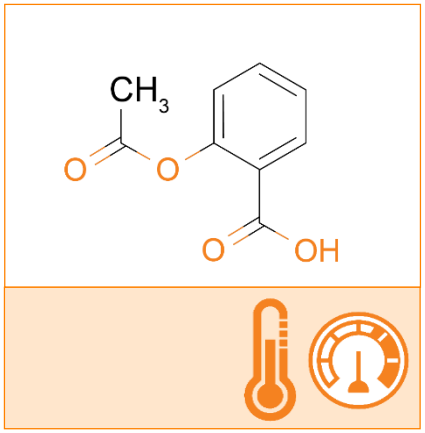
New Reaxys 使用介绍

Reaxys解决方案咨询师
俞靓

提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
  - Reaxys的基本检索模式
  - 如何利用Reaxys结构面板实现复杂结构定义
  - 如何利用Reaxys进行物质检索和物质分析
  - 如何利用Reaxys进行反应检索和条件筛选
  - 如何利用Reaxys制作合成计划
- Reaxys检索小结

什么是Reaxys?



>105 M 物质记录
>500 M 实验数据
物理的，化学的, 光谱数据，生态学, 生物活性数据

>42 M 反应记录
以及这些反应的条件，溶剂，催化剂，收率，反应中心，反应类型

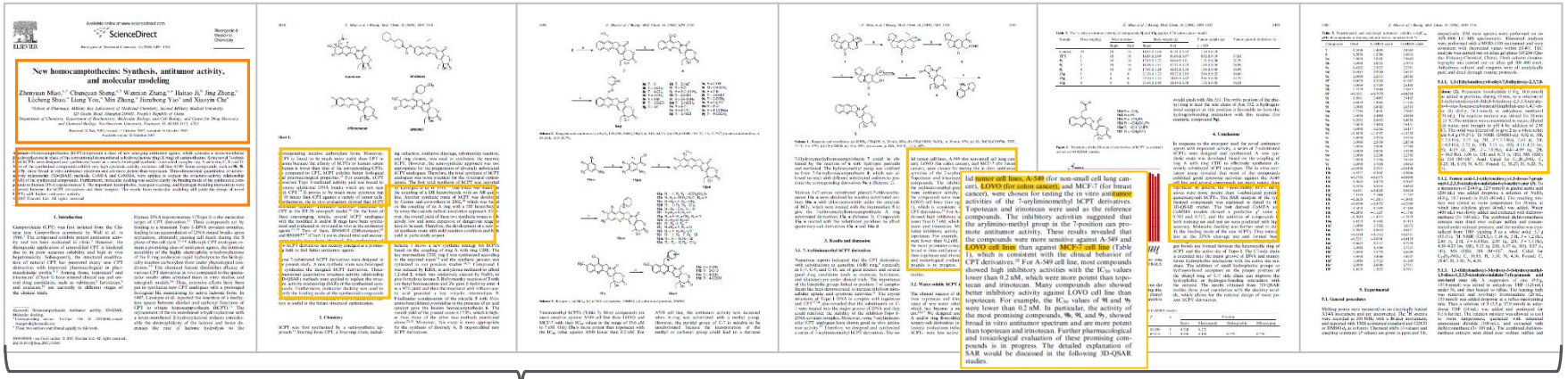
Linked to

>54 M 文献记录
>16,000 期刊，专利
涉及有机化学，材料化学，生物医药，地球科学，工程等多种领域

Chemistry fundamentals

Uses across disciplines

Reaxys索引的内容—文献内容



Reaxys提炼了文献的书目信息，摘要，题录，并用不同角度的索引词对文献内容进行描述。

bibliographic

New homocamptothecins: Synthesis, antitumor activity, and molecular modeling — Cited 23 times

Miao, Zhenyuan; Sheng, Chunquan; Zhang, Wannian; Ji, Haitao; Zhang, Jing; Shao, Luecheng; You, Liang; Zhang, Min; Yao, Jianzhong; Che, Xiaoyin - Bioorganic and Medicinal Chemistry, **2008**, vol. 16, # 3, p. 1493 - 1510

Abstract | Index Terms | Substances 124 | Reactions 78 | Full Text

Abstract

Homocamptothecins (hCPTs) represent a class of new emerging antitumor agents, which contains a seven-membered β-hydroxylactone in place of the conventional six-membered α-hydroxylactone ring (E ring) of camptothecins. Some novel 7-substituted hCPTs were designed and synthesized based on a newly developed synthetic route which couples ring A with ring C, E and D. Most of the synthesized compounds exhibit very high cytotoxic activity on tumor cell line A549. Some compounds, such as 9b, 9l, and 9y, show broad in vitro antitumor spectrum and are more potent than topotecan. Three-dimensional quantitative structure-activity relationship (3D-QSAR) methods, CoMFA and CoMSIA, were applied to explain the structure-activity relationship (SAR) of the synthesized compounds. Furthermore, molecular docking was used to clarify the binding mode of the synthesized compounds to human DNA topoisomerase I. The important hydrophobic, base-pair stacking, and hydrogen-bonding interactions were observed between the hCPT derivatives and their receptor. The results from molecular modeling will guide the design of novel hCPTs with higher antitumor activity.

Manual [digital] Indexing

Index terms

EMTREE drug term: 10 methyl 11 chloro 7 (pyridiniummethyl)homocamptothecin chloride, 7 (2 bromophenyl)iminomethyl methoxyphenyl)iminomethylhomocamptothecin, 7 (2 methylphenyl)iminomethylhomocamptothecin, 7 (2,4 dichlorophenyl) dichlorophenyl)iminomethylhomocamptothecin, 7 (3 chloro 4 fluorophenyl)iminomethylhomocamptothecin, 7 (3 chloro 4 r fluorophenyl)iminomethylhomocamptothecin, 7 (3 methylphenyl)iminomethylhomocamptothecin, 7 (3,4 dichlorophenyl)im dimethylphenyl)iminomethylhomocamptothecin, 7 (3,5 dichlorophenyl)iminomethylhomocamptothecin, 7 (3,5 dimethylphe chlorophenyl)iminomethylhomocamptothecin, 7 (4 cyanophenyl)iminomethylhomocamptothecin, 7 (4 methylphenyl)iminor phenyliminomethylhomocamptothecin, antineoplastic agent, camptothecin derivative, irinotecan, topotecan, unclassified d

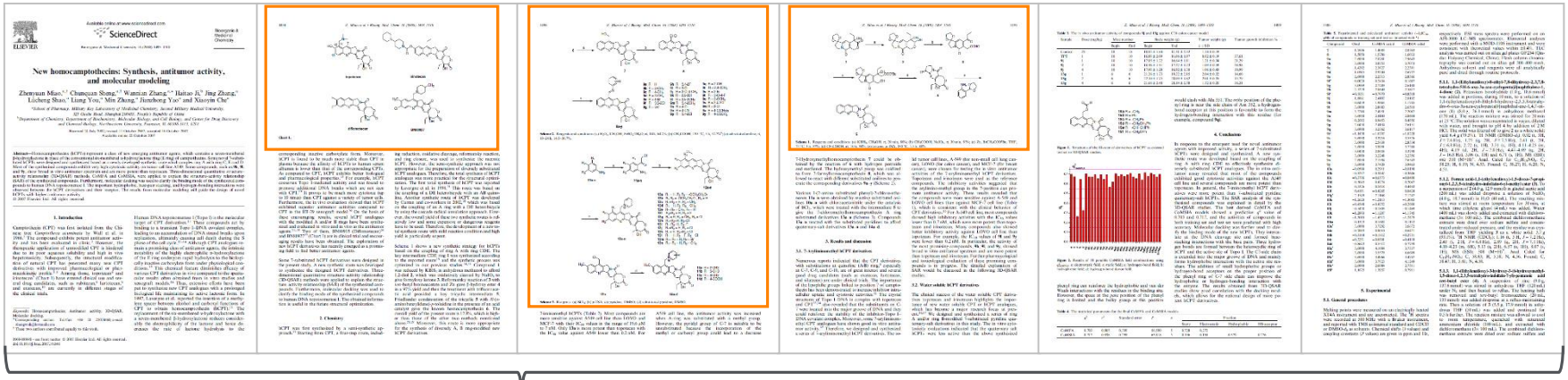
EMTREE medical term: animal experiment, animal model, antineoplastic activity, article, colon cancer, comparative molecu protein binding, drug structure, drug synthesis, human, human cell, hydrogen bond, hydrophobicity, male, molecular dock imaging, tumor cell

Author keyword: 3D amptothecins, Molecular docking

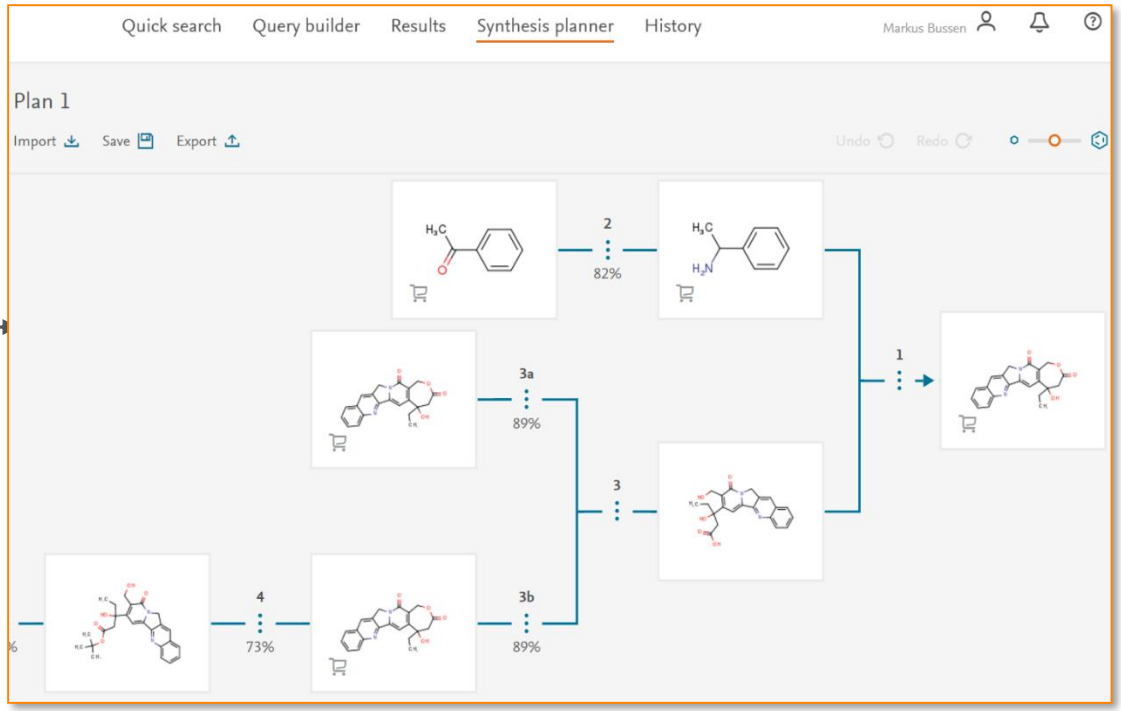
Reaxys Index Terms: hydrophobic surface

tumor cell line

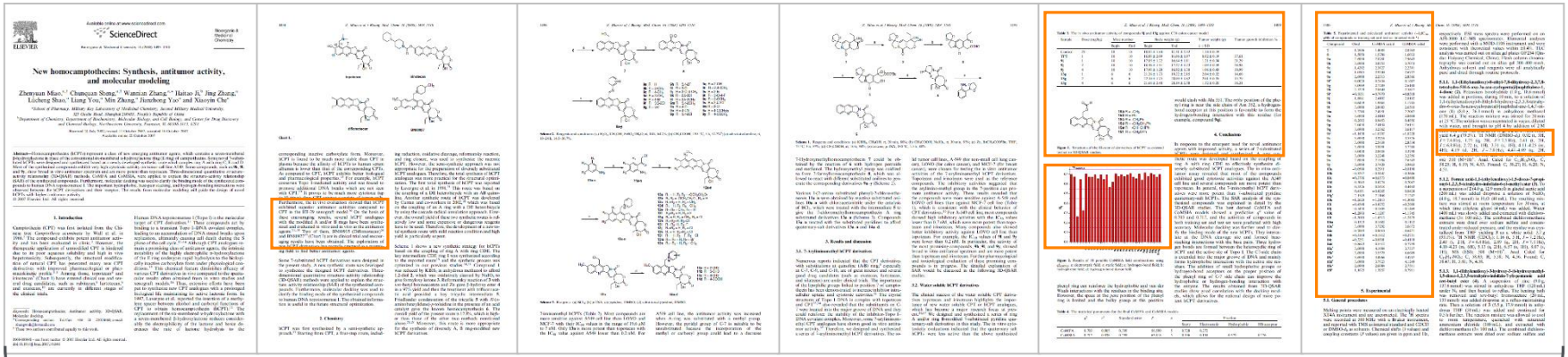
Reaxys索引的内容—结构与反应



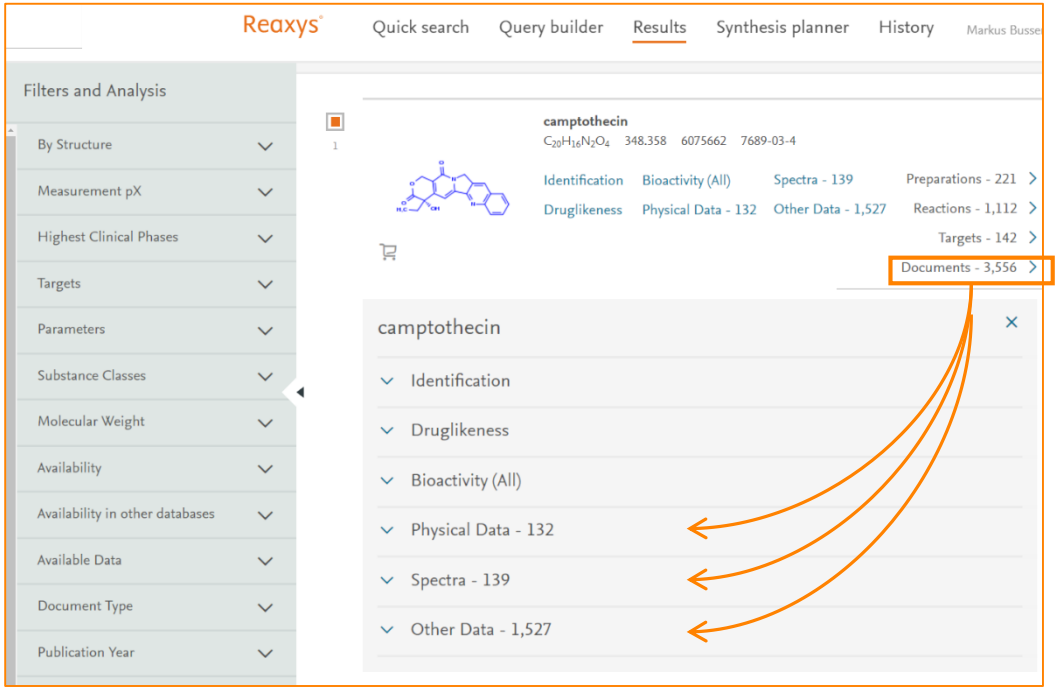
Reaxys的反应记录，抽提了所有相关的数据，包括收率，催化剂，溶剂，反应类型等



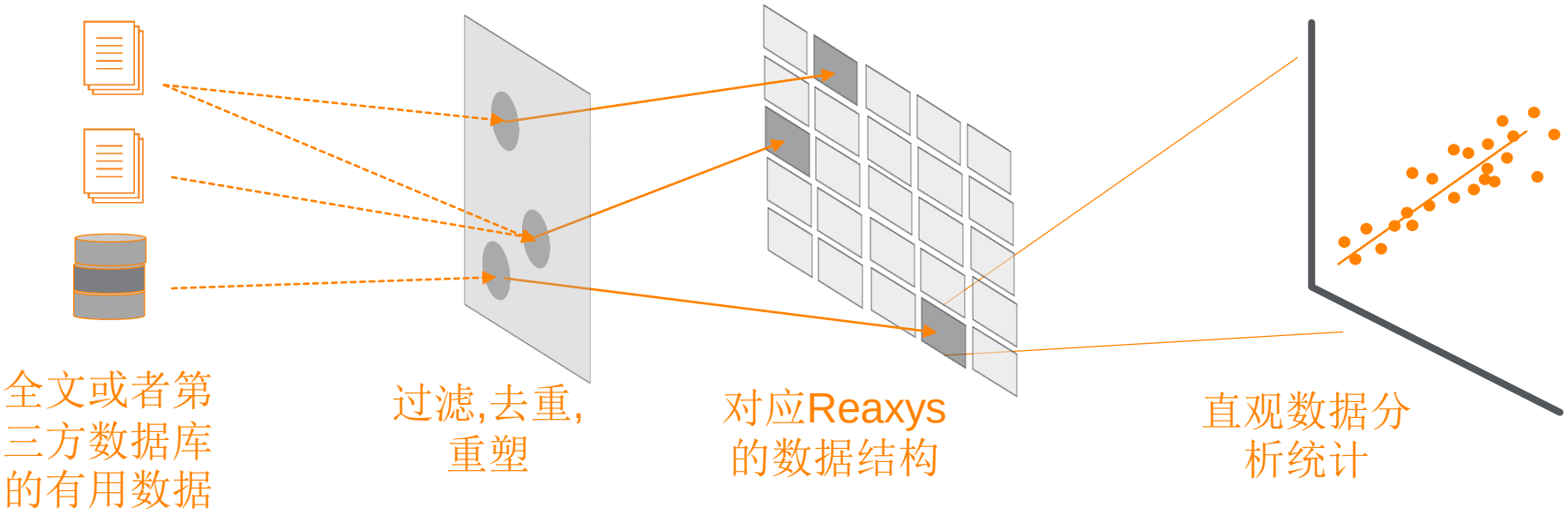
Reaxys索引的内容—文献中的数据



Reaxys的物性记录，抽提了超过500中不同的物性实验数据，生物活性数据，环境数据，以及谱图数据等等



Reaxys旨在弹指之间传递关键信息



重在索引文献中的有用信息

提纲

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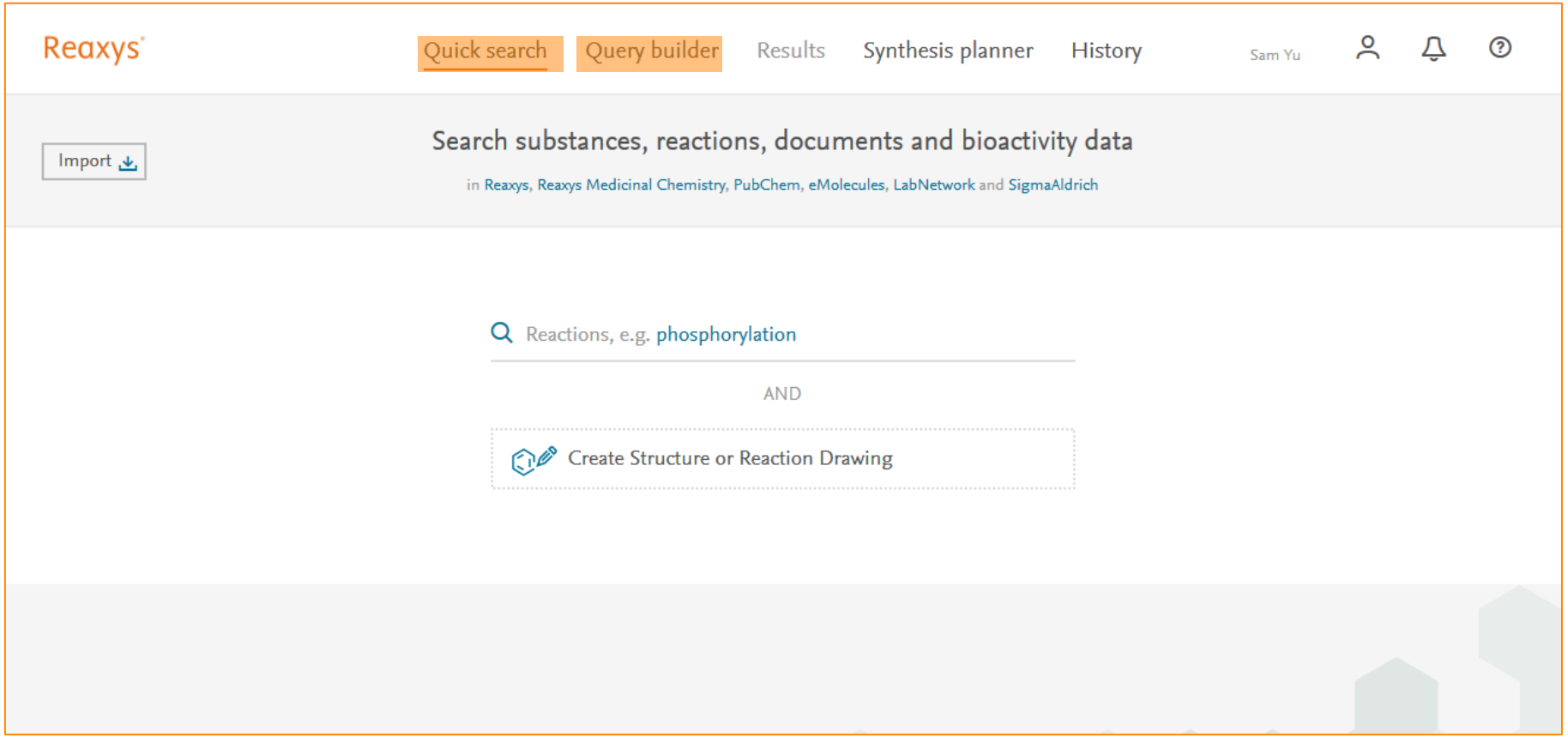
New Reaxys的界面

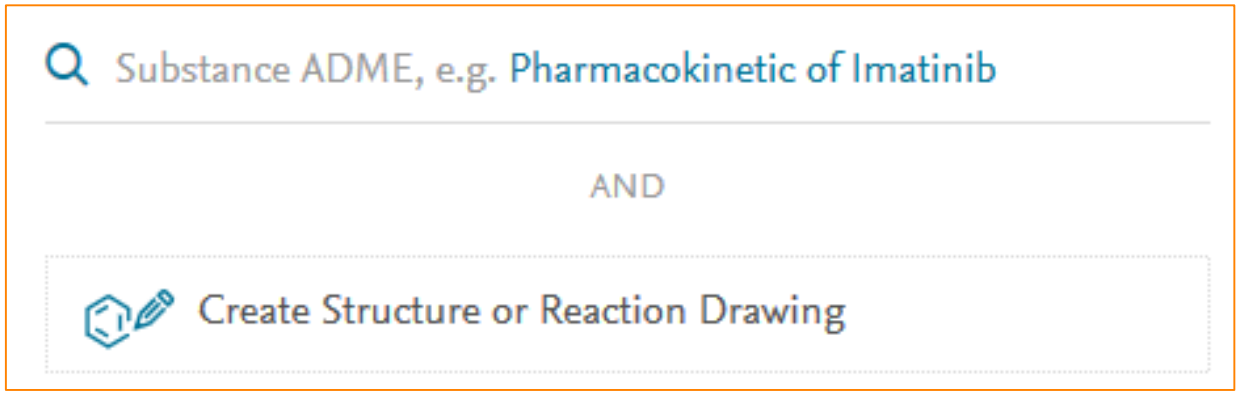
- Http://new.reaxys.com

Quick Search

Query Builder



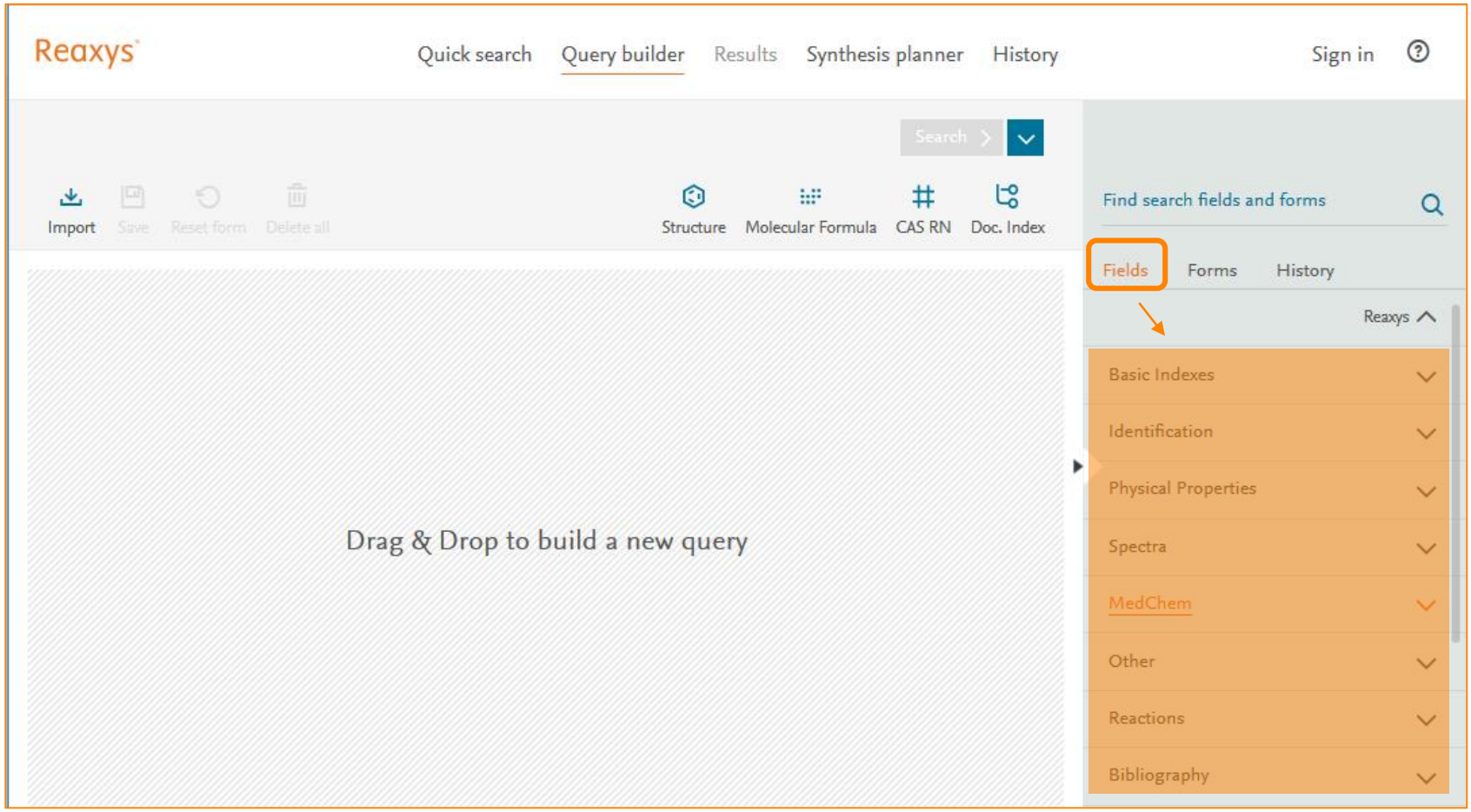
Reaxys的检索方式—Quick Search



Quick Search中可以使用的方式：

1. 物质名称，	Gefitinib
2. 反应名称，	Wittig Reaction
3. 物质理化性质，	Solubility of Gefitinib
4. 物质的谱图，	NMR of Gefitinib
5. 分子式，	C22H24ClFN4O3
6. 反应类型，	Substitution
7. 关键词，	Immunology Oncology
8. 反应结构，物质结构	

Reaxys的检索方式—Query Builder

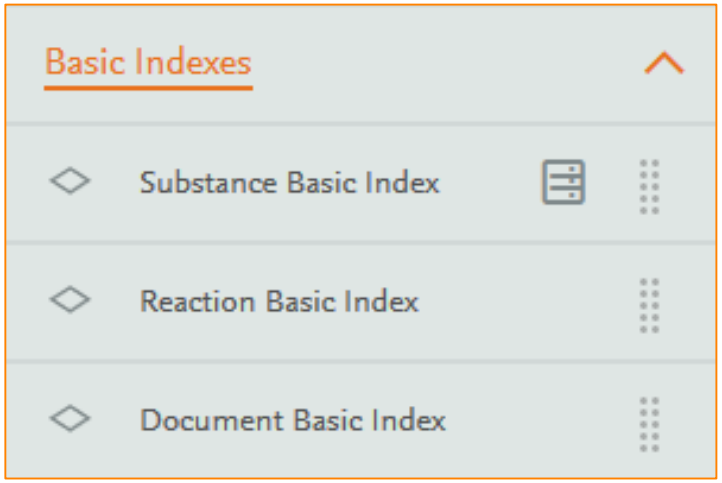


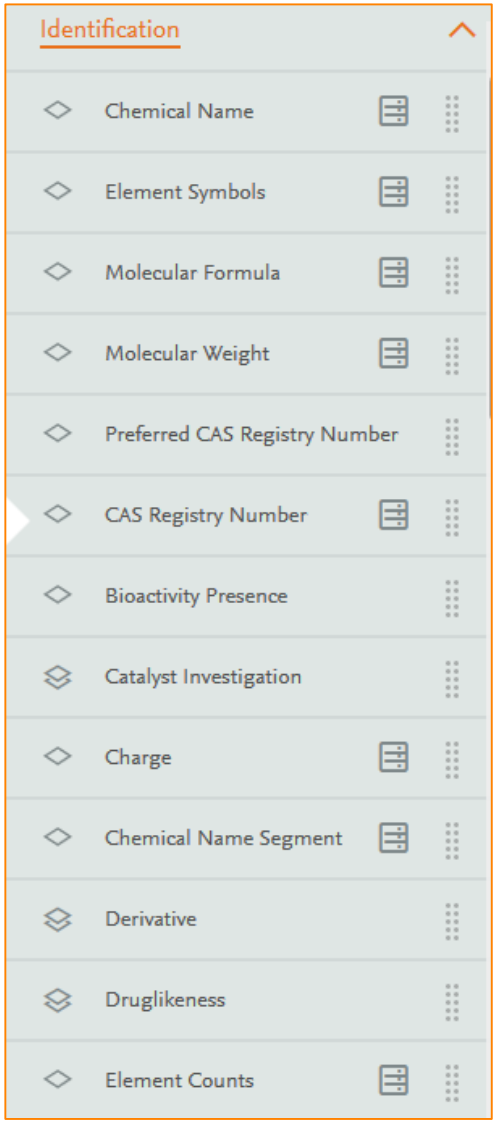
Query Builder模块下，Fields中可以选择不同类型的字段进行自由组合检索

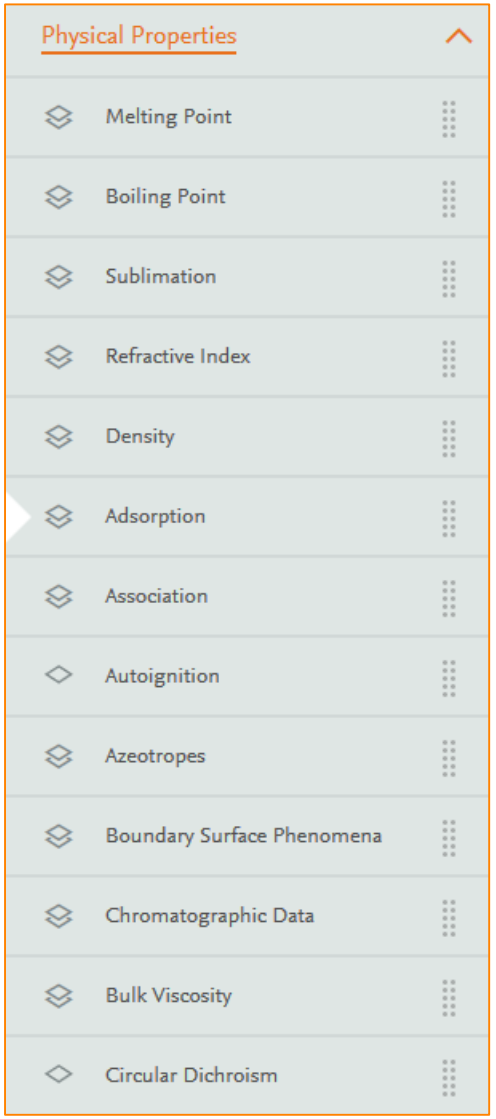
Reaxys中的字段检索

Tips:

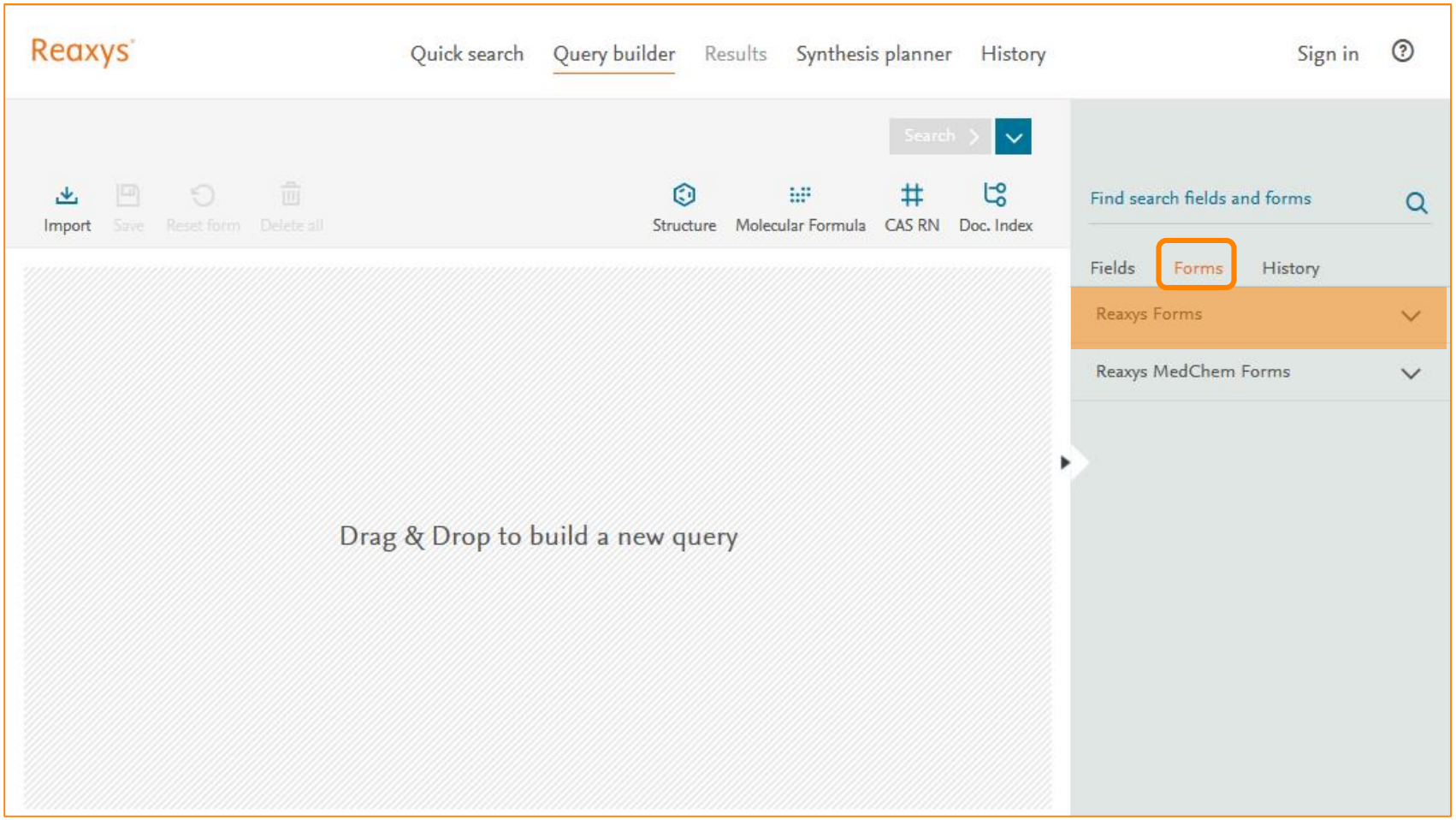
Reaxys提供8种不同的分类，每种分类中拥有和这种分类相关的多种字段，可以依据这些字段自由组合进行检索





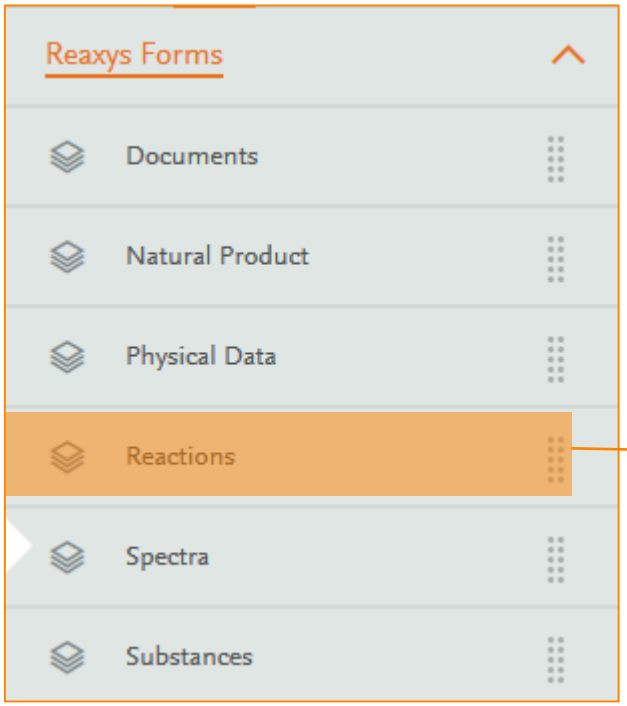


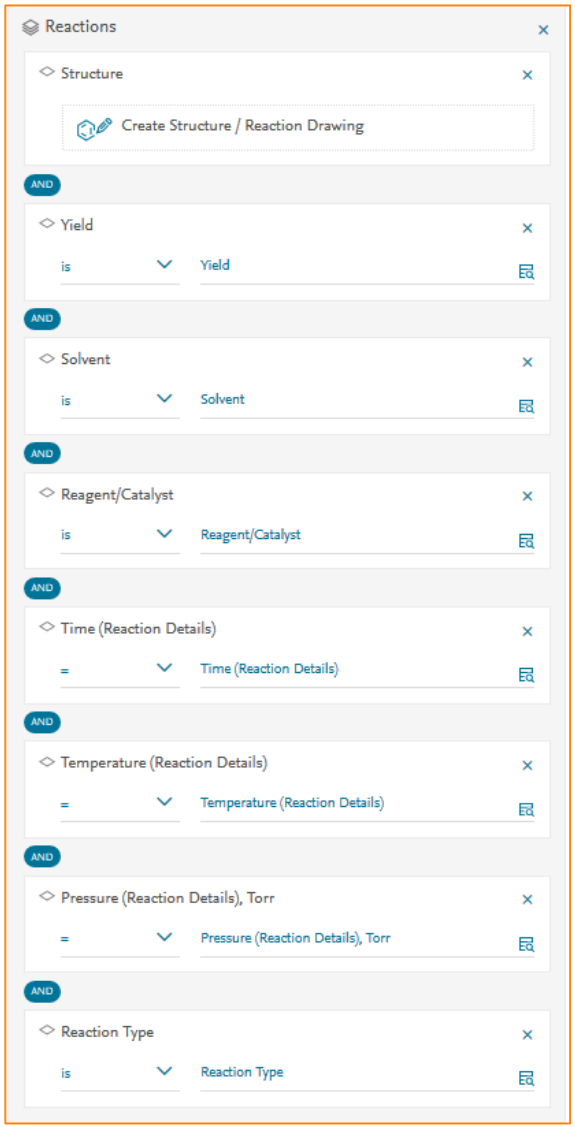
Reaxys检索方式—Query Builder Forms



Query Builder模块下，Forms中Reaxys的预设模块检索

Reaxys Form中的预设模块





反应结构

反应收率

反应溶剂

试剂催化剂

反应时间

反应温度

反应压力

反应类型

提纲

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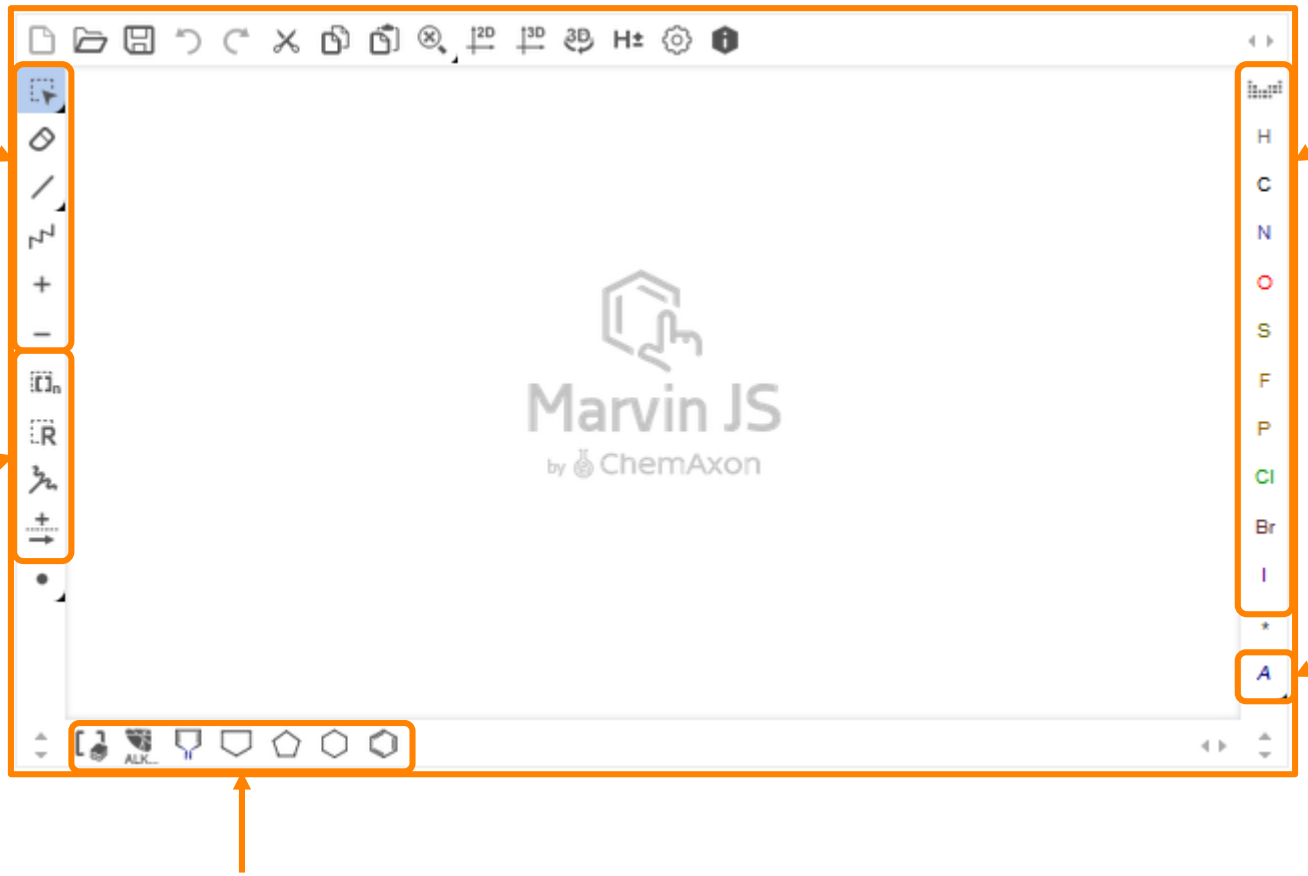
Reaxys中Marvin JS结构编辑器使用

选择工具，橡皮，键定义，链，正负电子

重复基团，R基团，R基团链接端，反应定义工具



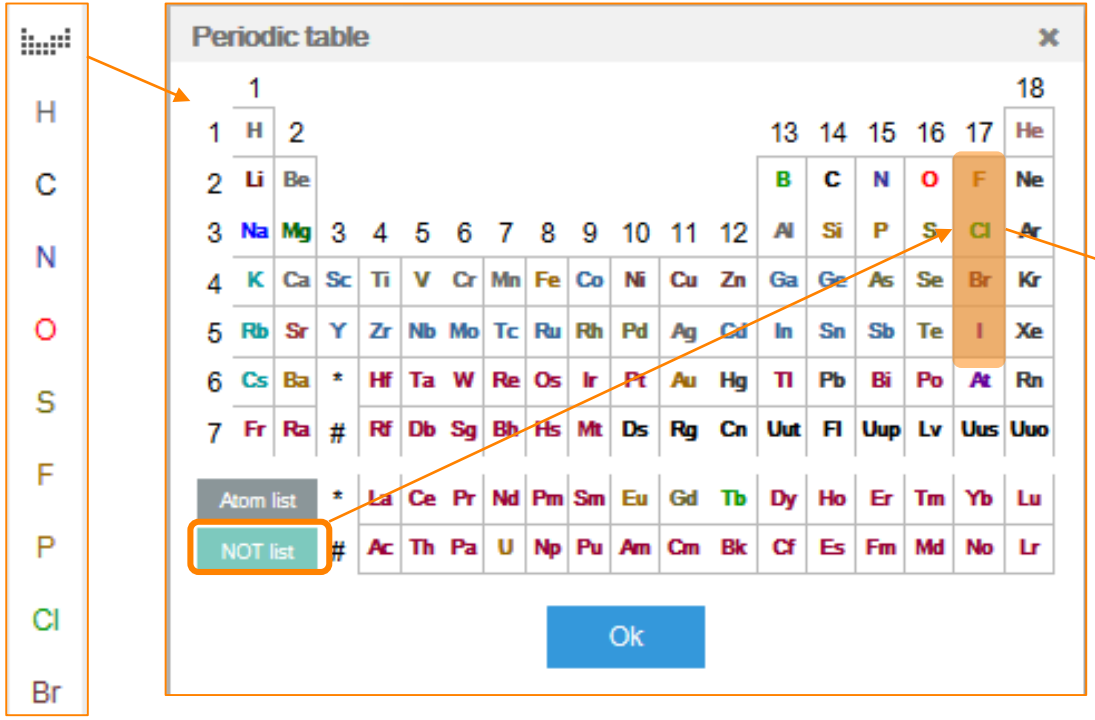
元素周期表以及常用原子

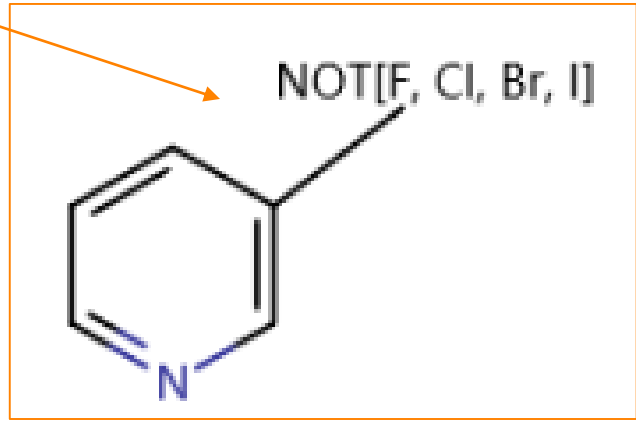
A：原子属性定义工具

常见的环，官能团，Reaxys的Generic Group定义

结构定义案例1—Not List的应用

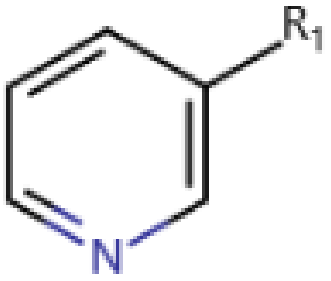
- 案例:
  - 定义某位点上不能发生F, Cl, Br, I取代



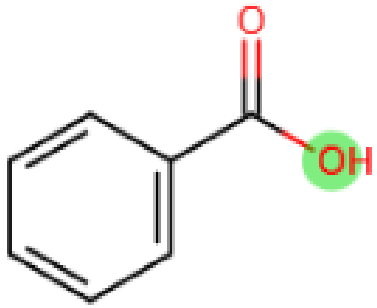


自定义R基团

- 案例
  - 定义一个结构A
  - R1分别是下面的这些结构，结构中绿色原子与A结构相连接

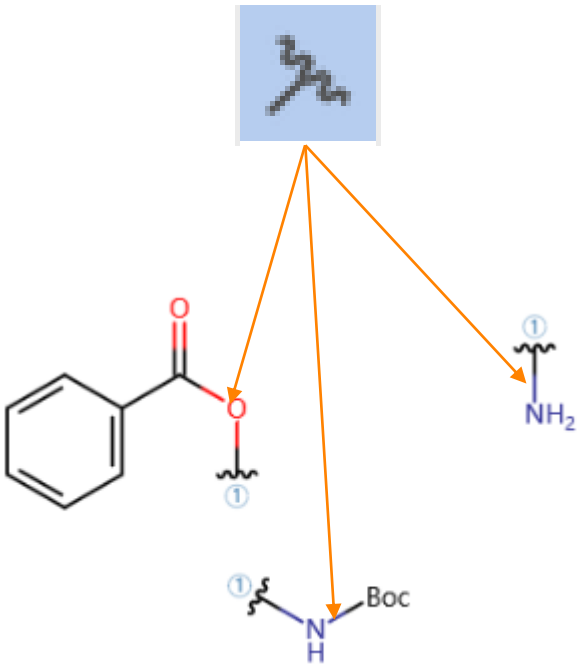


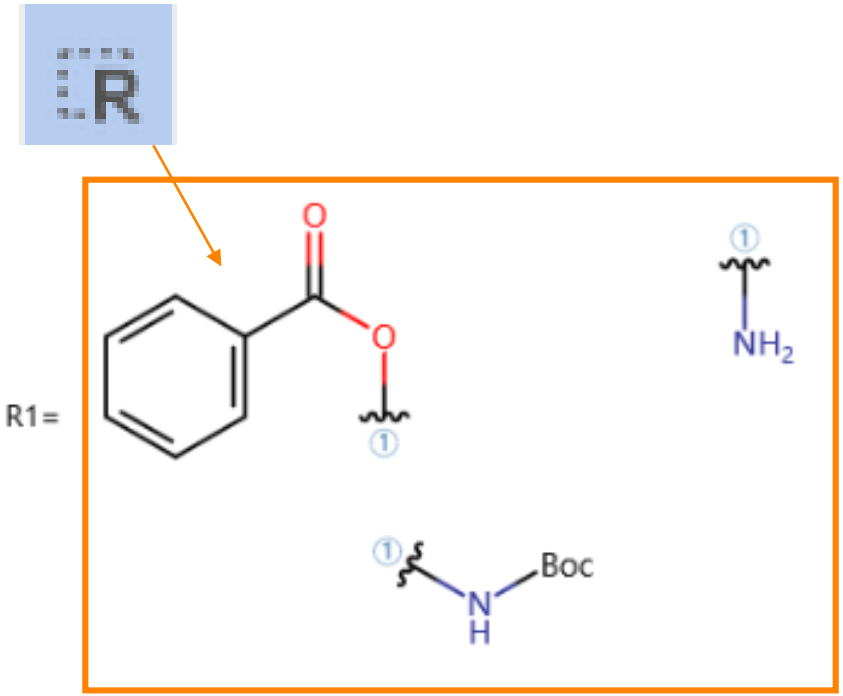
A



绘制方法

- 定义步骤：
  - 使用R基团末端定义工具定义绿色原子
  - 使用R基团定义工具，选择全部片段，即可完成R1的定义





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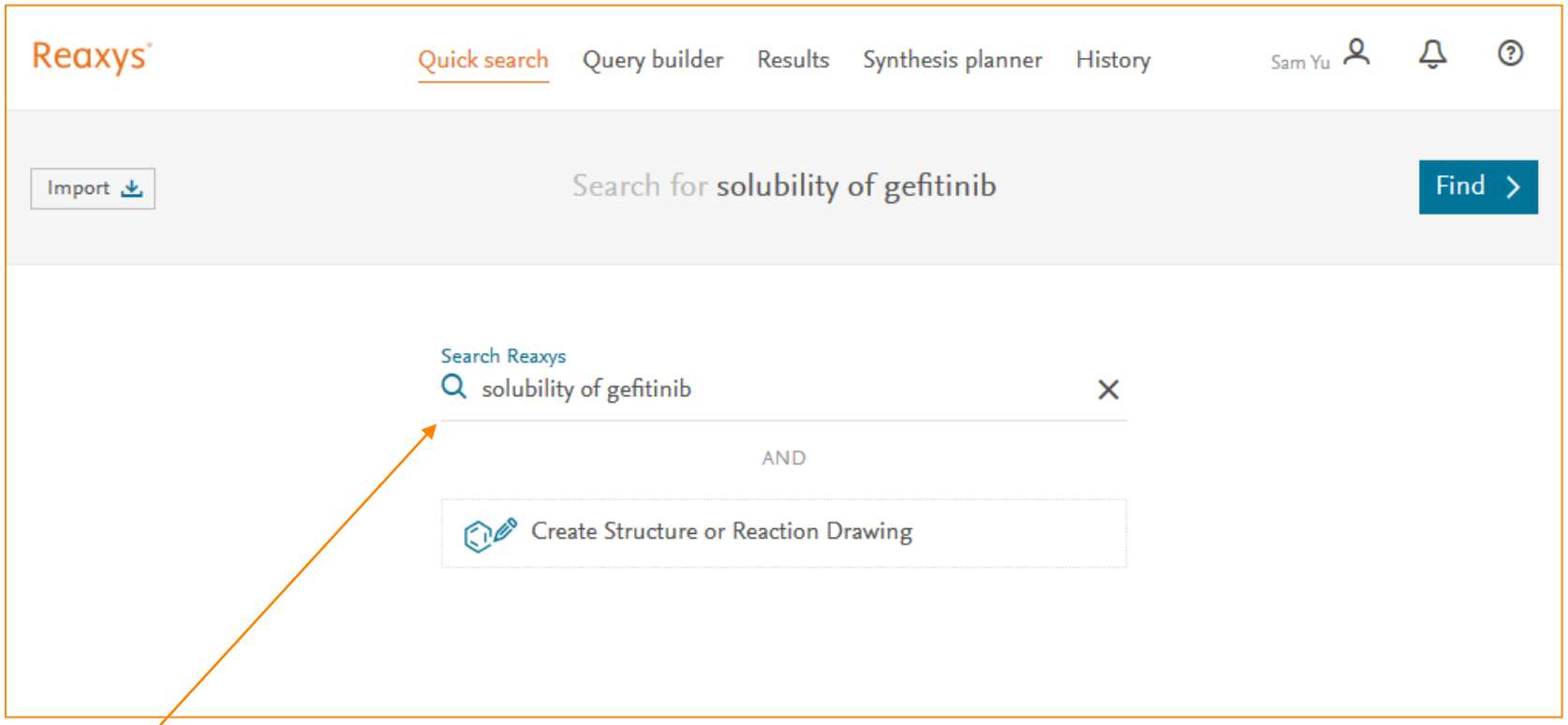
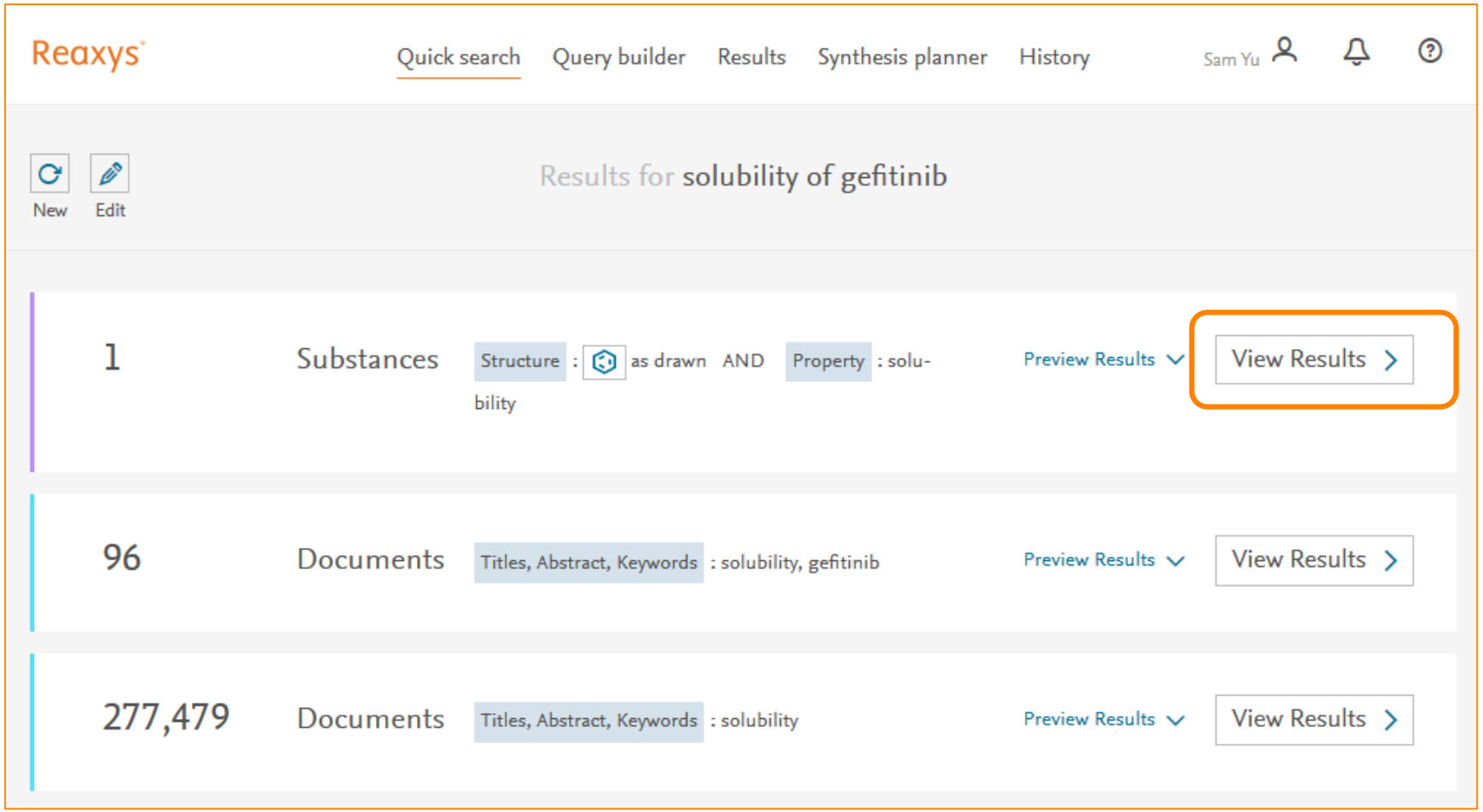
Case Study 1—快速获得物质的理化性质

- 检索吉非替尼的溶解性数据

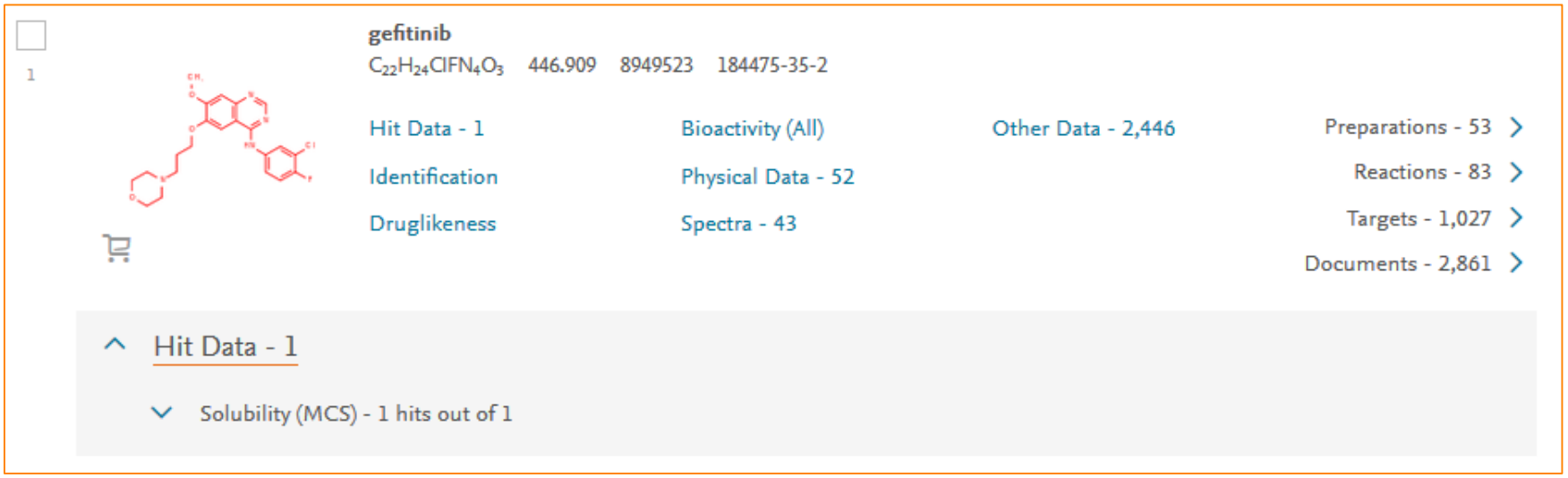


直接用自然语言在输入，solubility of gefitinib，检索

Reaxys直接给出结果

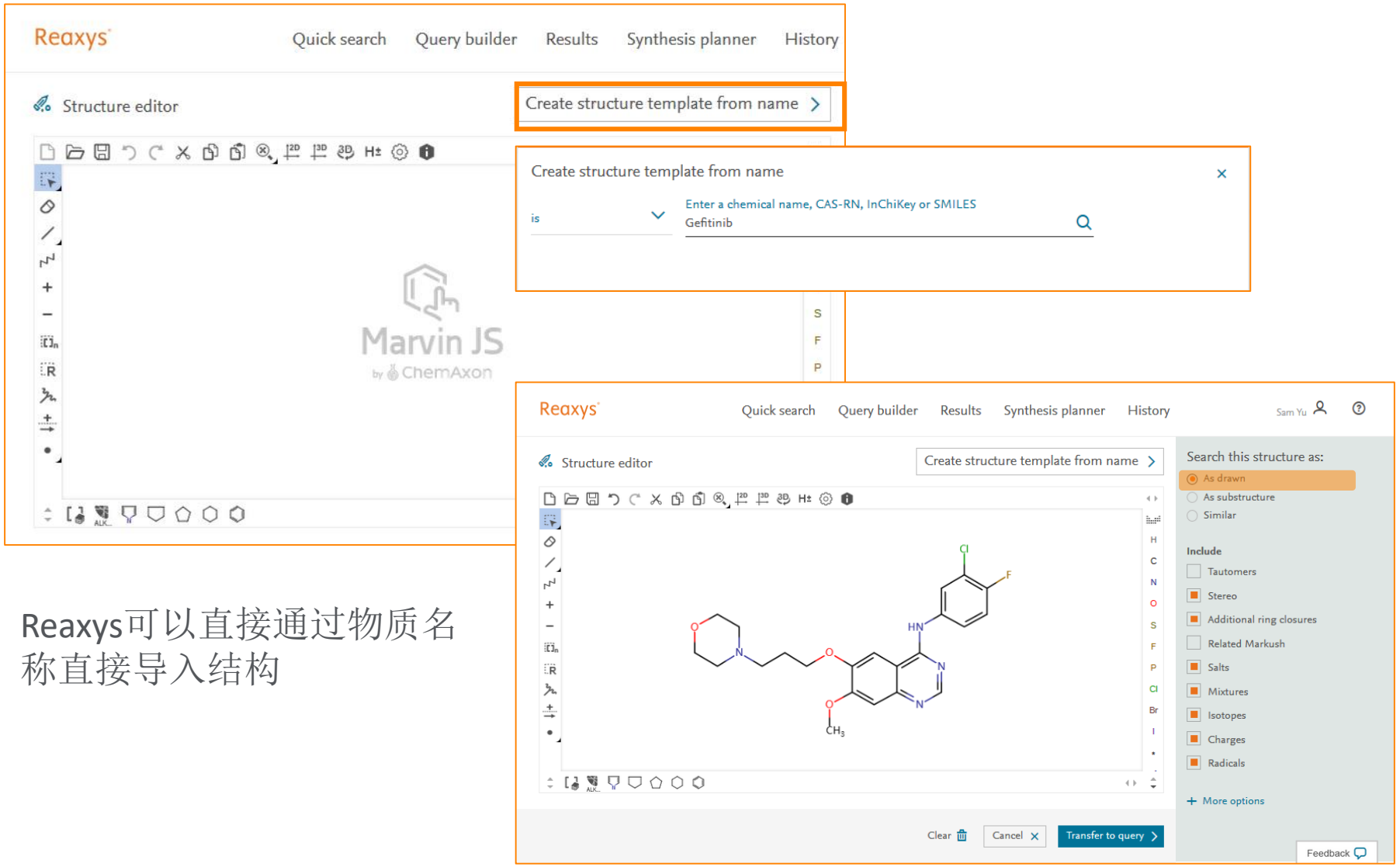


最后的结果



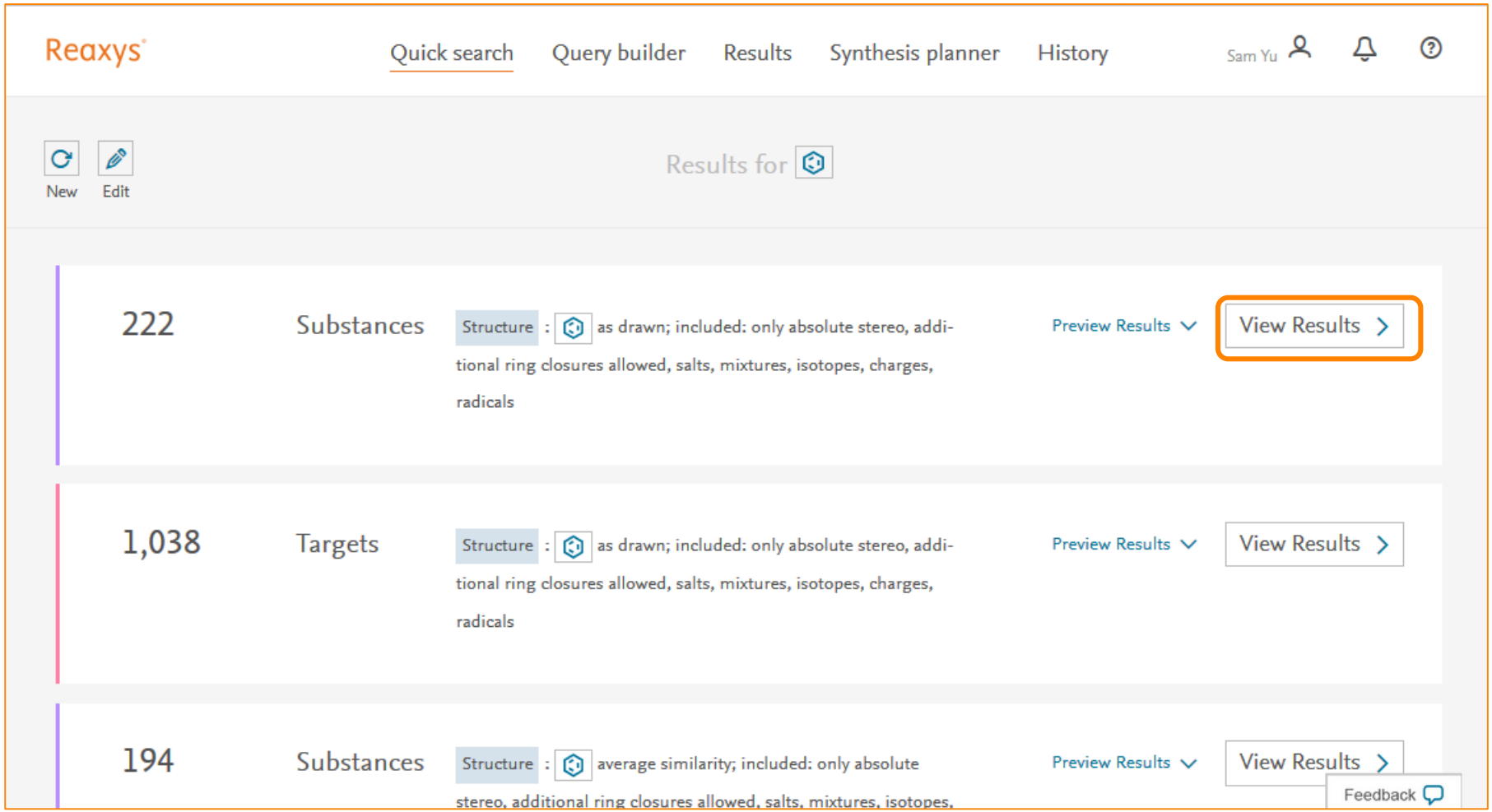
Hit Data直接给出具体的实验数据，以及检测条件和全文链接

Case Study 2—结构检索物质

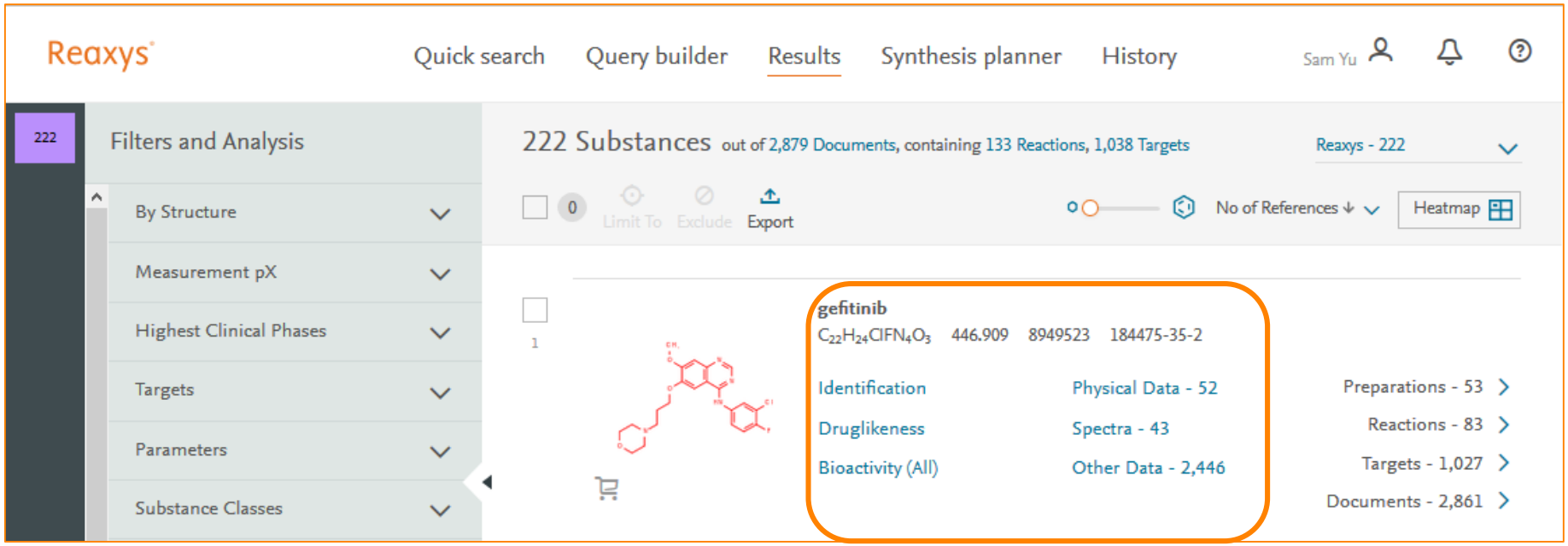


Reaxys可以直接通过物质名称直接导入结构

New Reaxys给出的结果



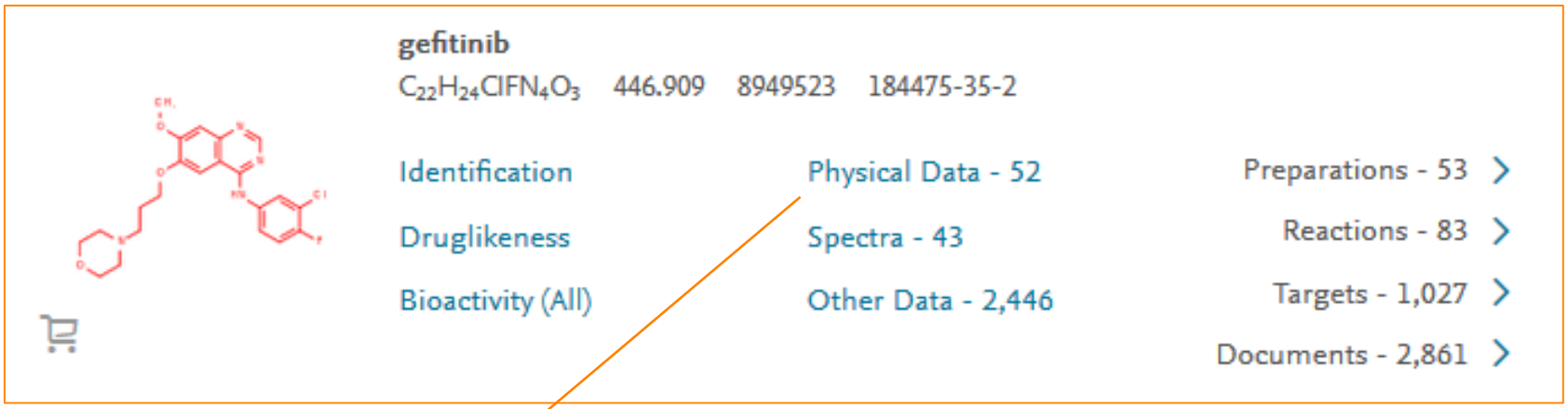
New Reaxys中的结果集

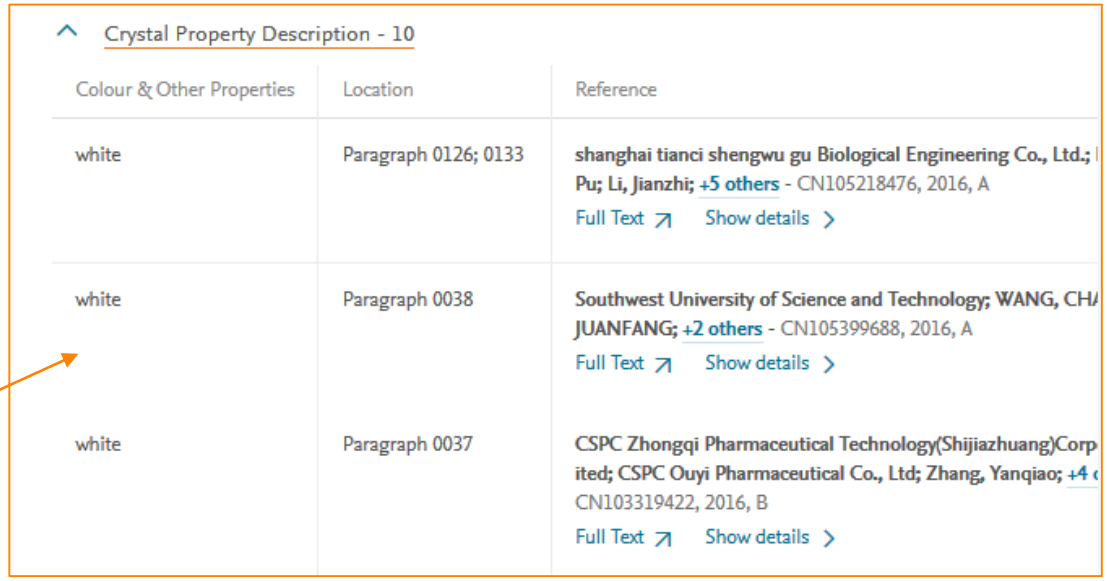


Tips：

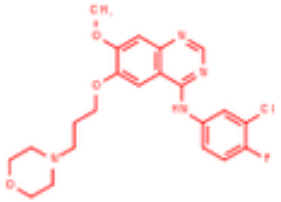
1. 每一个结构结果中，存在的理化性质数据可以直接打开，且可以直接看到对应文献的出处，
2. 物质对应的文献，可以进行进一步的分析，筛选

New Reaxys中的物质理化性质





New Reaxys中的谱图



gefitinib

$C_{22}H_{24}ClFN_4O_3$ 446.909 8949523 184475-35-2

Identification | Physical Data - 52

Druglikeness | Spectra - 43

Bioactivity (All) | Other Data - 2,446

Spectra - 43

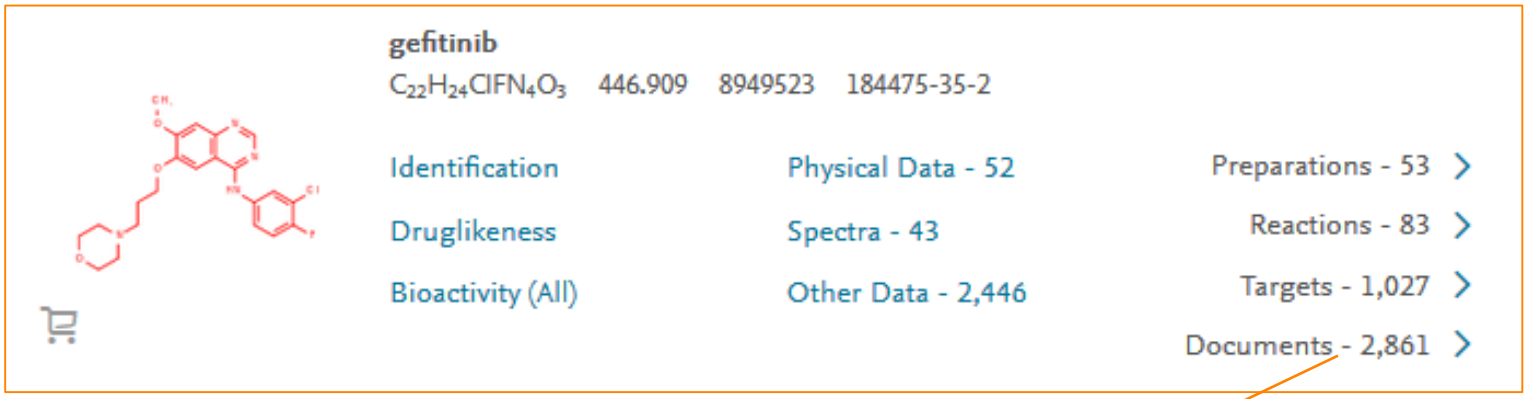
- NMR Spectroscopy - 27
- IR Spectroscopy - 4
- Mass Spectrometry - 7
- UV/VIS Spectroscopy - 4
- Raman Spectroscopy - 1

Tips：

Reaxys直接摘录原文中的NMR谱图描述，并提供原文中的位置

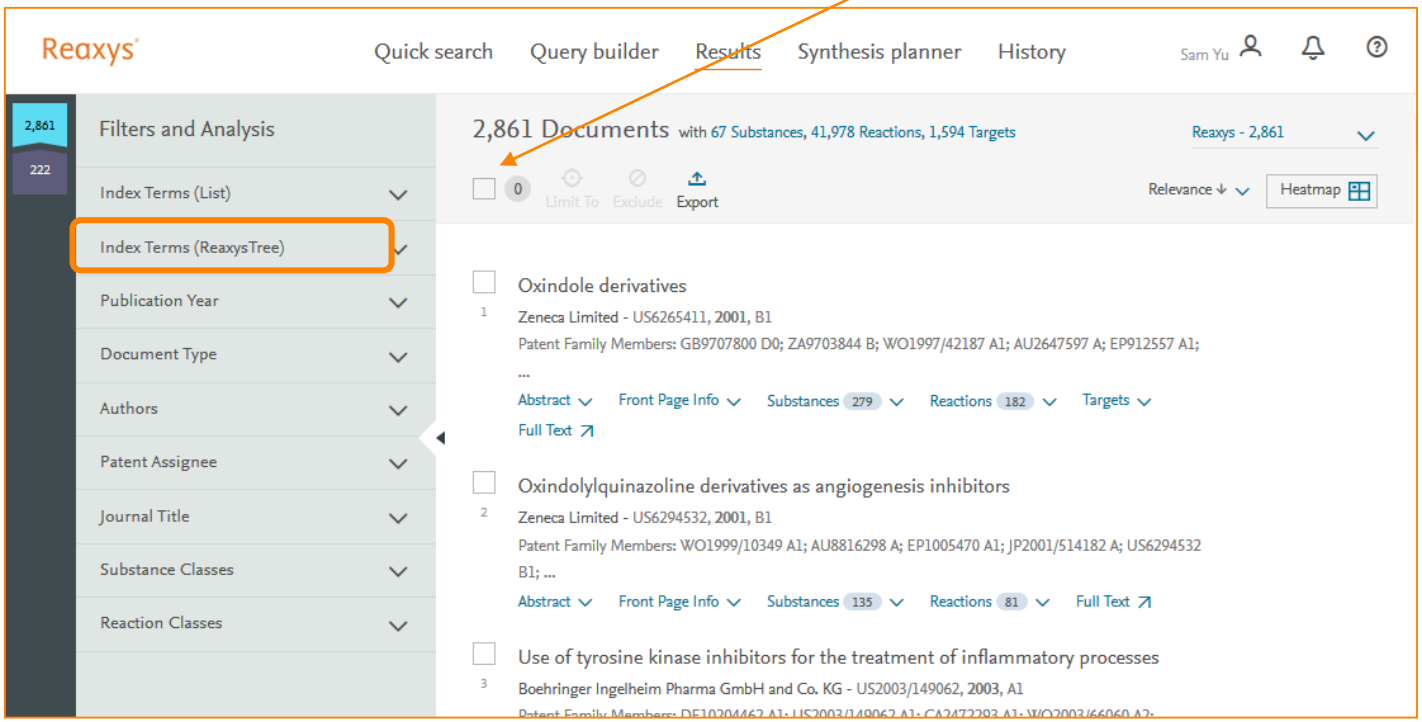
1H NMR (400 MHz, d6-DMSO) O 9.44 (5, 1H), 8.50 (5, 1H), 8.12 (dd, J= 6.9, 2.7 Hz,1H), 7.80 (m, 2H), 7.44 (t, 1H), 7.20 (5, 1H), 4.18 (t, J= 6.7 Hz, 2H), 3.94 (5, 3H), 3.59(t, J = 4.4 Hz, 4H), 2.49 (t, J = 6.9 Hz, 2H), 2.41 (bs, 4H), 2.00 (m, 2H).	Paragraph 0035	**SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou** - WO2015/188318, 2015, A1 Full Text ↗ Show details ›
13C NMR (100 MHz, d6-DMSO) O 156.48, 154.94, 153.57 (J = 241 Hz), 153.05,148.74, 147.43, 137.33 (J = 3 Hz), 123.91, 122.77 (J = 7 Hz), 119.19 (J = 19 Hz),116.90 (J=21 Hz), 109.26,107.72,103.14,67.59,66.43,56.31,55.35,53.73,26.13.	Paragraph 0035	**SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou** - WO2015/188318, 2015, A1 Full Text ↗ Show details ›

Reaxys中的分析文献的获取

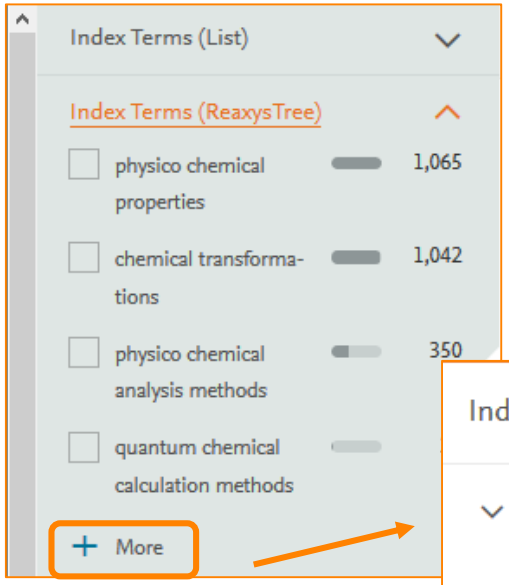


Tips:

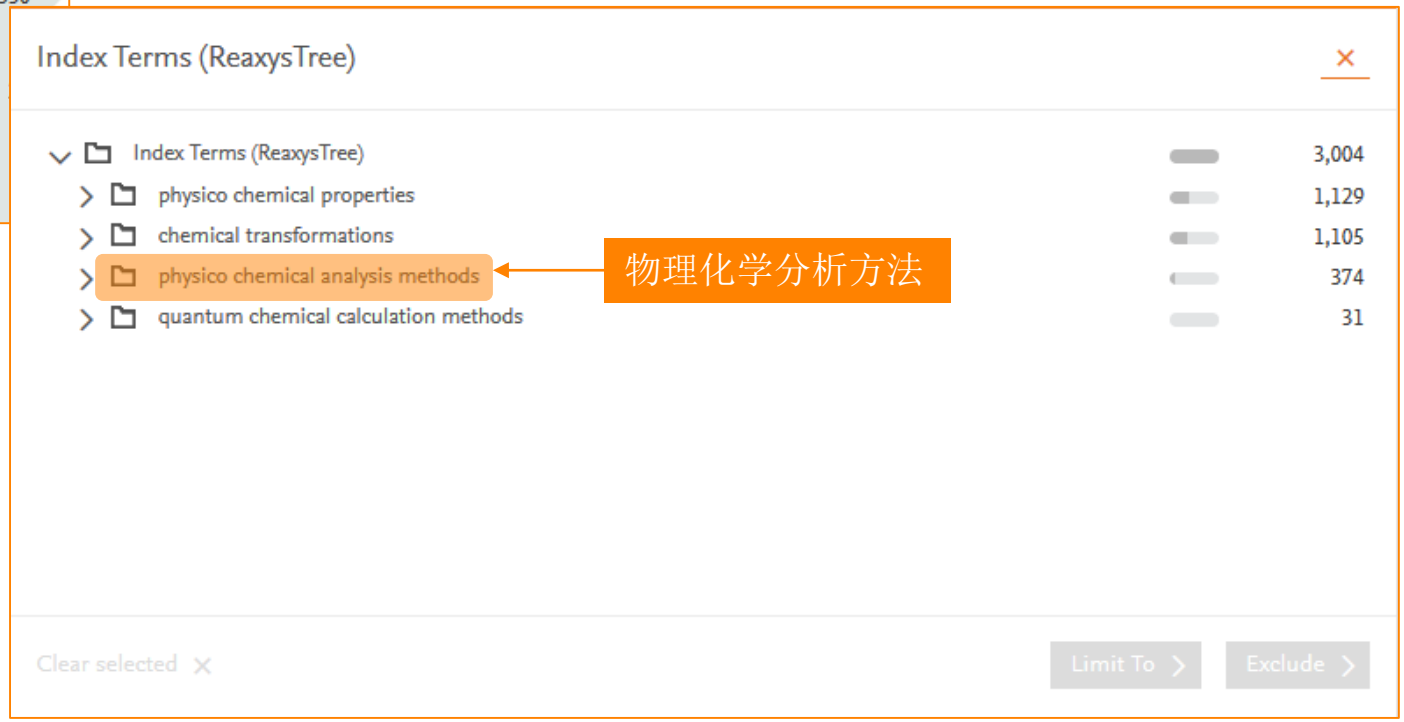
获得文献后，可以通过Reaxys的文献过滤工具对文献进行后处理



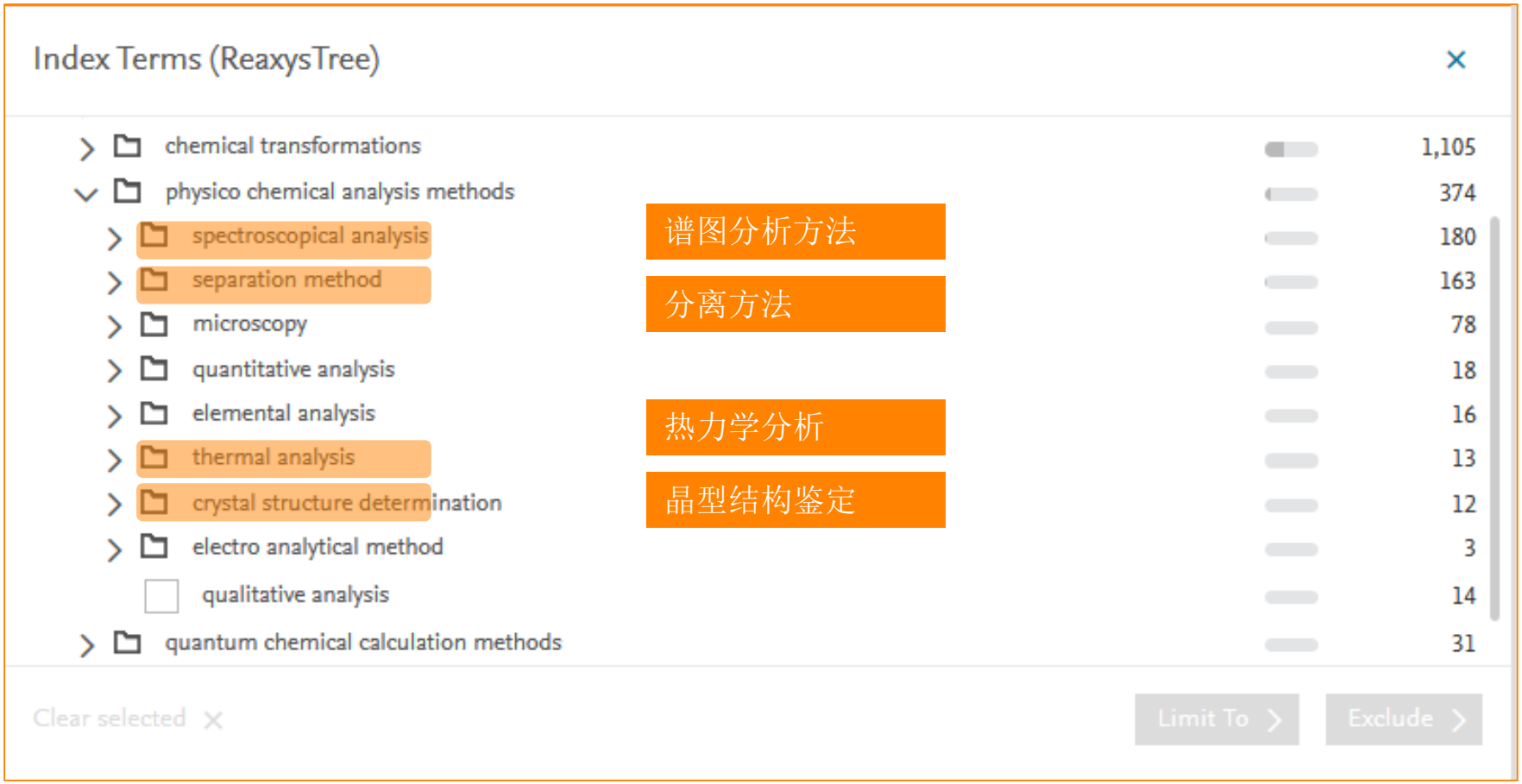
Index Term Reaxys Tree的应用



Reaxys通过Index Term Reaxys Tree的方式，将文献进行精确分类，帮助大家快速定位所需分析文献。

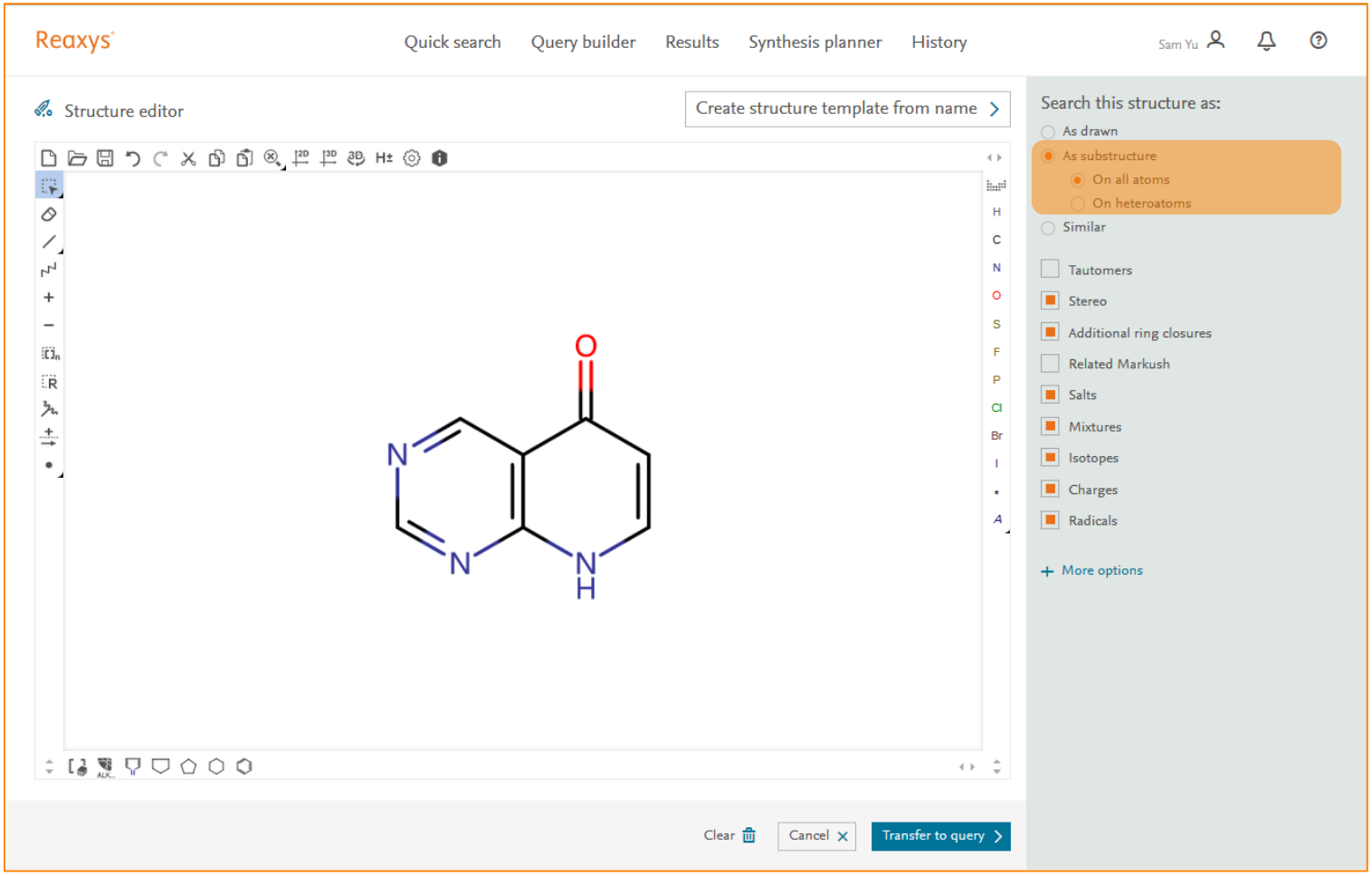


物理化学分析方法中的细节性分类

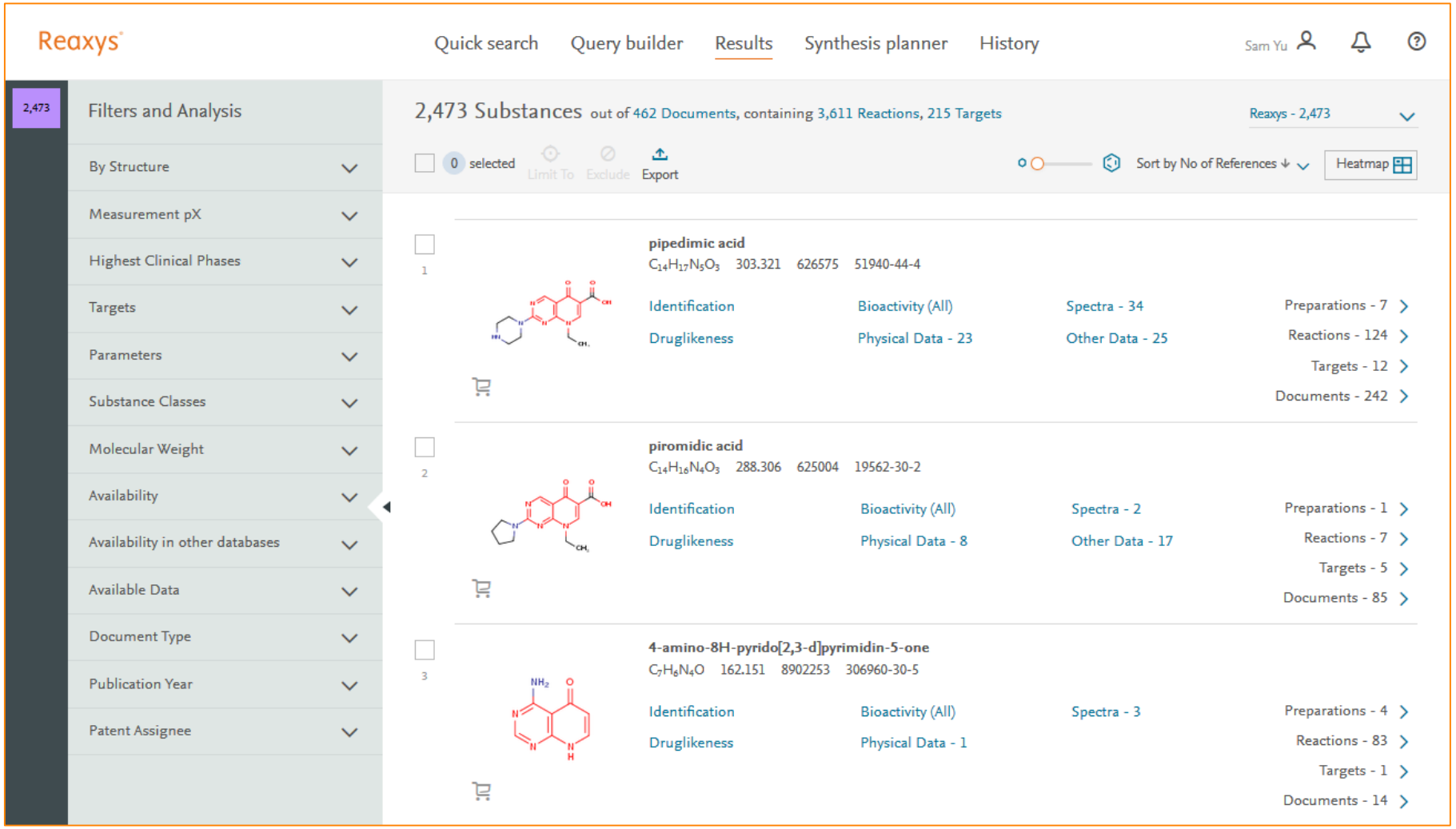


Case Study 3—母核结构检索

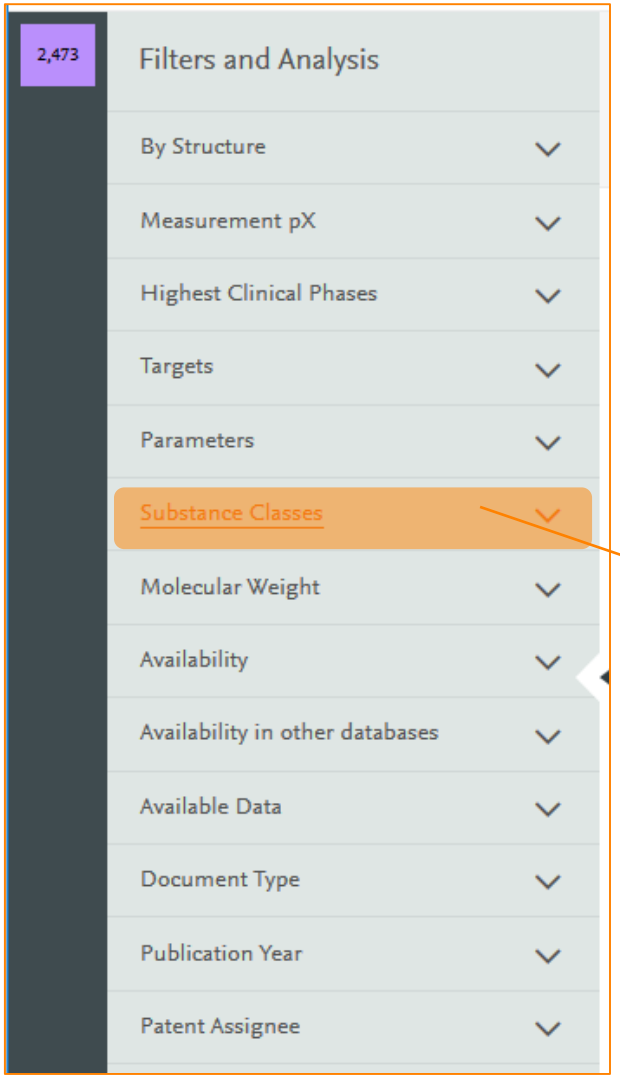
- 检索包含以下母核的结构



As Substructure检索结果

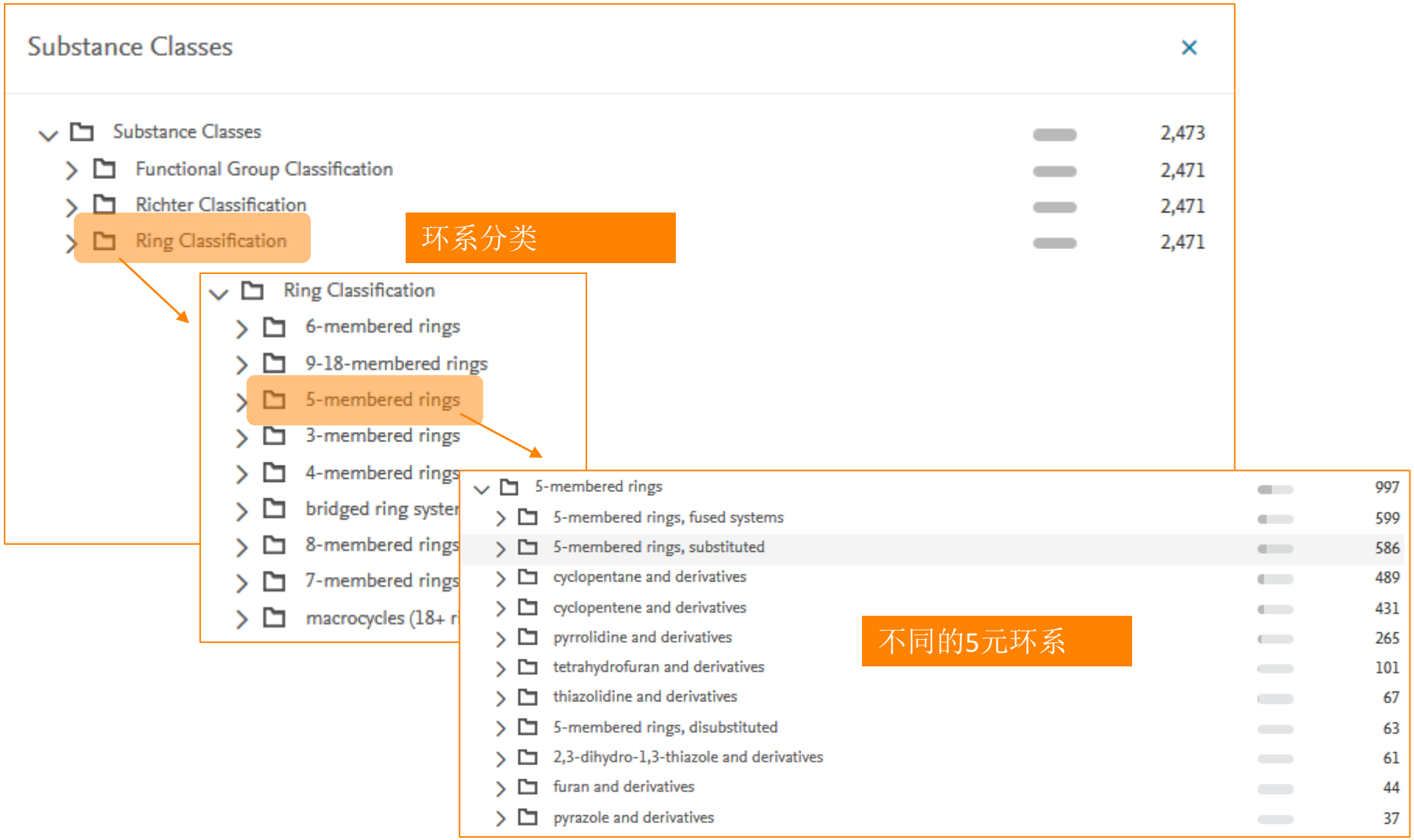


Reaxys中的筛选过程



结构的筛选工具，Substance Class帮助了解结构中的特殊片段

Reaxys中的结构分析

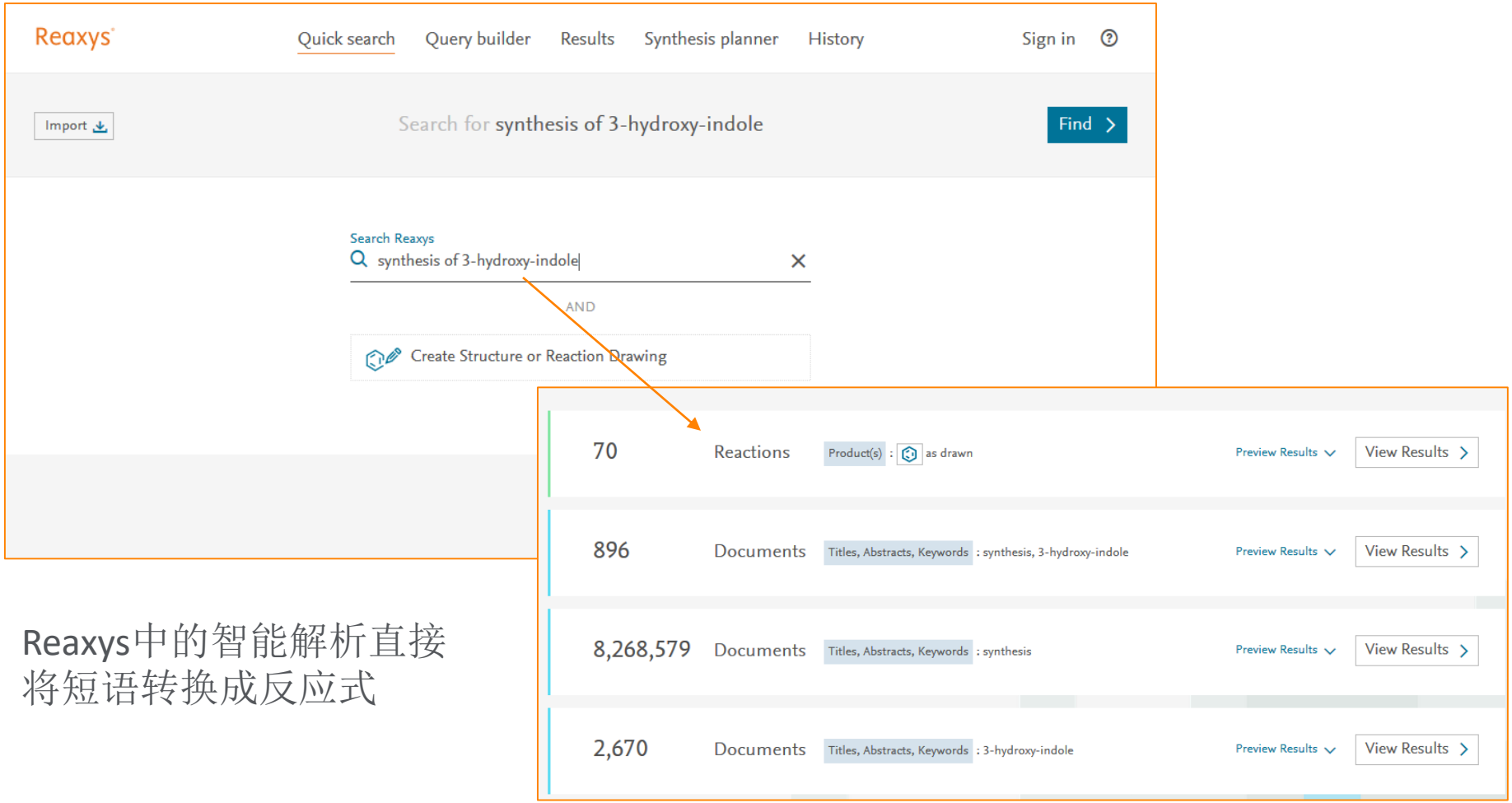


提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
  - Reaxys的基本检索模式
  - 如何利用Reaxys结构面板实现复杂结构定义
  - 如何利用Reaxys进行物质检索和物质分析
  - 如何利用Reaxys进行反应检索和条件筛选
  - 如何利用Reaxys制作合成计划
- Reaxys检索小结

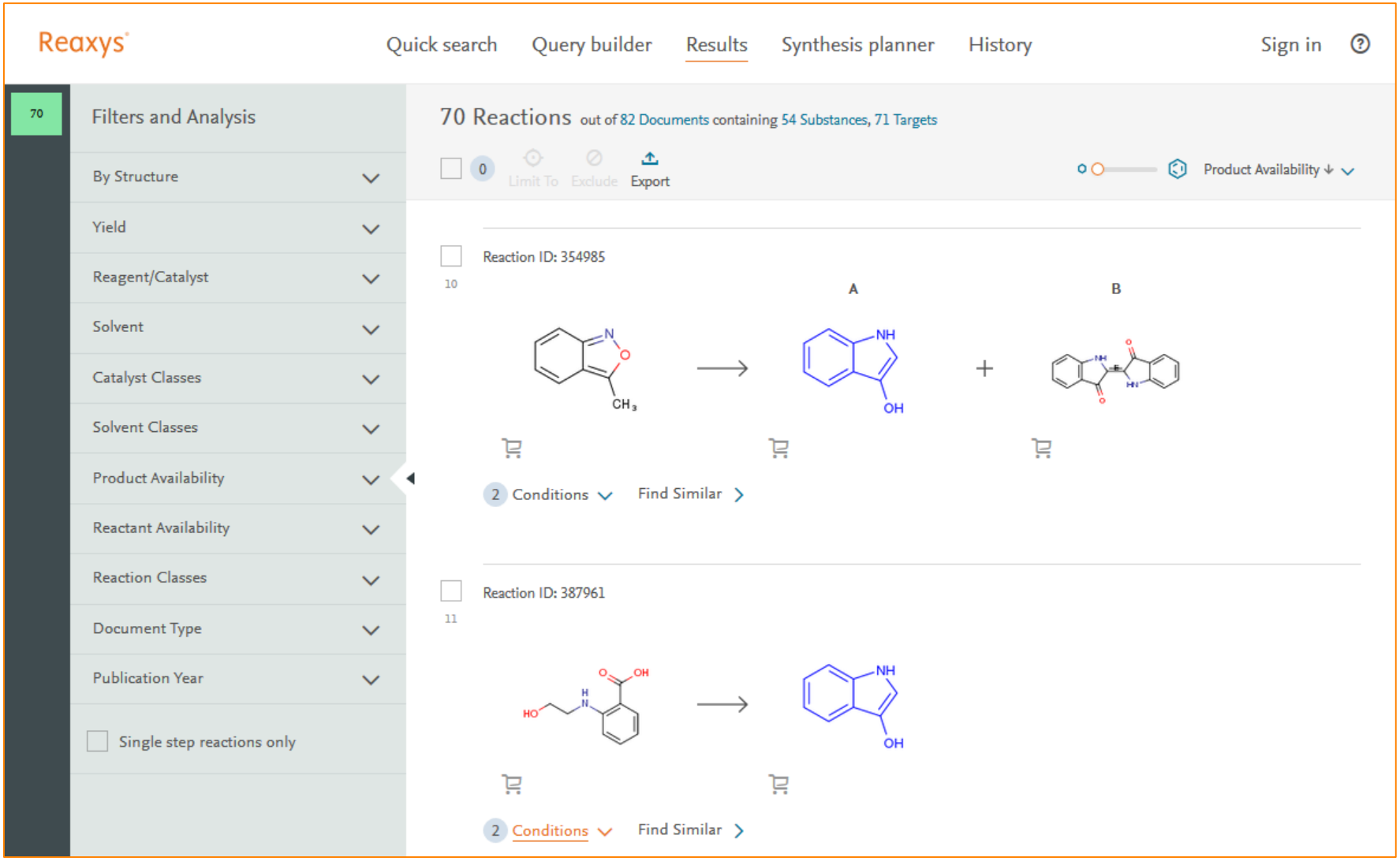
Case Study 4 关键词检索反应

- Synthesis of 3-hydroxy-indole



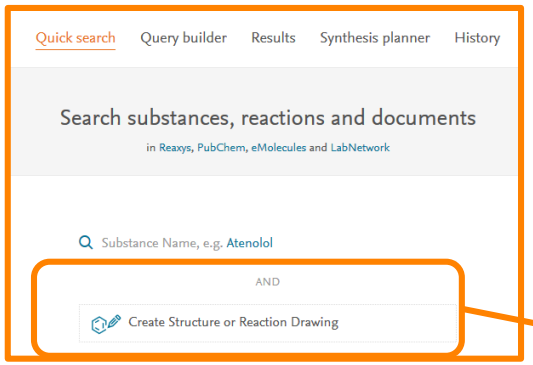
Reaxys中的智能解析直接将短语转换成反应式

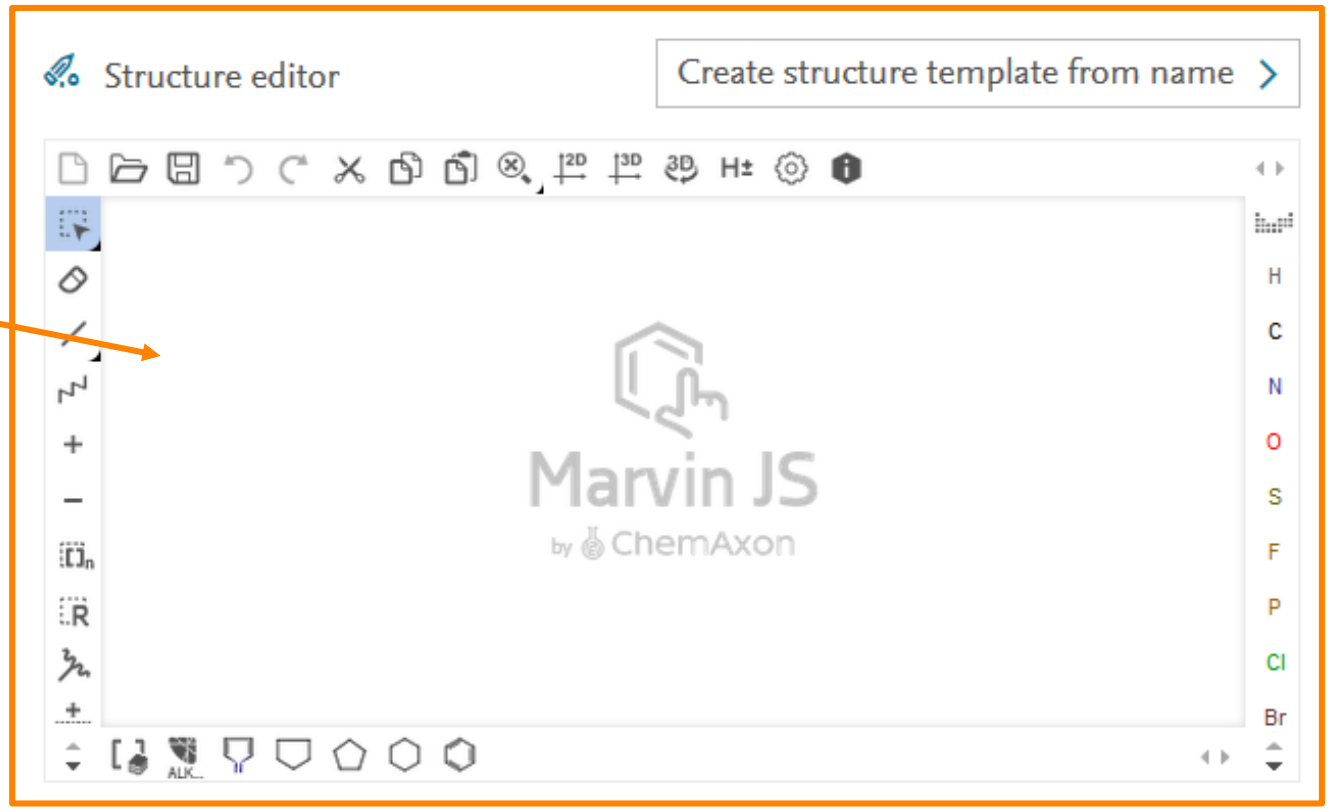
Reaxys中的结果


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Sign in
70
Filters and Analysis
By Structure
Yield
Reagent/Catalyst
Solvent
Catalyst Classes
Solvent Classes
Product Availability
Reactant Availability
Reaction Classes
Document Type
Publication Year
Single step reactions only
70 Reactions out of 82 Documents containing 54 Substances, 71 Targets
0
Limit To
Exclude
Export
Product Availability
Reaction ID: 354985
10
A
B
2 Conditions
Find Similar
Reaction ID: 387961
11
2 Conditions
Find Similar

Case Study 5 基本反应结构检索

- 检索以下的反应
  - 吡啶环2，3，4位上存在一个硝基还原成氨基
  - 吡啶环6位上存在一个Cl





检索Tips：

在Quick Search界面启动Marvin JS结构编辑器，进行结构编辑

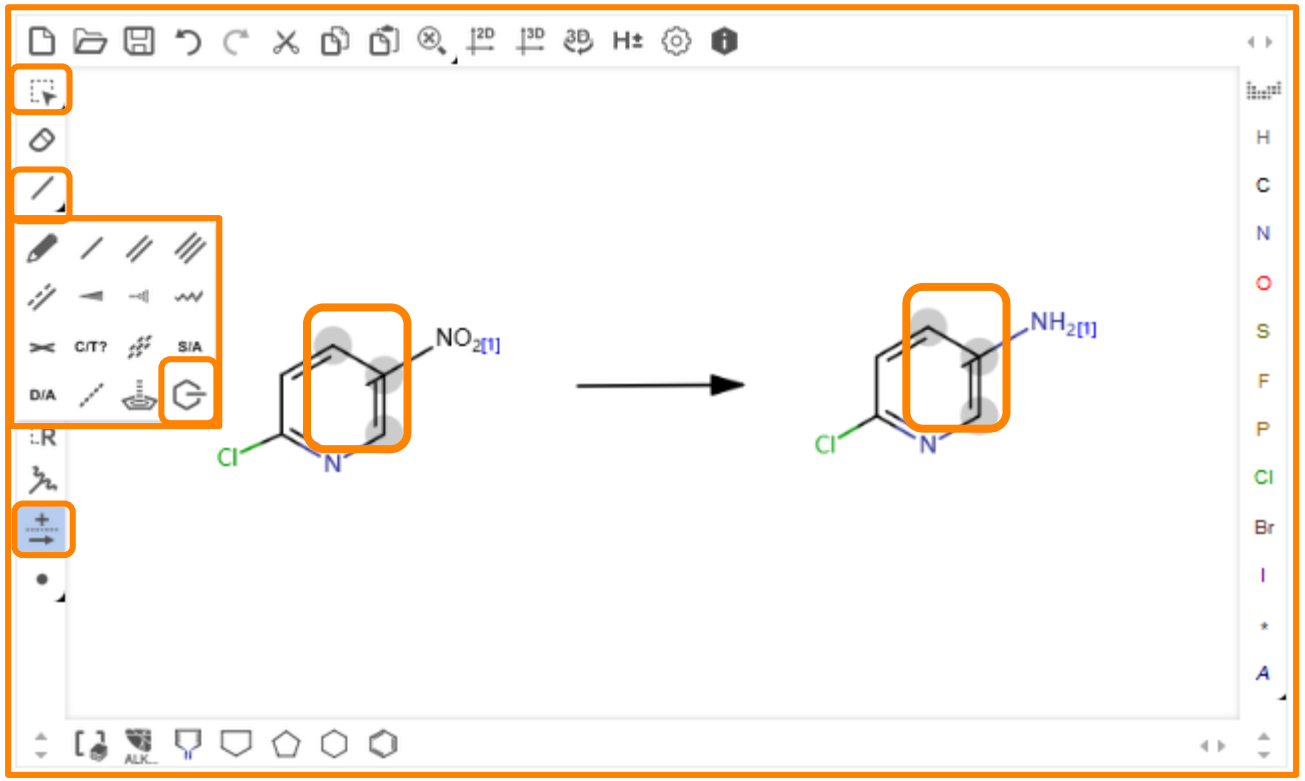
结构的定义

结构绘制步骤：

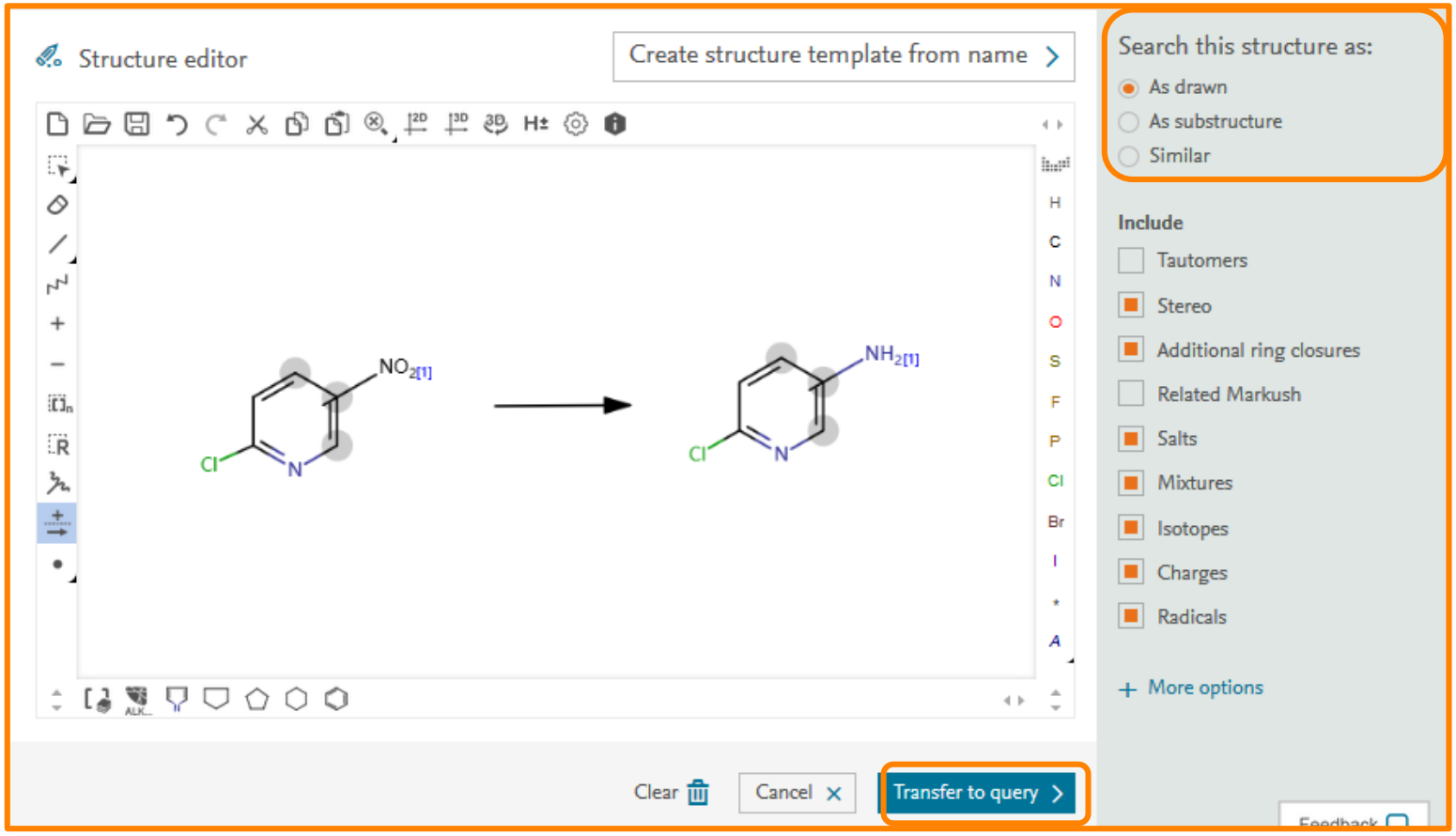
1：用套索选择工具选择吡啶上的3个C原子

2：用链工具中的不定位取代健将吡啶和NO2，NH2相接

3：用反应定义工具，指定反应前后NO2到NH2的变化



检索功能的选择和检索

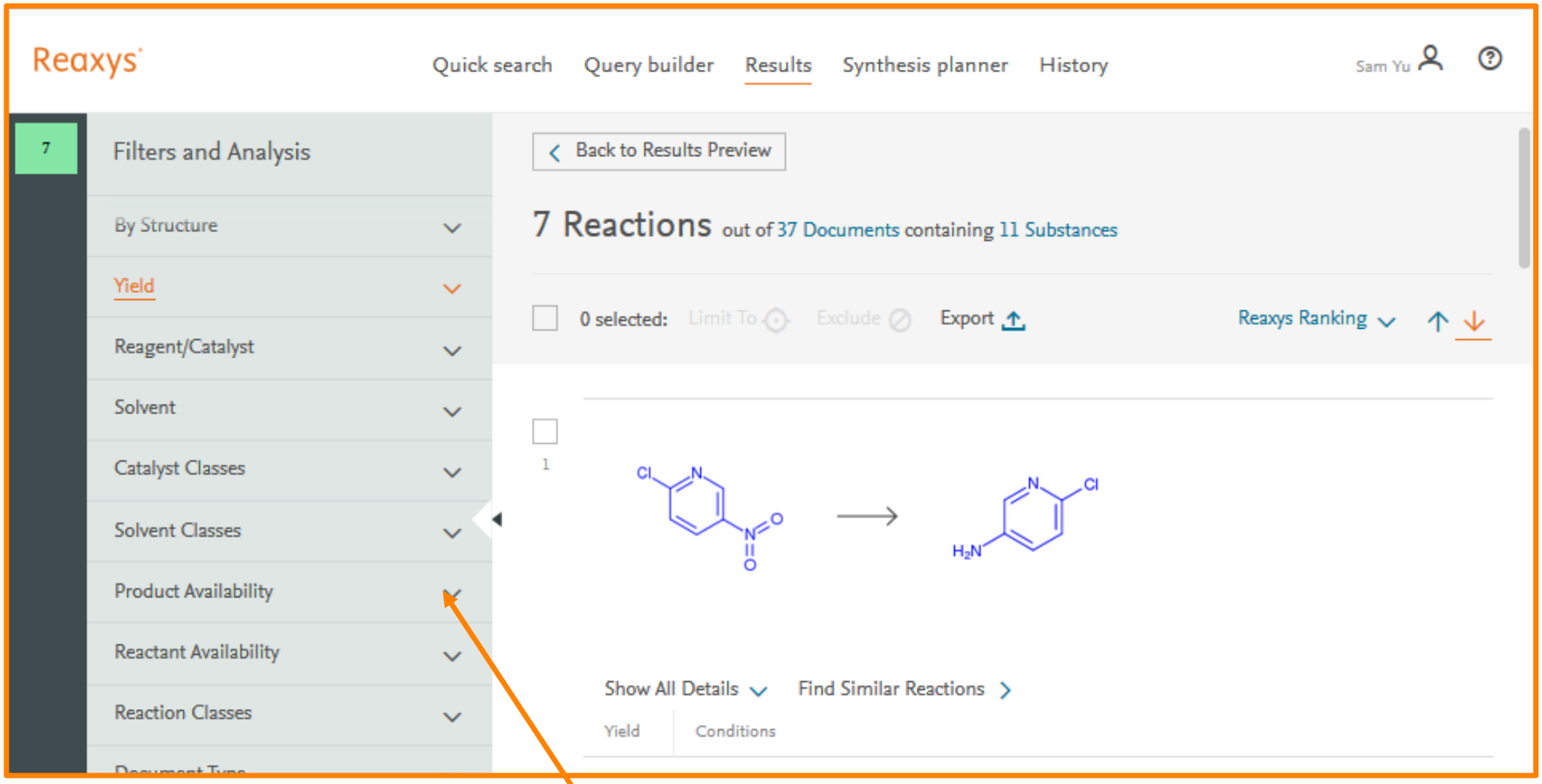


检索Tips:

1：As Drawn，和所画结构完全一致的反应

2：Substructure，亚结构反应检索，会展开所有H，可以设定所有原子开放还是杂原子开放

最终的结果

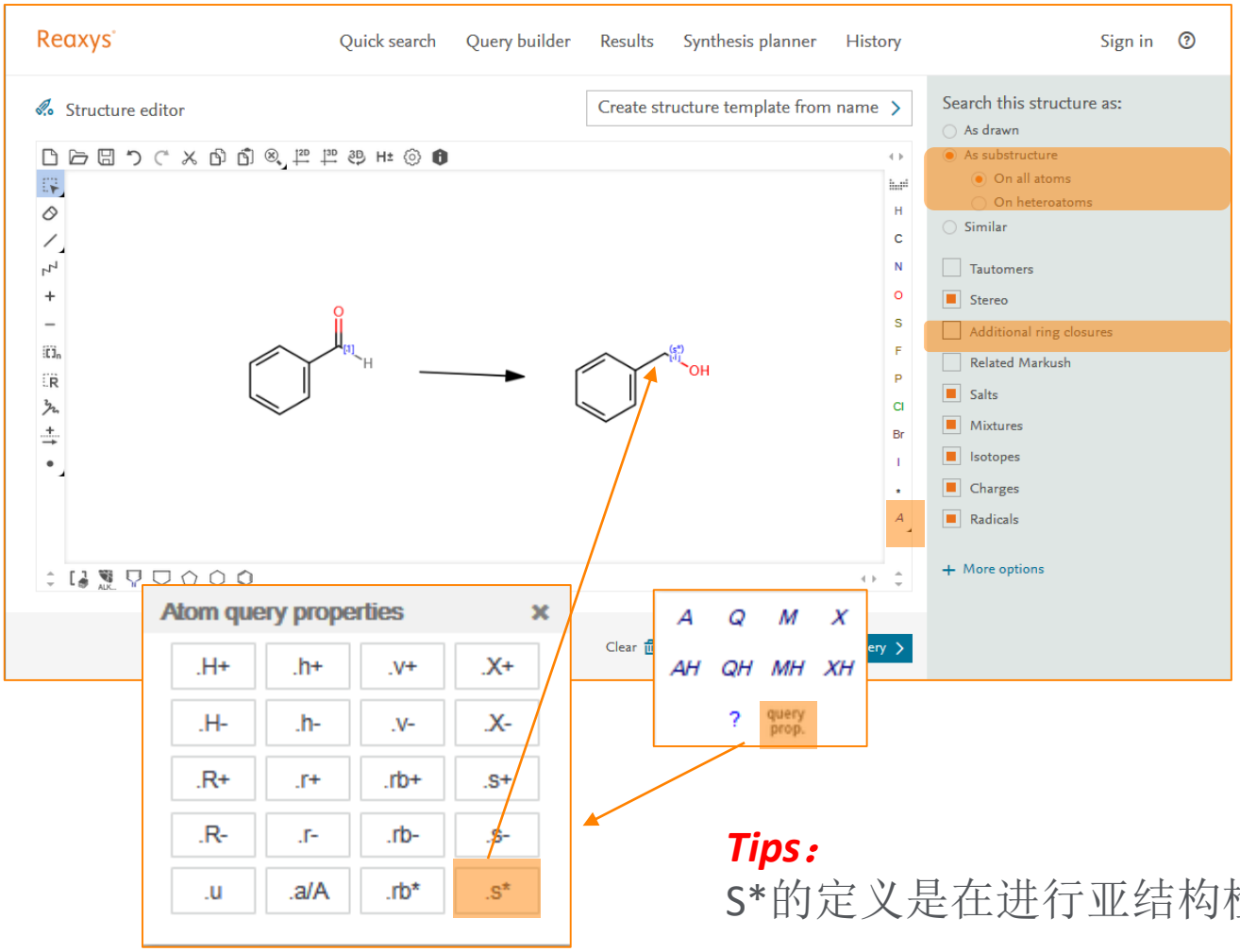


Tips：

检索到结果后，可以通过旁边的工具进行筛选

Case Study 5 反应条件筛选

- 检索包含以下核心结构的反应，并对条件进行筛选



亚结构检索，用于检索核心结构

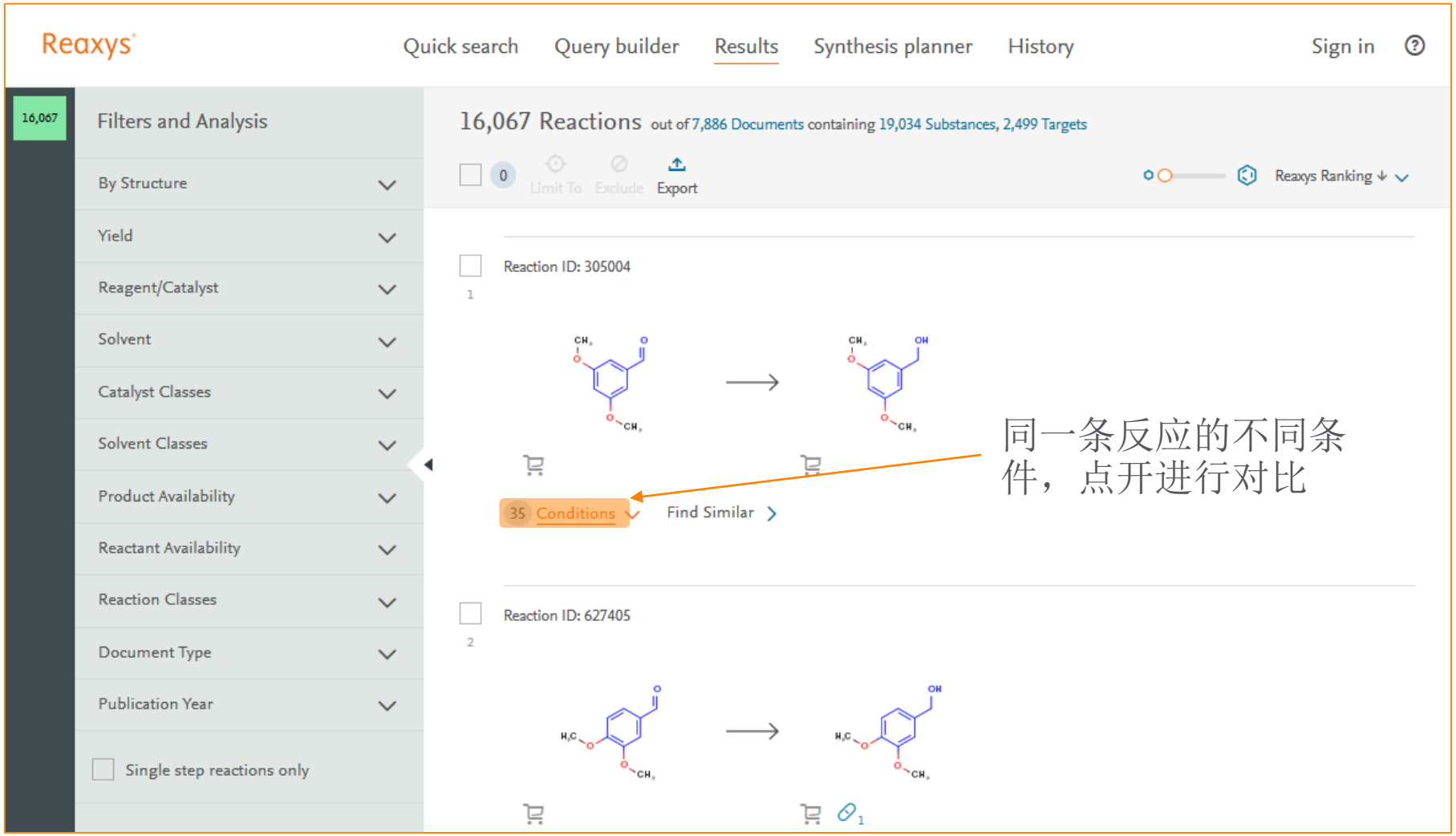
Tips：

Additional Ring Closures用于保护环系，在进行亚结构检索的时，不发生稠环

Tips：

S*的定义是在进行亚结构检索时没有取代

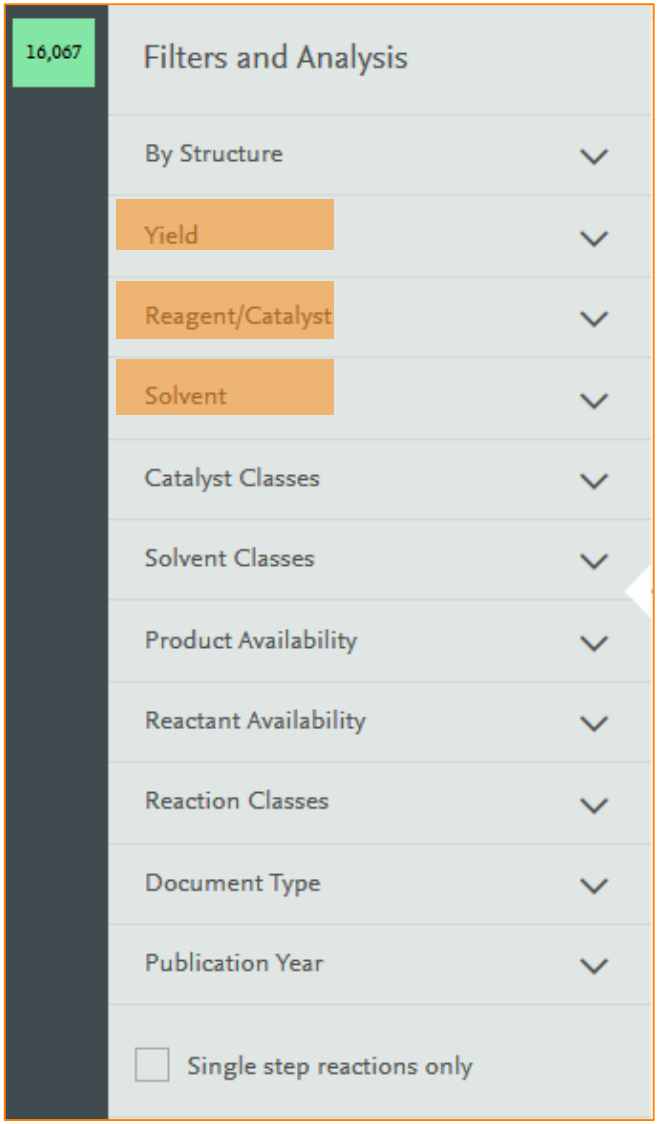
Reaxys中的结果

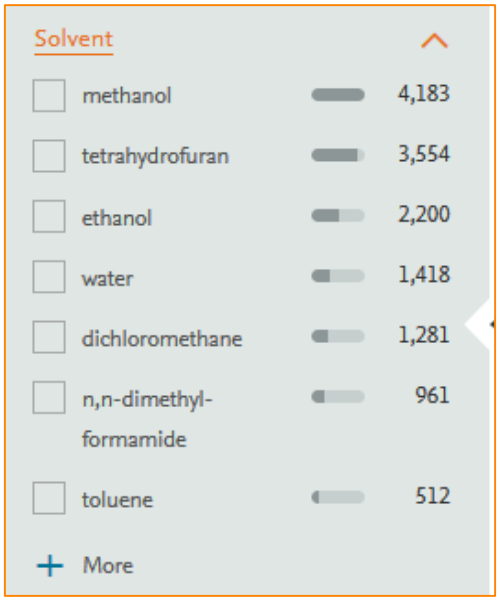

Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Sign in
16,067
Filters and Analysis
By Structure
Yield
Reagent/Catalyst
Solvent
Catalyst Classes
Solvent Classes
Product Availability
Reactant Availability
Reaction Classes
Document Type
Publication Year
Single step reactions only
16,067 Reactions out of 7,886 Documents containing 19,034 Substances, 2,499 Targets
0
Limit To
Exclude
Export
Reaxys Ranking
Reaction ID: 305004
1
35 Conditions
Find Similar
Reaction ID: 627405
2
同一条反应的不同条件，点开进行对比

Reaxys中的反应呈现形式

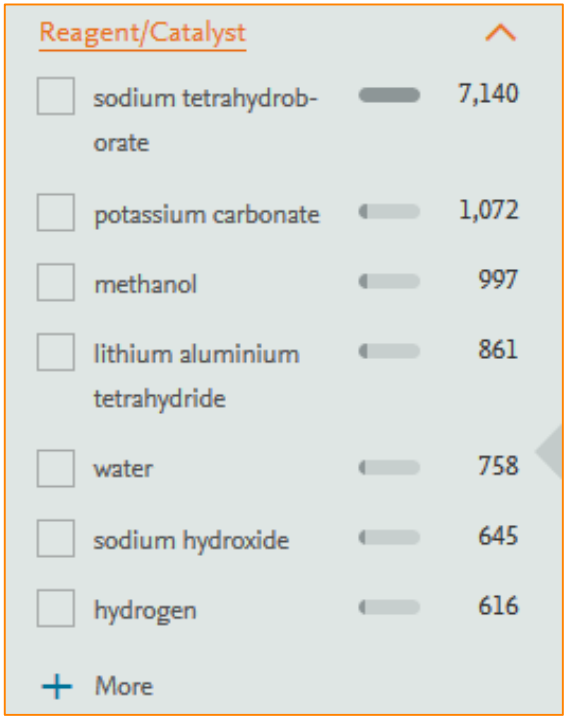
- 同底物，同产物的反应归并到一起，有利于科研工作者的评估

更多的筛选条件

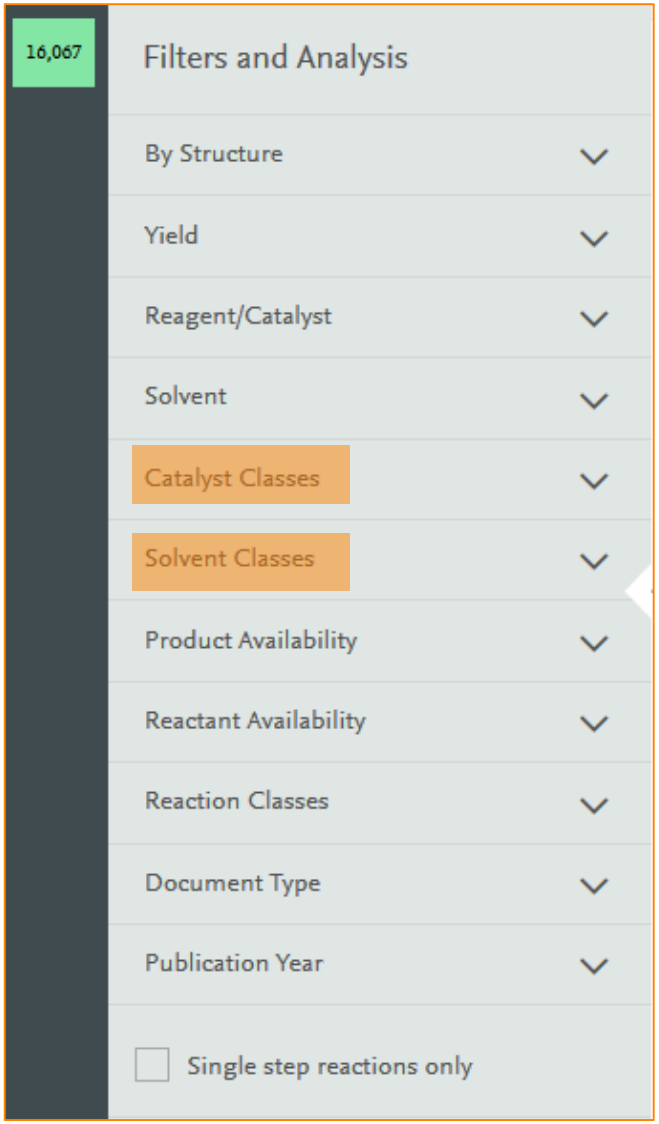


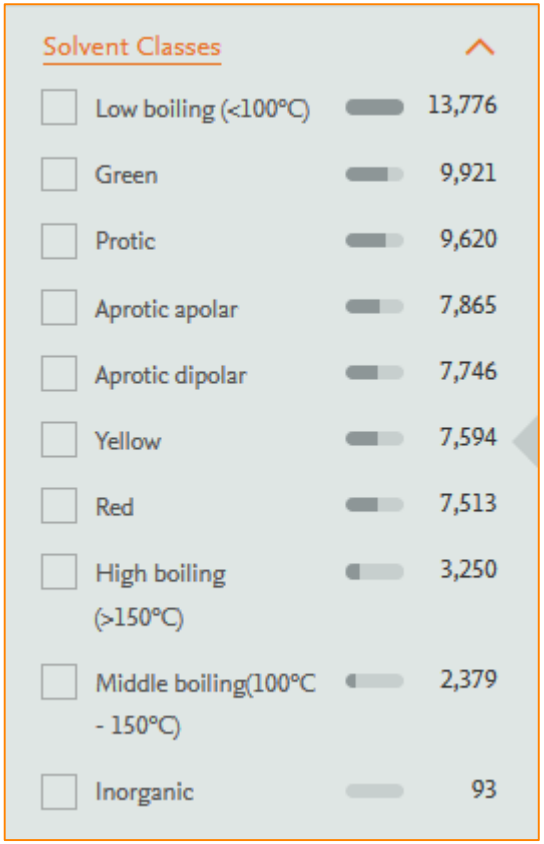


Reaxys提供多种反应条件过滤工具



类别条件筛选—溶剂类别，催化剂类别



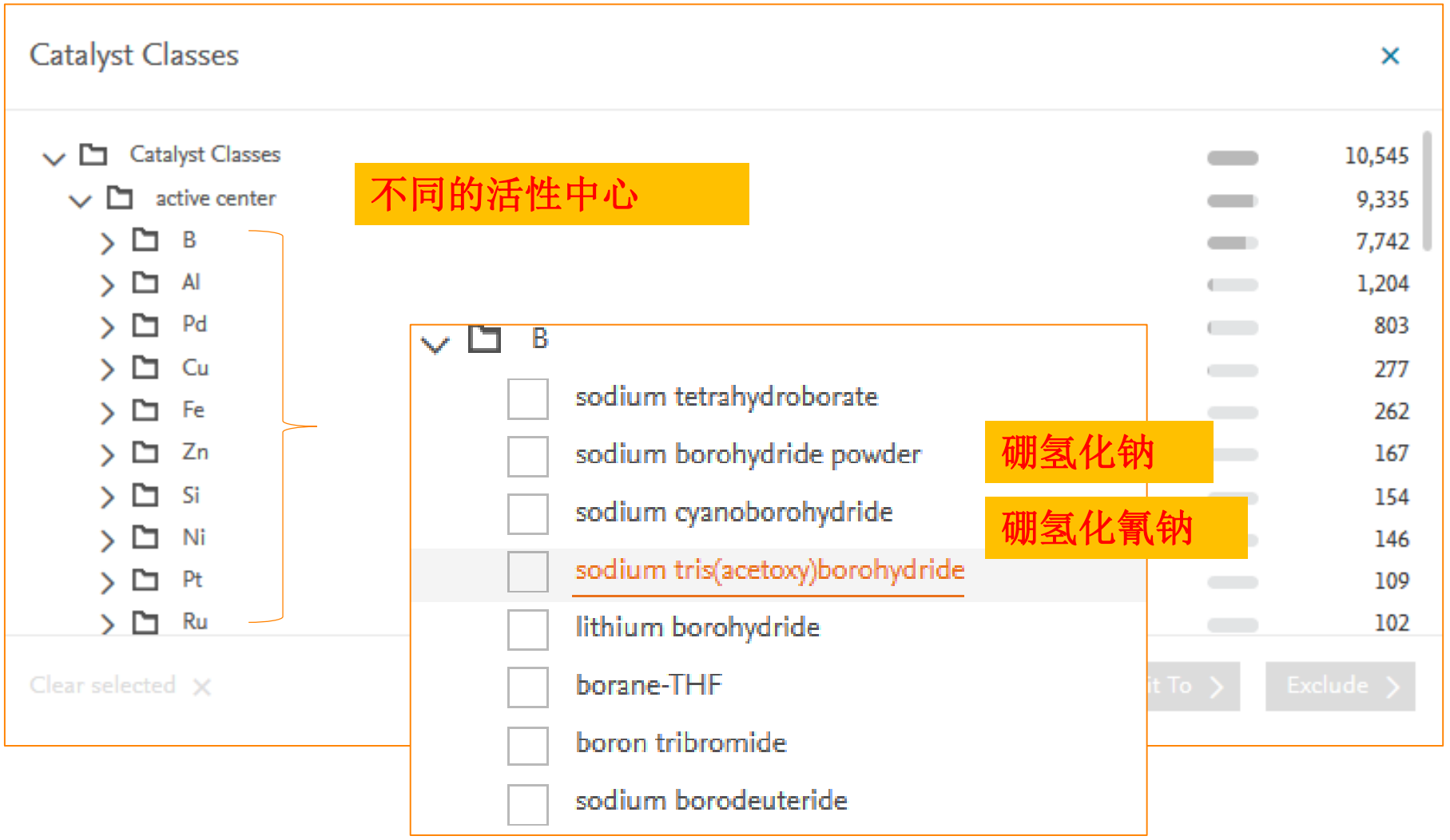


可以通过一些溶剂的类型进行筛选，高沸，中沸，低沸的溶剂，质子溶剂等等

Reaxys中独有的催化剂类别筛选工具

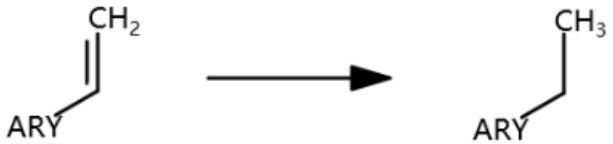
- 催化剂分类工具

活性中心分类

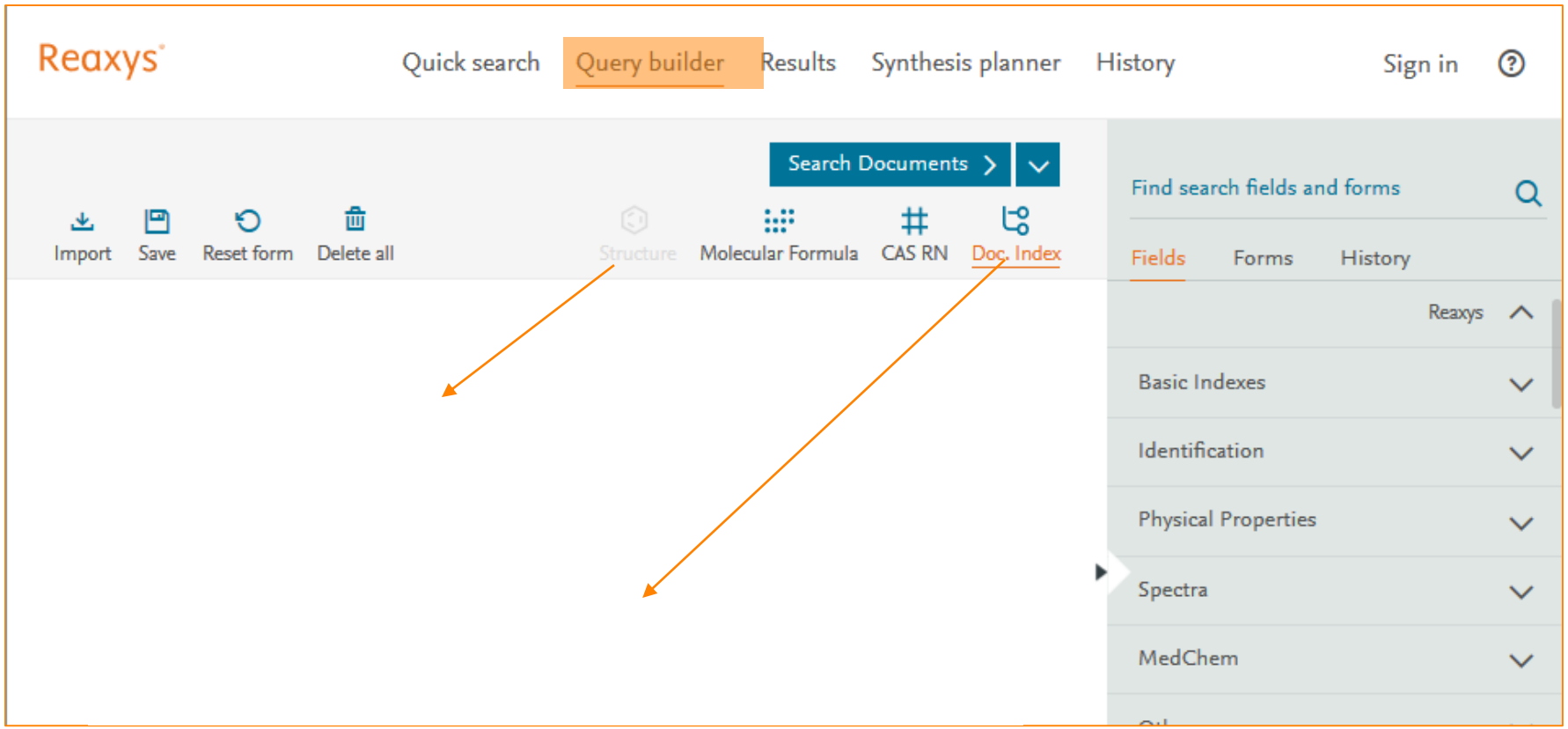

Catalyst Classes
Catalyst Classes
active center
B
Al
Pd
Cu
Fe
Zn
Si
Ni
Pt
Ru
不同的活性中心
10,545
9,335
7,742
1,204
803
277
262
167
154
146
109
102
B
sodium tetrahydroborate
sodium borohydride powder
硼氢化钠
sodium cyanoborohydride
硼氢化氰钠
sodium tris(acetoxy)borohydride
lithium borohydride
borane-THF
boron tribromide
sodium borodeuteride
Clear selected
Exclude

Case Study 6 反应组合检索, 关键词联合反应检索

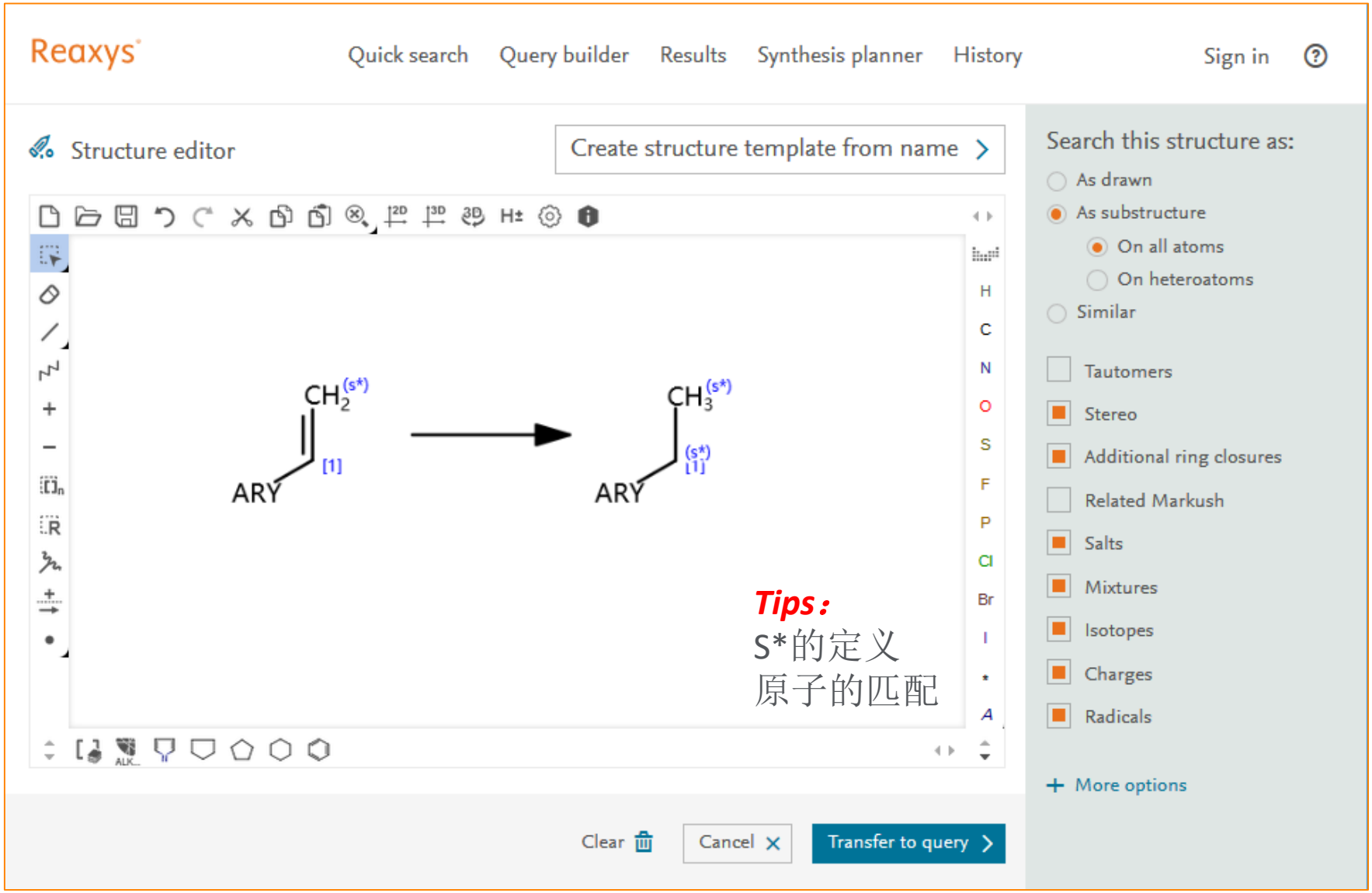
- 检索涉及以下反应机理的文献



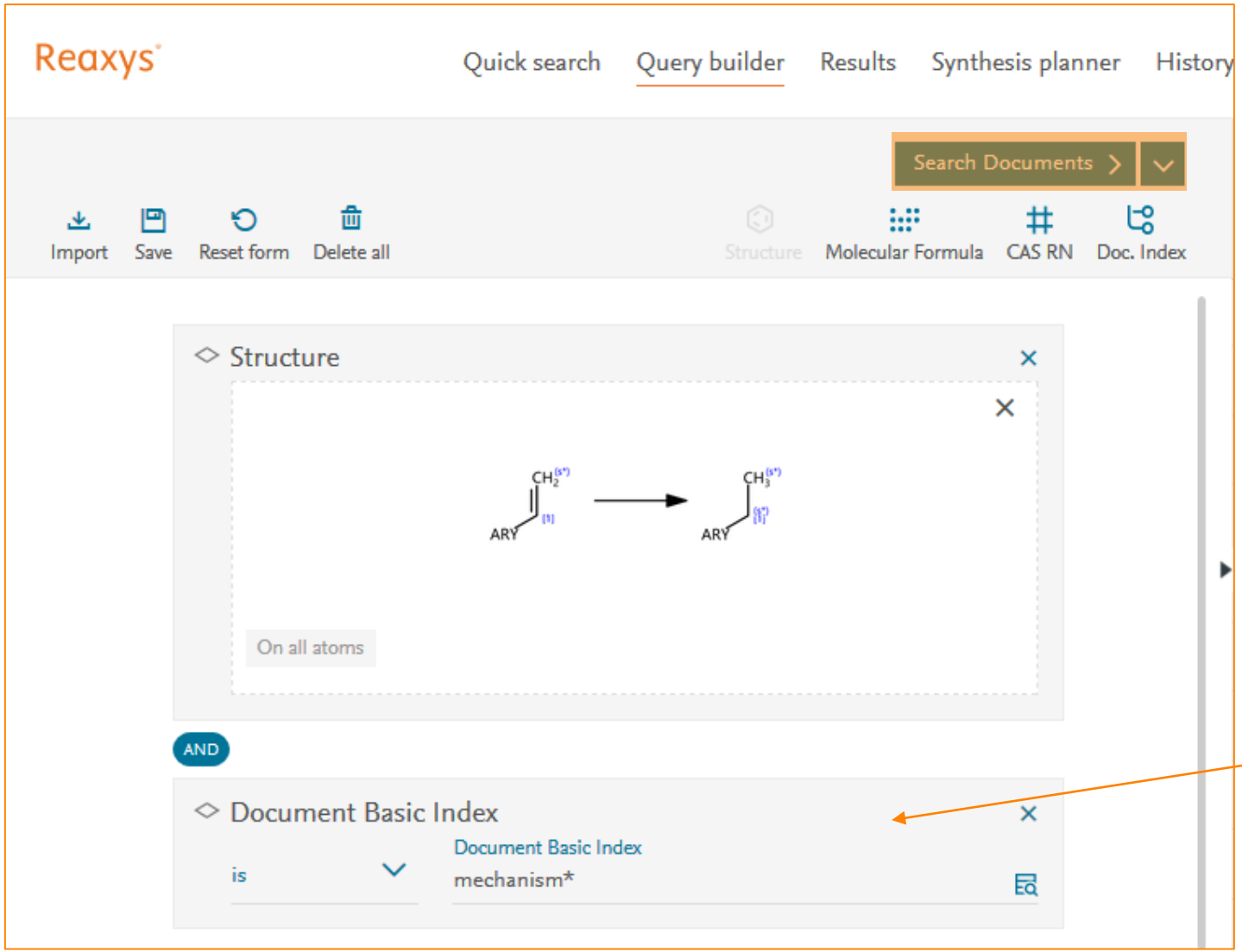
通过Query Builder创建组合检索式



反应结构的添加


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Sign in
Structure editor
Create structure template from name
CH2 (s*)
[1]
ARY
CH3 (s*)
(s*)
[1]
ARY
Tips：
S*的定义
原子的匹配
Search this structure as:
As drawn
As substructure
On all atoms
On heteroatoms
Similar
Tautomers
Stereo
Additional ring closures
Related Markush
Salts
Mixtures
Isotopes
Charges
Radicals
More options
Clear
Cancel
Transfer to query

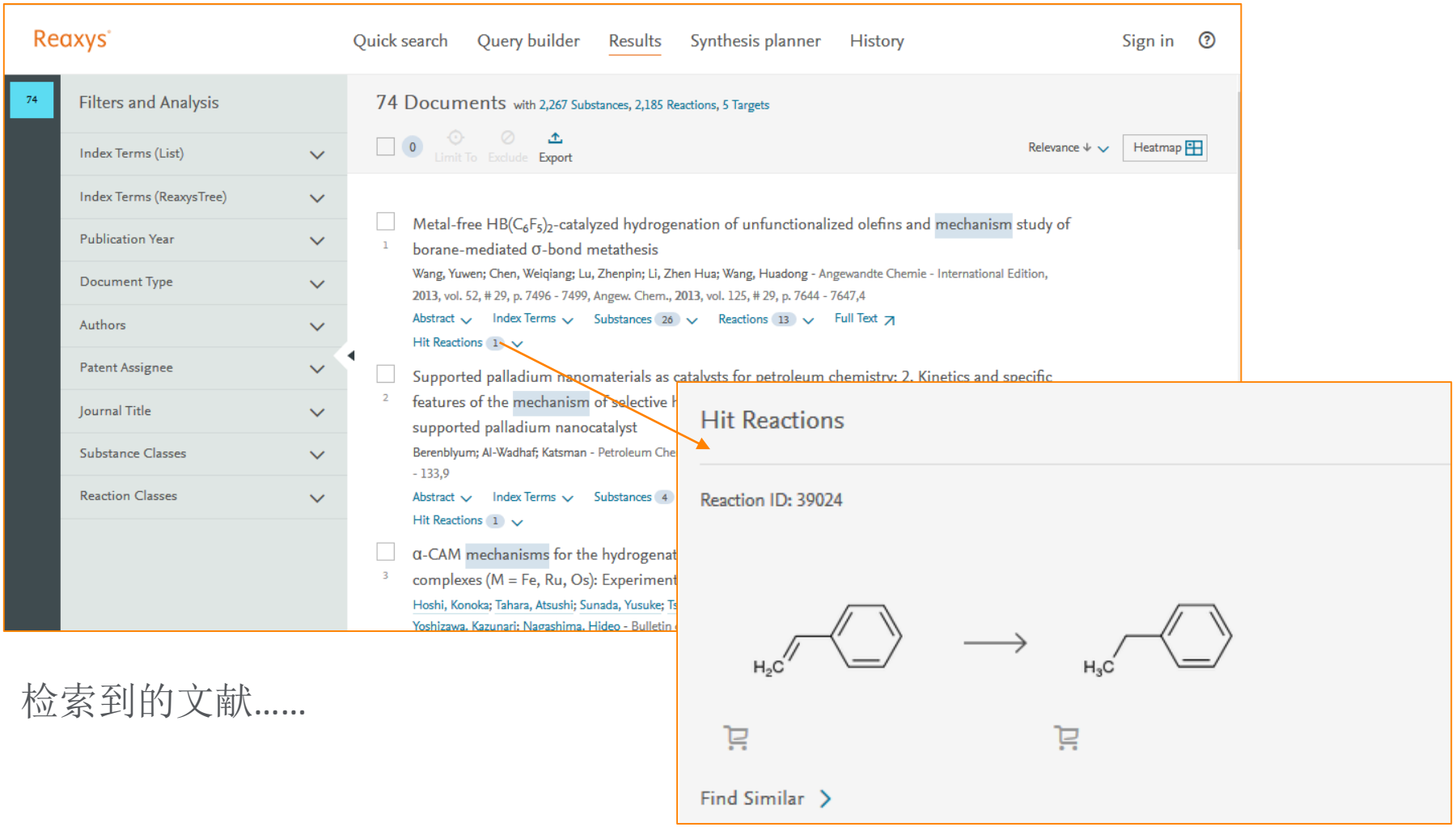
添加关键词后的检索式



检索文献

添加机理单词

最后的结果

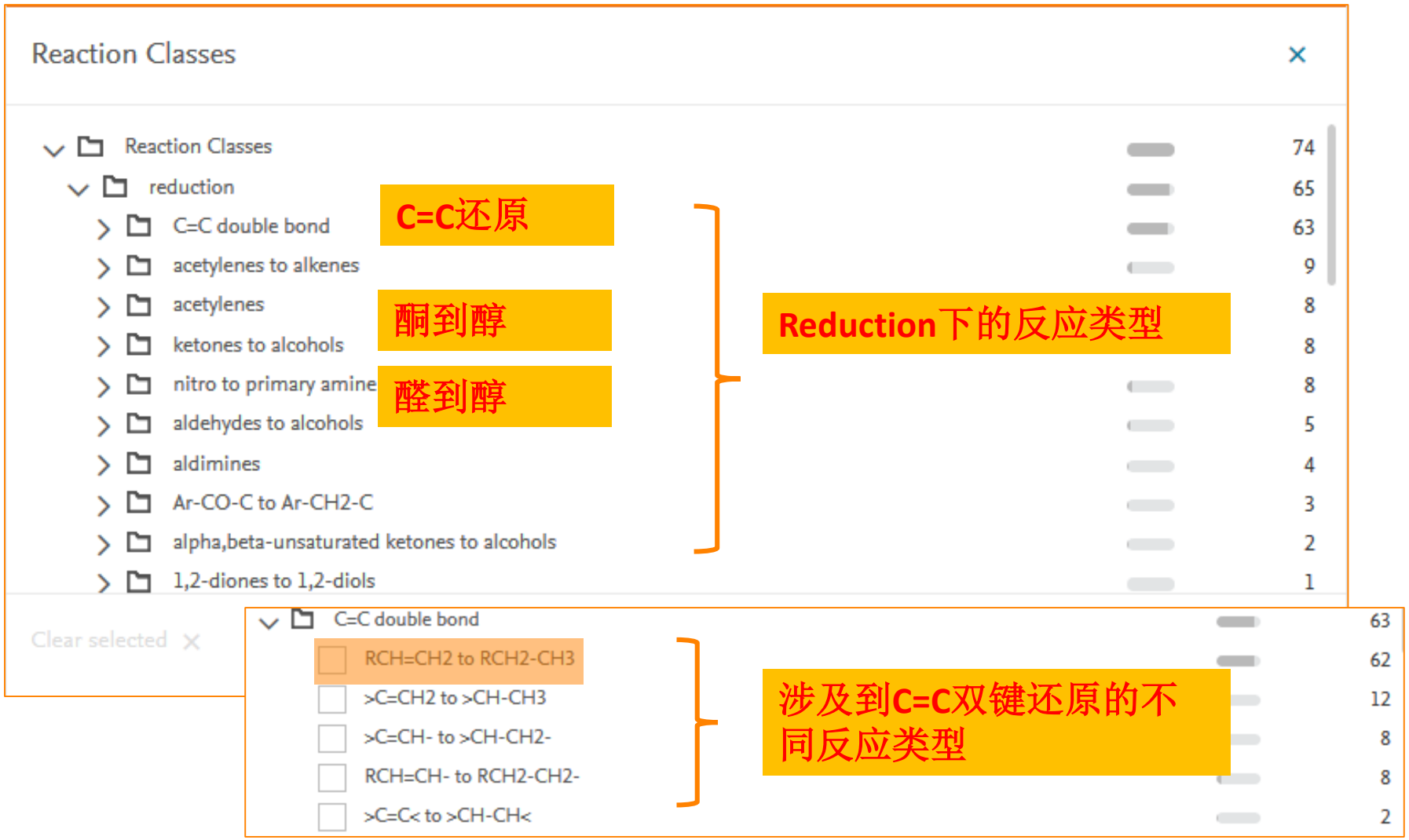


检索到的文献.....

文献中更多的内容—利用反应中心对文献进行筛选

Reaction Classes可以利用反应中心的类型进行筛选

更加细节性内容

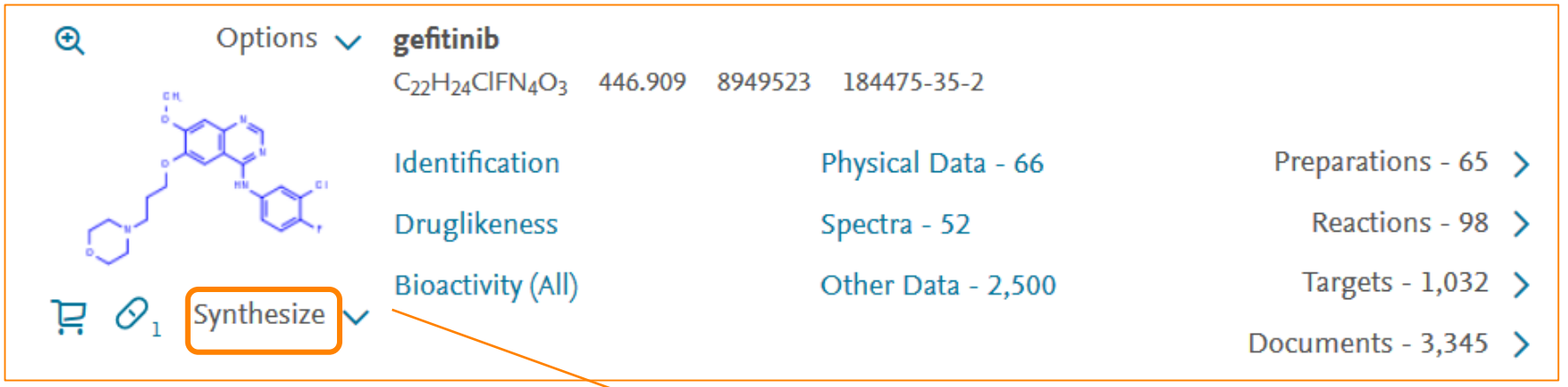

Reaction Classes
Reaction Classes
reduction
C=C double bond
acetylenes to alkenes
acetylenes
ketones to alcohols
nitro to primary amine
aldehydes to alcohols
aldimines
Ar-CO-C to Ar-CH2-C
alpha,beta-unsaturated ketones to alcohols
1,2-diones to 1,2-diols
74
65
63
9
8
8
8
5
4
3
2
1
C=C还原
酮到醇
醛到醇
Reduction下的反应类型
Clear selected
C=C double bond
RCH=CH2 to RCH2-CH3
>C=CH2 to >CH-CH3
>C=CH- to >CH-CH2-
RCH=CH- to RCH2-CH2-
>C=C< to >CH-CH<
63
62
12
8
8
2
涉及到C=C双键还原的不同反应类型

提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
  - Reaxys的基本检索模式
  - 如何利用Reaxys结构面板实现复杂结构定义
  - 如何利用Reaxys进行物质检索和物质分析
  - 如何利用Reaxys进行反应检索和条件筛选
  - 如何利用Reaxys制作合成计划
- Reaxys检索小结

Case Study 7 如何利用Reaxys制作合成计划

- 给吉非替尼制定合成计划
  - Step1：检索到吉非替尼
  - Step2：导入合成计划

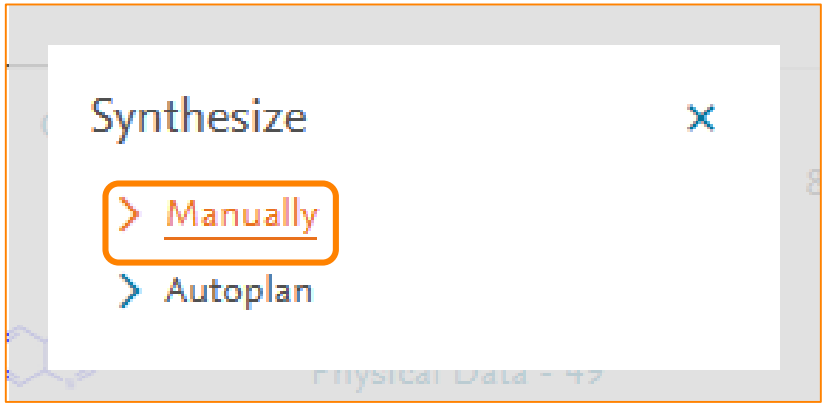


Tips：

1：通过前述的操作找到物质

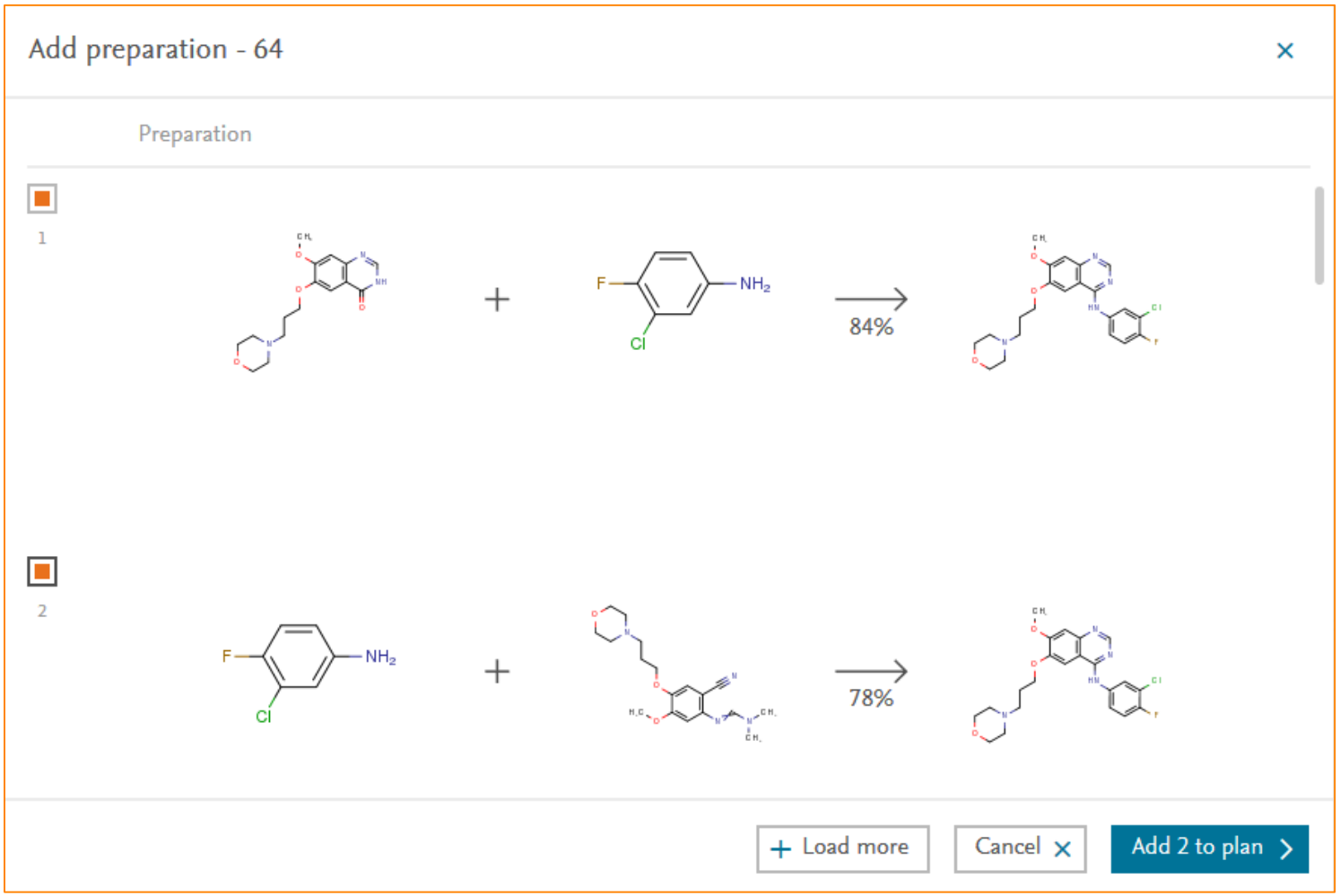
2：鼠标悬停在结构上，看到Synthesize

3：点击，打开Synthesis Plan，这里选择手动

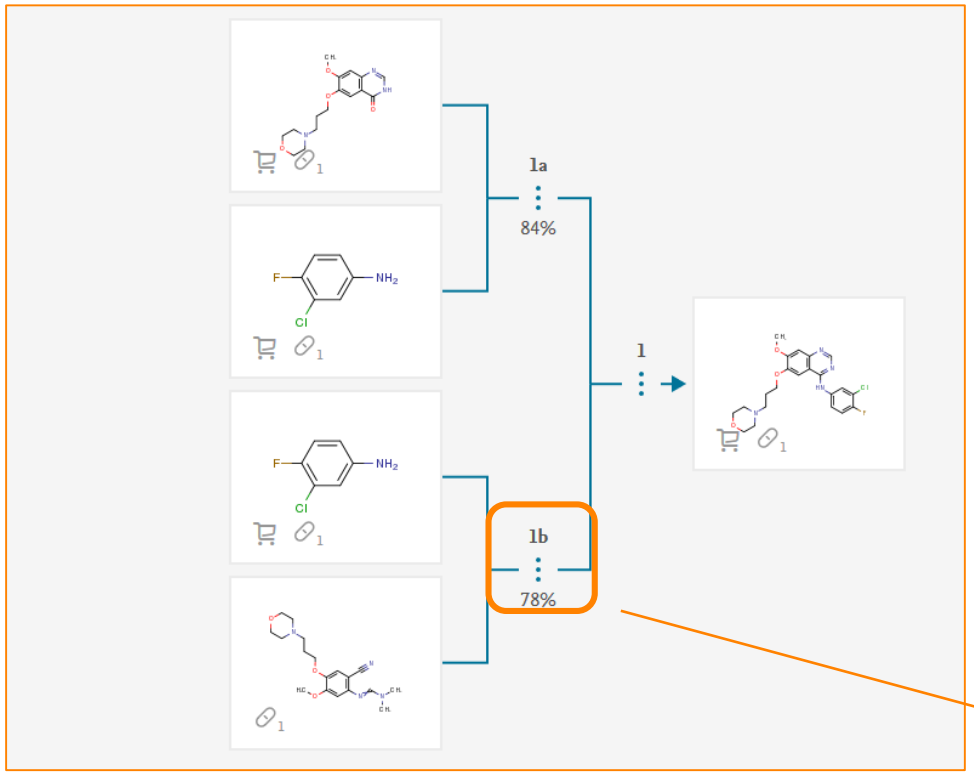


Synthesis Plan—添加感兴趣的反应

- 可以添加多条反应在一个Plan中，用于比较

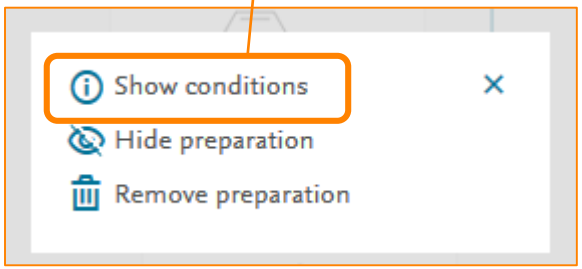


添加好的结果界面



Preparation - 1b

Yield	Conditions	Reference
78%	**With** acetic acid at 130°C; for 3h; Temperature; Experimental Procedure	Guangzhou Baiyunshan Pharmaceutical Group Co., Ltd. Baiyunshan Pharmaceutical Zong Factory; Chen Mao; Zhu Shaoxuan; Huang Xiaoguang - CN104072426, 2017, B Location in patent: Paragraph 0050; 0051; 0052; 0053; 0054; 0055 Full Text Details Abstract
71.1%	**With** acetic acid **In** 5,5-dimethyl-1,3-cyclohexadiene at 135°C; Experimental Procedure	Shaanxi Normal University; Li, Baolin; Ren, Yufei; Wang, Liuchang; Jia, Yucai; Ding, Siyi; Wang, Wei - CN103539702, 2016, B Location in patent: Paragraph 0094-0096 Full Text Details Abstract
70%	**With** acetic acid at 125 - 130°C; for 3h;	- Organic Process Research and Development, 2007, vol. 11, # 5, p. 813 - 816 Full Text Cited 51 times Details Abstract

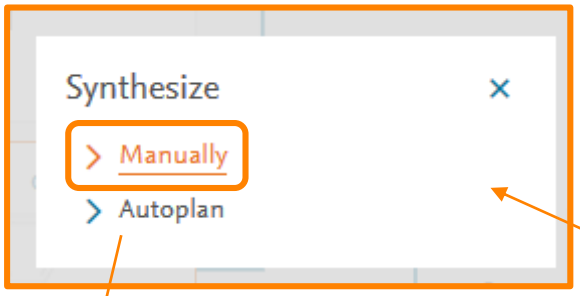


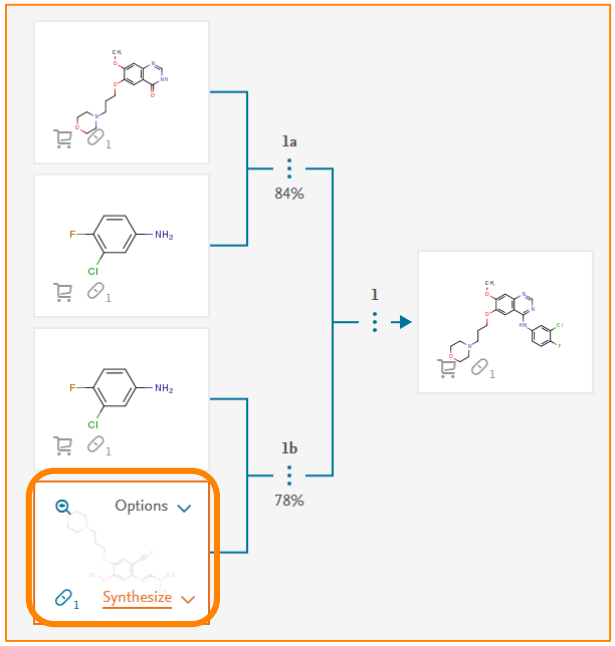
Tips：

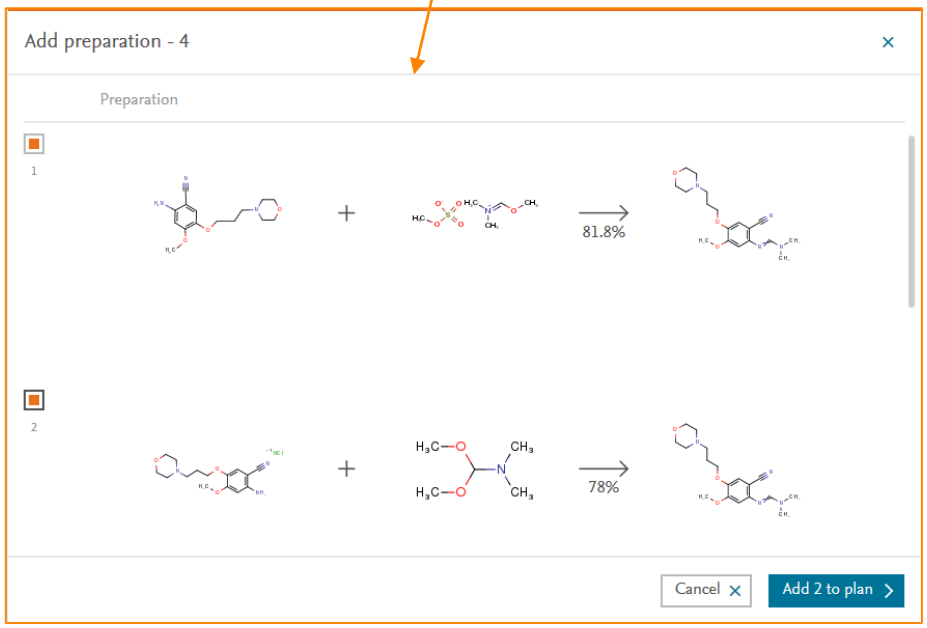
1：通过添加多条反应，可以用来评估反应信息

2：点击虚线的地方，可以查看条件，或者隐藏，移除反应

继续的扩充反应路线



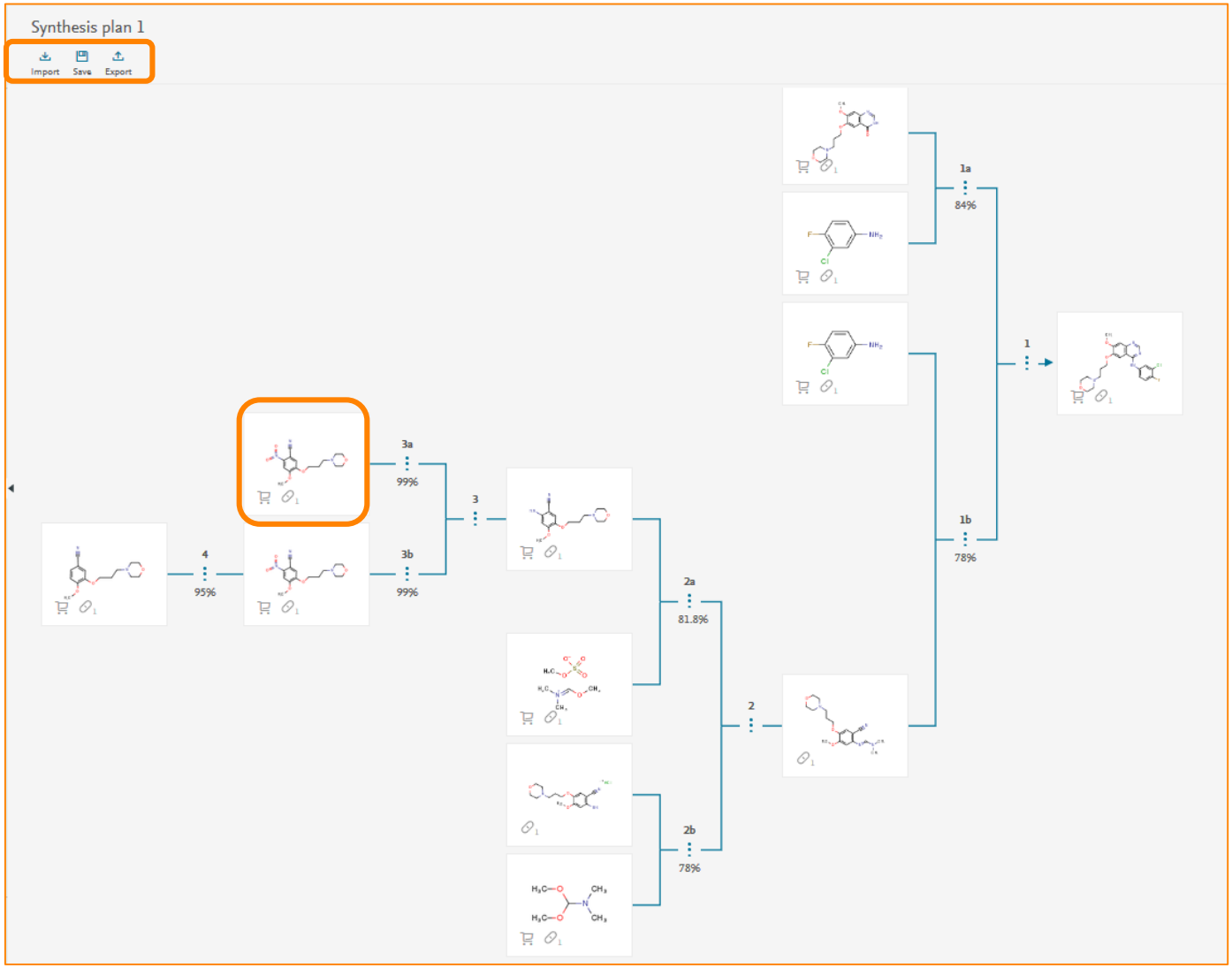




Tips：

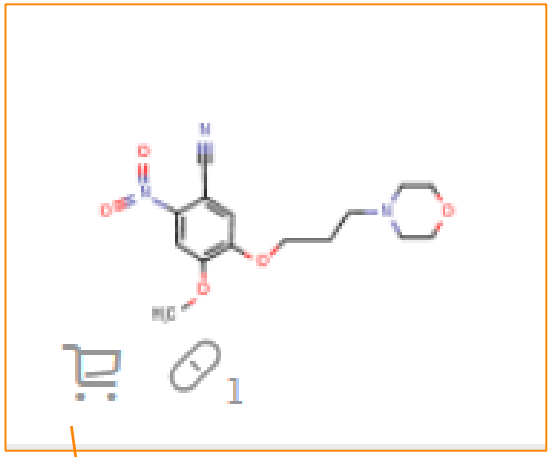
在Synthesis Plan上可以对任意一个物质进行同样的Synthesis的操作，可以将更多的反应添加进来

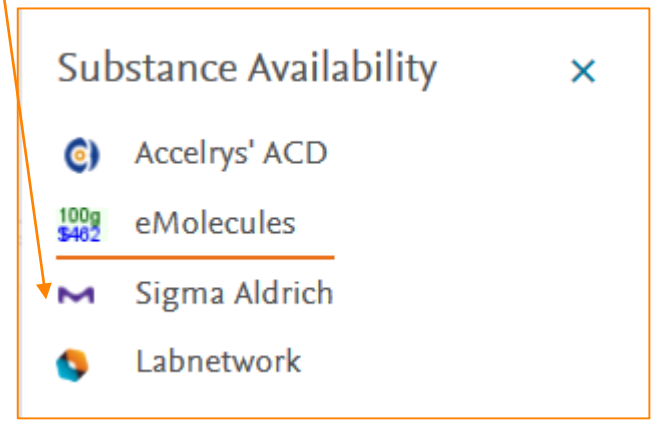
最后的结果

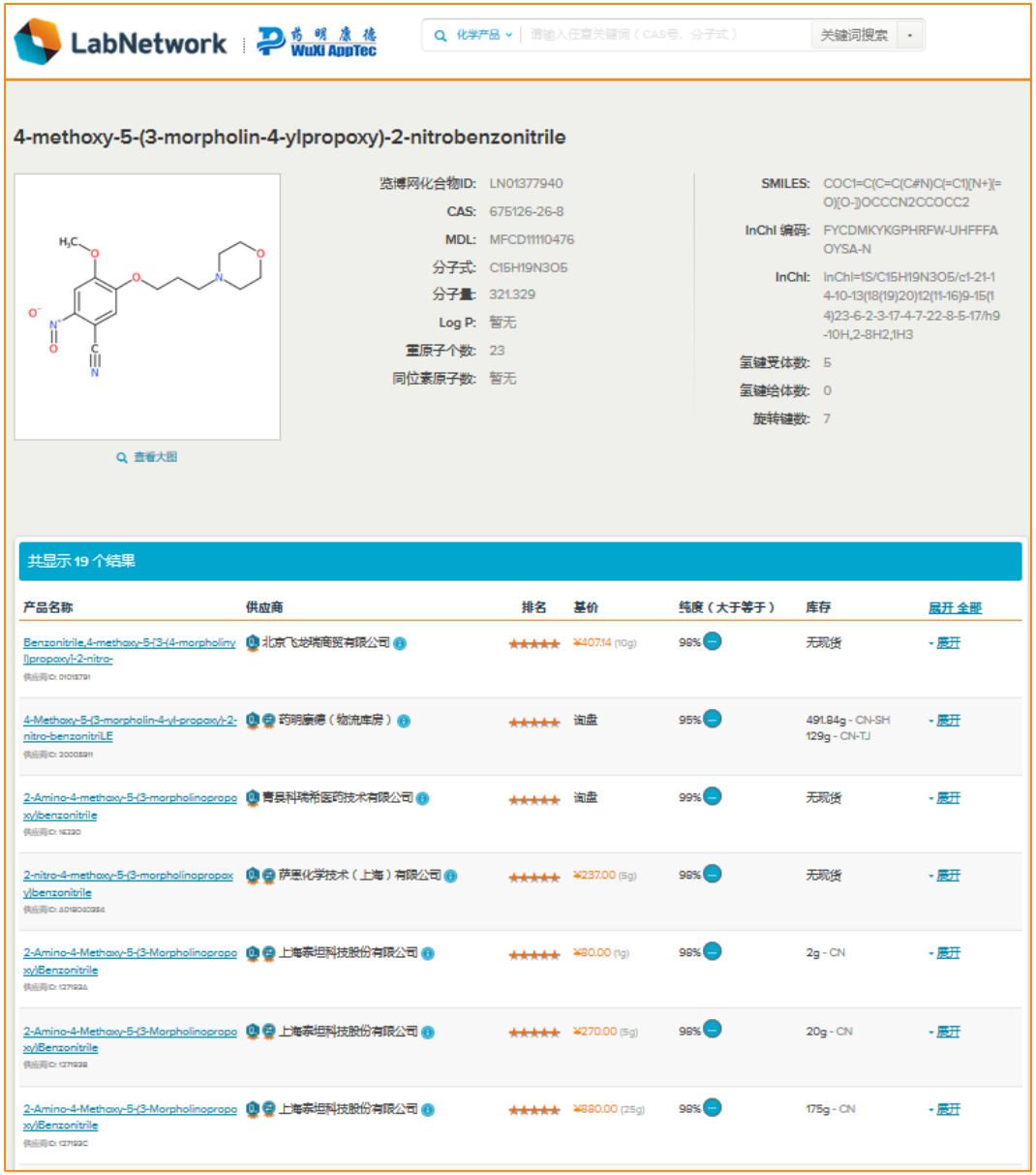


可以对Synthesis Plan进行导入，导出或者保存等操作。

获得物质的商业信息




Substance Availability
Accelrys' ACD
100g $462
eMolecules
Sigma Aldrich
Labnetwork


LabNetwork
WuXi AppTec
化学产品
关键词搜索
4-methoxy-5-(3-morpholin-4-ylpropoxy)-2-nitrobenzonitrile
查看大图
药明康德网化合物ID: LN01377940
CAS: 675126-26-8
MDL: MFCD11110476
分子式: C15H19N3O5
分子量: 321.329
Log P: 暂无
重原子个数: 23
同位素原子数: 暂无
SMILES: COC1=C(C=C(C#N)C(=C1)[N+](=O)[O-])OCCCN2CCOCC2
InChI 编码: FYCDMKYKGPHRFW-UHFFFAOYSA-N
InChI: InChI=1S/C15H19N3O5/c1-21-14-10-13(18(19)20)12(11-16)9-15(14)23-6-2-3-17-4-7-22-8-5-17/h9-10H,2-8H2,1H3
氢键受体数: 5
氢键给体数: 0
旋转键数: 7
共显示 19 个结果
产品名称
供应商
排名
基价
纯度（大于等于）
库存
展开 全部
Benzonitrile,4-methoxy-5-[3-(4-morpholinyl)propoxy]-2-nitro-
北京飞龙瑞商贸有限公司
¥407.14 (10g)
98%
无现货
展开
4-Methoxy-5-(3-morpholin-4-yl-propoxy)-2-nitro-benzonitriLE
药明康德（物流库房）
询盘
95%
491.84g - CN-SH
129g - CN-TJ
展开
2-Amino-4-methoxy-5-(3-morpholinopropoxy)benzonitrile
青岛科瑞希医药技术有限公司
询盘
99%
无现货
展开
2-nitro-4-methoxy-5-(3-morpholinopropoxy)benzonitrile
萨恩化学技术（上海）有限公司
¥237.00 (5g)
98%
无现货
展开
2-Amino-4-Methoxy-5-(3-Morpholinopropoxy)Benzonitrile
上海泰坦科技股份有限公司
¥80.00 (1g)
98%
2g - CN
展开
2-Amino-4-Methoxy-5-(3-Morpholinopropoxy)Benzonitrile
上海泰坦科技股份有限公司
¥270.00 (5g)
98%
20g - CN
展开
2-Amino-4-Methoxy-5-(3-Morpholinopropoxy)Benzonitrile
上海泰坦科技股份有限公司
¥880.00 (25g)
98%
175g - CN
展开

提纲

- Reaxys中的内容和数据索引介绍
- Reaxys中的检索
  - Reaxys的基本检索模式
  - 如何利用Reaxys结构面板实现复杂结构定义
  - 如何利用Reaxys进行物质检索和物质分析
  - 如何利用Reaxys进行反应检索和条件筛选
  - 如何利用Reaxys制作合成计划
- Reaxys检索小结

Reaxys中的检索小结

- Reaxys中的物质检索方法
  - Quick Search 物质名称
  - Quick Search 结构检索
  - Query Builder 组合检索
  - Quick Search 理化性质+物质名称/结构
- Reaxys中反应检索方法
  - Quick Search 关键词
  - Quick Search 结构式检索
  - Query Builder 组合检索

Reaxys检索小结

- New Reaxys从大量文献中摘取和物质性质相关的所有数据，帮助科研人员获得标准化，规范化，格式化的物性数据列表及参考文献

- New Reaxys中的Query Builder检索帮助科研人员通过简便的方式，获得精准，跨学科的精确答案

- New Reaxys中的结构面板，能实现科研人员绝大部分的结构绘制要求，帮助科研人员用最直接的方式获得相应的物质和反应

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