr, and 10h were Q₂ = 37.644-5.41X₁-3.25X₂-2.017X₁², Q₆ = 72.367-8.05X₁-4.4X₂-3.75X₁², and Q₁₀ = 90.844-5.8X₁-2.633X₂-2.8X₁X₂ resp. Optimized batch F019 shows good tablet properties like hardness (7-9kg/cm²), thickness (4.48mm), friability (0.024%), assay (99.3%) and nearly similar

1. 直接進行文獻檢索
2. 點擊 Formulus，可以獲得製劑（配方）的更多資訊（請諮詢美國化學文摘社台灣代表處 Taiwan@acs-i.org 獲取更多有關 Formulus 的資訊）
3. 在 Formulation Purpose 進行勾選感興趣的製劑（配方）資訊，點擊 View All 查看全部選項



1. 根據文獻數量對選項進行排序
2. 根據選項字母順序排序



1. 可以選擇一個或者幾個選項
2. 點擊題目查看文獻資訊詳情

Hydrolysed protein-polysaccharide complexes

By: Schmitt, Christophe Joseph Etienne

Abstract: Hydrolyzed protein-polysaccharide complexes, and more specifically those complexes formed by complex formation of a protein with a polysaccharide followed by hydrolysis are presented. The resulting complexes have good emulsifying and stabilizing properties and can be used in food, cosmetic or pharmaceutical products. The invention further relates to the method of manufacture of such complexes.

PATENTPAK Viewer

Full Text ▾

Patent Family

Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Number	Application Date
EP2196097	English	A1	1 PDF PDF+ Viewer	2010-06-16	EP2008-170653	2008-12-04
EP2196097	English	B1	PDF	2014-06-18	EP2008-170653	2008-12-04
ES2488098	Spanish	T3	PDF	2014-08-26	ES2008-170653	2008-12-04
AU2009324245	English	A1	PDF	2010-06-10	AU2009-324245	2009-11-30
CA2743101	English	A1		2010-06-10	CA2009-2743101	2009-11-30
WO2010063669	English	A1	PDF PDF+ Viewer	2010-06-10	WO2009-EP66038	2009-11-30
CN102227170	Chinese	A	PDF	2011-10-26	CN2009-80147598	2009-11-30
IL211972	English	A		2012-12-31	IL2009-211972	2009-11-30
NZ591979	English	A		2013-01-25	NZ2009-591979	2009-11-30
AU2009324245	English	B2	PDF	2014-11-20	AU2009-324245	2009-11-30
CN102227170	Chinese	B	PDF	2014-12-10	CN2009-80147598	2009-11-30
BR2009022290	Portuguese	A2		2015-08-11	BR2009-22290	2009-11-30
MY158625	English	A		2016-10-31	MY2011-1385	2009-11-30
US20110236554	English	A1	PDF	2011-09-29	US2011-13129501	2011-06-06
US8728556	English	B2	PDF PDF+ Viewer	2014-05-20	US2011-13129501	2011-06-06

[Expand All](#) | [Collapse All](#)

▾ Concepts

▾ Substances

▴ Formulations **2**

1. 點擊 PatentPak 可以直接閱讀或者獲取專利的 PDF 全文
2. 點擊 Formulations 查看製劑（配方）資訊

Hydrolyzed Protein-Polysaccharide Complex: Pharmaceutical Products or Cosmetic, Etc. 1

[View Formulus® Detail ?](#) 2

Location: example 3 3

Purpose: Cosmetics and Personal care products, Drugs 3

Component 4	Function 5	Amount Reported 6
Whey proteins	active agent	1 w %
Gum arabic 7	active agent	1 w %
Enzeco bromelain enzyme	enzymes	1 w %
Sunflower oil	-	10 g

Additional Components Reported in Full Text

1. 點擊 **View Formulus** 將進入 **CAS** 另一個解決方案 **Formulus** (關於 **Formulus** 的更多資訊，請諮詢美國化學文摘社台灣代表處 Taiwan@acs-i.org)
2. 該製劑（配方）在原文中出現的位置（示例為在實施例 3 中）
3. 製劑（配方）用途
4. 製劑（配方）中的成分
5. 各成分所起的作用
6. 成分含量
7. 點擊藍色超連結的物質名，可以獲取其物質資訊詳情

方法 2、從物質檢索開始，通過物質獲取文獻，然後在文獻結果頁面左側選擇 Formulation Purpose,獲得感興趣的製劑（配方）資訊（以獲取阿拉伯木聚糖製劑資訊為例）：

The screenshot shows the SciFinder search results page for 'arabinoxylan'. The search bar at the top contains 'arabinoxylan'. On the left, a sidebar lists filters: 'Substances (1)' (highlighted with a purple box labeled '1'), 'Reactions (20)', 'References (5,458)', and 'Suppliers (3)'. The main content area is titled 'All Answer Types' and shows 'Substances (1)'. A specific substance entry is displayed with the ID '9040-27-1' and a 'View Detail' link. Below the ID, it says 'Image Not Available'. The substance is labeled 'Unspecified Arabinoxylan'. At the bottom of the entry, there are three buttons: 'References' (3,515), 'Reactions' (20), and 'Suppliers' (3). A purple box labeled '2' is placed over the 'References' button.

1. 進行物質檢索，獲得物質檢索結果集
2. 由物質獲得文獻結果集

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References ▾ Enter a query...

Draw 🔍 ★ 🕒 👤

Filter by

- Document Type
- Substance Role
- Language
- Publication Year
- Available at My Institution
- Author
- Organization
- Publication Name
- Concept
- CAS Solutions
- Formulation Purpose **1**
 - Food (25)
 - Dietary supplements (16)
 - Drugs (14)
 - Drug delivery systems (10)
 - Antidiabetic agents (5)

[View All](#)

References (3,515)

Sort: Relevance ▾ View: Full Abstract ▾

Substances ▾ Reactions ▾ Cited By ▾

📄 📧 ★ Save

Cereal arabinoxylans: advances in structure and physiochemical properties

By: Izydorczyk, Marta S.; Billaderis, Costas G.
Carbohydrate Polymers (1995), 28(1), 33-48 | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: A review with 89 references They consist of a linear β -(1 \rightarrow 4) linked xylan backbone to which α -L-arabinofuranose units are attached as side residues via α -(1 \rightarrow 3) and/or α -(1 \rightarrow 2) linkages. Several structural models have been put forward based on enzymic degradation studies and structure elucidation of oligosaccharides by NMR, methylation, and periodate oxidation techniques. These tentative models present different substitution patterns of arabinoses along the xylan chain. Cereal arabinoxylans exhibit a great deal of structural heterogeneity with respect to ratio of Araf/Xylp, substitution pattern of arabinoses, content of feruloyl groups and mol. size. The conformation and physiochem. properties (viscosity, gelation potential, intermol. association) of arabinoxylans in aqueous solutions are dependent on the mol. features of these polysaccharides; specific structure-property relationships have been established in model and actual food systems. Wheat and rye arabinoxylans are important functional ingredients in baked products affecting the mech. properties of dough, as well as the texture and other end-product quality characteristics.

Full Text ▾ Substance (1) Reactions (0) Cited By (502) Citation Map

Arabinoxylans and Endoxylanases in Wheat Flour Bread-making

By: Courtin, C. M.; Delcour, J. A.
Journal of Cereal Science (2002), 35(3), 225-243 | Language: English, Database: CAplus
[View Reference Detail](#)

1. 在 Formulation Purpose 中勾選所需目標製劑資訊

SciFinder[®] 使用技巧 | 片段結構的物質檢索

如果希望某些重要的結構片段一定要出現在物質中，且對這些片段相互之間的連接方式和位置不明確要求的話，則可以在 SciFinder[®] 中用片段結構檢索來實現。

The screenshot displays the SciFinder search interface. On the left, a vertical navigation menu includes 'All', 'Substances', 'Reactions', 'References', and 'Suppliers'. The 'Substances' option is highlighted with a purple arrow and a purple box containing the number '1'. The main search area features a search bar with the placeholder text 'Enter a query...' and a search button with a magnifying glass icon. Above the search bar, it says 'Search by Substance Name, CAS RN, Patent Number, etc.' and below it, 'Use [Advanced Search](#) for Molecular Formula, Substance Property, or Experimental Spectra'. To the right of the search bar, there is an 'Edit' button with a pencil icon and a search button with a magnifying glass icon. A purple box with the number '3' is positioned above the search button. Below the search bar, a drawing tool is open, showing two chemical structures: a cyclohexane ring and a cyclohexane ring with a methyl group. A purple box with the number '2' is positioned to the left of the drawing tool. Below the drawing tool, there are buttons for 'Edit Drawing' and 'Remove', and a checkbox for 'Search Patent Markush'.

1. 選擇 **Substances** 檢索
2. 繪製片段結構
3. 點擊檢索

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A CAS SOLUTION

Substances ▾ Enter a query...

0 References 0 Reactions 0 Suppliers

1 Reference 0 Reactions 0 Suppliers

6 Reactions 3 Suppliers

3 References 0 Reactions 1 Supplier

1 Reference 0 Reactions 0 Suppliers

1 Reference 0 Reactions 0 Suppliers

1 Reference 3 Reactions 1 Supplier

89 References 0 Reactions 5 Suppliers

1 (261K) **1**

2 (12K)

3 (693)

4 (218)

5 or more (320)

Substance Class **2**

Organic/Inorganic Small Molecule (259K)

Coordination Compound (789)

Protein/Peptide Sequence (308)

Incompletely Defined Substance (265)

Nucleic Acid Sequence (249)

Polymer (148)

Radical Ion (2)

View Fewer

Isotopes

99361-68-9
View Detail

O=C1NC(=O)C(S(=O)(=O)c2ccccc2)C(=O)N1

$C_{10}H_8N_2O_5S$
5-Pyrimidinesulfonic acid, 1,2,3,4-tetrahydro-2,4-dioxo-, phenyl ester

3 References 0 Reactions 1 Supplier

211449-01-1
View Detail

O=C1NC(=O)C(=O)N(C1)C2=CC=CC=C2

$C_{10}H_8HgN_2O_3$
Mercury, (2-hydroxyphenyl)(2,4(1H,3H)-pyrimidinedionato-κN³)-

1 Reference 0 Reactions 0 Suppliers

000-11-3
View Detail

COC1=CC=C(C=C1)SCC2=CN(C(=O)NC2=O)C3=CC=CC=C3

$C_{12}H_{12}N_2O_3S$
2,4(1H,3H)-Pyrimidinedione, 5-[[[4-methoxyphenyl]thio]methyl]-

1 Reference 1 Reaction 3 Suppliers

211449-03-5
View Detail

O=C1NC(=O)C(=O)N(C1)C2=CC=C(O)C=C2

$C_{10}H_8HgN_2O_3$
Mercury, (4-hydroxyphenyl)(2,4(1H,3H)-pyrimidinedionato-κN³)-

1 Reference 0 Reactions 0 Suppliers

515824-66-5
View Detail

COC1=CC=C(C=C1)SCC2=CN(C(=O)NC2=O)C3=CC=CC=C3

$C_{12}H_{12}N_2O_3S$
2,4(1H,3H)-Pyrimidinedione, 5-[[[4-methoxyphenyl]methyl]thio]-

1 Reference 3 Reactions 1 Supplier

29050-86-0
View Detail

O=C1NC(=O)C(=O)N(C1)/N=N/C2=CC=C(O)C=C2

$C_{10}H_8N_4O_3$
6-[2-(4-Hydroxyphenyl)diazenyl]-2,4(1H,3H)-pyrimidinedione

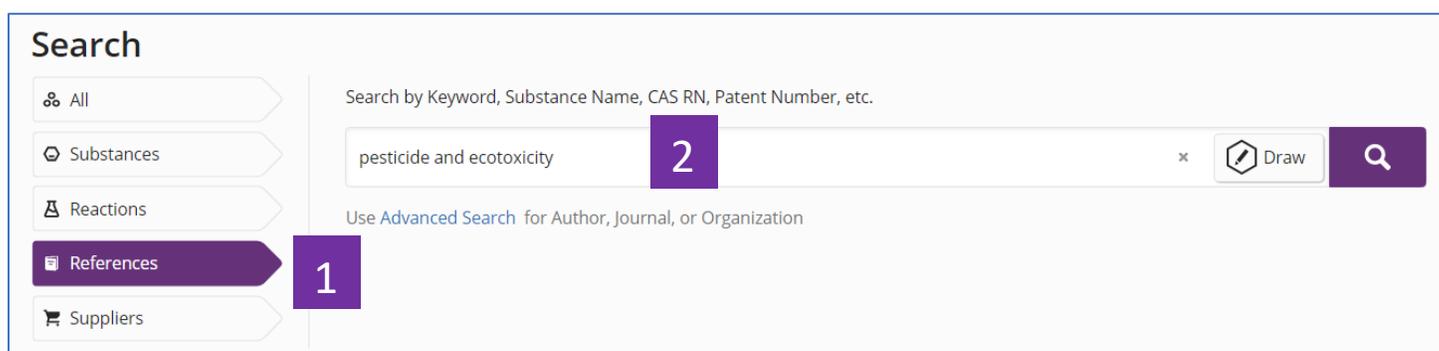
89 References 0 Reactions 5 Suppliers

1. 通過 **Number of Components**，限定被檢索的片段在同一個組分或多個不同組分中（如，選擇 **1**，表示被檢索片段在同一個組分中；選擇 **2**，表示被檢索片段分別在 **2** 個不同組分中等；以此類推）
2. 可繼續通過 **Substance Class**，篩選物質類型
3. 查看物質詳情

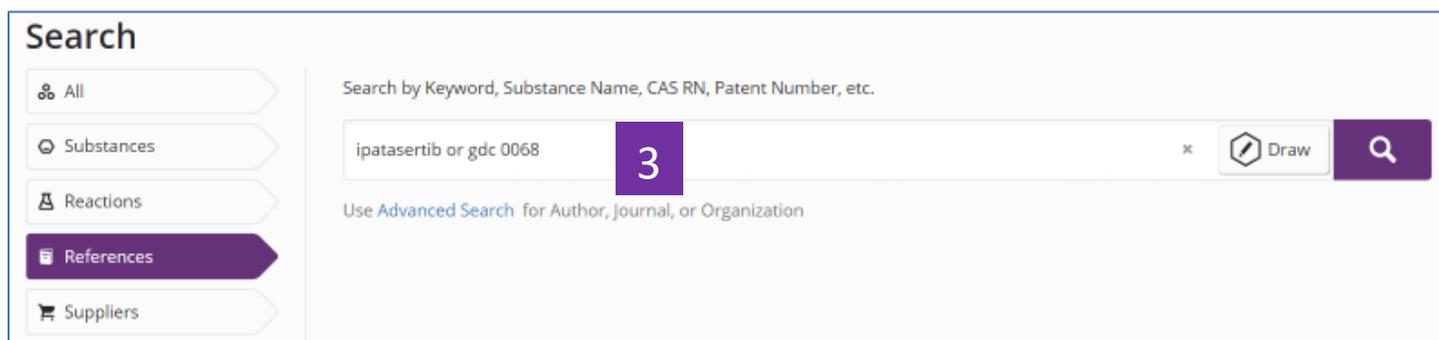
SciFinderⁿ 使用技巧 | 布林邏輯運算元在文獻檢索中的應用

在 SciFinder-n 中用文本詞語檢索文獻時，可使用以下布林邏輯運算元：

1. AND：表示兩個（多個）被檢索的詞語同時出現在檢索結果中；
2. OR：表示在檢索結果中出現任意一個被檢索詞即可；
3. NOT：排除某個被檢索詞出現在檢索結果中；
4. “ ”：表示被檢索的是一個確定的詞語或片語；
5. ()：在檢索式中有多個布林邏輯運算元時，可用括弧指定不同布林邏輯運算元間的運行順序。



1. 點擊 **References** 開始文獻檢索
2. 使用 **AND** 連接兩個檢索詞，如 **Pesticide and ecotoxicity**，表示在檢索結果中 **Pesticide** 和 **ecotoxicity** 同時出現



3. 使用 **OR** 連接兩個檢索詞，如 **ipatasertib or gdc 0068**，表示 **ipatasertib** 和 **gdc 0068** 任意一個出現即可

The screenshot shows a search interface with a sidebar on the left containing navigation options: All, Substances, Reactions, References (highlighted), and Suppliers. The main search area has a header "Search by Keyword, Substance Name, CAS RN, Patent Number, etc." and a search input field containing the query "thermally conductive not halogen-containing pd". A purple box with the number "4" is placed over the search input. A dropdown menu is visible below the input, listing search results such as "thermally conductive not Halogen-containing polymers", "thermally conductive not Halogen-containing polyamide-polyesters", and "thermally conductive not Halogen-containing polycarbonate-polysulfones". The interface also includes a "Recent Search History" section at the bottom left showing the date "October 12, 2019".

4.使用 NOT 連接兩個單詞或片語，如 thermally conductive not halogen-containing polymers，則只能得到 thermally conductive 出現的結果。

The screenshot shows a search interface similar to the one above. The search input field contains the query "high efficiency and low toxicity and (pesticide or herbicide)". A purple box with the number "5" is placed over the search input. A dropdown menu is visible below the input, listing search results such as "high efficiency and low toxicity and (pesticide or herbicide)", "high efficiency and low toxicity and (pesticide or herbicides)", and "high efficiency and low toxicity and (pesticide or herbicide M)". The interface also includes a "Recent Search History" section at the bottom left showing the date "October 12, 2019".

5.當使用多個布林邏輯運算元時，可使用括弧()，指定邏輯運算元的運算順序。如 high efficiency and low toxicity and (pesticide or herbicide)，此時表示優先運算 pesticide or herbicide。

Search

All
Substances
Reactions
References
Suppliers

Search by Keyword, Substance Name, CAS RN, Patent Number, etc.

"total synthesis" and taxol **6** × Draw 🔍

Use [Advanced Search](#) for Author, Journal, or Organization

6. 引號“”，表示被檢索的詞（片語）為確定的，不能出現不同拼寫或片語被拆分的情況，如“total synthesis” and taxol。此時指 total synthesis 是一個固定片語

SCIFINDERⁿ A CAS SOLUTION

References ▾ "total synthesis" and taxol × Draw 🔍 ★ 🕒 👤

← Return to Home

References (298) Sort: Relevance ▾ View: Partial Abstract ▾

Substances ▾ Reactions ▾ Cited By ▾ 📄 📧 ★ Save

Total synthesis of taxol.

By: Nicolaou, K C; Yang, Z; Liu, J J; Ueno, H; Nantermet, P G; Guy, R K; Claiborne, C F; Renaud, J; Couladouros, E A; Paulvannan, K
Nature (1994), 367(6464), 630-4 | Language: English, Database: MEDLINE
[View Reference Detail](#)

Abstract: Taxol, a substance originally isolated from the Pacific yew tree (*Taxus brevifolia*) more than two decades ago, has recently been approved for the clinical treatment of cancer patients. Hailed as having provided one of the most significant advances in cancer therapy, this molecule exerts its anticancer activity by inhibiting mitosis through enhancement of the polymerization of tubulin and consequent stabilization of microtubules. The scarcity of taxol and the ecological impact of harvesting it have prompted extensive searches for alternative sources including semisynthesis, cell-free culture, and

[View More ▾](#)

Full Text ▾ Substance (1) Reactions (0) Cited By (718) Citation Map

Total synthesis of taxol

By: Nicolaou, K. C.; Yang, Z.; Liu, J. J.; Ueno, H.; Nantermet, P. G.; Guy, R. K.; Claiborne, C. F.; Renaud, J.; Couladouros, E. A.
Nature (London, United Kingdom) (1994), 367(6464), 630-4 | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: The total synthesis of taxol (I) from the benzofuranone II by a convergent strategy, which opens a chem. pathway for the production of both I and a variety of designed taxoids is reported.

[View More ▾](#)

Full Text ▾ Substances (26) Reactions (23) Cited By (718) Citation Map

Filter by

Relevance

- Best (69)
- Good (174)
- Fair (55)

[Learn more about Relevance...](#)

Document Type

- Journal (222)
- Patent (11)
- Review (86)
- Commentary (1)
- Conference (42)

[View All](#)

Language

- English (256)
- Japanese (15)
- Chinese (12)
- German (4)
- French (2)

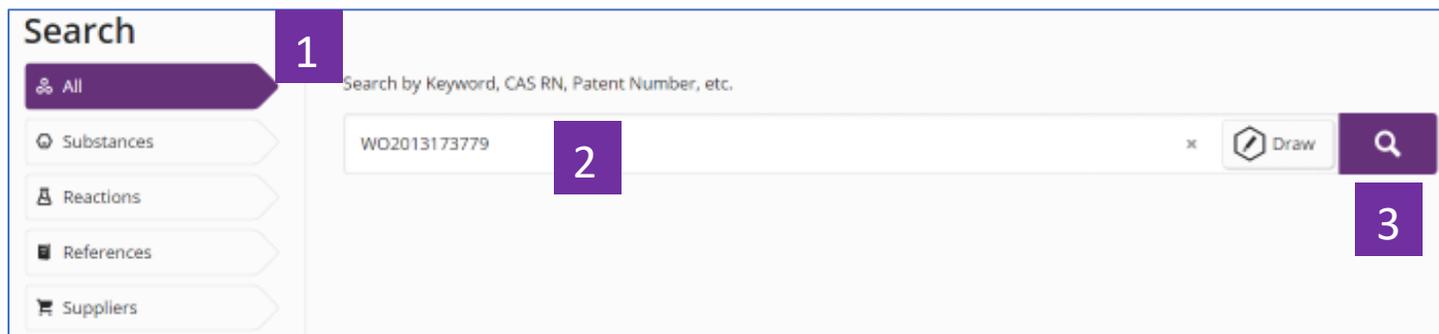
[View All](#)

Publication Year

SciFinderⁿ 使用技巧 | 利用專利號進行檢索

當用專利號進行檢索時，可以選擇 All 或分別選擇 Substances、Reactions 和 References 進行檢索。

注：專利號中的國家代碼和數字間不能用空格隔開，如 WO2013173779



1. 選擇 All，同時獲取該專利中披露的反應、物質、本專利文獻及其披露的物質的供應商資訊
2. 輸入專利號
3. 進行檢索


All WO2013173779 Draw Search Star Clock User

[Return to Home](#)

Show only **4**

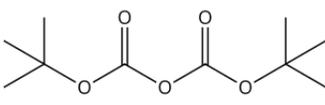
- Substances (18)
- Reactions (35)
- References (2)
- Suppliers (0)

All Answer Types

Top two answers by relevance from each answer type.

Substances (18)

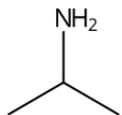
24424-99-5
[View Detail](#)



C₁₀H₁₈O₅
Di-tert-butyl dicarbonate

49K References
136K Reactions
144 Suppliers

75-31-0
[View Detail](#)



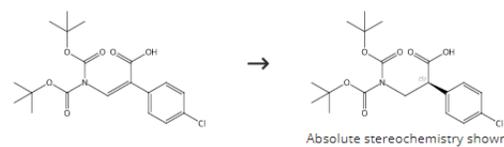
C₃H₉N
Isopropylamine

20K References
24K Reactions
68 Suppliers

[View All Substances](#)

Reactions (35)

Scheme 1 (1 Reaction) [View](#)



Steps: 1
Yield: 99%

Absolute stereochemistry shown

4. 本專利披露的物質、反應和本專利文獻資訊及其披露的物質的供應商資訊

SCI FINDERⁿ
A CAS SOLUTION

References WO2013173779

Draw

5

Return to Home

Filter by

- Relevance
- Document Type
 - Patent (2)
- Language
- Publication Year

2009 2019

No Min to No Max Apply

View Larger
- Author
- Organization
- Publication Name
- Concept
- Database
- Search Within Results

References (2) Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

Process for making amino acid compounds

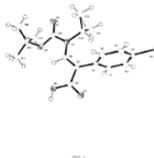
By: Remarchuk, Travis
United States, US9278917 B2 2016-03-08 | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: The invention provides new processes for making and purifying amino acid compounds, which are useful in the preparation of AKT inhibitors used in the treatment of diseases such as cancer, including the compound (S)-2-(4-chlorophenyl)-1-(4-((5R,7R)-7-hydroxy-5-methyl-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-yl)piperazin-1-yl)-3-(isopropylamino)propan-1-one.

PATENTPAK Full Text Substances (17) Reactions (12) Cited By (0) Citation Map

Process for making amino acid compounds using enantioselective hydrogenation reactions

By: Remarchuk, Travis
World Intellectual Property Organization, WO2013173779 A1 2013-11-21 | Language: English, Database: CAplus
[View Reference Detail](#)



Abstract: The invention provides processes for making and purifying amino acid compounds of formula I [R¹ and R² are independently H, C₁₋₁₂ alkyl, and amino-protecting group] and their salts, which are useful in the preparation of AKT inhibitors, including the compound (S)-2-(4-chlorophenyl)-1-(4-((5R,7R)-7-hydroxy-5-methyl-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-yl)piperazin-1-yl)-3-(isopropylamino)propan-1-one. Compound I [R¹ = H; R² = Boc] was prepared by condensation of Et 4-chlorophenylacetate with Et formate and isopropylamine followed by Boc-protection; the resulting (E)-Et 3-(tert-butoxycarbony...

View More

PATENTPAK Full Text Substances (18) Reactions (23) Cited By (1) Citation Map

5.選擇 References，獲得該專利及其同族資訊

SciFINDERⁿ
A CAS SOLUTION

Substances WO2013173779

Draw

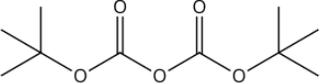
6

Substances (18)

Sort: Relevance View Partial

References Reactions Suppliers Save

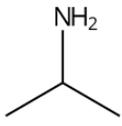
24424-99-5
View Detail



C₁₀H₁₈O₅
Di-*tert*-butyl dicarbonate

49K References 136K Reactions 144 Suppliers

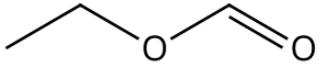
75-31-0
View Detail



C₃H₉N
Isopropylamine

20K References 24K Reactions 68 Suppliers

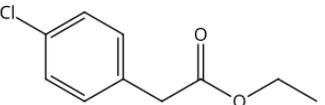
109-94-4
View Detail



C₃H₆O₂
Ethyl formate

13K References 13K Reactions 72 Suppliers

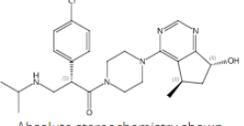
14062-24-9
View Detail



C₁₀H₁₁ClO₂
Benzeneacetic acid, 4-chloro-, ethyl ester

254 References 244 Reactions 68 Suppliers

1001264-89-6
View Detail

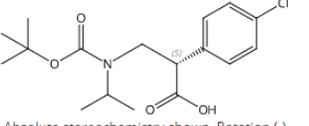


Absolute stereochemistry shown

C₂₄H₃₂ClN₅O₂
GDC 0068

131 References 254 Reactions 71 Suppliers

1001179-33-4
View Detail



Absolute stereochemistry shown, Rotation (-)

C₁₇H₂₄ClNO₄
(αS)-4-Chloro-α-[[[(1,1-dimethylethoxy)carbonyl](1-methylethyl)amino]methyl] benz...

24 References 156 Reactions 9 Suppliers

6. 選擇 Substances，獲得該專利披露的物質資訊

SCIFINDER[®]
A CAS SOLUTION

Reactions WO2013173779

Draw

7

Return to Home

Filter by

- Yield
- Number of Steps
- Experimental Protocols
- Reaction Type
- Stereochemistry
- Reagent
- Catalyst
- Solvent
- Commercial Availability
- Reaction Notes
- Search Within Results

Source Reference

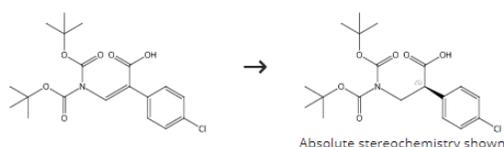
- Publication Year
- Document Type
- Language

Reactions (35)

View Collapsed

References

Scheme 1 (1 Reaction) View

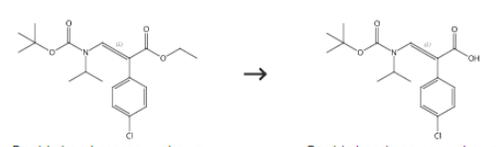


Steps: 1
Yield: 99%

Absolute stereochemistry shown

Expand Scheme

Scheme 2 (1 Reaction) View



Steps: 1
Yield: 91%

Double bond geometry shown

Supplier (1)

Suppliers (30)

7.選擇 Reactions，獲得該專利披露的反應資訊

SciFinder[®] 使用技巧 | 獲取化學品供應商資訊

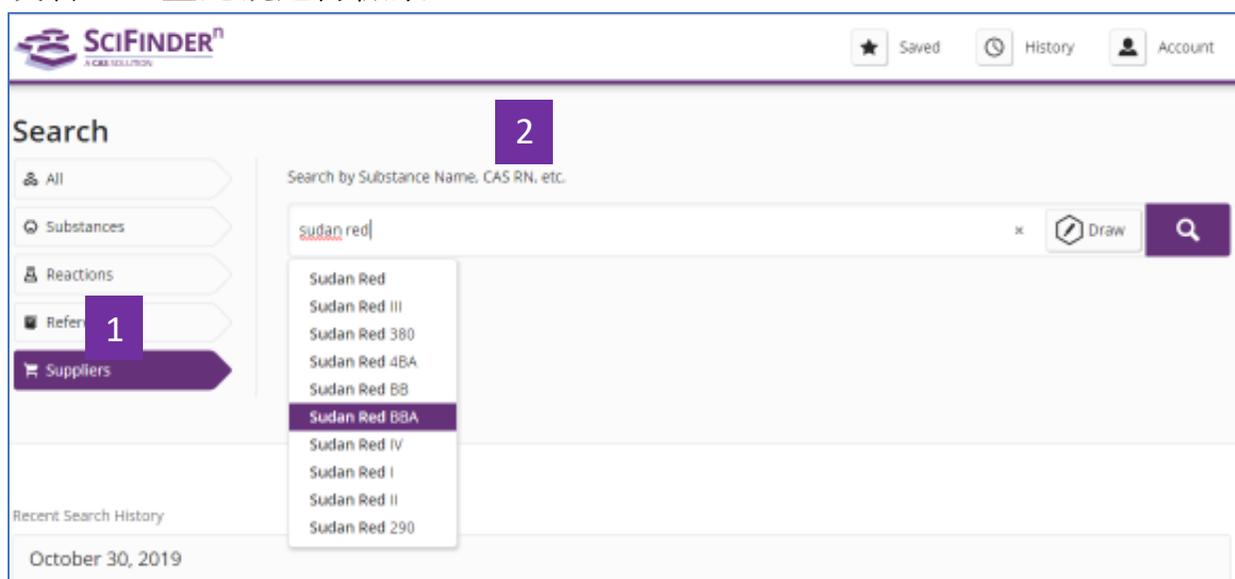
在 SciFinder[®] 中可通過以下三種方式獲取化學品供應商的資訊：

直接在 Suppliers 檢索框中輸入所需化學品的物質名稱（包括商品名、俗名等）或者 CAS 登記號進行檢索。

在物質結果集頁面，點擊相應的 suppliers 獲得供應商資訊

在反應結果集中頁面點擊相應的 Suppliers 獲取供應商資訊

方法一、直接在 Suppliers 檢索框中輸入所需化學品的物質名稱（包括商品名、俗名等）或者 CAS 登記號進行檢索



1. 點擊 Suppliers
2. 輸入所需化學品的物質名稱（包括商品名，俗名等），或者 CAS 登記號

化學品供應商資訊結果

SCIFINDERⁿ A CAS SOLUTION

Suppliers Sudan Red BBA

Draw

Return to Home

Filter by **1**

- Preferred Suppliers
 - No Preference (69)
- Supplier
 - Synnovator Product List (3)
 - Carbosynth Product List (2)
 - FUJIFILM Wako Chemicals Europe GmbH Product List (2)
 - FUJIFILM Wako Chemicals U.S.A. Corporation Product List (2)
 - FUJIFILM Wako Pure Chemical Corporation Product List (2)
 - [View All](#)
- Purity
 - ≥99% (1)
 - 95-98% (32)
 - 90-94% (5)
 - <90% (1)
- Quantity
 - Milligrams (17)
 - Grams (48)
 - Kilograms or greater (10)
 - Bulk (35)
 - Screening (9)
- Ships Within
 - 1 week (24)
 - 2 weeks (12)
 - 4 weeks (6)
 - 8 weeks (1)

Suppliers (69) Sort: Supplier: A to Z

Supplier: A to Z
Supplier: Z to A
Ships Within
Purity

Supplier	Substance	Purity	Purchasing D	
1Click CHEMISTRY 1Click Chemistry Stock Products United States	2 1-(2-methyl-4-[[2-methyl(phenyl)diazenyl]-phenyl]azo)-2-naphthol	95-98%	4 Order From Supplier USD 65.70 250.00 G, USD 97.40 1.00 KG, USD 230.80 2.50 KG, USD 461.60 View all Bulk	Maintained in stock Ships within 1 week
aablocks AA BLOCKS LLC Product List United States	85-83-6 2-Naphthalenol, 1-[[2-methyl-4-[[2-methyl(phenyl)azo]phenyl]azo]-	95-98%	Order From Supplier 25g, USD 39 100g, USD 75	Maintained in stock Ships within 1 week
abcr abcr GmbH Product List Germany	85-83-6 Sudan IV		5 Product Information EUR 79.20 EUR 1.0 kg, EUR 284.10	
Accel Pharmtech Accel Pharmtech Product List United States	85-83-6 1-((2-Methyl-4-(o-tolyldiazenyl)phenyl)diazenyl)naphthalen-2-ol	95-98%	1g 10g 100g 1kg	
AK Scientific AK Scientific Product Catalog United States	85-83-6 Solvent Red 24	95-98%	Order From Supplier 25g, USD 21 100g, USD 54	Maintained in stock Ships within

- Stock Status
 - Maintained in stock (34)
 - Typically in stock (17)
 - Intermittently available (3)
 - Synthesis on demand (3)
- Order From Supplier
 - Link Available (30)
- Country
 - United States (48)
 - Germany (12)
 - Japan (12)
 - China (10)
 - United Kingdom (10)
 - [View All](#)

aldlab Aldlab Chemicals In Stock Product List United States	85-83-6 Sudan IV:Solvent red 24	95-98%	Bulk Screening 1g 5g Bulk	1 week Typically in stock Ships within 2 weeks
Merck KGaA Darmstadt, Germany ALDRICH United States	85-83-6 Sudan IV		Order From Supplier 25 g 100 g Bulk	Maintained in stock
Alfa Aesar Alfa Aesar United States	85-83-6 Sudan IV		Order From Supplier 25g, USD 25.10 100g, USD 63.20 Bulk Screening	Typically in stock Ships within 1 week

1. 供應商篩選選項，可以根據：優選供應商、供應商名稱、產品純度、產品量級、運送時間、儲存狀態、是否有直達訂購連結、國家等對供應商結果進行篩選。
2. 可以選擇  或  來設置優選或者非優選供應商。
3. 可以按照供應商名稱的字母排列順序、運送時間或產品純度對供應商進行重新排序。
4. 點擊 **order from suppliers**，直接訪問產品訂購頁面。
5. 點擊 **product information**，訪問該供應商對此產品的描述資訊。

點擊 order from suppliers 所獲介面

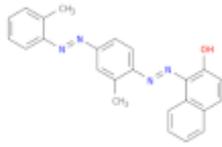
sales@aablocks.com +1 858-523-8231 Login | Register

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Home About Us Products Support Contact Us

Home / Other Building Blocks / 85-83-6

Catalog No.: AA00IDF7 **85-83-6 | 2-Naphthalenol, 1-[[2-methyl-4-[(2-methylphenyl)azo]phenyl]azo]-**



Pack Size	Purity	Availability	Price(USD)	Quantity	
25g	≥88% (dye content)	1 week	\$52.00	- 1 +	<input type="button" value="Add To Cart"/> <input type="button" value="Order Now"/>
100g	≥88% (dye content)	1 week	\$66.00	- 1 +	<input type="button" value="Add To Cart"/> <input type="button" value="Order Now"/>
250g	≥88% (dye content)	1 week	\$93.00	- 1 +	<input type="button" value="Add To Cart"/> <input type="button" value="Order Now"/>

Technical Information

Properties	Catalog Number: AA00IDF7
Literature	Chemical Name: 2-Naphthalenol, 1-[[2-methyl-4-[(2-methylphenyl)azo]phenyl]azo]-
Request for Quotation	CAS Number: 85-83-6
	Molecular Formula: C24H20N4O

點擊 Product Information 所獲介面



Search by CAS# / CAT# / Product Name

SEARCH

Home

About Us

Products v

Services v

Resources v

Order Center

Contact Us

NAVIGATION

> Products

> Services

> Hot Products HOT

> Order

CONTACT US

Email: info@alfa-chemistry.com

Tel: 1-201-478-8534

1-516-662-5404

Fax: 1-516-927-0118

Address: 2200 Smithtown Avenue, Room 1 Ronkonkoma, NY 11779-7329 USA

For product inquiries, please use our online system or send an email to inquiry@alfa-chemistry.com



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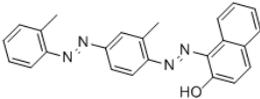


Home > Product > Dyes > Solvent Dyes > Solvent Red 24



Solvent Red 24

PRICE INQUIRY

Catalog Number	ACM85836
Product Name	Solvent Red 24
Structure	
CAS Number	85-83-6
IUPAC Name	(1Z)-1-[[2-methyl-4-(2-methylphenyl)diazenylphenyl]hydrazinylidene]naphthalen-2-one
Synonyms	Scharlachrot, Lipid crimson, Scarlet oil, Scarlet red, Oil Scarlet, Hidaco Oil Red, Resoform Red G, Waxoline Red O, Fat Ponceau R, Lacquer Red V, Organol Red B, Rubrum scarlatinum, Waxoline Red OM, Waxoline Red OS, Candle Scarlet B, Candle Scarlet G, Tertrogras Red N, Lacquer Red VS, Somalia Red IV, Sudan P
Molecular Formula	C ₂₄ H ₂₀ N ₄ O
Molecular Weight	380.45
Exact Mass	380.16400
Boiling Point	260°C
Melting Point	199°C
Flash Point	424.365°C
Density	1.192 g/cm ³
Purity	PURIFIED
Appearance	dark red to brown crystals or powder
InChIKey	KMDLOETUWUPGMB-BXCCFQQFSA-N

H-Bond Donor	1
H-Bond Acceptor	5
Safety Description	S24/25
Hazard Statements	Xi: Irritant; T: Toxic;
WGK Germany	3
Stability	Stable. Incompatible with strong oxidizing agents.
MSDS	Download MSDS
COA	Download COA
Spec Sheet	Download Spec Sheet

Return to Home

Filter by

- Preferred Suppliers
 - No Preference (69)
- Supplier
 - Synnovator Product List (3)
 - Carbosynth Product List (2)
 - FUJIFILM Wako Chemicals Europe GmbH Product List (2)
 - FUJIFILM Wako Chemicals U.S.A. Corporation Product List (2)
 - FUJIFILM Wako Pure Chemical Corporation Product List (2)
 - View All
- Purity
 - ≥99% (1)

Suppliers (69) Sort: Supplier: A to Z

Supplier	Substance	Pur	Price	Availability
	85-83-6 1-[(2-Methylphenyl)diazenyl]-2-naphthol	95-	25.00 G, USD 54.30 100.00 G, USD 65.70 250.00 G, USD 97.40 1.00 KG, USD 230.80 2.50 KG, USD 461.60 View all Bulk	Ships within 1 week

Download Results
Excel (.xlsx) (max 100)
PDF

1. 供應商結果集可以匯出為 **Excel** 或者 **PDF** 格式檔。
2. 點擊 **CAS** 登記號，查看物質資訊詳情。

點擊 CAS 登記號所獲介面

CAS RN
85-83-6
[View Detail](#)

CAS Name
Solvent Red 24

- Substance Detail
- Reactions (22)
- Synthesize (2)
- Create Retrosynthesis Plan
- References (1,301)
- Suppliers (69)

Edit Structure - Reset +

方法二：在物質結果集頁面，點擊相應的 Suppliers 獲得供應商資訊

The screenshot displays a search results page for substances. On the left, a sidebar titled 'Structure Match' contains filters such as 'As Drawn (74)', 'Substructure (282K)', and 'Similarity (7,473)'. Below these are various filter categories like 'Commercial Availability', 'Reaction Role', and 'Stereochemistry'. The main area shows a grid of substance cards under the heading 'Substances (66)'. Each card includes a chemical structure, a name, a molecular formula, and buttons for 'References', 'Reactions', and 'Suppliers'. Two purple callout boxes with the number '1' are positioned over the 'Commercial Availability' filter and the 'Suppliers' button of the first card. A purple callout box with the number '2' is positioned over the 'Suppliers' button of the second card.

1. 在物質結果集中，篩選有供應商資訊的物質
2. 點擊 Suppliers 按鈕，查看供應商資訊

方法三：在反應結果集中頁面點擊相應的 Suppliers 獲取供應商資訊

The screenshot displays a search interface for chemical reactions. On the left is a 'Filter by' sidebar with categories like Substance Role, Yield, Number of Steps, Experimental Protocols, Reaction Type, Stereochemistry, Reagent, Catalyst, Solvent, Commercial Availability, Reaction Notes, and Search Within Results. The main area is titled 'Reactions (4,604)' and shows 'Scheme 1 (1 Reaction) View'. The reaction scheme depicts the conversion of a complex starting material to a 5-methylimidazole product. Below the reaction, there are two 'Suppliers' buttons: one for the starting material with 2 suppliers (marked with a purple '1') and one for the product with 110 suppliers (marked with a purple '2'). Below the reaction scheme is a 'Reaction Summary' table with columns for Reagents, Catalysts, Solvents, and Conditions, and a summary box showing 'Steps: 1' and 'Yield: 100%'. To the right of the summary is a reference entry: '7,7a-Dihydroimidazo[1,2-d]-1,2,4-oxadiazoles from imidazoles and benzonitrile oxide', 'By: Foti, Francesco; et al', and 'Journal of Chemical Research, Synopses (1983), (9), 230-1'. A 'Full Text' button is also present.

1. 在反應結果集中，篩選起始物或者產物有供應商資訊的反應
2. 點擊 Suppliers 按鈕，查看供應商資訊

SciFinder[®] 使用技巧 | 將物質結果匯出為可以編輯的結構資料檔案

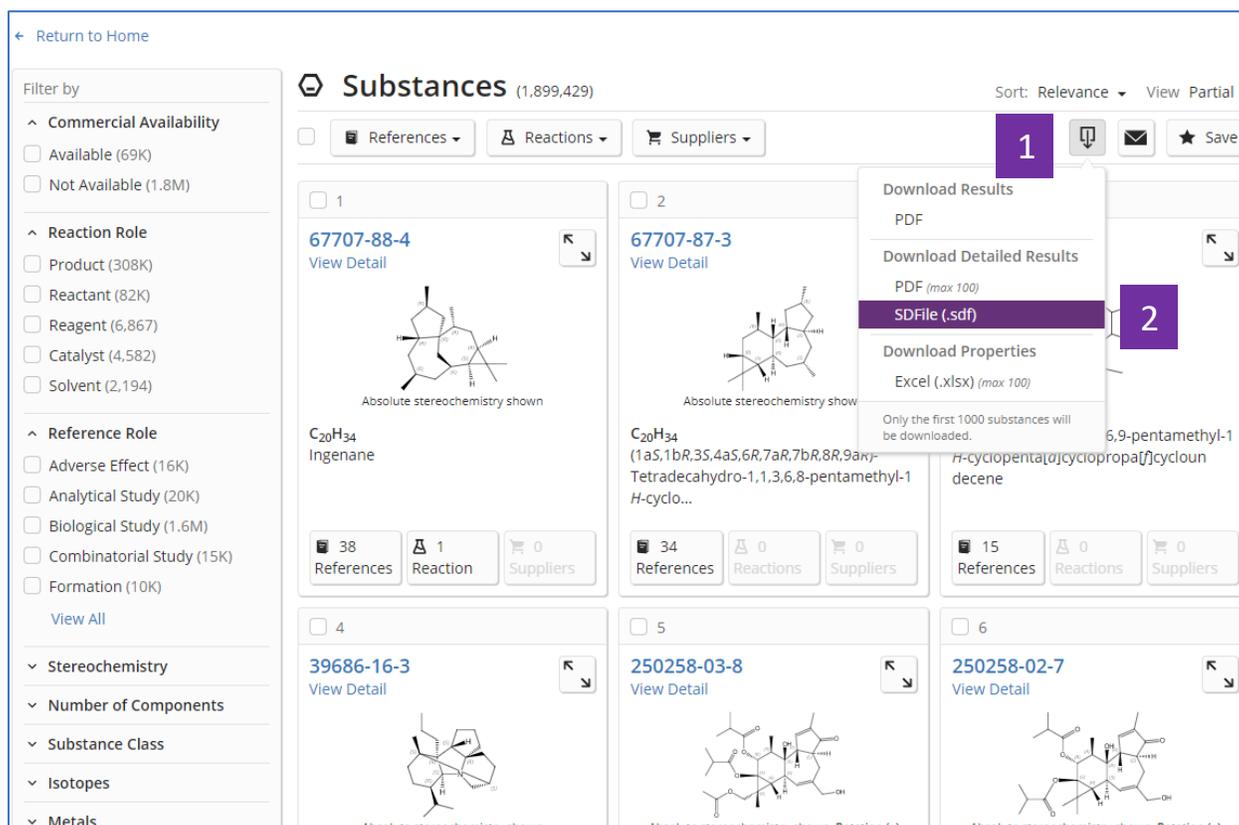
有以下三種方法可以將物質結果匯出為可以編輯的結構資料檔案：

直接在物質結果集中點擊 ，選擇 SDFFile，可以批量匯出可編輯的結構資料檔案。

若需要匯出某一物質結構資料檔案，則可以點擊該物質結構，在新視窗中點擊 ，選擇所需下載的結構資料檔案格式(CXF, MOL, SDF)

若需要匯出某一物質結構資料檔案及其屬性值，則可以點擊 substance detail，在新視窗中點擊 ，同時下載的結構資料檔案格式(CXF, MOL, SDF)和屬性值 (EXCEL) 檔。

方法一：直接在物質結果集中點擊 ，選擇 SDFFile，可以批量匯出可編輯的結構資料檔案。

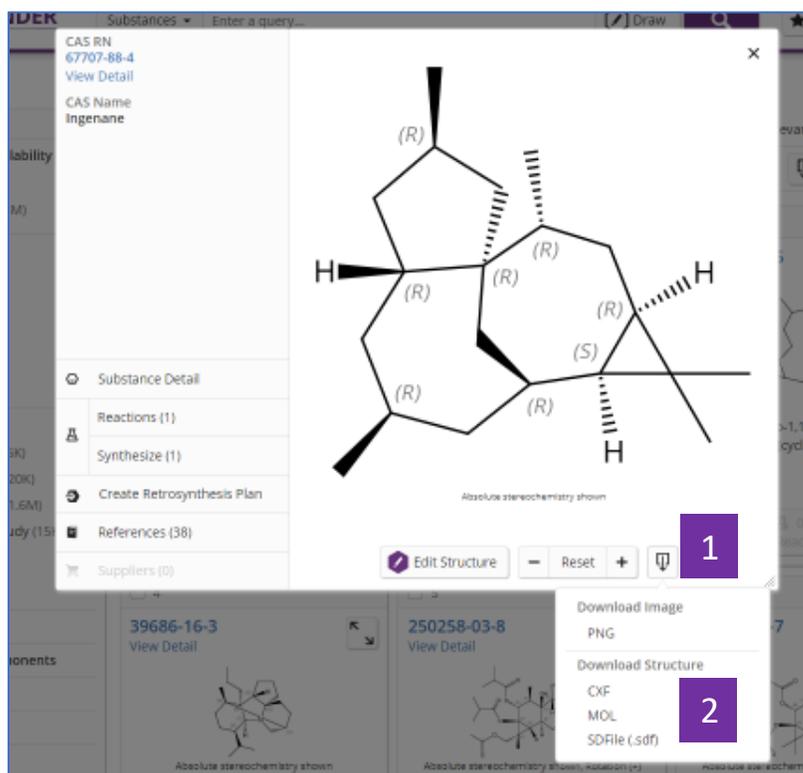


The screenshot displays the SciFinder 'Substances' search results page. On the left, there is a 'Filter by' sidebar with categories like Commercial Availability, Reaction Role, Reference Role, Stereochemistry, Number of Components, Substance Class, Isotopes, and Metals. The main area shows a grid of substance cards. A dropdown menu is open over the grid, with a purple box '1' highlighting the download icon and another purple box '2' highlighting the 'SDFFile (.sdf)' option. The menu also includes options for PDF, Detailed Results, Properties, and Excel. A note at the bottom of the menu states: 'Only the first 1000 substances will be downloaded.'

Substance ID	Name	Chemical Formula	References	Reactions	Suppliers
67707-88-4	Ingenane	C ₂₀ H ₃₄	38	1	0
67707-87-3	6,9-pentamethyl-1 H-cyclopenta[<i>a</i>]cyclopropa[<i>f</i>]cycloundecene	C ₂₀ H ₃₄	34	0	0
39686-16-3					
250258-03-8					
250258-02-7					

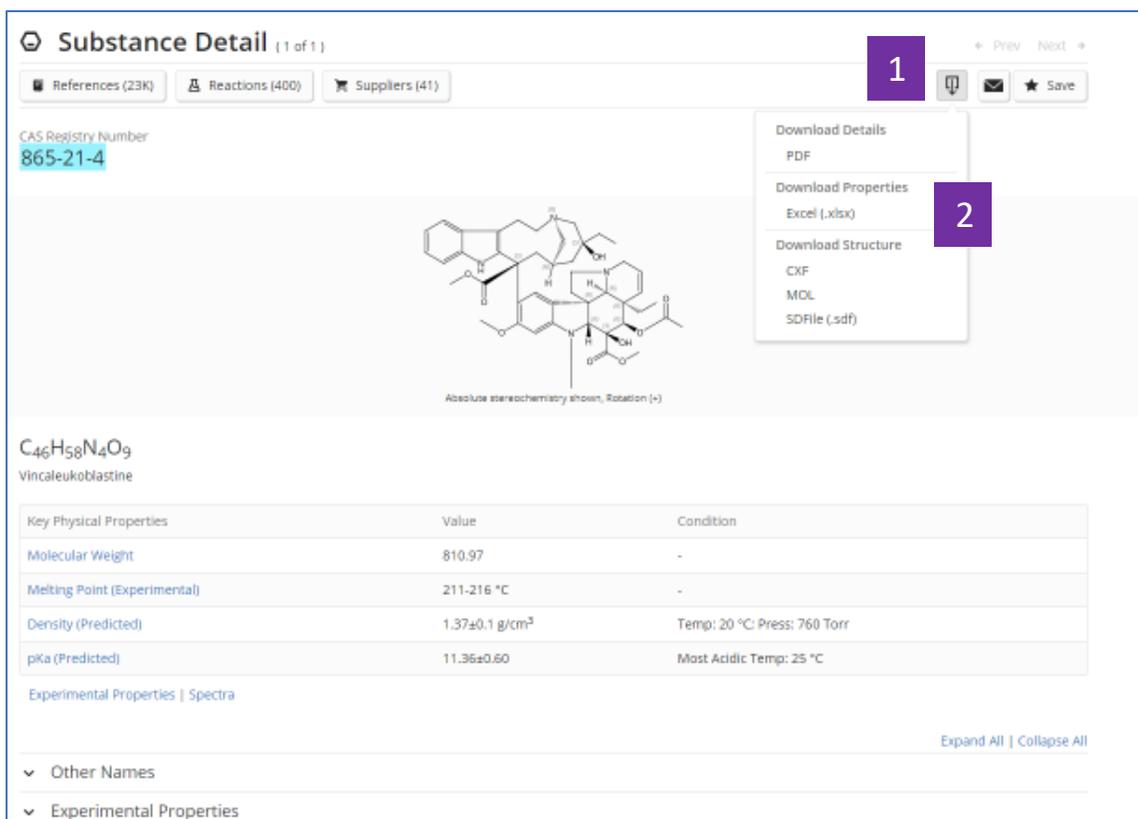
1. 點擊  按鈕
2. 選擇 SDFFile

方法二：若需要匯出某一物質結構資料檔案，則可以點擊該物質結構，在新視窗中點擊 ，選擇所需下載的結構資料檔案格式(CXF, MOL, SDF)



1. 點擊  按鈕
2. 選擇所需下載的結構資料檔案格式(CXF, MOL, SDF)

方法三：若需要匯出某一物質結構資料檔案及其屬性值，則可以點擊 substance detail，在新視窗中點擊 ，同時下載的結構資料檔案格式(CXF, MOL, SDF)和屬性值（EXCEL）檔。



Substance Detail (1 of 1)

References (23K) Reactions (400) Suppliers (41)

CAS Registry Number
865-21-4

C46H58N4O9
Vincalukoblastine

Absolute stereochemistry shown, Rotation (-)

Key Physical Properties	Value	Condition
Molecular Weight	810.97	-
Melting Point (Experimental)	211-216 °C	-
Density (Predicted)	1.37±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	11.35±0.60	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

Other Names

Experimental Properties

1. 點擊  按鈕
2. 所需下載的結構資料檔案格式(CXF, MOL, SDF)和屬性值檔 EXCEL

請注意：如果物質沒有結構或無法建模，則將無法使用此下載選項。

```
865-21-4 (1).sdf - Notepad
File Edit Format View Help
Vincal leukoblastine
C46H58N4O9
865-21-4 Copyright (C) 2019 ACS
 62 70 0 0 1 0 0 0 0 0999 V2000
75193.548426691.5323 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
80891.129029975.8065 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63326.612912592.7419 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
69024.1935 9308.4677 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57629.0323 9308.4677 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
74721.774212592.7419 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
69024.193515895.1613 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50969.7581 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
75193.548419487.9032 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
84302.419424750.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
90000.000021465.7258 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
84302.419431336.6935 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26764.112919487.9032 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19306.451623788.3065 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20594.758136762.0968 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14897.177440046.3710 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20594.758130175.4032 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 8637.096836435.4839 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
60895.161354090.7258 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
66592.741950806.4516 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59770.161346070.5645 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57157.258129975.8065 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63326.612933586.6935 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57157.258122772.1774 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44800.403229975.8065 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50969.758133586.6935 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
69495.967729975.8065 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

結構式資料 SDF 檔下載示例

```
 57 58 2 0 0 0 0
M END
> <cas.rn>
865-21-4

> <cas.index.name>
Vincal leukoblastine

> <molecular.formula>
C46H58N4O9

> <molecular.weight>
810.97

> <melting.point.experimental>
211-216 °C

> <density.predicted>
1.37±0.1 g/cm3 Temp: 20 °C; Press: 760 Torr

> <pka.predicted>
11.36±0.60 Most Acidic Temp: 25 °C

$$$$
```

屬性值 EXCEL 檔下載示例：

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CAS Registry Number: 865-21-4
CAS Display Name: Vinblastine

Type	Category	Property	Value and Units	Temperature	Pressure	pH
Experimental	Biological	Median Lethal Dose	15 mg/kg			
Experimental	Biological	Median Lethal Dose	15 mg/kg			
Experimental	Biological	Median Lethal Dose	7.3 mg/kg			
Experimental	Biological	Median Lethal Dose	5.6 mg/kg			
Experimental	Biological	Median Lethal Dose	3.12 mg/kg			
Experimental	Biological	Median Lethal Dose	0.34 mg/kg			
Experimental	Optical and Scattering	Optical Rotatory Power	+42 deg	26 °C		
Experimental	Optical and Scattering	Optical Rotatory Power	+42 deg	26 °C		
Experimental	Optical and Scattering	Optical Rotatory Power	+42 deg	26 °C		
Experimental	Optical and Scattering	Optical Rotatory Power	+40 deg	23 °C		
Experimental	Optical and Scattering	Optical Rotatory Power	+40 deg	23 °C		
Experimental	Optical and Scattering	Optical Rotatory Power	+31 deg	25 °C		
Experimental	Optical and Scattering	Optical Rotatory Power	-22 deg	25 °C		
Experimental	Optical and Scattering	Optical Rotatory Power	-32 deg	23 °C		
Experimental	Thermal	Melting Point	211-216 °C			
Experimental	Thermal	Melting Point	211-216 °C			
Experimental	Thermal	Melting Point	201-211 °C (decomp)			
Experimental	Thermal	Melting Point	201-211 °C			
Predicted	Biological	Bioconcentration Factor	1.0	25 °C		pH 1
Predicted	Biological	Bioconcentration Factor	1.28	25 °C		pH 2
Predicted	Biological	Bioconcentration Factor	1.50	25 °C		pH 3
Predicted	Biological	Bioconcentration Factor	2.04	25 °C		pH 4
Predicted	Biological	Bioconcentration Factor	13.9	25 °C		pH 5

SciFinder[®] 使用技巧 | 特定反應類型的獲取及指定反應資訊來源

The screenshot shows the SciFinder interface with search results for 'sofosbuvir'. The left sidebar contains filters for 'Reaction Type' and 'Reaction Notes'. The main area displays three reaction schemes with chemical structures and yields.

Reaction Type Filters:

- Full (545)
- Product Only (32)

Reaction Notes Filters:

- Stereoselective (134)
- Regioselective (33)
- Prophetic Reaction (13)
- High Pressure (10)
- Anaerobic (6)
- Biotransformation (1)
- Enzymic (1)

Reaction Schemes:

- Scheme 1:** Absolute stereochemistry shown. Yield: 100%. Steps: 1.
- Scheme 2:** Absolute stereochemistry shown. Yield: 89%. Steps: 1.
- Scheme 3:** Absolute stereochemistry shown.

1. 在反應結果集頁面，通過左側 **Reaction Type**，查看反應性質為完整反應或僅有產物的反應
2. 在反應結果集頁面，通過左側 **Reaction Notes**，流覽或選擇感興趣的反應類型

SCIFINDERⁿ
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Reactions 1190307-88-0 Draw

Document Type

Language

Publication Name **1**

- World Intellectual Property Organization (266)
- China (138)
- United States (73)
- India (43)
- European Journal of Organic Chemistry (36)
- Bioorganic & Medicinal Chemistry (5)
- Journal of Organic Chemistry (4)
- Organic Letters (4)
- Journal of Medicinal Chemistry (3)
- European Patent Organization (2)
- IP.com Journal (2)
- Czech Republic (1)
- Journal of the American Chemical Society (1)
- Topics in Heterocyclic Chemistry (1)

[View Fewer](#)

Yield: 89%

Suppliers (77)

Expand Scheme

Scheme 4 (8 Reactions) [View All](#)

Steps: 1
Yield: 83-88%

Suppliers (63) Suppliers (102) Suppliers (77)

Expand Scheme

Scheme 5 (1 Reaction) [View](#)

Steps: 1
Yield: 87%

1. 在反應結果集頁面，通過左側的 **Publication Name**，可以選擇自己感興趣的反應來源

Combine 的應用

Combine功能：可用於對多個檢索結果集（包括文獻、物質和反應的檢索結果集）進行邏輯處理（包括合併、取交集和排除）。

The screenshot shows the SciFinder web interface. At the top, there is a search bar with the text "Substances" and "Enter a query...". Below the search bar, there are several icons: "Edit", "Search", "Star", "Clock", and "User". The main content area is titled "Substances (143)". On the left, there is a sidebar with filters: "Structure Match" (As Drawn (3), Substructure (143), Similarity (1,841), Analyze Structure Precision), "Filter by" (Commercial Availability, Reaction Role, Reference Role). The main area displays three substance cards. Each card has a chemical structure, a CAS number, a molecular formula, and a name. The first card is labeled "1" in a purple box. The second card is labeled "2" in a purple box. The third card is labeled "1" in a purple box. A "Save" button is highlighted with a "1" in a purple box. A "Combine" button is highlighted with a "2" in a purple box.

1 點擊Save，保存檢索結果

2 打開保存的檢索結果，進行Combine操作

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References cataract and Metformin

Filter by

- Result Type
 - Patent Markush (2)
 - Reactions (38)
 - References (79)
 - Retrosynthesis (4)
 - Substances (46)
- Alerts
 - Unviewed (13)
- Tags
 - patent, Chinese, EOC (1)

Combine Saved Results

Combine

★ Saved (169)

cataract and Metformin---Medline

November 26, 2019, 12:08 PM

References cataract and Metformin + Filters

Rerun Search

View Saved

Alerts Add Tags

cataract and Metformin---CAplus

November 26, 2019, 12:05 PM

References cataract and Metformin + Filters

Rerun Search

View Saved

3 點擊Combine, 進行多個結果的邏輯處理

Combine Saved Results

1

Select a Result Type:

Substances

Reactions

References

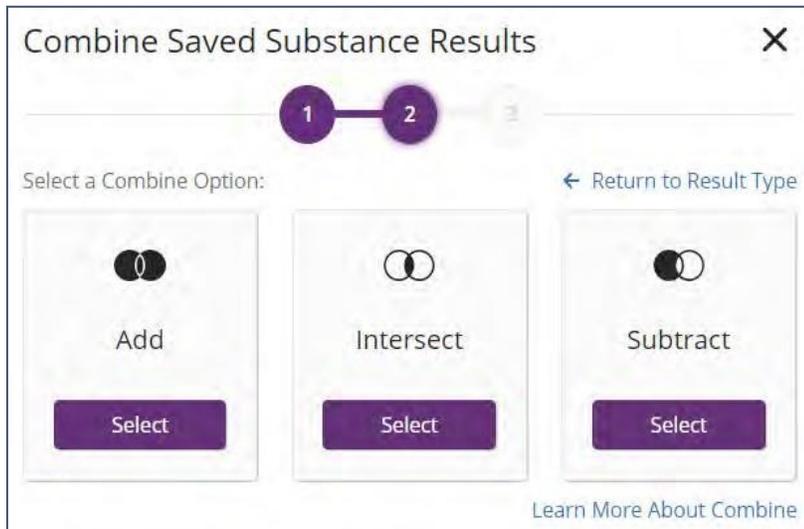
Select

Select

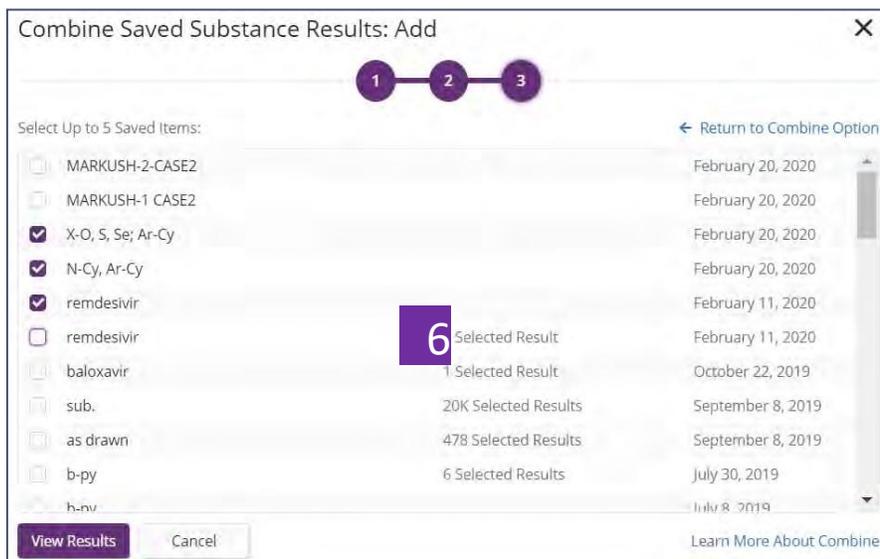
Select

Learn More About Combine

4 選擇需要處理的結果集類型



5 選擇需要進行的邏輯操作



6 選擇需要combine的結果集

7 點擊View Results，獲得combine后的結果集

