CAS SciFinder^{n}

反应信息的获取

程小燕博士

2022年3月15日

ACS International | CAS A division of the American Chemical Society

2022年CAS SciFinder^{n}论坛直播日程表

	日期	主题	主讲人
基础培训	3月1日	文献信息的获取	刘萌萌
	3月8日	物质信息的获取	钱欣
	3月15日	反应信息的获取	程小燕
	3月22日	生物序列的获取	刘萌萌
	3月29日	利用CAS SciFinder^{n}顺利开题、进行文献综述	钱欣
检索策略详解	4月25日	聚合物相关信息获取策略	程小燕
	5月24日	无机与金属有机化合物相关信息获取策略	钱欣
	6月14日	光电材料相关信息获取策略	程小燕
	7月5日	农化相关信息获取策略	钱欣
	9月13日	药物结构设计与合成	程小燕
	10月11日	天然植物化学相关信息获取策略	钱欣
	11月8日	稀土材料相关信息获取策略	程小燕
	11月29日	纳米材料相关信息获取策略	钱欣
	12月20日	催化合成信息获取策略	程小燕

直播时间：

18:00 – 19:00

关注公众号：ACS美国化学会
随时观看回放，了解直播信息

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提纲

- CAS和CAS SciFinder^{n}简介
- CAS SciFinder^n 反应检索方法
- 反应案例分享
- 在线演示以及Q&A

CAS具有最全面的学科连接内容合集

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CAS SciFinder^{n}中覆盖的内容合集

来源：
https://www.cas.org/cas-data
https://www.cas.org/about/cas-content

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提纲

- CAS和CAS SciFinder^{n}简介
- **CAS SciFinder^n 反应检索方法**
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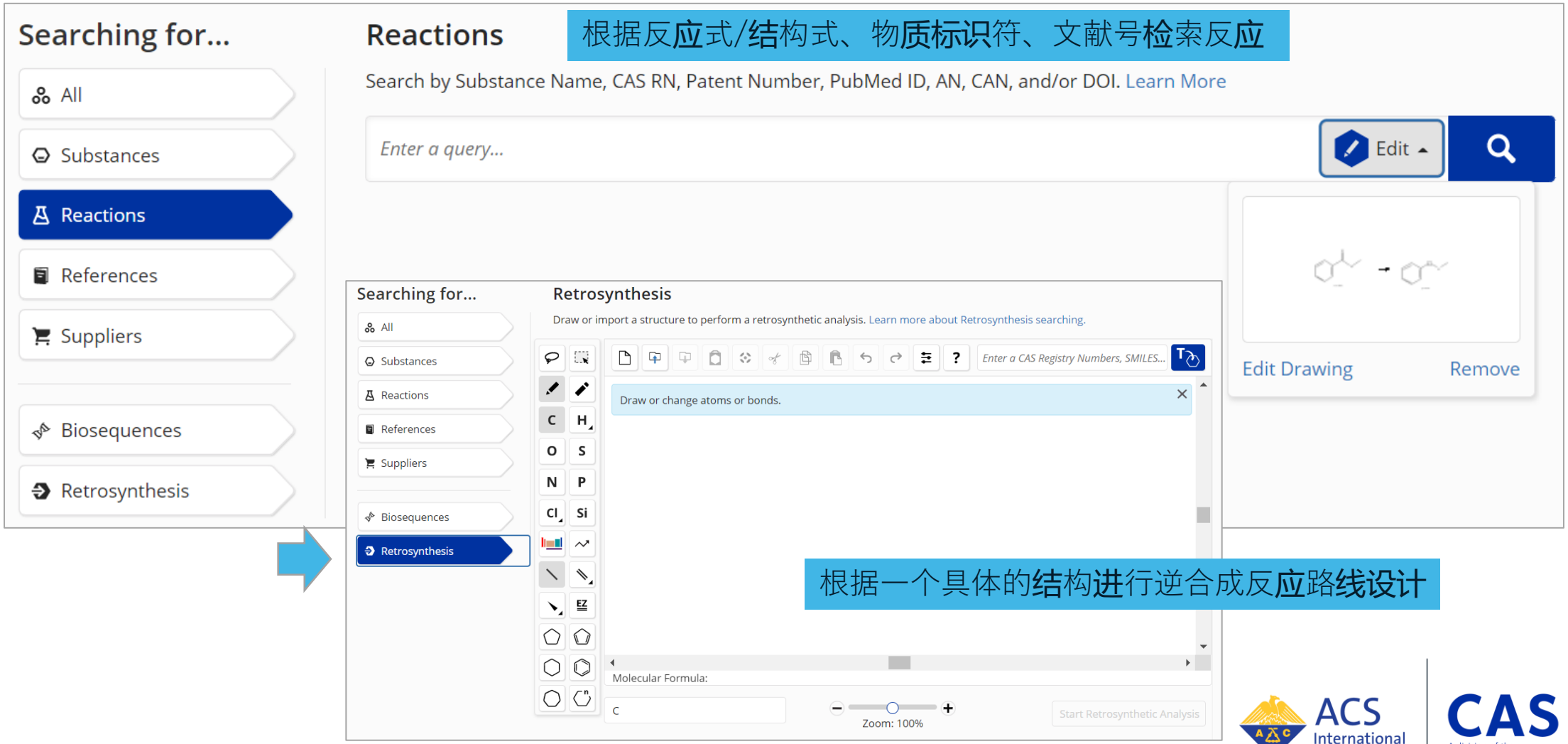
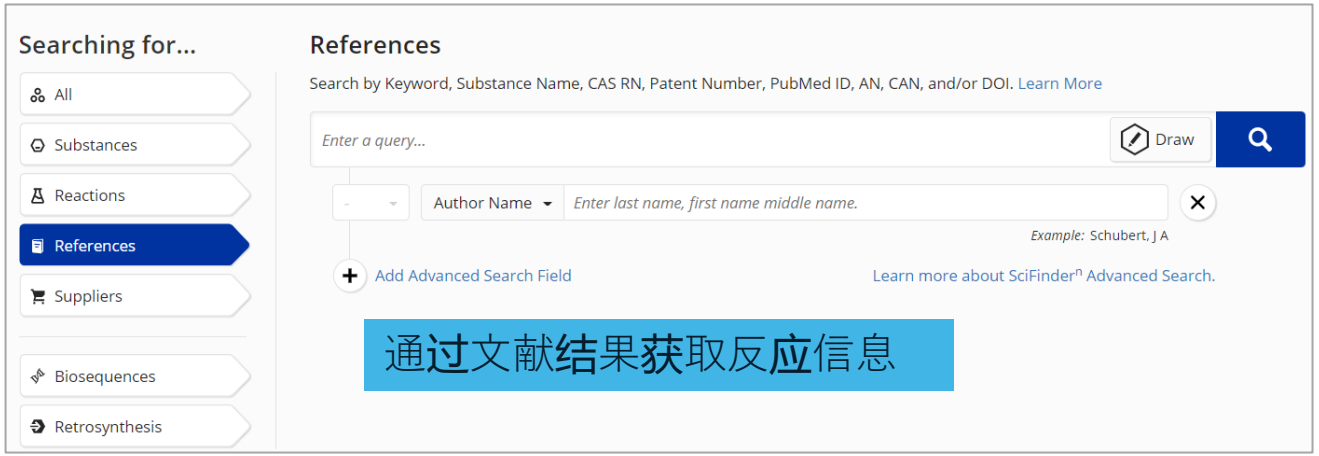
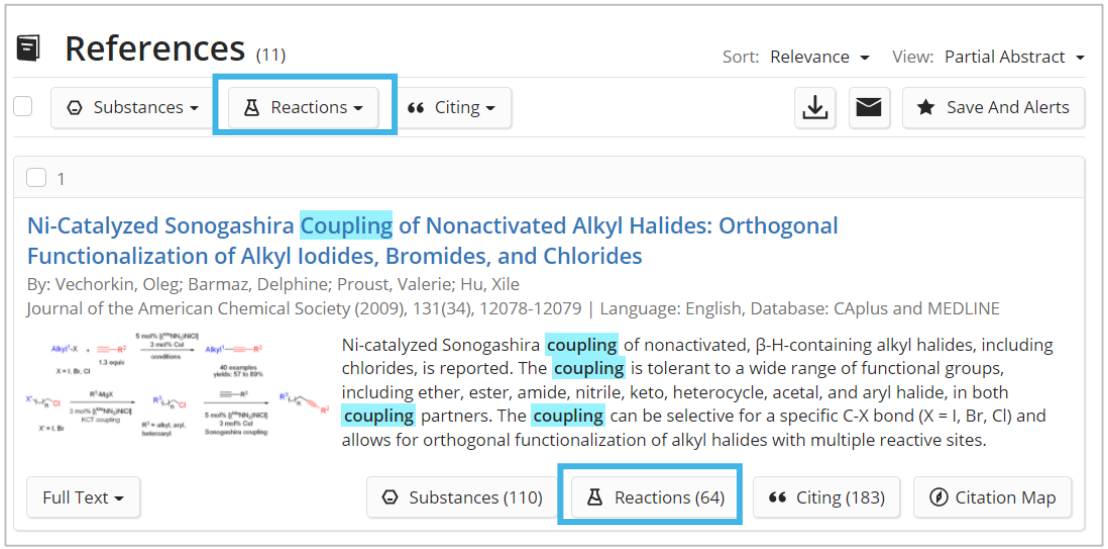
- 在线演示以及Q&A

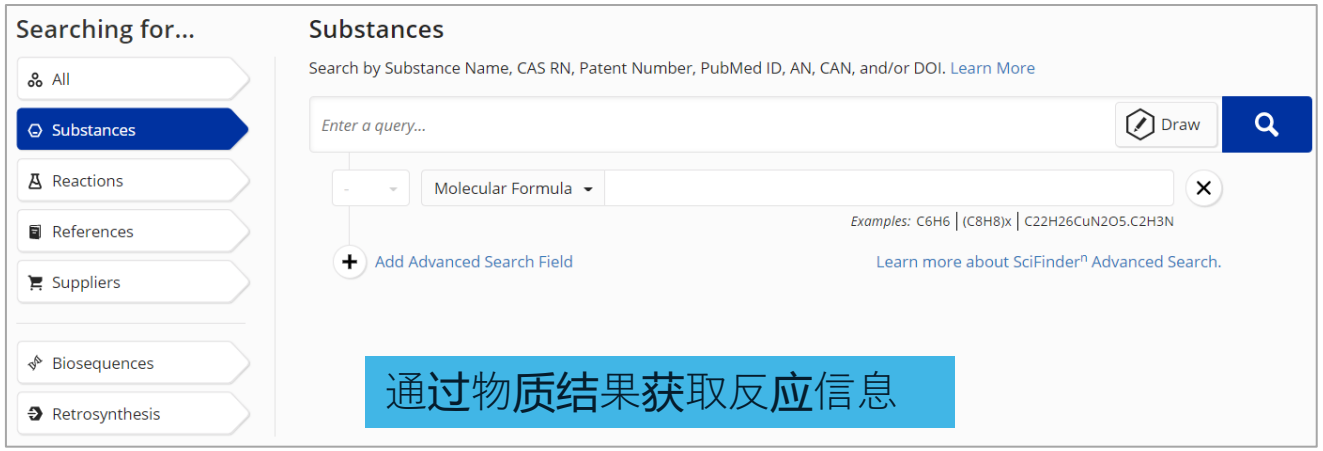
反应检索方法——直接检索

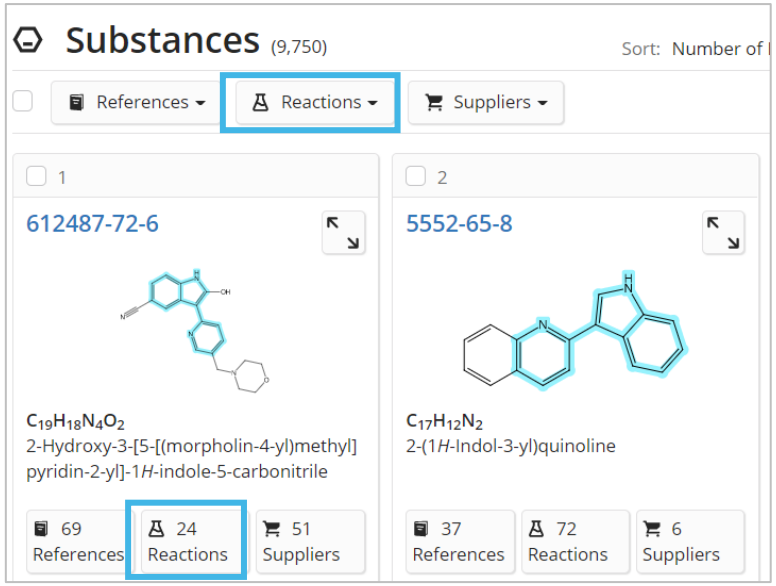


反应检索方法——间接检索









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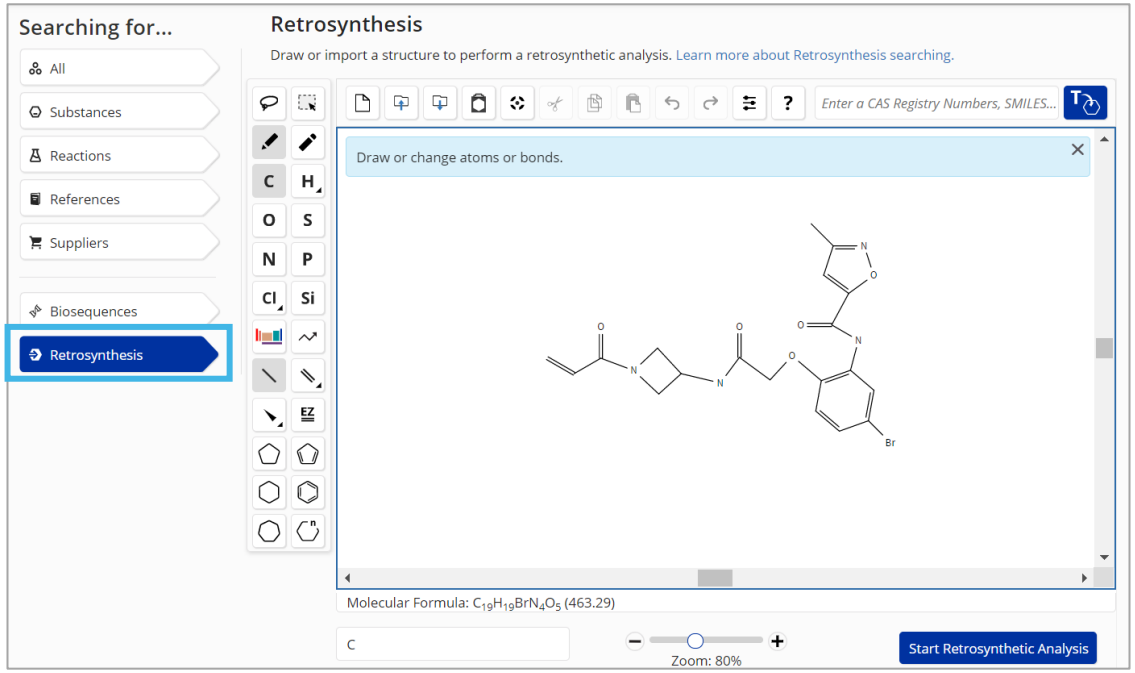
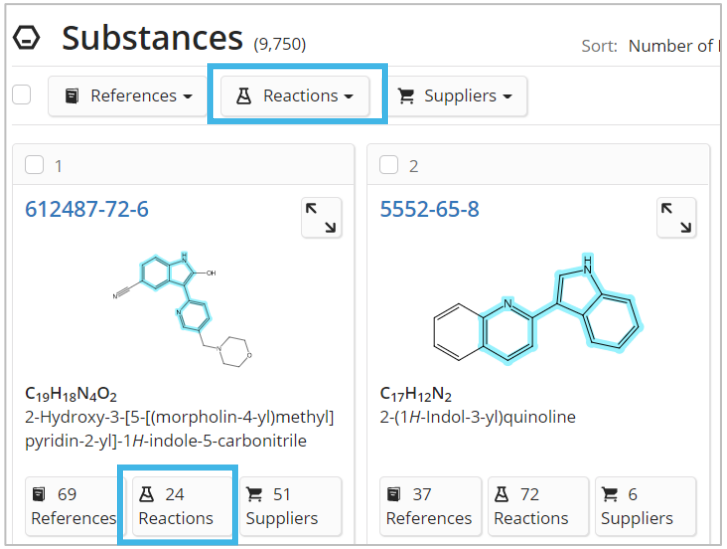
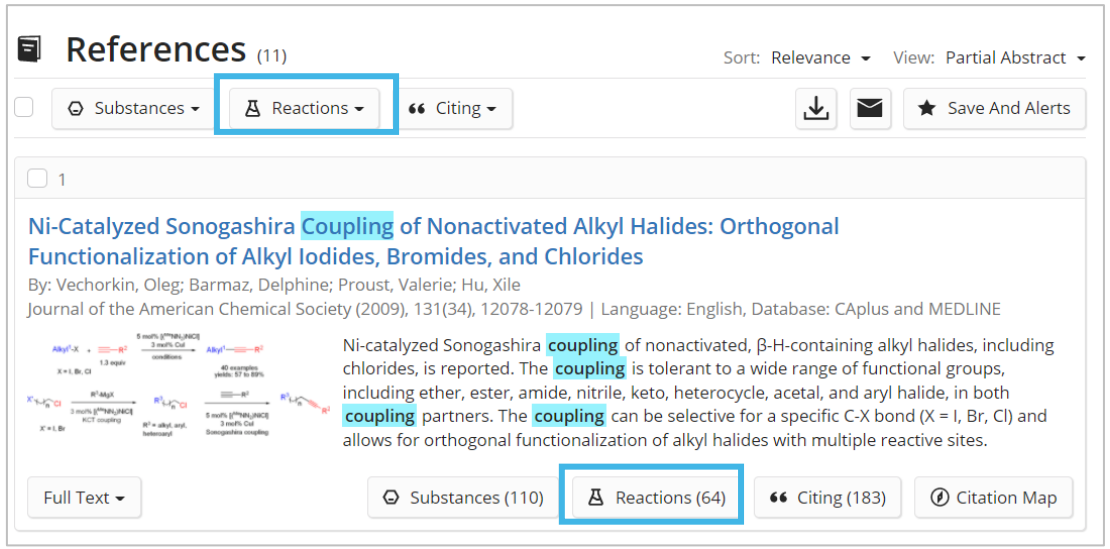
反应检索方法汇总



1. 直接进行Reaction检索
2. 通过Retrosynthesis Plan 获取逆合成反应路线
3. 通过物质获取反应
4. 通过文献获取反应





反应检索场景及检索方法建议

1. 直接进行Reaction检索——根据反应式/结构式、物质标识符、文献号检索反应
   - ✓ 已知反应式，或者反应物/产物/反应试剂的结构式
   - ✓ 已知物质标识符（包括名称、CAS RN等）
   - ✓ 已知文献号或专利号等
2. 通过Retrosynthesis Plan获取逆合成反应路线——依据一个确定结构的物质进行设计
   - ✓ 有报道且结构明确的物质，无论是否有反应信息报道
   - ✓ 未有报道且结构明确的物质
3. 通过物质获取反应——先检索物质，再通过物质结果获取反应信息
   - ✓ 需要先对物质结果进行结构、属性或反应角色等筛选，然后再看反应
   - ✓ 某些物质（手性分子、多片段结构组成的物质）和盐类化合物、聚合物等多组分物质的反应
4. 通过文献获取反应——先检索文献，再通过文献结果获取反应
   - ✓ 通过结构检索没有得到反应结果
   - ✓ 需要通过关键词精炼感兴趣的反应信息

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反应绘制工具介绍

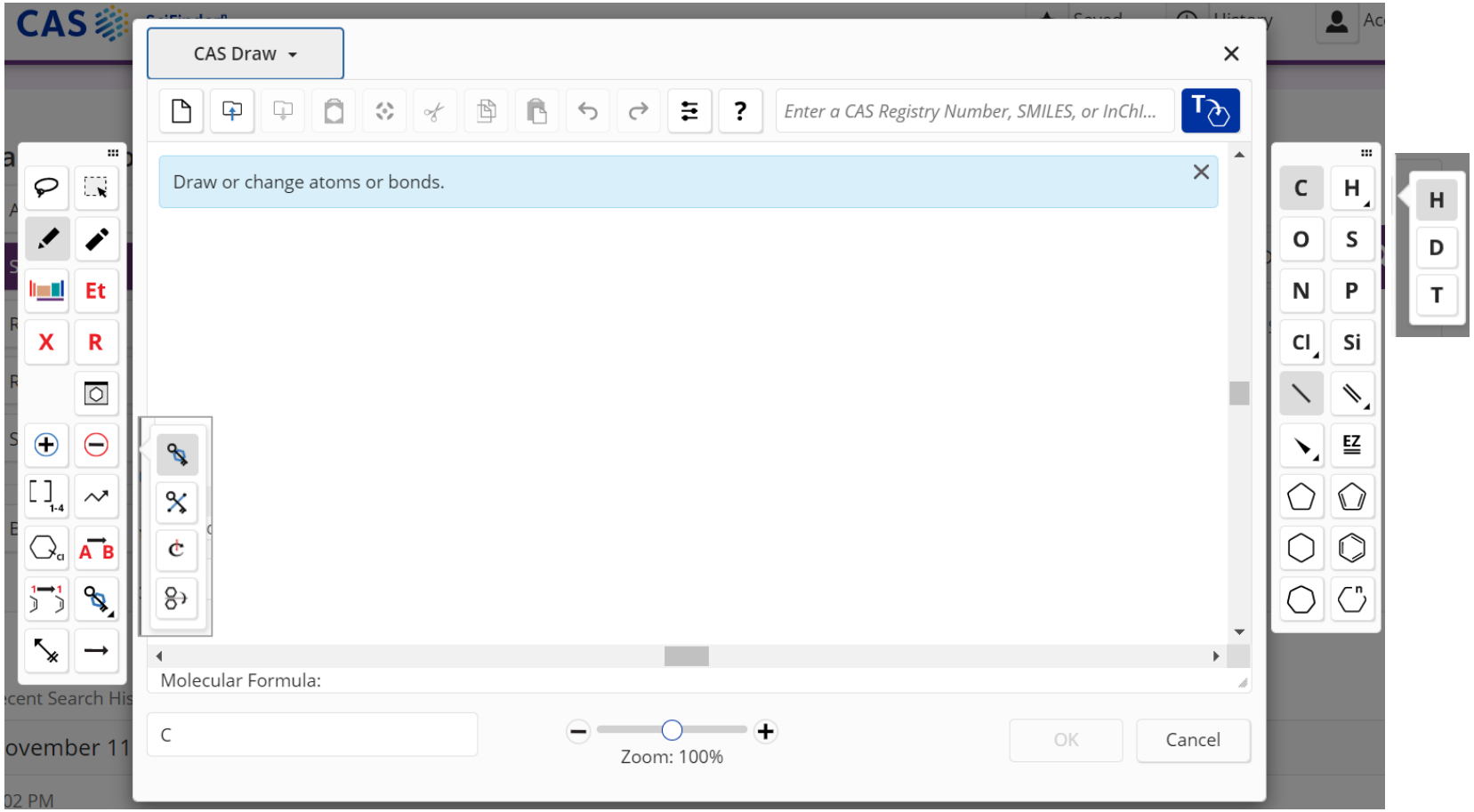
反应绘制工具注释

反应箭头

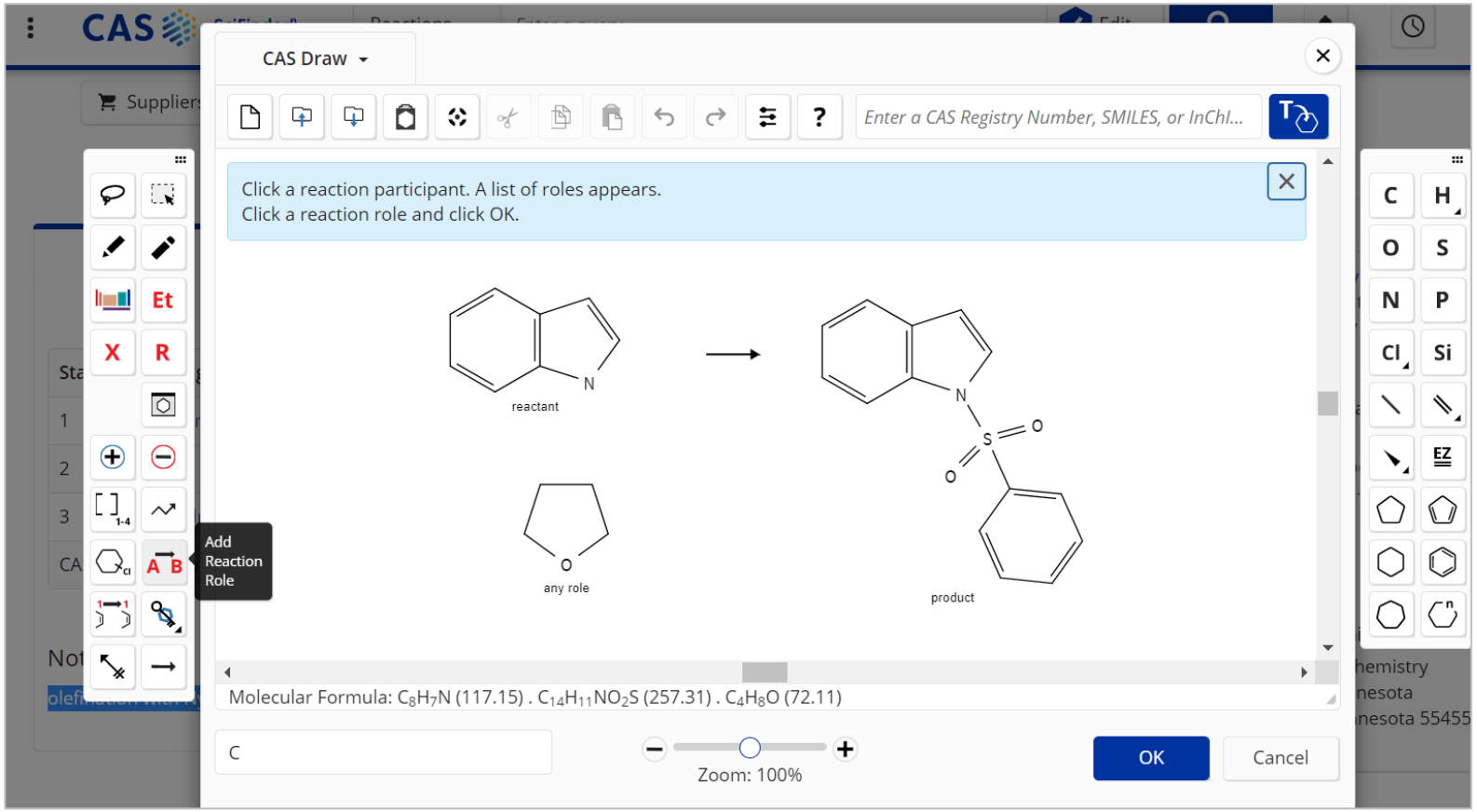
反应角色标记

原子标记

化学键标记

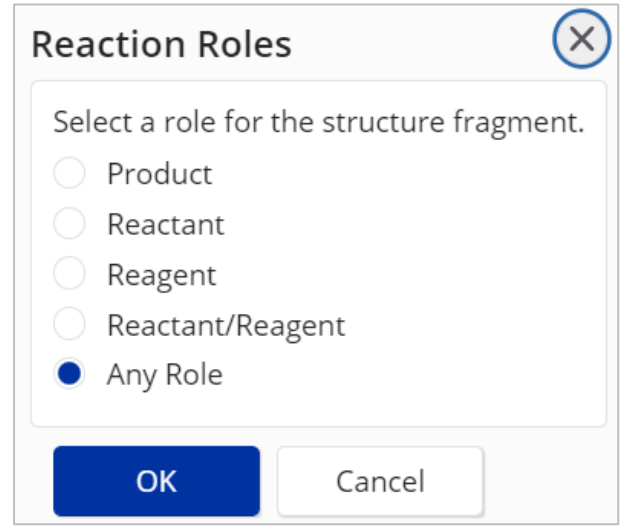


反应箭头和反应角色标记



反应箭头

反应角色标记



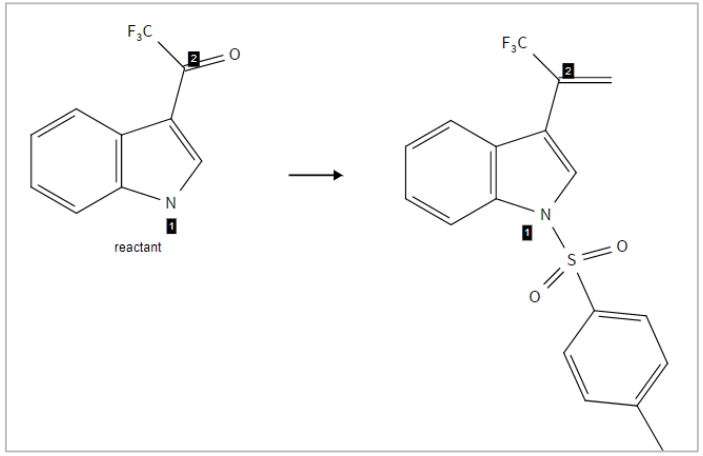
Reagent：参与反应，但不构成产物的碳原子

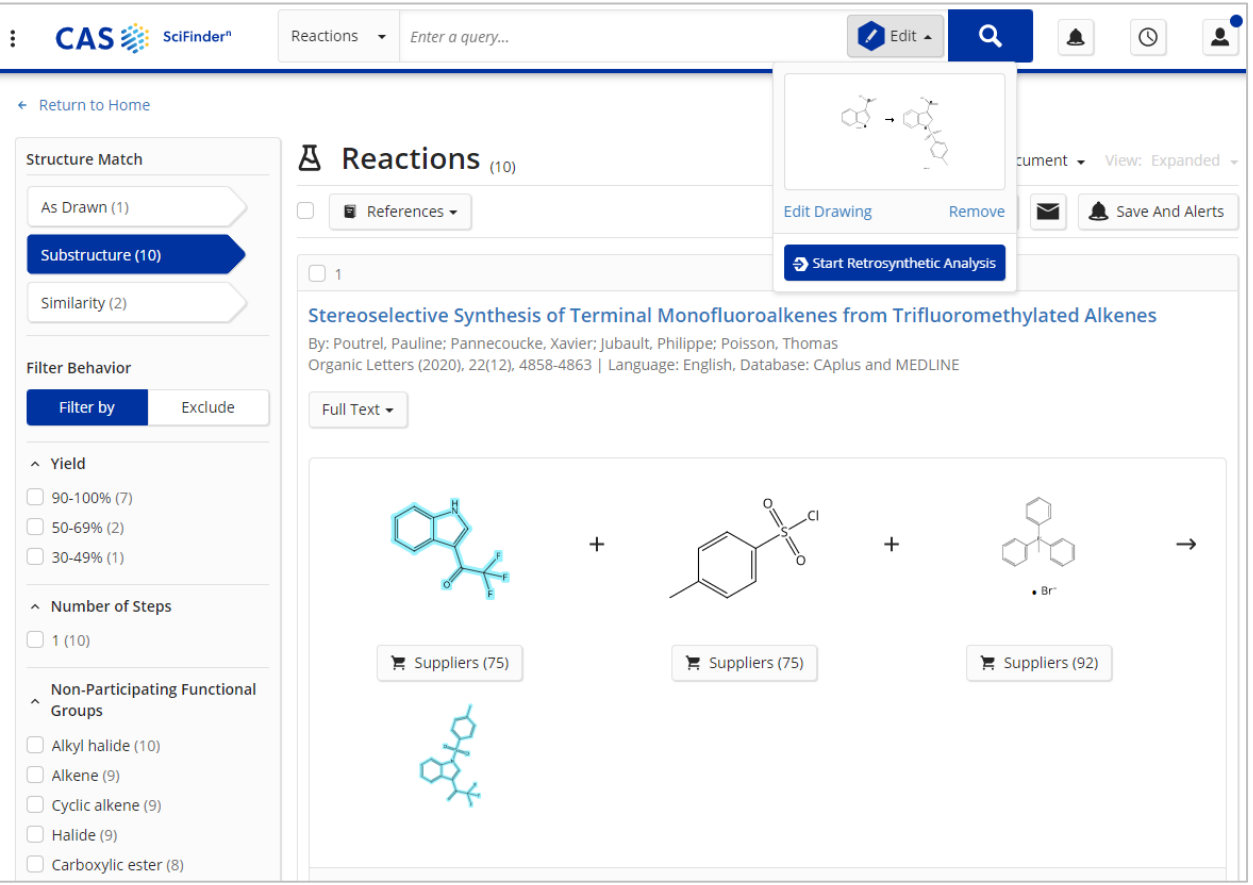
Any Role: 指reactant、reagent或product中的一种

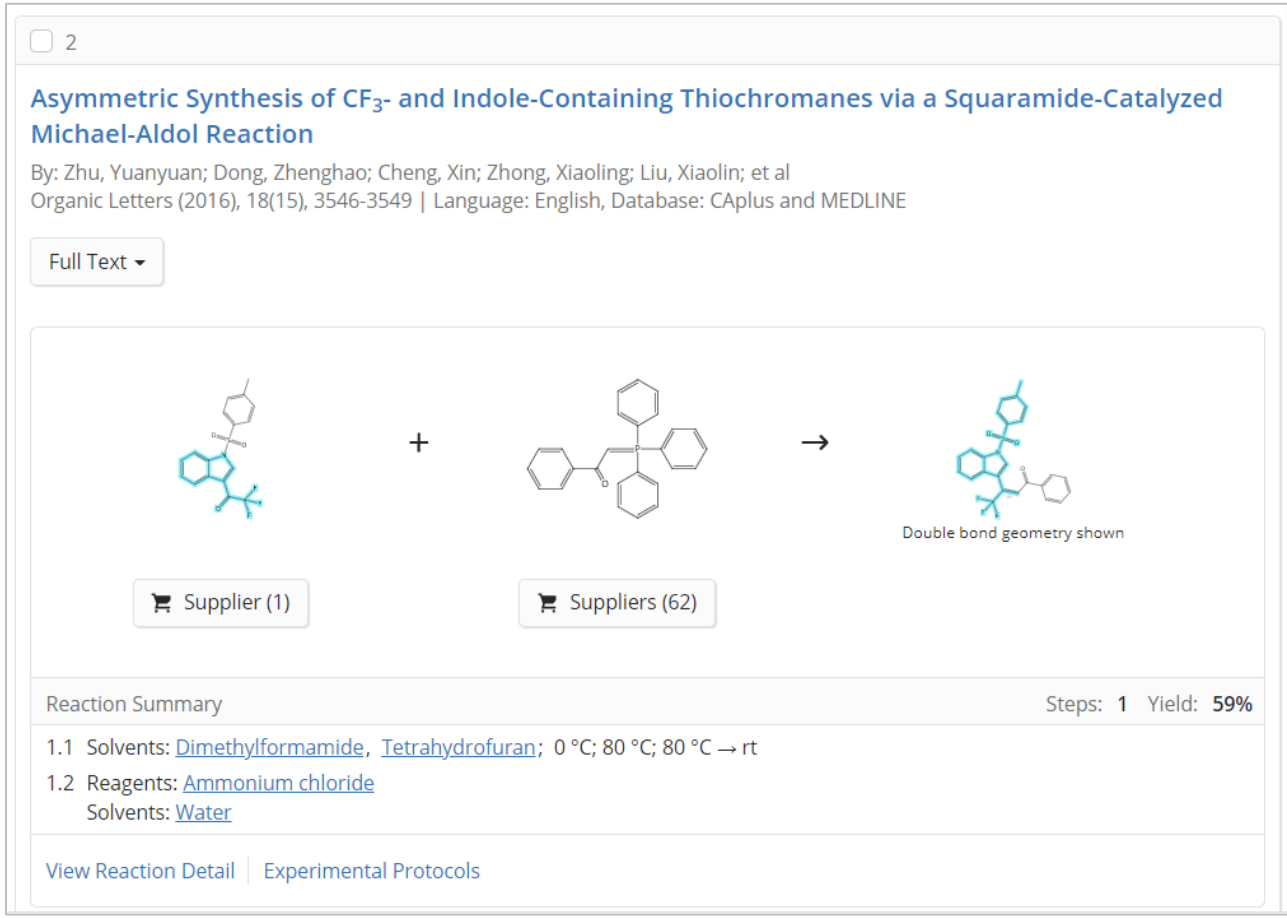
原子标记

原子标记

标记反应物和产物中的同一个原子



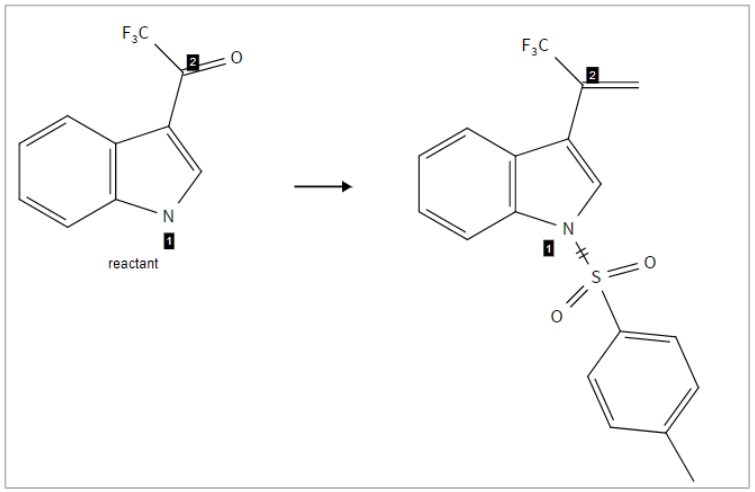


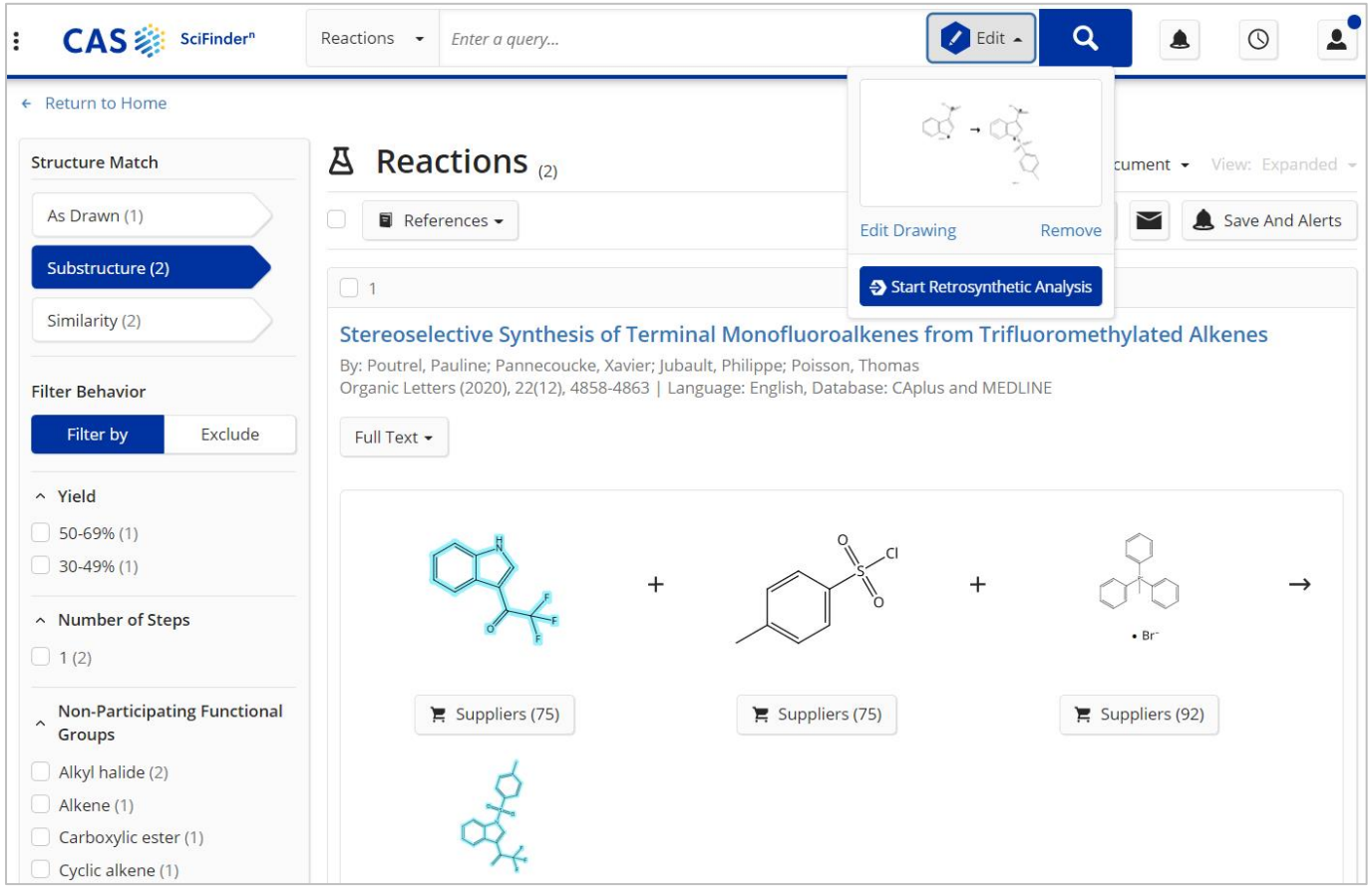


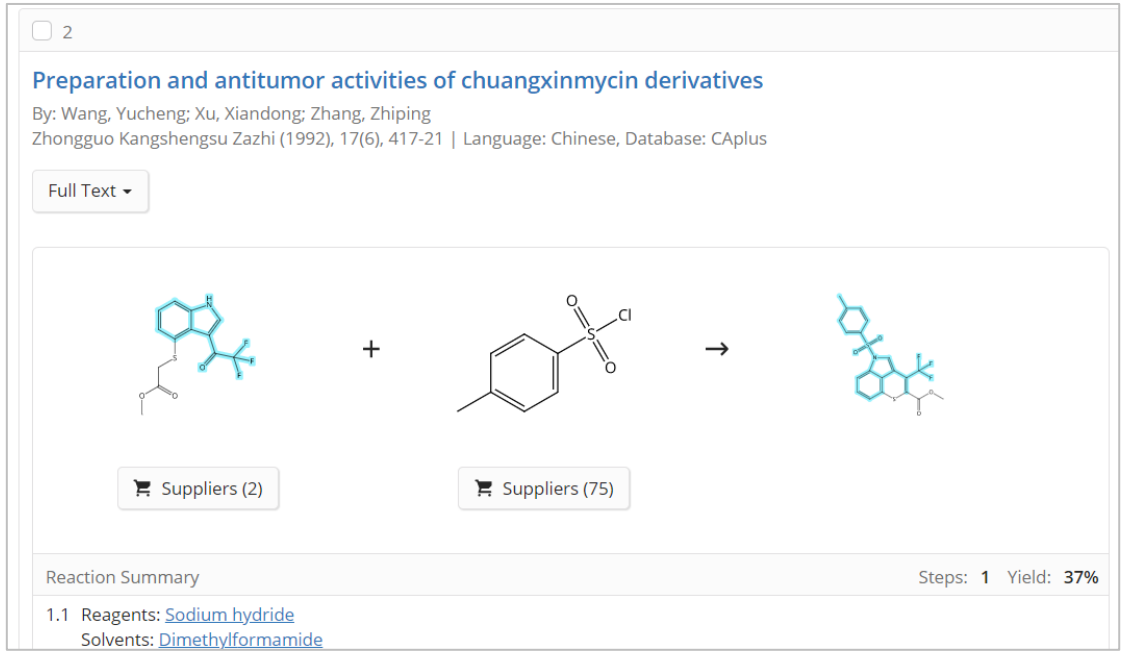
化学键标记

化学键标记 

标记反应中发生变化的键（断裂、生成或键级变化）







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小结：

- 反应检索方法：直接检索（Reaction Search, Retrosynthesis），间接获取反应（通过物质或文献获取）
- 反应检索场景及检索方法建议：基于四种检索方法下的多个应用场景，考虑检索前已知哪些信息，检索中的具体需求
- 反应绘制工具介绍：反应箭头、反应角色标记、原子标记和化学键的标记
- 数据关联支持灵活检索：文献、物质和反应数据已经CAS科学家进行深度关联

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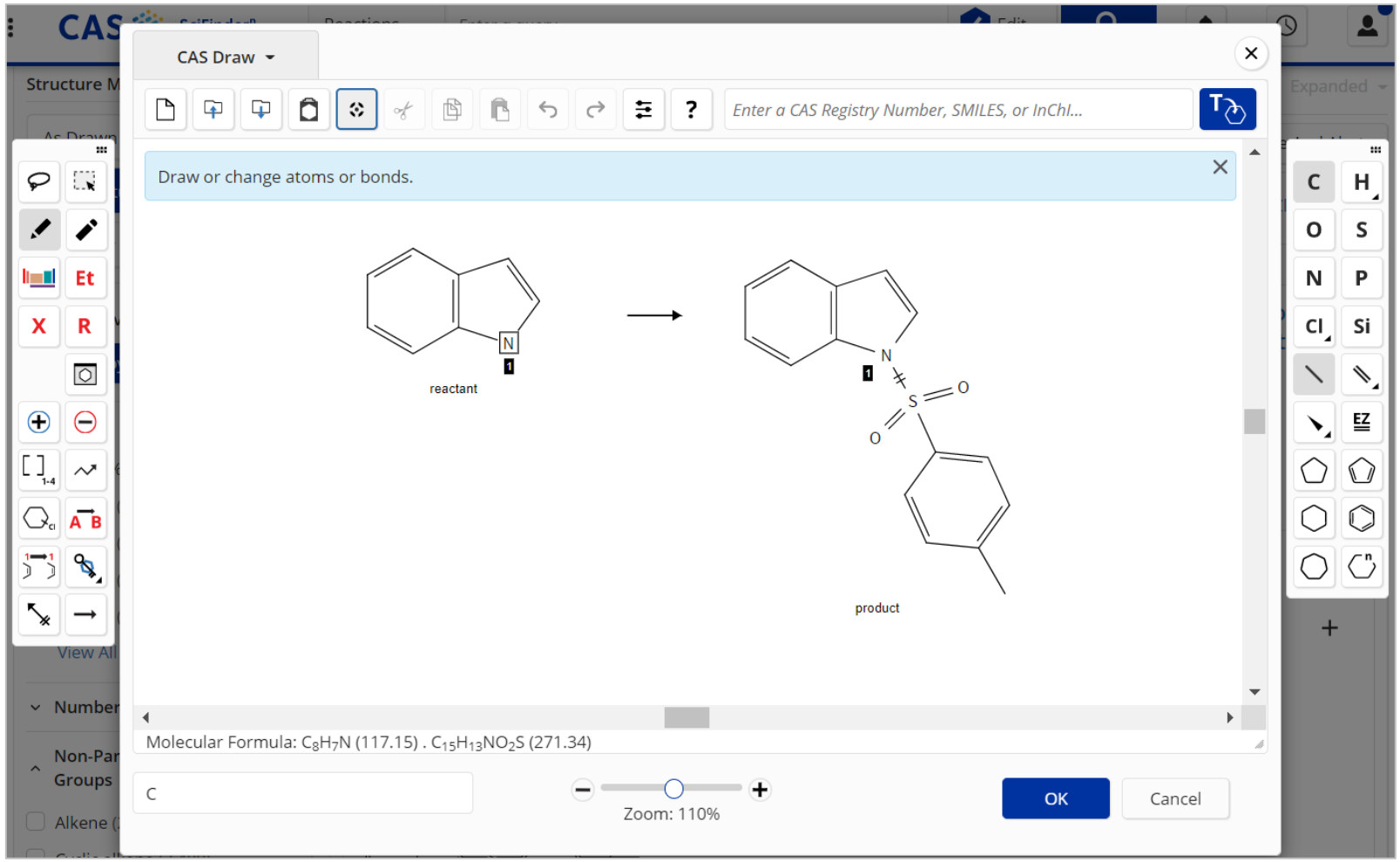
提纲

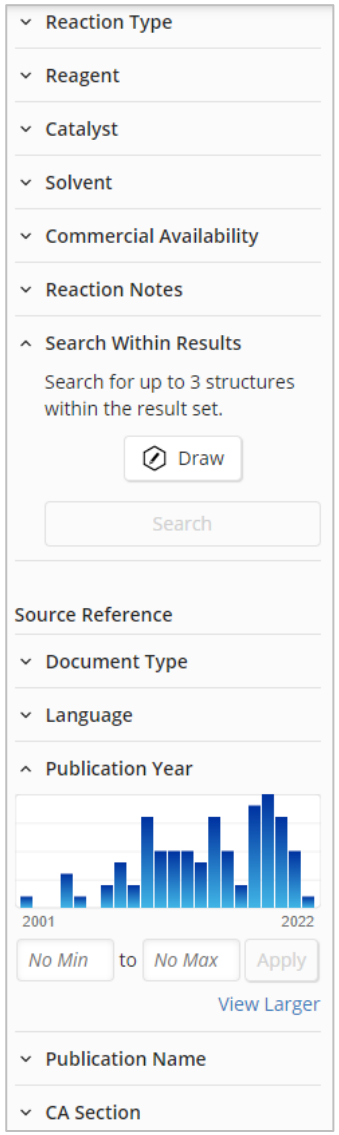
- CAS和CAS SciFinder^{n}简介
- CAS SciFinder^n 反应检索方法
- **反应案例分享**
- 在线演示以及Q&A

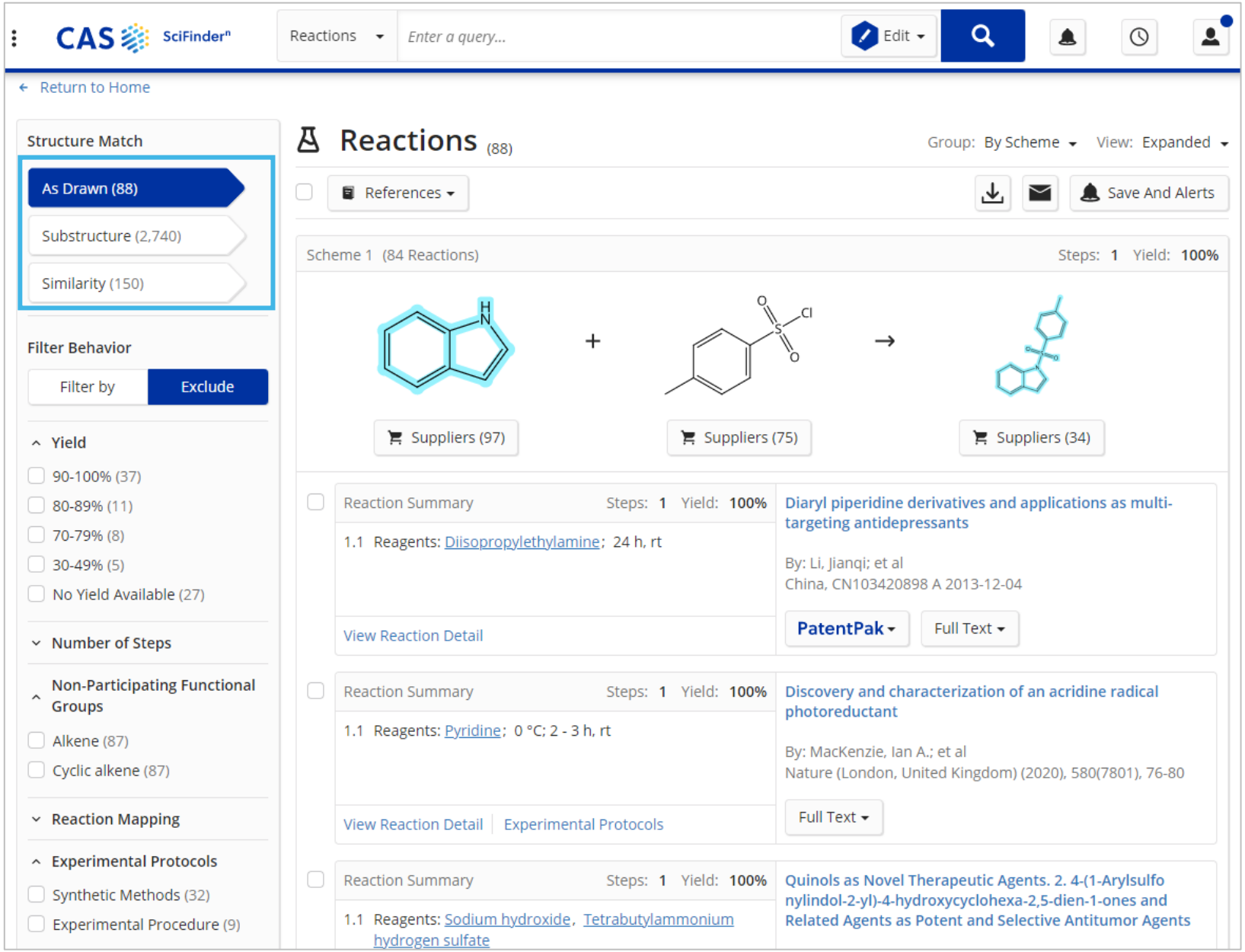
例1：直接通过反应式检索反应



反应结果分析与精炼

产率
步数
不参与反应官能团
实验详情
反应类型
试剂
催化剂
溶剂
供应商信息
反应分类
二次结构检索
文献类型
语言
发表年份
刊物名
CA学科领域





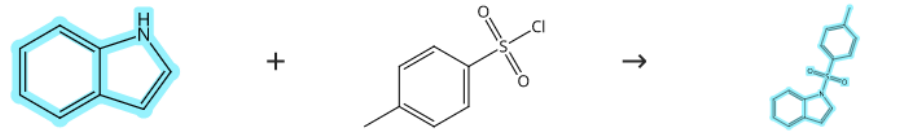
Group by Scheme/Document：选择反应结果的呈现方式

Reactions (88)

Group: By Scheme | View: Expanded

References | Save And Alerts

Scheme 1 (84 Reactions) Steps: 1 Yield: 100%



Suppliers (97) | Suppliers (75) | Suppliers (34)

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Diisopropylethylamine; 24 h, rt

View Reaction Detail

Diaryl piperidine derivatives and applications as multi-targeting antidepressants

By: Li, Jianqi; et al
China, CN103420898 A 2013-12-04

PatentPak | Full Text

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Pyridine; 0 °C; 2 - 3 h, rt

View Reaction Detail | Experimental Protocols

Discovery and characterization of an acridine radical photoreductant

By: MacKenzie, Ian A.; et al
Nature (London, United Kingdom) (2020), 580(7801), 76-80

Full Text

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Sodium hydroxide, Tetrabutylammonium hydrogen sulfate
Solvents: Toluene, Water; 0 °C; 16 h, rt

Quinols as Novel Therapeutic Agents. 2. 4-(1-Arylsulfonylindol-2-yl)-4-hydroxycyclohexa-2,5-dien-1-ones and Related Agents as Potent and Selective Antitumor Agents

By: Berry, Jane M.; et al
Journal of Medicinal Chemistry (2005), 48(2), 639-644

Reactions (88)

Group: By Document | View: Expanded

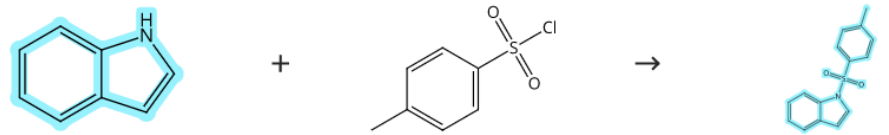
References | Save And Alerts

1

Discovery and characterization of an acridine radical photoreductant

By: MacKenzie, Ian A.; Wang, Leifeng; Onuska, Nicholas P. R.; Williams, Olivia F.; Begam, Khadiza; et al
Nature (London, United Kingdom) (2020), 580(7801), 76-80 | Language: English, Database: CAplus and MEDLINE

Full Text



Suppliers (97) | Suppliers (75) | Suppliers (34)

Reaction Summary Steps: 1 Yield: 100%

1.1 Reagents: Pyridine; 0 °C; 2 - 3 h, rt

View Reaction Detail | Experimental Protocols

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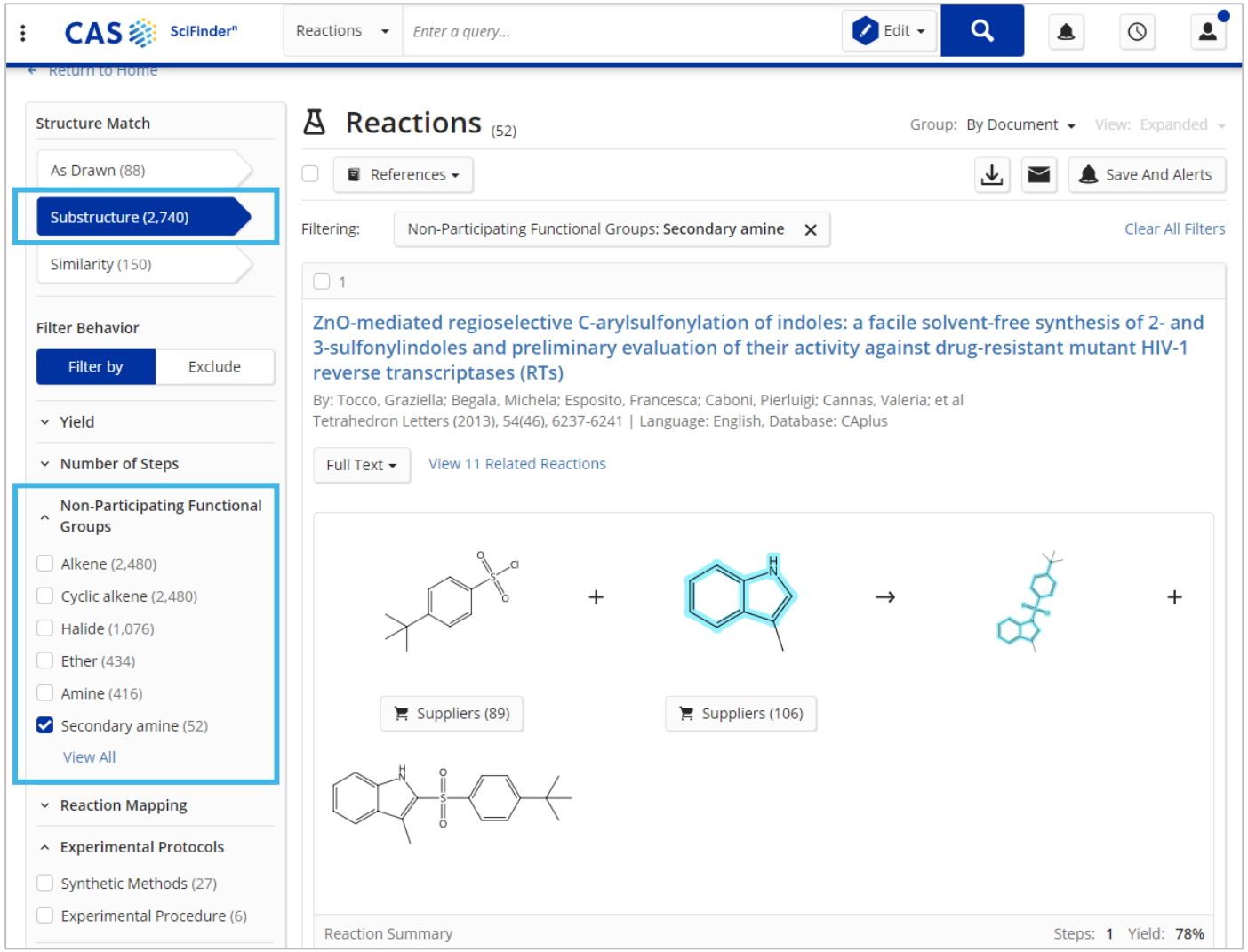
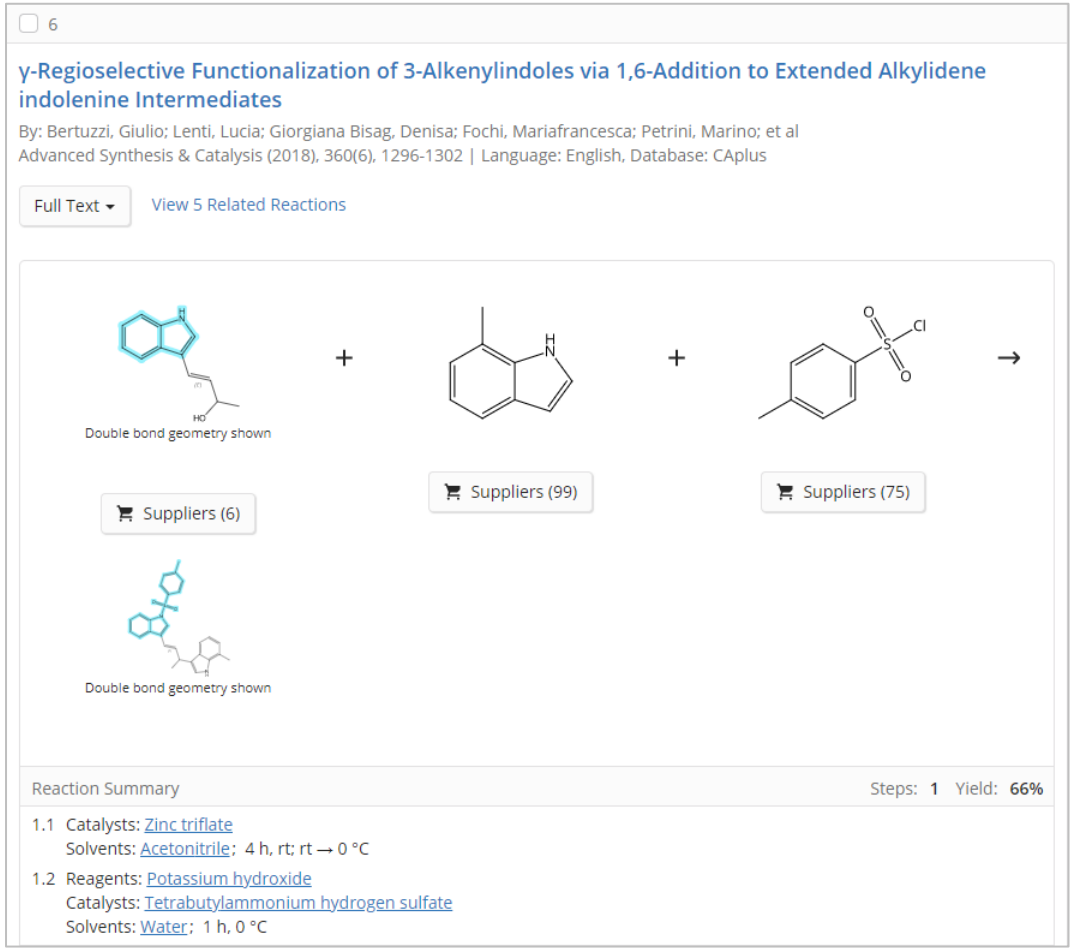
Non-participating Functional Group: 浏览或筛选不参与反应官能团

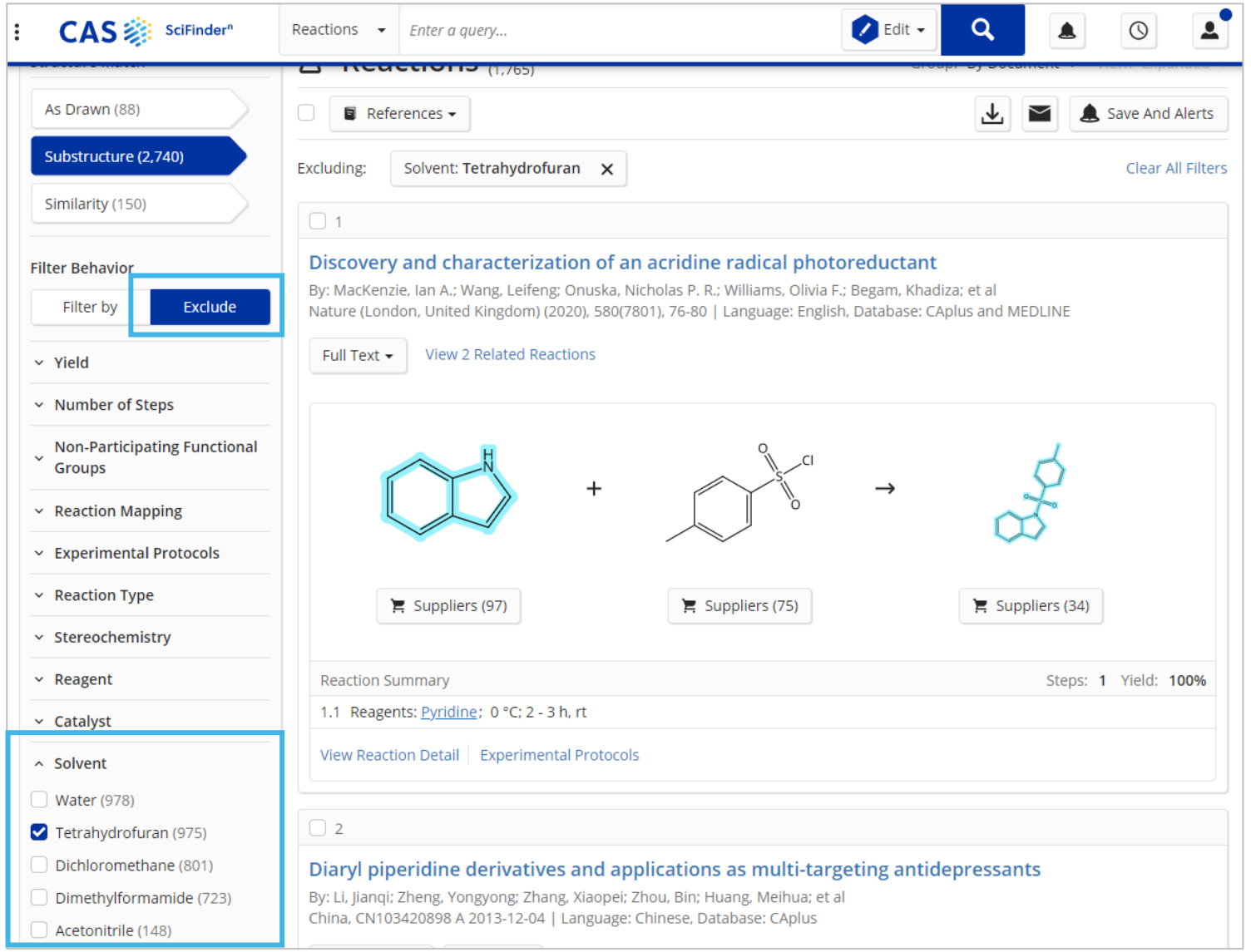
出现在反应前后，但未发生变化的官能团

同时考虑分子间和分子内的官能团





使用Exclude，一键排除不感兴趣的反应



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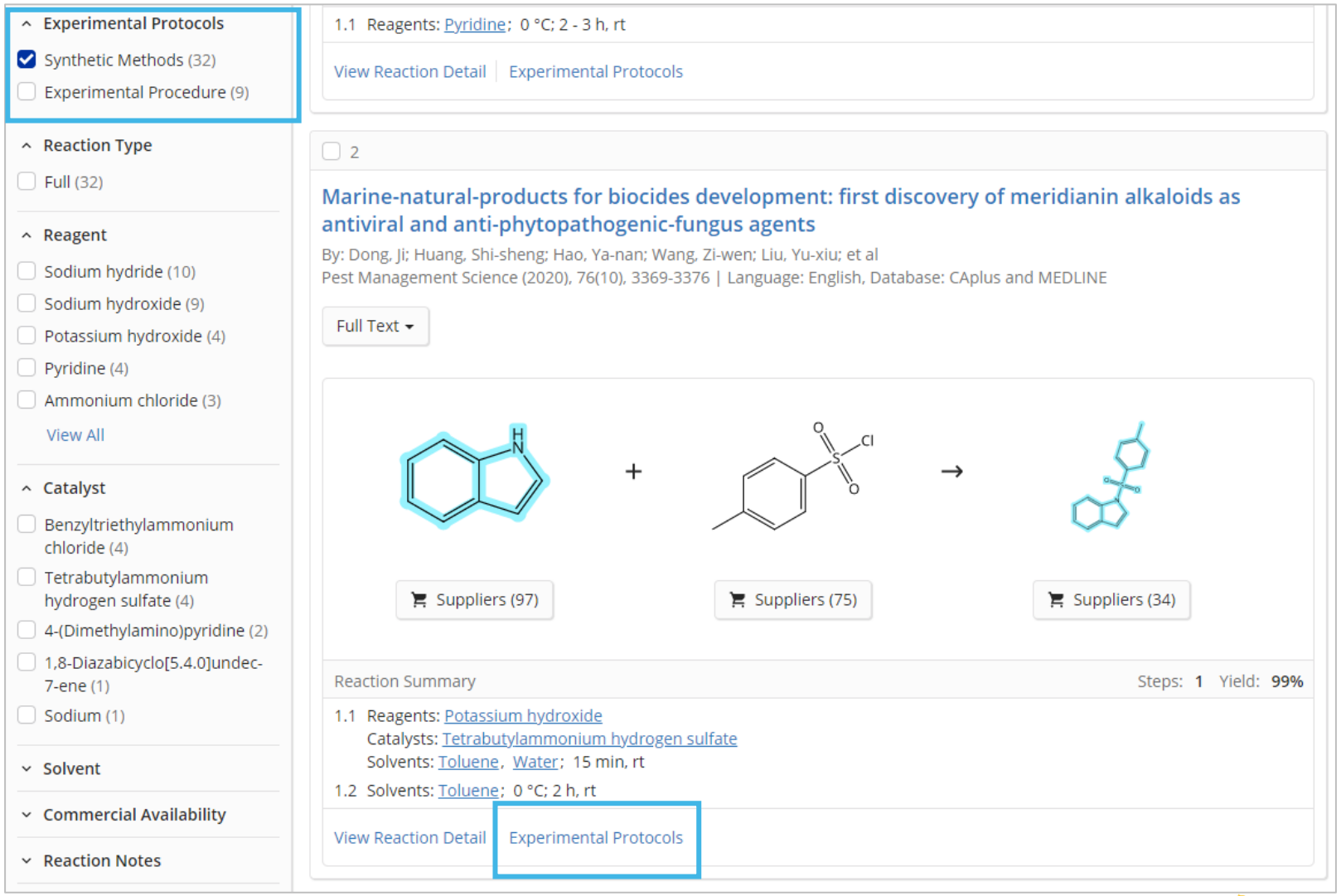
Experimental Protocols获取反应详情



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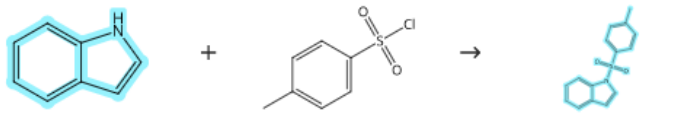
Synthetic Methods获取增值的反应详情

← Return to Results

Reaction Detail (Document 2, Reaction 1 of 1)

← Prev Next →

Save



Steps: 1
Yield: 99%

Suppliers (97) | [Stage 2] Suppliers (75) | 99% Suppliers (34)

Step 1

Alternative Steps (83)

Stage	Reagents	Catalysts	Solvents	Conditions
1	Potassium hydroxide	Tetrabutylammonium hydrogen sulfate	Toluene Water	15 min, rt
2	-	-	Toluene	0 °C; 2 h, rt

CAS Reaction Number: 31-081-CAS-22650181

Experimental Protocols

Synthetic Methods

Products	1-[(4-Methylphenyl)sulfonyl]-1*H*-indole, Yield: 99%
Reactants	Indole Tosyl chloride
Reagents	Potassium hydroxide
Catalysts	Tetrabutylammonium hydrogen sulfate
Solvents	Toluene Water
Procedure	1. Add tetrabutylammonium hydrogen sulfate (0.95 g, 3 mmol) and 50% KOH aqueous solution (50 mL) to a solution of substituted indole (40 mmol) in toluene (50 mL). 2. Stir the reaction mixture at room temperature for 15 minutes. 3. Add TsCl (9.2 g) in toluene (100 mL) at 0 °C. 4. Stir the reaction at room temperature for 2 hours. 5. After completion of the reaction, extract the mixture with ethyl acetate (200 mL×3). 6. Wash the combined organic phase with brine (200 mL). 7. Dry the combined organic phase over anhydrous Na_2SO_4. 8. Concentrate the combined organic phase.
Transformation	Sulfonation of Aromatic Compounds Formation of Sulfonamides
Scale	milligram

JOURNAL

Marine-natural-products for biocides development: first discovery of meridianin alkaloids as antiviral and anti-phytopat hogenic-fungus agents

By: Dong, Ji; et al
View All

Pest Management Science (2020), 76(10), 3369-3376

Full Text

Company/Organization

Tianjin Key Laboratory of Structure and Performance for Functional Molecules, MOE Key Laboratory of Inorganic-Organic Hybrid Functional Material Chemistry, College of Chemistry
Tianjin Normal University
Tianjin
China

Characterization Data

1-[(4-Methylphenyl)sulfonyl]-1*H*-indole

Proton NMR Spectrum	(400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H, Ar-H), 7.75 (d, *J* = 8.3 Hz, 2H, Ar-H), 7.55 (d, *J* = 3.6 Hz, 1H, Ar-H), 7.51 (d, *J* = 7.8 Hz, 1H, Ar-H), 7.30 (t, *J* = 7.6 Hz, 1H, Ar-H), 7.24-7.20 (m, 1H, Ar-H), 7.17 (d, *J* = 8.4 Hz, 2H, Ar-H), 6.63 (d, *J* = 3.6 Hz, 1H, Ar-H), 2.29 (s, 3H, CH_3).
Carbon-13 NMR	(100 MHz, $CDCl_3$) δ 145.0, 135.3, 134.8, 130.8, 129.9, 126.8, 126.4, 124.6, 123.3, 121.4, 113.6, 109.1, 21.8.
Melting Point	77-78 °C.
State	white solid.

CAS Method Number 3-081-CAS-22650181

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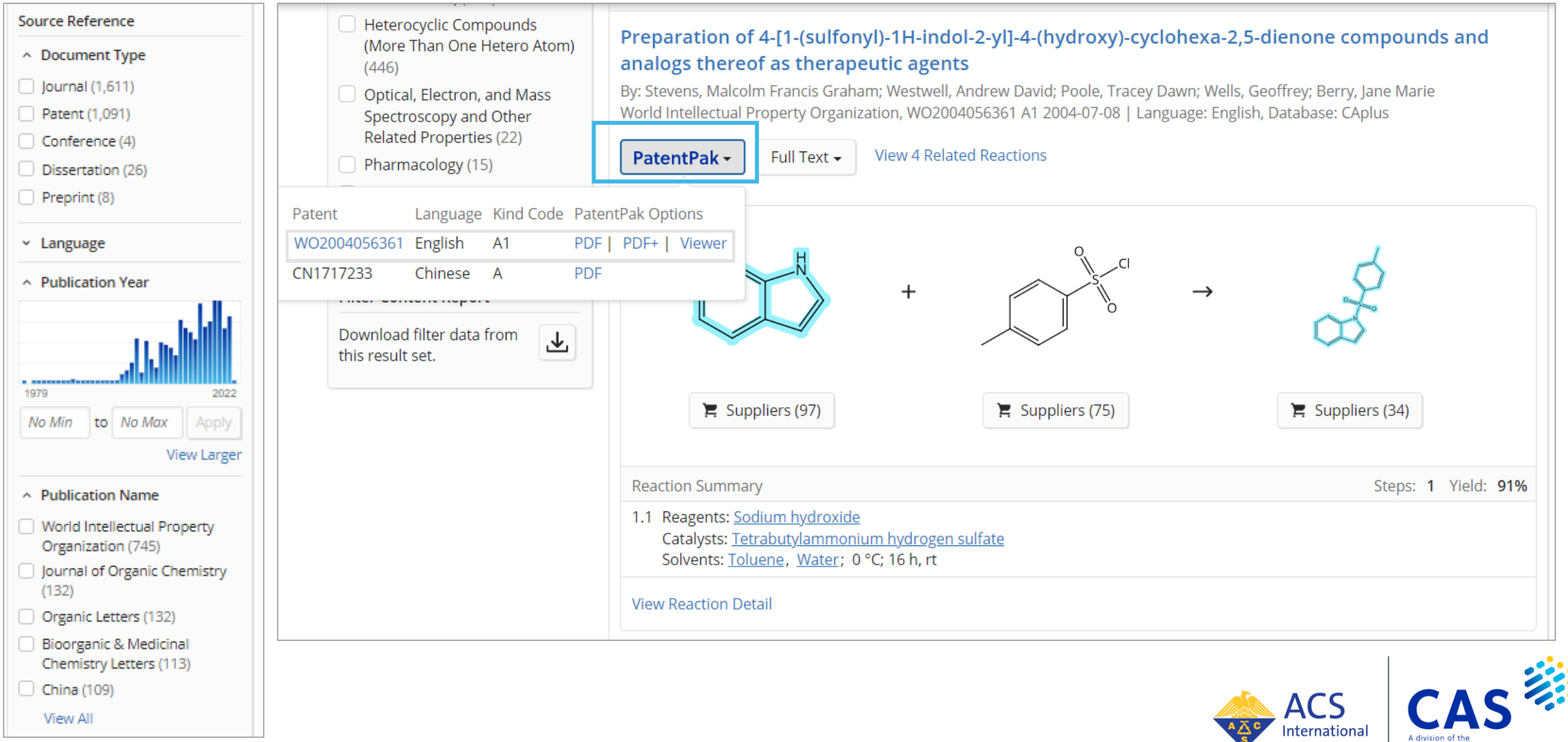
CAS PatentPak：高效获取专利详情



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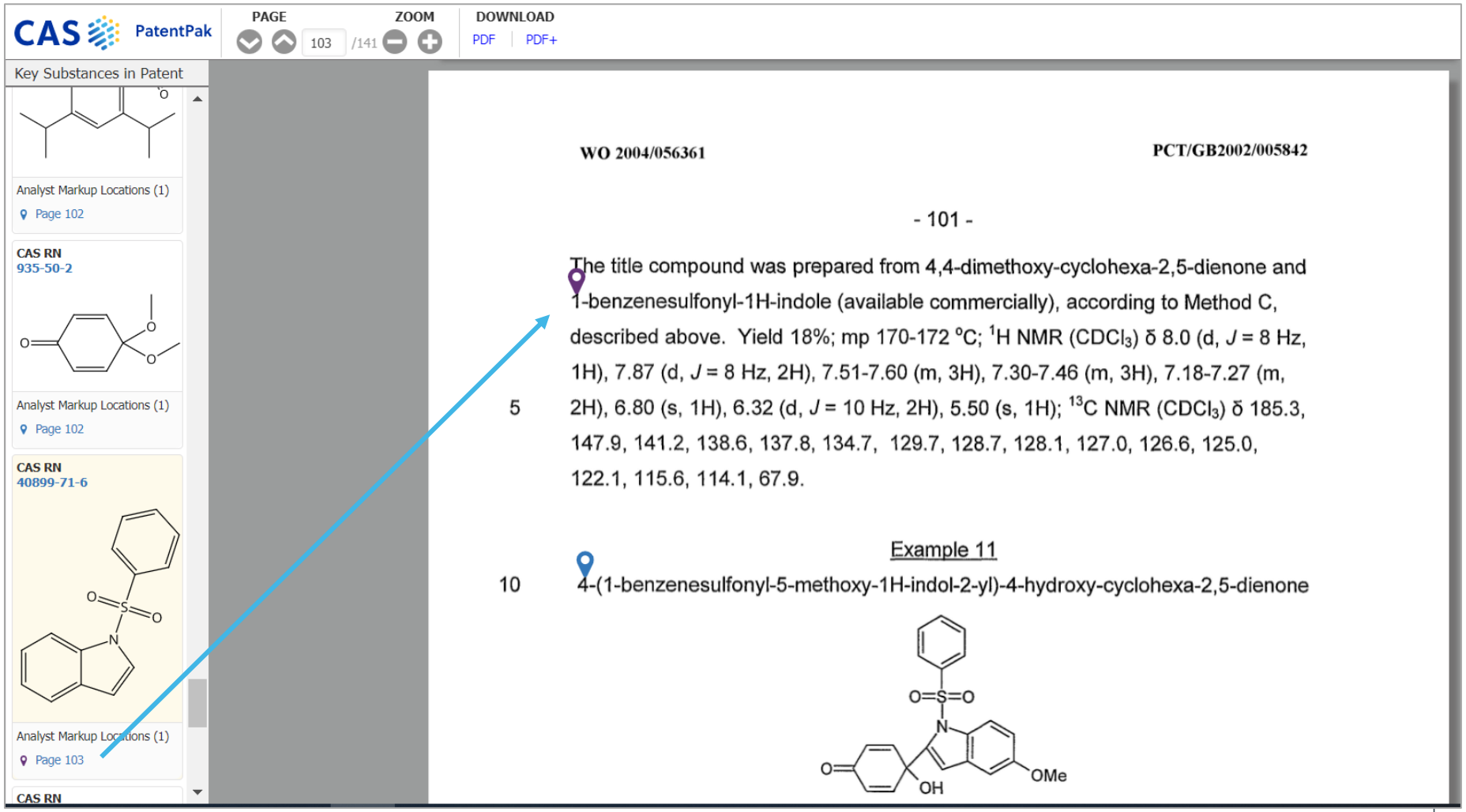
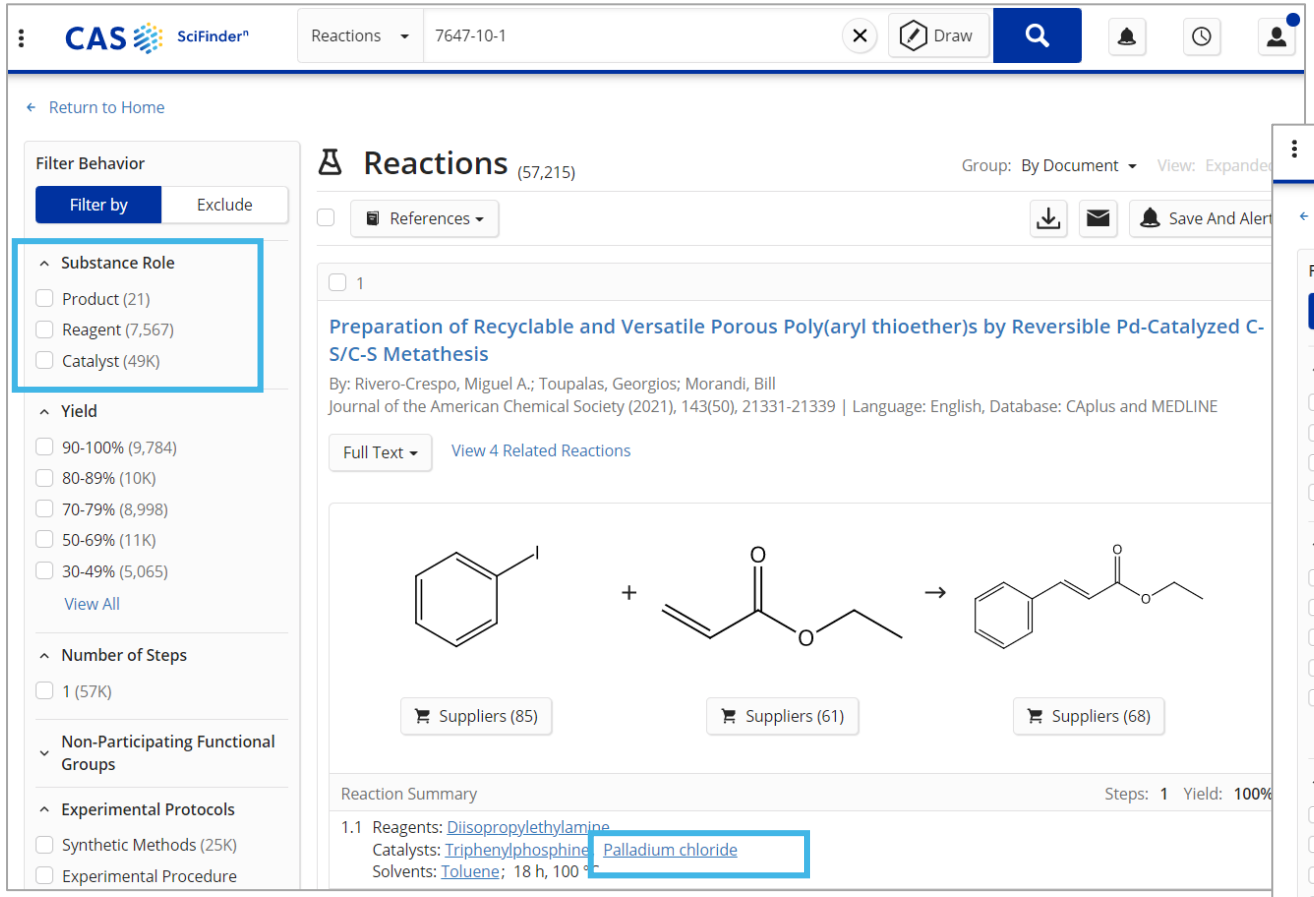
CAS PatentPak：一键定位专利中重要的物质

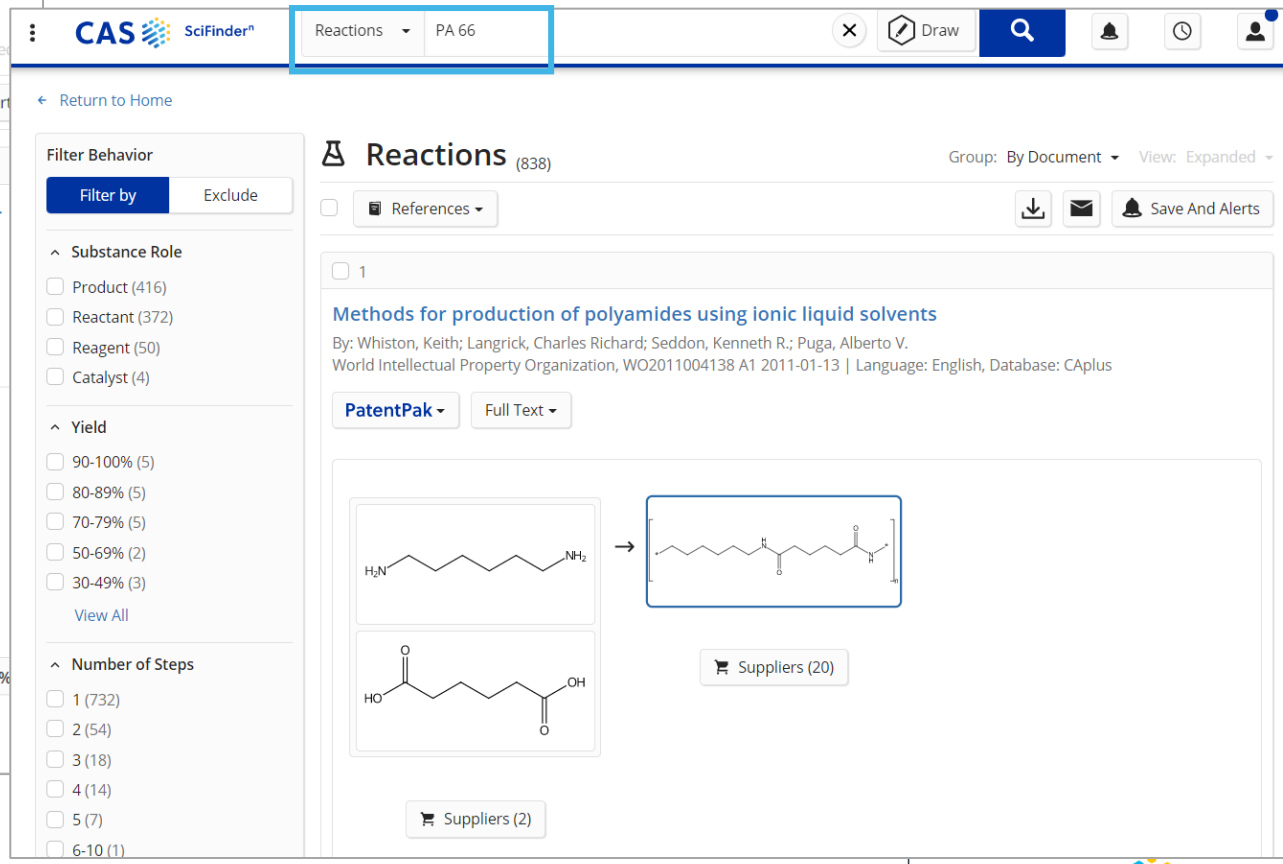


小结：

- 直接通过反应式检索反应：绘制反应式，并根据需要使用原子标记或化学键标记工具等
- 反应结果聚类分析工具：Filter by/Exclude——Yield、Steps 、Reagent 、Catalyst 、 Solvent 、 Commercial Availability 、 Non-participating Functional Groups 、 Reaction Note 、Experimental Protocols 、Search Within Results 、Source Reference
- 反应结果分组：Group by Scheme/Document
- 反应详情的查看： Experimental Protocols——Synthetic Methods、Experimental Procedures, CAS PatentPak

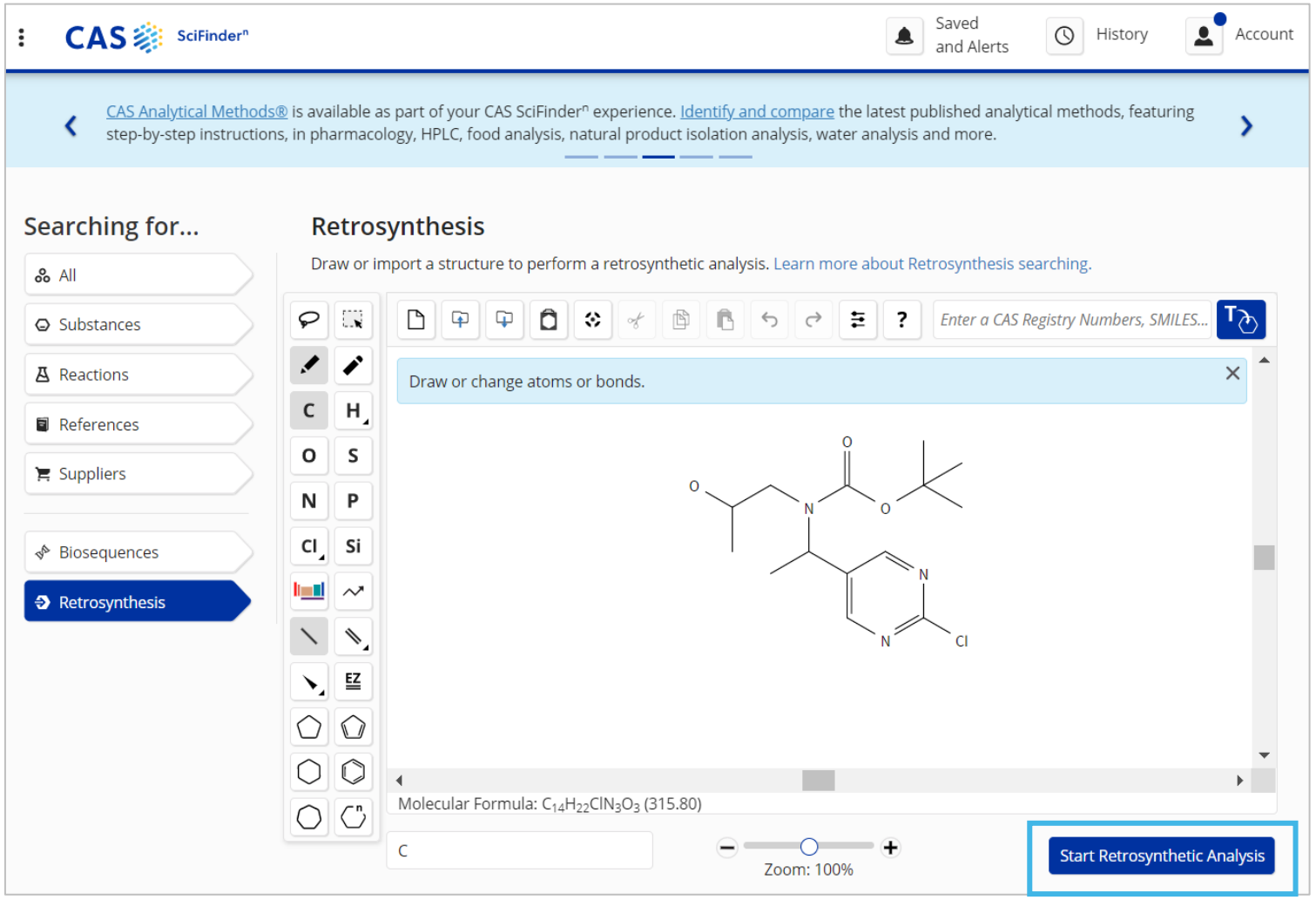
例2：直接通过物质标识符检索反应





Substance Role：浏览物质在反应中的角色

例3：通过Retrosynthesis工具设计逆合成反应路线，获得更多启发



Retrosynthesis Tool：可用于未知化合物或已知化合物和的逆合成路线设计

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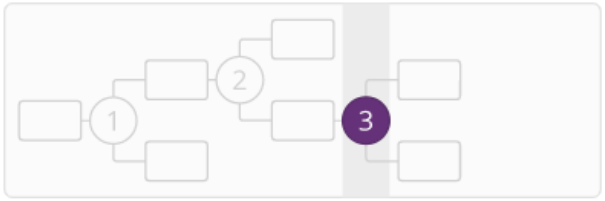
预设参数

Retrosynthesis Plan Options

Powered by ChemPlanner®

Select Synthetic Depth Learn more.

- 1
- 2
- 3
- 4



Set Rules Supporting Predicted Reactions Learn more.

- Common
- Uncommon *(includes Common Rules)*
- Rare *(includes Common and Uncommon Rules)*

Set Starting Materials Cost Limit Learn more.

10 USD/mol

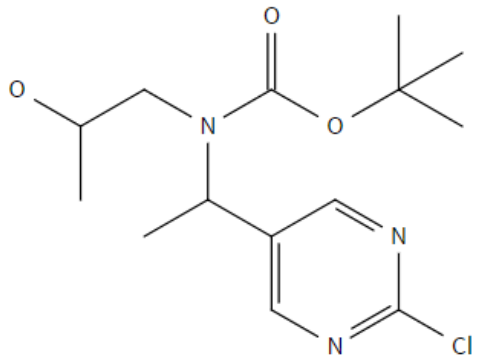
USD/mol
USD/g

Email me when my plan is complete

Create Retrosynthesis Plan

Break and Protect Bonds Learn more.

Break Bond | Protect Bond | Clear All Bond Selections



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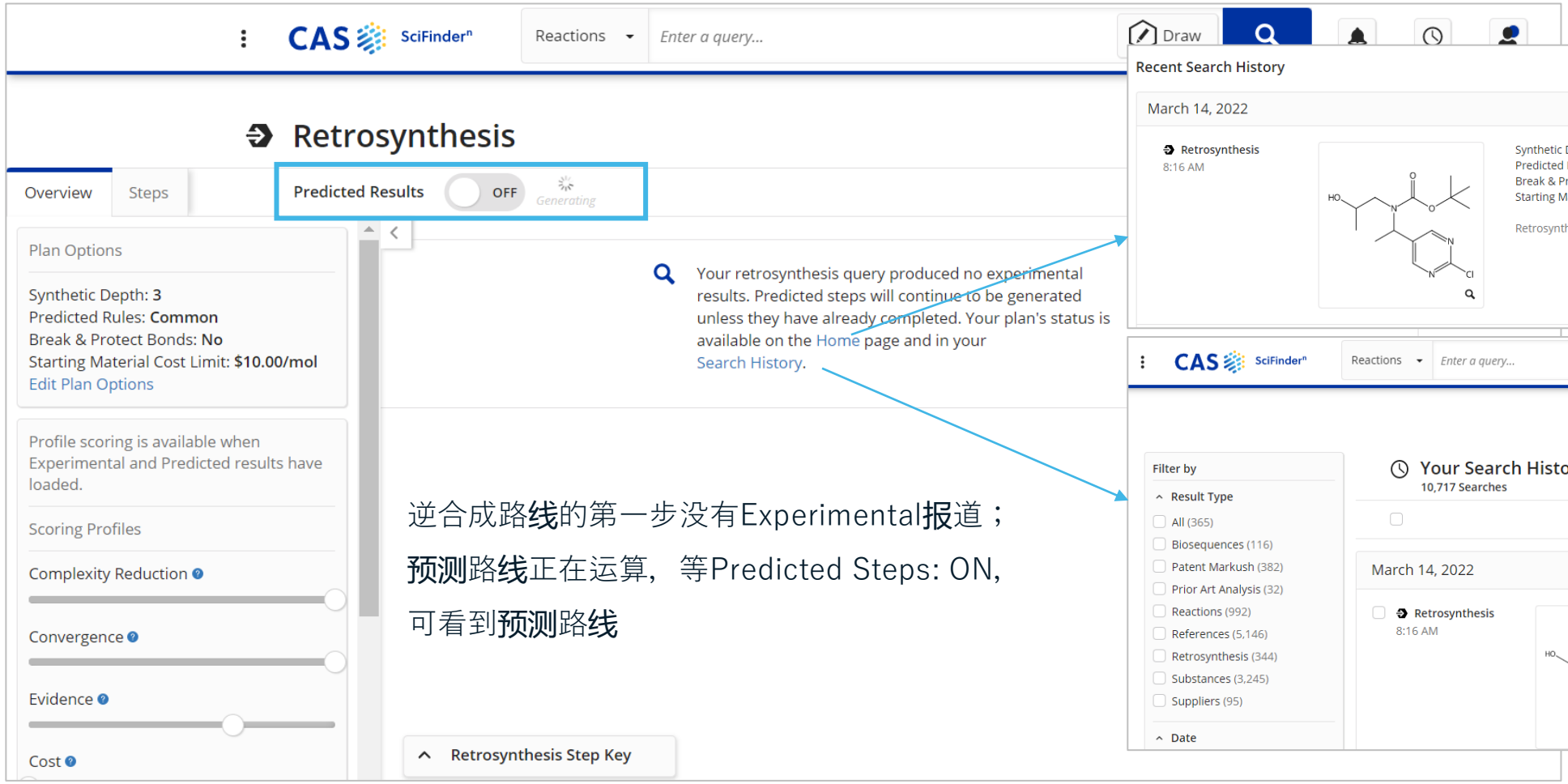
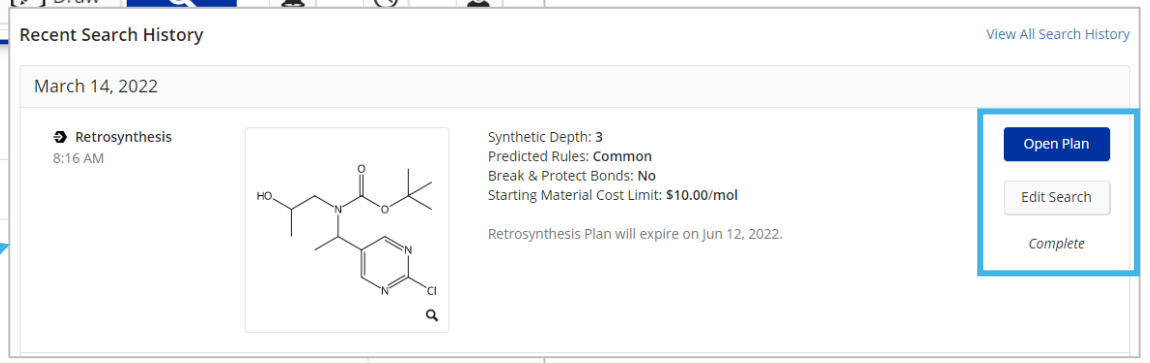
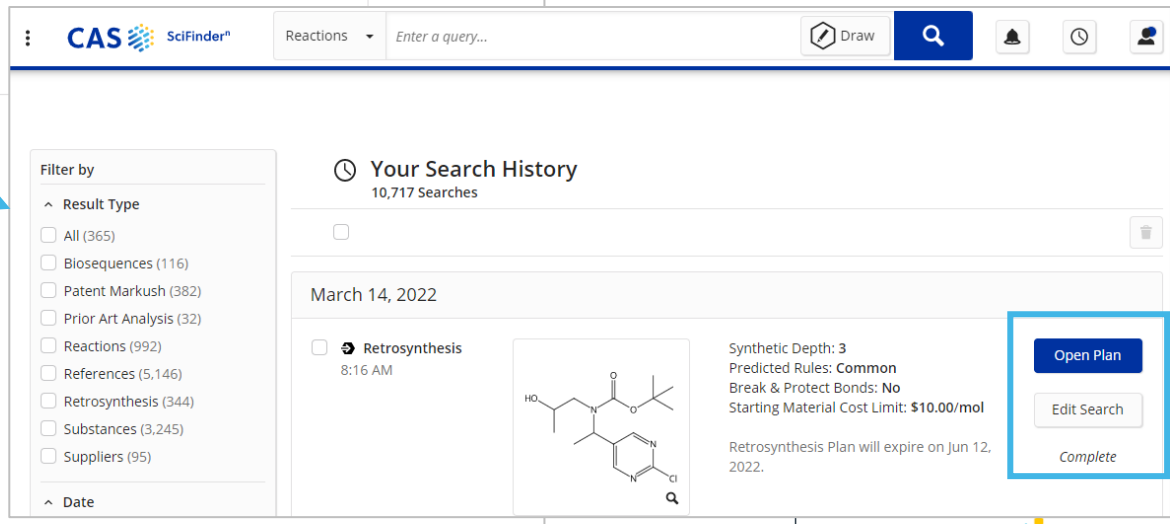
结果查看







逆合成路线的第一步没有Experimental报道；

预测路线正在运算，等Predicted Steps: ON,

可看到预测路线

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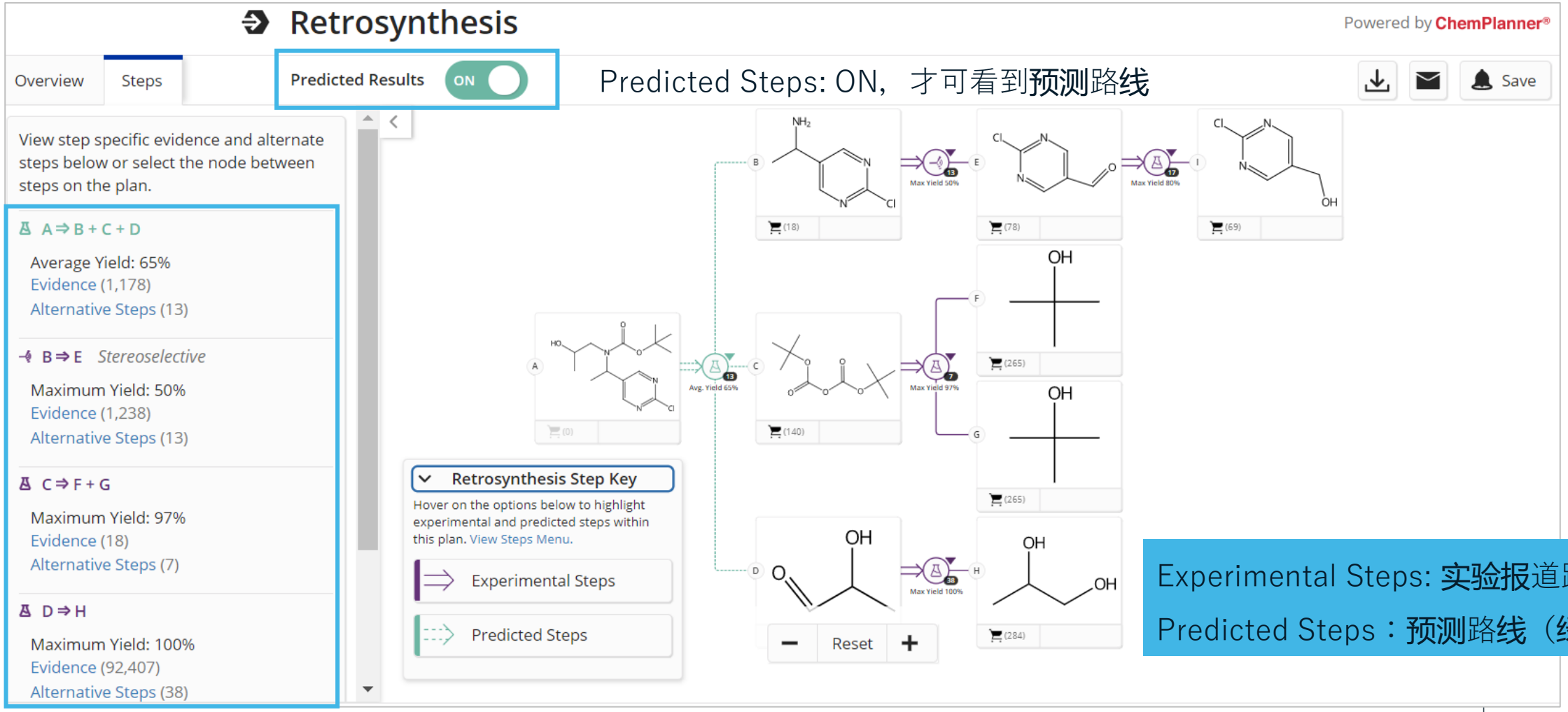
获得逆合成反应路线结果



Experimental Steps: 实验报道路线（紫色）

Predicted Steps：预测路线（绿色）

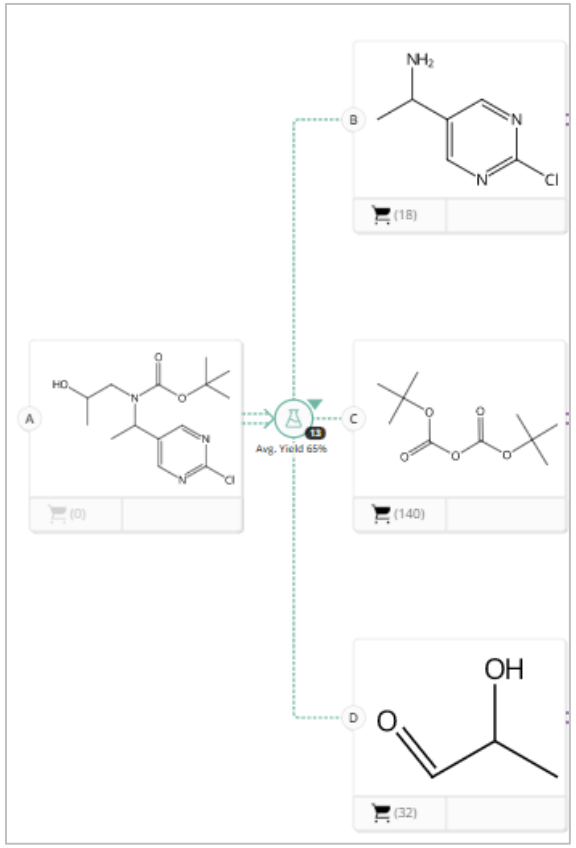
Predicted steps

A ⇒ B + C + D

Average Yield: 65%

Evidence (1,178)

Alternative Steps (13)



Filter Behavior

Filter by | Exclude

Yield

- 90-100% (97)
- 80-89% (117)
- 70-79% (147)
- 50-69% (201)
- 30-49% (106)

View All

Number of Steps

- 1 (1,178)

Non-Participating Functional Groups

Experimental Protocols

- Synthetic Methods (262)
- Experimental Procedure (320)

Reaction Type

Stereochemistry

Reagent

Reactions (1,178)

Group: By Document | View: Expanded

References | A ⟹ B+C+D的Evidence | Save

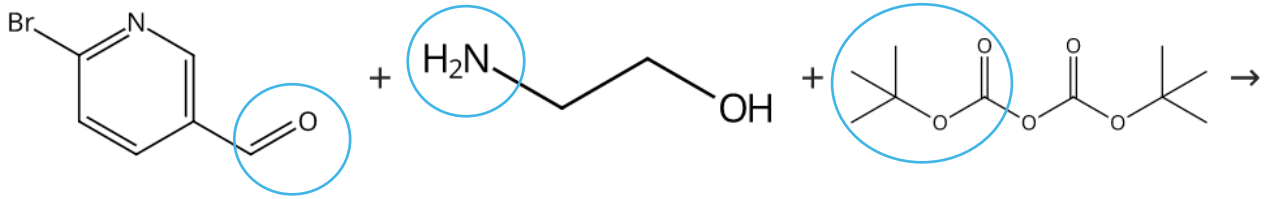
1

Preparation of substituted thiophene-2-hydroxamic acids as histone deacetylase inhibitors useful against disorders involving increased cell proliferation

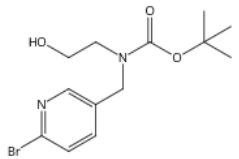
By: Dyke, Hazel Joan; Price, Stephen; Van den Heuvel, Marco; Sutton, Jonathan Mark; Mackenzie, Robert Edward; et al

World Intellectual Property Organization, WO2005014588 A1 2005-02-17 | Language: English, Database: CAplus

PatentPak | Full Text | View 5 Related Reactions



Suppliers (110) | Suppliers (119) | Suppliers (140)



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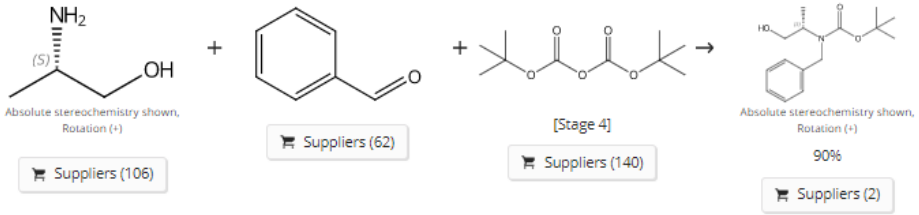
参考实验详情

Reaction Detail (Document 1, Reaction 1 of 5)

Prev Next

Save



Steps: 1
Yield: 90%

Suppliers (106) | Suppliers (62) | Suppliers (140) | 90% | Suppliers (2)

Step 1

Alternative Steps (0)

Stage	Reagents	Catalysts	Solvents	Conditions
1	-	-	Methanol	2 h, rt; rt → 0 °C
2	Sodium borohydride	-	-	0 °C; 1 h, 0 °C → rt; rt → 0 °C
3	Ammonium chloride	-	Water	-
4	Triethylamine	-	Tetrahydrofuran	16 h, rt
5	Hydrochloric acid	-	Water	-

CAS Reaction Number: 31-313-CAS-16424766

JOURNAL

Substrate-Controlled Diastereoselectivity Reversal in NHC-Catalyzed Cross-Benzoin Reactions Using N-Boc-N-Bn-Protected α-Amino Aldehydes

By: Haghshenas, Pouyan; et al
View All

Journal of Organic Chemistry (2016), 81(24), 12075-12083

Full Text

Company/Organization

Department of Chemistry
University of Saskatchewan
Saskatoon, Saskatchewan S7N 5C9
Canada

Experimental Protocols

Synthetic Methods

Products	1,1-Dimethylethyl *N*-[(1*S*)-2-hydroxy-1-methylethyl]-*N*-(phenylmethyl)carbamate, Yield: 90%
Reactants	Benzaldehyde L-Alaninol Di-*tert*-butyl dicarbonate
Reagents	Sodium borohydride Ammonium chloride Triethylamine Hydrochloric acid
Solvents	Methanol Water Tetrahydrofuran

Procedure

1. Add freshly distilled benzaldehyde (1 equivalent) to a solution of the α-amino alcohol (1 equivalent) in dry MeOH (0.25M) at room temperature.
2. Stir the resulting solution for 2 hours.
3. Cool the resulting solution to 0 °C using an ice bath.
4. Add $NaBH_4$ (5 equivalents) slowly to the mixture in three portions.
5. Warm the resulting suspension to room temperature.
6. Stir the resulting suspension for 1 hour.
7. Cool the suspension once again to 0 °C.
8. Quench the suspension with the addition of saturated NH_4Cl (aqueous).
9. Extract the reaction mixture with EtOAc (×3).
10. Dry the combined organic layers over $MgSO_4$.
11. Reduce the crude mixture in vacuo.
12. Add triethylamine (1 equivalent) to a solution of N-Bn-amino alcohol (1 equivalent) in THF (0.3M) at room temperature.
13. Add di-tert-butyl dicarbonate (Boc_2O) (1.1 equivalents) to the solution.
14. Stir the solution at ambient temperature for 16 hours.
15. Quench the reaction mixture by addition of HCl (1M).
16. Extract reaction mixture with Et_2O (×3).
17. Wash the combined organic layers with brine.
18. Dry the combined organic over $MgSO_4$.
19. Purify the crude product by column chromatography.

Transformation

Reductive Alkylation of Ammonia or Amines
Acylation of Nitrogen Nucleophiles by Anhydrides or Dicarbonates

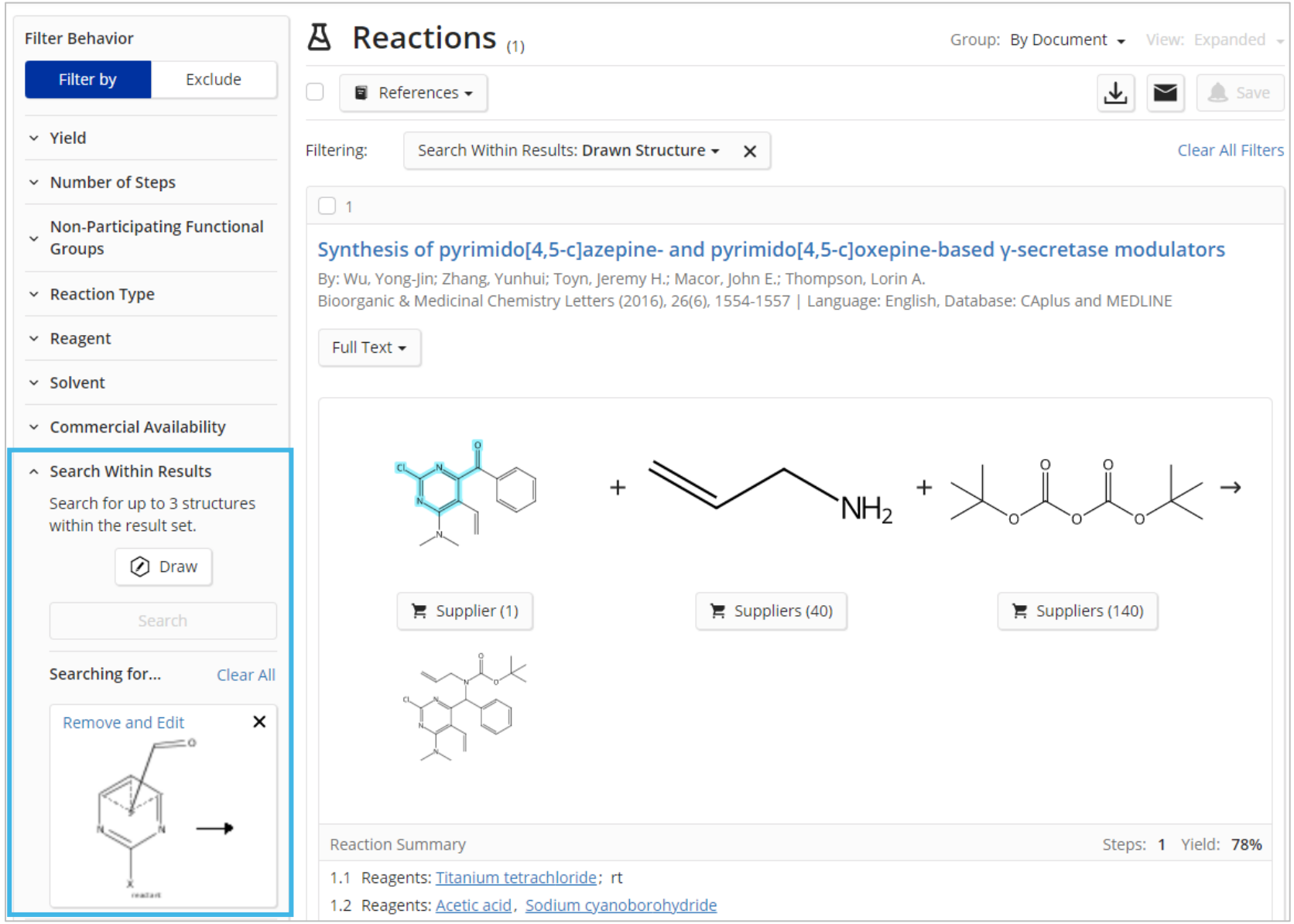
Characterization Data

1,1-Dimethylethyl *N*-[(1*S*)-2-hydroxy-1-methylethyl]-*N*-(phenylmethyl)carbamate

Proton NMR Spectrum	(500 MHz, $CDCl_3$) δ 7.35-7.26 (m, 4H), 7.26-7.22 (m, 1H), 4.39 (br s, 2H), 4.05-3.90 (m, 1H), 3.73-2.85 (m, 1H), 2.93 (br s, 1H), 1.43 (s, 9H), 1.14 (br d, *J*= 4.9 Hz, 3H).
R_f	0.21 (25% EtOAc in hexane).
State	clear colorless oil.

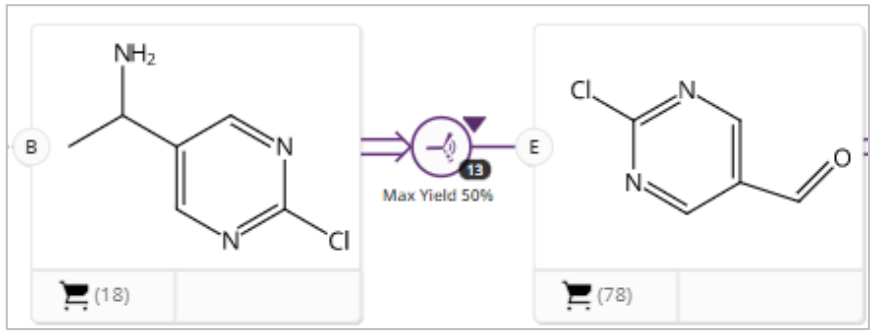
CAS Method Number 3-313-CAS-16424766

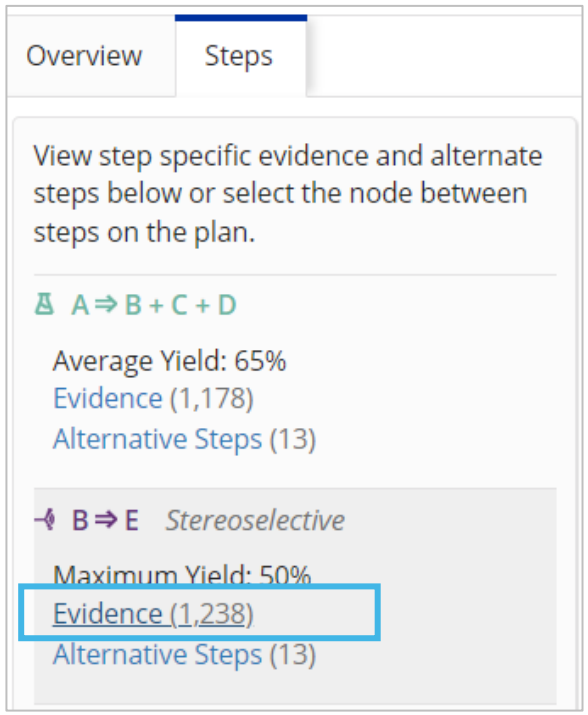
精炼反应物结构

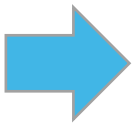


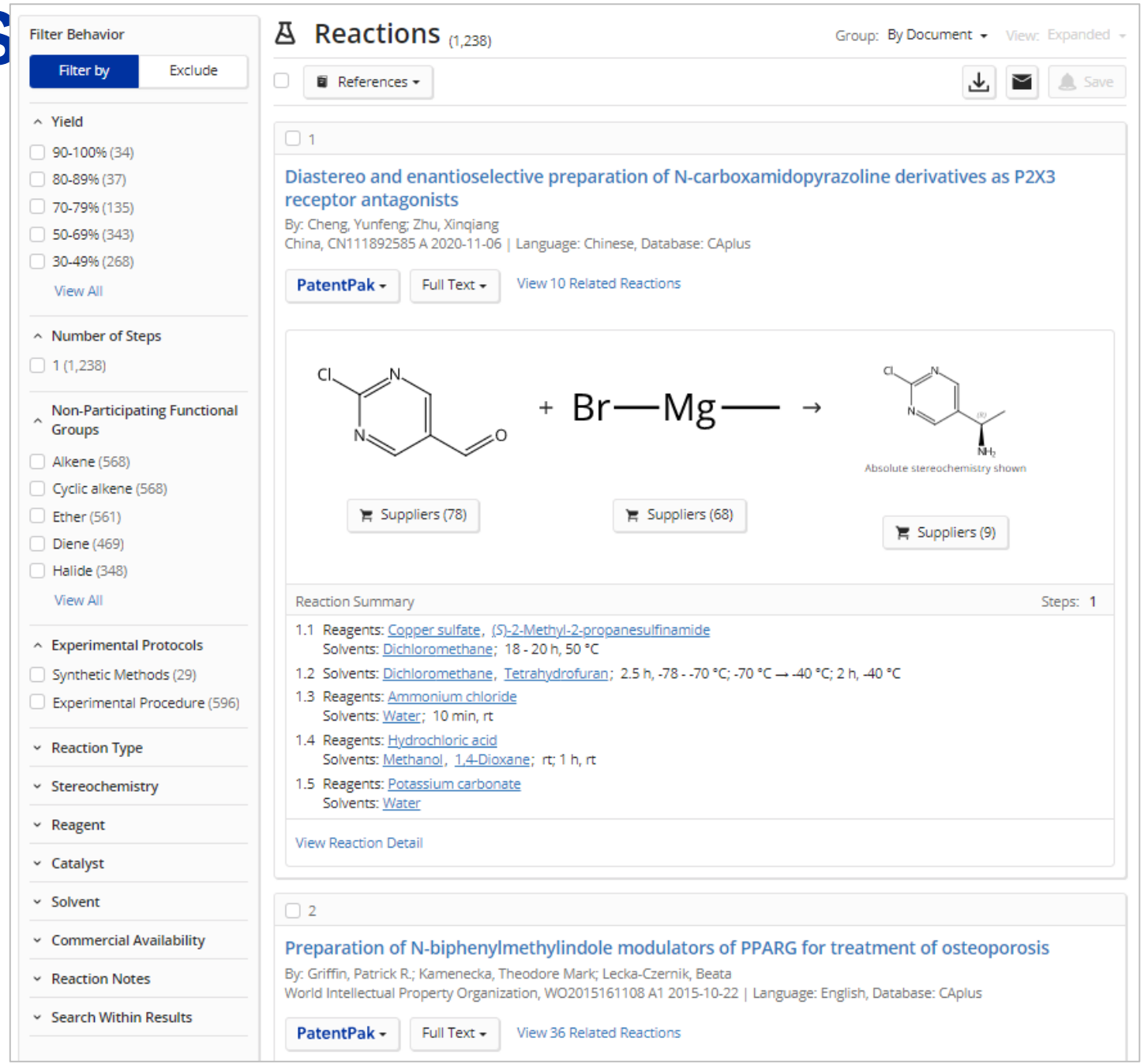
通过Search Within Results，二次限定参考文献（Evidence）中最相关的原料结构

Experimental Steps

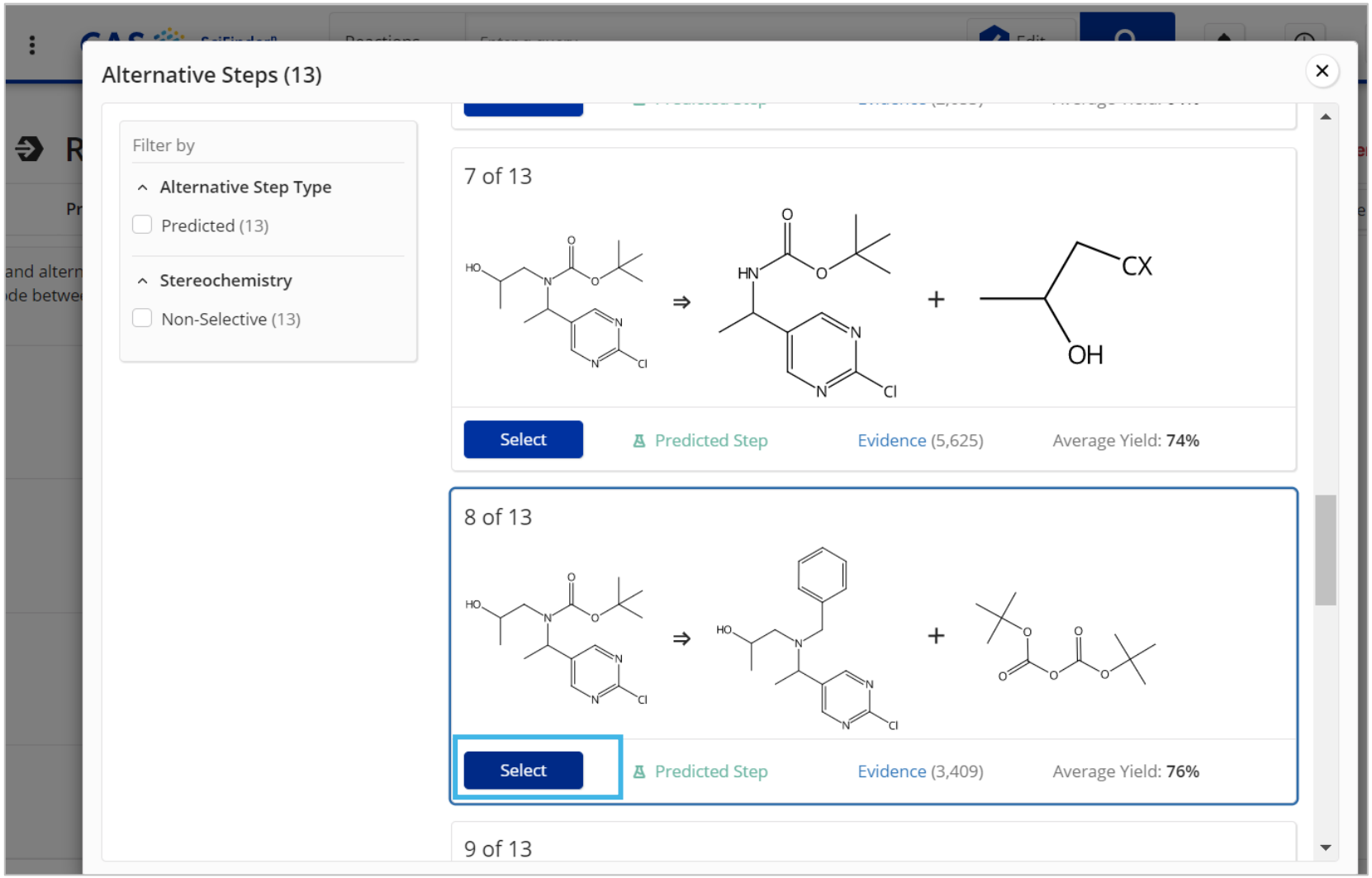




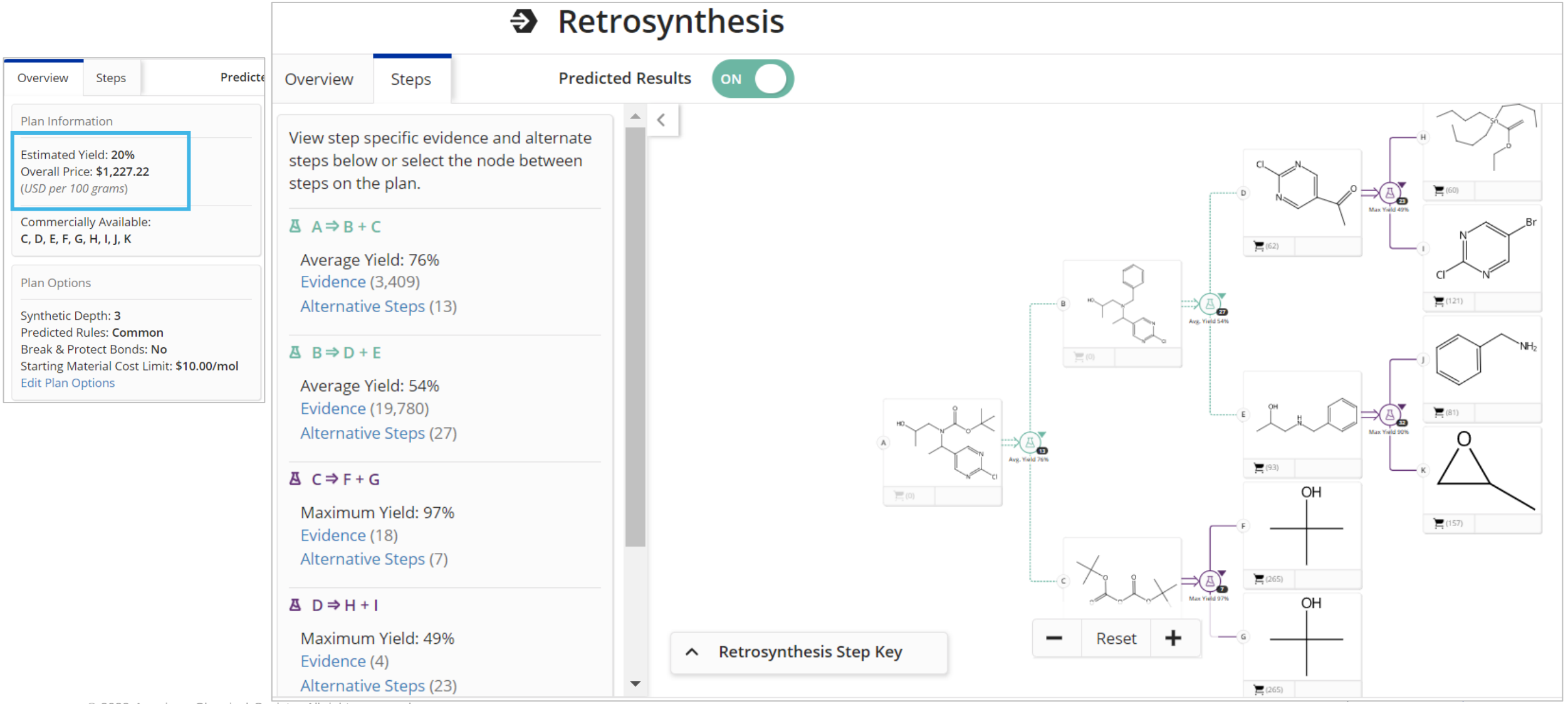




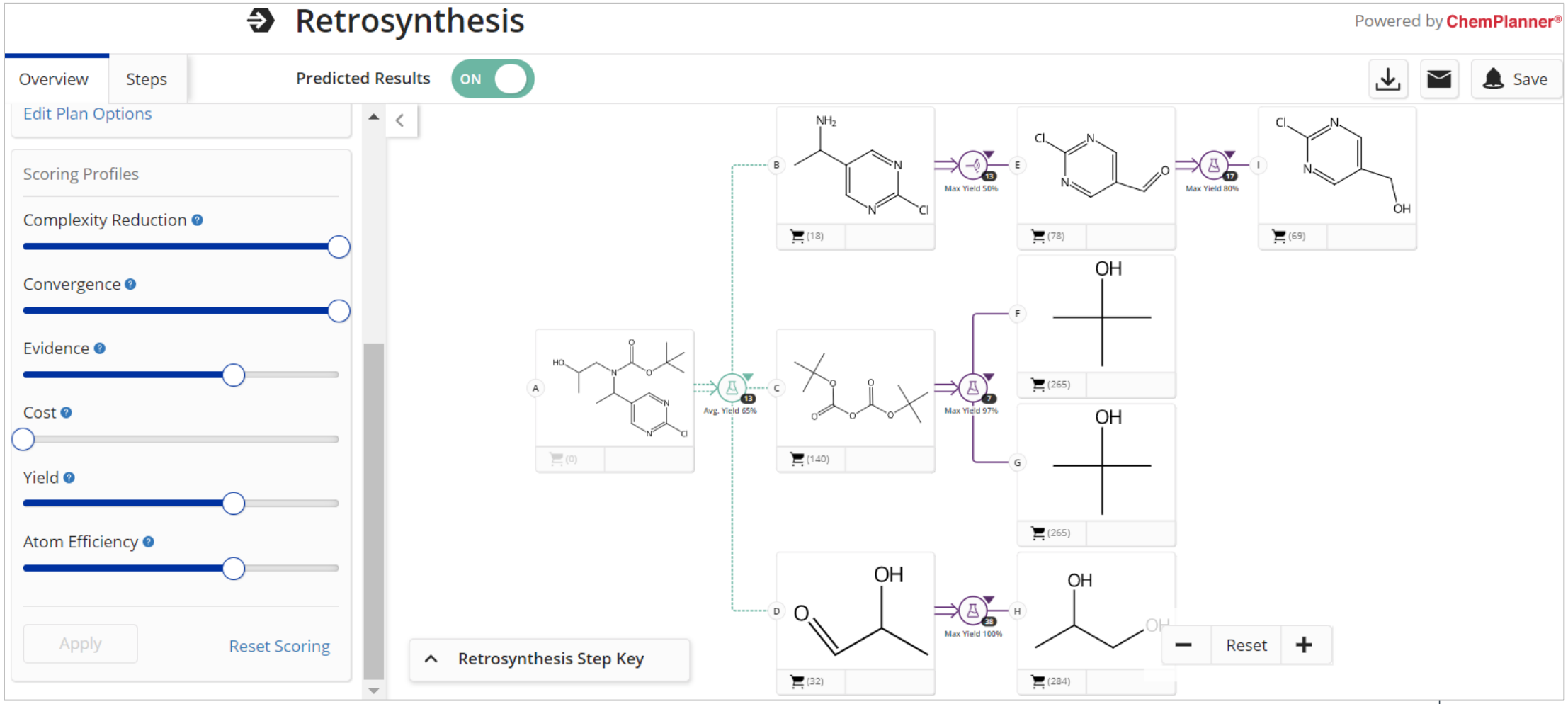
浏览Alternative Steps，获取其他合成方法



获得新的逆合成路线



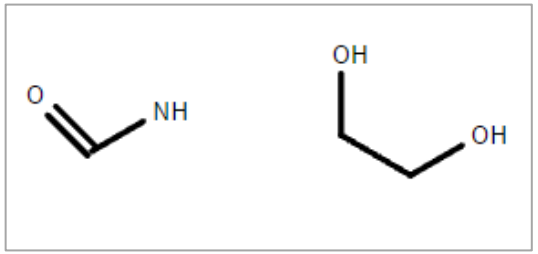
通过Scoring Profiles重新调整逆合成路线



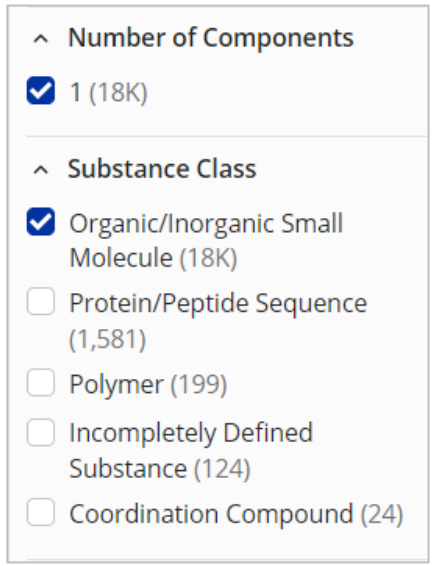
小结：

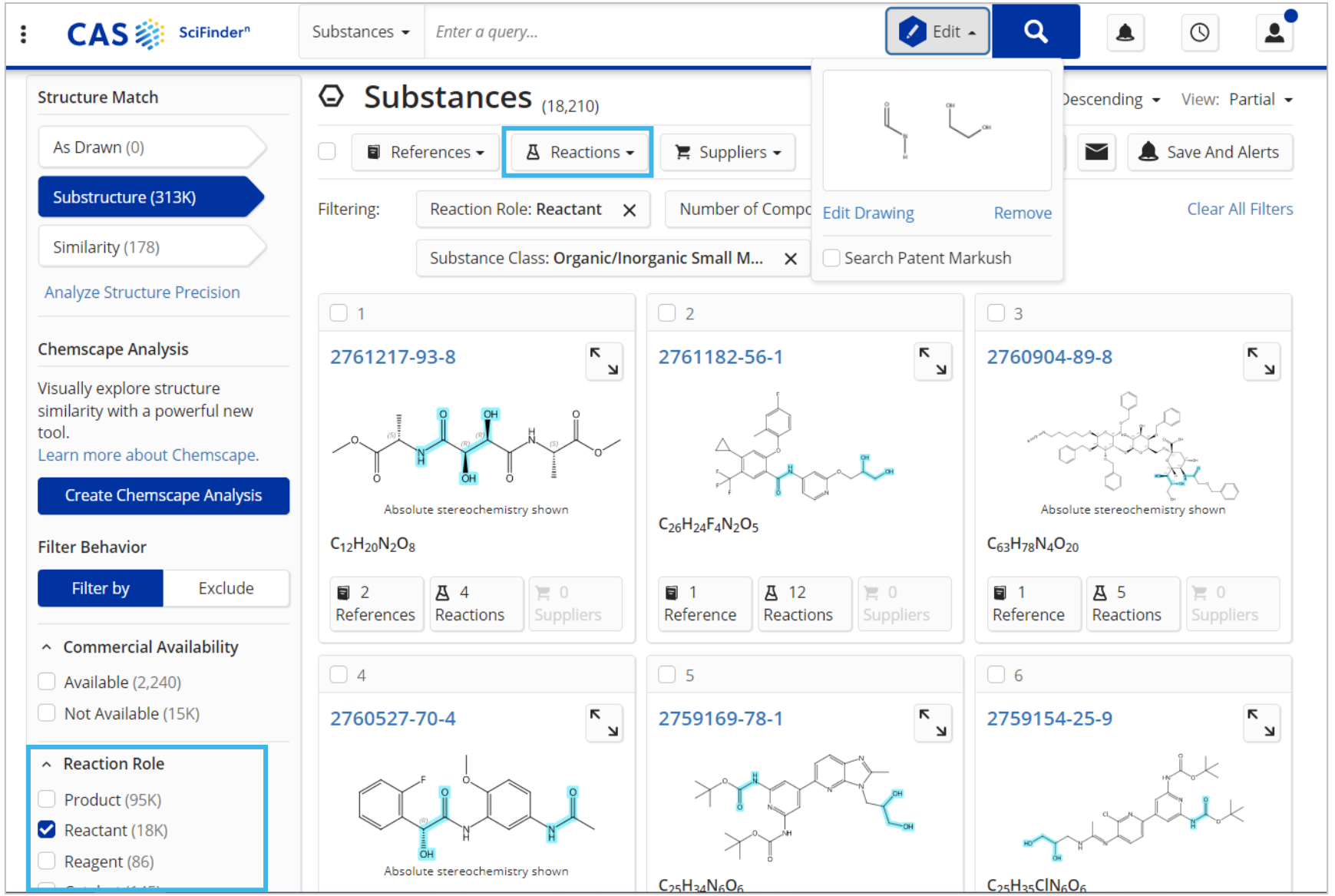
- 逆合成反应路线支持的物质：有具体且单一结构的未知化合物或已知化合物
- 预设参数：Synthetic Depth、Set Rules、Starting Material Cost、Break/Protect Bond
- 结果查看：执行逆合成路线设计的当前界面、主界面上的Recent Search History处、检索历史界面
- 预测路线/实验路线：Predicted Steps（绿色）, Experimental Steps（紫色）
- 查看相关反应和替代反应：Evidence, Alternative Steps
- 精炼相关反应结果：利用Synthetic Methods和Search within Results从反应详情和反应物的结构来精炼Evidence中提供的支持反应
- 评分介绍Scoring Profile：Complexity Reduction, Convergence, Evidence, Cost, Yield, Atom Efficiency

例4: 通过片段结构信息获取反应

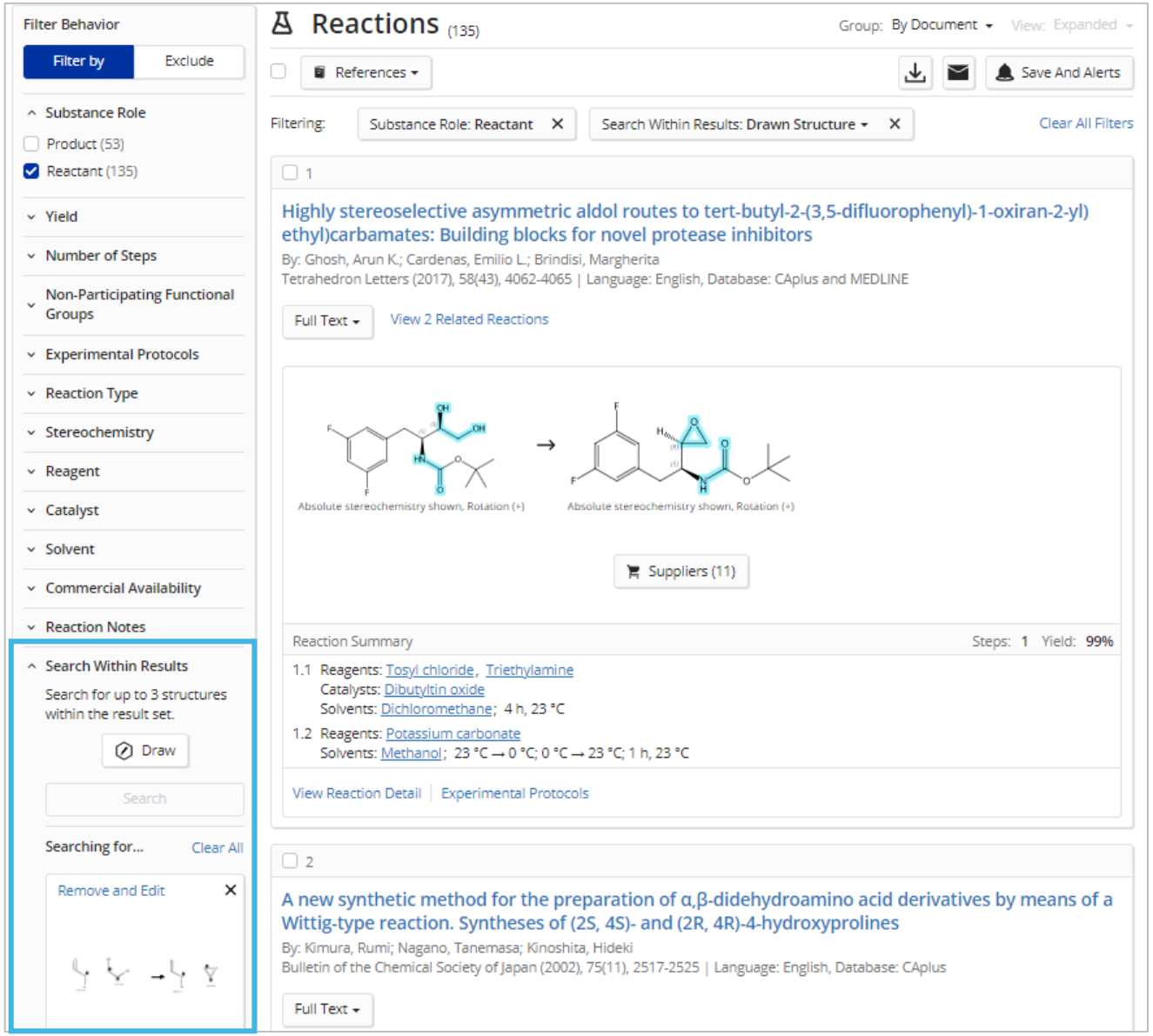


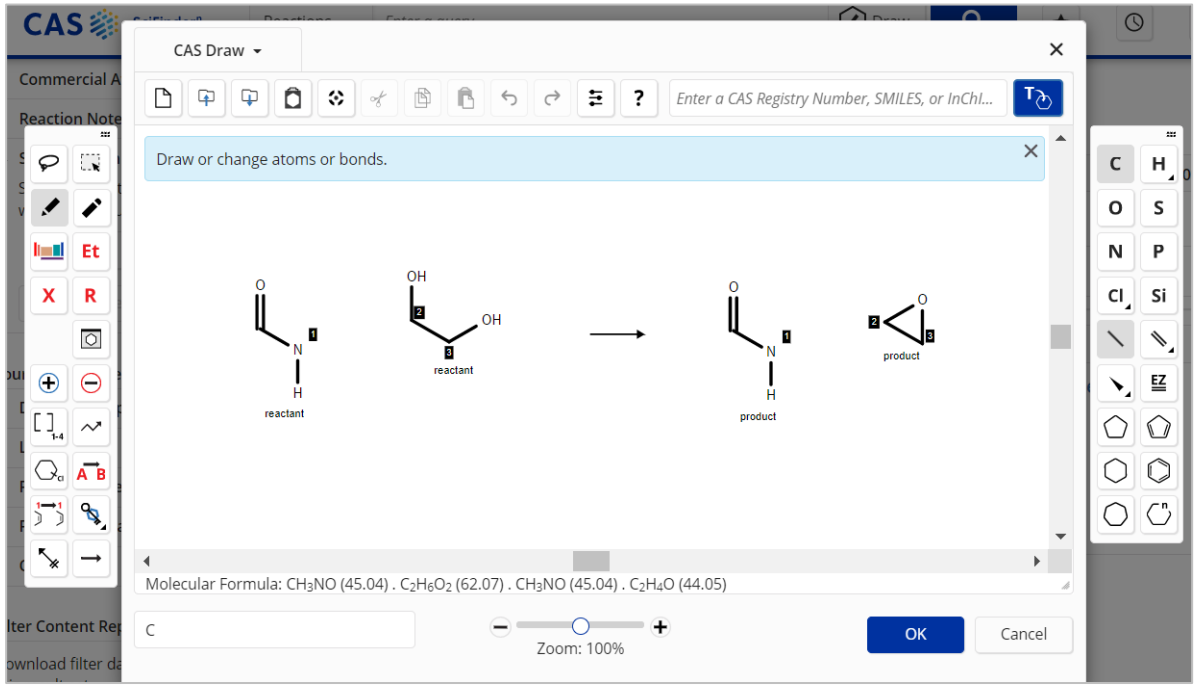
片段结构的反应检索：先从结构出发进行物质检索，再通过物质获取反应





Search Within Results：精炼产物结构





使用原子**标记**工具精准定位原料和**产**物中的同一原子

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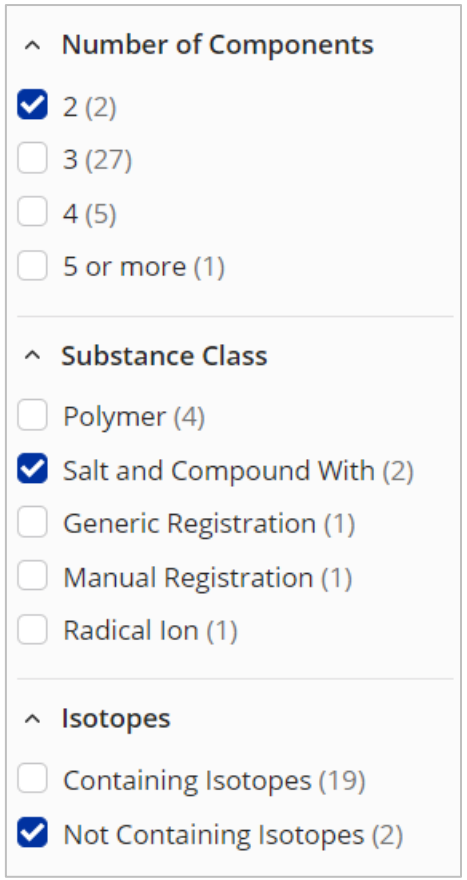
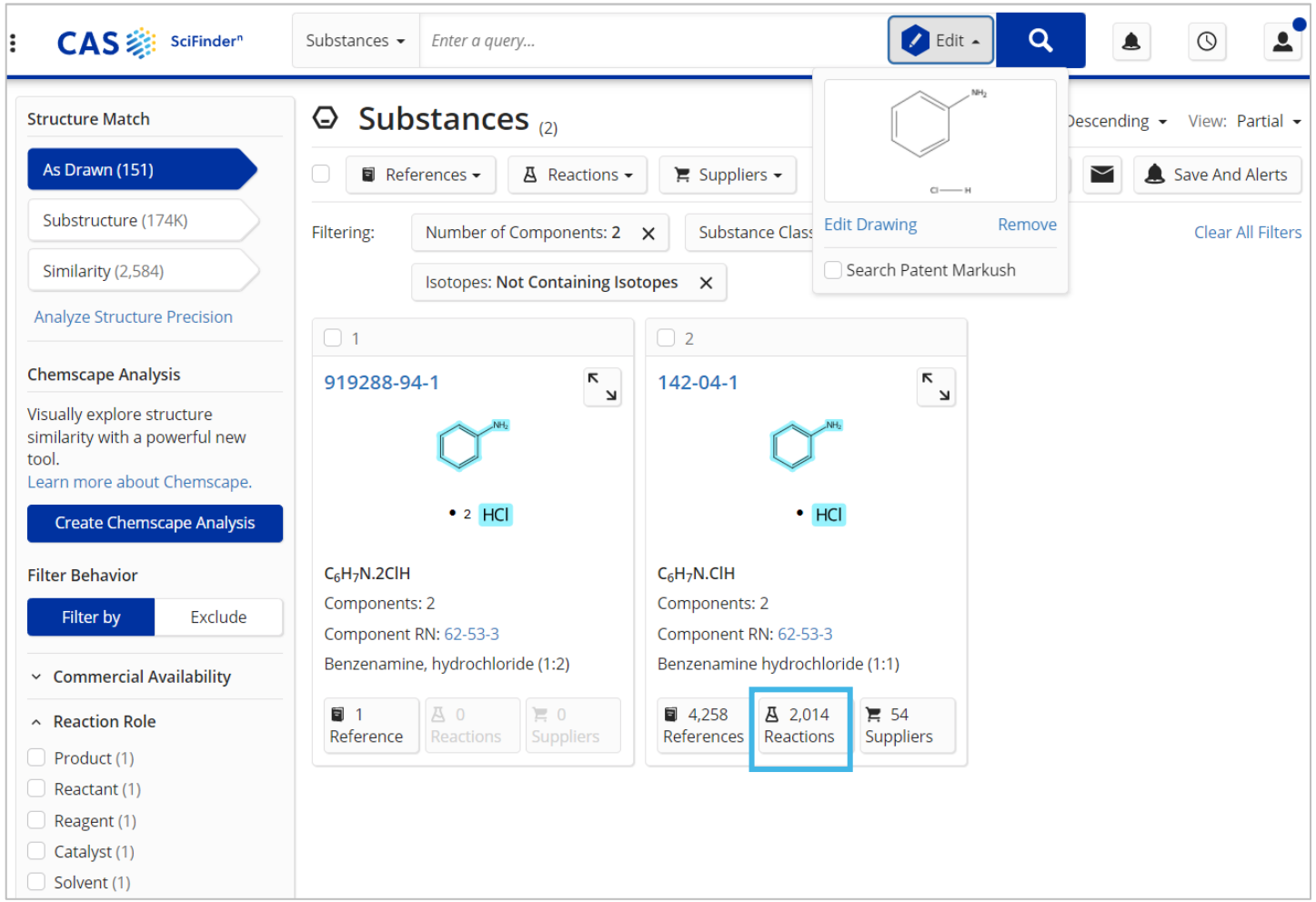
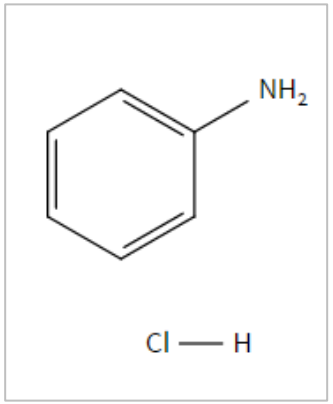
例5：通过多组分物质的结构信息获取反应

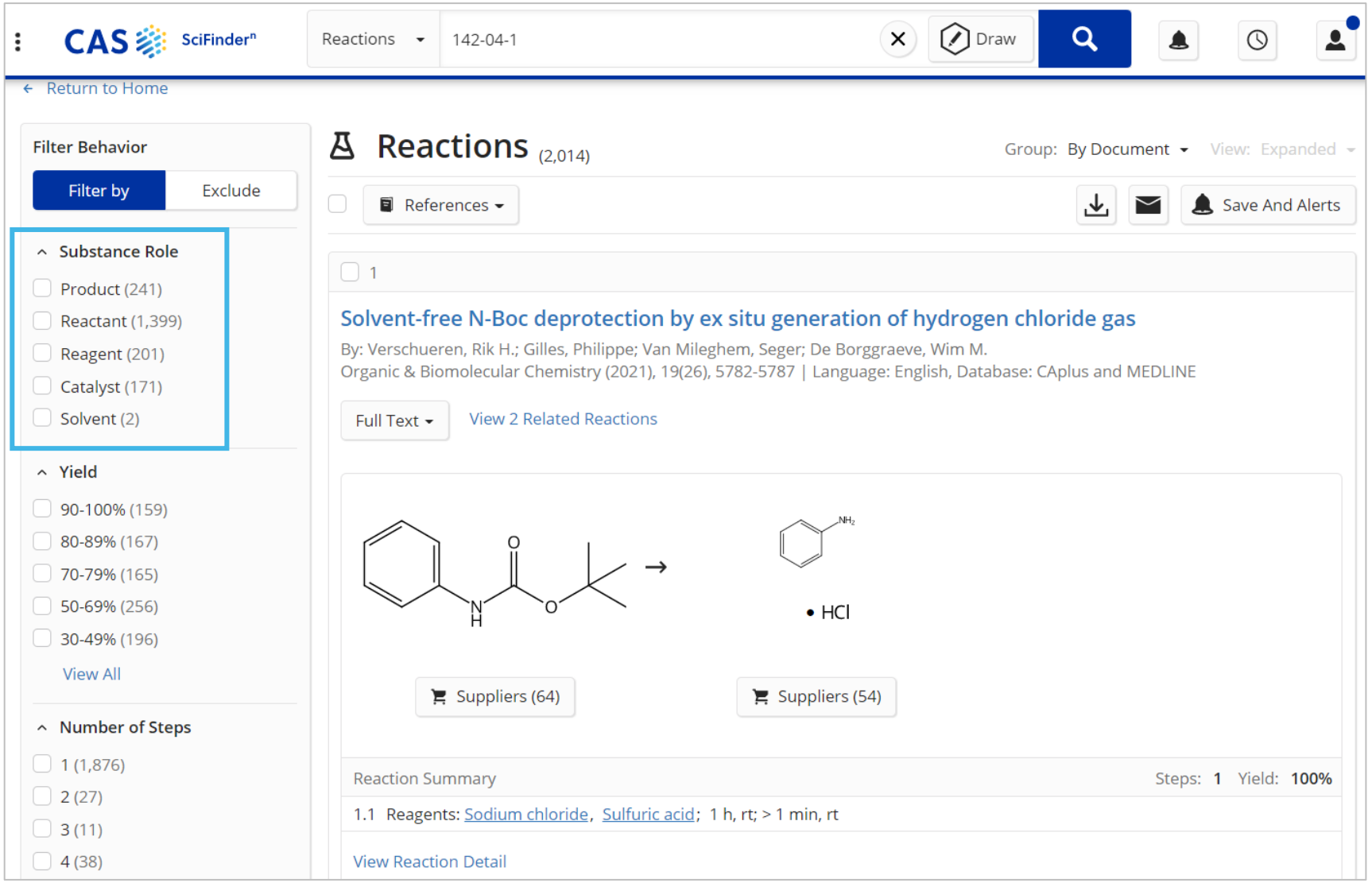






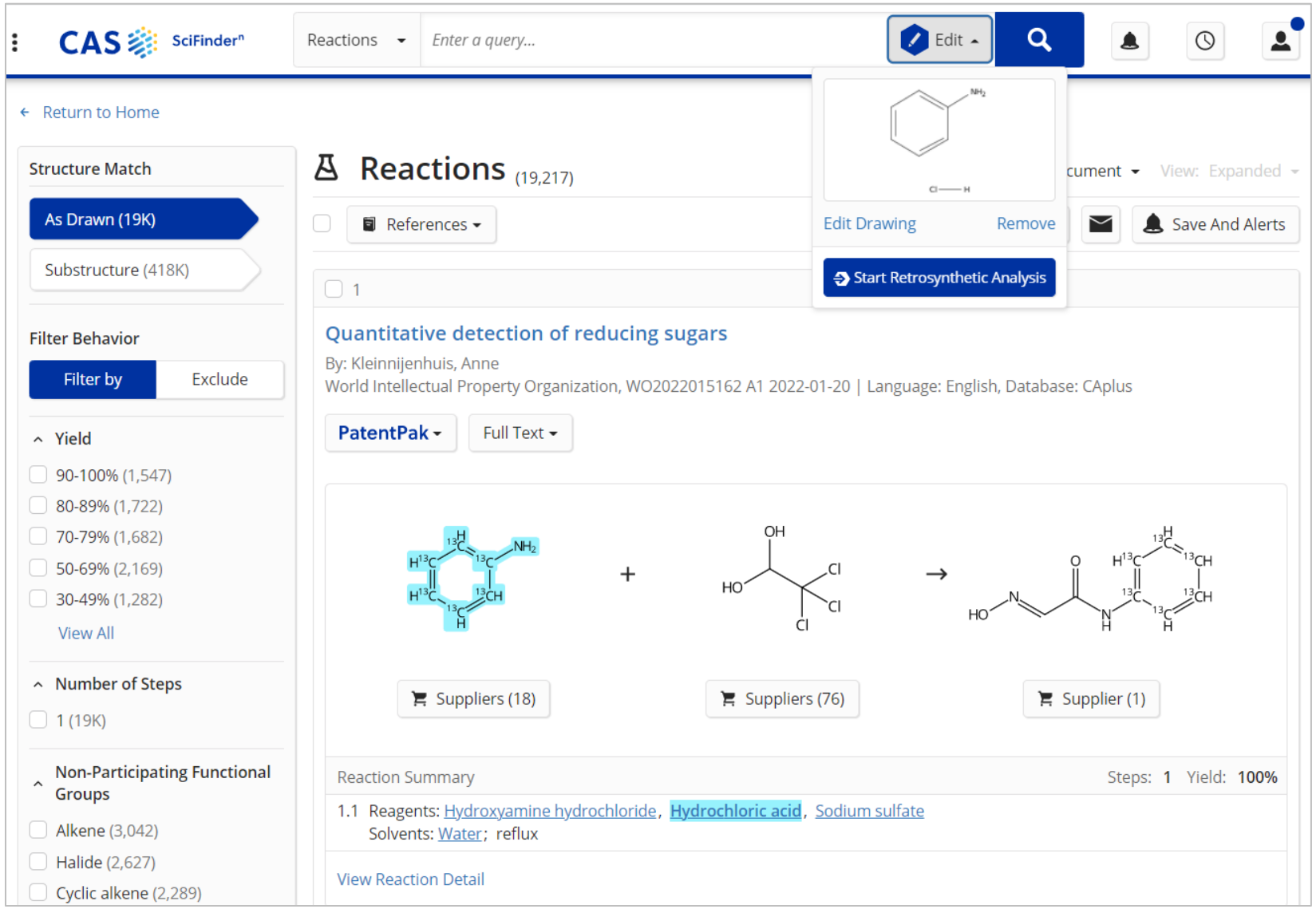
可提前精炼组分数、物质类型、排除同位素标记物等，再通过物质获取反应

获得多组分物质参与的各种角色的反应



通过Substance Role，浏览或筛选此物质参与的反应角色

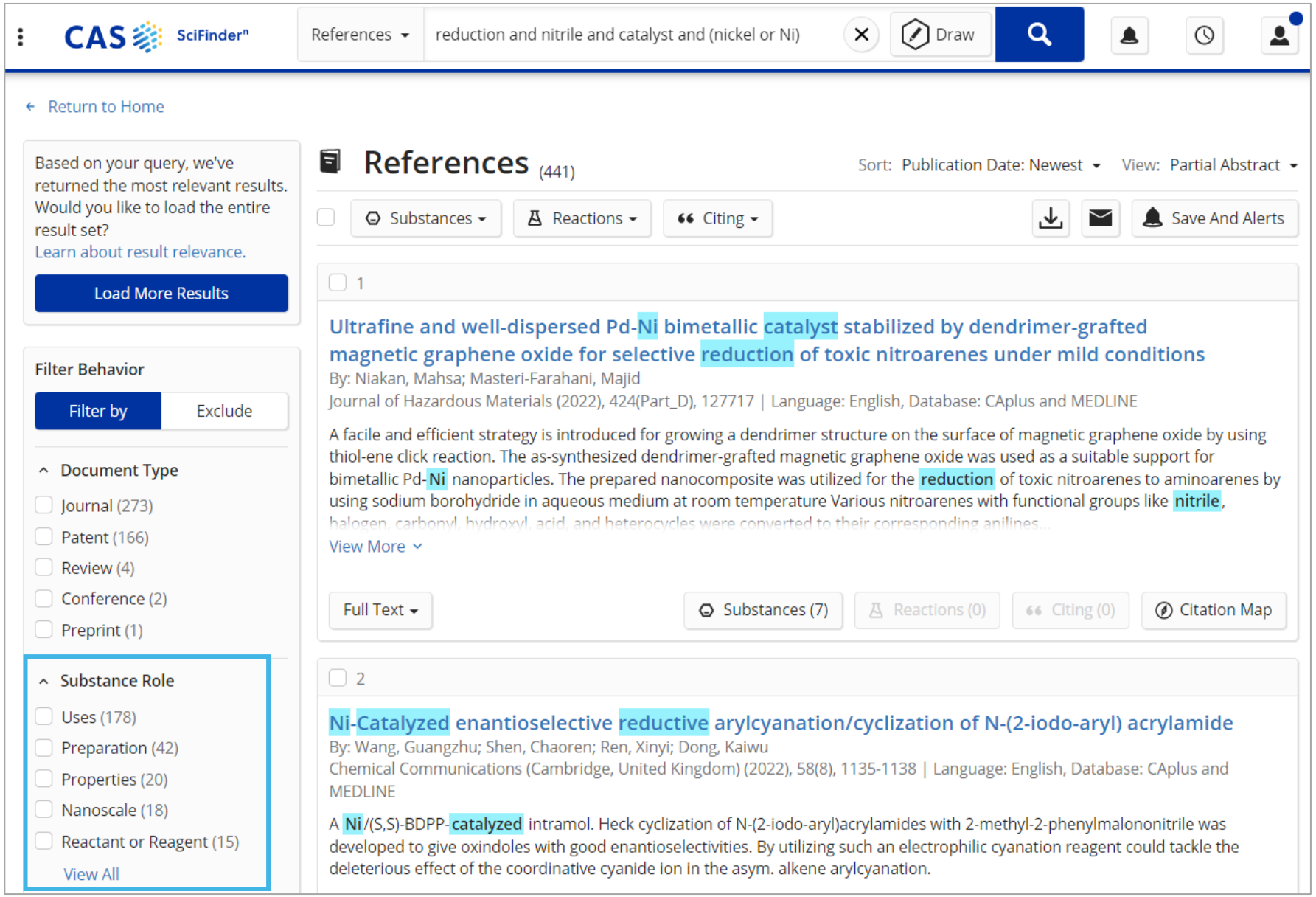
对比直接通过多组分物质的结构信息获取反应



各种As Drawn的结果都会出现，包括同位素标记物等

多组分物质中的多个组分会出现在不同的物质中

例6：通过文献获取反应



- 主题词：reduction and nitrile and catalyst and (nickel or Ni)
- Substance Role & Concept精炼
- 通过文献获取反应

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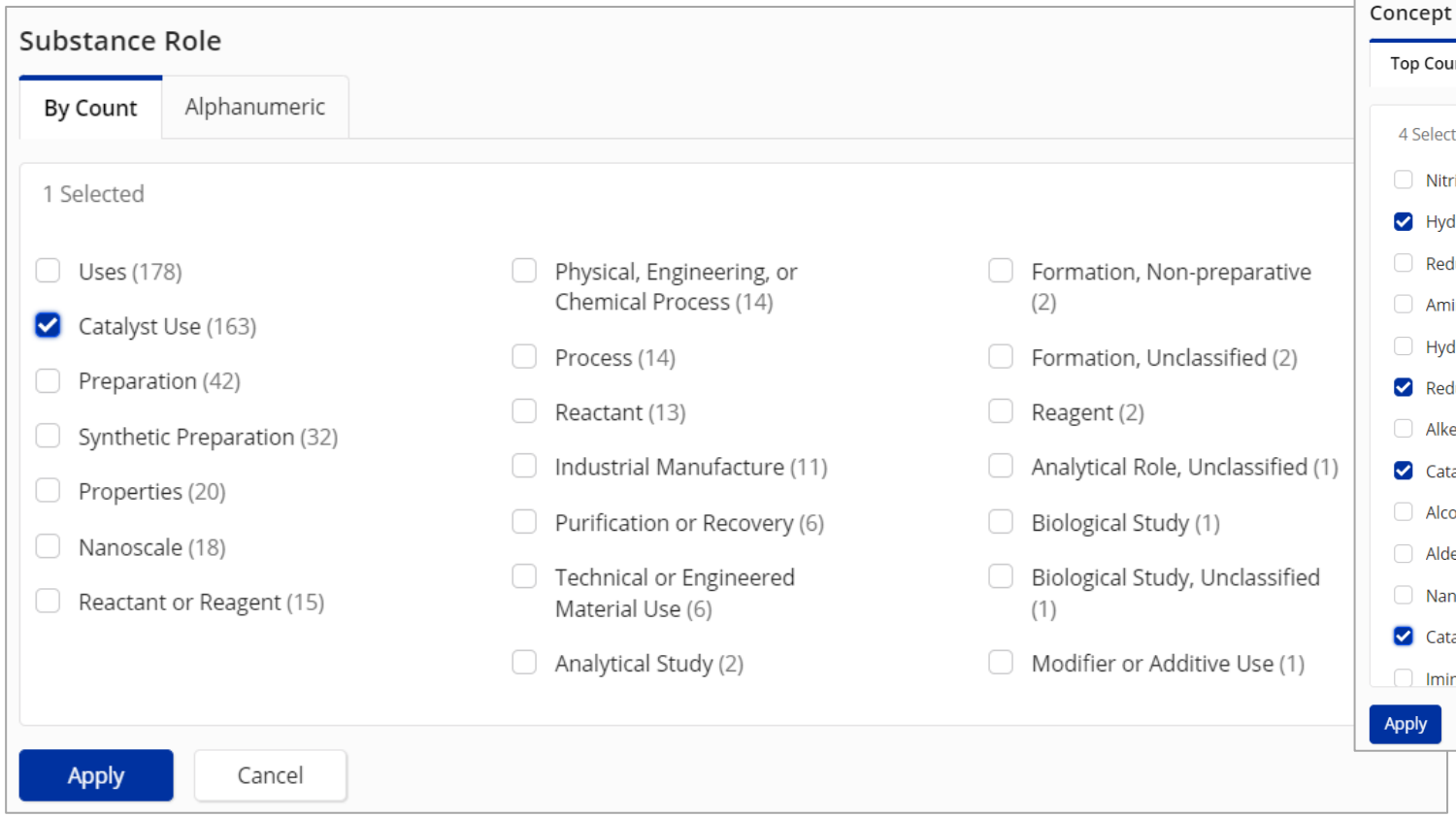
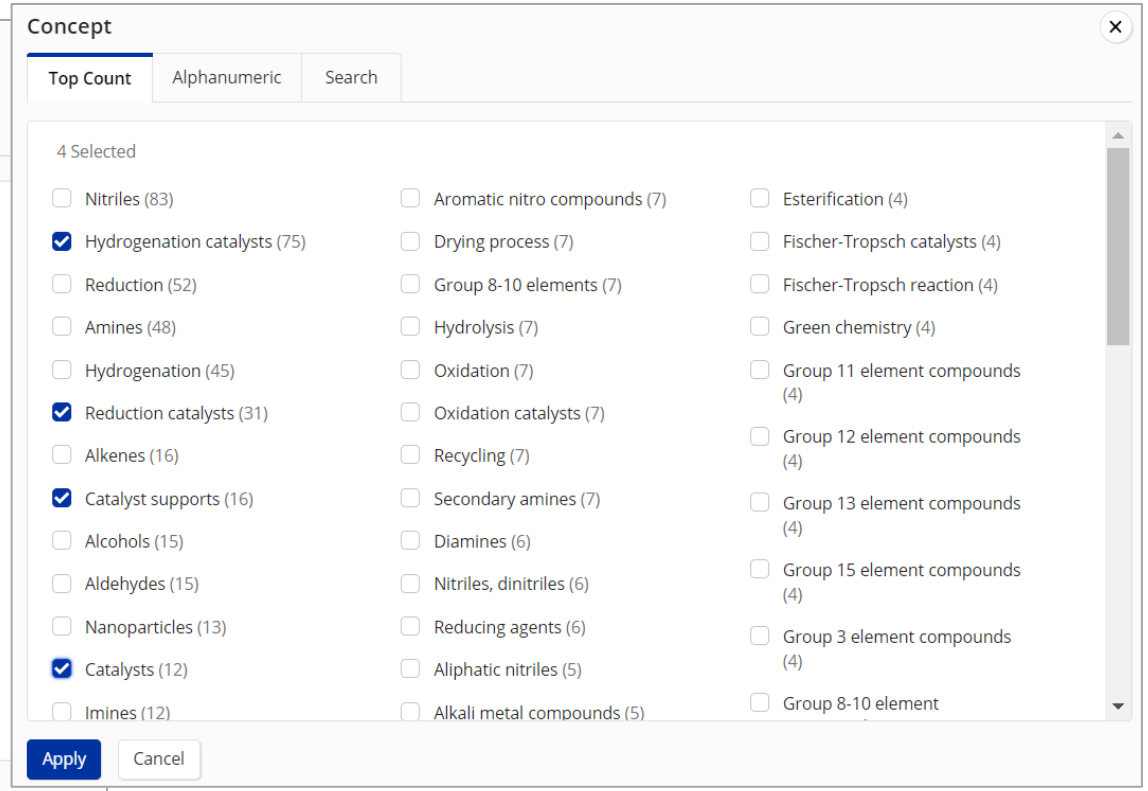
Substance Role：精炼检索主题中的物质在文献中最相关的研究角色；Concept：纵览并精炼文献核心研究点





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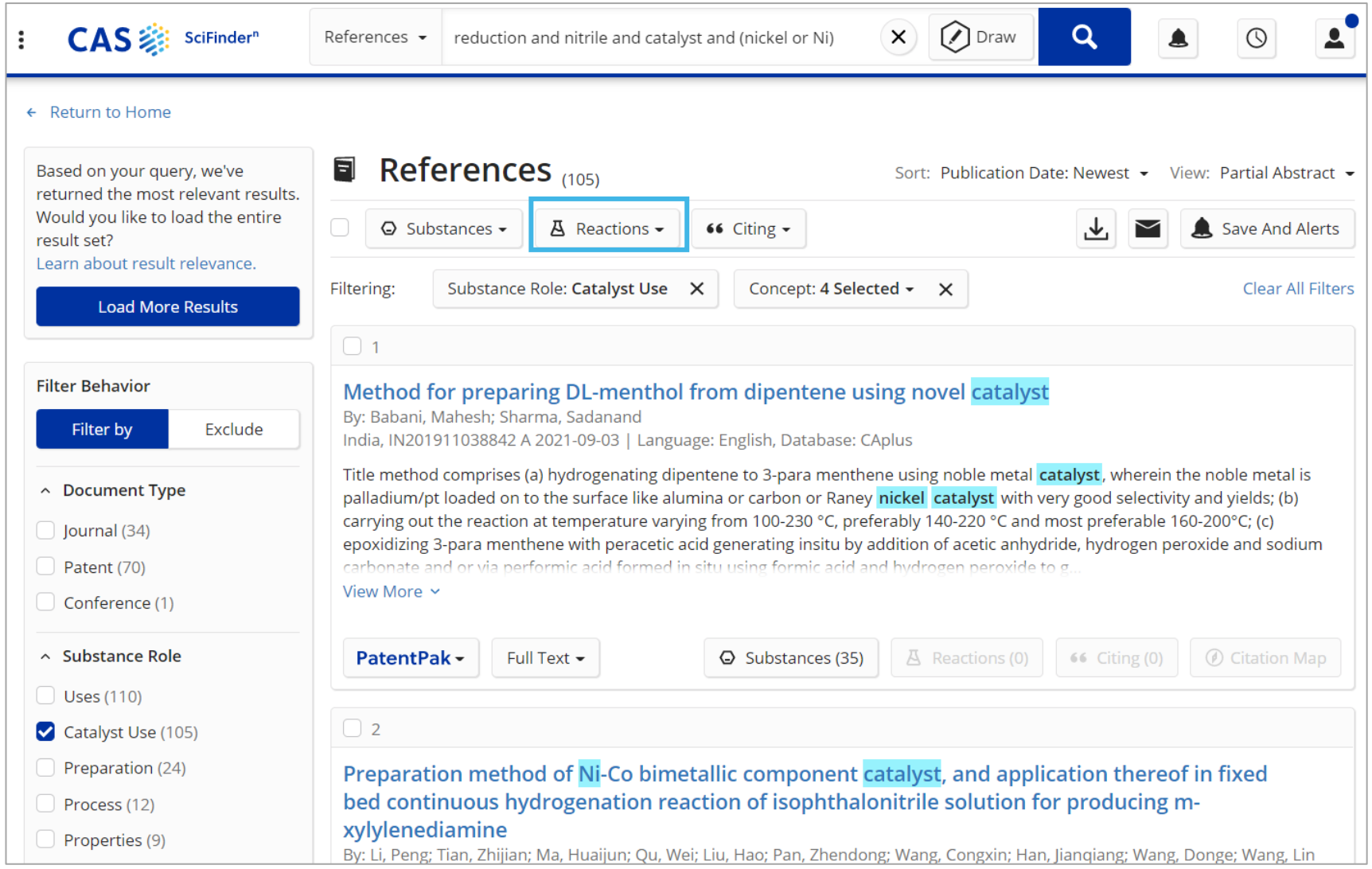
基于精炼后的文献获取反应信息



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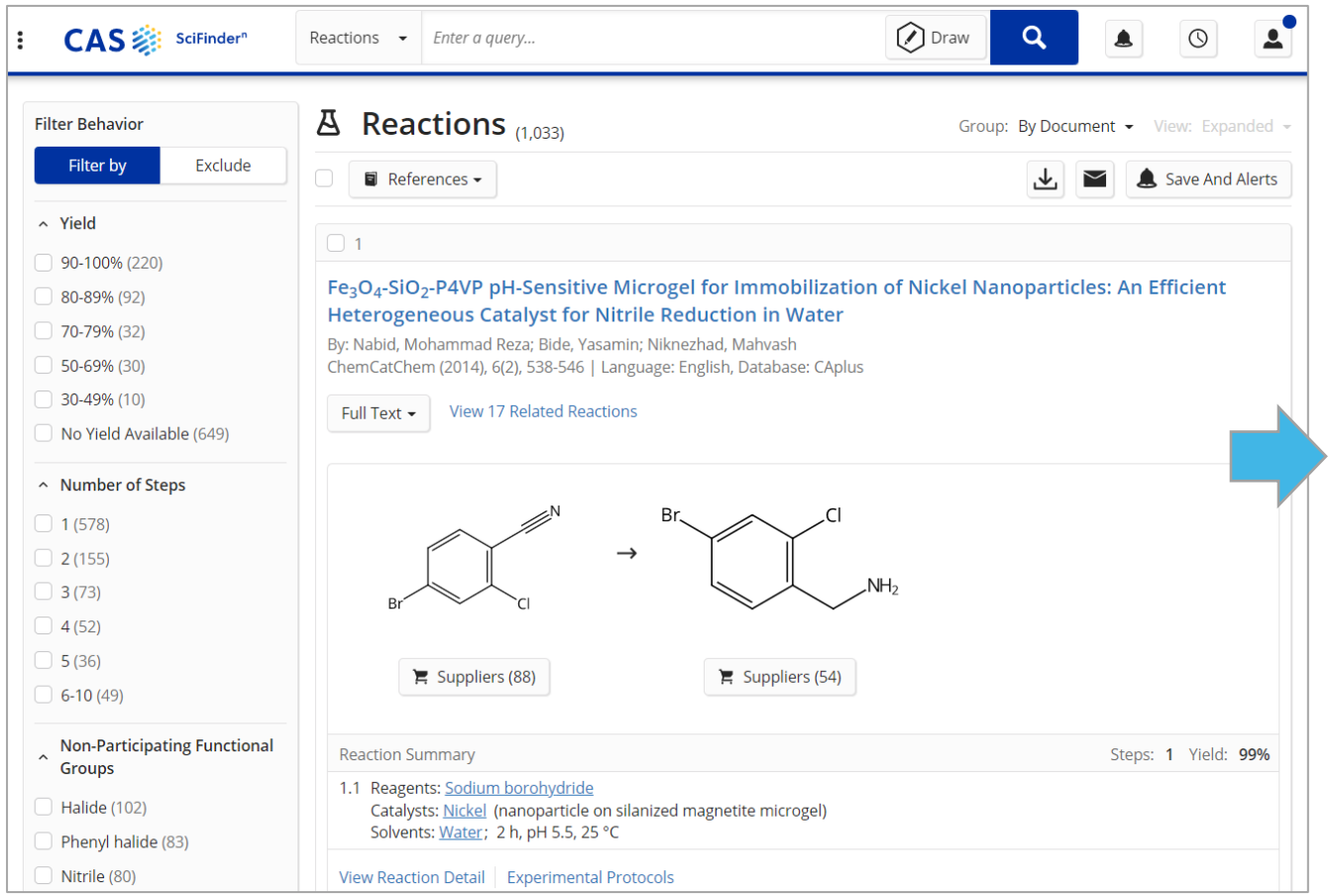
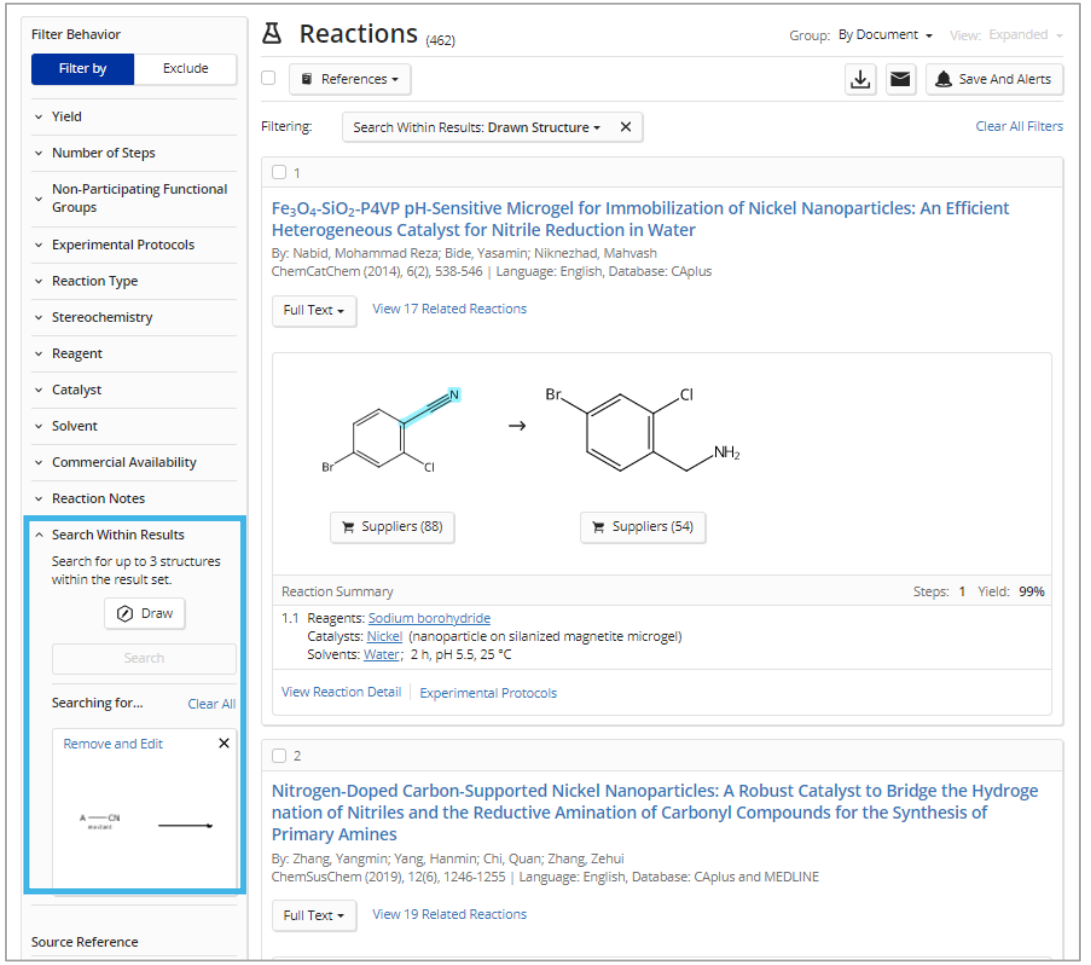
进一步精炼反应结果





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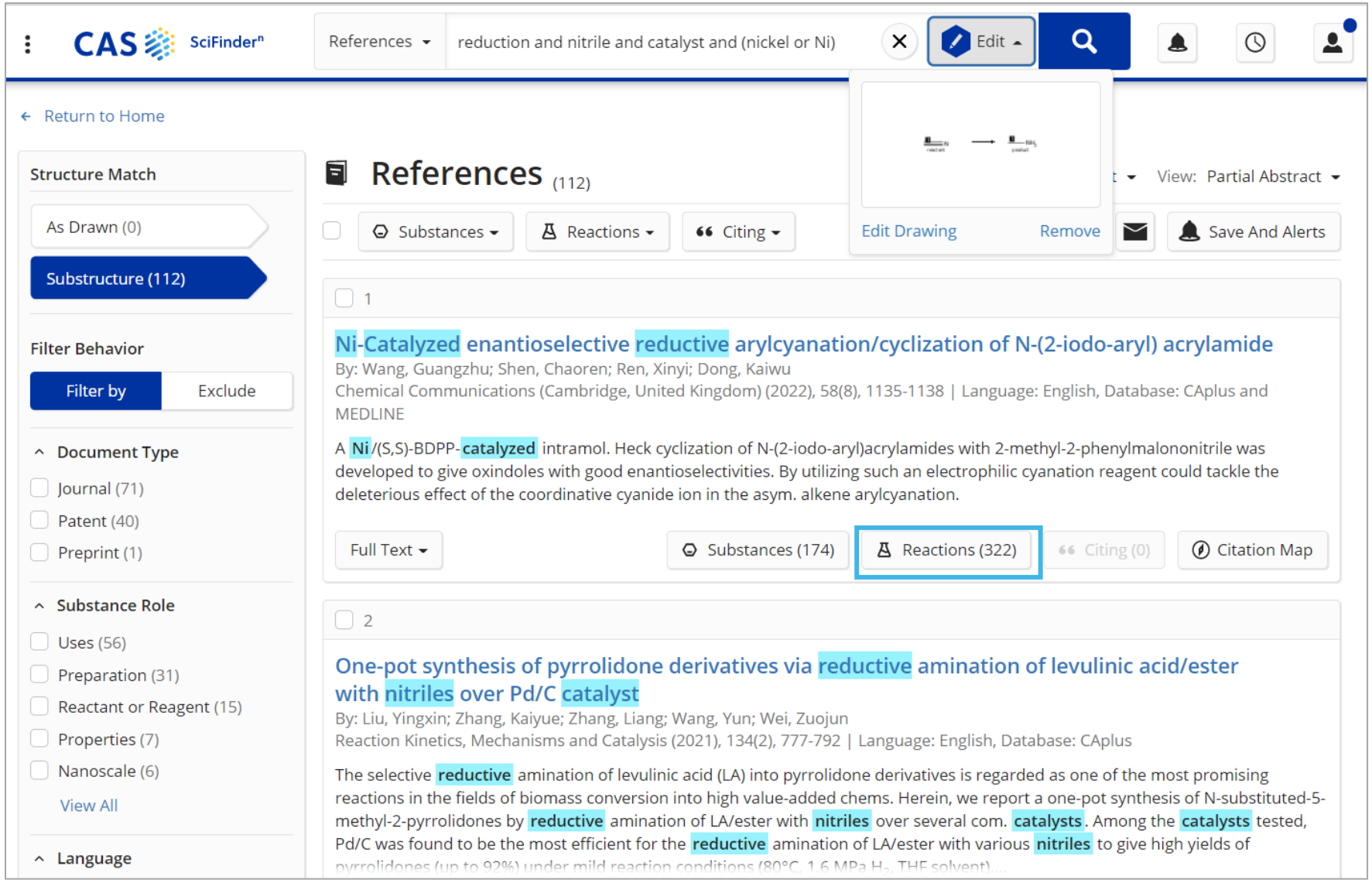
主题词与反应式联用检索



Reference支持主**题词**和反**应**式**联**用**检**索，同**时识**别主**题词**和反**应**式

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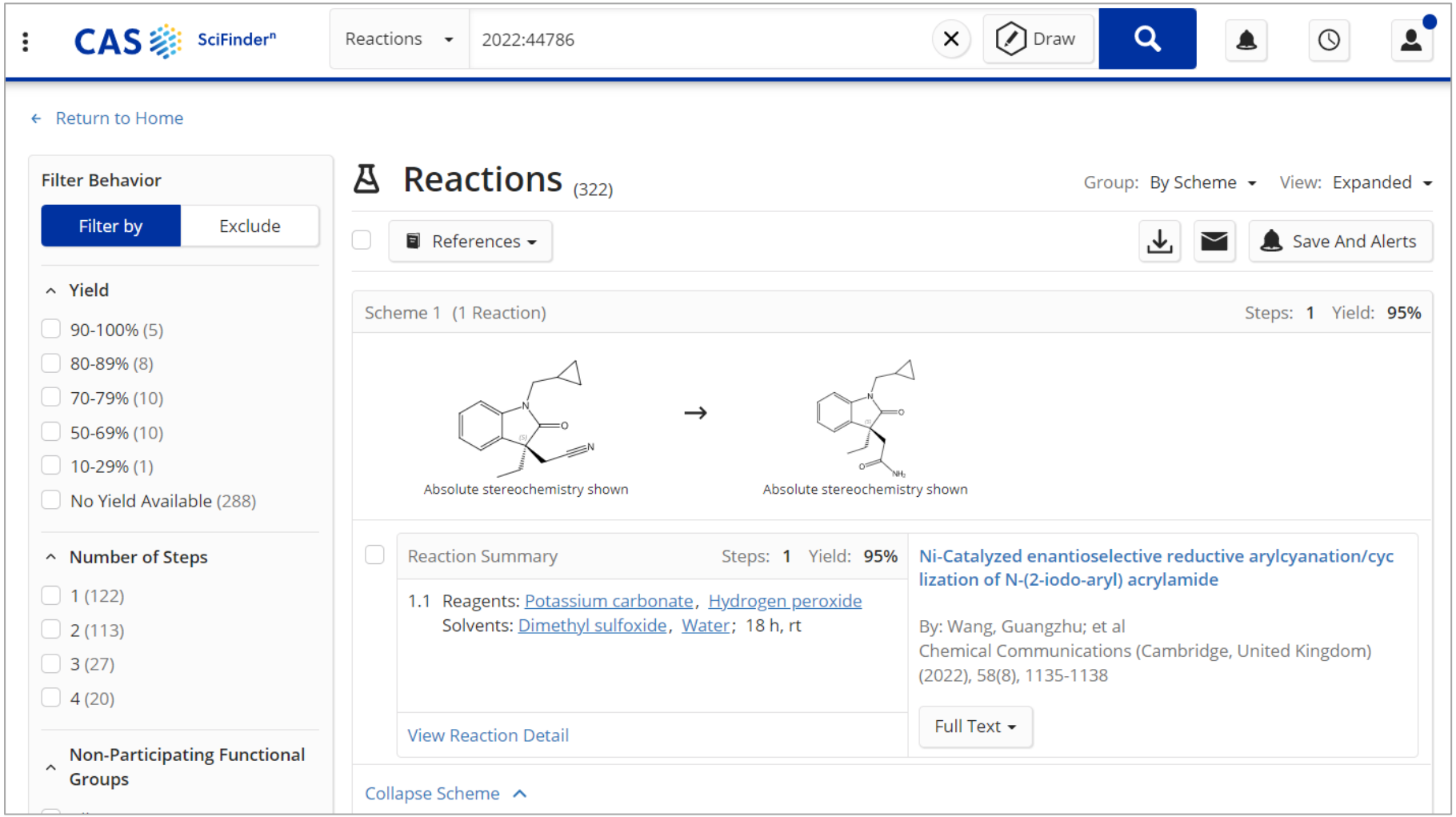
获得关联文献中的反应结果



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小结：

- 通过文献获取反应：基于需要检索的反应信息，形成检索词，并通过逻辑符构建检索主题词
- Reference检索：支持文献主题与反应式联合检索反应文献
- 文献结果精炼：Substance Role物质在文献中的角色、Concept核心研究点
- 数据关联支持灵活获取信息：通过文献获取反应
- 反应结果精炼：可通过Search Within Results等工具精炼反应结果

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总结：

- **反应信息的获取方法**：
  - ✓ 直接进行Reaction检、通过Retrosynthesis Plan获取逆合成反应路线、通过物质或文献获取反应。
  - ✓ 根据检索前掌握的信息和检索目的，灵活选择不同的检索方式。文献、物质和反应三者的数据已经CAS科学家进行高度关联。
- **反应结果聚类分析工具**：Filter by/Exclude
  - ✓ Yield, Steps, Reagent, Catalyst, Solvent, Commercial Availability
  - ✓ Non-participating Functional Groups, Reaction Note, Experimental Protocols, Search Within Results
  - ✓ Source Reference
- **反应详情的查看**： Experimental Protocols——Synthetic Methods、Experimental Procedures, CAS PatentPak
- **逆合成反应路线设计工具Retrosynthesis**：预设参数、查看每一步的Evidence详情、浏览并根据需要调整Alternative Steps、如有必要进一步使用Scoring Profile。

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美国艾赛思国际有限公司北京代表处

(ACS International Ltd Beijing Rep Office)

china@acs-i.org

010-62508026/7

记住本次讲座口令：

反应检索

30天内微信公众号回复讲座口令，获得PPT分享链接

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学习资源

1. 关注“ACS美国化学会”微信公众号，搜索**SciFinder-n**，查看检索技巧、检索视频，以及论坛回放视频

2. CAS SciFinder^{n}网络在线演示培训资料
https://www.cas.org/about/events/scifinder-webinars

3.CAS官网上的培训资料
https://www.cas.org/support/training/scifinder-n

4.CAS SciFinder^{n} Help使用指南
https://scifinder-n.cas.org/help/#t=Searching_in_SciFinder-n%2FIntroduction_to_searching.htm

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2022年CAS SciFinder^{n}论坛直播日程表

	日期	主题	主讲人
基础培训	3月1日	文献信息的获取	刘萌萌
	3月8日	物质信息的获取	钱欣
	3月15日	反应信息的获取	程小燕
	3月22日	生物序列的获取	刘萌萌
	3月29日	利用CAS SciFinder^{n}顺利开题、进行文献综述	钱欣
检索策略详解	4月25日	聚合物相关信息获取策略	程小燕
	5月24日	无机与金属有机化合物相关信息获取策略	钱欣
	6月14日	光电材料相关信息获取策略	程小燕
	7月5日	农化相关信息获取策略	钱欣
	9月13日	药物结构设计与合成	程小燕
	10月11日	天然植物化学相关信息获取策略	钱欣
	11月8日	稀土材料相关信息获取策略	程小燕
	11月29日	纳米材料相关信息获取策略	钱欣
	12月20日	催化合成信息获取策略	程小燕

直播时间：

18:00 – 19:00

扫描下方二维码
即可注册各期论坛：

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谢谢关注!

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美国化学文摘社北京代表处
ACS International, Ltd. – Representing CAS
Unit 1010, Tower B, Raycom InfoTech Park
2 Kexueyuan Nanlu, Haidian District, Beijing, China
+86-10-6250 8026/7
cas.org

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