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通过SciFinder高效获取合成制备信息

SCIFINDER®
A CAS SOLUTION

提纲

- SciFinder中获取化合物制备信息的方法
- 反应相关信息获取方法
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何通过反应式检索反应，精炼结果并获得实验详情
  - 利用SciPlanner实现反应路线设计
  - 反应检索案例分享
- 通过文献主题检索合成制备相关信息的方法

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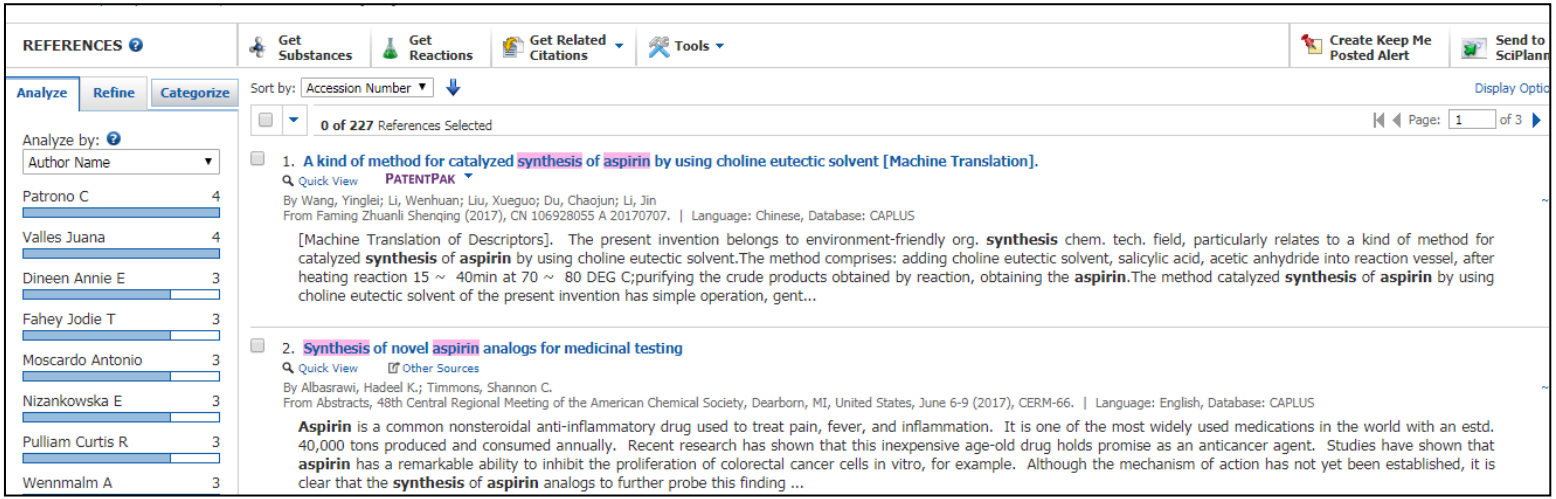
在SciFinder中，检索化合物制备信息主要有4种方式：

方法1：在文献检索Research Topic中输入preparation of 50-78-2或者synthesis of aspirin进行检索



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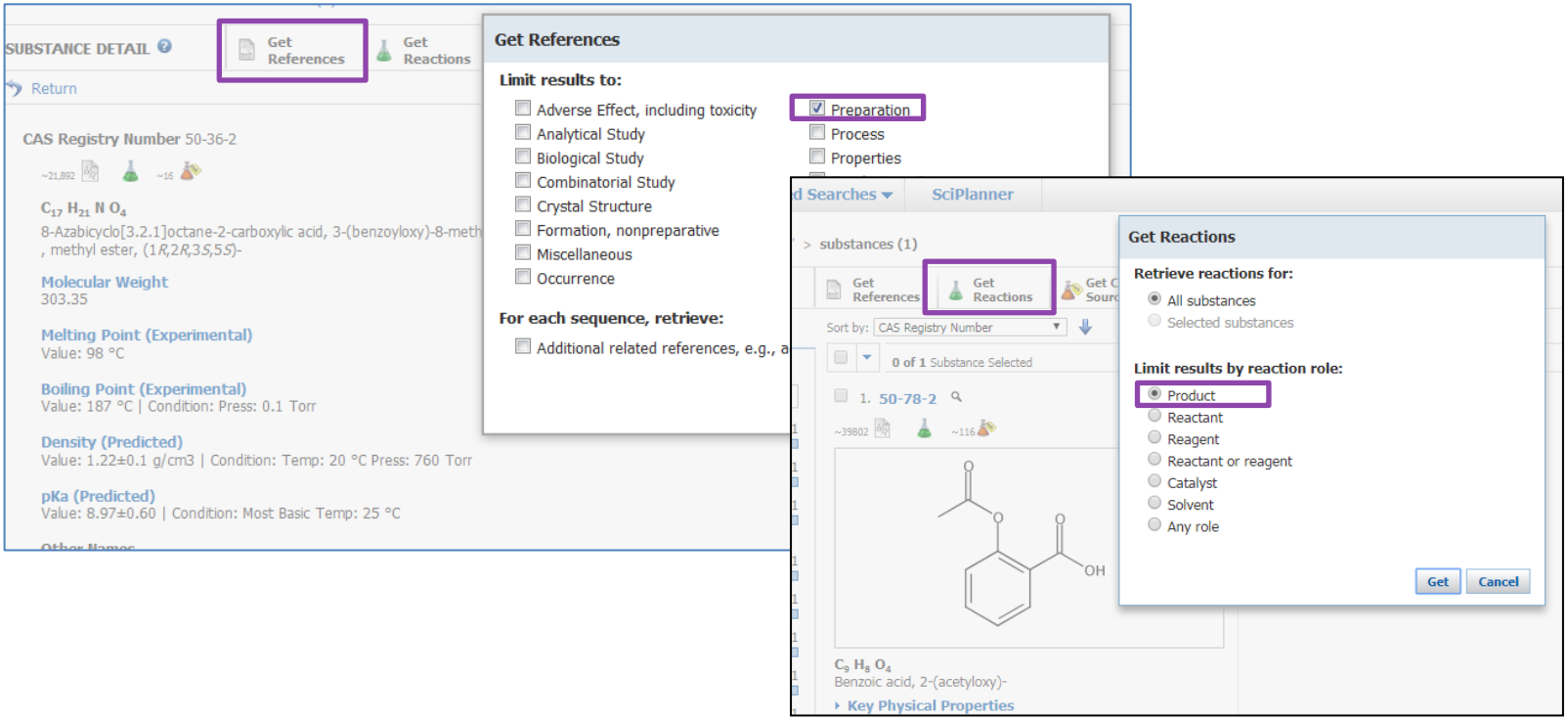
方法2：检索物质后，在物质信息详情页面，可以由此物质获得制备(preparation)相关文献或者产物为此物质的反应。



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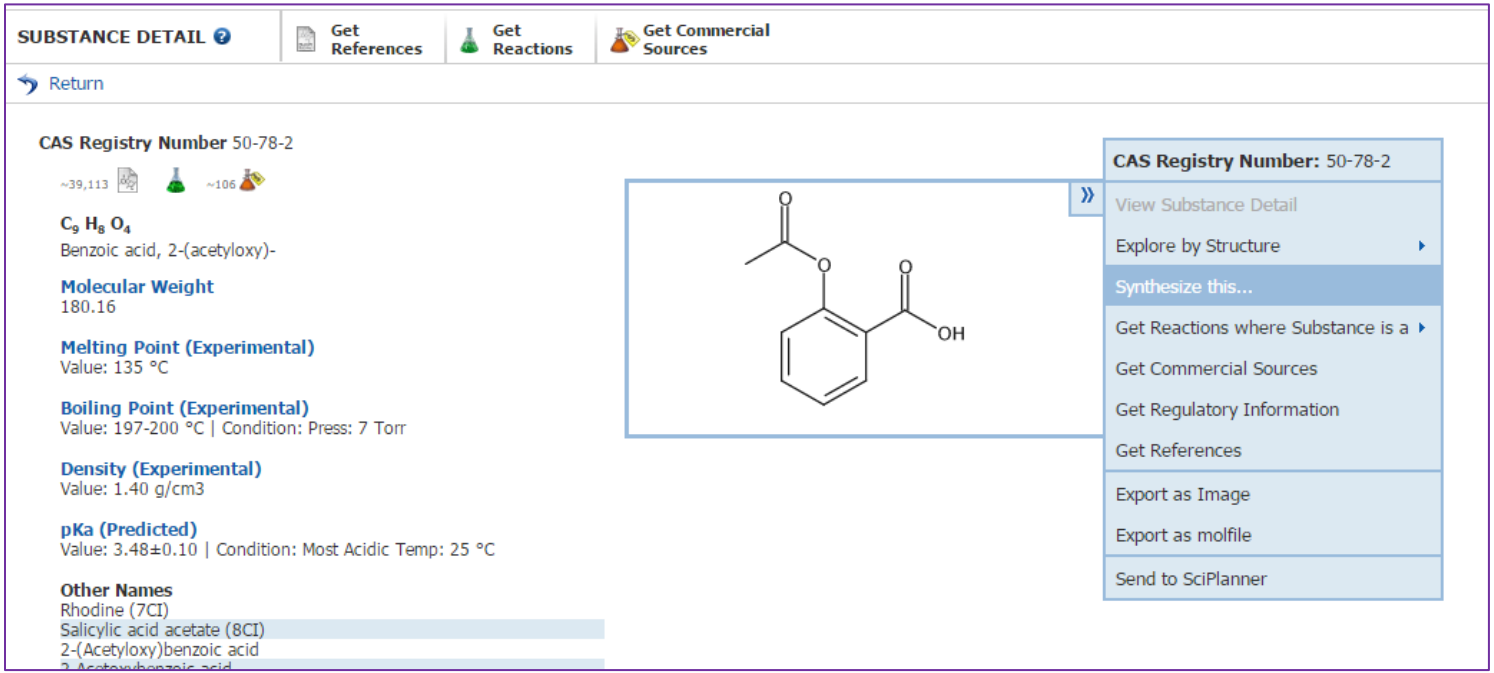
方法3：也可以点击物质结构右上角的蓝色双箭头，点击Synthesis this，获得相关反应



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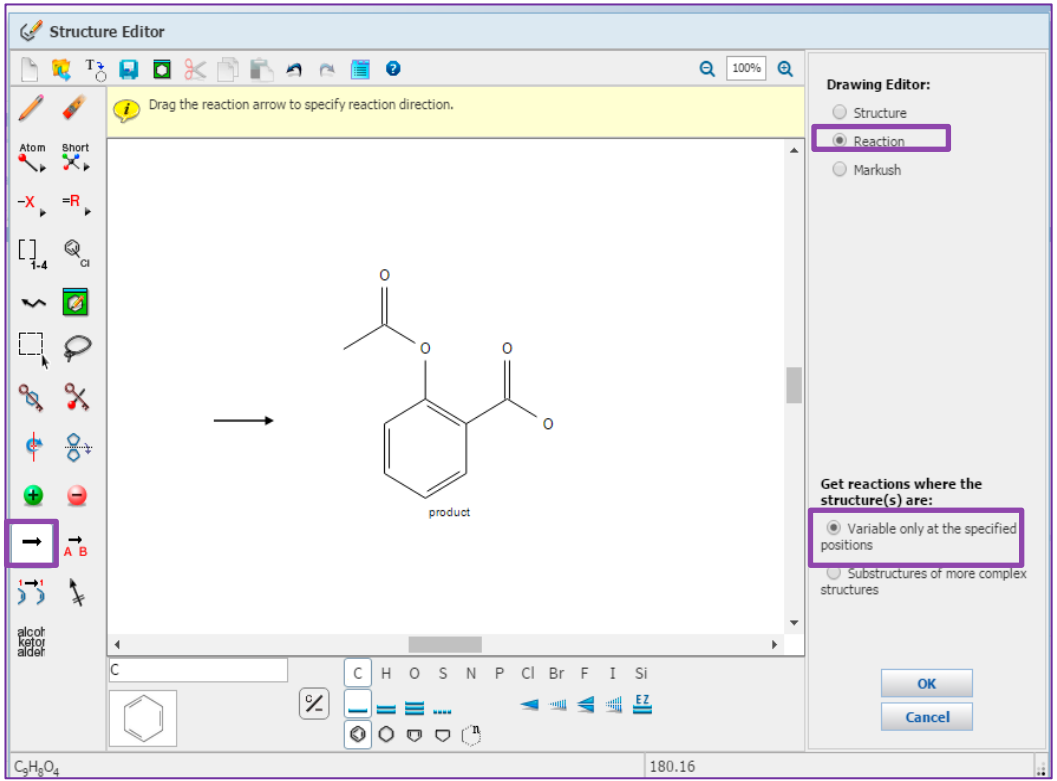
方法4：在SciFinder反应检索编辑器中绘制结构，获得反应。



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小结：获取化合物制备信息的方法

方法1：基于物质名称和主题词获取到合成制备信息；

方法2：基于物质的CAS号检索合成制备信息；

方法3：在CAS REACT中获取到该结构的精确合成信息；

方法4：在CAS REACT中获取到该结构的精确反应信息、该结构的盐、同位素、立体构型等合成信息。

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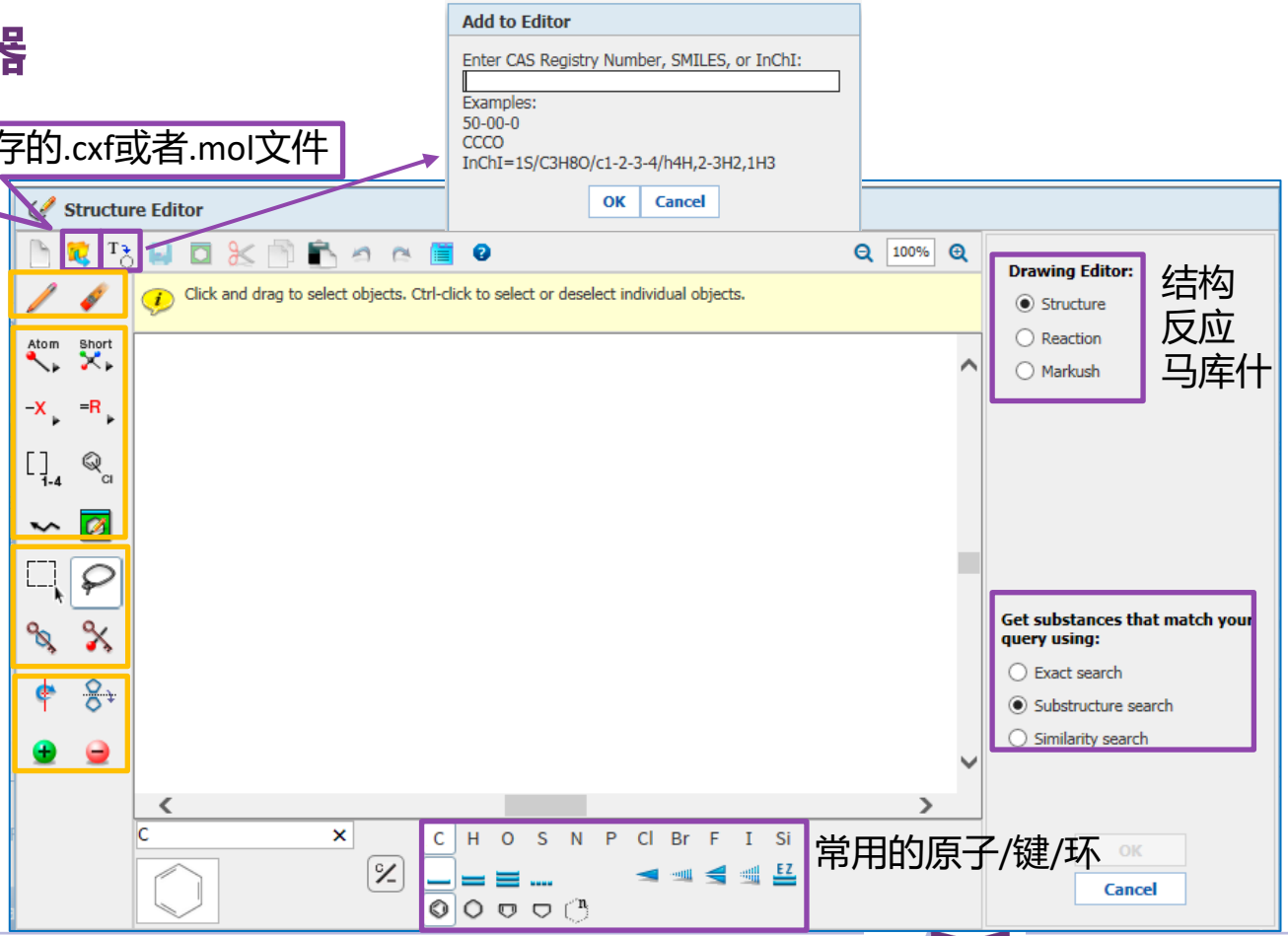
结构编辑器

直接导入已保存的.cxf或者.mol文件



画笔/橡皮

画图工具

选中工具
锁定工具

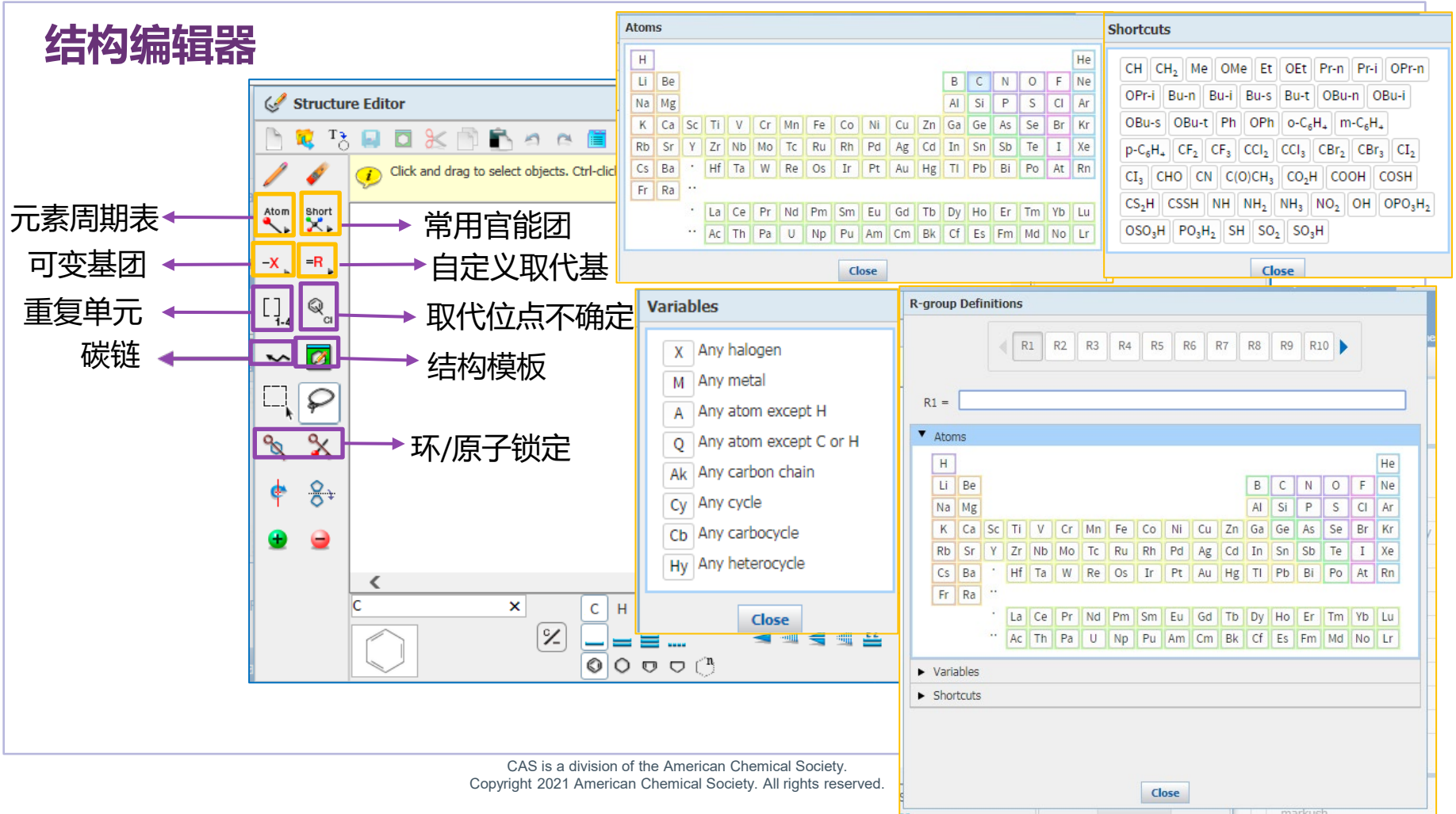
旋转/翻转
阴阳离子

结构
反应
马库什

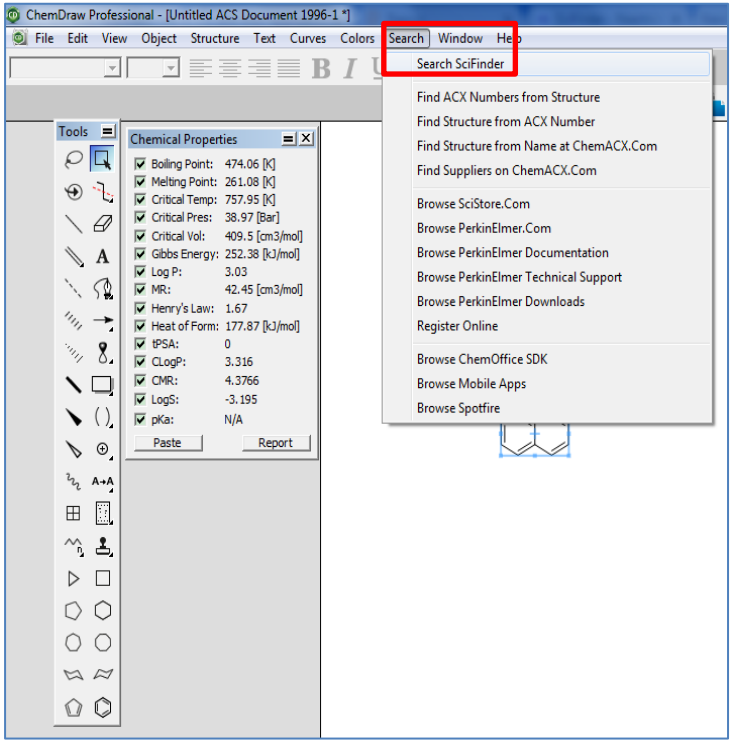
常用的原子/键/环

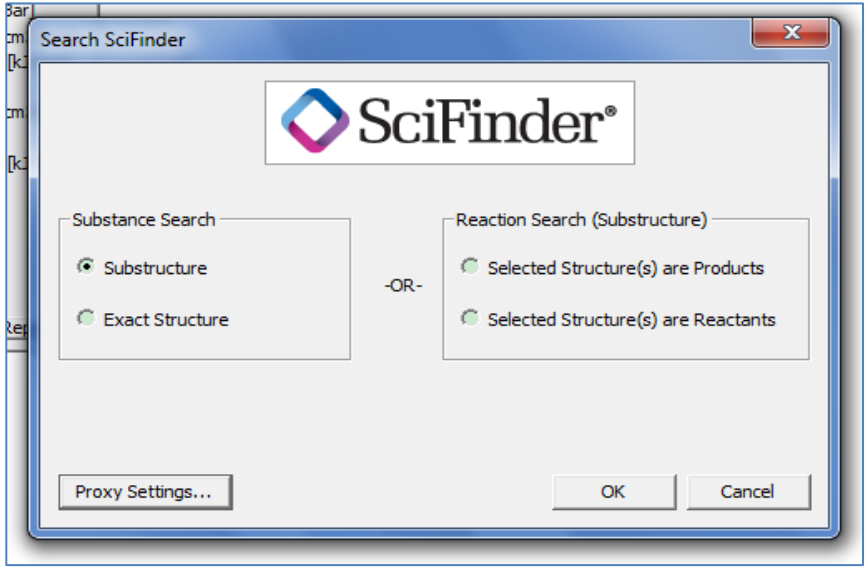
A CAS SOLUTION

结构编辑器



Chemdraw 14.0以上正版用户可以直接在chemdraw里边画结构然后在SF中检索





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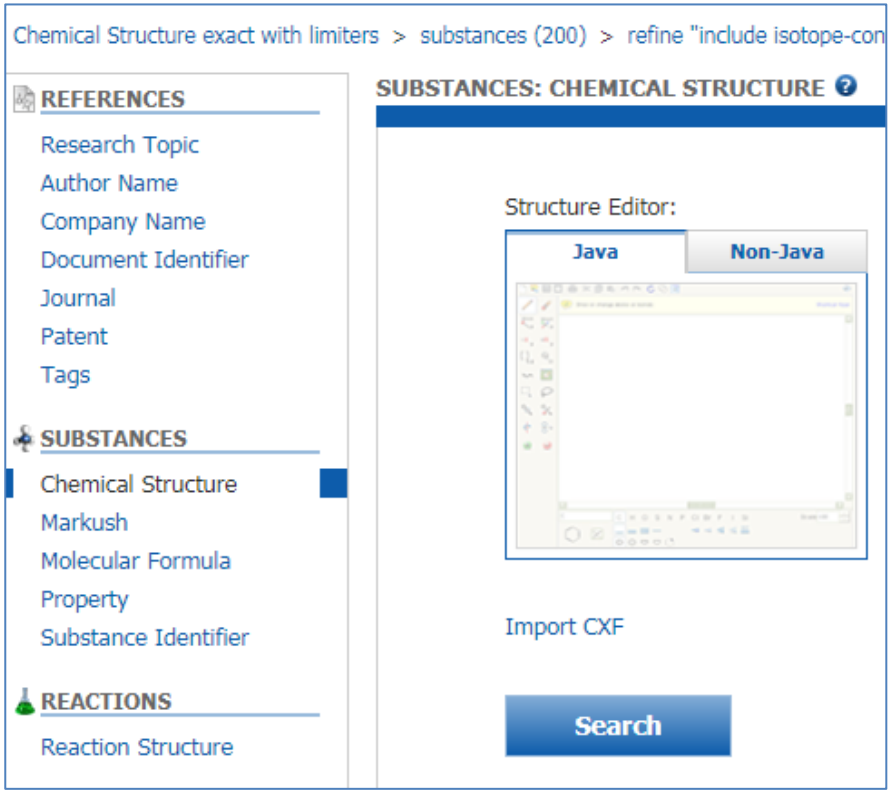
如果想用复制/粘贴功能，请在java条件下运行结构编辑器，并且保证Java及时更新



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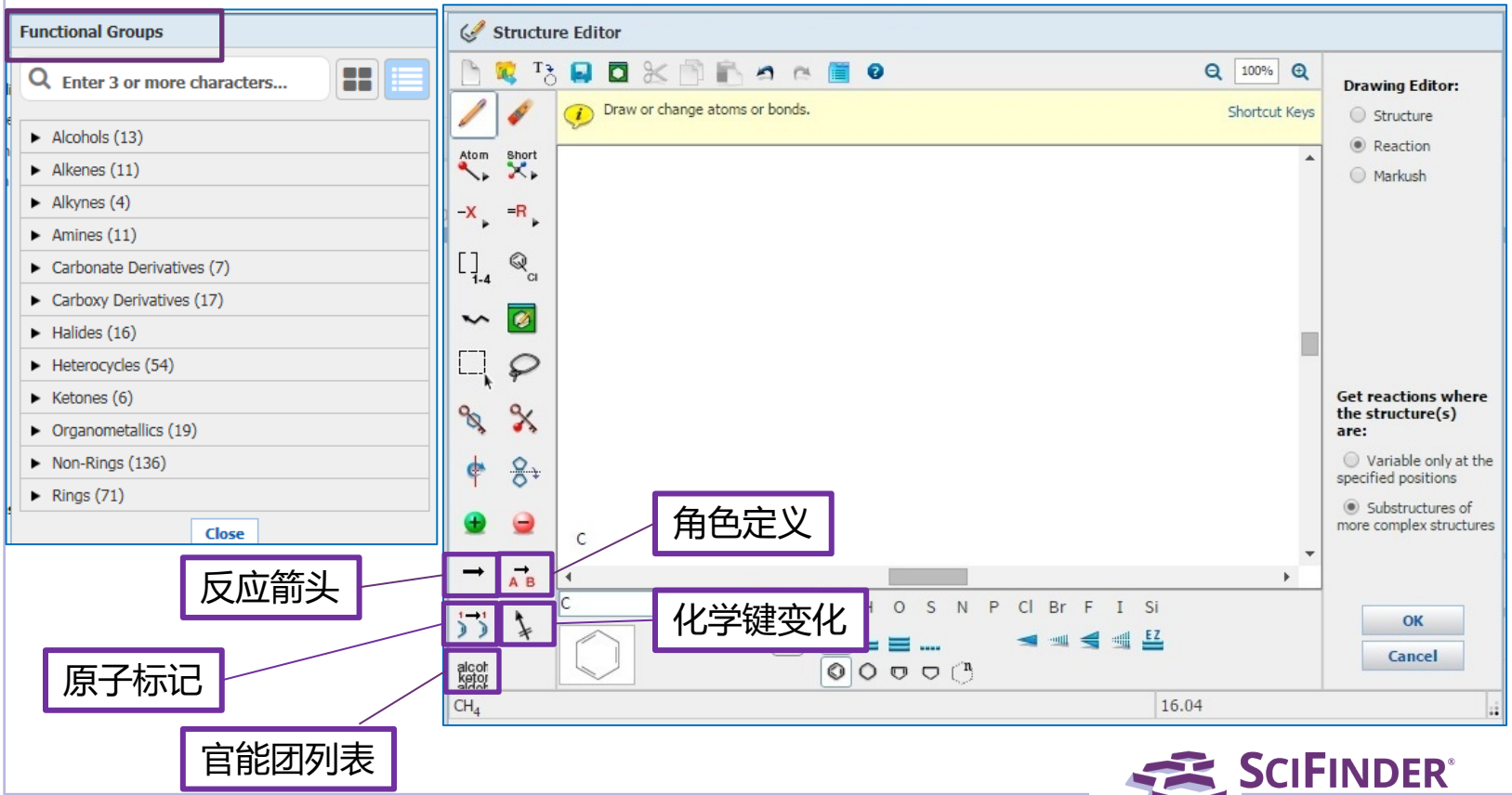
结构编辑器：绘制反应工具



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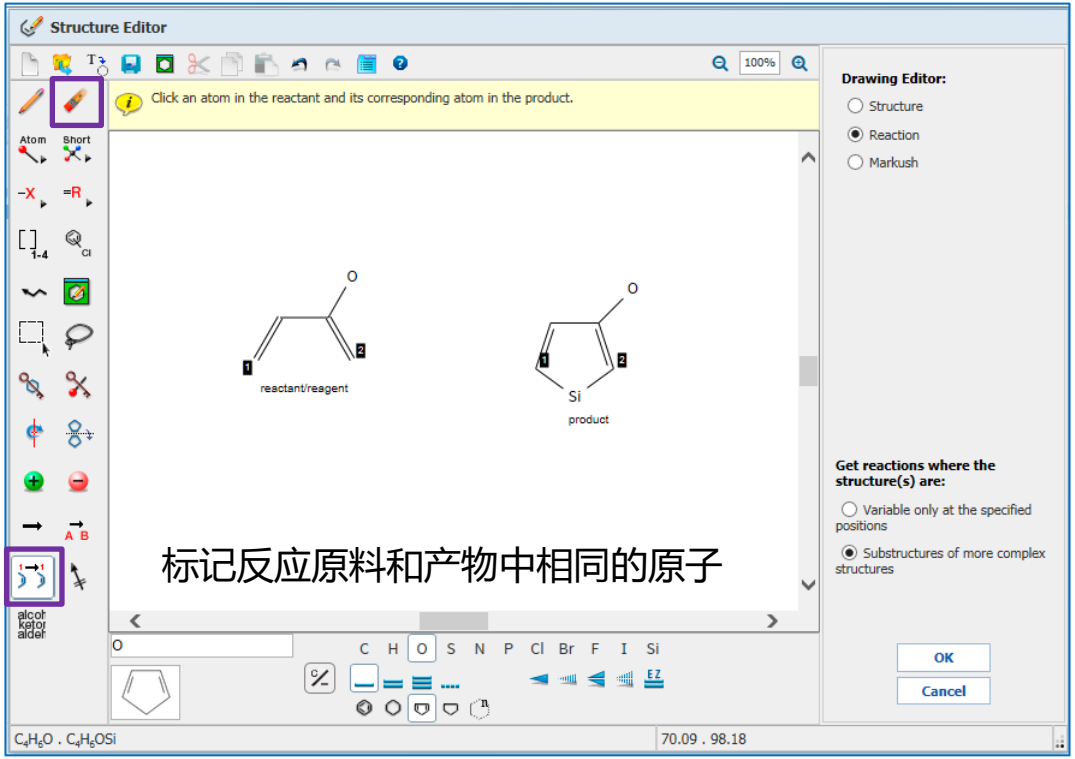
例：反应前后物质中的原子标记



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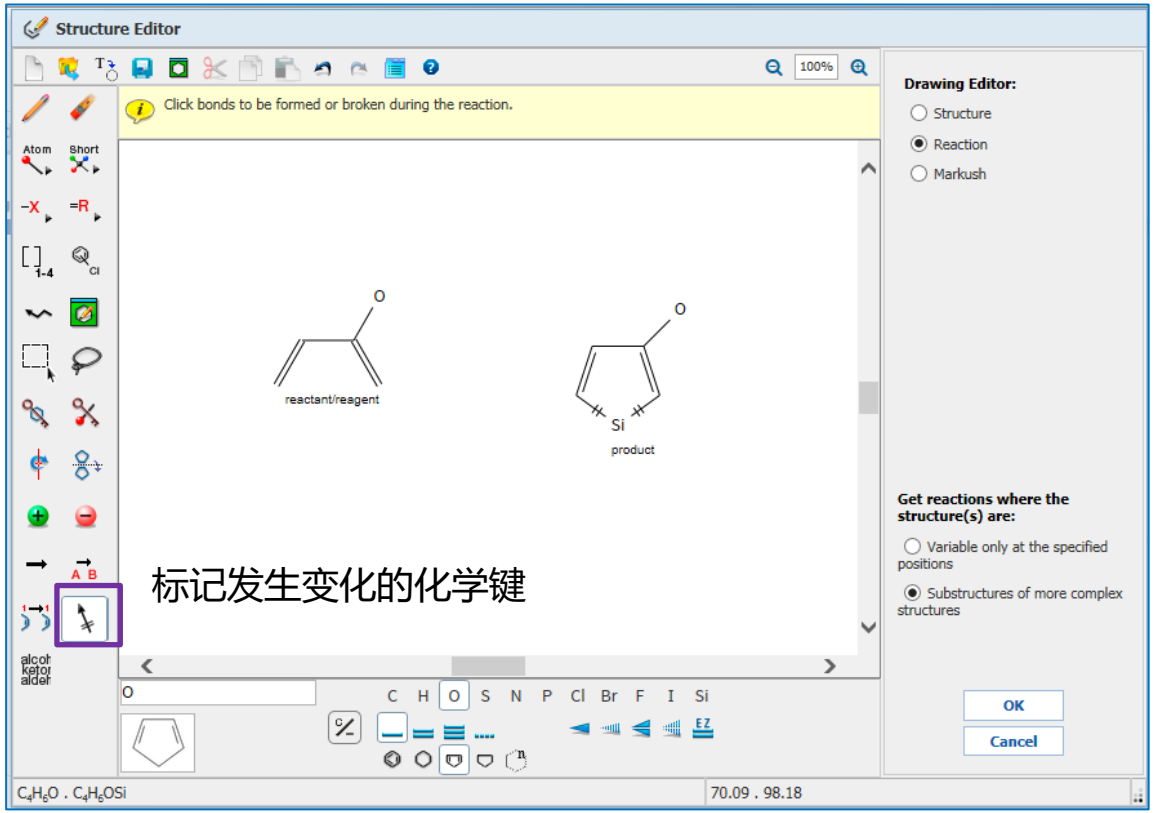
例：发生变化的化学键标记



标记发生变化的化学键

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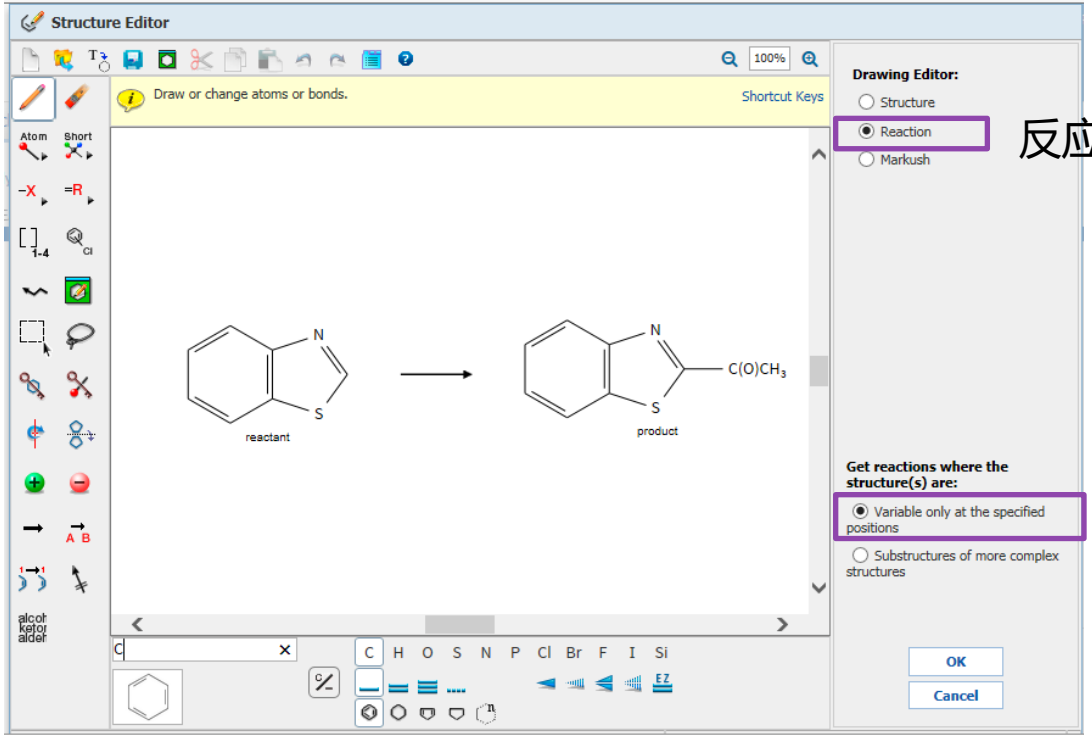
精确结构反应检索：绘制反应式



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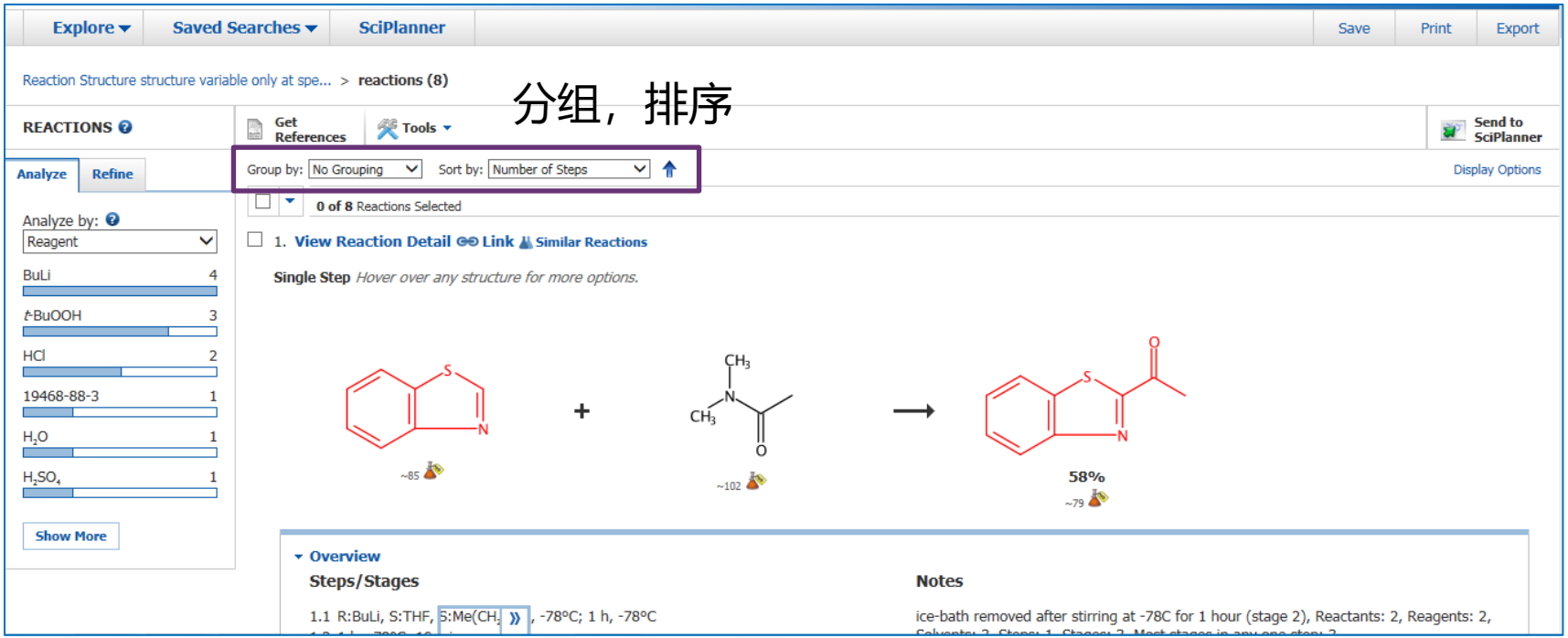
精确结构反应检索：查看反应结果集



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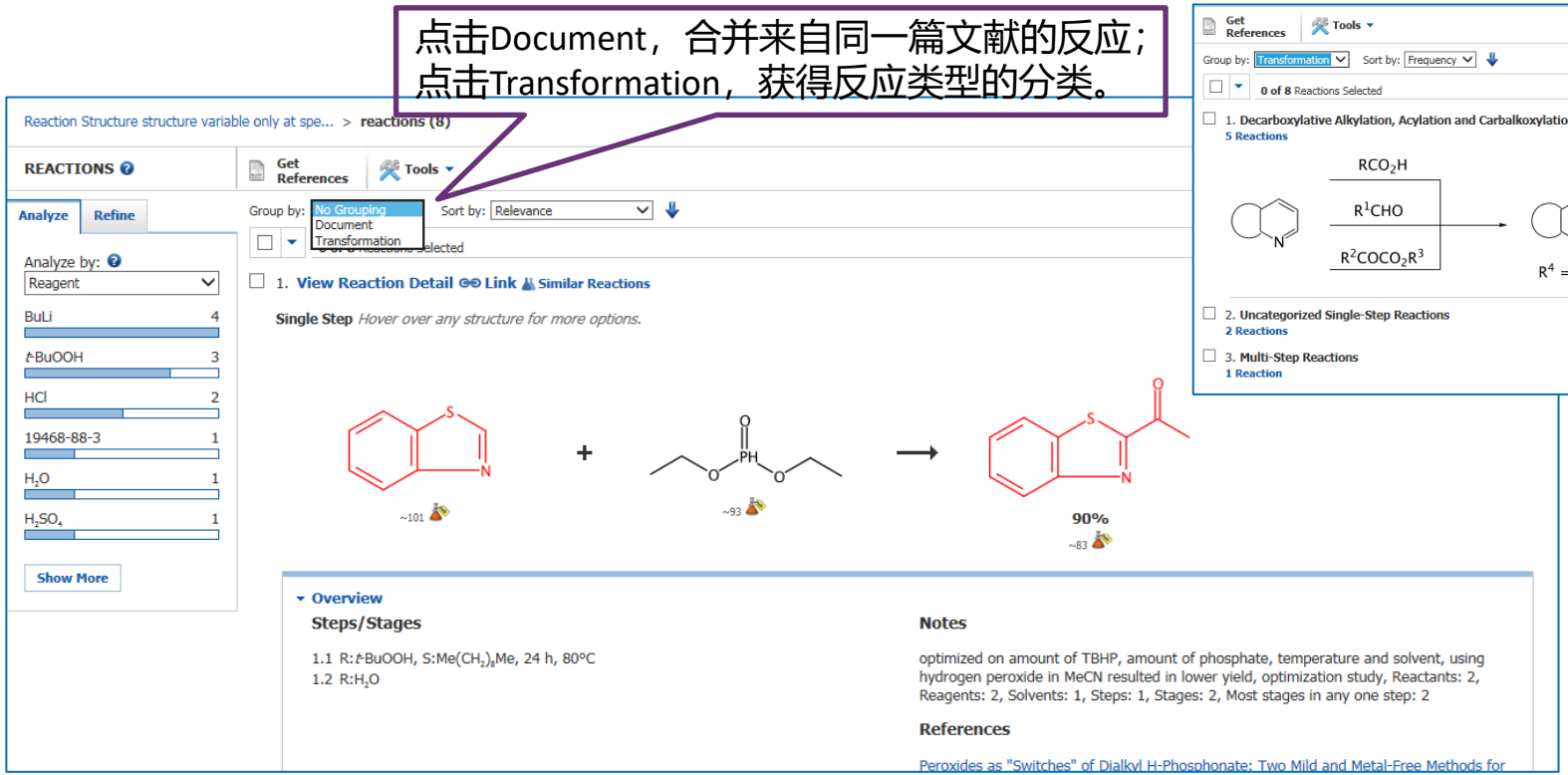
精确结构反应检索：查看反应结果集

点击Document，合并来自同一篇文献的反应；
点击Transformation，获得反应类型的分类。



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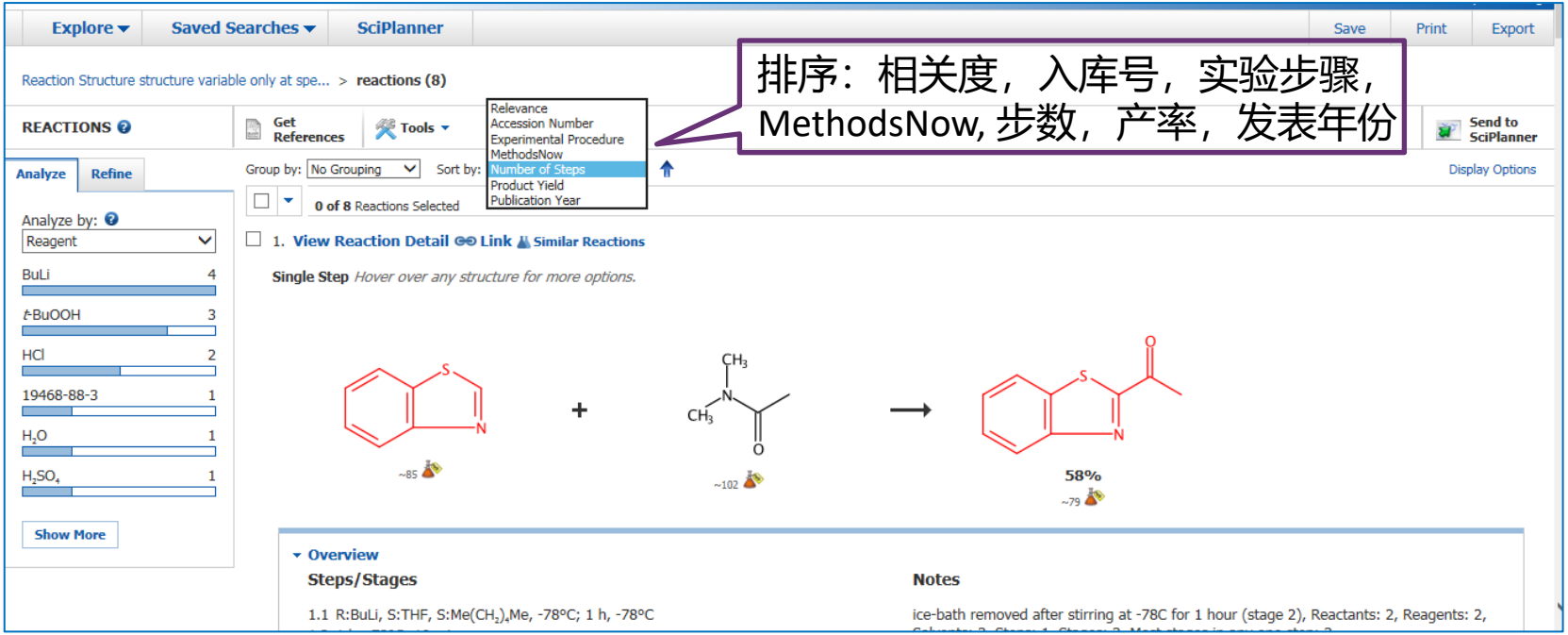
精确结构反应检索：查看反应结果集



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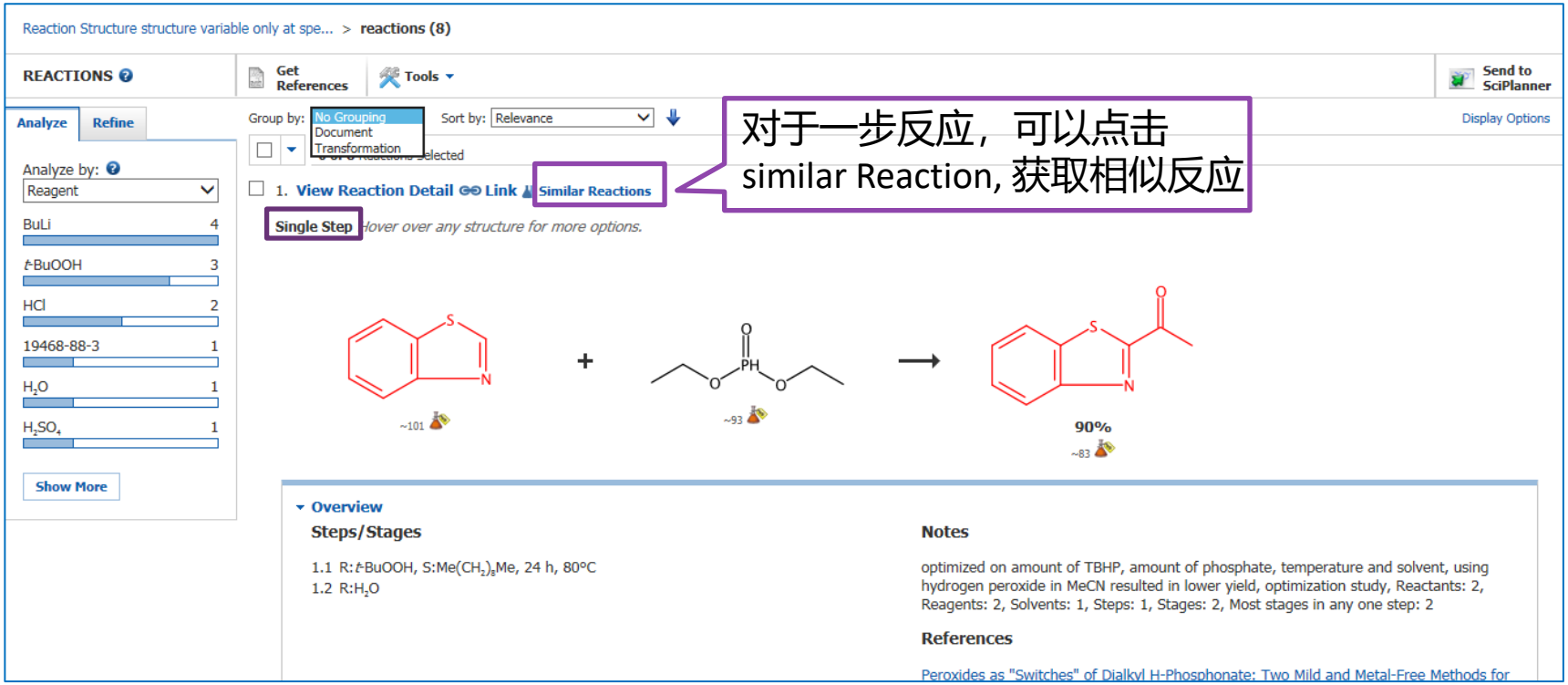
精确结构反应检索：查看反应结果集



对于一步反应，可以点击similar Reaction, 获取相似反应

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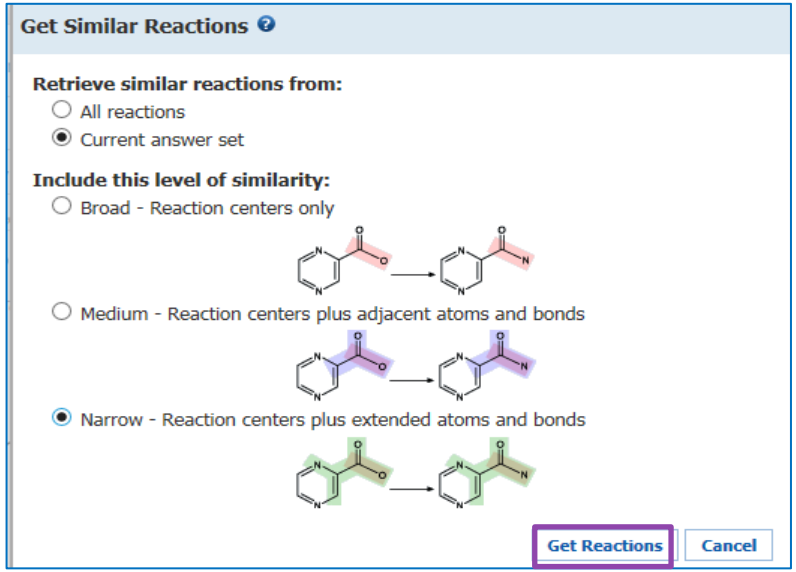
精确结构反应检索：获取相似反应



相似度限制：
Broad：仅反应中心相似
Medium：反应中心及附属原子和键
Narrow：反应中心及扩展的原子和键

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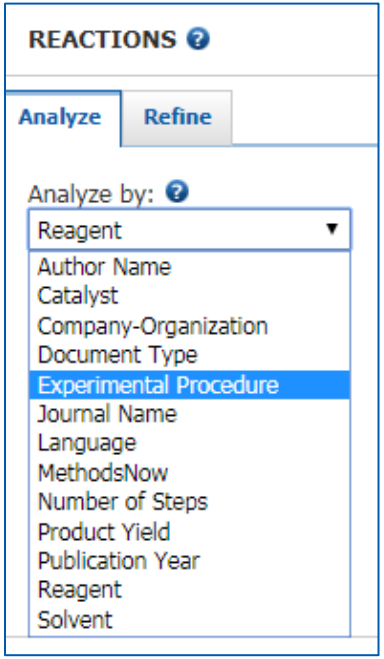
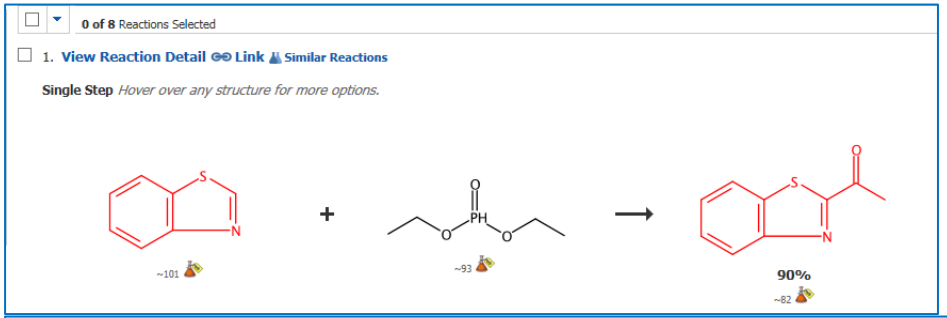
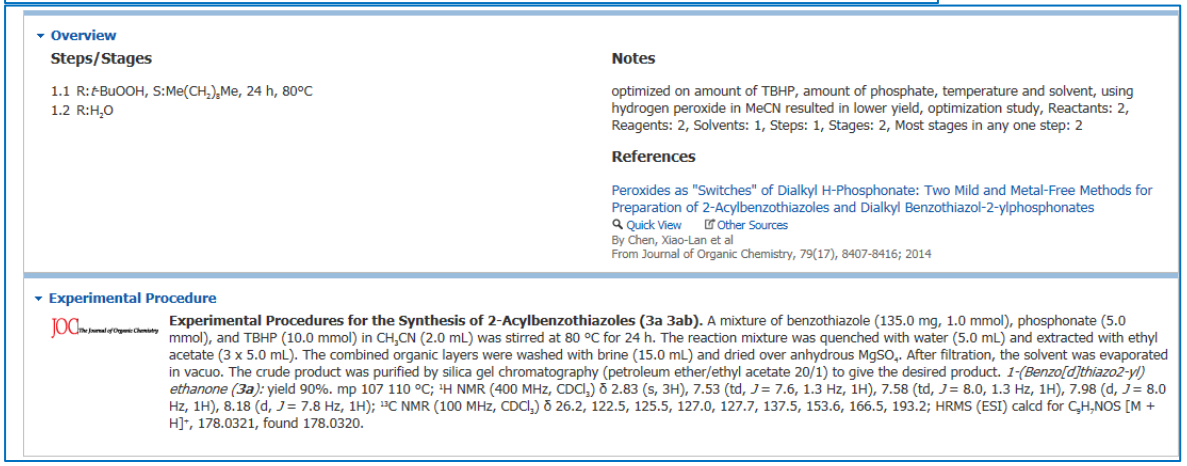
精确结构反应检索：查看感兴趣的反应信息







实验步骤

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MethodsNow Synthesis——人工标引的反应信息，节省您宝贵的时间

- 详细、明确的物质信息
- 全面、有条理的实验过程信息
- 更好的阅读体验——表格形式
- 无需查看原文直接获取实验详情——反应物，反应条件，步骤，产物性质，谱图等

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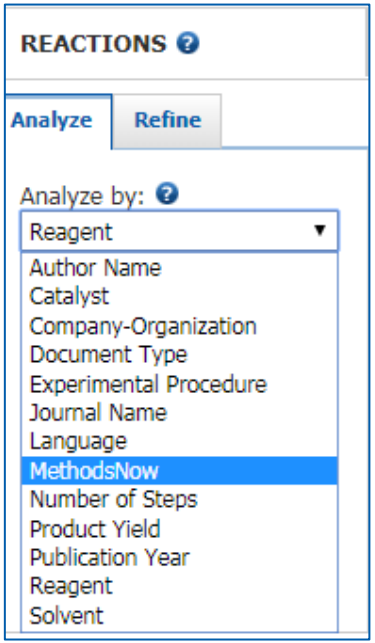
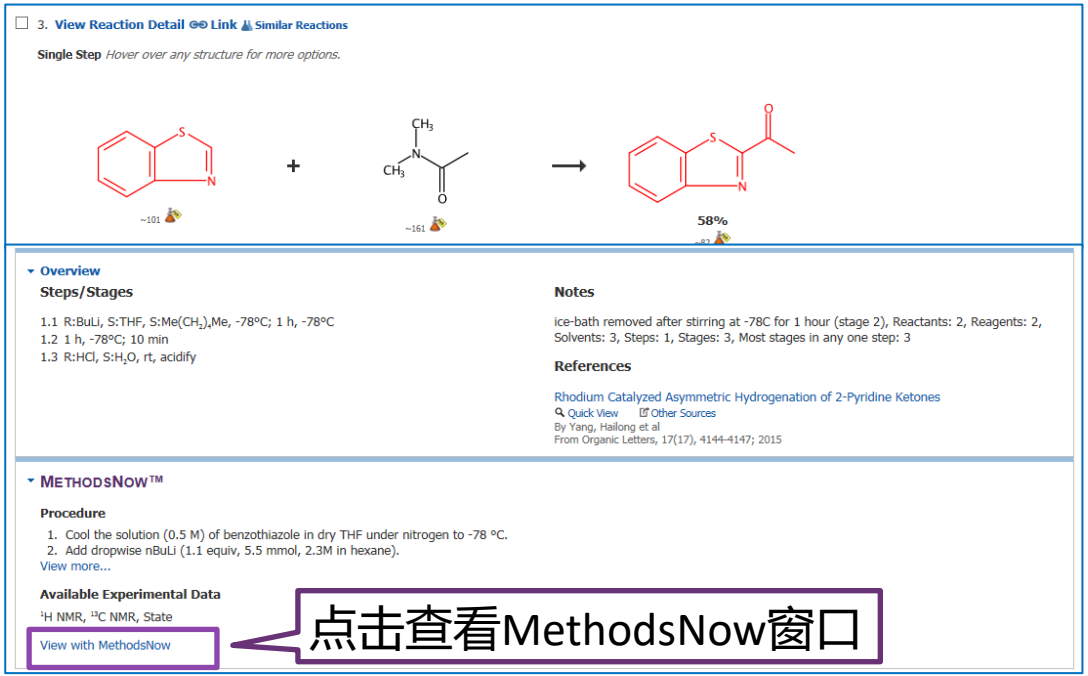
MethodsNow Synthesis: 通过Analyze，选择有MethodsNow标引的反应，点击MethodsNow查看实验详情





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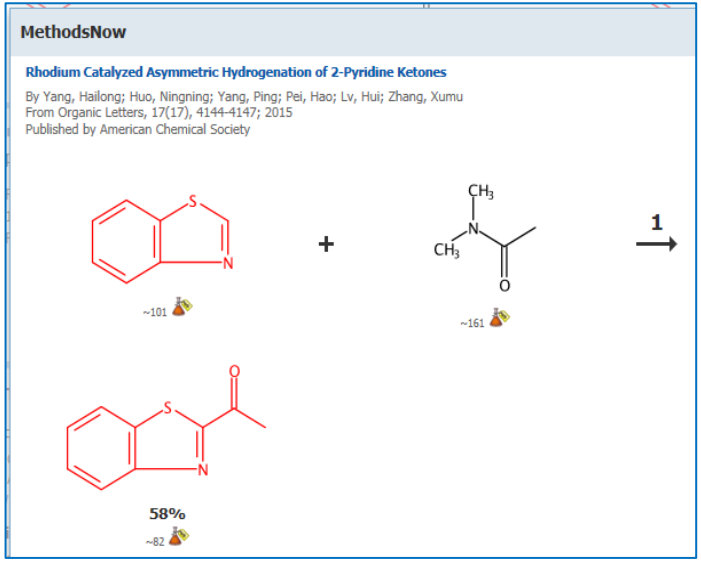
MethodsNow Synthesis: 实验详情展示窗口



Products	Ethanone, 1-(2-benzothiazolyl)-, 58%, CAS RN: 1629-78-3
Reactants	Benzothiazole, CAS RN: 95-16-9 Dimethylacetamide, CAS RN: 127-19-5
Reagents	Butyllithium, CAS RN: 109-72-8 Hydrochloric acid, CAS RN: 7647-01-0
Solvents	Tetrahydrofuran, CAS RN: 109-99-9 Hexane, CAS RN: 110-54-3 Water, CAS RN: 7732-18-5
Procedure	1. Cool the solution (0.5 M) of benzothiazole in dry THF under nitrogen to -78 °C. 2. Add dropwise nBuLi (1.1 equiv, 5.5 mmol, 2.3M in hexane). 3. Keep the resulted mixture for 1 h under -78 °C. 4. Add N,N-dimethylacetamide (1 equiv, 5 mmol) to the stirred solution at -78 °C. 5. Stir the mixture was continuously for 1 h. 6. Remove the cold bath and stir the mixture for additional 10 min. 7. Hydrolyze with concd hydrochloric acid (1 mL). 8. Stir the acidic solution continuously until the temperature reach to room temperature. 9. Pour the mixture into same amount of water. 10. Extract the aqueous mixture with ethyl acetrate 3 times. 11. Dry the combined organic solution with Na_2SO_4. 12. Purify by flash column chromatography to afford product.
Transformation	Decarboxylative Alkylation, Acylation and Carbalkoxylation of Nitrogen Heterocycle
^{1}H NMR	(400 MHz, $CDCl_3$)δ8.22 (d,J = 8.0Hz,1H), 8.01 (d, J = 7.6Hz, H), 7.55-7.63 (m, 2H), 2.87 (s, 3H);
^{13}C NMR	(101MHz, $CDCl_3$)δ193.2, 166.5, 153.6, 137.4, 127.7, 127.0, 125.5, 122.5, 26.2.
State	white solid
CAS Method Number	3-219-CAS-1662290

点击CAS RN，即时查看物质

产物，反应物，试剂，溶剂，步骤，反应类型，规模，核磁氢谱，核磁碳谱，产物状态，CAS方法号

PDF or XLS格式

Print/Export　Close

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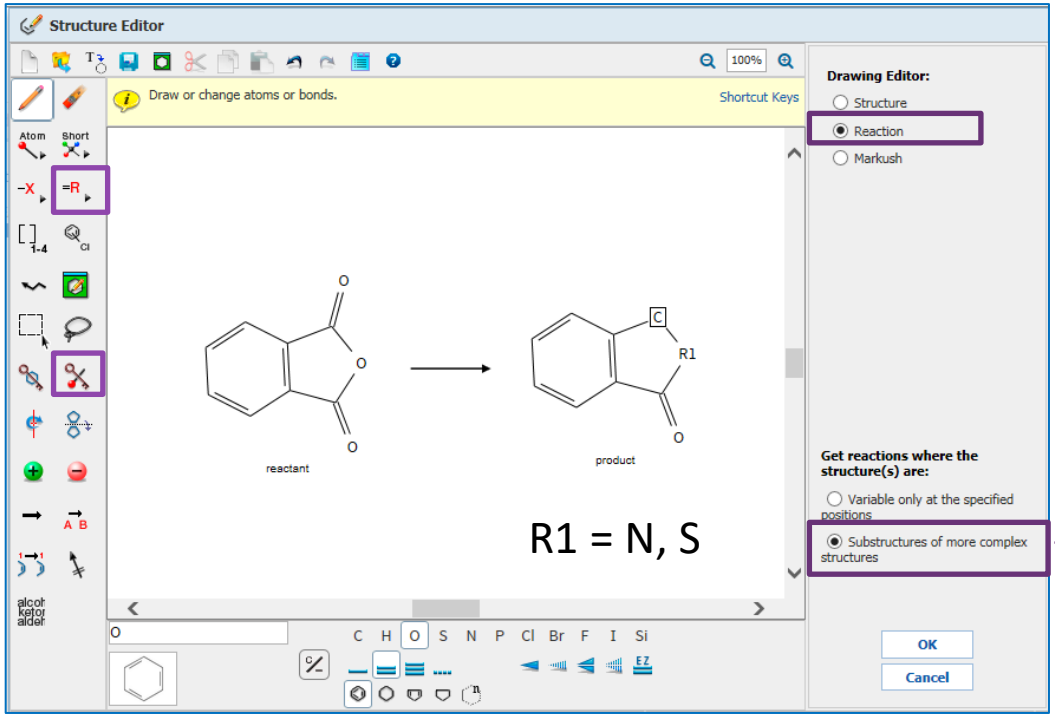
亚结构反应检索: 绘制反应式



输入的反应物和产物结构可以被修饰，但母体结构不变

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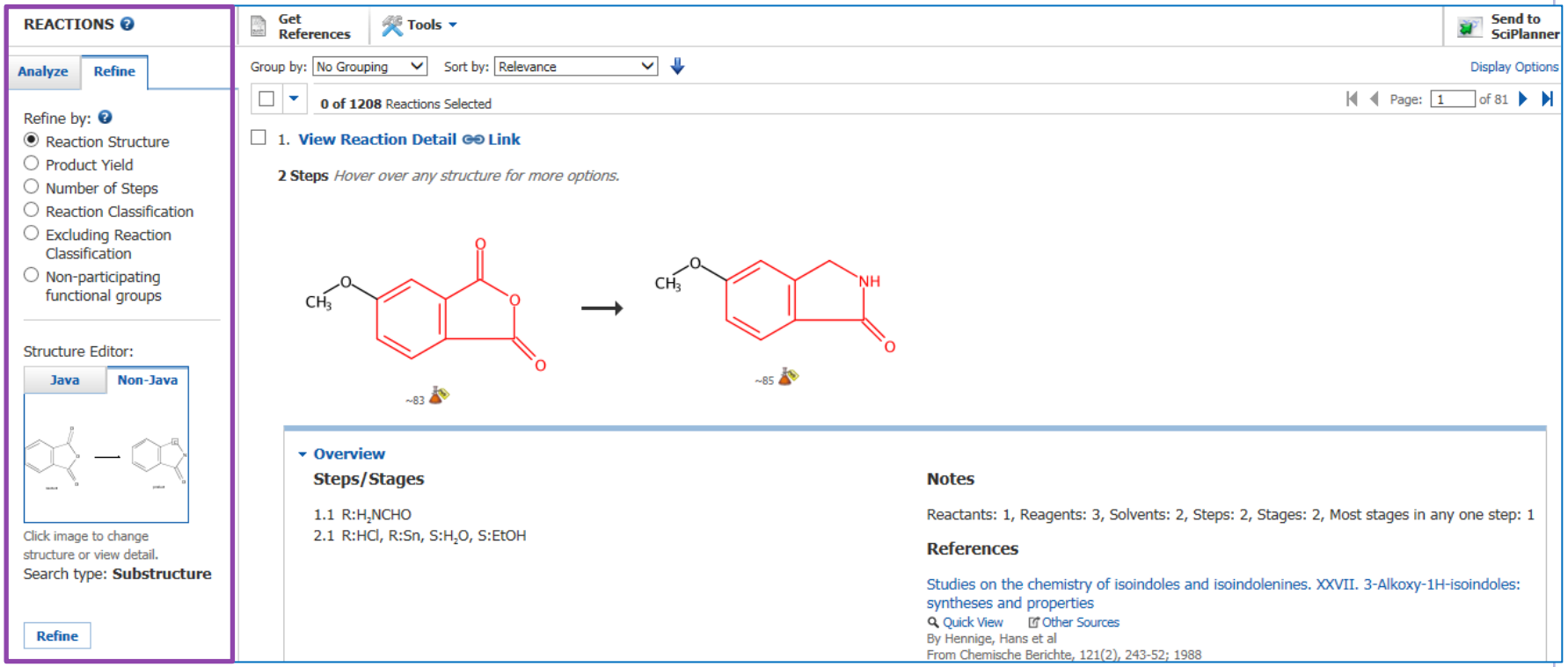
亚结构反应检索：获得反应结果集



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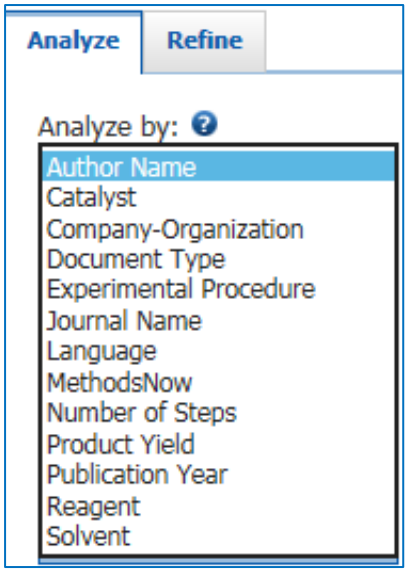
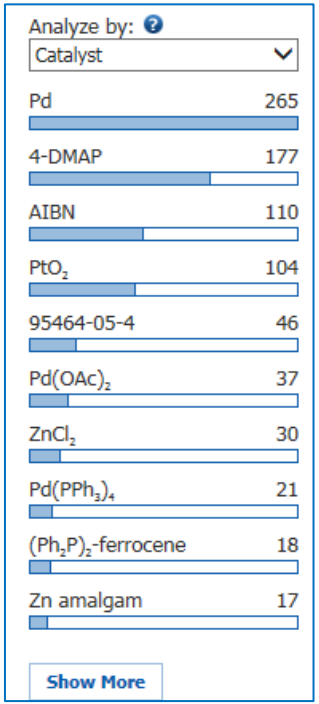
亚结构反应检索：分析处理

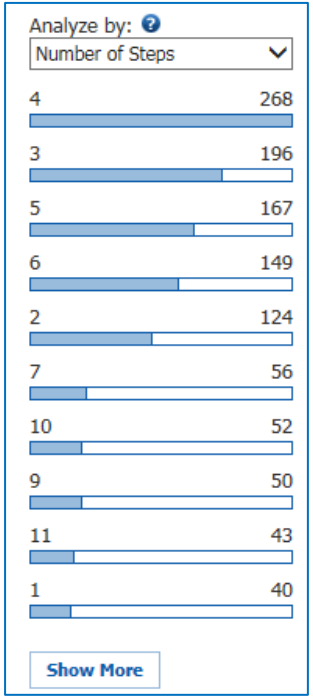
13种分析选项



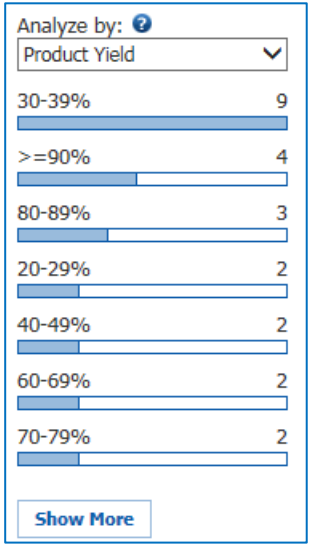
催化剂



反应步数



产率



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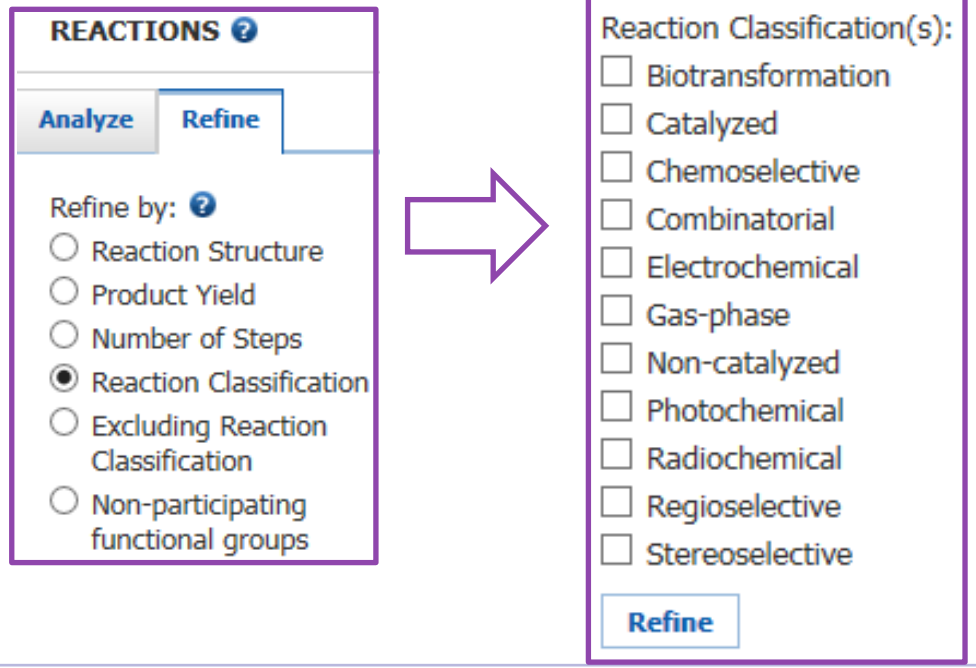
亚结构反应检索：筛选处理

6种筛选选项：反应结构、产率、反应步数、包含/排除的反应类型(11种)、不参与反应官能团(217种)



- ❑ 生物转化
- ❑ 催化反应
- ❑ 化学选择性
- ❑ 组合化学
- ❑ 电子化学
- ❑ 气相反应
- ❑ 非催化反应
- ❑ 光化学
- ❑ 放射化学
- ❑ 区域选择反应
- ❑ 立体选择反应

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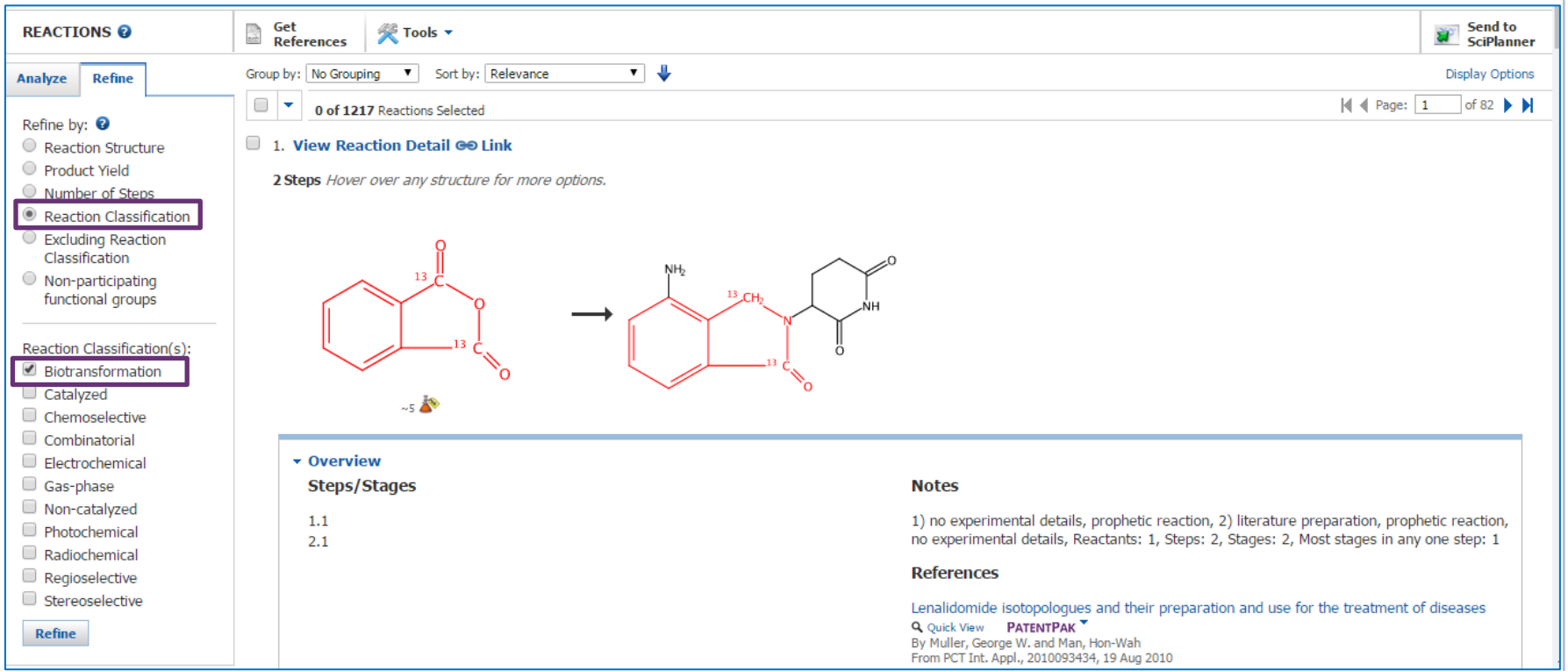
亚结构反应检索：勾选反应类型



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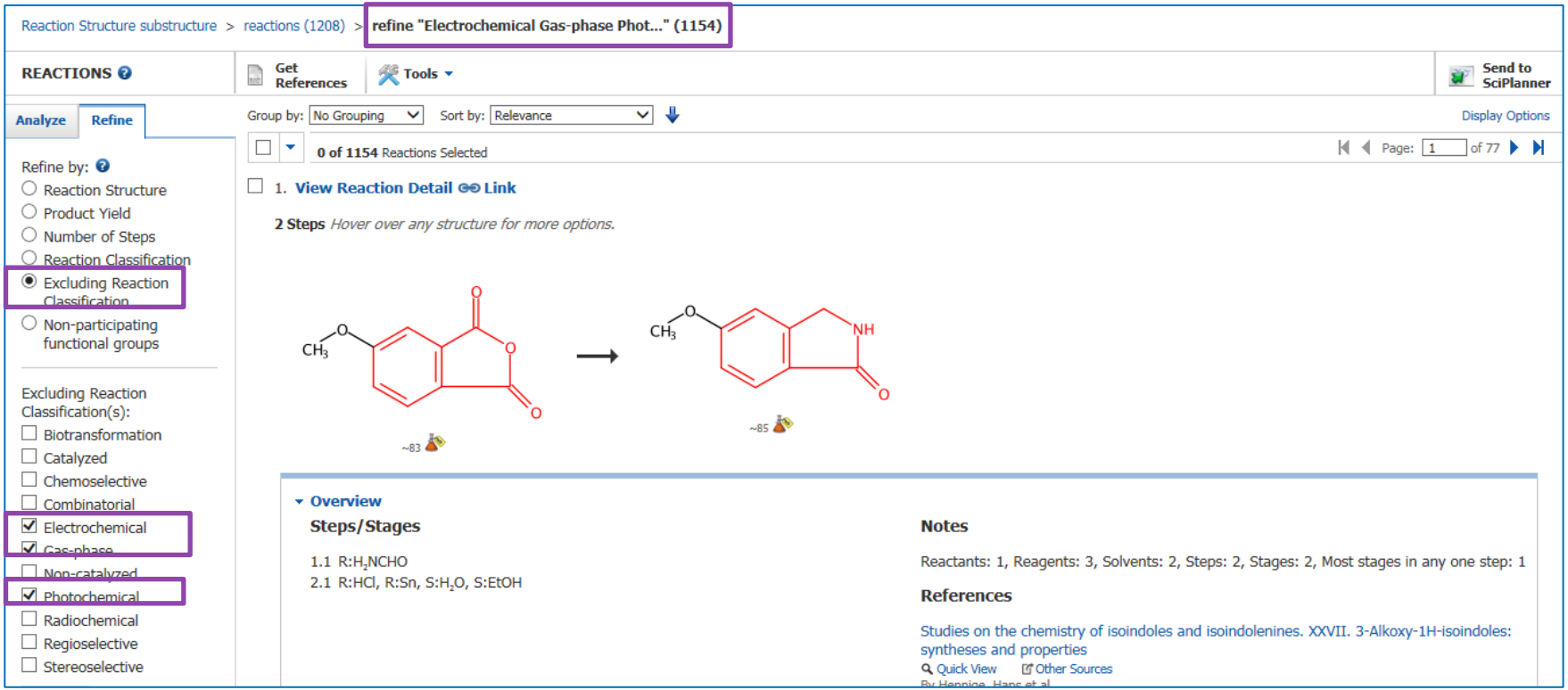
亚结构反应检索：排除反应类型



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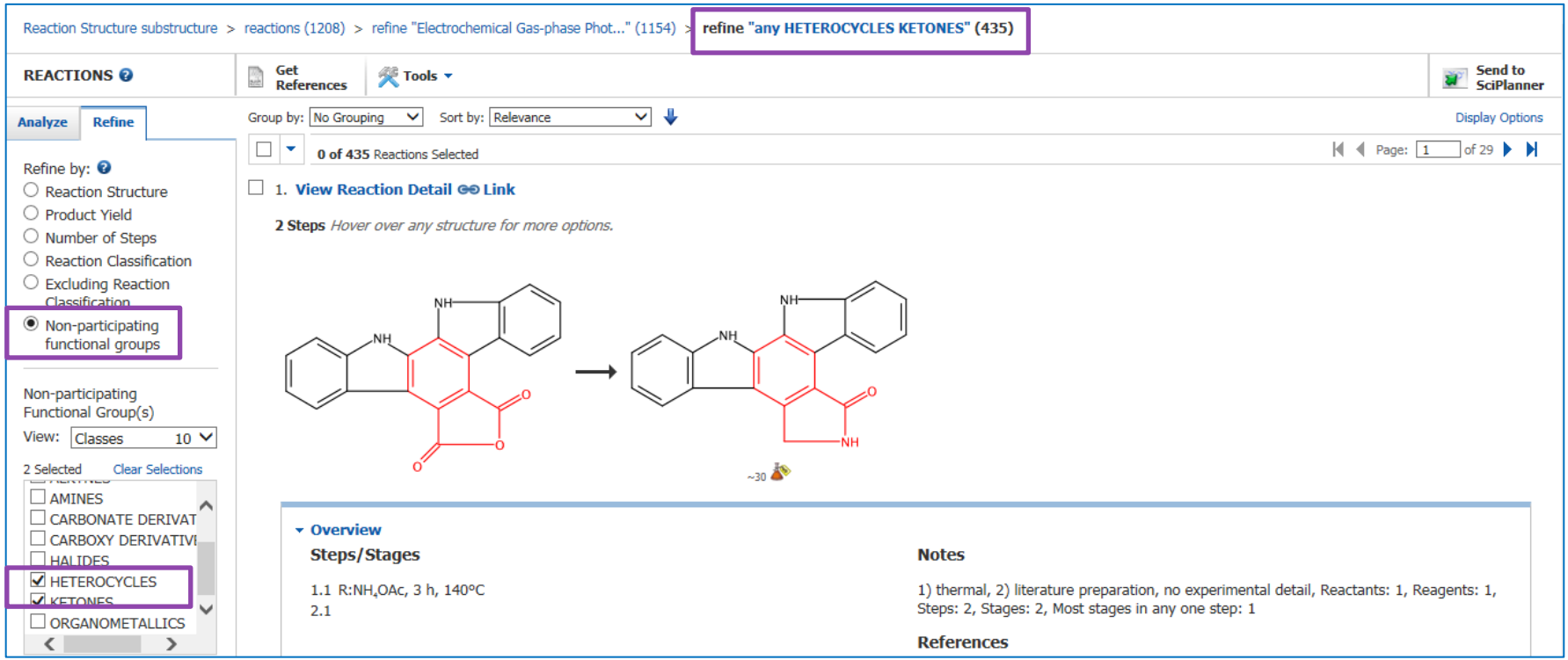
亚结构反应检索：筛选官能团



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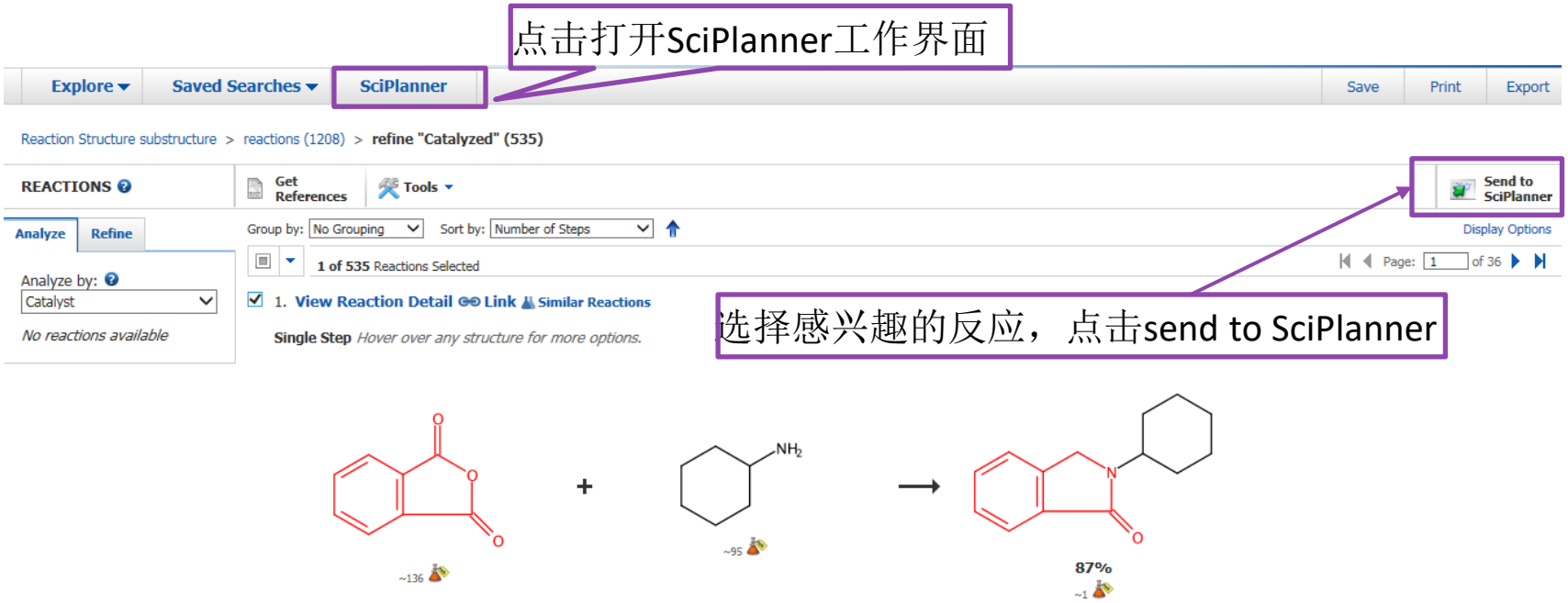
利用SciPlanner设计拟合成反应路线



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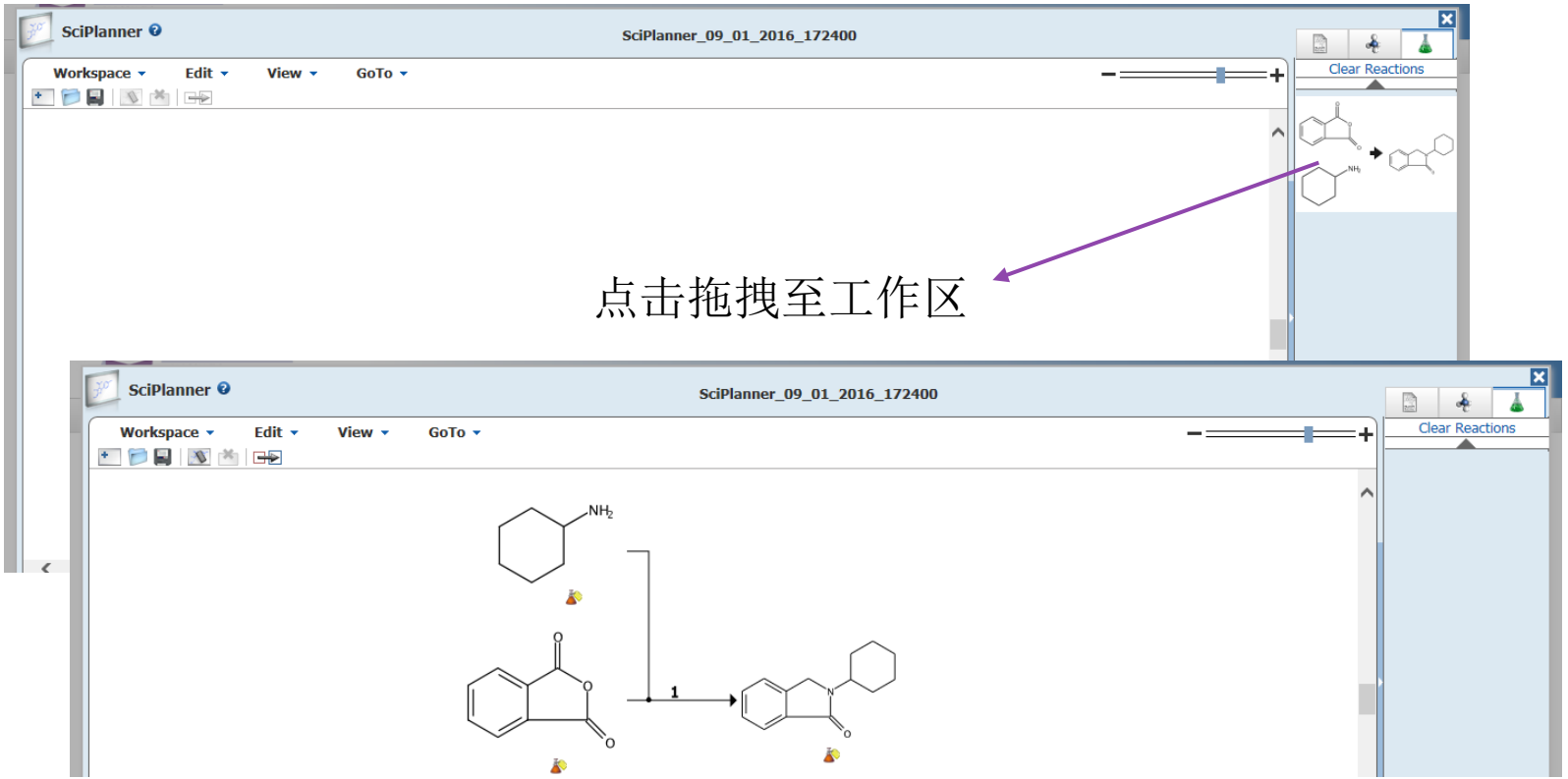
SciPlanner工作界面



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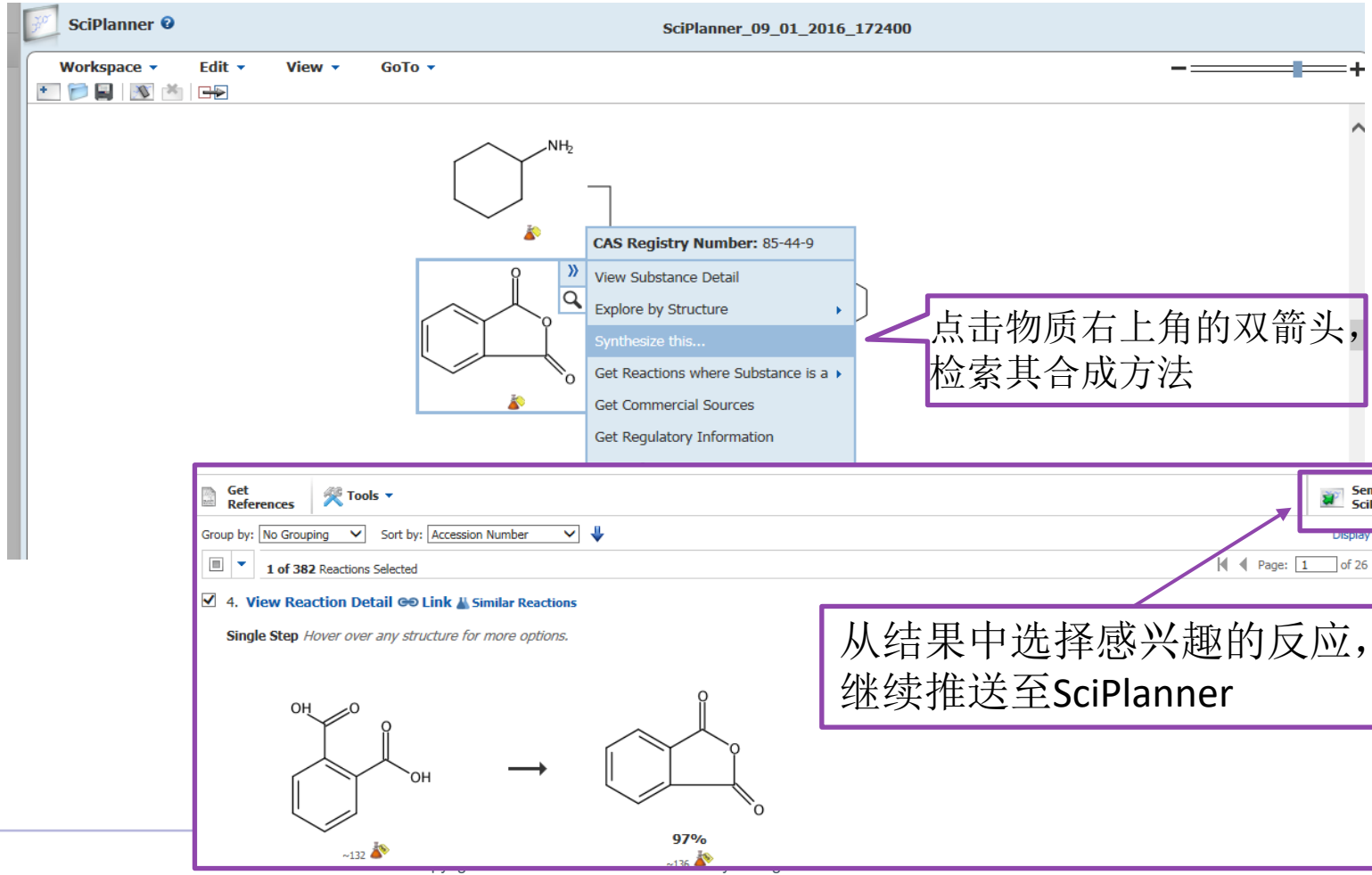
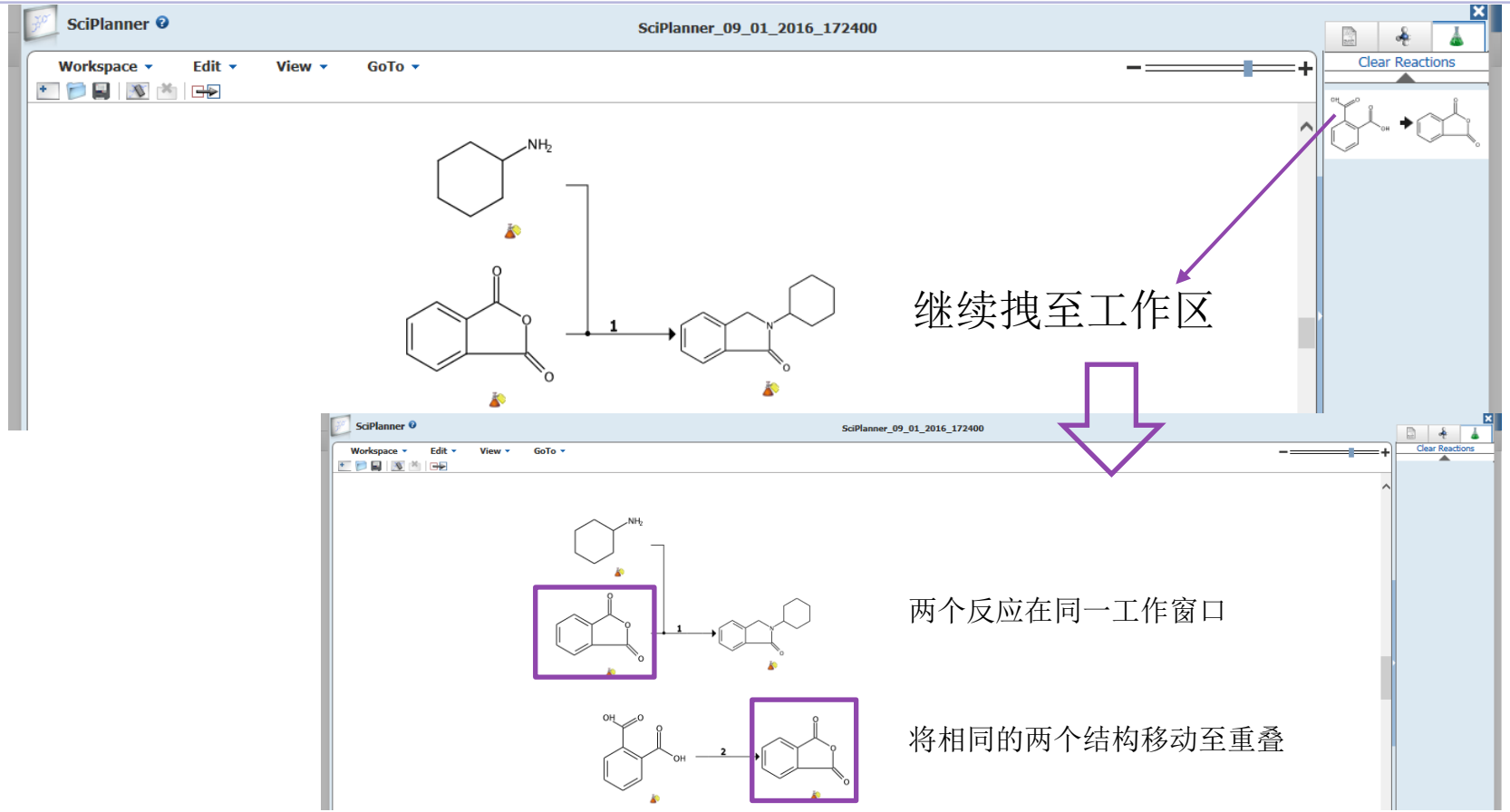

SciPlanner
SciPlanner_09_01_2016_172400
Workspace
Edit
View
GoTo
NH2
CAS Registry Number: 85-44-9
View Substance Detail
Explore by Structure
Synthesize this...
Get Reactions where Substance is a
Get Commercial Sources
Get Regulatory Information
点击物质右上角的双箭头，检索其合成方法
Get References
Tools
Send to SciPlanner
Group by: No Grouping
Sort by: Accession Number
Display Options
1 of 382 Reactions Selected
Page: 1 of 26
4. View Reaction Detail Link Similar Reactions
Single Step Hover over any structure for more options.
OH
OH
97%
从结果中选择感兴趣的反应，继续推送至SciPlanner



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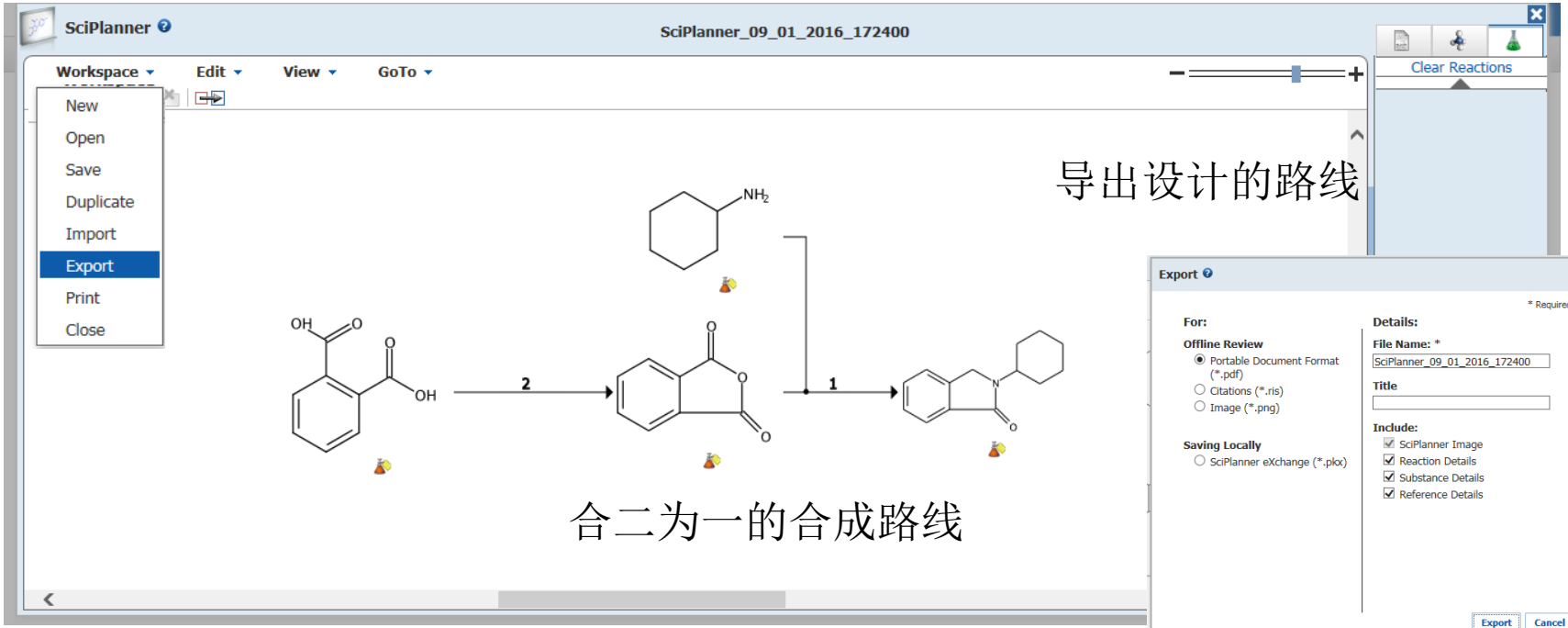
SciPlanner——设计拟合成的反应路线



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提纲

- SciFinder中获取化合物制备信息的方法
- 反应相关信息获取方法
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何通过反应式检索反应，精炼结果并获得实验详情
  - 利用SciPlanner实现反应路线设计
  - 反应检索案例分享
- 通过文献主题检索合成制备相关信息的方法

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提纲

- 反应检索案例：
  - 金属有机物质的反应
  - 溴代杂芳环与炔烃的 Sonogashira偶联反应检索
  - 片段结构的化学选择性反应
  - 检索某物质作为试剂的反应
  - 系列化合物的反应

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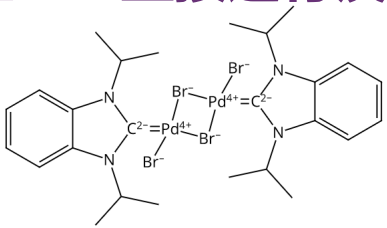
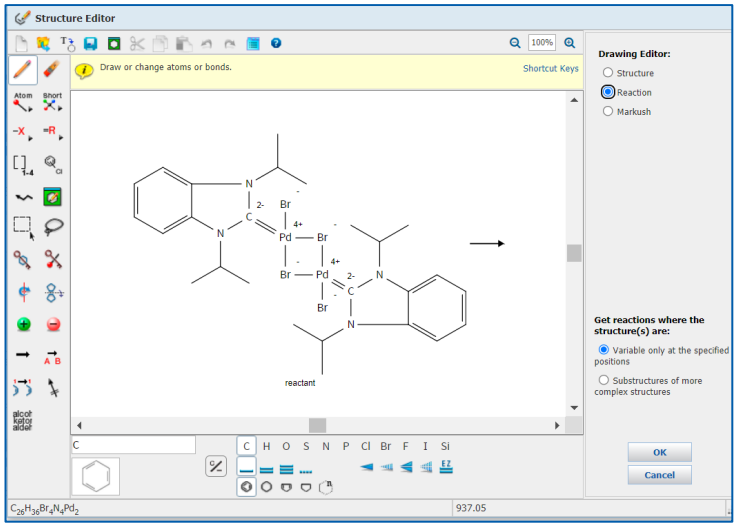
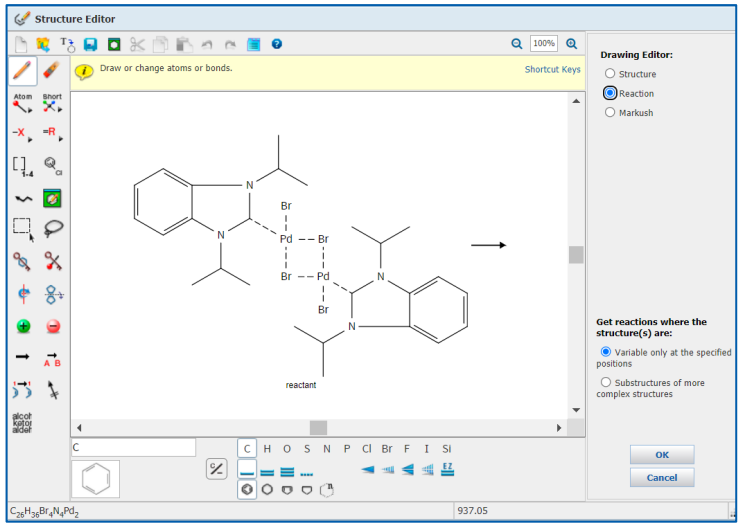
例1：金属有机化合物的反应——直接进行反应检索







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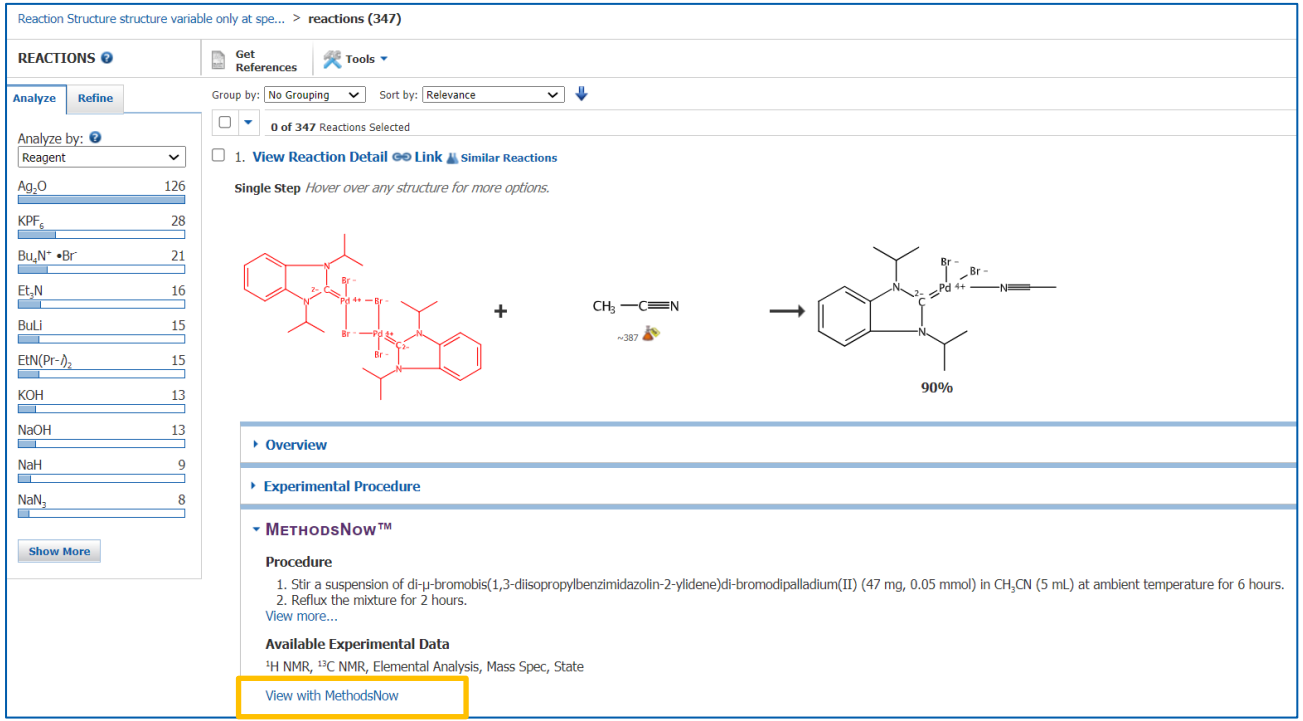
通过MethodsNow Synthesis获取合成实验详情



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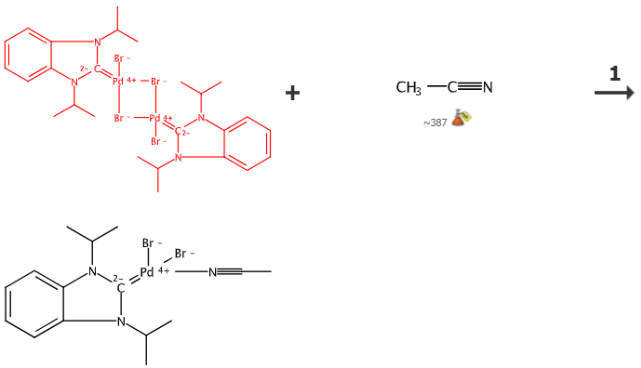
MethodsNow Synthesis合成实验详情

MethodsNow

Palladium(II) complexes of a sterically bulky, benzannulated N-heterocyclic carbene with unusual intramolecular C-H···Pd and Ccarben...

By Huynh, Han Vinh; Han, Yuan; Ho, Joanne Hui Hui; Tan, Geok Kheng
From Organometallics, 25(13), 3267-3274; 2006
Published by American Chemical Society



90%

Products	(*SP*-4-1)-(Acetonitrile)dibromo[1,3-dihydro-1,3-bis(1-methylethyl)-2*H*-benzimidazol-2-ylidene]palladium, 90%, CAS RN: 895632-20-9
Reactants	Stereoisomer of di-μ-bromodibromobis[1,3-dihydro-1,3-bis(1-methylethyl)-2*H*-benzimidazol-2-ylidene]dipalladium, CAS RN: 895632-19-6 Acetonitrile, CAS RN: 75-05-8
Solvents	Acetonitrile, CAS RN: 75-05-8

Procedure	1. Stir a suspension of di-μ-bromobis(1,3-diisopropylbenzimidazolin-2-ylidene)di-bromodipalladium(II) (47 mg, 0.05 mmol) in CH_3CN (5 mL) at ambient temperature for 6 hours. 2. Reflux the mixture for 2 hours. 3. Filter the reaction mixture over Celite. 4. Remove the solvent in vacuo to afford trans-dibromo(acetonitrile)(1,3-diisopropylbenzimidazolin-2-ylidene)palladium(II).
Transformation	Coordination of a Metal to Carbon and Heteroatom Ligand Substitution
Scale	milligram
^{1}H NMR	(300 MHz, CD_3CN): δ 7.73 (dd, 2 H, Ar-H), 7.29 (dd, 2 H, Ar-H), 6.14 (m, ^{3}J(H,H) = 7.1 Hz, 2 H, $NCH(CH_3)_2$), 1.96 (s, CH_3CN, correct integration is not possible due to ligand exchange with the solvent), 1.70 (d, ^{3}J(H,H) = 7.1Hz, 12 H, CH_3).
^{13}C NMR	(75.47 MHz, CD_3CN): 158.4 (s, NCN), 133.8, 123.9 (s, Ar-C), 118.3 (s, CN), 113.9 (s, Ar-C), 55.8 (s, $NCH(CH_3)_2$), 20.5 (s, CH_3), 1.32 (m, CH_3CN, assignment is tentative due to overlap with solvent signals).
Elemental Analysis	Anal. Calc for $C_{15}H_{21}Br_2N_3Pd$: C, 35.36; H, 4.15; N, 8.25. Found: C, 35.64; H, 4.08; N, 8.06.
Mass Spec	MS (ESI): = 471 [M - Br + CH_3CN]$^+$.
State	yellow powder
CAS Method Number	3-562-CAS-8549846

Print/Export Close

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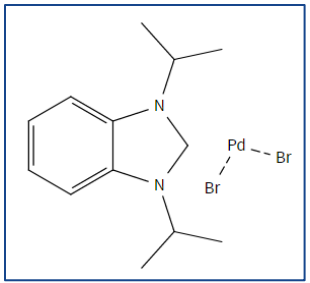
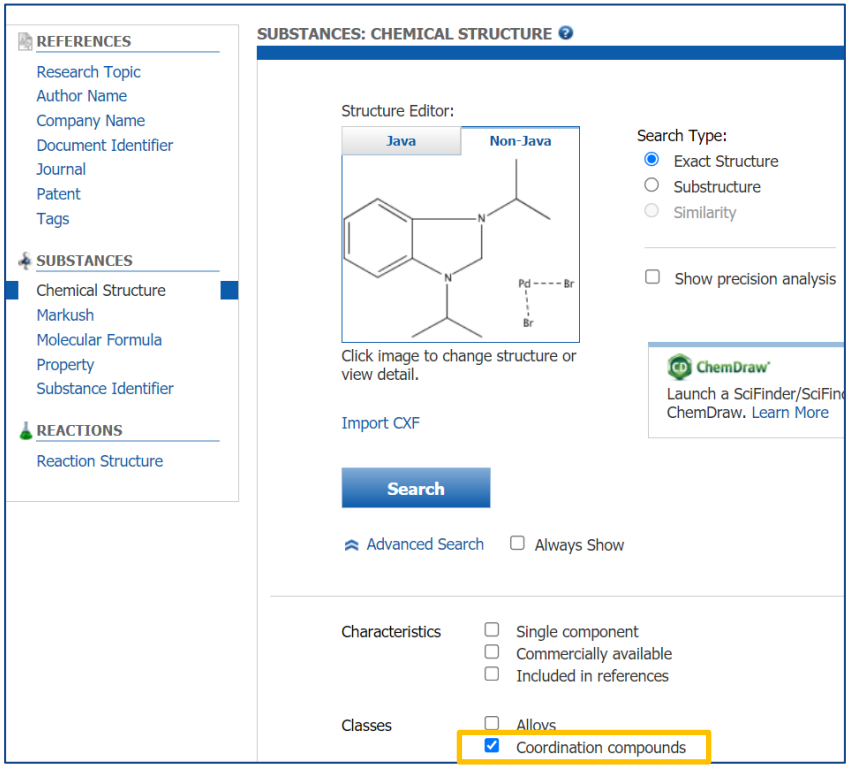
根据物质获取反应——金属有机化合物的的检索





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iters > **substances (7)**

Get References | Get Reactions | Get Commercial Sources | Tools | Create Keep Me Posted Alert | Send to SciPlanner

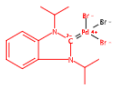
Sort by: CAS Registry Number | Display Options

0 of 7 Substances Selected

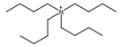
1. **2095501-02-1**

~1

895632-21-0
$C_{13}H_{18}Br_3N_2Pd$



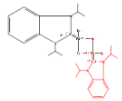
10549-76-5
$C_{16}H_{36}N$



$C_{16}H_{36}N \cdot C_{13}H_{18}Br_3N_2Pd$
INDEX NAME NOT YET ASSIGNED

2. **1189146-19-7**

~2

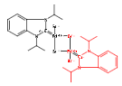


$C_{26}H_{36}Br_4N_4Pd_2$
Palladium, di-μ-bromodibromobis[1,3-dihydro-1,3-bis(1-methylethyl)-2*H*-benzimidazol-2-ylidene-2-^{13}C]di-, stereoisomer

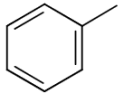
3. **896142-63-5**

~1

895632-19-6
$C_{26}H_{36}Br_4N_4Pd_2$



108-88-3
C_7H_8

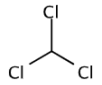


$C_{26}H_{36}Br_4N_4Pd_2 \cdot C_7H_8$
Palladium, di-μ-bromodibromobis[1,3-dihydro-1,3-bis(1-methylethyl)-2*H*-benzimidazol-2-ylidene]di-, stereoisomer, compd. with methylbenzene (1:1) (9CI)

4. **895632-25-4**

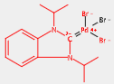
~1

67-66-3
$CHCl_3$

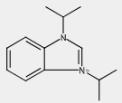


895632-22-1
$C_{13}H_{19}N_2 \cdot C_{13}H_{18}Br_3N_2Pd$

895632-21-0
$C_{13}H_{18}Br_3N_2Pd$



736926-78-6
$C_{13}H_{19}N_2$



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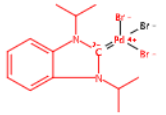
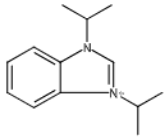
5. **895632-22-1**

~2

895632-21-0
$C_{13}H_{18}Br_3N_2Pd$



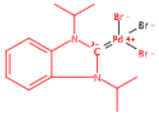
736926-78-6
$C_{13}H_{19}N_2$



$C_{13}H_{19}N_2 \cdot C_{13}H_{18}Br_3N_2Pd$
1*H*-Benzimidazolium, 1,3-bis(1-methylethyl)-, (*SP*-4-2)-tribromo[1,3-dihydro-1,3-bis(1-methylethyl)-2*H*-benzimidazol-2-ylidene] palladate(1-) (9CI)

6. **895632-21-0**

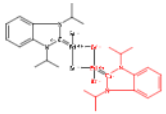
~0



$C_{13}H_{18}Br_3N_2Pd$
Palladate(1-), tribromo[1,3-dihydro-1,3-bis(1-methylethyl)-2*H*-benzimidazol-2-ylidene]-, (*SP*-4-2)-

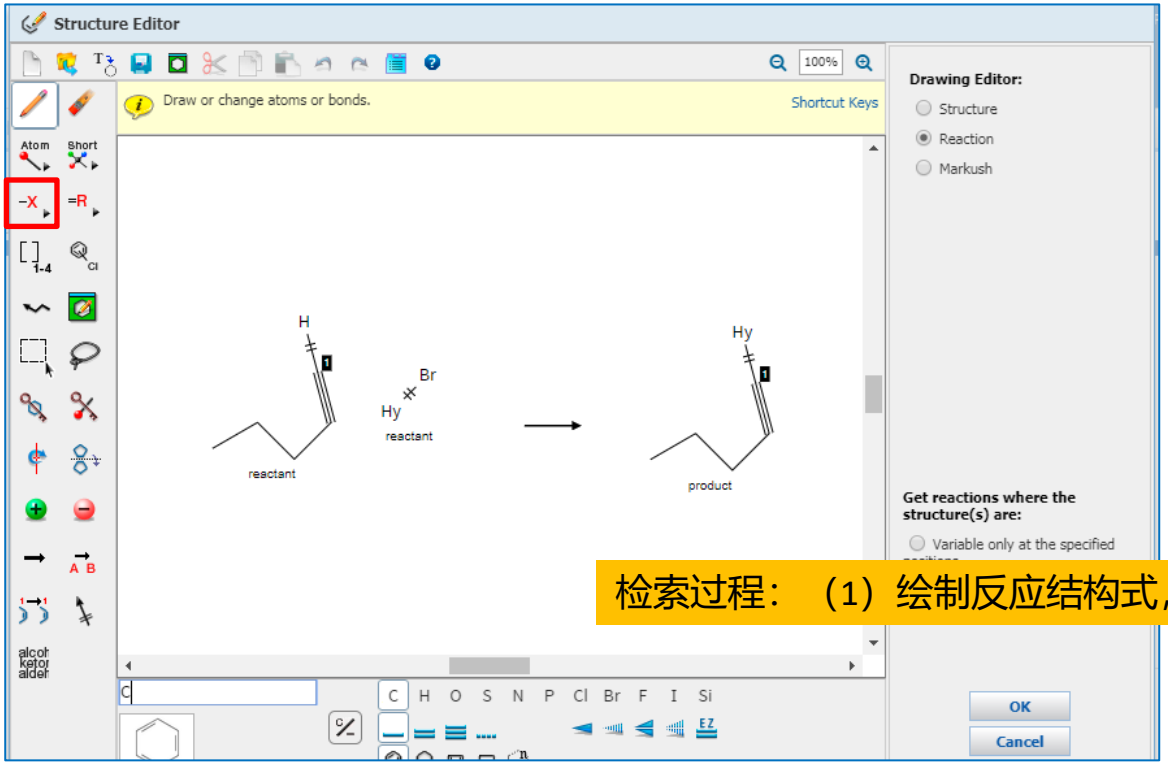
7. **895632-19-6**

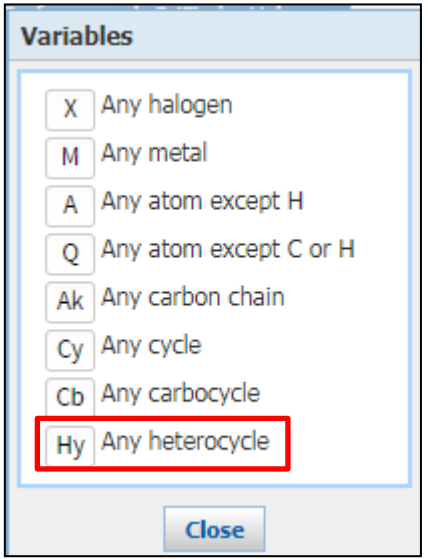
~32



$C_{26}H_{36}Br_4N_4Pd_2$
Palladium, di-μ-bromodibromobis[1,3-dihydro-1,3-bis(1-methylethyl)-2*H*-benzimidazol-2-ylidene]di-, stereoisomer

例2：溴代杂芳环与炔烃的 Sonogashira偶联反应检索





检索过程：（1）绘制反应结构式，杂环用-X中的Hy表示即可

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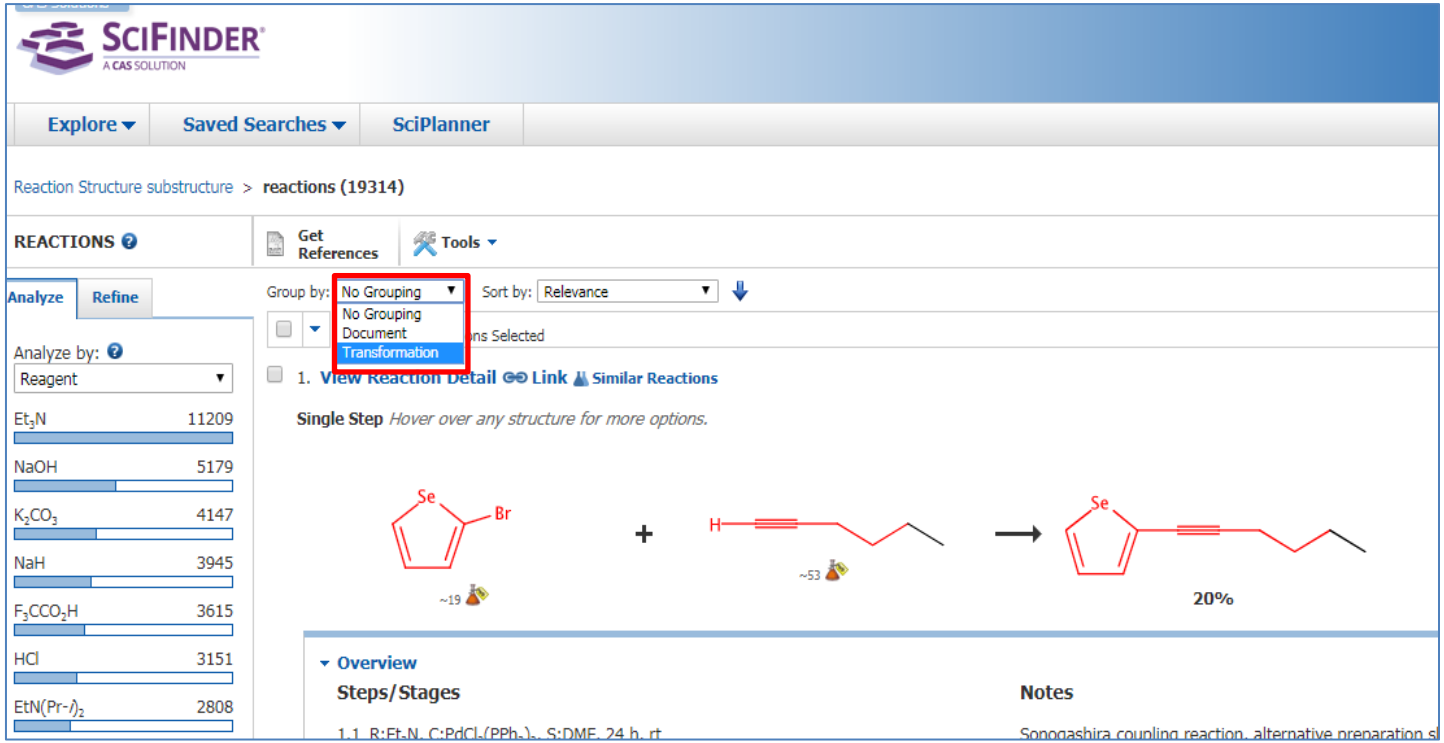
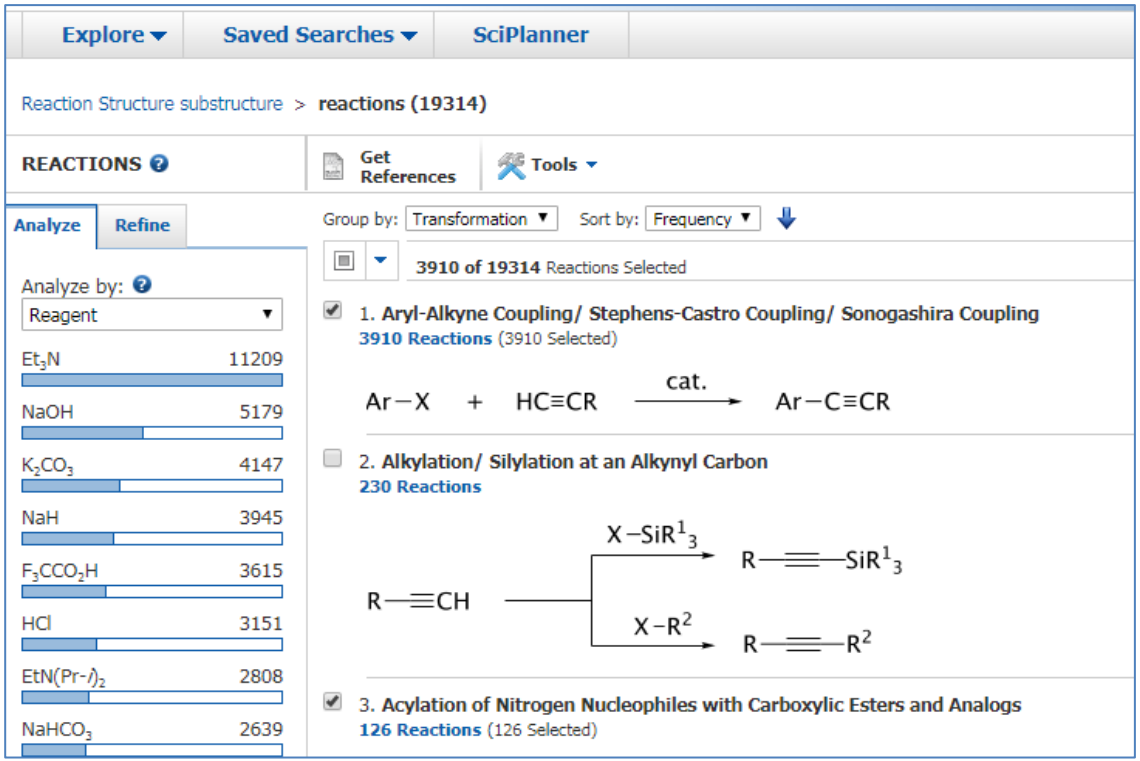
在反应结果集中选择group by transformation



根据需求，选择相应的反应类型（如，aryl-alkyne sonogashira偶联）



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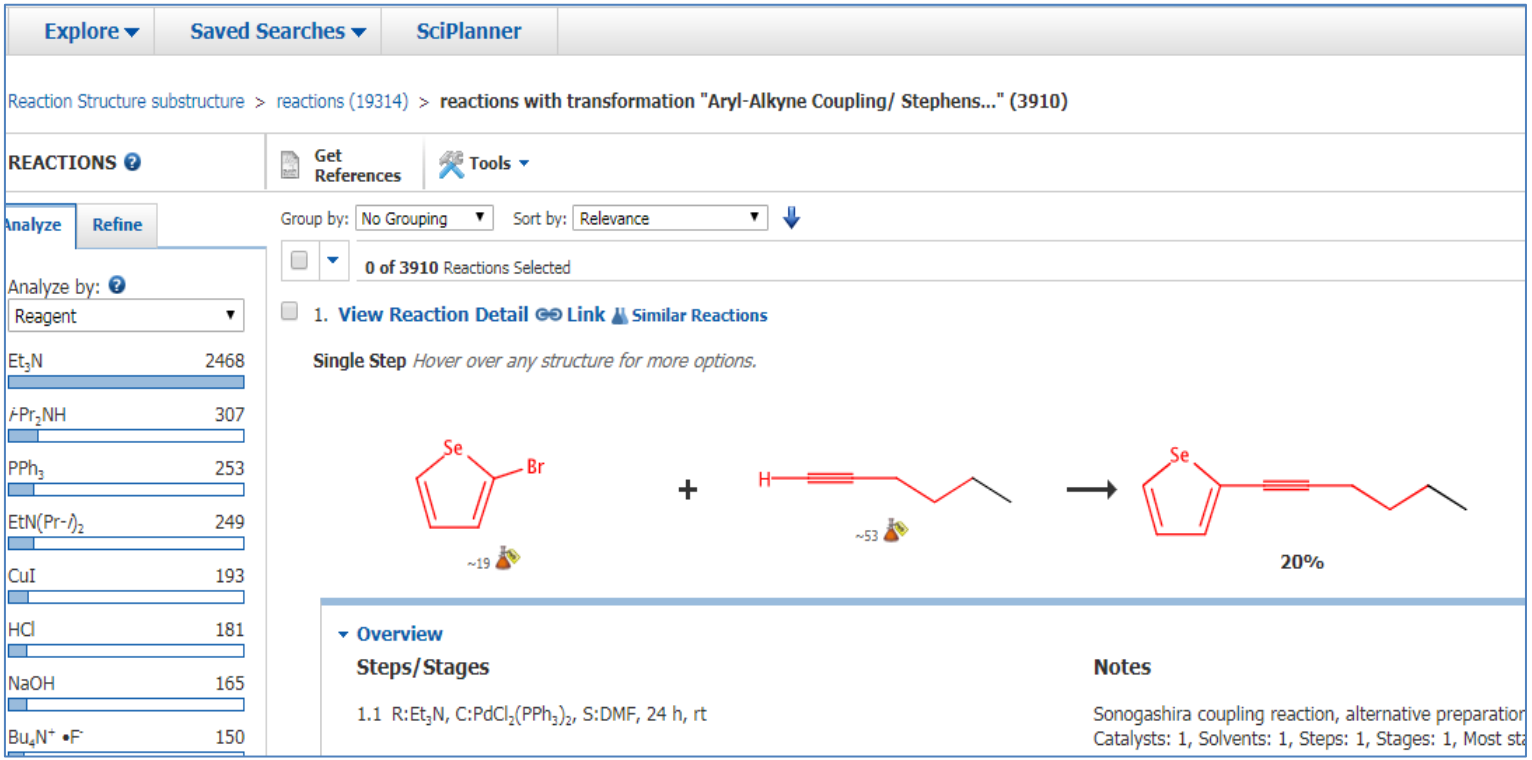
获得全面、准确的反应



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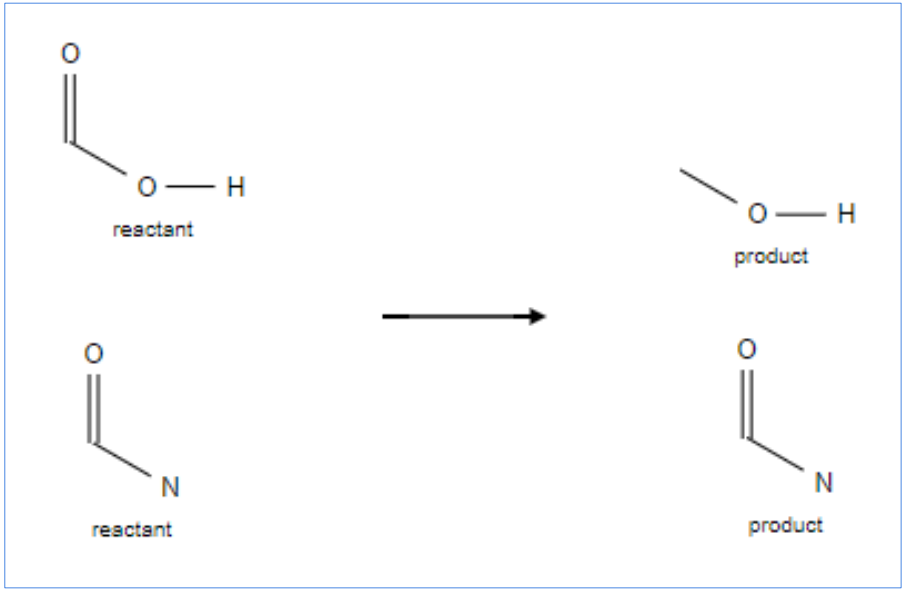
例3：片段结构的化学选择性反应



检索要求：

1. 反应物中含有羧基和酰胺基团；
2. 反应物种的羧基被还原为产物中的羟基；
3. 反应物中的酰胺基在反应后没有发生变化。

分析：
化学选择性反应可以使用non-participating functional groups来限定不参与反应的官能团。

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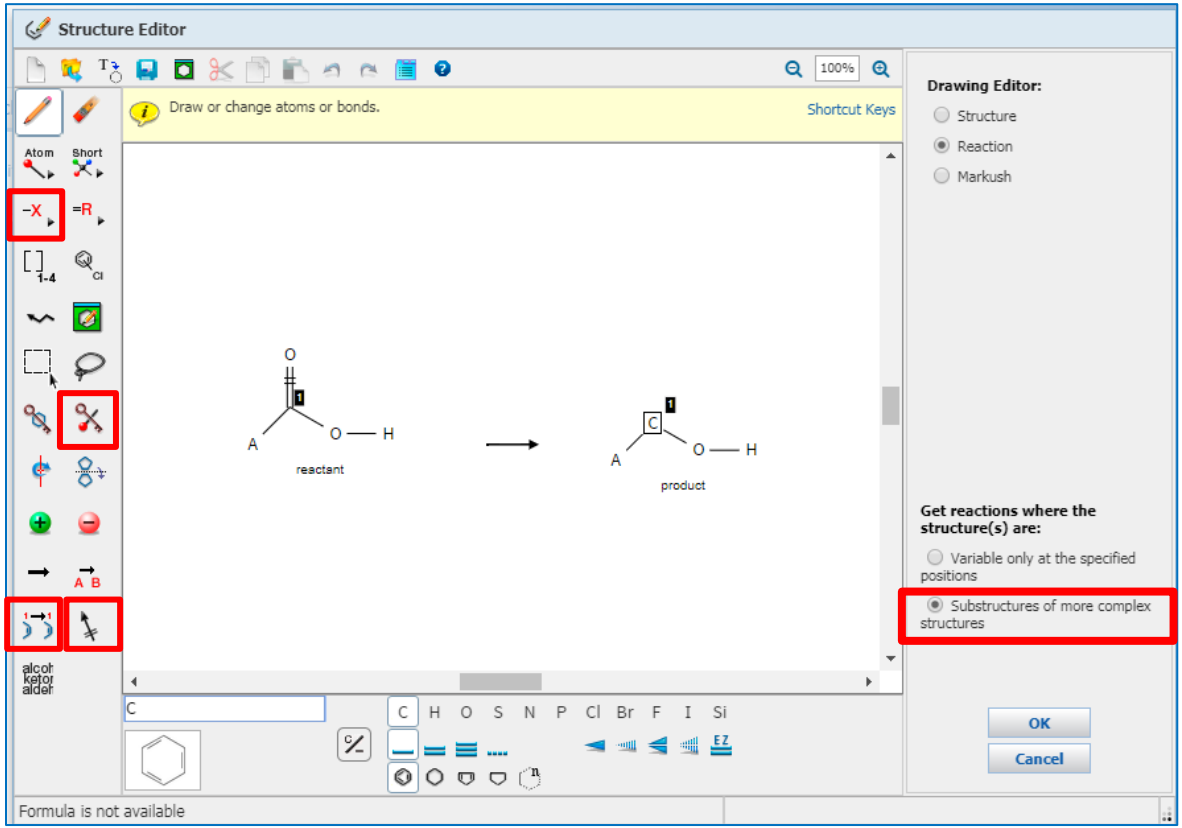
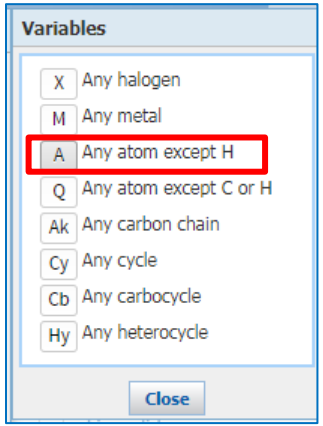
使用标亮的工具，绘制如下反应式，进行亚结构反应检索





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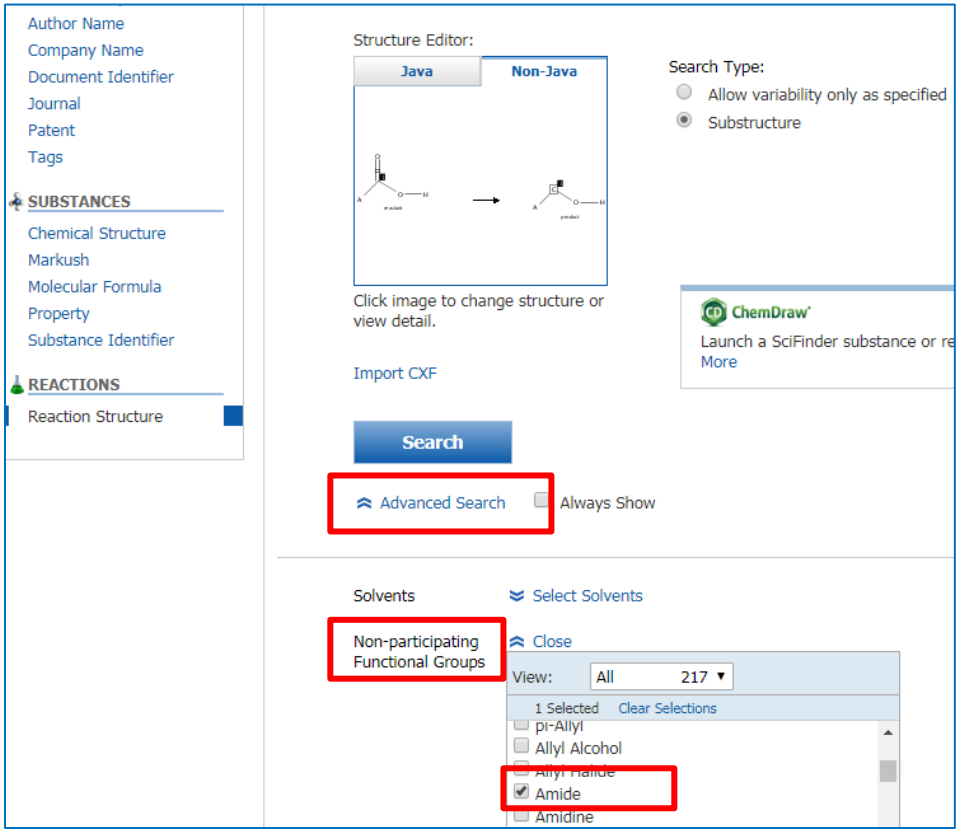

1. 点击高级检索；

2. 点击不参与反应官能团；

3. 选择酰胺amide。

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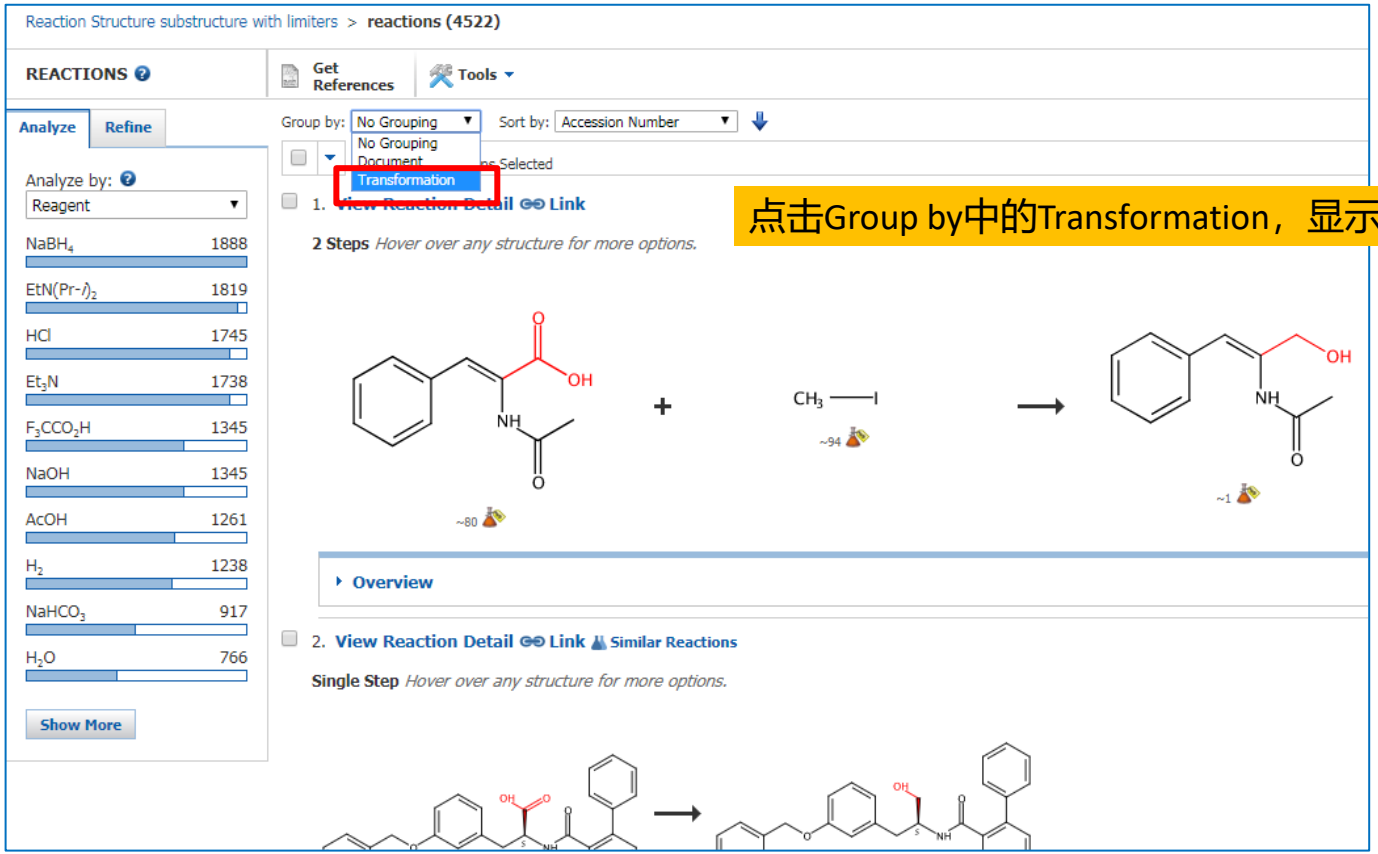

点击Group by中的Transformation，显示反应类型

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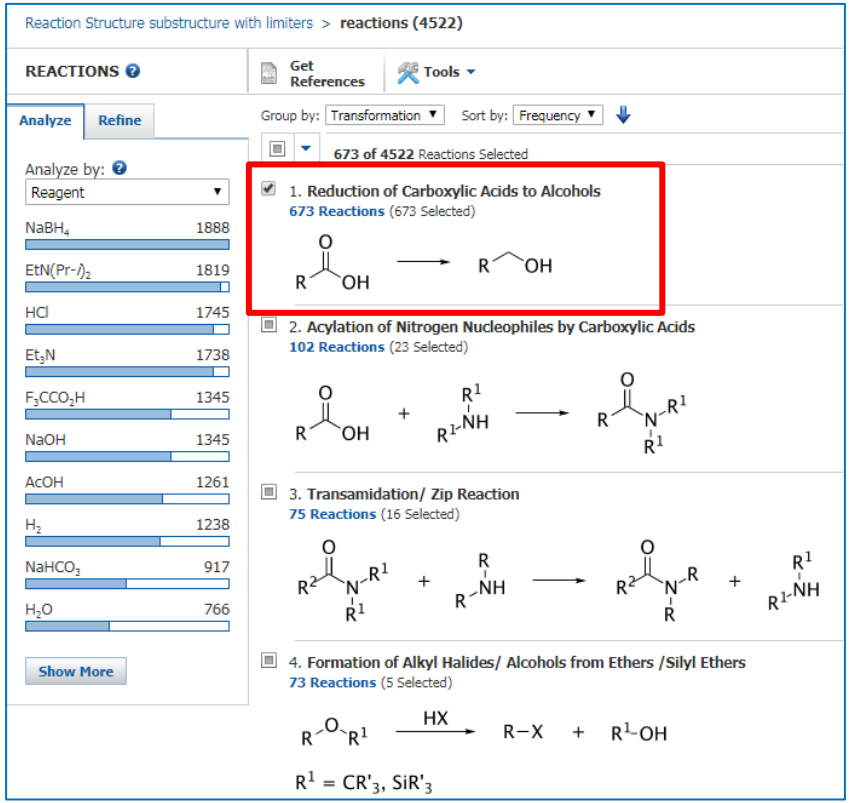

选择羧酸还原为醇的这类反应

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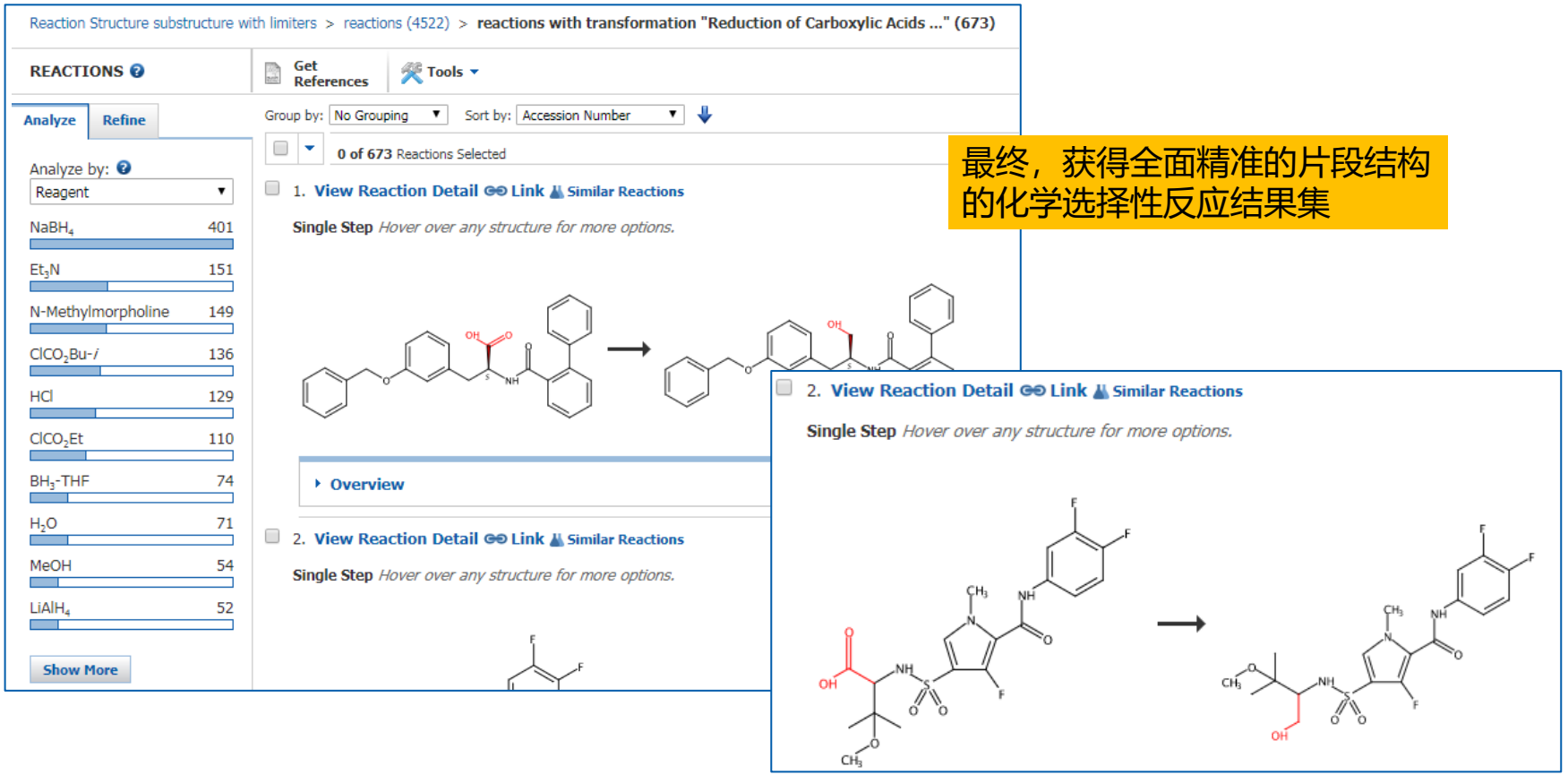

最终，获得全面精准的片段结构的化学选择性反应结果集

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例4：检索使用$Na_2S_2O_4$作为试剂的反应

思路：先检索物质，然后通过物质获取反应

- 分子式检索无机物，要按照Hill排序规则检索。具体为，不含碳化合物，按照元素符号字母顺序排序。含碳化合物， 碳在前，氢紧随其后，其他元素按照字母排序。
- 无机含氧酸盐，按照多组分物质检索（比如Na2S2O4，就按照相应的酸和钠的混合物标引，阳离子有多少个阳离子，阴离子部分用H补齐），所用分子式为: H2O4S2.2Na

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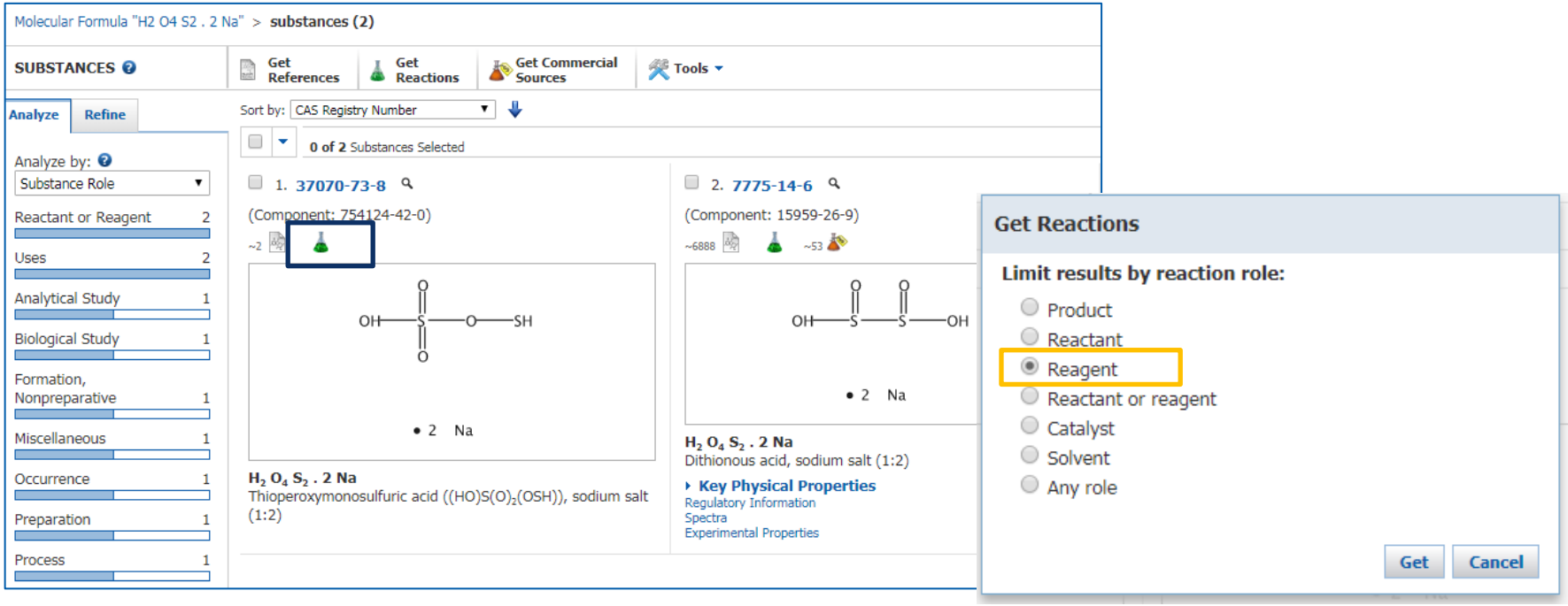
通过物质获取反应，并限制反应角色为Reagent



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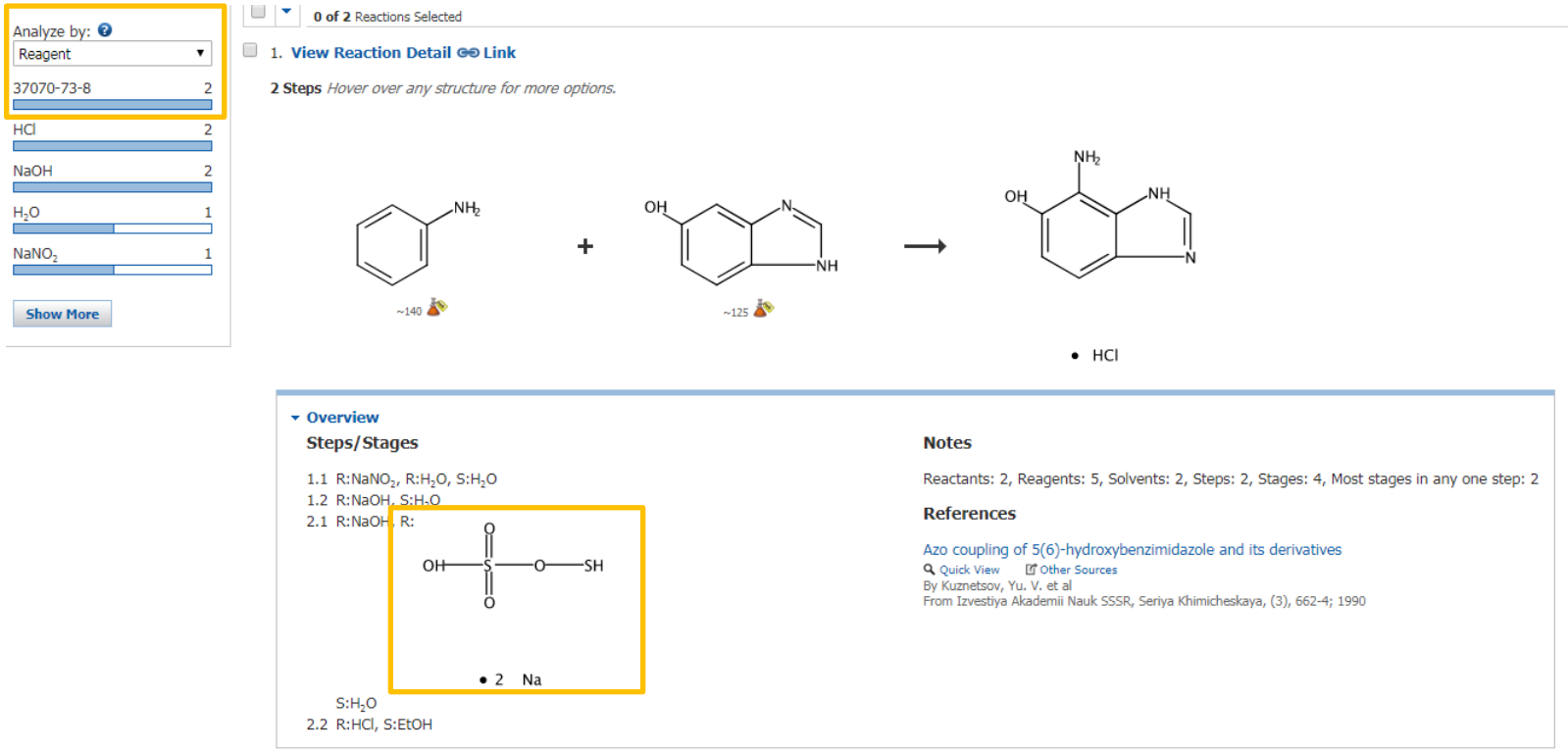
获得使用$Na_2S_2O_4$作为试剂的反应



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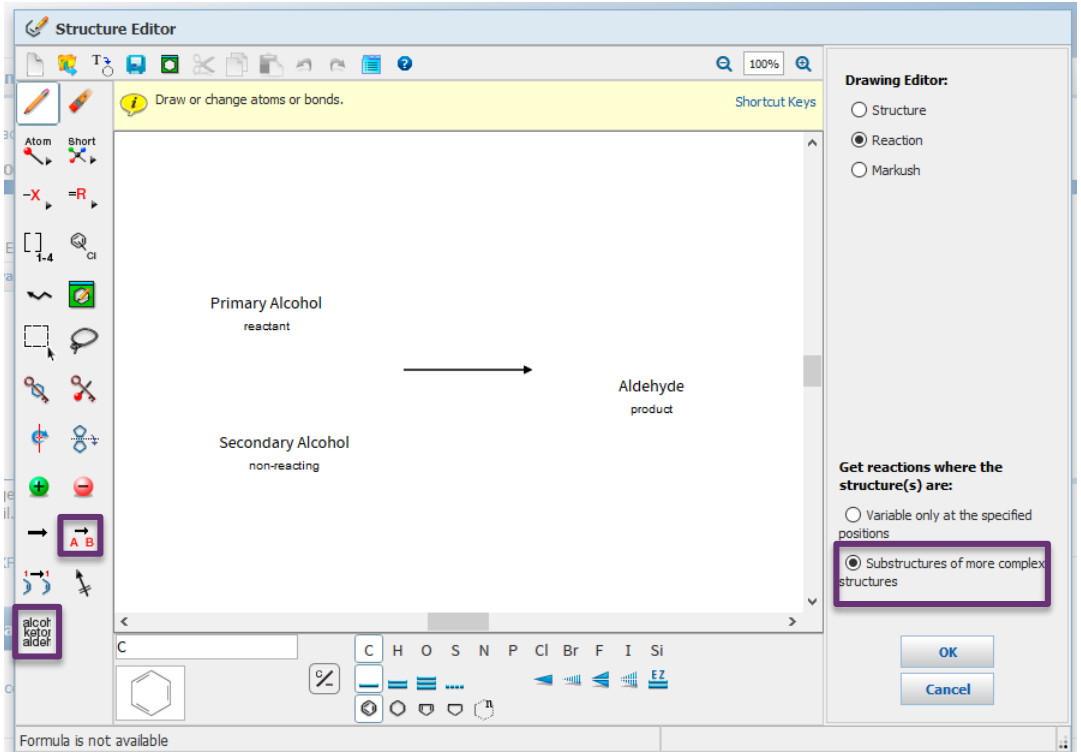
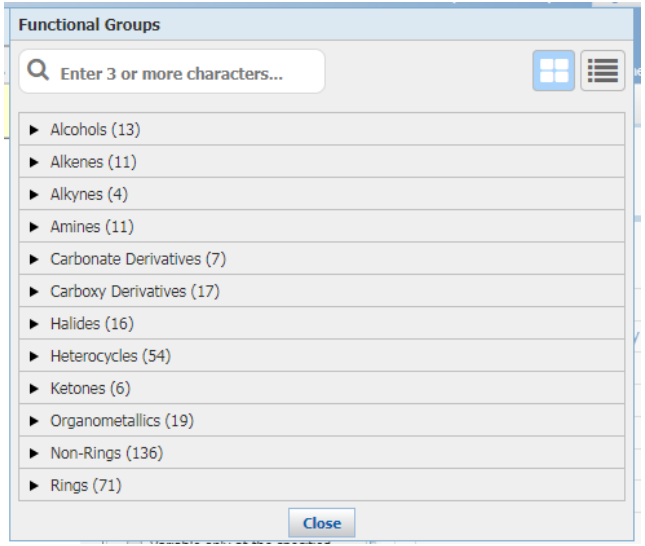
例5：在非反应仲醇存在的条件下，将伯醇转换为醛





使用反应角色定义工具和官能团列表

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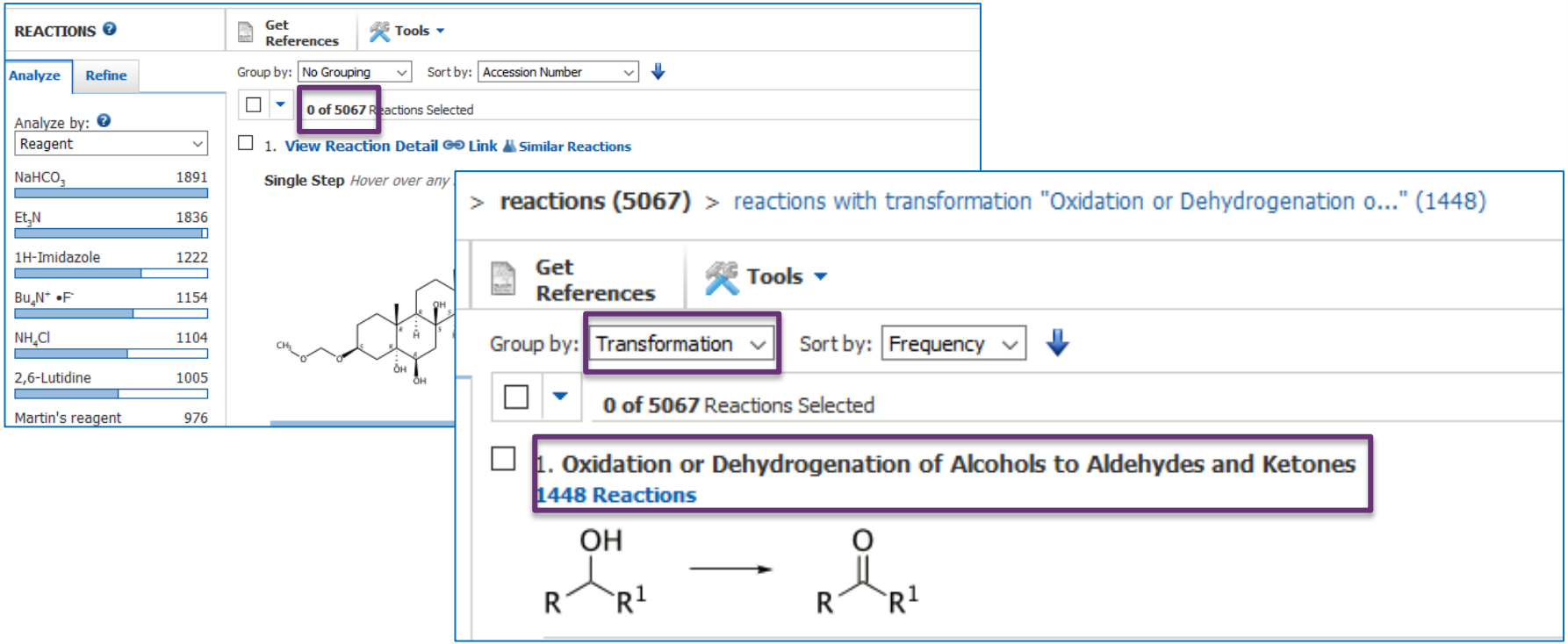
通过Group by: Transformation，筛选需要的反应类型



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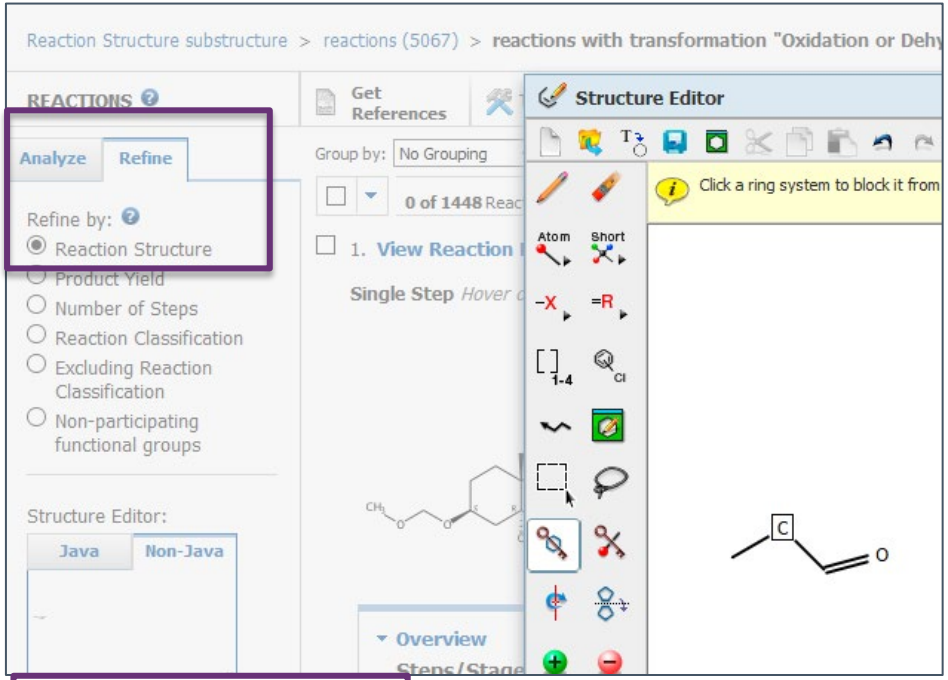
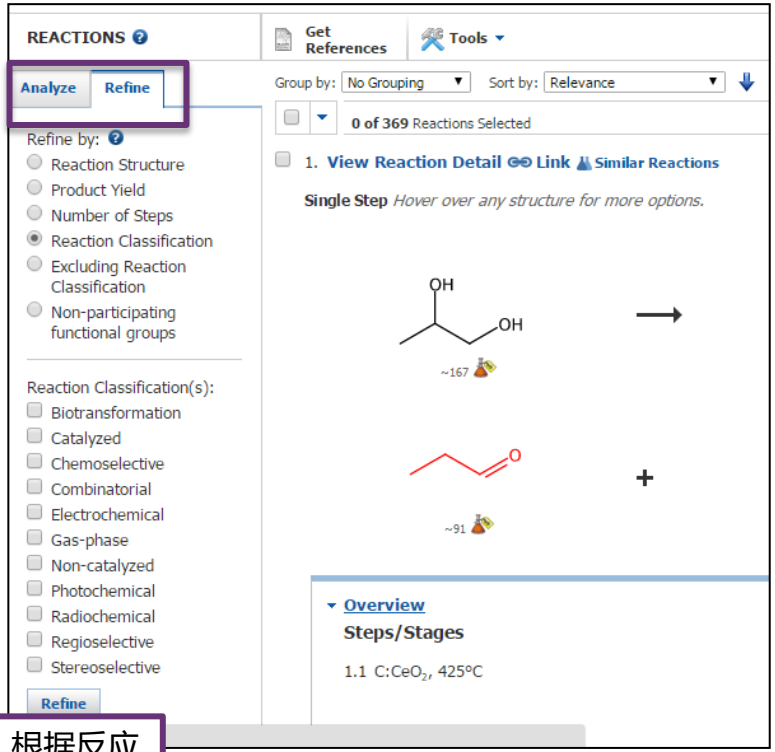


继续用“丙醛”这个结构对结果进行限定获得



使用限定功能，根据反应类型选择反应

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提纲

- SciFinder中获取化合物制备信息的方法
- 反应相关信息获取方法
  - 结构编辑器的使用（绘图、限定反应的工具）
  - 如何通过反应式检索反应，精炼结果并获得实验详情
  - 利用SciPlanner实现反应路线设计
  - 反应检索案例分享
- 通过文献主题检索合成制备相关信息的方法

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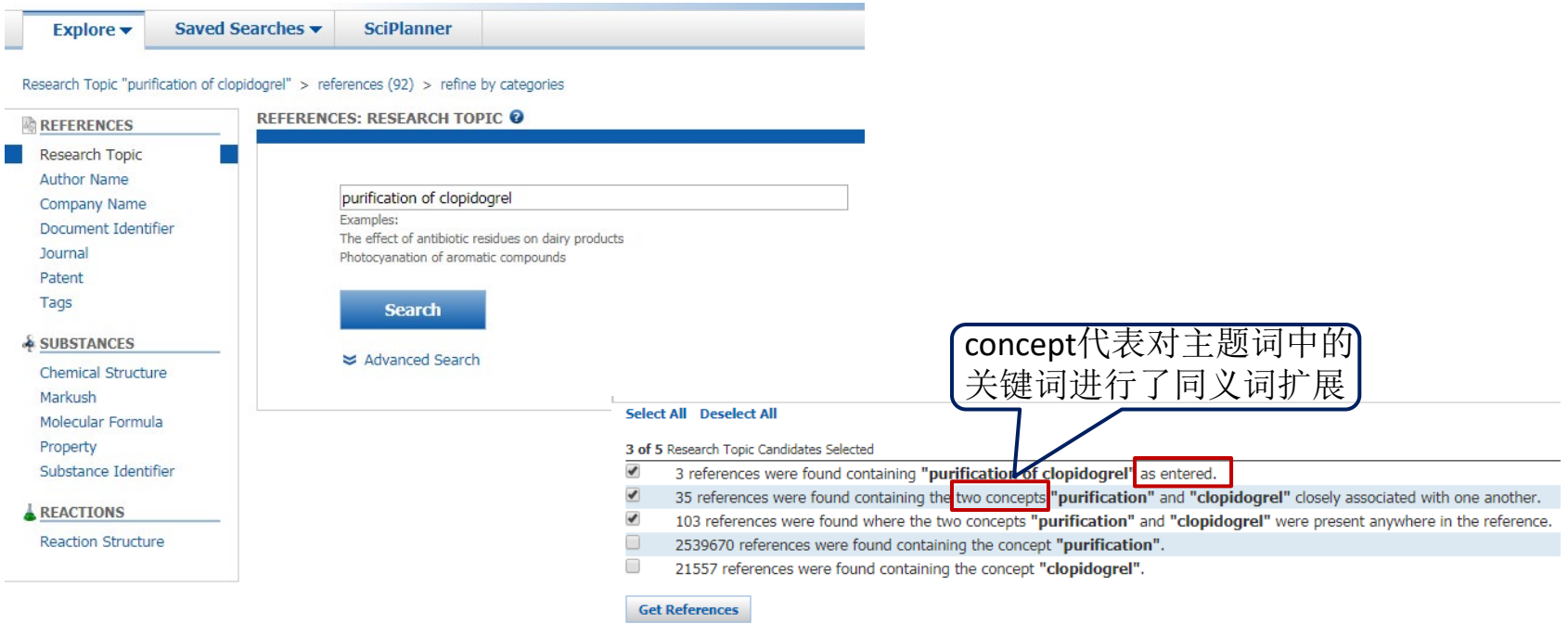
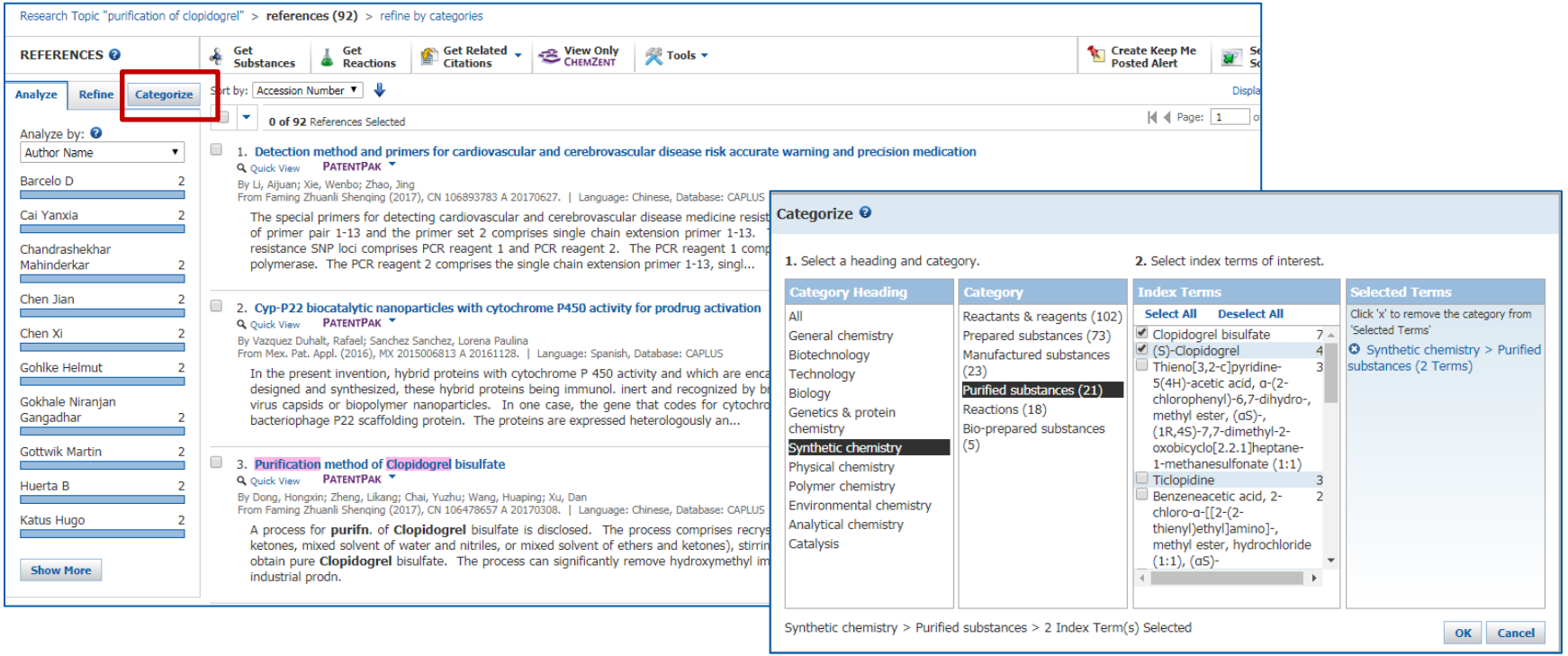
例1. 通过文献主题词检索，获取有关氯吡格雷纯化方面的文献



在文献结果集中，可通过Categorize精准定位“purified substances”



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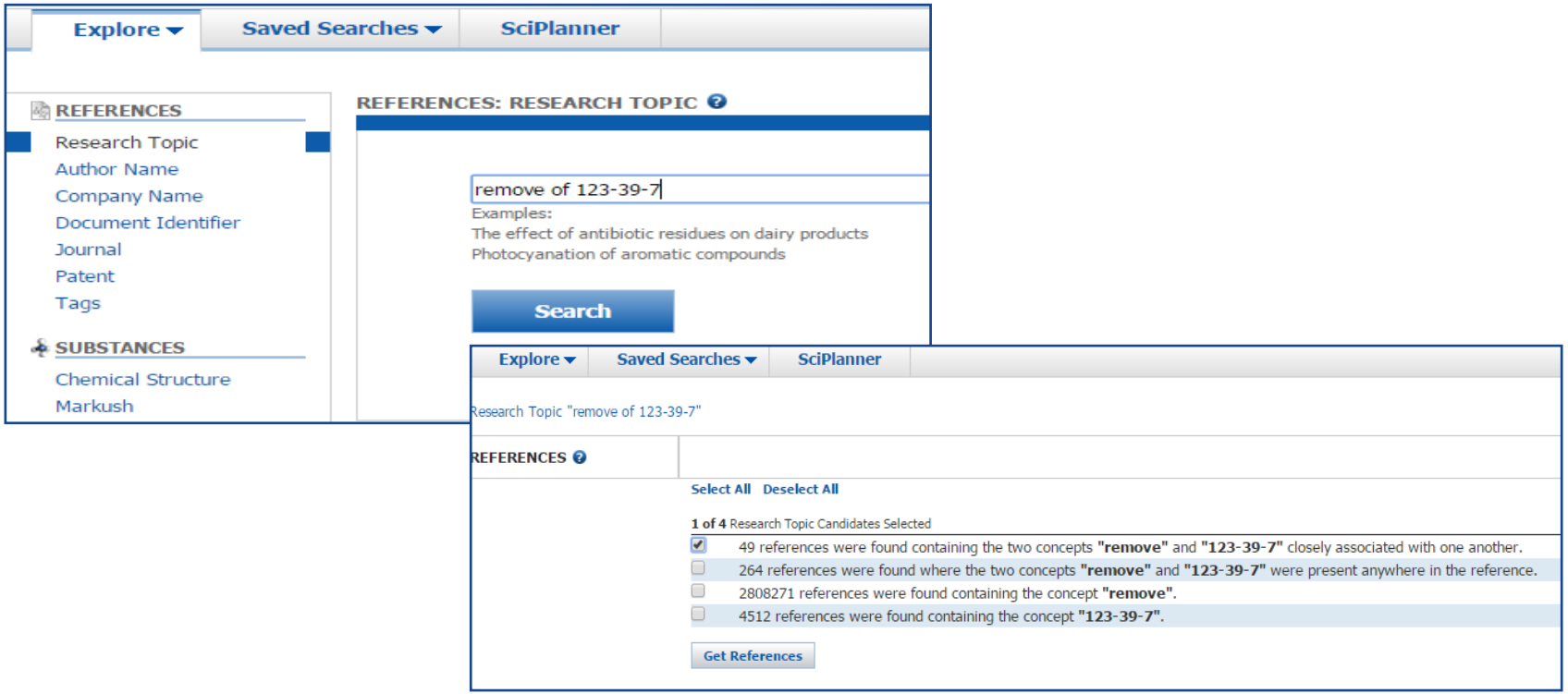
例2：去除N-甲基甲酰胺（123-39-7）



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文献详情中的Substance标引，指出物质在文献中的作用

1. Removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

By: Wang, Wenzheng; Fan, Xing; Zhu, Tianle; Wang, Haining; Ye, Daiqi; Hong, Xiaowei

Dimethylamine (DMA) and N,N-dimethylformamide (DMF) are typical N-VOCs exhausted from manufg. factories. In the present study, the behavior of non-thermal plasma (NTP) was systematically investigated for removal of gas-phase DMA and DMF in a link tooth wheel-cylinder plasma reactor. Exptl. results show that DMA is much easier to be decompd. by NTP than DMF. Coexisting DMF has no effect on DMA conversion while DMF conversion is significantly promoted by the addn. of DMA. Regardless of initial gas compns. as well as DMA and DMF concn., CO_x selectivity increased monotonously with increasing ED. But CO_x selectivity of 100% cannot be obtained even with ED higher than 70 J L^{-1}, indicating the formation of org. intermediates during DMA and DMF decompn. Based on org. products anal. with GC-MS and mol. optimization results with d. functional theory calcn., possible mechanisms on DMA and DMF degrdn. were proposed. The org. products from DMA and DMF decompn. by NTP were found to have great soly. and high biodegradability. Thus, NTP enhanced absorption/biol. method is suggested for complete removal of DMA and DMF.

Indexing

Air Pollution and Industrial Hygiene (Section59-4)

Concepts

Absorption
Air pollution control
Bond energy
Bond length
Decomposition
Decomposition catalysts
Plasma
Waste gas treatment

removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

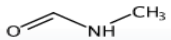
Volatile organic compounds

removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

Removal or disposal; Process

Substances

56-40-6 Glycine, formation (nonpreparative)
64-18-6 Formic acid, formation (nonpreparative)
75-12-7 Formamide, formation (nonpreparative)
79-20-9 Methyl acetate
105-37-3 Ethyl propionate
107-31-3 Methyl formate
123-39-7 N-Methyl formamide



144-62-7 Oxalic acid, formation (nonpreparative)

removal of gas phase dimethylamine and N,N-dimethylformamide using non-thermal plasma

Formation, unclassified; Formation, nonpreparative

需要的文献

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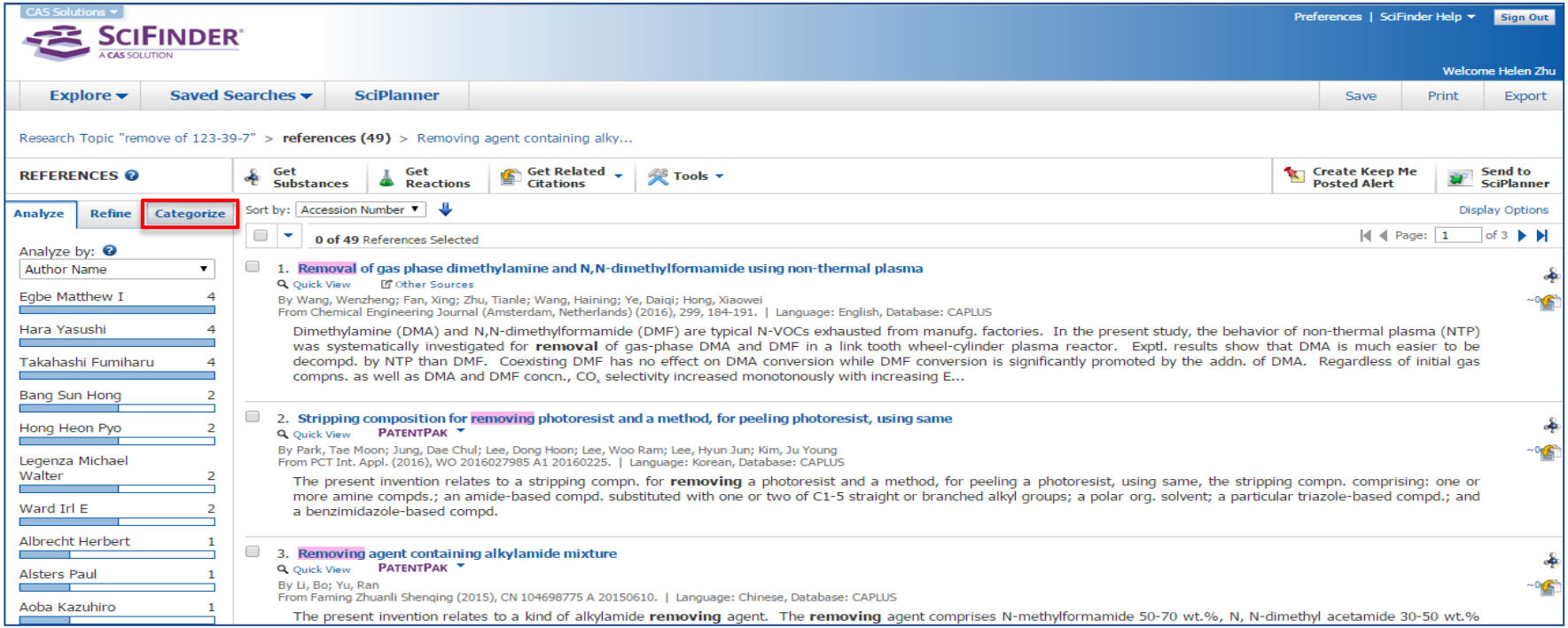
通过Categorize，精准获取所需文献



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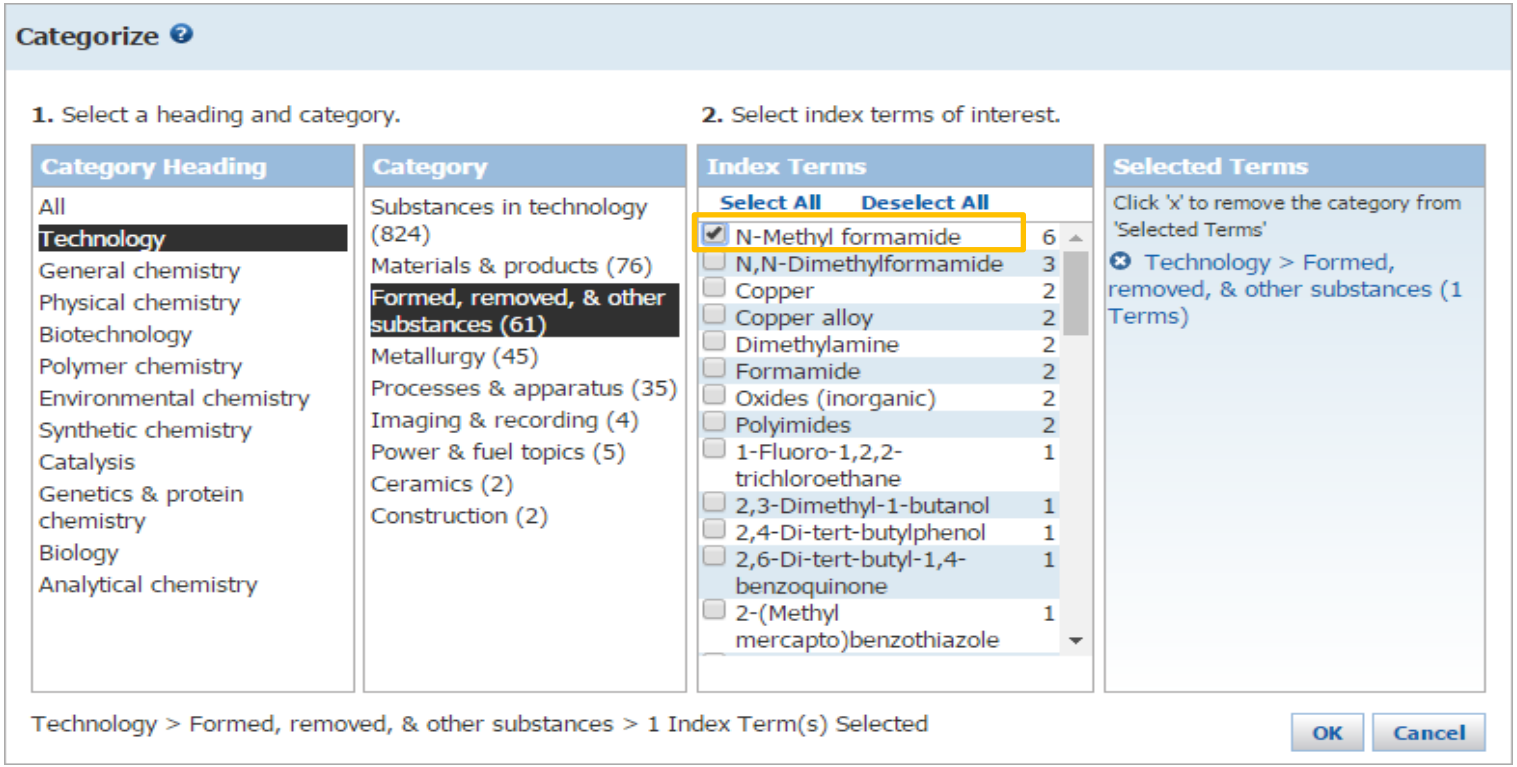
通过Categorize，精准获取所需文献



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