



CAS SciFinder 使用手冊

用 CAS SciFinder 完成反應搜尋、逆合成、光譜、文獻與 AI 探索
以Aspirin為例

從名稱或結構開始搜尋

輸入 Aspirin，或按 Draw 畫出目標結構。

The screenshot displays the CAS SciFinder web interface. At the top, the CAS SciFinder logo is visible on the left, and user information (YENCHEN LEE) and a notification bell are on the right. A greeting "Good Afternoon, YENCHEN" is shown. Below this is a search bar containing the text "Aspirin". To the right of the search bar is a "Draw" button, which is highlighted with a blue arrow. Below the search bar is a button labeled "Ask CAS Newton".

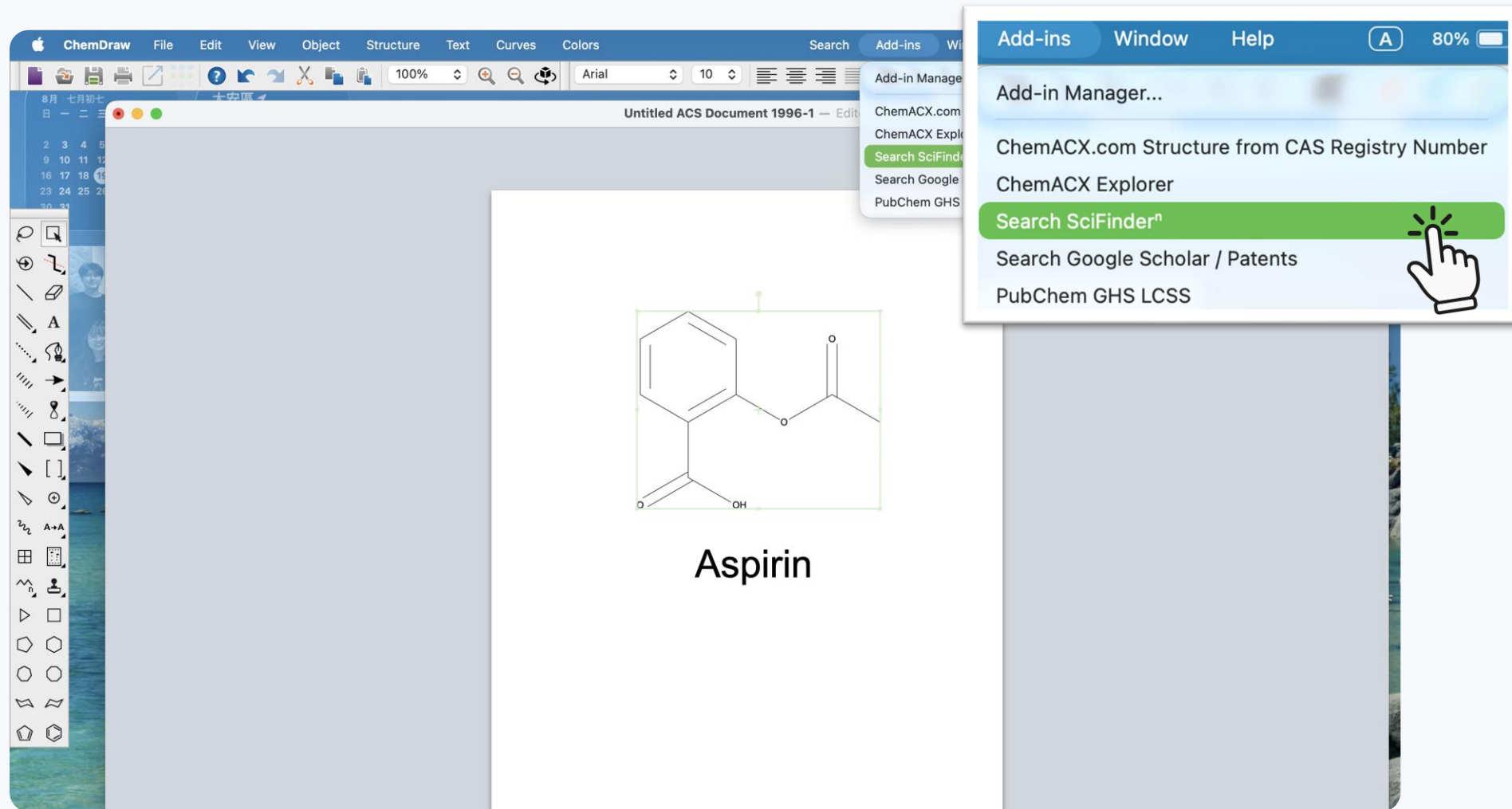
Under the "Featured Search" section, there are two main options:

- Advanced Search**: Select data fields and search operators to create a focused query.
- Search CAS Lexicon**: Build powerful searches using CAS concepts, chemical classes, and taxonomy.

The "CAS Draw" window is open, showing a chemical structure of Aspirin (Acetylsalicylic acid). The structure is a benzene ring with a carboxylic acid group (-COOH) and an acetoxy group (-O-C(=O)-CH₃). The molecular formula is displayed as C₉H₈O₄ (180.16). The interface includes a toolbar on the left with various drawing tools and a zoom slider at the bottom.

ChemDraw 一鍵帶入 SciFinder

畫好結構後，從 Add-ins 選擇 Search SciFinder。



找到目標化合物Aspirin

CAS SciFinder Aspirin

← Return to Home

Substances search for "Aspirin"

Query Interpretation ?

CAS Newton NEW All Substances Reactions References Suppliers Patent Markush

View Related Results ▾

Filter Results

Analyze Results

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

6 Results

1

50-78-2

CC(=O)Oc1ccccc1C(=O)O

C₉H₈O₄
Aspirin

97K 2,598 132

2

2410093-58-0

Image Not Available

Notes: An aspirin deriv.
Unspecified
ATB 340

3 0 0

3

2243982-77-4

Image Not Available

Notes: A medication contg. aspirin
Unspecified
Aspocid

4 0 0

Sort: Relevance ▾ View: Partial ▾

物質頁面是所有功能的入口

反應、合成、文獻、供應商與逆合成都能從這裡展開。

CAS Registry Number
50-78-2

CAS Name
Aspirin

Get Substance Details

Get Life Science Data

Get Reactions (2,598)

Synthesize (473)

Start Retrosynthetic

Get References (97K)

Get Suppliers (132)

View in [CAS BioFinder](#)

Chemical structure of Aspirin (Acetylsalicylic acid) is displayed. The structure shows a benzene ring with a carboxylic acid group (-COOH) and an acetoxy group (-O-C(=O)-CH₃) attached to adjacent carbons.

查詢合成條件

Edit Structure

Reset

Download

把大量合成方法按「反應類型」分組

Group by Transformation 會把相同化學轉換集中在一起。

Reactions search for "synthesis of 50-78-2"

Query Interpretation ?

View Related Results ▾



Filter Results

Behavior

Filter by

Exclude

Search Within Results

Search for up to 3 structures within the result set.



Search

Reagent

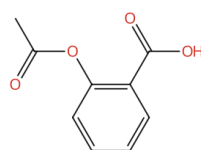
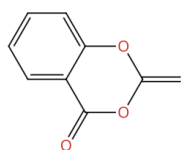
Yield

☐ 90-100% (71)

☐ 80-89% (54)

☐ 473 Results

Scheme 1 (1 Reaction)



Suppliers (3)

Suppliers (132)

☐

31-614-CAS-26606265

Steps: 1 Yield: 100% ...

1.1 Solvents: [Water](#)

2-Alkylidene-benzo[1,3]dioxin-4-ones: a new class of
By: Babin, P.; et al
Tetrahedron Letters (2001), 42(31), 5231-5233

Full Text ▾

[Collapse Scheme](#) ^

Group: By Scheme ▾

Sort: Relevance ▾

View: Expanded ▾

Group: By Scheme ▴

By Scheme

By Document

By Transformation

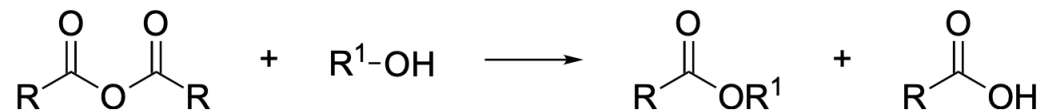
先看有哪些反應能生成 Aspirin

最常見路徑：醋酸酐對酚羟基的乙酐化（酸酐的酚解）。


☐ 1

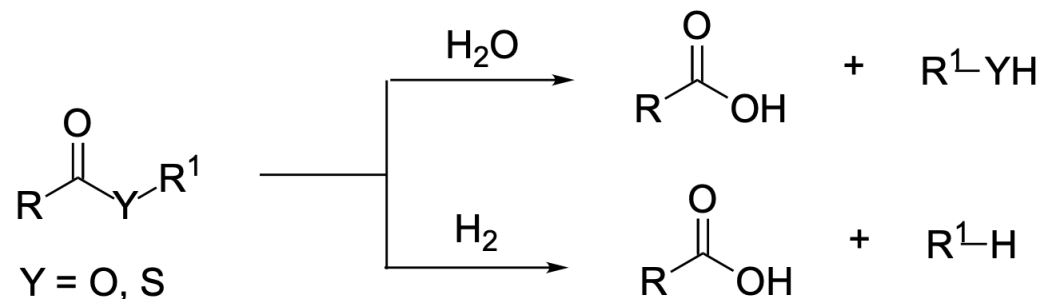
Alcoholysis of Anhydrides

[View 183 Related Reactions](#)


☐ 2

Hydrolysis or Hydrogenolysis of Carboxylic Esters or Thioesters

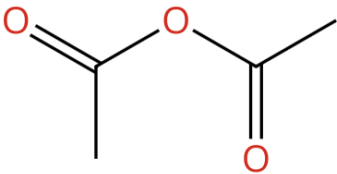
[View 18 Related Reactions](#)



點進反應方案，直接比較條件與產率

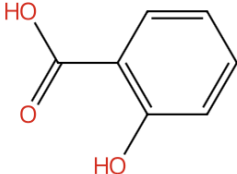
優先找有 Experimental Procedure、產率高且試劑容易取得的方法。

Scheme 1 (172 Reactions) Steps: 1 Yield: 99-100% ...



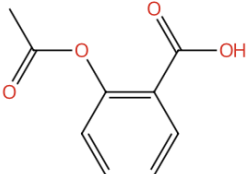
 Suppliers (83)

+



 Suppliers (167)

→



 Suppliers (132)

☐	31-355-CAS-6514481 Steps: 1 Yield: 100% ... 1.1 Catalysts: Silica , 12-Tungstosilicic acid ; 3 min, 25 °C 1.2 Reagents: Water ; 25 °C	Acetylation of alcohols and phenols using continuous-flow, tungstosilicic acid-supported, monolith microreactors with scale-up capability By: He, Ping; et al Journal of Flow Chemistry (2012), 2, 47-51 Full Text ▾
☐	31-355-CAS-3933172 Steps: 1 Yield: 100% ... 1.1 Reagents: Sulfuric acid	Preparation of acetylsalicylic acid, acetanilide and p-acetophenetidide By: Manicke, I. P.; et al Archiv der Pharmazie und Berichte der Deutschen Pharmazeutischen Gesellschaft (1926), 264, 322-4 Full Text ▾

指定反應物與產物角色，降低無關結果

在結構編輯器中設定 Reactant、Reagent 與 Product。

The image illustrates the process of assigning reaction roles in the CAS Draw software. It features a main window with a toolbar and a chemical reaction scheme. A hand icon labeled '1' points to the 'A → B' button in the toolbar. A hand icon labeled '2' points to a chemical structure (acetic acid) in the reaction scheme, which is labeled 'reactant'. A 'Reaction Roles' dialog box is open, showing a list of roles: Product, Reactant (selected), Reagent, Reactant/Reagent, and Any Role. The dialog box also includes 'OK' and 'Cancel' buttons. The reaction scheme shows acetic acid reacting with a substituted benzene ring to form a product.

1

2

reactant

reactant

product

Reaction Roles

Select a role for the structure fragment.

- ☐ Product
- ☒ Reactant
- ☐ Reagent
- ☐ Reactant/Reagent
- ☐ Any Role

OK Cancel

調整反應搜尋範圍

As Drawn：只看完全符合所畫結構的反應

適合已知確切反應物與產物時，範圍最精準。

CAS SciFinder

Enter a query...

Edit

15

[Return to Home](#)

Reactions search for drawn structure

CAS Newton NEW

All

Substances

Reactions

References

Suppliers

Patent Markush

View Related Results

Filter Results

Structure Match

As Drawn (194)

Substructure (4,706)

Similarity (330K)

194 Results

Group: By Transformation

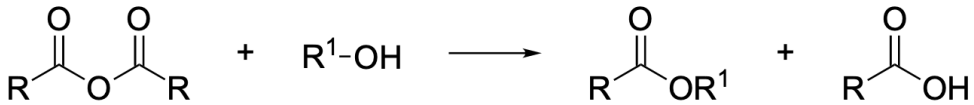
Sort: Reaction Count: Descending

View: Expanded

1

Alcoholysis of Anhydrides

[View 187 Related Reactions](#)



調整反應搜尋範圍

Similarity：尋找相似化學轉換，拓展至其他分子的合成

門檻愈低，結果愈多；適合找相似化學轉換。

CAS SciFinder

Enter a query...

Edit

Q

15

Filter Results

Structure Match

As Drawn (194)

Substructure (4,706)

Similarity (330K)

Similarity

Broad (330K) Medium (12K) Narrow (11K)

Behavior

Filter by

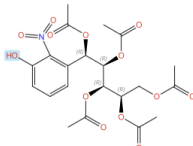
Exclude

330,896 Results

Group: By Scheme Sort: Relevance View: Expanded

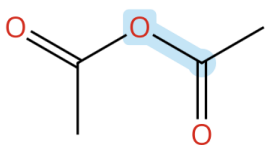
Scheme 1 (1 Reaction)

Steps: 1 Yield: 100%



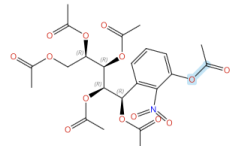
Absolute stereochemistry shown, Rotation (-)

+



Suppliers (83)

→



Absolute stereochemistry shown, Rotation (-)

31-355-CAS-15100699

Steps: 1 Yield: 100%

1.1 Reagents: [Pyridine](#)

New C-aryl aldittols from Diels-Alder adducts of sugar nitroalkenes

By: Araujo, Noelia; et al

ARKIVOC (Gainesville, FL, United States) (2008), (11), 175-186

Full Text

Collapse Scheme

調整物質結構搜尋範圍

Substructure：保留核心骨架，外圍可延伸

會納入鹽類、混合物、複合物及在核心外加上取代基的衍生物。

Filter Results

Analyze Results

Structure Match

As Drawn (951)

Substructure (24K)

Similarity (811)

Analyze Structure Precision

Behavior

Filter by

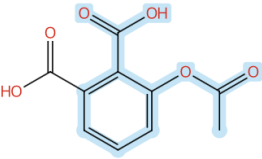
Exclude

Search Within Results

1 0 1

313

21872-44-6



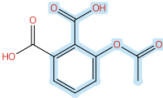
$C_{10}H_8O_6$
3-(Acetyloxy)-1,2-benzenedicarboxylic acid

3 1 1

1 0 0

314

93839-98-6



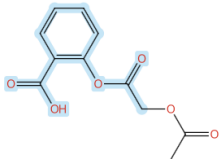
$C_{10}H_8O_6 \cdot Pb$
Components: 2
Component RN: 21872-44-6
1,2-Benzenedicarboxylic acid, 3-(acetyloxy)-, lead(2+) salt (1:1)

0 0 1

53 16 34

315

861368-59-4



$C_{11}H_{10}O_6$
2-[[2-(Acetyloxy)acetyl]oxy]benzoic acid

1 0 6

調整物質結構搜尋範圍

Similarity：整體結構相近，不一定含完整核心

CAS SciFinder

Enter a query...

Edit

15

Structure Match

As Drawn (951)

Substructure (24K)

Similarity (811)

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Similarity

>=99 (260)

75-79 (8)

70-74 (78)

65-69 (115)

8 12 6 7 10 14 4 4 5

407 65

3545-41-3

ClC(=O)Oc1ccccc1C(=O)O

$C_9H_6Cl_2O_4$

Benzoic acid, 2-[(2,2-dichloroacetyl)oxy]-

4 3 7

408 65

65594-66-3

CC(=O)Oc1ccccc1C(=O)Oc2ccccc2C(=O)OC(C)=O

$C_{17}H_{14}O_5$

Bis[2-(acetyloxy)phenyl]methanone

3 2 2

409 65

364-71-6

FC(=O)Oc1ccccc1C(=O)O

$C_9H_7FO_4$

2-[(2-Fluoroacetyl)oxy]benzoic acid

3 0 17

410 65

2750250-22-5

CC(=O)Oc1ccccc1C(=O)OSeC

$C_{10}H_{10}O_3Se$

Se-Methyl 2-(acetyloxy)benzenecarboselenoate

2 1 0

411 65

74736-86-0

CC(=O)Oc1ccccc1C(=O)C=C

$C_{11}H_{10}O_3$

1-[2-(Acetyloxy)phenyl]-2-propen-1-one

2 3 3

412 65

3098350-99-0

CC(=O)Oc1ccccc1C(=O)OC(=O)C

$C_{10}H_8D_2O_4$

1 2 0

從 Aspirin 物質頁啟動逆合成分析

只有目標分子，也能反推可能的起始物與路徑。

CAS Registry Number
50-78-2

CAS Name
Aspirin

Get Substance Details

Get Life Science Data

Get Reactions (2,598)

Synthesize (473)

Start Retrosynthetic Analysis

Get References (97K)

Get Suppliers (132)

View in [CAS BioFinder](#)

CC(=O)Oc1ccccc1C(=O)O

Edit Structure

Reset

+

Download

逆合成一次提出多條可行路徑

每一步都可查看預測反應或已報導的實驗證據。

CAS SciFinder

Retrosynthesis Plan for drawn structure

Build Status: Complete ✓ Estimated Yield: 95% Overall Price: \$3

Customize Plan

Selected Options [Edit](#)

Predicted Rules: Common

Break and Protect Bonds: None

Filters

[View Excluded Options](#)

Step Type

☒ Experimental Steps

☐ Predicted Steps

At least one step type must be turned on to display a plan.

Starting Material Cost Limit

9 USD/mol [Apply](#)

Retrosynthesis Plan:

Structure A (182 \$10.81) → Structure B (83 \$0.55) → Structure C (98 \$4.76)

Max Yield: 95%

點按中間燒杯

[Return to All Steps](#)

A ⇒ B + C

顯示所有可能路線與參考文獻

Evidence [Alternative Steps \(38\)](#) [Exclude Step](#)

Filters

1 of 38 [Experimental Step](#) | Max Yield: 95%

Evidence [Current Step](#)

2 of 38 [Experimental Step](#) | Max Yield: 84%

Evidence [Replace Step](#)

鎖定斷鍵位置，讓路徑更符合你的想法

Break Bond / Protect Bond 可引導模型切斷或保留指定鍵。

鎖定斷鍵位置

Customize Plan

Selected Options

Predicted Rules: **Common**

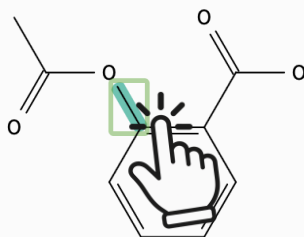
Break and Protect Bonds: **None**

Edit

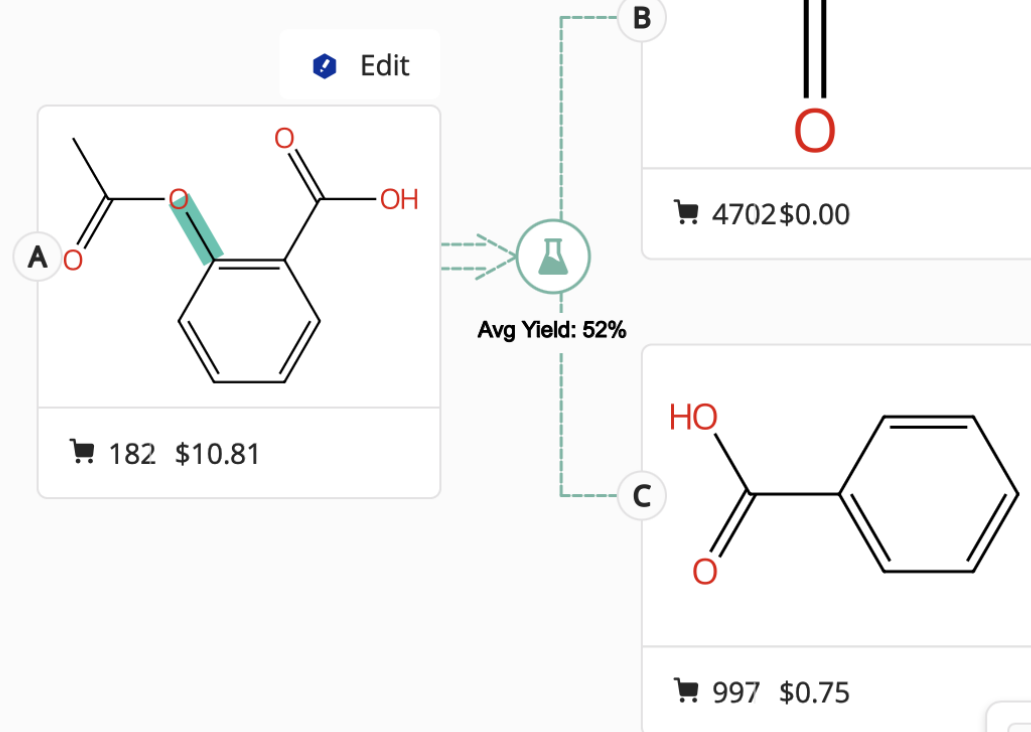
Break Bond

Protect Bond

Clear All Bond Selections



顯示特定斷鍵位置的合成方法



從物質紀錄連接光譜與文獻

以 Aspirin 為中心，繼續查找 NMR、文獻與相關反應。

CAS Registry Number
50-78-2

CAS Name
Aspirin

Get Substance Details

Get Life Science Data

Get Reactions (2,598)

Synthesize (473)

Start Retrosynthetic Analysis

Get References (97K)

Get Suppliers (132)

View in [CAS BioFinder](#)

Chemical structure of Aspirin (Acetylsalicylic acid) is displayed. The structure shows a benzene ring with a carboxylic acid group (-COOH) and an ester group (-O-C(=O)-CH₃) attached to adjacent carbons.

Edit Structure

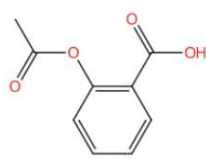
Reset

Download

快速找到 NMR 光譜與實驗條件

先確認溶劑、頻率、溫度與資料來源，再用於比對。

50-78-2



CC(=O)Oc1ccccc1C(=O)O

C₉H₈O₄

CAS Name
Aspirin

Conditions
Working Frequency
400 MHz

Solvent
DMSO-*d*₆ (2206-27-1)

Spectrum Summary
Spectrum ID
Not Available

Peak Data
2.8, 7.1-8.1, 11.5 ppm

Experimental Properties | Spectra

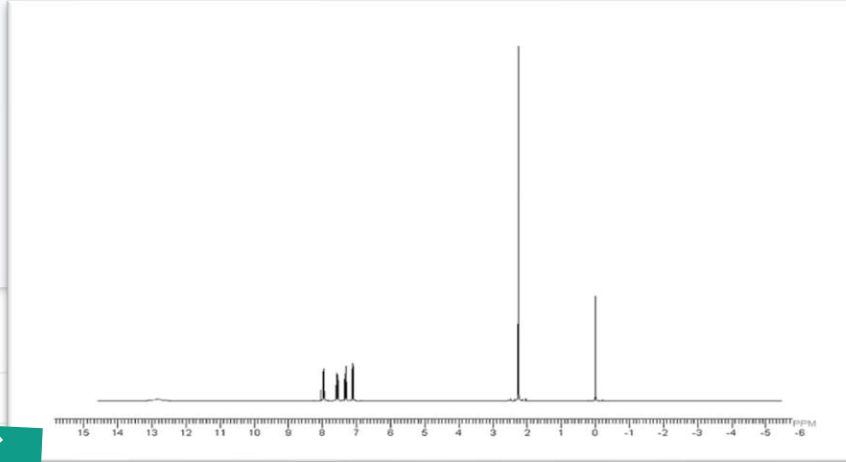
Other Names and Identifiers

Experimental Properties

Experimental Spectra

¹ H NMR	¹³ C NMR	Hetero NMR	IR	Mass	Raman	UV and Visible	X-Ray	Additional Spectra
Solvent								
Source								
View Proton NMR Spectrum (Image Available)								(1) WSA
View Proton NMR Spectrum (Image Available)								(2) BIORAD
View Proton NMR Spectrum (Image Available)								(2) BIORAD
View Proton NMR Spectrum (Image Available)								(3) AIST
View Proton NMR Spectrum (Image Available)								(4) ACD-A
View Proton NMR Spectrum								(5) CAS
View Proton NMR Spectrum								(6) CAS
View Proton NMR Spectrum								(7) CAS
Proton NMR Spectrum - 5 Sources								(8-12) CAS

Sources



15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6

Collapse All

Download

Up

文獻搜尋後，先用圖表看研究輪廓

用文獻類型圖表快速判斷研究目前的發展

點擊分析結果

← Return to Home

References search for drawn structure

CAS Newton **NEW** All Substances Reactions **References** Suppliers Patent Markush

View Related Results ▾

Filter Results <

Analyze Results

Structure Match

As Drawn (98K)

Substructure (108K)

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

98,504 Results

Sort: Relevance ▾ View: Partial Abstract ▾

1

Clonidine versus aspirin for secondary prevention of coronary artery disease: a systematic review and individual patient data meta-analysis

By: Valgimigli, Marco; Choi, Ki Hong; Giacompo, Daniele; Gragnano, Felice; Kimura, Takeshi; Watanabe, Hirotohi; Kim, Hyo-Soo; Kang, Jeehoon; Park, Kyung Woo; Pettersen, Alf-Age; et al
Lancet (2025), 406(10508), 1091-1102 | Language: English, Database: CAlplus and MEDLINE

Meta-anal. of aspirin monotherapy is recommended indefinitely for patients with established coronary artery disease (CAD). The aim of this individual patient level meta-anal. was to provide a comprehensive evaluation of the comparative efficacy and safety of clonidine vs. aspirin monotherapy in patients with established CAD, most of whom had undergone percutaneous coronary intervention or had acute coronary syndrome. We conducted a systematic search in PubMed, Scopus, Web of Science, and Embase to identify randomised trials published from database inception to Apr. 12, 2025, comparing clonidine...

View More ▾

Full Text ▾ 2 0 44

2

Analyze Results

Top Document Types

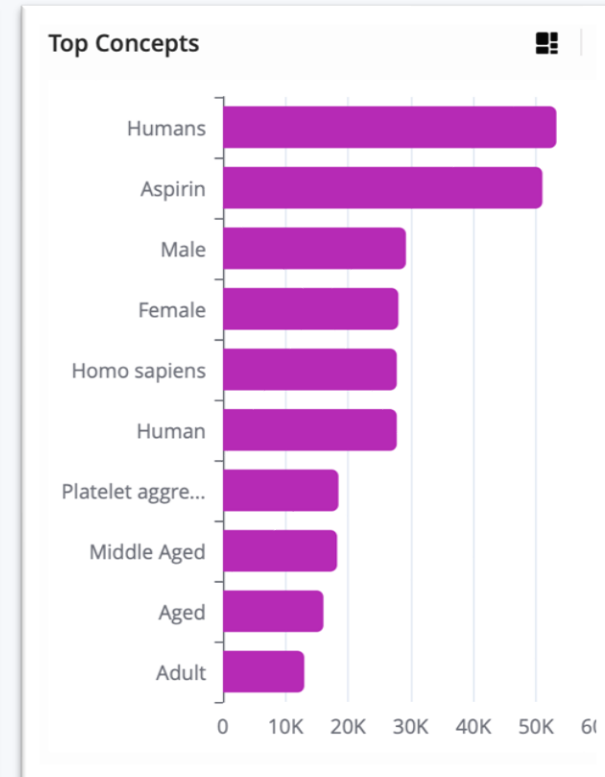
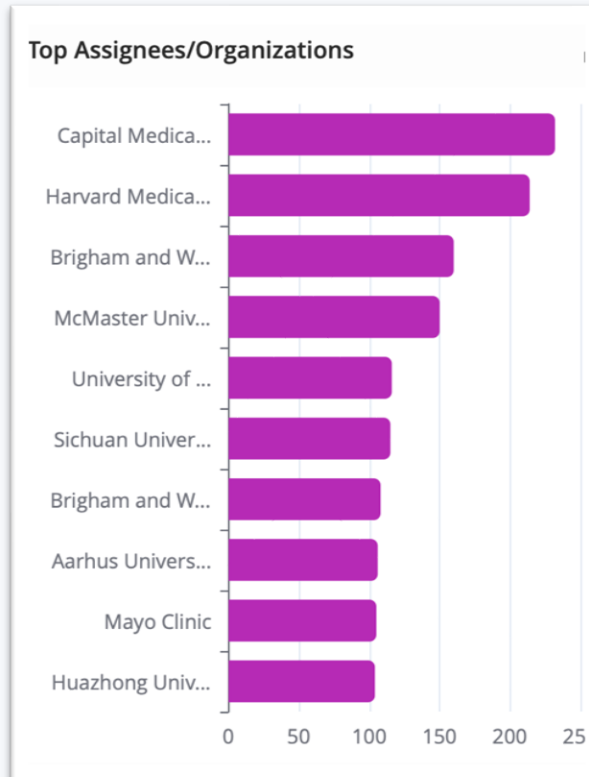
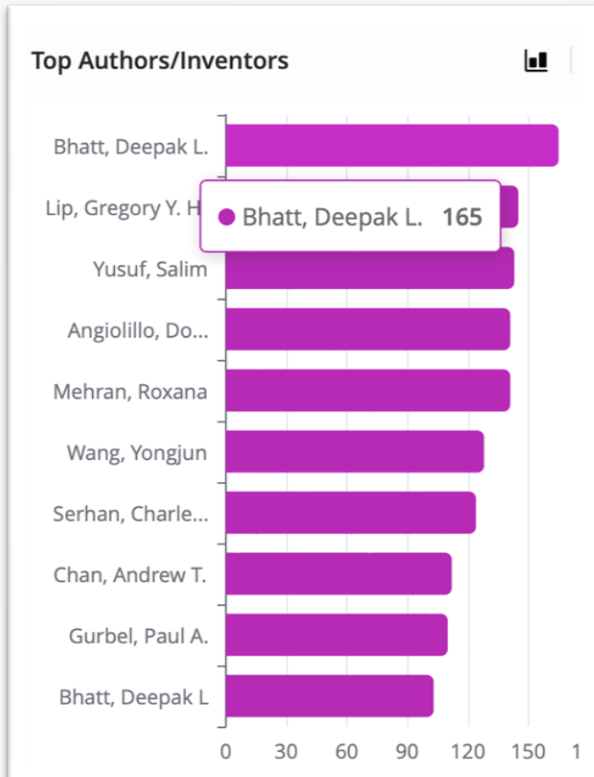
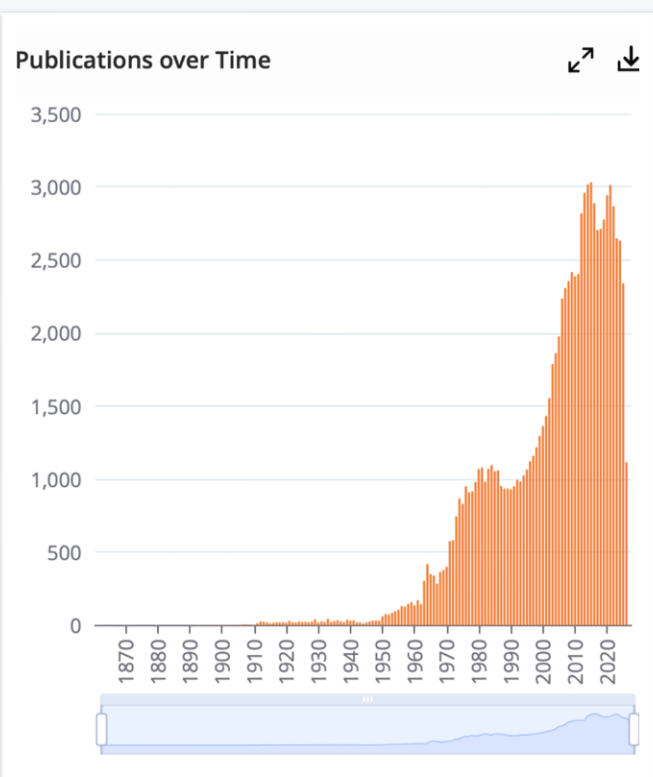
Document Type	Count
Journal	98
Patent	108
Clinical Trial	10
Review	10
Report	10
Let	10
C	10
Ed...	10

右側會出現統計圖表

分析圖表揭示研究熱度與主要貢獻者

年份、作者、機構與主題圖適合找經典文獻和活躍研究群。

點擊統計數據可以鎖定搜尋文獻結果



By: Valgimigli, Marco; Choi, Ki Hong; Giacoppo, Daniele; Gragnano, Felice; Kimura, Takeshi; Watanabe, Hirotoshi; Kim, Hyo-Soo; Kang, Jeehoon; Park, Kyung Woo; Pettersen, Alf-Age; et al
Lancet (2025), 406(10508), 1091-1102 | Language: English

Full Text ▾  2  0  44 

反應

Substances for AN 2025:2699107

Filter Results <

Behavior

Filter by

Exclude

^ Search Within Results

Search for up to 3 structures within the result set.

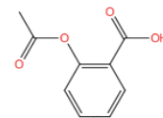
 Draw[^] Reaction Role

2 Results

Sort: Relevance ▾ View: Partial ▾

0 1

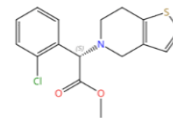
50-78-2



$C_9H_8O_4$
Aspirin

□ 2

113665-84-2



Absolute stereochemistry shown,
Rotation (+)

C₁₆H₁₆ClNO₂S
Clopidogrel

SciFinder AI：用CAS Newton開始探索研究主題

適合不知道關鍵字、想先掌握研究方向時使用。

CAS SciFinder

Good Evening, YENCHEN

Pauling, Linus

Ask CAS Newton

Featured Search

Advanced Search
Select data fields and search operators to create a focused query.

Search CAS Lexicon
Build powerful searches using CAS concepts, chemical classes, and taxonomy.

Patent Markush
Search Patent Markush by structure and view associated references.

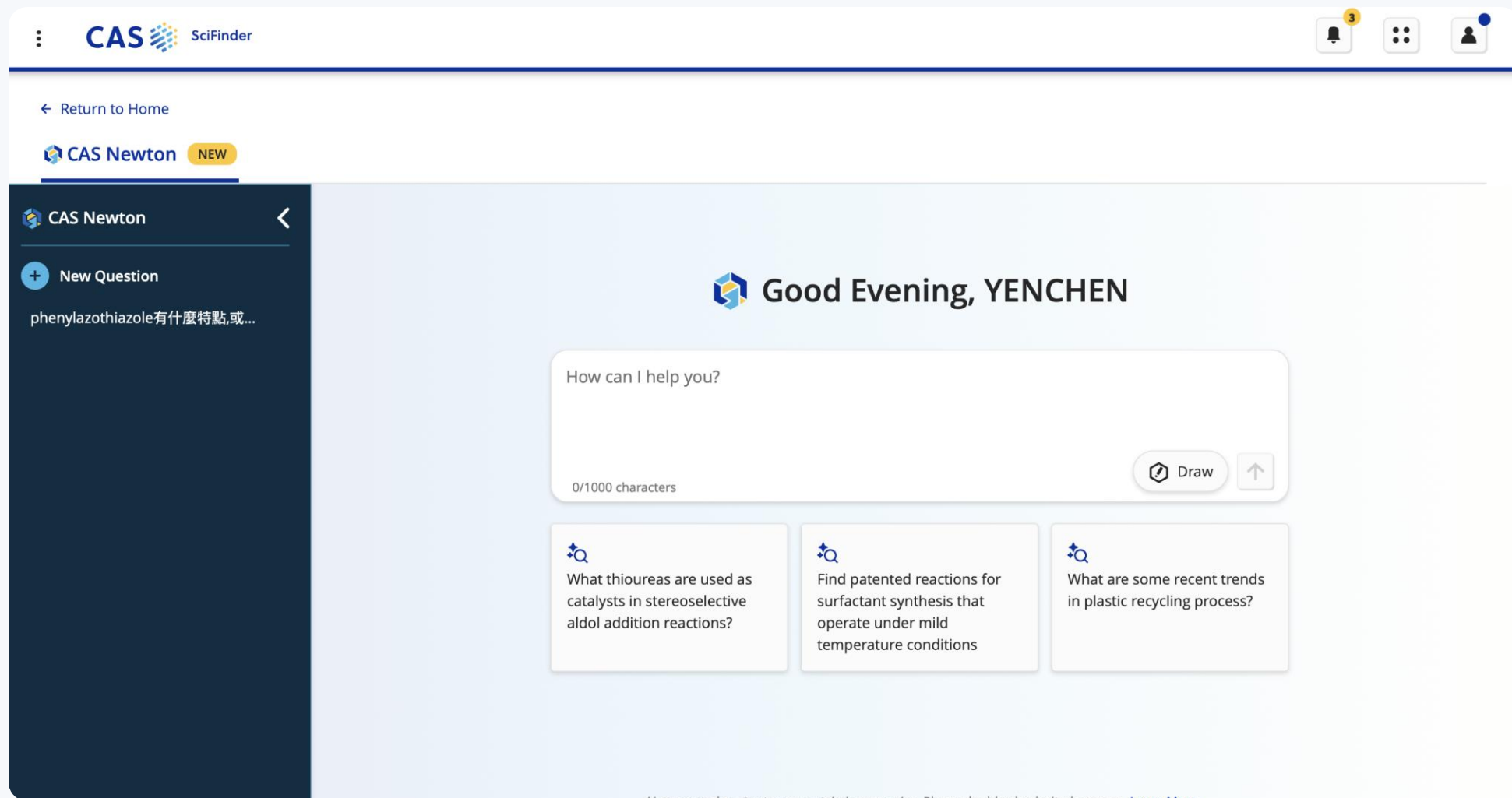
Retrosynthetic Analysis
Make reaction plans with conditions, yields, catalysts, and experimental procedures.

History For You NEW

Recent Search History

View All Search History

CAS Newton 頁面



為什麼 Aspirin 放久會有醋味？

為什麼 aspirin 放久了會出現像醋一樣的味道？發生了什麼有機反應？



阿司匹林放久了產生醋味的原因

您觀察到的現象非常正確！阿司匹林放久了會產生醋味，這是因為發生了**酯水解反應**（ester hydrolysis）。

化學結構與反應機制

Aspirin (CAS 50-78-2) 的化學結構是**乙醯水楊酸**（acetylsalicylic acid），分子式為 $C_9H_8O_4$ ，結構式為 CC(=O)Oc1ccccc1C(=O)O。

關鍵的是，阿司匹林分子中含有一個**酯基**（ $-OCOCH_3$ ），這個酯基在以下條件下容易發生水解：

1. 濕氣（水分）的存在
2. 時間的累積
3. 溫度的影響（溫度越高，水解越快）

Newton 給出整理答案，可連回相關物質

Aspirin 水解會生成 salicylic acid 與 acetic acid；醋味來自醋酸。

水解反應

反應式：

阿司匹林 + H_2O → 水楊酸 + 乙酸

具體來說：

- 反應物：Aspirin (CAS 50-78-2) (乙醯水楊酸)
- 產物：
 - Salicylic acid (CAS 69-72-7) (水楊酸)
 - Acetic acid (CAS 64-19-7) (乙酸)

根據 CAS 資料庫的記錄，這個水解反應可以在室溫 (25°C) 下進行。

為什麼會聞到醋味？

產生的 Acetic acid (CAS 64-19-7) (乙酸) 就是食用醋的主要成分！

- 強烈的刺激性氣味
- 揮發性高

• 反應物：Aspirin (CAS 50-78-2) (乙醯水楊酸)

• 產物：

◦ Salicylic acid (CAS 69-72-7) (水楊酸)

◦ Acetic acid (CAS 64-19-7) (乙酸)

根據 CAS

為什麼

產生的 A

• 強烈

• 揮發

four daily

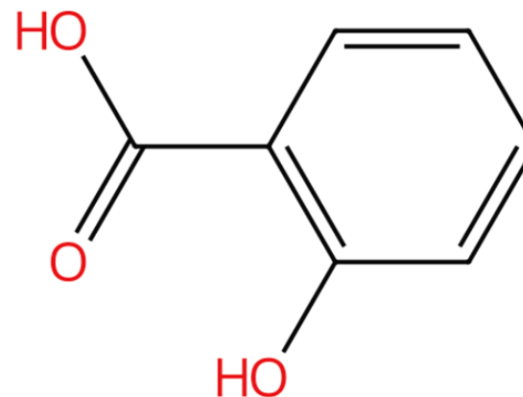
Please come

an I help

Substance Details

69-72-7

Salicylic acid



Molecular Weight

138.12

Newton可以連結scifinder文獻資料庫

有文獻討論嗎

Scientific Literature on Aspirin Hydrolysis

I found extensive scientific literature discussing the hydrolysis of aspirin to salicylic acid and acetic acid. Here's a comprehensive overview:

Overview

The CAS Content Collection contains [7,148 references on aspirin hydrolysis, degradation, and stability](#), covering various aspects including degradation mechanisms, stability studies, kinetics, and environmental fate.

點擊搜尋出來的文獻結果



Newton可以提供完整References清單

CAS SciFinder

Enter a query...

Draw

15

[Return to Home](#)

References

View Related Results ▾

Filter Results

Analyze Results

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 text strings within the result set.

Enter a query...

Search

Document Type

Journal (5,575)

Patent (1,480)

Review (363)

Biography (1)

Clinical Trial (467)

View All

7,148 Results

Sort: Relevance ▾ View: Partial Abstract ▾

1

Stability Indicating Assay Method and LC-MS Characterization of Forced Degradation Products of Pantoprazole and Aspirin

By: Patel, Tinkal S.; Chaudhary, Ankit B.

Journal of Chromatographic Science (2025), 63(5), bmaf029 | Language: English, Database: CAplus and MEDLINE

To assess the degradation of the drug under forced degradation, stability experiments with aspirin and pantoprazole were performed. Under the guidelines set forth by the International Conference on Harmonization, pantoprazole and aspirin were exposed to oxidation, alk. and acidic hydrolysis and thermal stress. Under basic and acidic hydrolysis stress, the drug combination demonstrated significant degradation Under conditions of oxidative stress and heat, however, it remained stable. A mobile phase, containing methanol: ammonium acetate buffer (0.01 M) (70: 30% volume/volume) was employed. a co...

View More ▾

Full Text ▾ 2 0 1

2

Magnesiothermal reduction and doping strategies in engineered TiO₂ for pharmaceutical degradation and CO₂ conversion

By: Gao, Junguang; Alsaab, Hashem O.; Zare, Masoud Habibi; Shirazian, Saeed

npj Clean Water (2025), 8(1), 76 | Language: English, Database: CAplus

Analyze Results

Top Document Types

Journal

Patent

Clinical Trial

Review

Re

Publications over Time

300

可以優先看Newton建議讀的paper

Key Research Areas

1. Hydrolysis Mechanism and Kinetics

Waugh Type Polyoxometalate Study [2024:483135](#)

- **Authors:** Mujawar et al. (2024)
- **Key Findings:**
 - Aspirin undergoes **acid-catalyzed hydrolysis** prior to oxidation
 - The hydrolysis is catalyzed by both acids (HClO_4) and certain oxidants
 - Mechanism involves ester bond cleavage generating salicylic acid
 - Rate laws were derived for the hydrolysis process
 - **DOI:** 10.14233/ajchem.2024.30296

DFT and Experimental Studies [2017:411222](#)