CAS SCIFINDER DISCOVERY PLATFORM™

反应检索策略及典型案例

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5/23/2025

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提纲

- CAS SciFinder Discovery Platform简介
- 反应检索策略及典型案例
  - 反应检索策略
  - 典型反应检索案例
- Q&A

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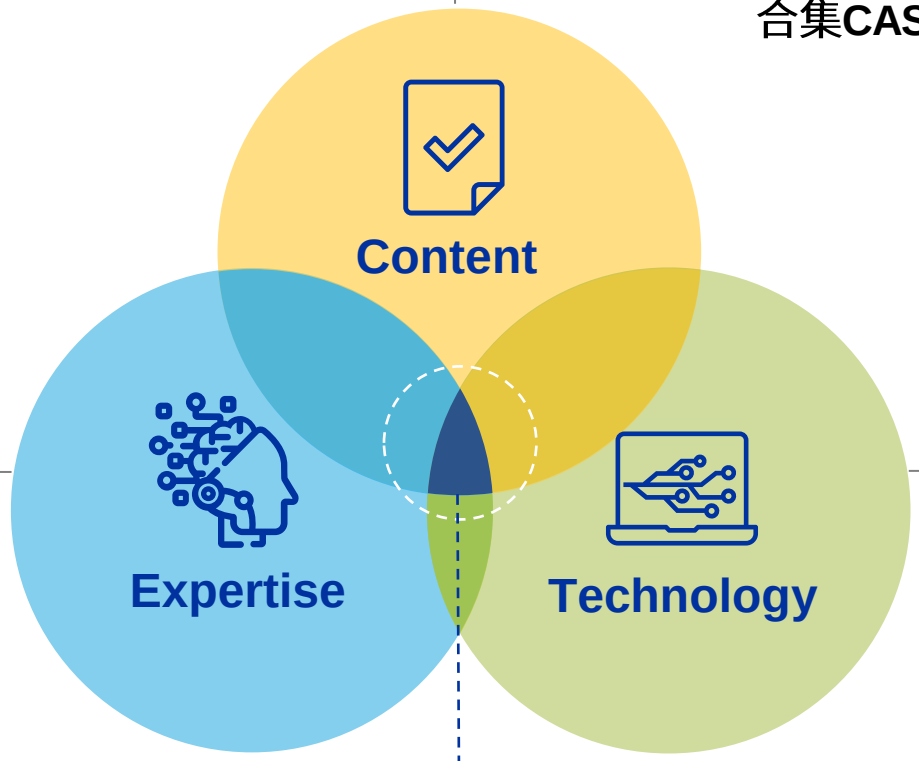

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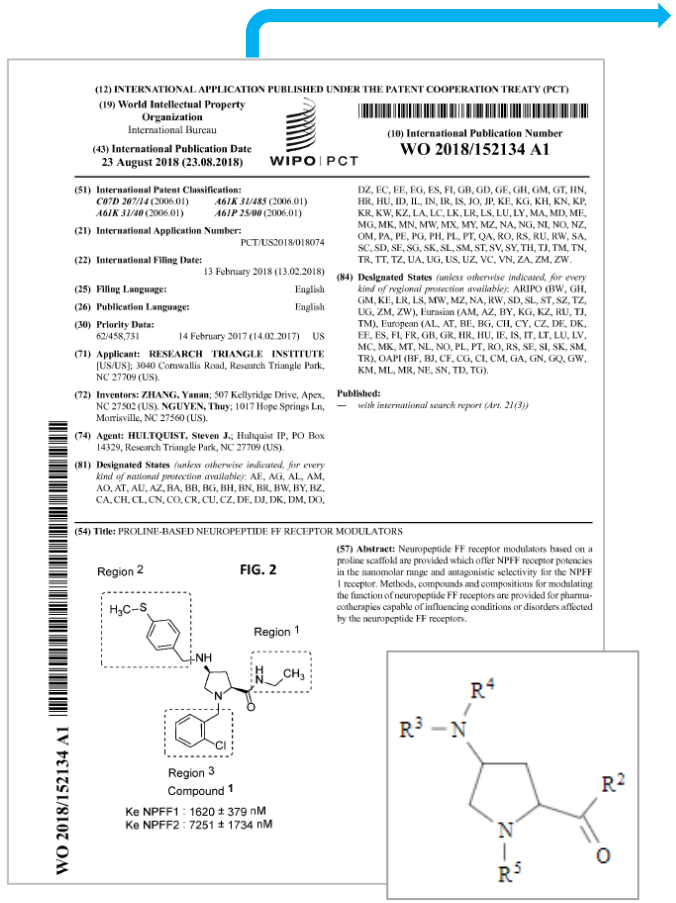
CAS 对文献的独特解读

以专利WO2018152134为例

改写的标准和摘要，尽可能揭示专利核心价值

丰富的增值标引信息：

- ***19** Concepts*
- ***163** Substances*
- ***625** Reactions*
- ***15** Patent Family Members*
- ***3** Formulations*
- ***1** Markush structure*
- ***18** SAR data points*
- ***141** ADME data points*



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(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

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(54) Title: PROLINE-BASED NEUROPEPTIDE FF RECEPTOR MODULATORS

(57) Abstract: Neuropeptide FF receptor modulators based on a proline scaffold are provided which offer NPFF receptor potencies in the nanomolar range and antagonistic selectivity for the NPFF 1 receptor. Methods, compounds and compositions for modulating the function of neuropeptide FF receptors are provided for pharmacotherapies capable of influencing conditions or disorders affected by the neuropeptide FF receptors.

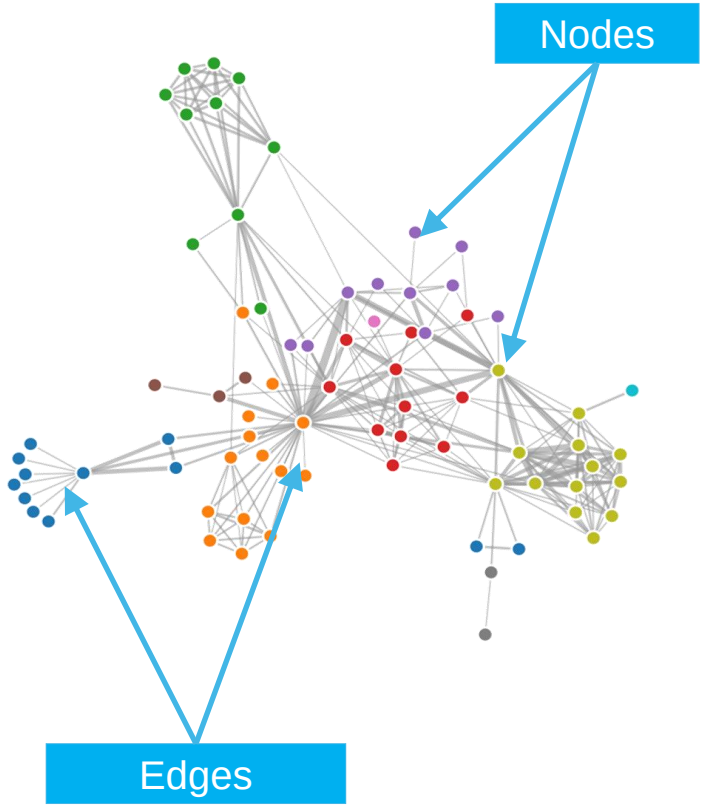
FIG. 2

Region 2 Region 1 Region 3

Compound 1

Ke NPFF1 : 1620 ± 379 nM
Ke NPFF2 : 7251 ± 1734 nM

WO 2018/152134 A1



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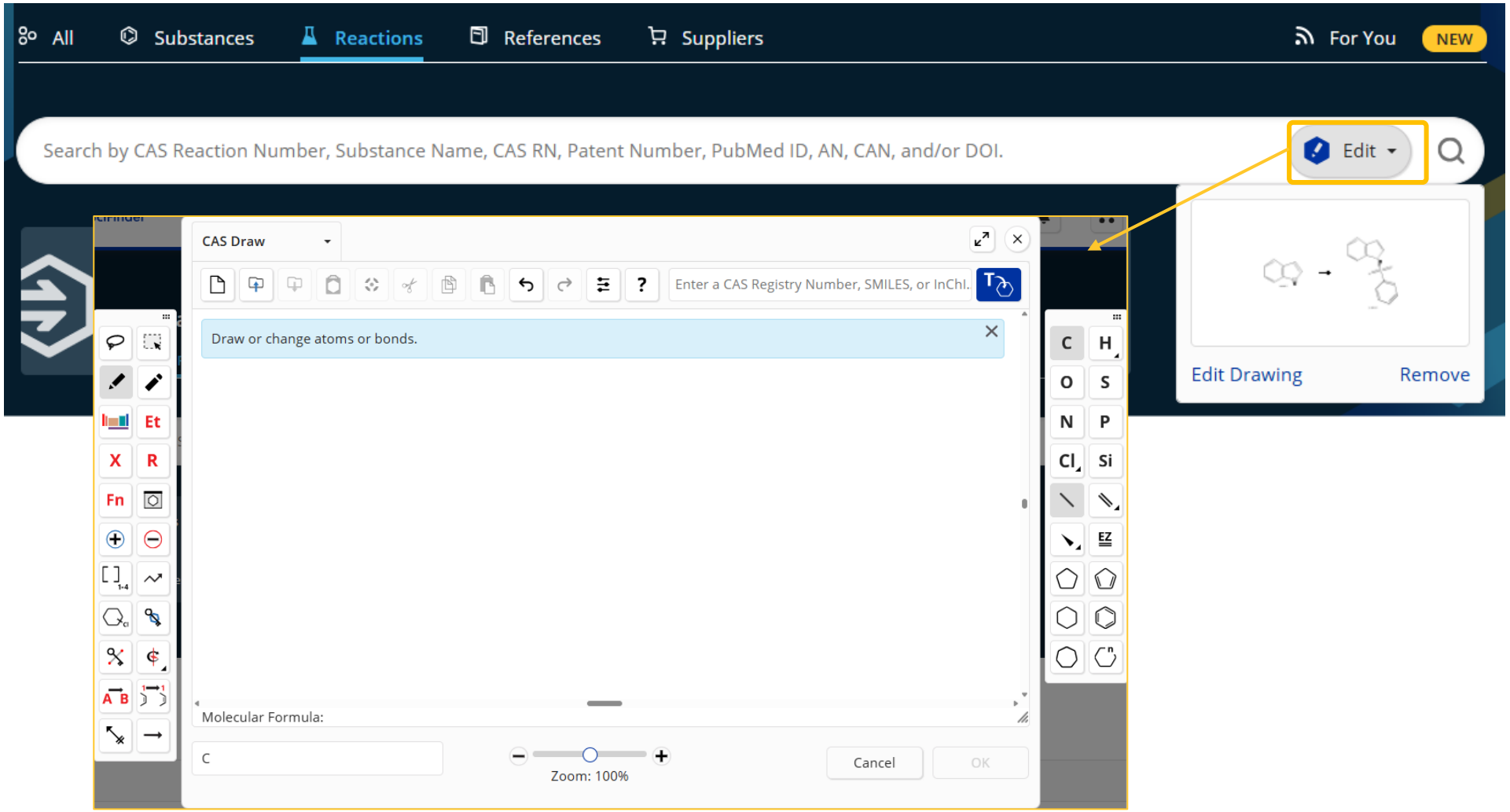
- CAS SciFinder Discovery Platform简介
- 反应检索策略及典型案例
  - 反应检索策略
    - 1.通过物质标识符、结构、自然语言等，直接检索反应
    - 2.通过相似反应拓展，物质/文献关联，间接检索反应
    - 3.通过逆合成路线分析获取反应路线
  - 典型反应检索案例
- Q&A

1. 反应的检索方法——直接检索

根据CAS反应方法号、反应式/结构式、物质标识符、文献号、自然语言检索反应



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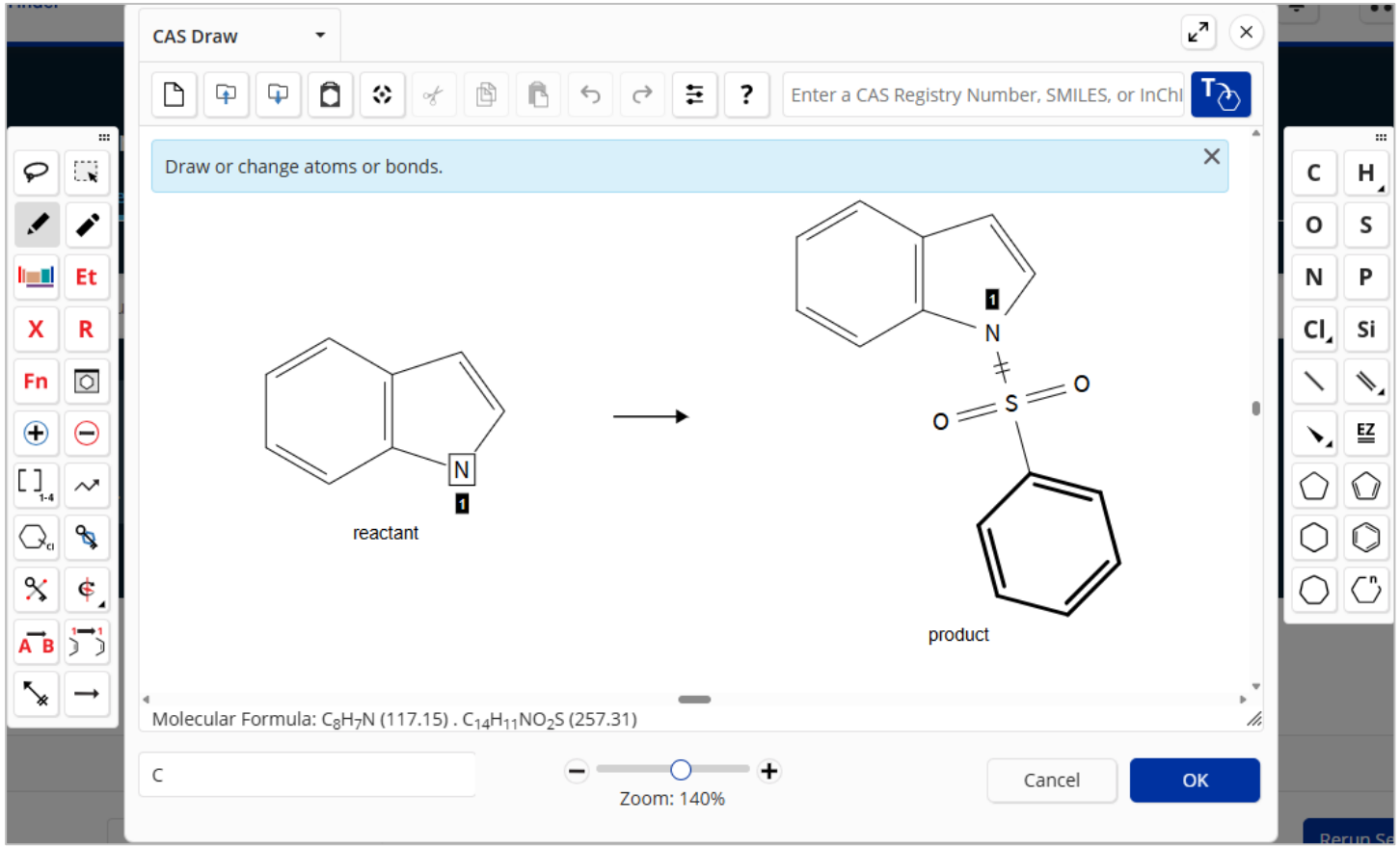
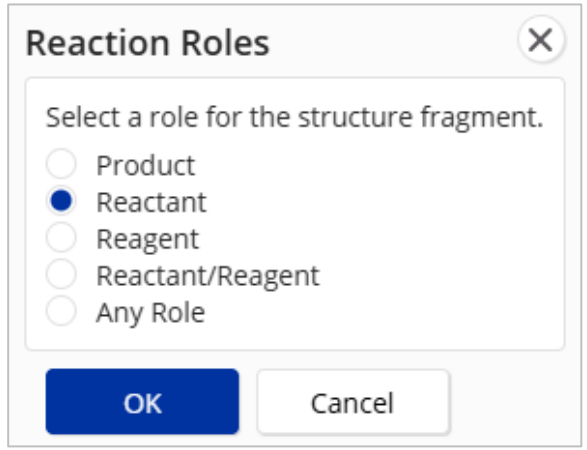
（续）1. 反应的检索方法——直接检索

使用绘制反应式、底物或产物检索反应



反应绘制工具注释：

- 反应角色定义工具
- 反应原子标记工具
- 化学键标记工具
- 反应箭头
- 环锁定工具
- 原子锁定工具



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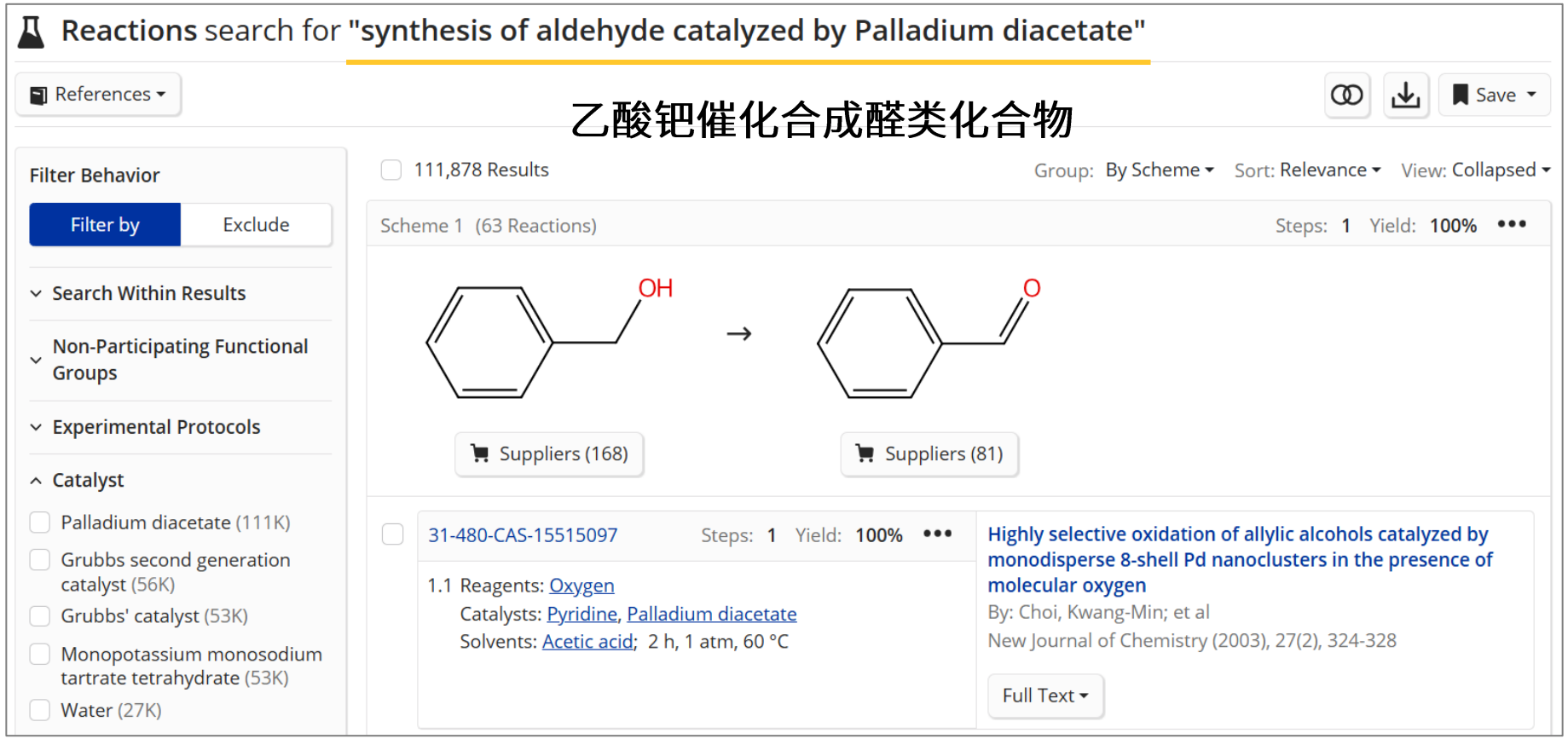
（续）1. 反应的检索方法——直接检索

利用自然语言，检索某一类反应



产物：synthesis/preparation/manufacture of

反应物：from

溶剂：in

催化剂：catalyzed by

试剂：mediated by

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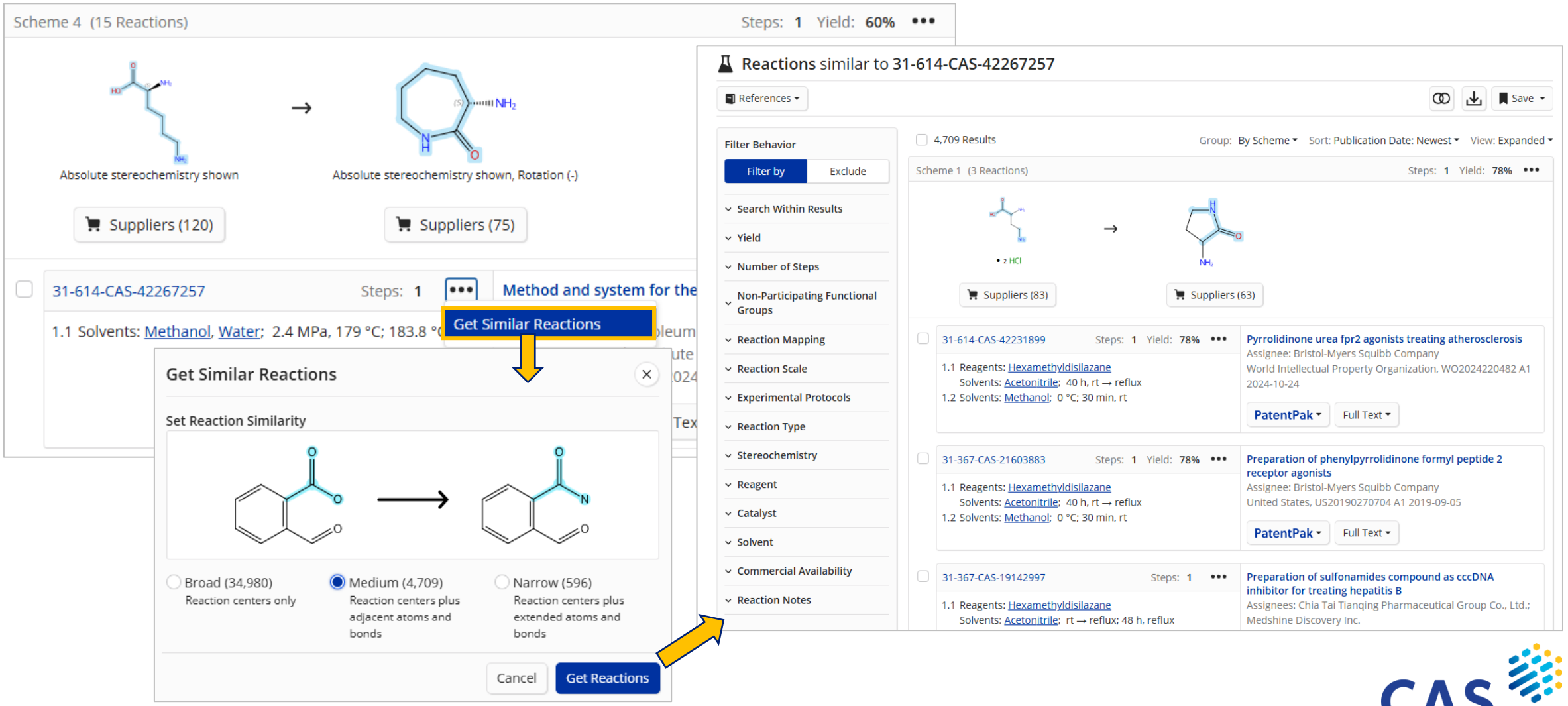
2. 反应的检索方法——间接检索

获取相似反应，拓展实验设计思路



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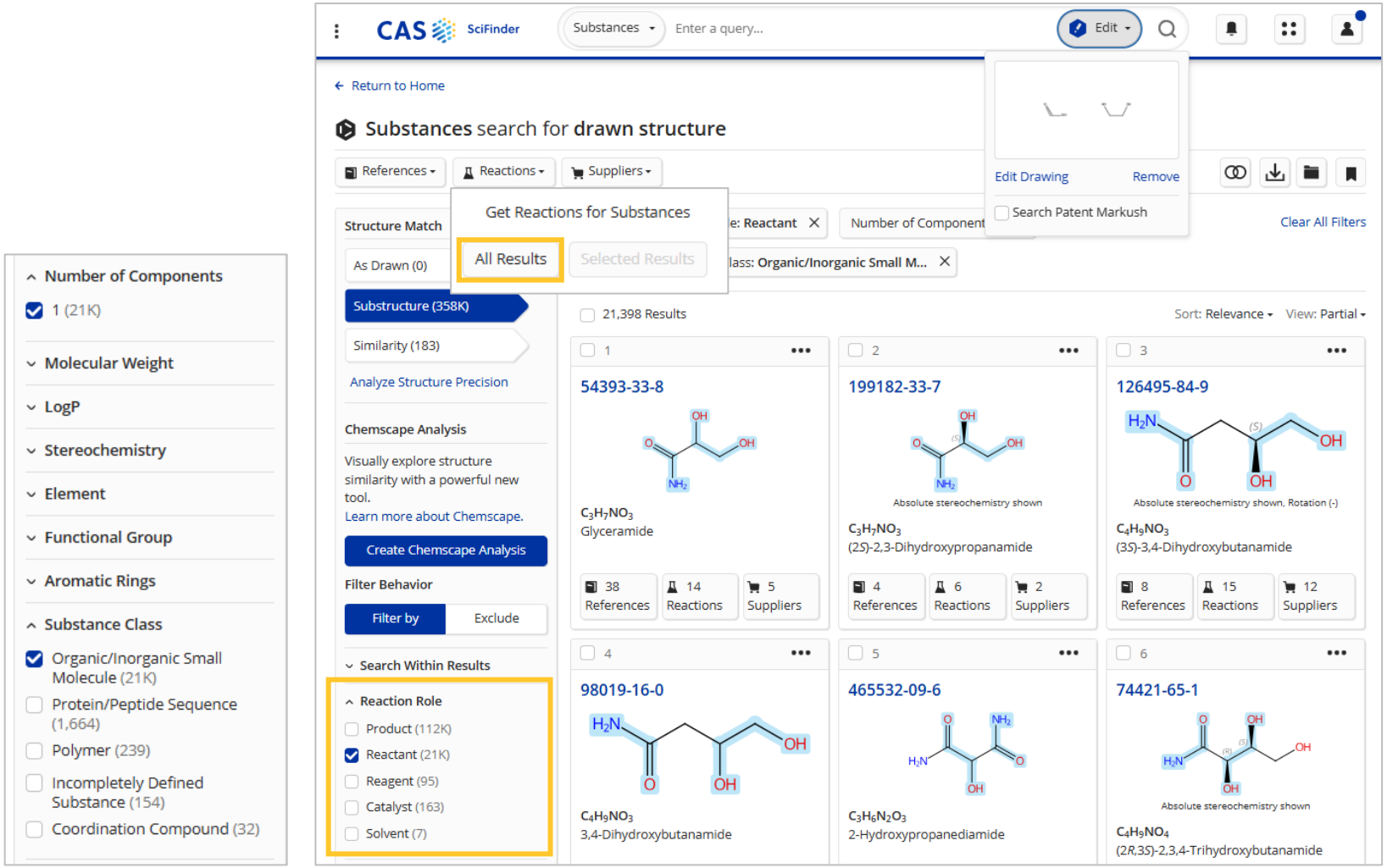
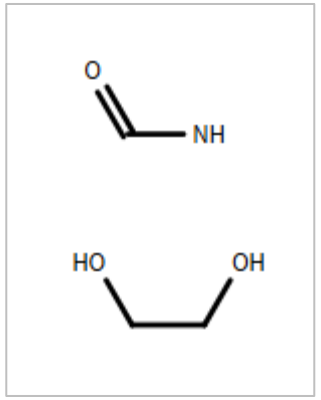
（续）2. 反应的检索方法——间接检索

先从结构出发进行物质检索，再获取反应





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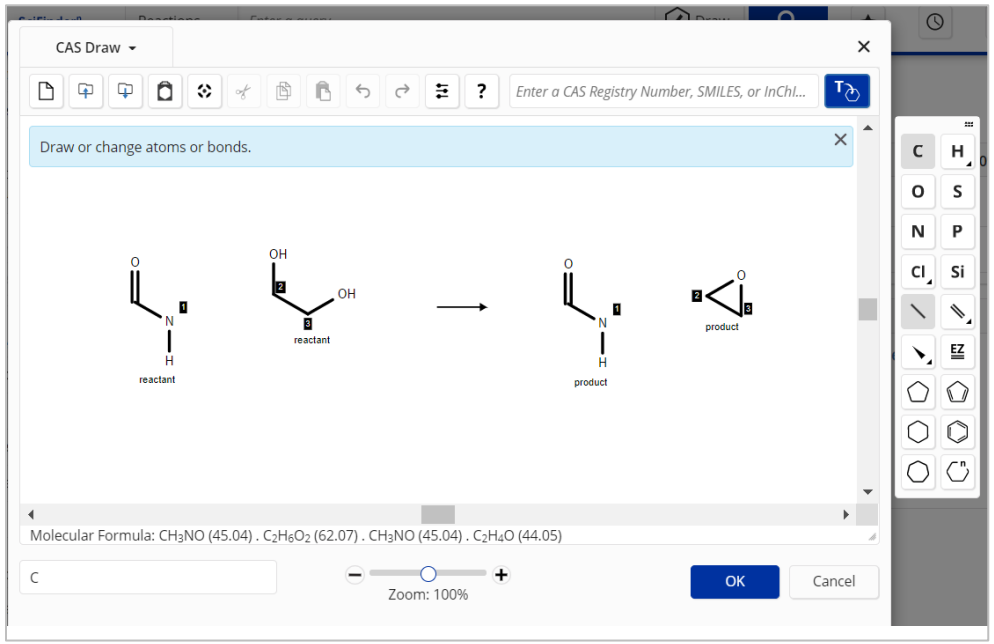
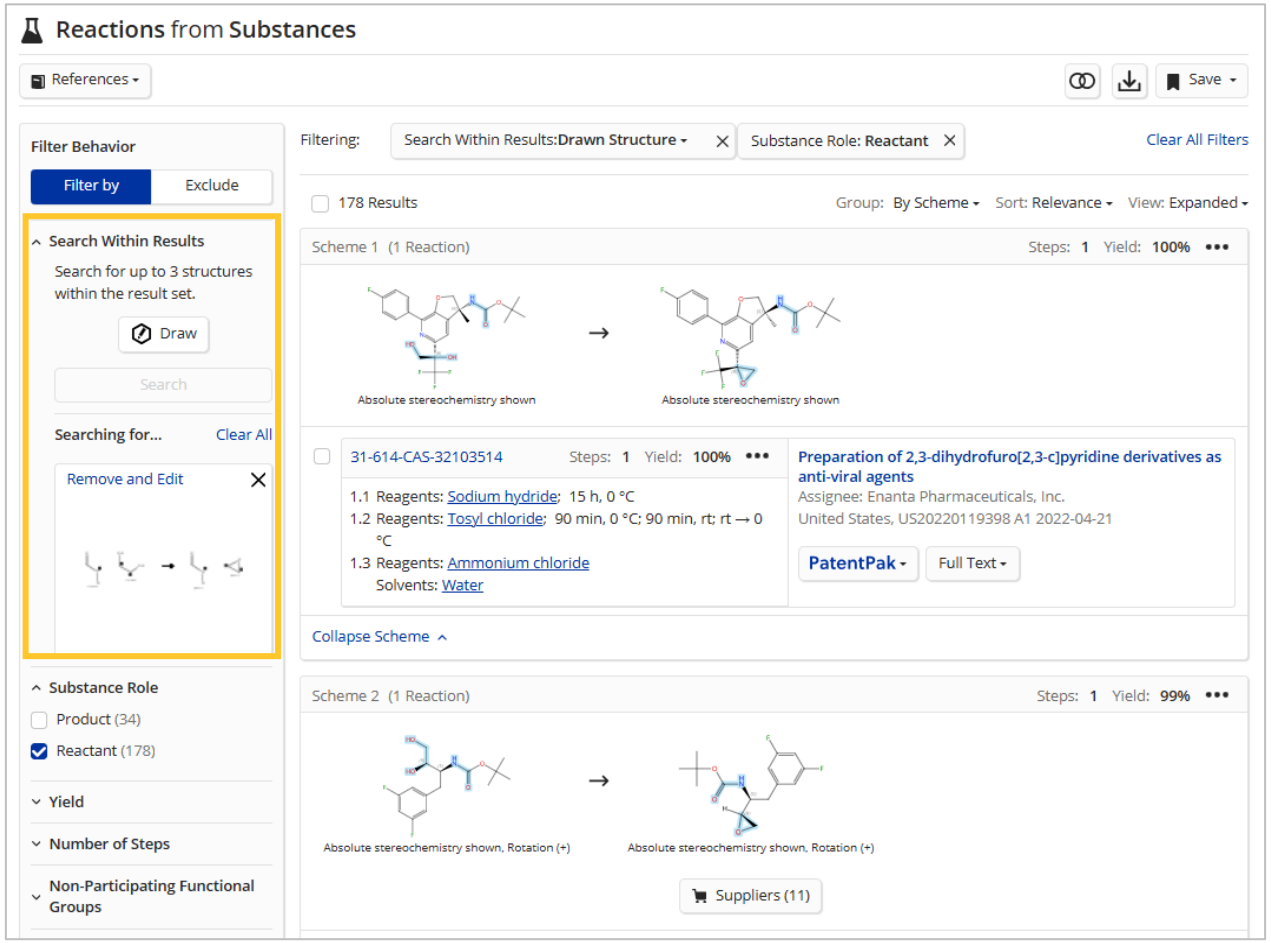
（续）2. 反应的检索方法——间接检索

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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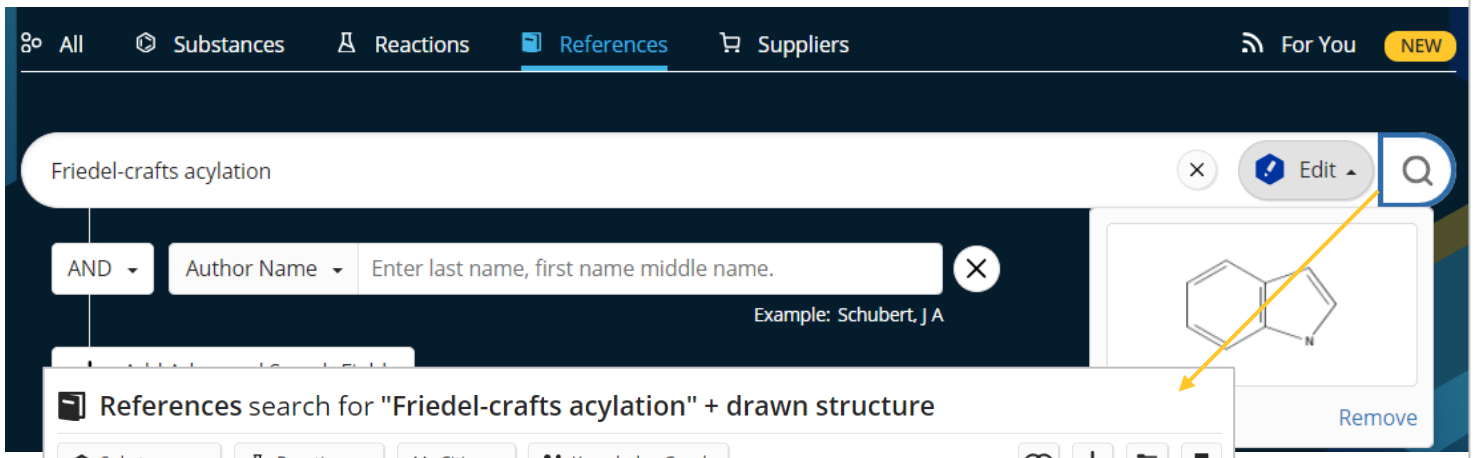
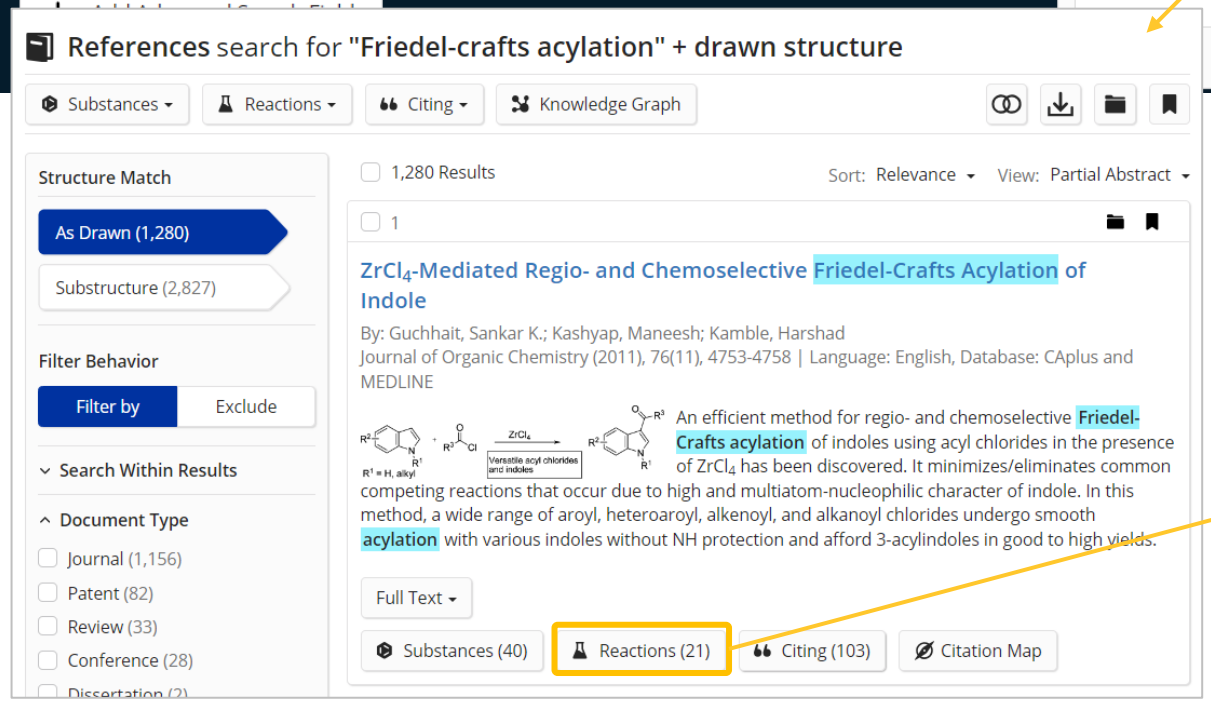
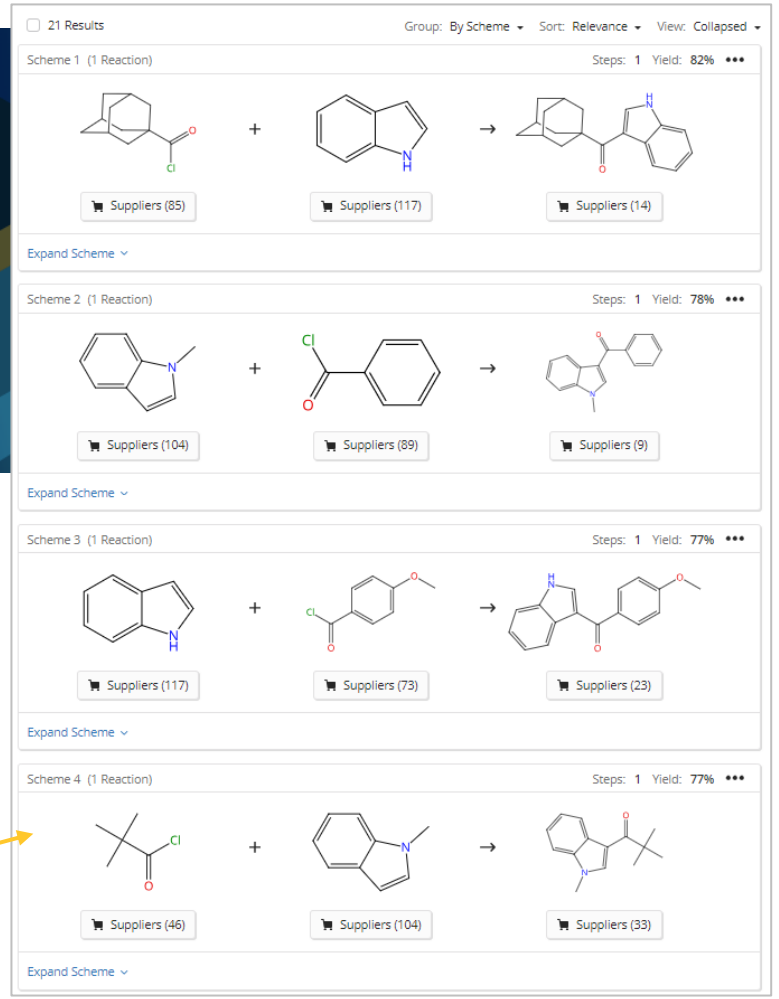
（续）2. 反应的检索方法——间接检索

主题词与结构联用检索

联用检索提高检索效率







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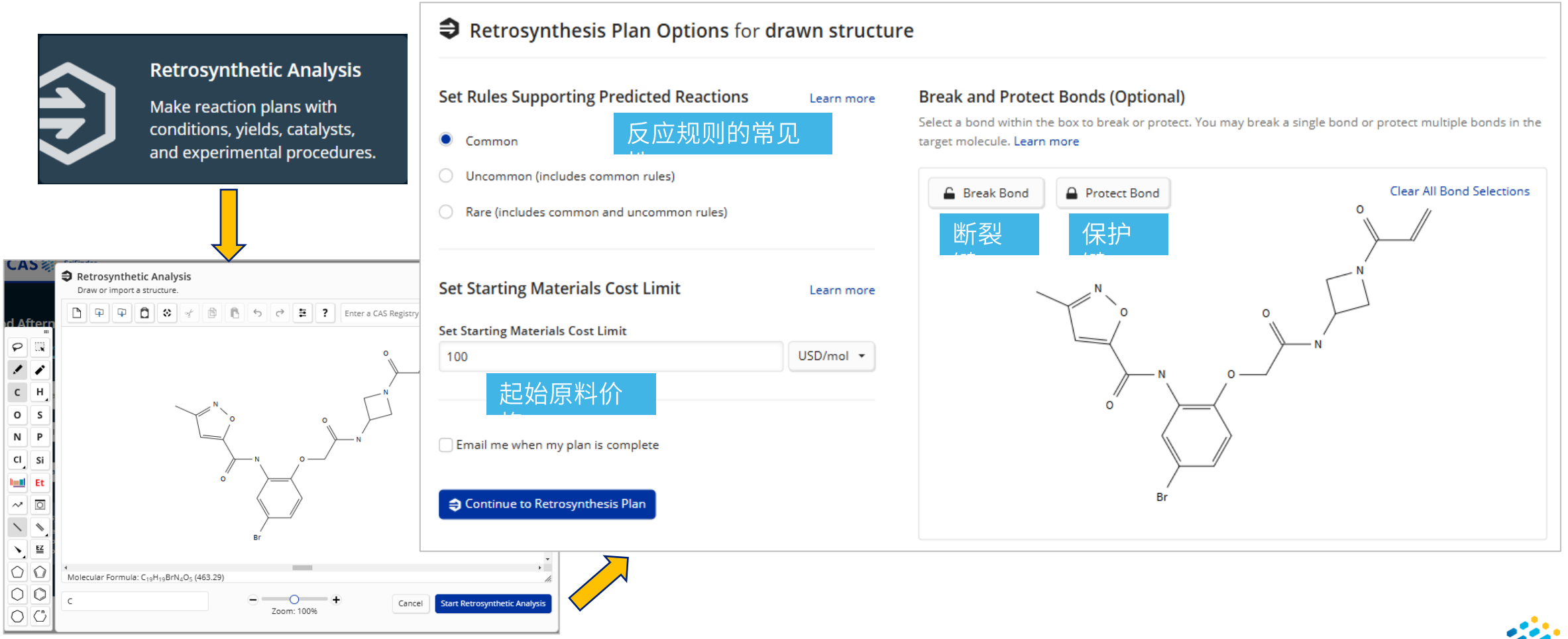
3. 反应的检索方法——Retrosynthetic Analysis

结合先进的AI技术和CAS科学家标引的高质量反应数据，为已知或未知分子设计合成路线



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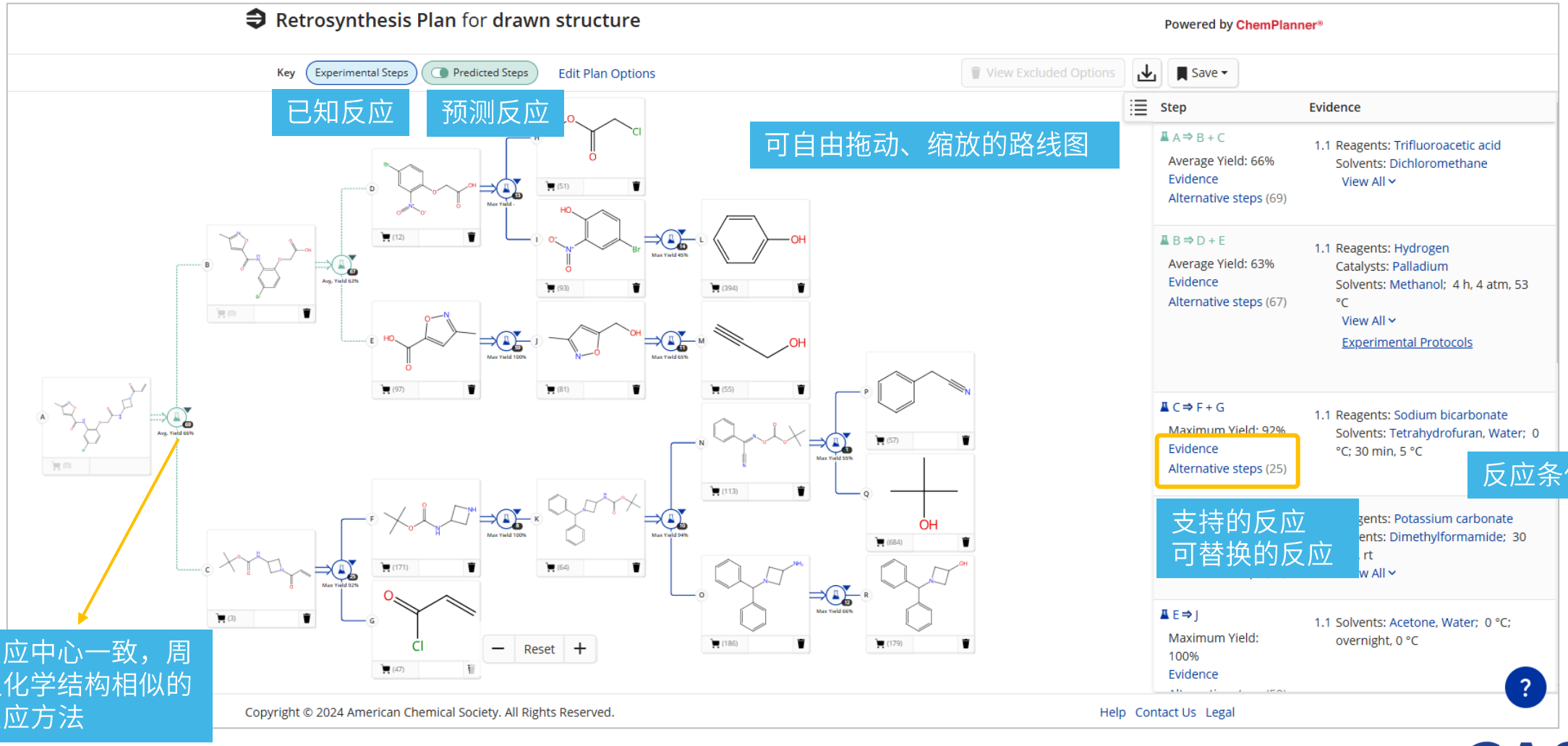
（续）3. 反应的检索方法——Retrosynthetic Analysis

可查看每步反应的文献支持与详细条件



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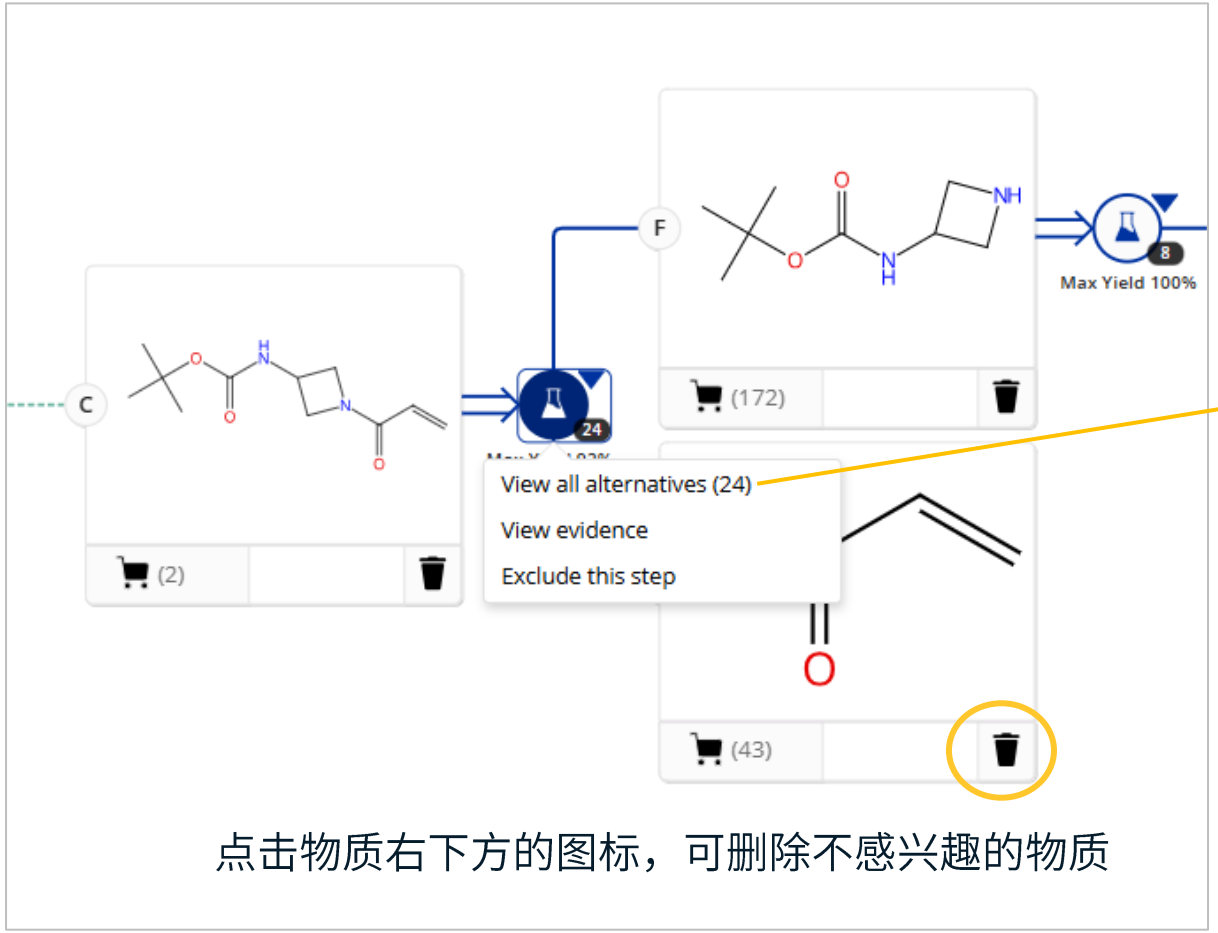
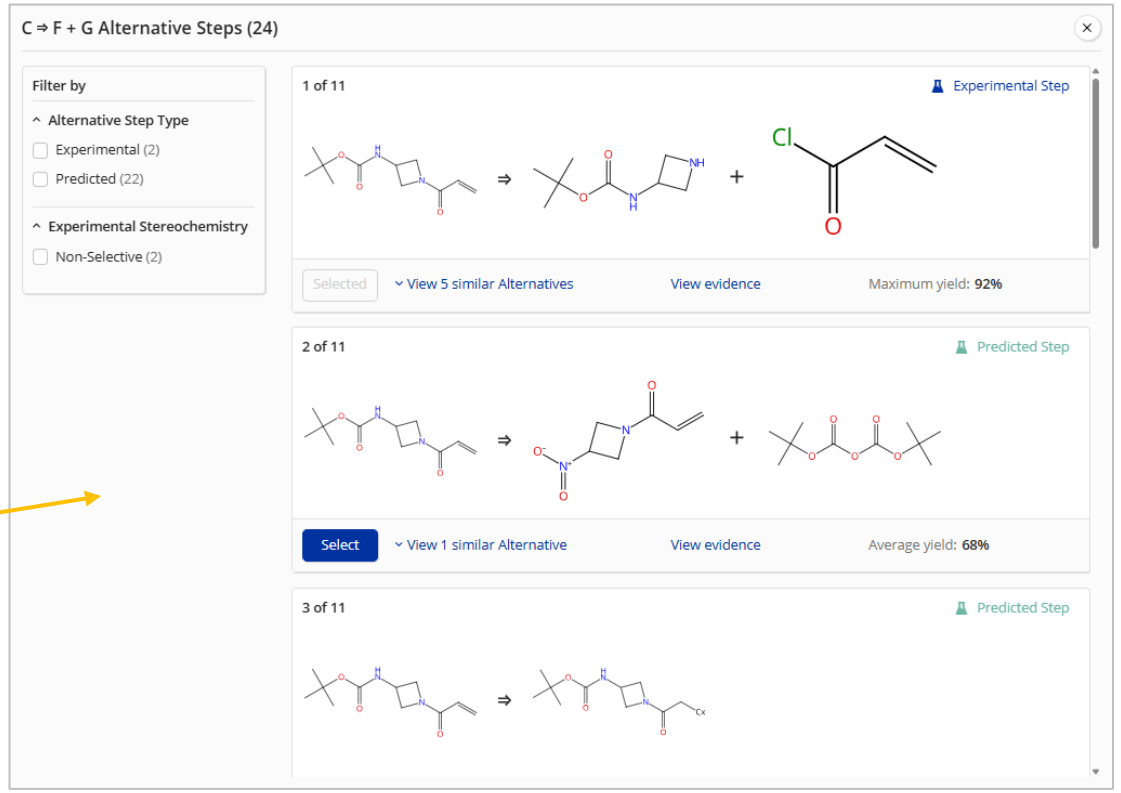
（续）3. 反应的检索方法——Retrosynthetic Analysis

反应路线的拓展与优化



点击物质右下方的图标，可删除不感兴趣的物质



View All Alternatives：查看所有的替代反应路线

View Evidence：查看某步路线的支持报道

Exclude This Step：删除不感兴趣的步骤

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小结

1. 反应的直接检索：
   - ✓ 通过反应式，或者反应物/产物/反应试剂的结构式，进行反应检索。
   - ✓ 通过物质标识符（包括名称、CAS RN等）、文献号或专利号等，进行反应检索。
   - ✓ 通过自然语言进行反应信息检索。
2. 反应的间接检索：
   - ✓ 通过相似反应拓展，获取更多相似反应路线支持。
   - ✓ 针对某类关注物质，进行结构、属性或反应角色等筛选，再关联到相关反应。
   - ✓ 通过关键词或关键词与结构联用，精炼感兴趣的文献信息，并获取相关反应。
3. 通过Retrosynthetic Analysis获取逆合成反应路线
   - ✓ 利用AI技术和CAS科学家标引的反应信息，提供已知或未知结构的已有或预测合成路线。

提纲

- CAS SciFinder Discovery Platform简介
- 反应检索策略及典型案例
  - 反应检索策略
  - 典型反应检索案例
    - 1. 目标化合物的合成工艺调研
    - 2. 手性化合物的制备与拆分
    - 3. 聚合物材料改性研究
    - 4. 生物转化与生物发酵反应检索
- Q&A

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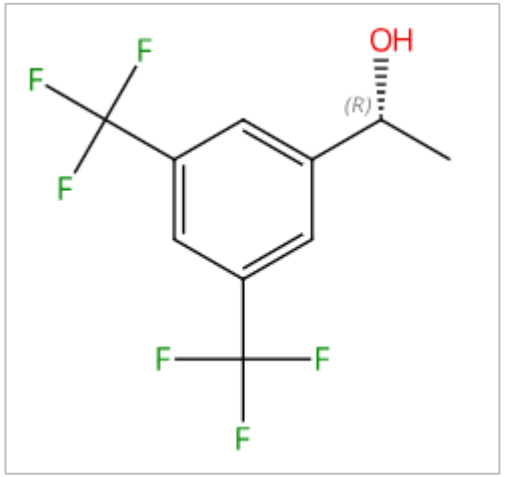
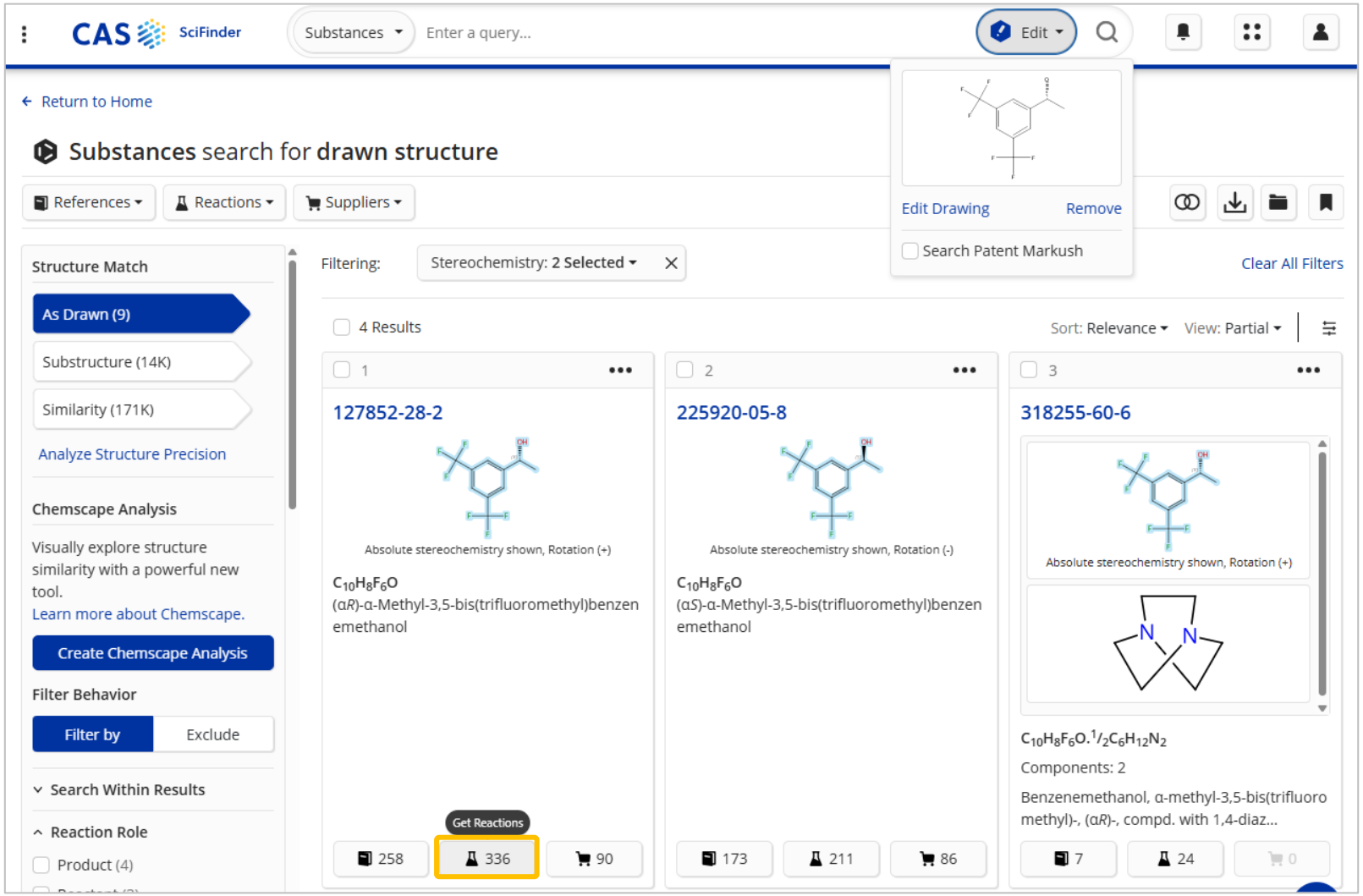
案例1：目标化合物的合成工艺调研

示例：

含氟中间体(R)-1-[3,5-二(三氟甲基)苯基]乙醇的合成工艺



- 通过物质结构、名称或其他物质标识符检索物质
- 一键链接到相关反应



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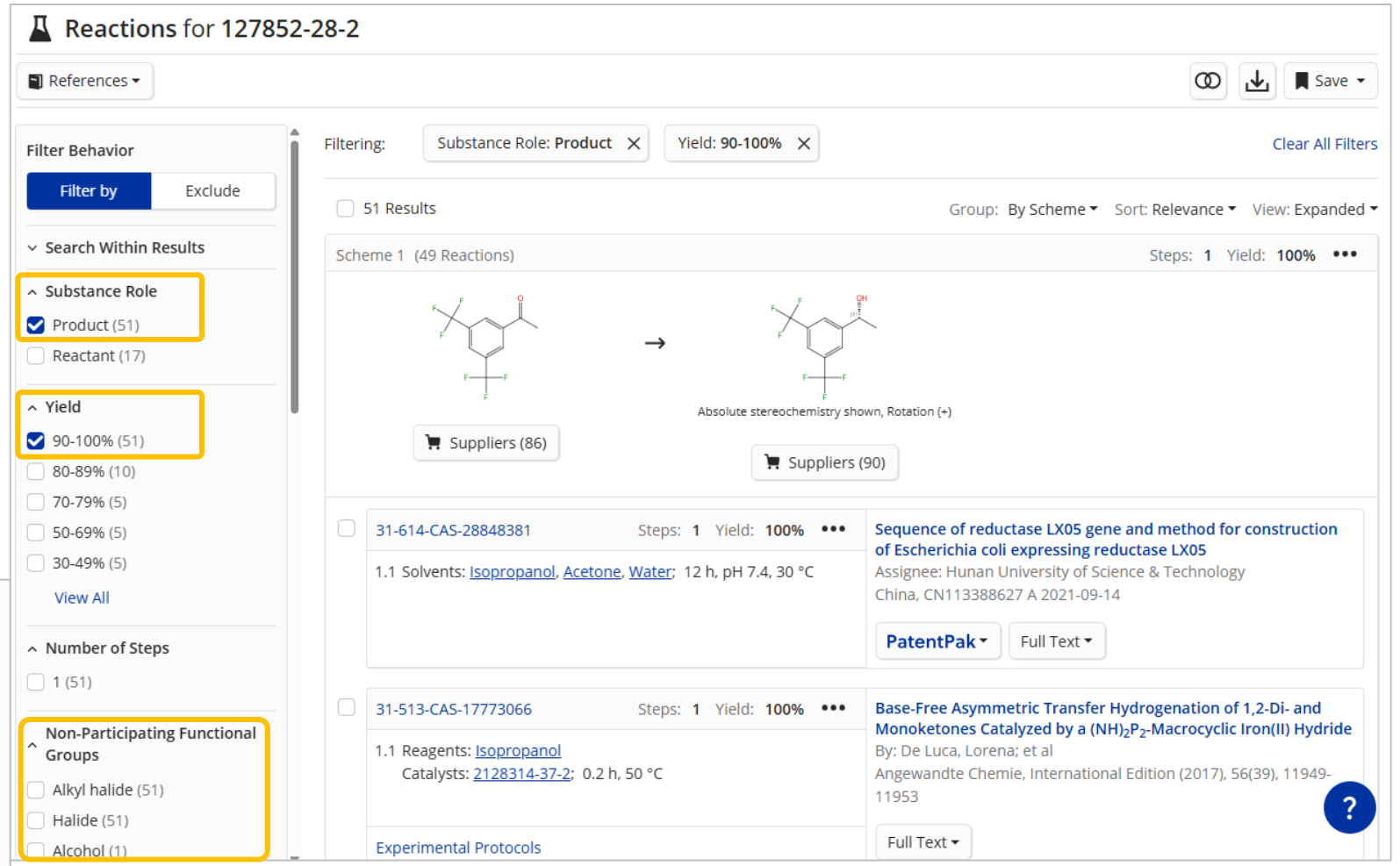
（续）案例1：目标化合物的合成工艺调研

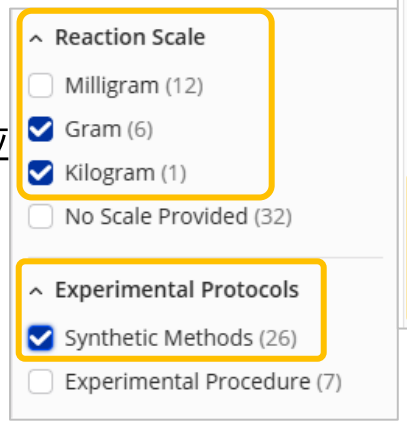
示例：

含氟中间体(R)-1-[3,5-二(三氟甲基)苯基]乙醇的合成工艺

- 限定物质角色为产物，通过产率筛选较优的反应条件
- 可进一步筛选反应规模、实验详情等



关注放大反应



筛选不参与反应官能团

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（续）案例1：目标化合物的合成工艺调研

Synthetic Methods——CAS科学家增值标引的合成制备详情

易于阅读的实验操作流程

产物表征数据

反应转化类型

反应注释

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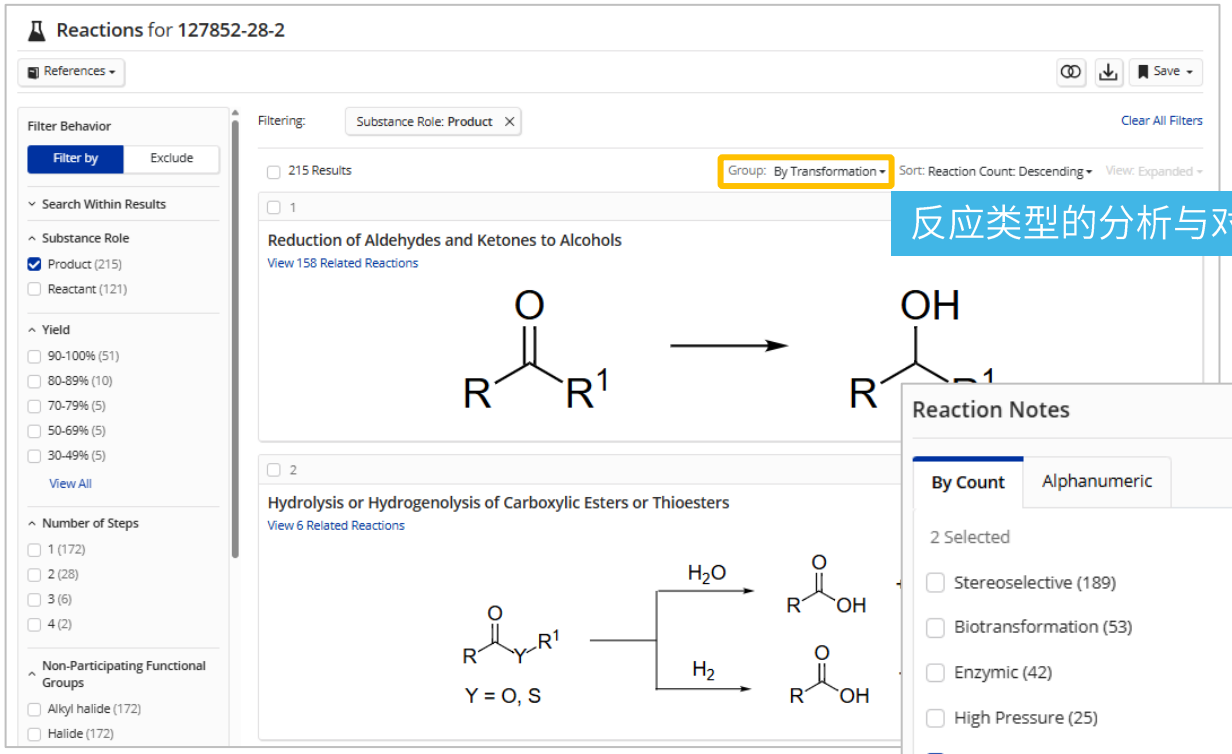
（续）案例1：目标化合物的合成工艺调研

关注反应转化类型与反应注释



反应类型的分析与对比

反应注释

通过反应注释，精炼筛选感兴趣的反应，如：绿色化学

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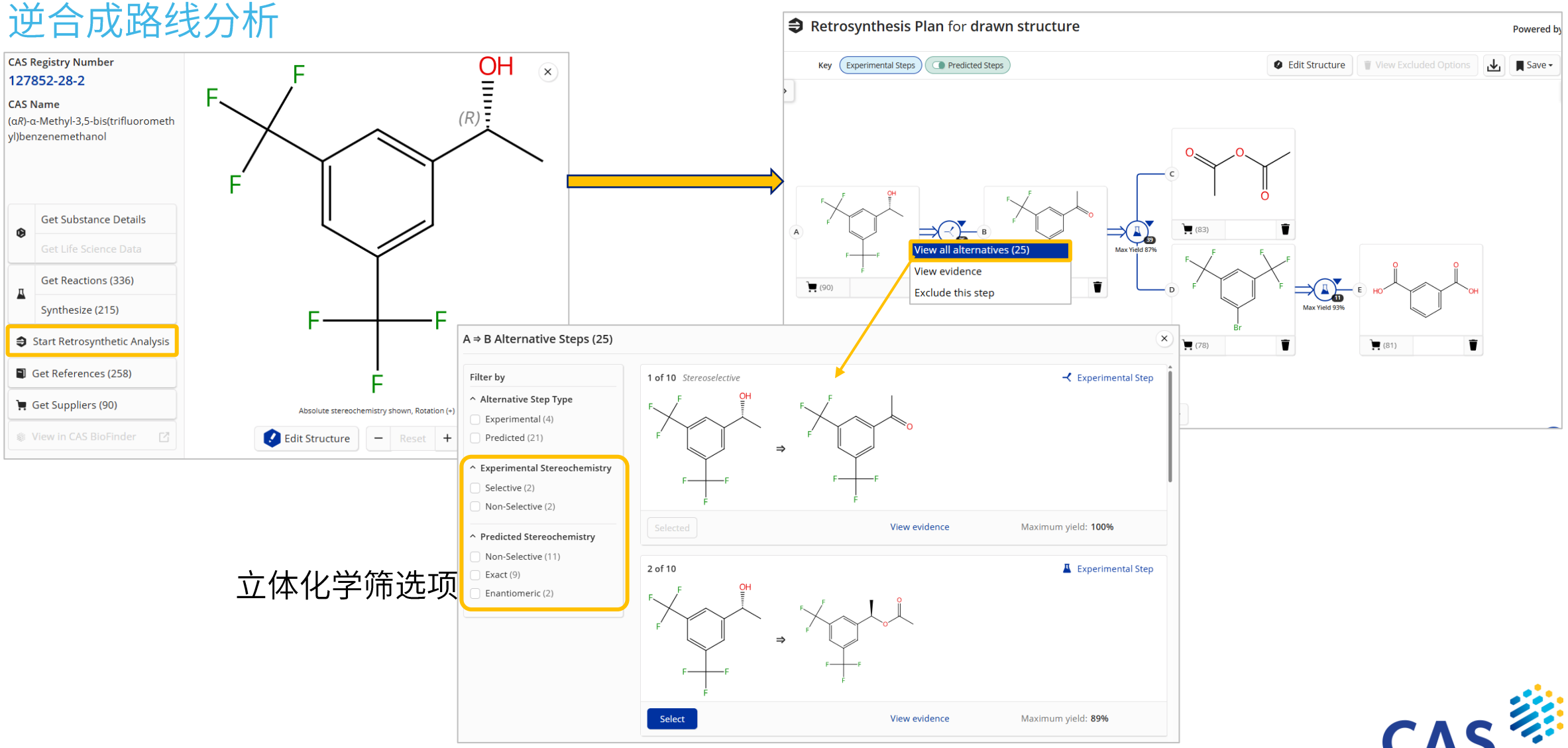
（续）案例1：目标化合物的合成工艺调研

逆合成路线分析



立体化学筛选项

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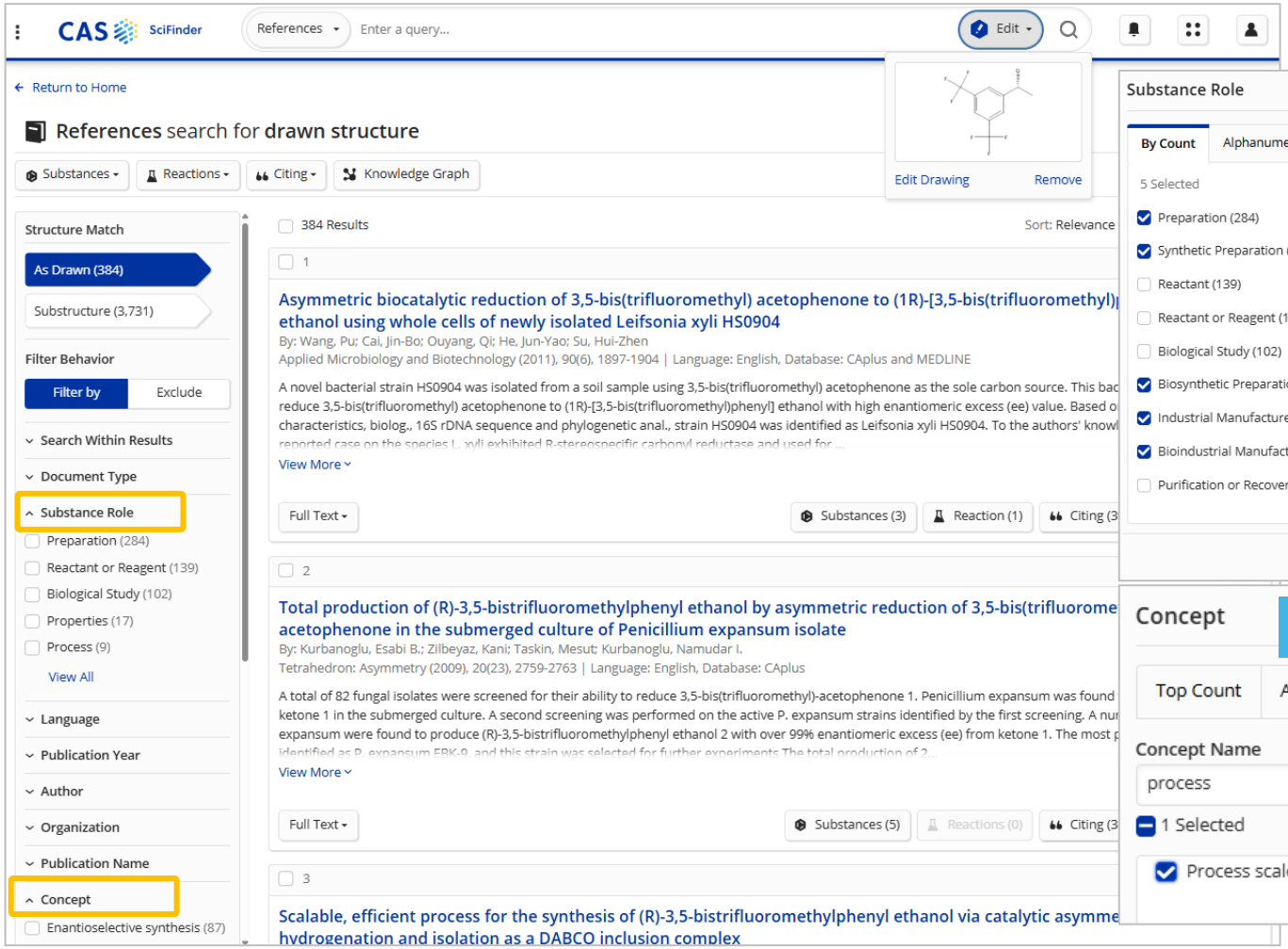
（续）案例1：目标化合物的合成工艺调研

获取目标化合物的合成工艺报道文献

- 对结构进行文献检索
- 对物质角色进行筛选
- 对核心研究点进行筛选
- 深入查看感兴趣的文献



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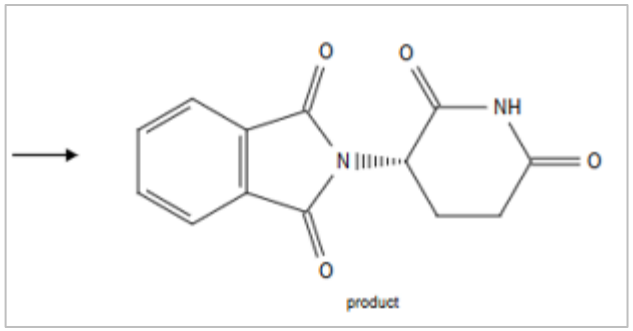
案例2：手性化合物的制备与拆分

直接绘制包含立体结构的反应式进行检索



Stereochemistry

- [x] Absolute Stereo Match (51)
- [x] Absolute Stereo Mirror Image (24)
- [ ] Stereo that Doesn't Match Query (61)
- [ ] No Stereo in Answer Structure (173)

Reactions search for **drawn structure**

References ▾ | Save ▾

Structure Match

As Drawn (297) | Substructure (294K)

Filter Behavior

Filter by | Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw | Search

Yield

Number of Steps

Non-Participating Functional Groups

Reaction Mapping

Reaction Scale

Experimental Protocols

Filtering: Stereochemistry: 2 Selected ▴ ×

Absolute Stereo Match

Absolute Stereo Mirror Image

Clear All Filters

63 Results | Group: By Scheme ▾ | Sort: Relevance ▾ | View: Expanded ▾

Scheme 1 (2 Reactions) Steps: 1 Yield: 75-90% •••

Absolute stereochemistry shown

Absolute stereochemistry shown, Rotation (-)

Suppliers (40) | Suppliers (49)

31-367-CAS-622921 Steps: 1 Yield: 90% •••

1.1 Reagents: 1,1'-Carbonyldiimidazole, 4-(Dimethylamino)pyridine
Solvents: Tetrahydrofuran

Preparation of non-polypeptide imides as inhibitors of TNFα
Assignee: Celgene Corporation
United States, US5463063 A 1995-10-31

PatentPak ▾ | Full Text ▾

31-367-CAS-4058441 Steps: 1 Yield: 75% •••

1.1 Reagents: 1,1'-Carbonyldiimidazole
Catalysts: 4-(Dimethylamino)pyridine
Solvents: Tetrahydrofuran; 20 h, reflux

Synthesis of conjugate of thalidomide and folic acid
By: Wang, Shu-yan; et al
Huaxue Yanjiu Yu Yingyong (2012), 24(3), 469-473

Full Text ▾

Collapse Scheme ▴

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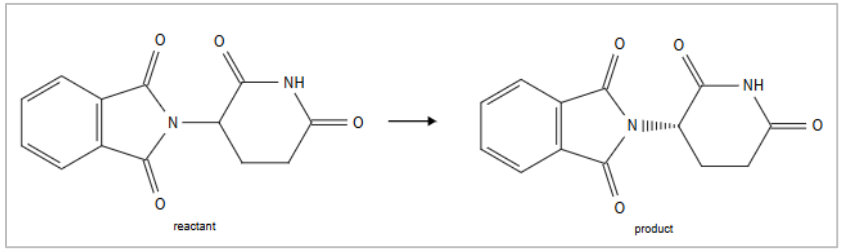
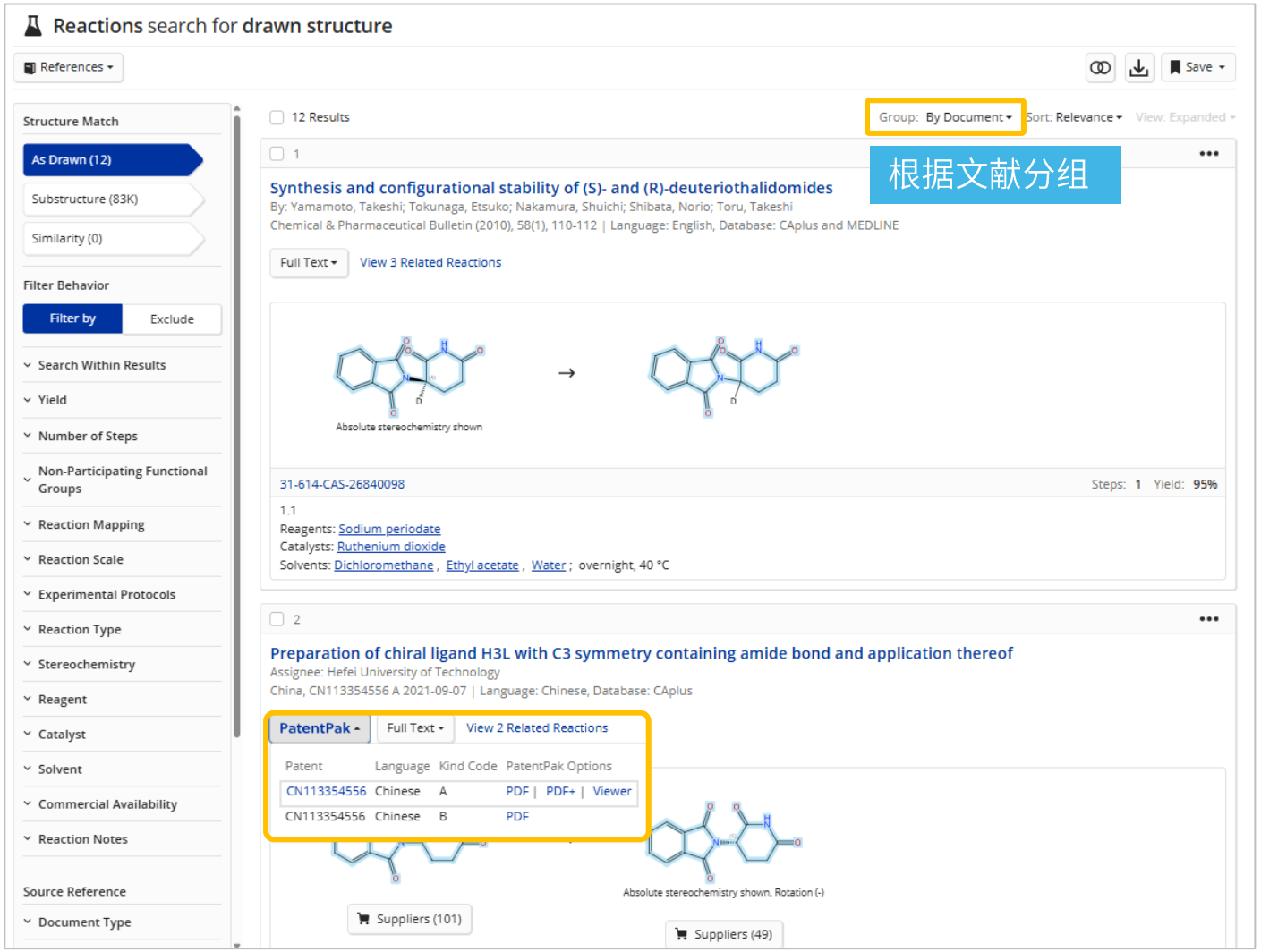
（续）案例2：手性化合物的制备与拆分

快速获取各类手性拆分反应



直接绘制反应式，检索手性拆分反应



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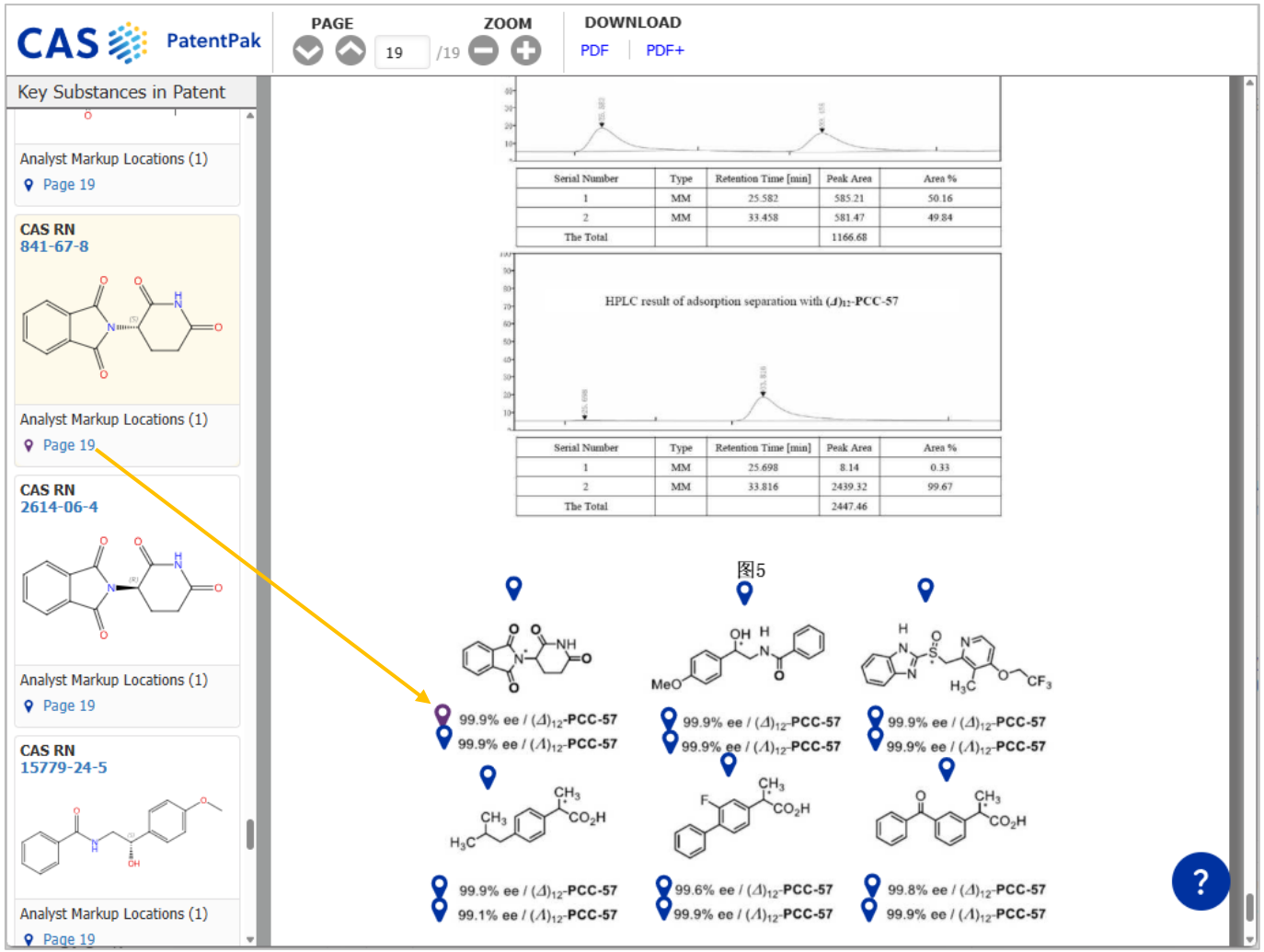
（续）案例2：手性化合物的制备与拆分

高效定位专利中重点物质信息——CAS PatentPak



CAS PatentPak：

- 快速理解专利
- 一键下载原文
- 快速定位专利中的物质
- 阅读其他语言撰写的等同专利

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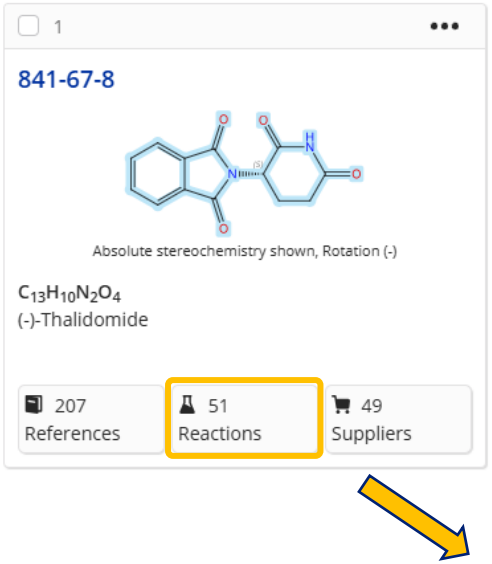
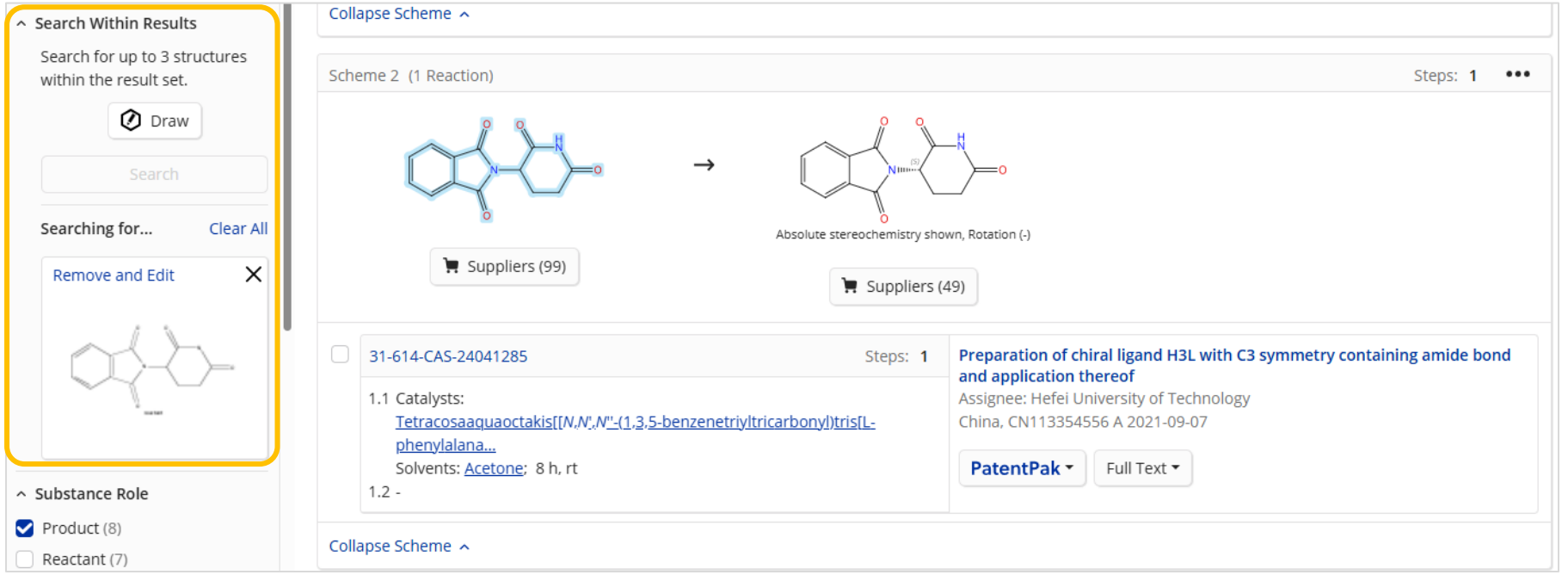
（续）案例2：手性化合物的制备与拆分

先检索产物，再链接到反应，并限定底物



在二次检索中，
绘制底物结构



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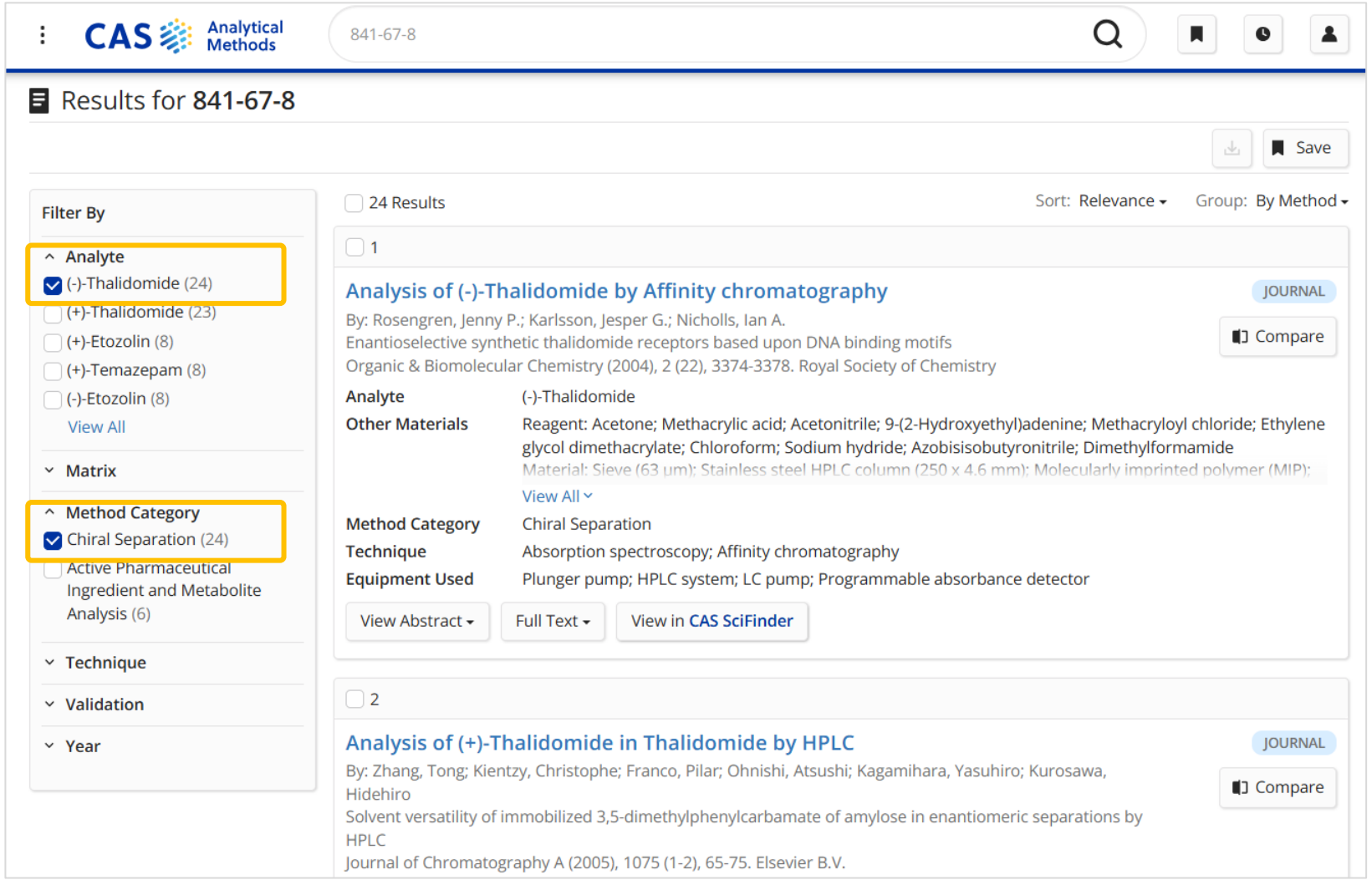
（续）案例2：手性化合物的制备与拆分

使用CAS Analytical Methods获取手性化合物拆分方法：https://methods.cas.org/

分析物

方法类别



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（续）案例2：手性化合物的制备与拆分

分析方法详情页

CAS Method Number
1-116-CAS-18769

Method Category
Chiral Separation

Technique
UV-visible spectroscopy; HPLC

Analyte	Matrix	Material	Reagent	Biological Reagent
(-)-Thalidomide (+)-Thalidomide	Thalidomide	Chiralpak IA	-	-

分析物　基质　所用材料

Equipment Used

HPLC system, D-7000, Merck Hitachi

Auto-sampler, L- 7200, Merck Hitachi

Pump, L-7100, Merck Hitachi

Ultraviolet detector, L-7400, Merck Hitachi

Column oven, L-7300, Merck Hitachi

HPLC system, 1100, Agilent

Quaternary pump, Agilent

Vacuum degasser, Agilent

Column oven, Agilent

Multiple wavelength UV detector, Agilent

Auto-sampler, Agilent

所用仪器

Instructions

High performance liquid chromatography - UV detection procedure using methyl *t*-butyl ether (MtBE)/1,4-dioxane 90/10 v/v as mobile phase

1. Analyze the sample using HPLC unit Agilent 1100 series apparatus equipped with a quaternary pump, a vacuum degasser, a column oven, a multiple wavelength UV detector, an auto-sampler and a HP Chemstation software.
2. Perform separation on analytical CHIRALPAK IA column (250 mm x 4.6 mm (I.D.)) by Daicel Chemical Industries Ltd. (Japan).
3. Use methyl *t*-butyl ether (MtBE)/1,4-dioxane 90/10 v/v as mobile phase.
4. Set the flow rate at 1.0 mL/min.
5. Maintain the temperature at 25 °C.
6. Perform detection at a wavelength of 300 nm.

实验步骤

Validation

数据验证

Separation Factor 1.65, (+)-Thalidomide/(-)-Thalidomide

Conditions

仪器测试条件

Instrument

Mobile phase - methyl *t*-butyl ether (MtBE)/1,4-dioxane 90/10 v/v; flow rate - 1.0 mL/min; temperature - 25 °C

Detection wavelength - 300 nm

Source

文献来源

JOURNAL

Solvent versatility of immobilized 3,5-dimethylphenylcarbamate of amylose in enantiomeric separations by HPLC
Zhang, Tong; Kientzy, Christophe; Franco, Pilar; Ohnishi, Atsushi; Kagamihara, Yasuhiro; Kurosawa, Hidehiro

Journal of Chromatography A (2005), 1075 (1-2), 65 - 75. Elsevier B.V.

CODEN : JCRAEY | ISSN : 00219673 | DOI : 10.1016/j.chroma.2005.03.116

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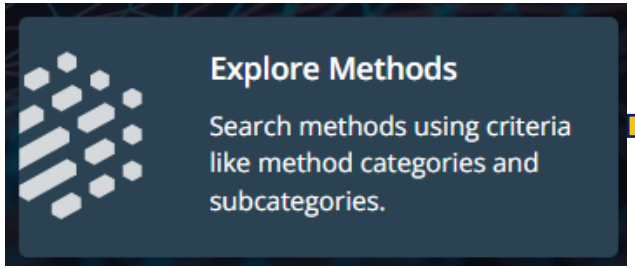
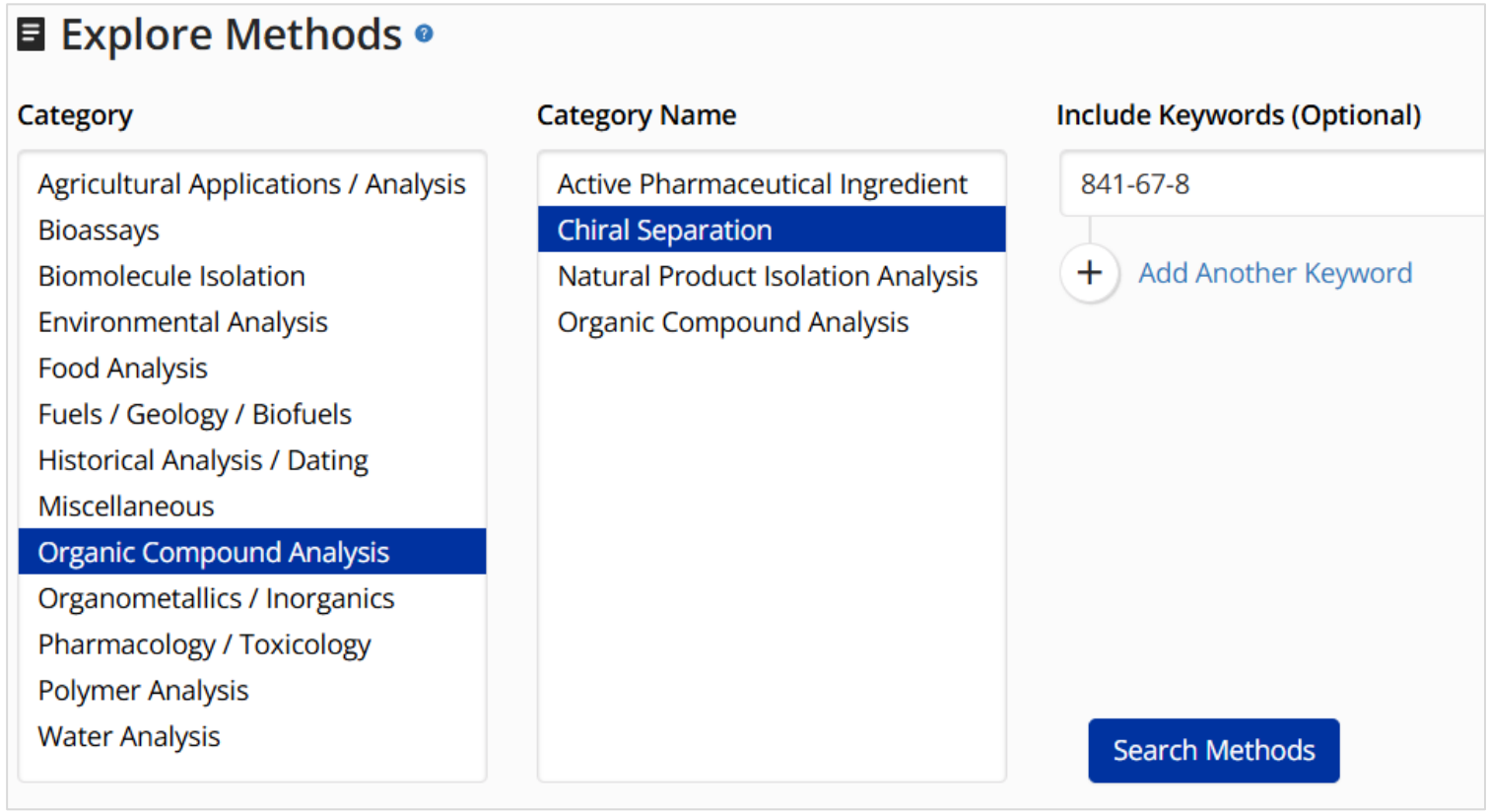
（续）案例2：手性化合物的制备与拆分

通过CAS Analytical Methods浏览分析方法类别，获取手性拆分分析方法实验





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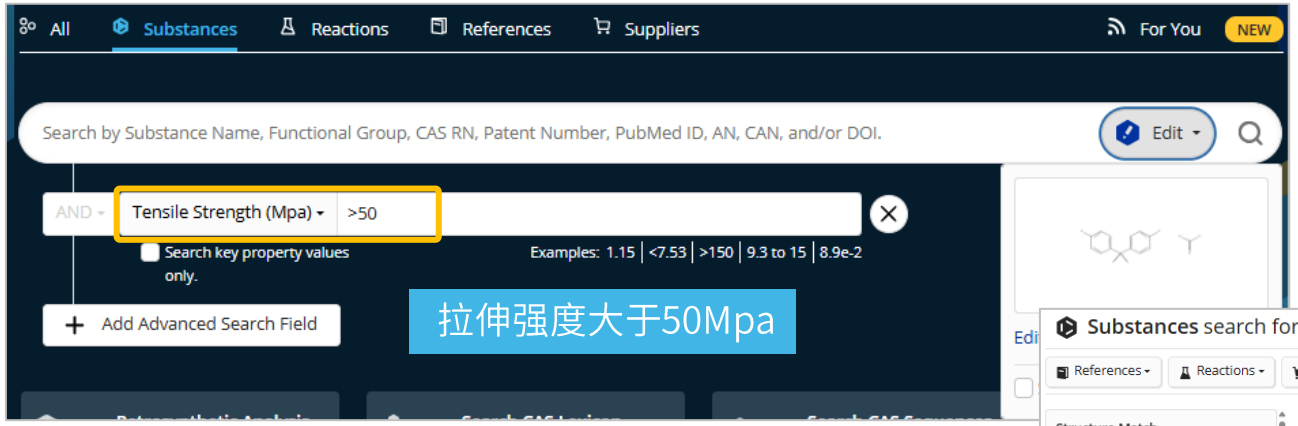
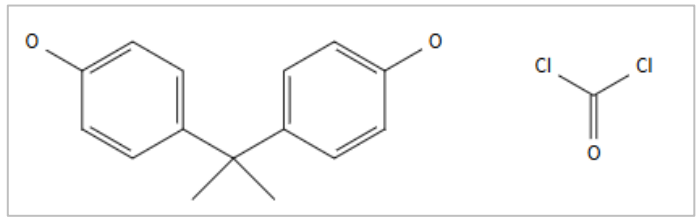
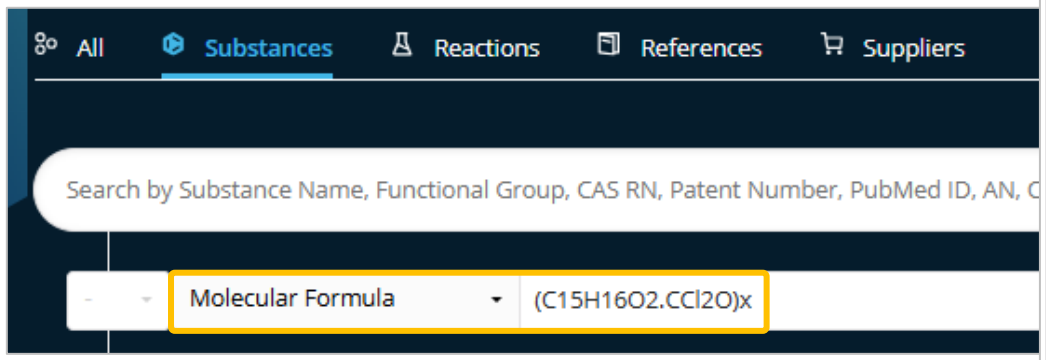
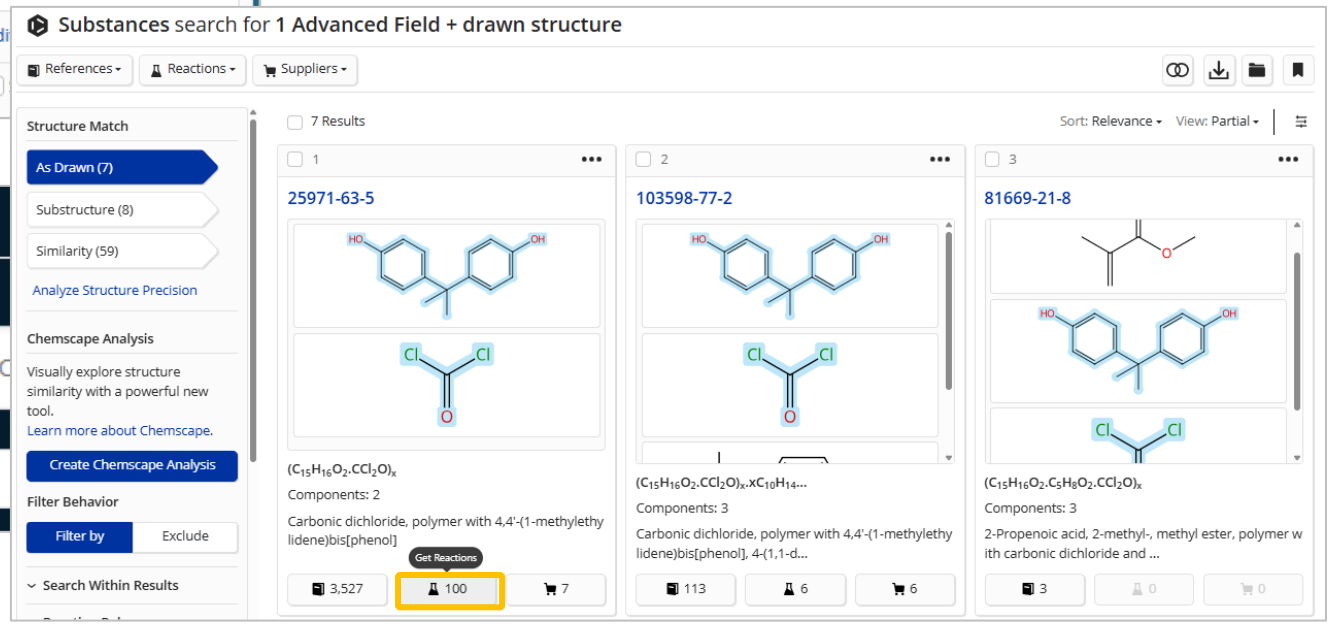
案例3：聚合物材料改性研究

通过单体结构、重复结构单元、分子式、属性等，多角度检索聚合物信息









(C2H4O)nC4H8O: 括号中是重复结构单元，括号外为n

(C15H16O2.CCl2O)x: 括号中是单体，括号外为x

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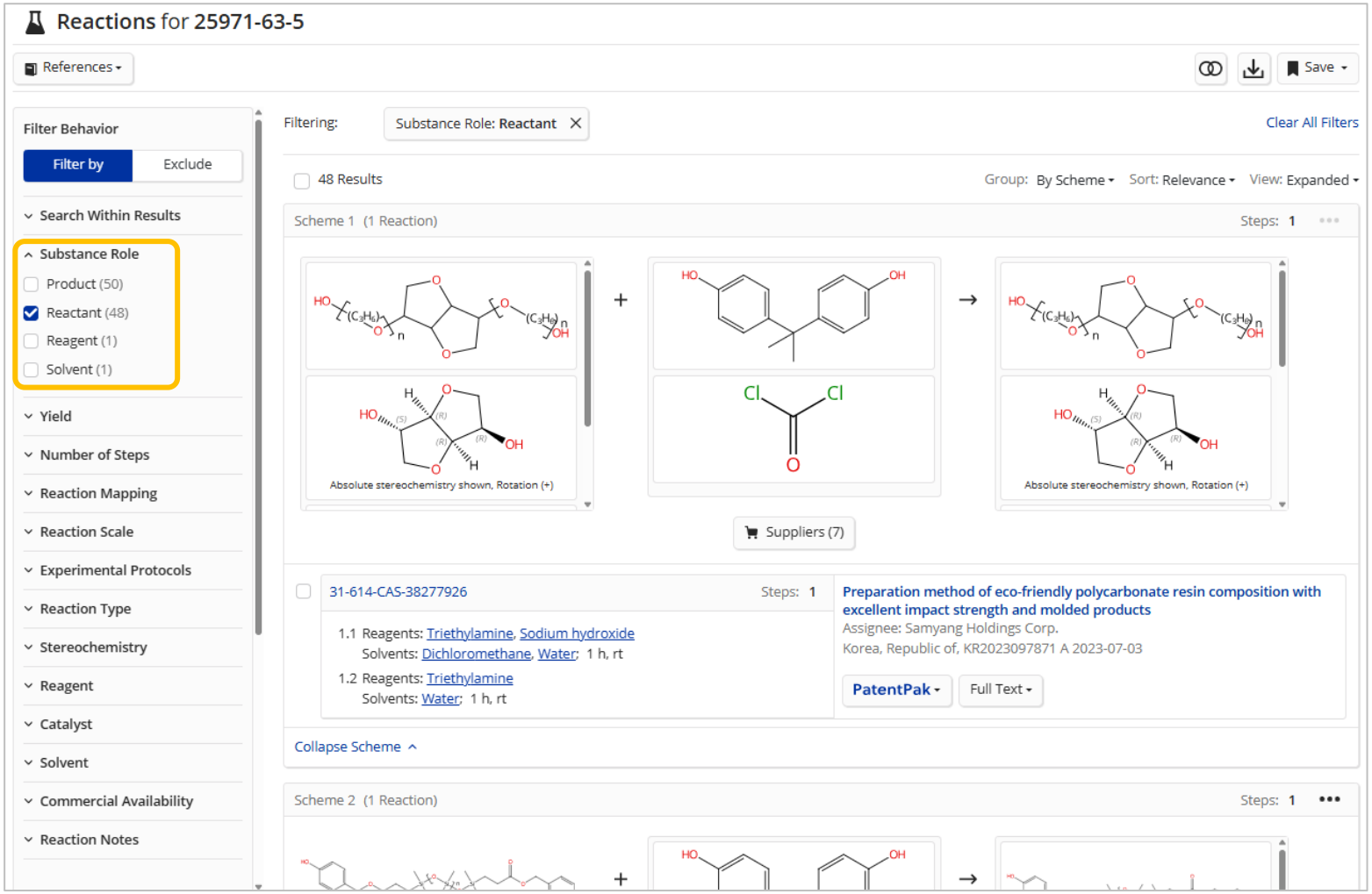
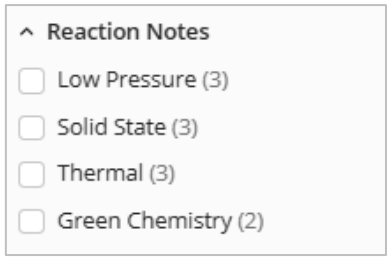
（续）案例3：聚合物材料改性研究

从聚碳酸酯物质出发，获取改性反应





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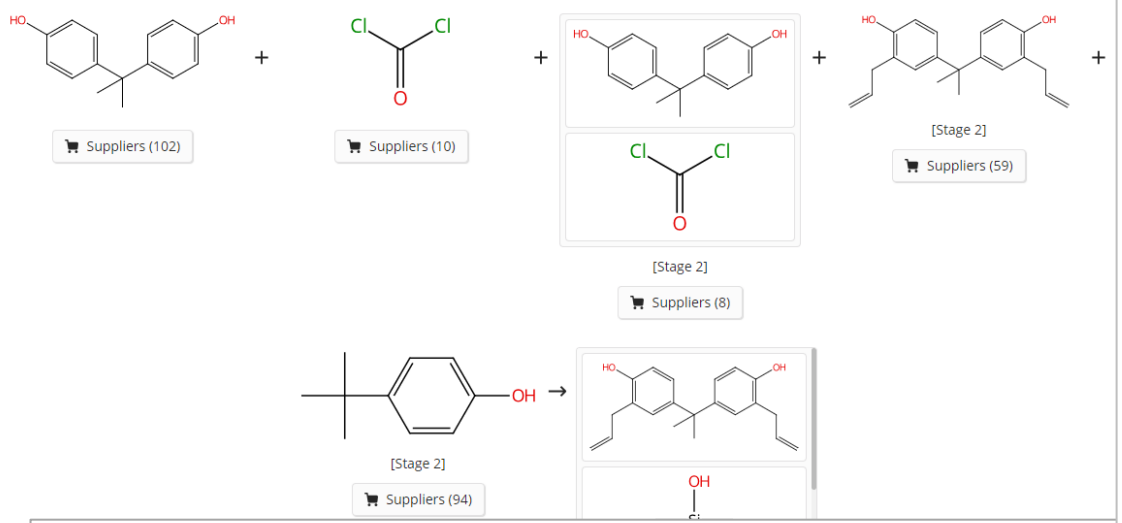
（续）案例3：聚合物材料改性研究

改性反应详情

CAS Reaction Number: 31-614-CAS-30579494



Step 1

Stage	Reagents	Catalysts	Solvents	Conditions
1	Sodium hydroxide	-	Dichloromethane Water	rt; 30 min, rt
2	Triethylamine Sodium hydroxide	-	Dichloromethane	3 h, rt
3	Triethylamine Sodium hydroxide	-	Dichloromethane Water	3 h, rt
4	Hydrochloric acid	-	Water	neutralized

Synthetic Methods | Experimental Procedure

Products	Carbonic dichloride, polymer with 1,1-dimethylsilanediol, 4,4'-(1-methylethylidene)bis[phenol] and 4,4'-(1-methylethylidene)bis[2-(2-propen-1-yl) phenol], graft
Reactants	Phosgene 2,2-Bis(4-hydroxyphenyl)propane 4-*tert*-Butylphenol *o,o'*-Diallylbisphenol A Carbonic dichloride, polymer with 4,4'-(1-methylethylidene)bis[phenol]
Reagents	Sodium hydroxide Triethylamine Hydrochloric acid
Solvents	Dichloromethane Water
Procedure	1. Add bisphenol A (114 g) and 5.4 wt% aqueous NaOH solution (44.8 g, 1.12 mol) to a 3 L of three-necked round bottomed flask that is filled with a nitrogen inlet and ice jacket. 2. Add phosgene (64.35 g) dissolved in 950 mL of methylene chloride slowly to the solution. 3. Stir the mixture for 30 minutes. 4. Separate the methylene chloride and water layers. 5. Place 50 mL of methylene chloride layer (bischloroformate 0.061 mol, 95 mol%) and 75 mL of aqueous layer in a 500 mL of three necked round bottomed flask. 6. Add 30 µL of triethylamine (15%, w/v), 0.988 g of diallyl bisphenol A (0.00321 mol, 5 mol%) dissolved in a 10 mL of NaOH solution (0.32 g, 8 mmol) and 0.2516 g of p-tert-butyl phenol (1.68 mmol), which is also dissolved in a 10 mL of NaOH solution (0.08 g, 2 mmol) to the reaction mixture. 7. Use p-tert-butyl phenol as a molecular weight controller. 8. Stir the reaction mixture for 3 hours at room temperature by using a mechanical stirrer (stirring speed 500 r.p.m). 9. Separate the methylene chloride layer. 10. Add 37 µL of triethylamine, 10 mL of methylene chloride and 2.05 g of NaOH in 15 mL of distilled water to the separated methylene chloride solution. 11. Stir the mixture for 3 hours at room temperature. 12. Wash the polymer solution with distilled water. 13. Neutralize the polymer solution with HCl. 14. Precipitate the polymer solution into a mixture of acetone and distilled water (50:50, v/v).
Scale	gram

反应中的重要物质及角色

详细的实验步骤、操作过程与表征信息

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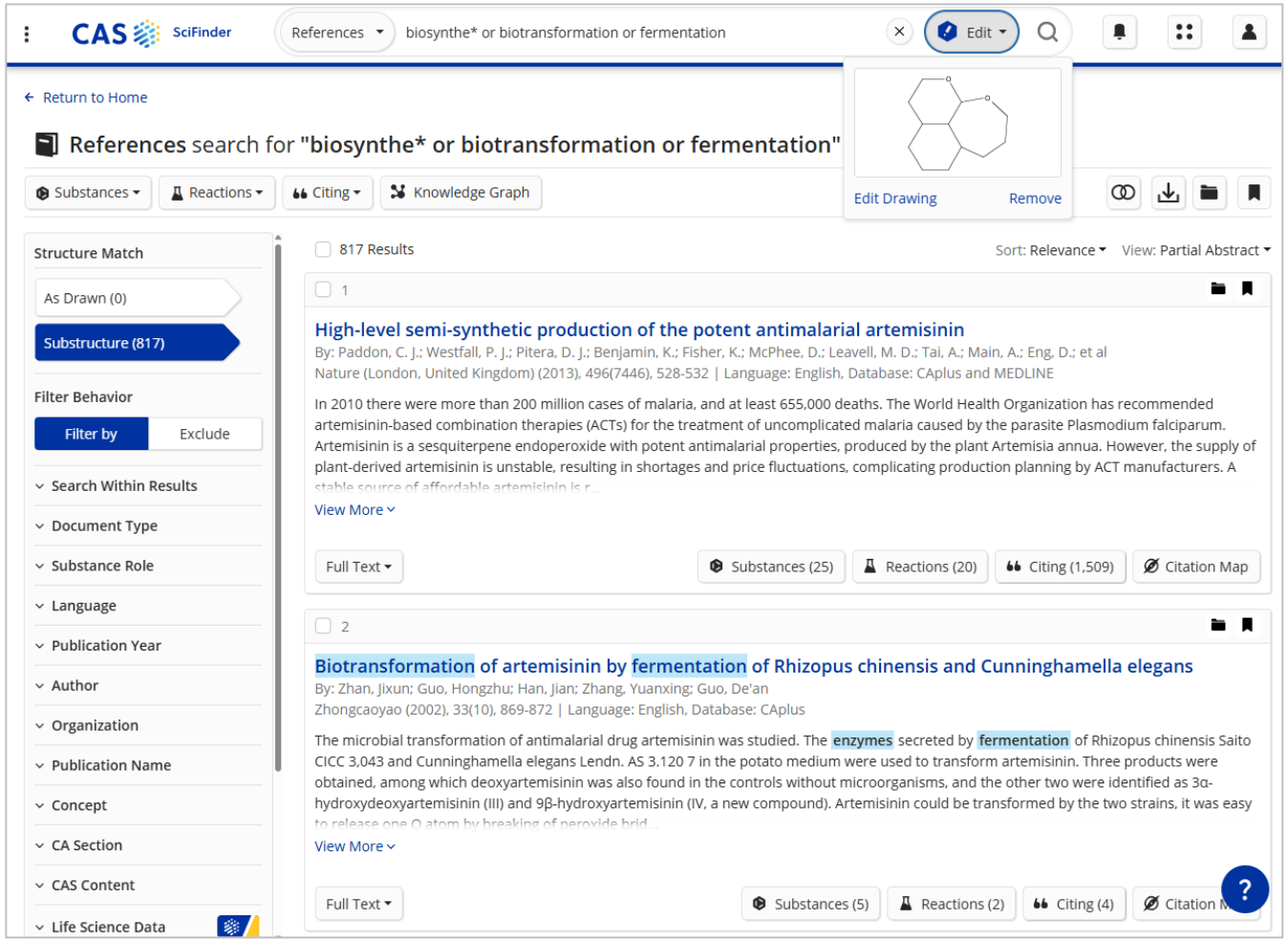
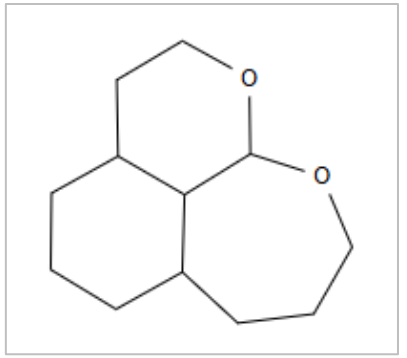
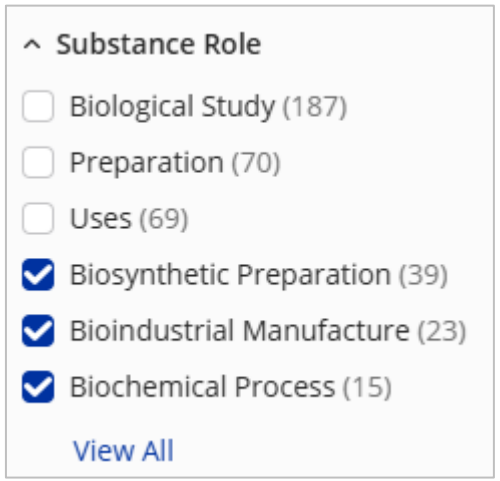
案例4：生物合成与生物转化反应检索

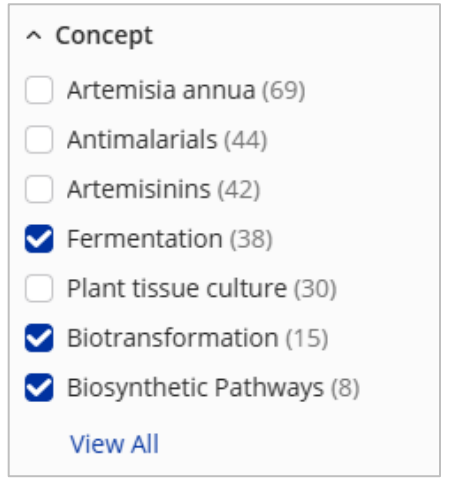
结构+关键词联用，精确查找与发酵/生物合成/生物转化相关，并涉及特定化合物结构的文献



例：biosynthe* or biotransformation or fermentation







浏览CAS科学家标引的信息，聚焦物质在文献中的研究角色及文献核心研究点

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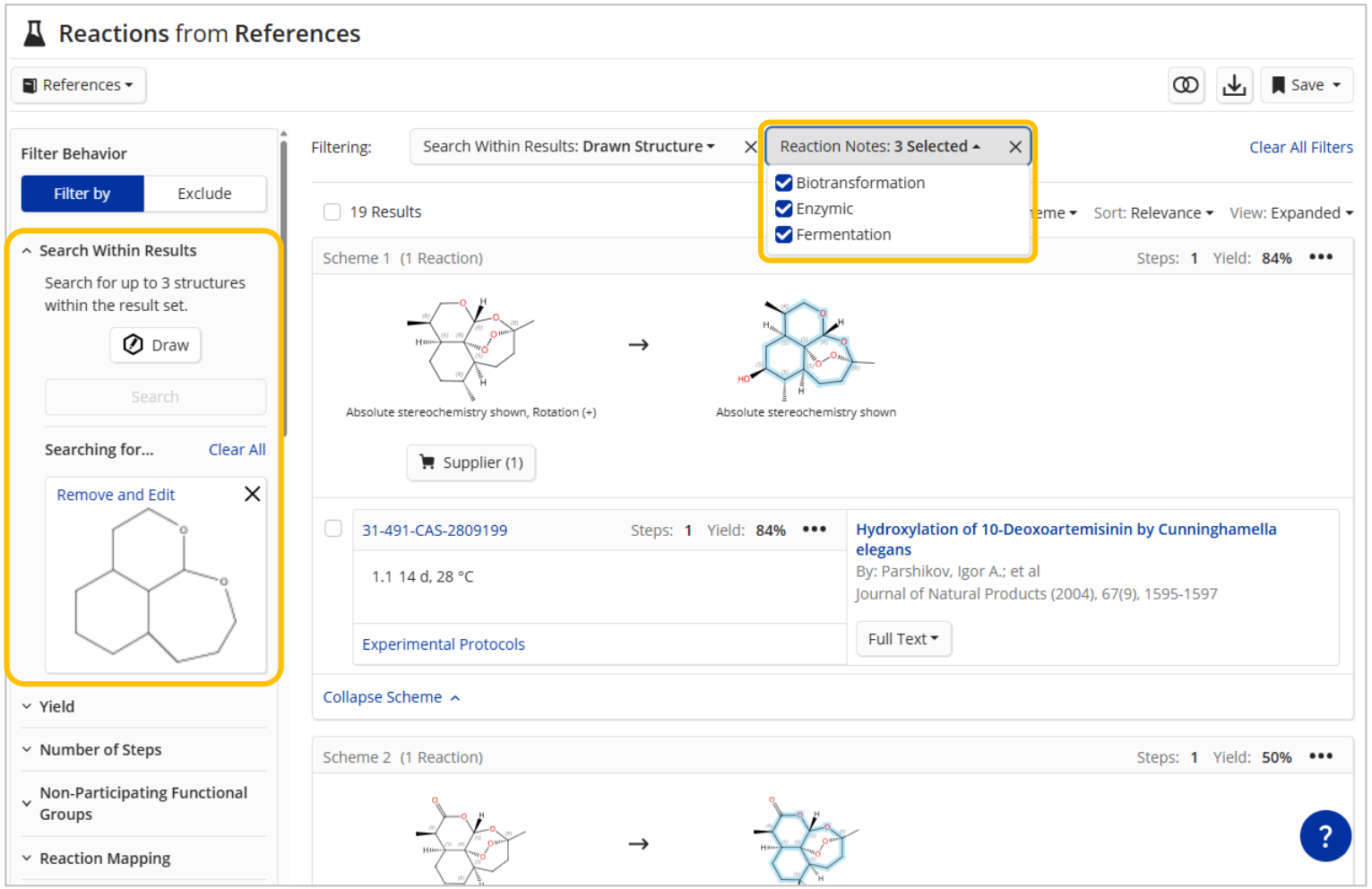
（续）案例4：生物合成与生物转化反应检索

获取文献相关反应：便捷筛选生物反应



Reaction Notes中Biotransformation、Enzymic、Fermentation等助力快捷获取生物转化类反应

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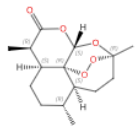
（续）案例4：生物合成与生物转化反应检索

获取反应步骤对应的科学家标引的注释和反应条件，助力快速了解生物转化过程

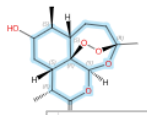
CAS Reaction Number: 31-491-CAS-429775

Get Similar Reactions

Save



Absolute stereochemistry shown



Suppliers (96)

Synthetic Methods

Products	(3*R*,5a*S*,6*S*,8a*S*,9*R*,12*S*,12a*R*)-Octahydro-7-hydroxy-3,6,9-trimethyl-3,12-epoxy-12*H*-pyrano[4,3-*j*]-1 -one
Reactants	Artemisinin
Solvents	Ethanol Water
Procedure	1. Grow elegans at 28°C in 20 500 mL culture flasks with each flask containing 200 mL of medi 2. Distribute a total of 1000 mg of artemisinin (in 40 mL of ethanol) among the 24 h-old stage l 3. Pool the incubation mixtures and filter to remove the cells. 4. Extract the filtrate (4 L) three times with ethyl acetate. 5. Dry the combine extracts over anhydrous Na_2SO_4 and evaporate to dyness at 35°C under re obtain crude product. 6. Purify the residue with a silica gel column (30 g, 25 cm) using a petroleum ether (60-90°C) -e mixture as the eluting system to obtain product.
Transformation	Hydroxylation at an Aliphatic Carbon
Scale	gram

Characterization Data

(3*R*,5a*S*,6*S*,8a*S*,9*R*,12*S*,12a*R*)-Octahydro-7-hydroxy-3,6,9-trimethyl-3,12-epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one

Proton NMR Spectrum	($CDCl_3$, 300 MHz): δ5.94 (1 H, s), 3.37 (1 H, m), 3.24 (1 H, m), 2.43 (1 H, m), 2.1 (1 H, m), 1.9-2.1 (1 H, m), 1.9-2.1 (2 H, m), 1.3-1.6 (1 H, m), 1.3-1.6 (2 H, m), 1.47 (3 H, s), 1.0-1.2 (2 H, m), 1.19 (3 H, d), 1.10 (3 H, d);
Carbon-13 NMR	($CDCl_3$, 75 MHz): δ171.6, 105.4, 93.4, 78.6, 73.5, 47.9, 44.4, 42.1, 35.7, 32.5, 32.1, 25.7, 24.7, 15.4, 12.3
HRMS	(ES) calcd for $C_{15}H_{22}NaO_6$ $(M + Na)^+$ 321.1309, found, 321.1313;
State	bown residue

CAS Method Number 3-491-CAS-429775

Transformations
1. Hydroxylation at an Aliphatic Carbon

Reaction Notes
biotransformation, literature preparation, whole cells of Cunninghamella elegans used, described medium

科学家标引的Notes帮助快速了解生物转化过程，包括：菌种、介质、代谢途径、酶等

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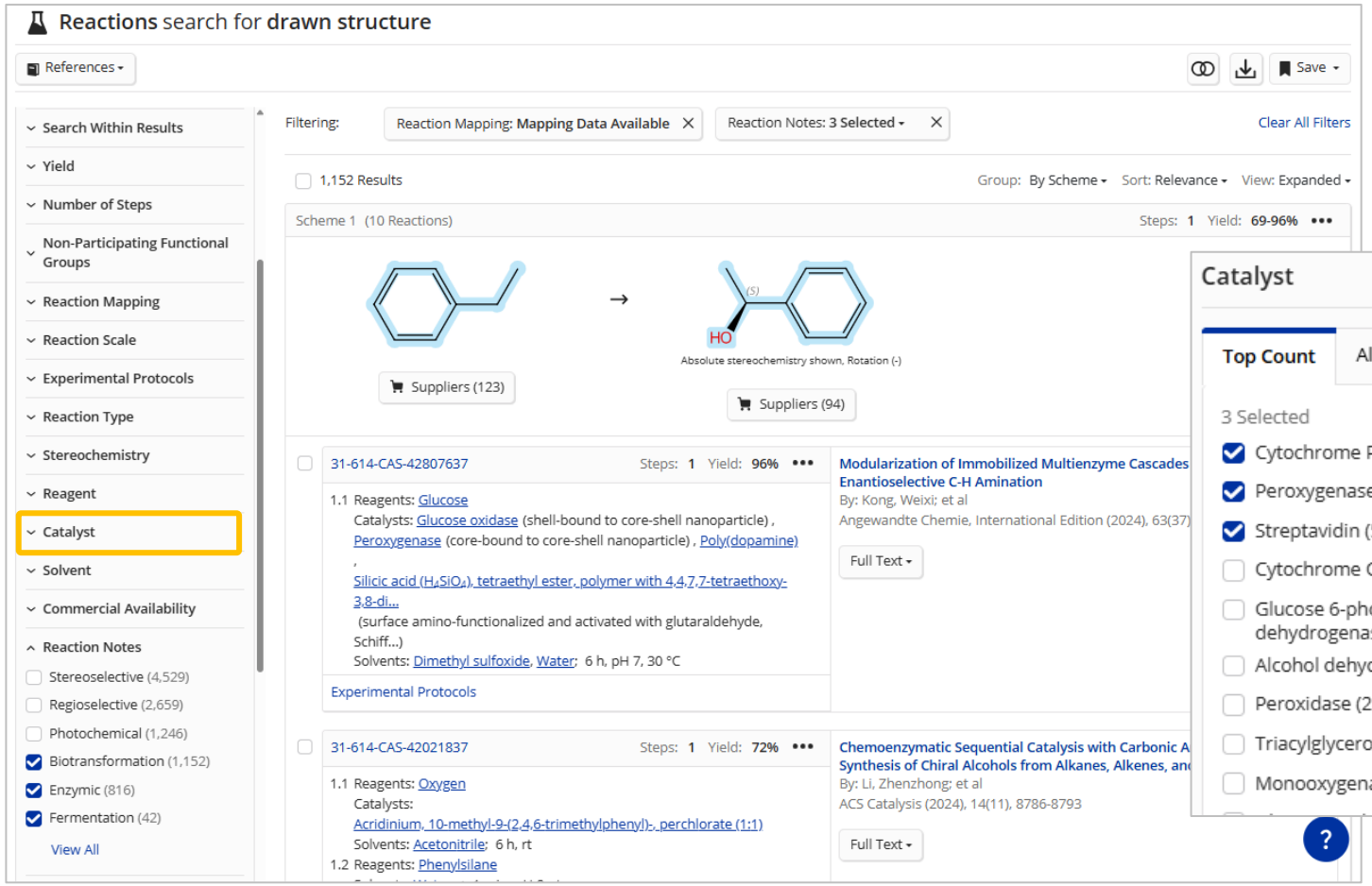
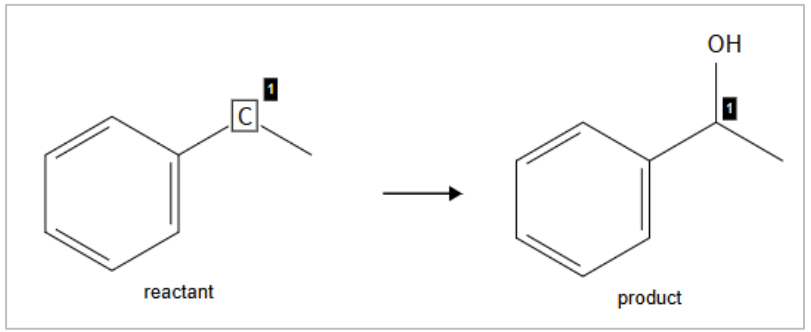
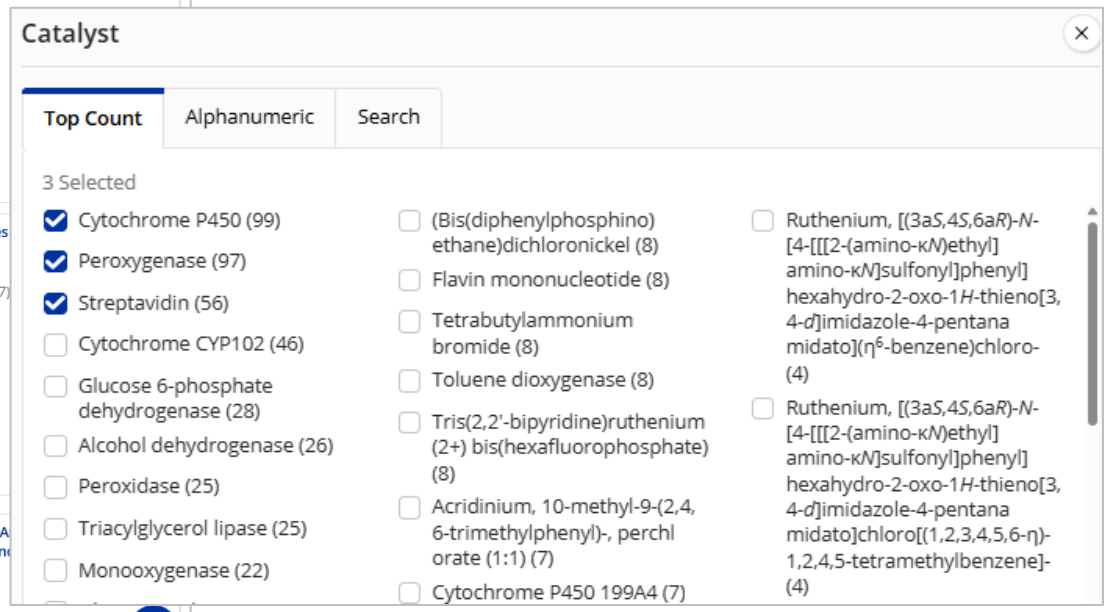
（续）案例4：生物合成与生物转化反应检索

浏览&聚焦感兴趣的生物反应催化剂







酶、菌、肽/蛋白、或其他化学催化剂

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总结

反应检索策略

- 灵活通过物质标识符、文献号、构建结构式或反应式等多种策略，满足各种场景下的反应检索需求。
- 支持通过自然语言，高效便捷检索某种或某一类目标化合物的反应。
- 通过相似反应拓展，获取更多相似反应路线支持，助力获取最合适的反应。
- 利用数据关联，从物质或文献出发，灵活获取不同物质种类或不同研究领域的反应信息。
- 获取已知化合物或新化合物的逆合成路线，进行更多反应路线与合成工艺拓展。

反应结果分析策略

- 利用丰富的反应结果分组与聚类分析选项，可多维度查看反应结果，助力全方位纵览所有报道反应的技术全貌，并进行筛选聚焦。
- 通过CAS科学家标引的Synthetic Methods，无需阅读原文，直接获取实验步骤详情及产物表征等信息。
- 基于反应、物质、文献之间的深度关联，并通过CAS科学家标引的聚类分析选项，高效完成关注领域的信息检索。

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Between problems and progress are connections that matter

are connections that matter

谢 谢!

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