Elsevier
Reaxys中化学信息的获取

俞靓（Sam Yu）
Elsevier Life Science Customer Consultant
Mail:S.yu.2@Elsevier.com
Phone: 18930408012

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
  - Reaxys对文献的提炼
  - Reaxys中物质与物性数据获取反向检索
  - Reaxys中结构面板与反应数据获取
  - Reaxys中的实用小案例
- Q&A

什么是Reaxys

Reaxys是Elsevier旗下Life Science产品线中基于数据深度提炼与挖掘的化学及相关学科的科研信息平台

6,000万文献

(Elsevier, ACS, Nature-Springer, Blackwell, Taylor and Francis,etc)

105家专利机构专利

WPO, USPO, EPO [≈ mid 70´s >]

PO: JP, KR, CN, TW [2015 >]

2021年底前完成105家专利机构专利回溯与抽提

38万书的章节

Beilstein, Gmelin,….

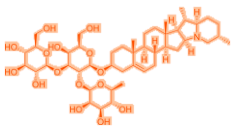
16,300 期刊

(journals, books and patents)

[自动抽提]

≈ 450 journals + PO

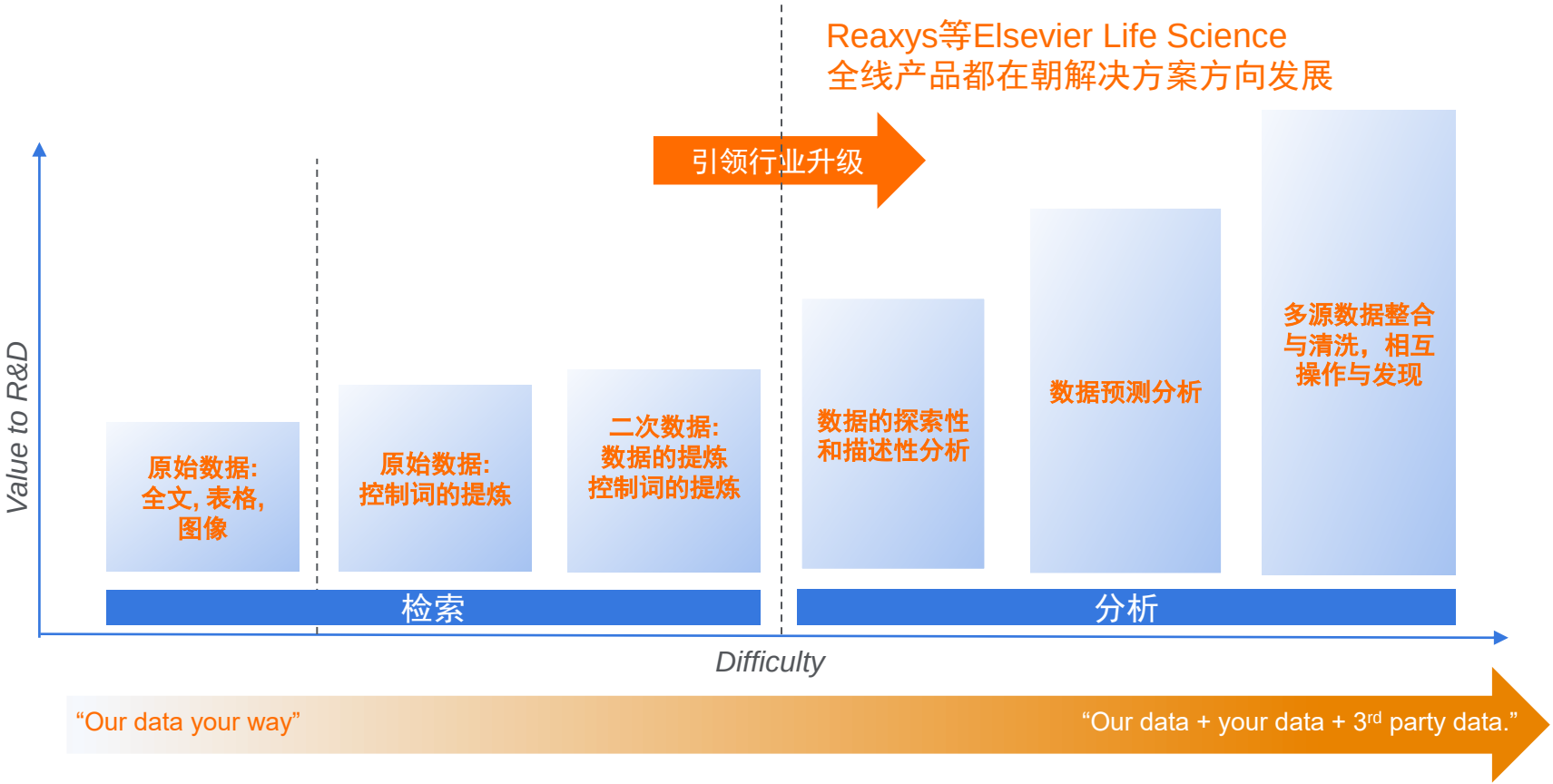
[人工抽提]



Reaxys

ELSEVIER

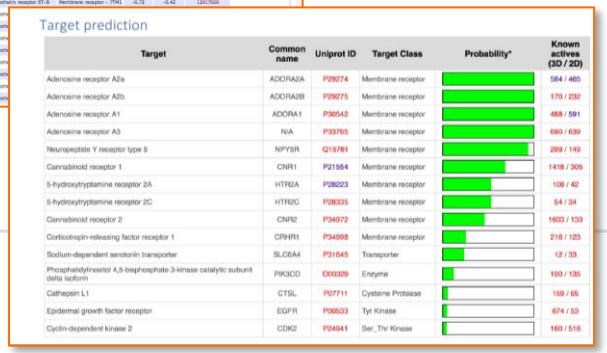
Reaxys已经在不断利用AI/ML技术， 引领数据库到解决方案的行业升级



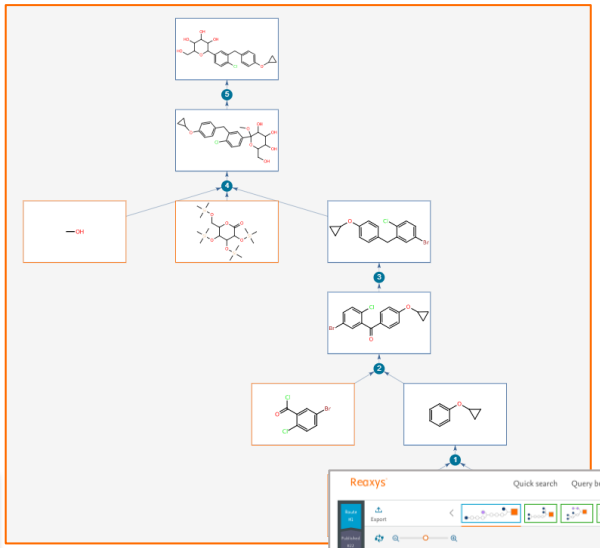
越来越多的AI/ML技术融入到数据库中

MMP分析

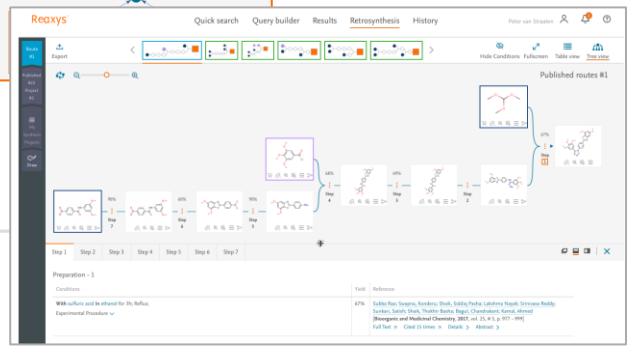
靶点预测



AI合成预测



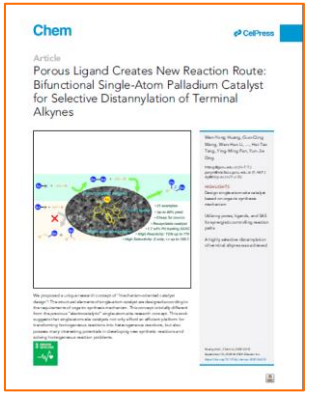
2021年将于现有Synthesis Plan整合到一个平台

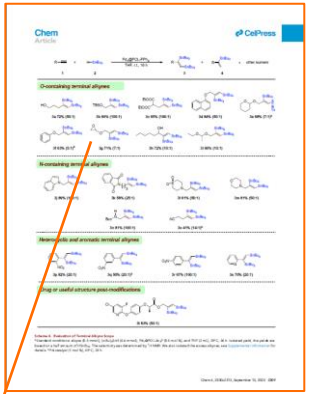


Agenda

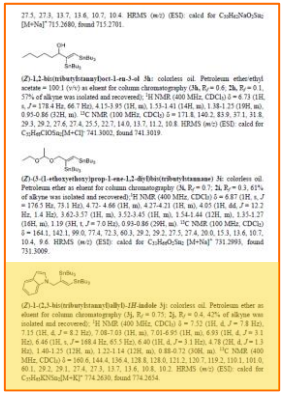
- Reaxys内容与发展规划
- Reaxys中的检索
  - Reaxys对文献的提炼
  - Reaxys中物质与物性数据获取反向检索
  - Reaxys中结构面板与反应数据获取
  - Reaxys中的实用小案例
- Q&A

一篇常见的化学相关文献的构成

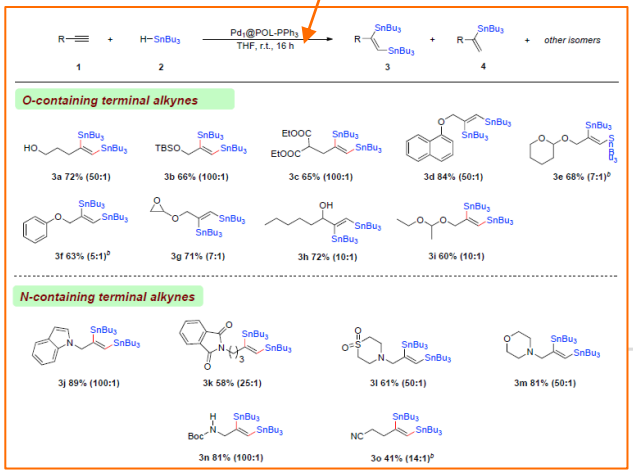


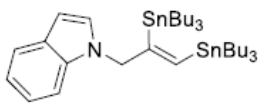


实验过程



一篇全文以及Support Information中有大量的数据，科研人员如果要获取，需要花费多的时间去阅读全文。





Support Information中的化合物理化性质描述

(*Z*)-1-(2,3-bis(tributylstannyl)allyl)-*1H*-indole 3j: colorless oil. Petroleum ether as eluent for column chromatography (**3j,** R_f = 0.75; **2j,** R_f = 0.4, 42% of alkyne was isolated and recovered); ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.52 (1H, d, *J* = 7.8 Hz), 7.15 (1H, d, *J* = 8.2 Hz), 7.08-7.03 (1H, m), 7.01-6.95 (1H, m), 6.93 (1H, d, *J* = 3.1 Hz), 6.46 (1H, s, *J* = 168.4 Hz, 65.5 Hz), 6.40 (1H, d, *J* = 3.1 Hz), 4.78 (2H, d, *J* = 1.3 Hz), 1.40-1.25 (12H, m), 1.22-1.14 (12H, m), 0.88-0.72 (30H, m). ^{13}C NMR (400 MHz, $CDCl_3$) δ = 160.6, 144.4, 136.4, 128.8, 128.0, 121.2, 120.7, 119.2, 110.1, 101.0, 60.1, 29.2, 29.1, 27.4, 27.3, 13.7, 13.6, 10.8, 10.2. HRMS (*m/z*) (ESI): calcd for $C_{35}H_{63}KNSn_2[M+K]^+$ 774.2630, found 774.2654.

Reaxys对这篇全文的提炼

1 Porous Ligand Creates New Reaction Route: Bifunctional Single-Atom Palladium Catalyst for Selective Distannylation of Terminal Alkynes

Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie [Chem, 2020, vol. 6, # 9, p. 2300 - 2313]

Abstract | Index Terms | Substances 58 | Reactions 29 | Full Text

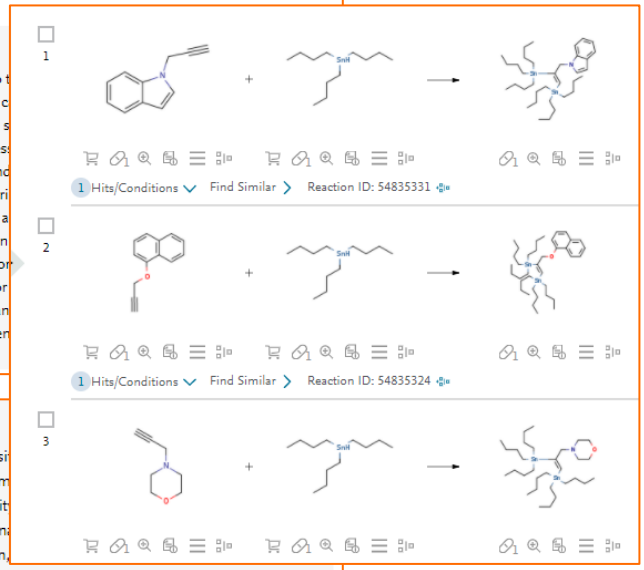
Abstract

We proposed a unique research concept of "mechanism-oriented catalyst design": The structural elements of single-atom catalyst are designed according to t mechanism. This concept is totally different from the previous "electrocatalytic" single-atom-site research concept. This work suggests that single-atom-site c transforming homogeneous reactions into heterogeneous reactions, but also possess many interesting potentials in developing new synthetic reactions and s Single-atom-site (SAS) catalyst, as a highly reactive heterogeneous catalytic system, is one of the effective tools for complex organic synthesis. However, exces metal atoms has led to the neglect of the role of supports and ligands. Here, we employed a P-doped porous organic polymer as a support, as well as a ligand enrichment of the substrates by the pores, ligand action of the support, and high chemoselectivity and anti-agglomeration of SAS catalysts were the most stri selective distannylation of terminal alkynes with a new mechanism was achieved by using the multiple properties of SAS catalyst. This catalytic system offers a the substrate by the pores to regulate the reaction mechanism, which opens a new frontier to use pores, ligands, and SASs for synergistic controlling reaction applications in organic synthesis. However, most of the research models related to organic synthesis still stay in the mode of "pursuing higher catalytic perfor article provides a reasonable design of the catalyst in accordance with the characteristics and reaction requirements of organic synthesis and finally uses it for distannylation of alkynes is very useful in the construction of complex molecules. In the past, only a few terminal alkynes could be achieved by selective distan reaction, the porous organic polymer catalyst with triarylphosphonate as the backbone was designed and prepared with advantages including pore enrichmen regulation. This catalyst solved all the problems in this reaction, such as narrow substrate scope, poor selectivity, and low catalytic efficiency.

Index Terms

Author keyword: chemoselectivity, distannylation, organic synthetic methodology, porous organic polymer, SDG3: Good health and well-being, single-atom-si

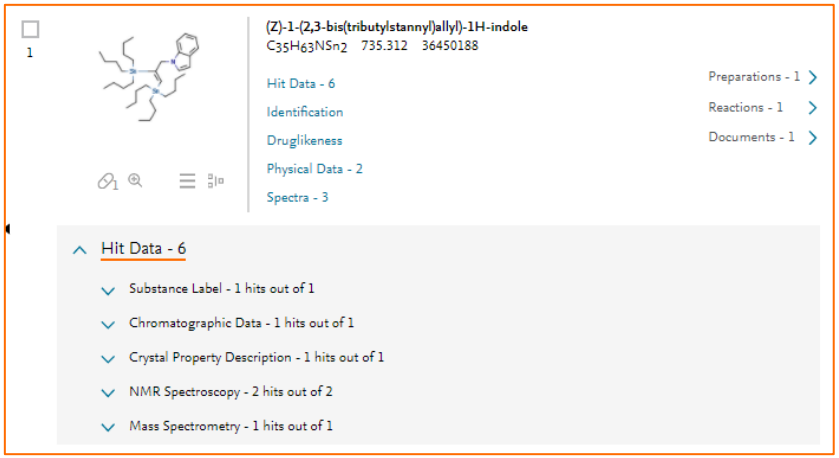
Reaxys Index Terms: Heck reaction, Migita-Kosugi-Stille coupling, Stereochemistry, Steric hindrance, X-ray diffraction, X-ray photoelectron spectroscopy, atom reaction, chemoselectivity, cross metathesis, cross-coupling reaction, cyclization reaction, decarbonylation, decarboxylation, dehydrogenation, enantioselectivit spectrum, heterogeneous catalysis, heterogeneous catalyst, homogeneous catalysis, homogeneous catalyst, hydroaminomethylation, hydroboration, hydrogen inorganic reaction, metathesis reaction, micro porosity, nanoporosity, noble metal, occurrence in nature, one pot reaction, organic reaction, oxidation reaction, porosities, reactivity, regioselectivity, side reaction, stannylation, stereoselectivity, total synthesis



ELSEVIER

Reaxys对于文献中的结构与反应都做了提炼

Reaxys对文献中的化合物的结构化数据提炼



Label	Reference
3j	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie[Chem, 2020, vol. 6, # 9, p. 2300 - 2313] Full Text ↗ Details > Abstract >

Colour & Other Properties	Location	Reference
colourless	supporting information	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie[Chem, 2020, vol. 6, # 9, p. 2300 - 2313] Full Text ↗ Details > Abstract >

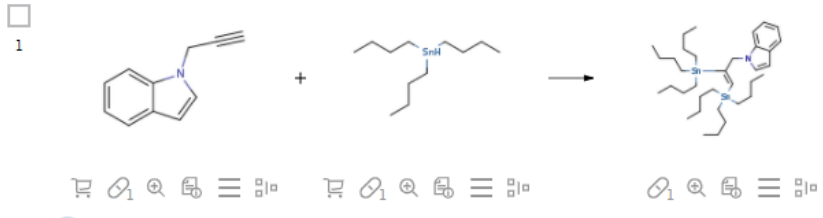
Show/Hide columns

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Frequency (NMR Spectroscopy), MHz	Location	Reference
Chemical shifts, Spectrum	1H	chloroform-d1	400	supporting information	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie[Chem, 2020, vol. 6, # 9, p. 2300 - 2313] Full Text ↗ Details > Abstract >
Chemical shifts, Spectrum	13C	chloroform-d1		supporting information	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie[Chem, 2020, vol. 6, # 9, p. 2300 - 2313] Full Text ↗ Details > Abstract >

文献中出现的化合物性质，全部直接抽提，或者给出文献中出现的位置，方便科研人员直接获取，或节省查找阅读全文的时间。

ELSEVIER

Reaxys对原文反应的提炼（3J)



1 Conditions Find Similar Reaction ID: 54835331

Conditions	Yield	Reference
With porous vinyl functionalized tri(2-methoxyphenyl)phosphine derived polymer supported palladium **In** tetrahydrofuran at 25°C; Schlenk technique; Sealed tube; stereoselective reaction; Experimental Procedure	89%	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie [**Chem, 2020**, vol. 6, # 9, p. 2300 - 2313] Full Text Details Abstract

General Procedure for Distannylation of Terminal Alkynes

General procedure: A flame-dried Schlenk tube was flushed under an atmosphere of ... added followed by addition of the alkyne (0.5 mmol). Tributyltin hydride (0.5 mmol, 1 ... (monitored by TLC), the solution was filtered and washed with EtOAc. The filtered sol... acetate, and 1% triethylamine to afford the corresponding product.

General Procedure for Distannylation of Terminal Alkynes

A flame-dried Schlenk tube was flushed under an atmosphere of nitrogen and charged with 15.5 mg of Pd_1@POL-5 (0.0025 mmol, 0.005 equiv-). The vial was sealed with a rubber septum and 2 mL of distilled THF was added followed by addition of the alkyne (0.5 mmol). Tributyltin hydride (0.5 mmol, 1 equiv) was added dropwise to the reaction vial. The reaction mixture was left to stir for 24–36 h at room temperature. When the reaction was completed (monitored by TLC), the solution was filtered and washed with EtOAc. The filtered solution was evaporated under vacuum. The crude product was purified directly by silica gel column chromatography eluting with petroleum ether, ethyl acetate, and 1% triethylamine to afford the corresponding product.

ELSEVIER

Reaxys从文献中提炼出来的内容

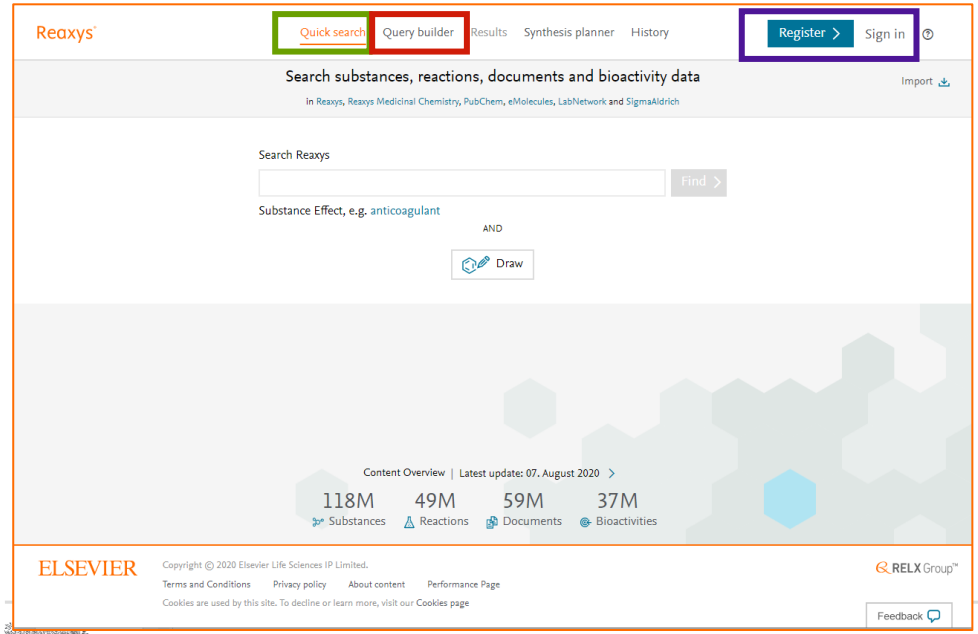
数据更新时间：2021/2/22

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
  - Reaxys对文献的提炼
  - Reaxys中物质与物性数据获取反向检索
  - Reaxys中结构面板与反应数据获取
  - Reaxys中的实用小案例
- Q&A

Reaxys的登录界面

- IP范围内，浏览器输入www.Reaxys.com，可以直接进行检索，推荐Chrome，Firefox浏览器，
- 收藏夹收藏的链接建议只收藏www.Reaxys.com



Tips:

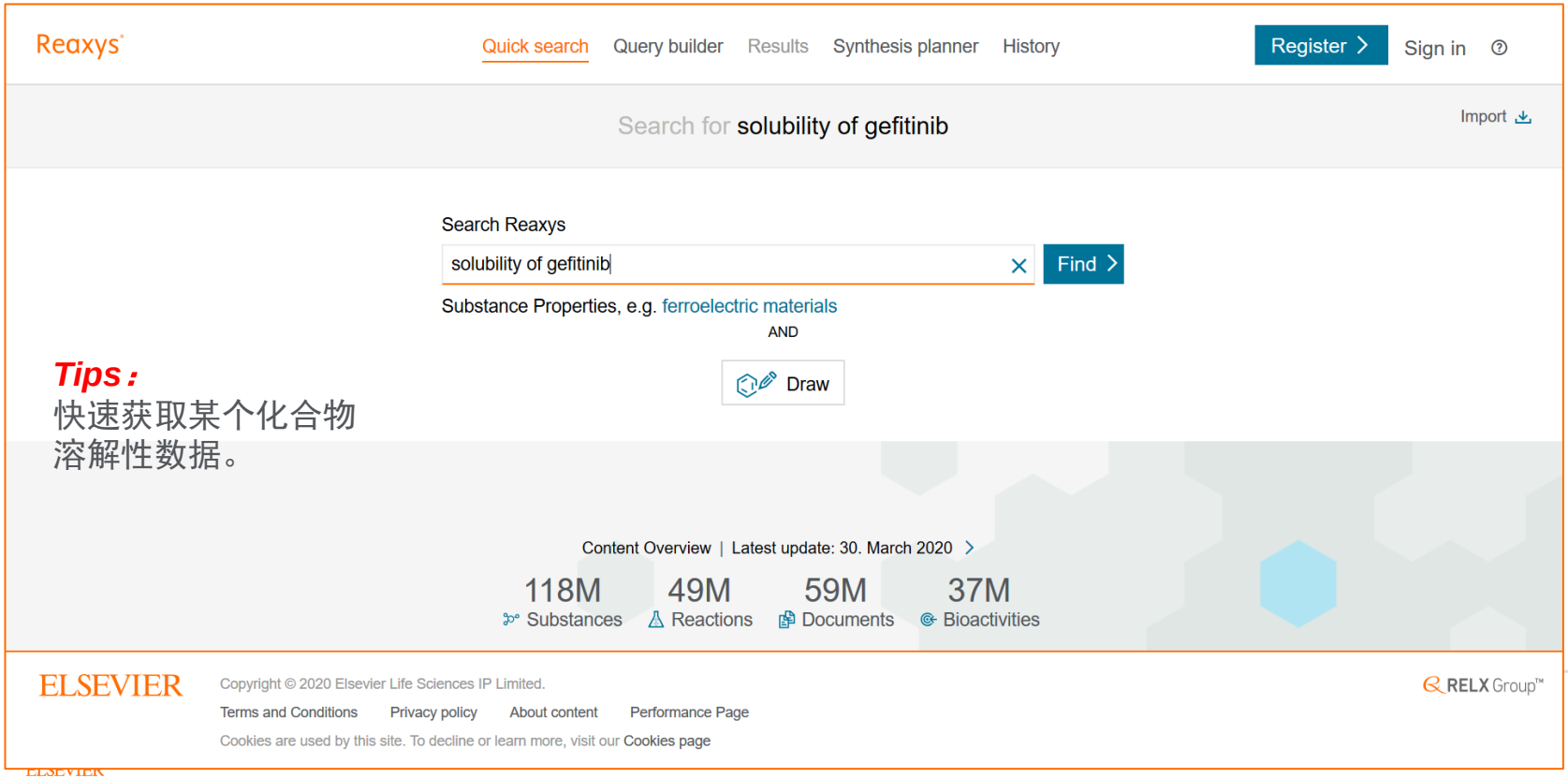
1. 账号注册（可选），注册帐号后，可以使用提醒，结果集保存，结果导出功能（2020.8以后）
2. Quick Search，快速检索，结构反应检索，或者输入自然语言，Reaxys智能分析语义进行检索。
3. Query Builder，组合检索，利用Reaxys中的各种字段进行组合，实现不同检索需求。

视频介绍：

1. Reaxys主界面：https://www.bilibili.com/video/BV1T5411L7Ec
2. Quick Search：https://www.bilibili.com/video/BV1az4y1C7ZL
3. Query Builder：https://www.bilibili.com/video/BV1UK4y1774Q
4. Reaxys账号注册与应用 https://www.bilibili.com/video/BV1NA41147if

ELSEVIER

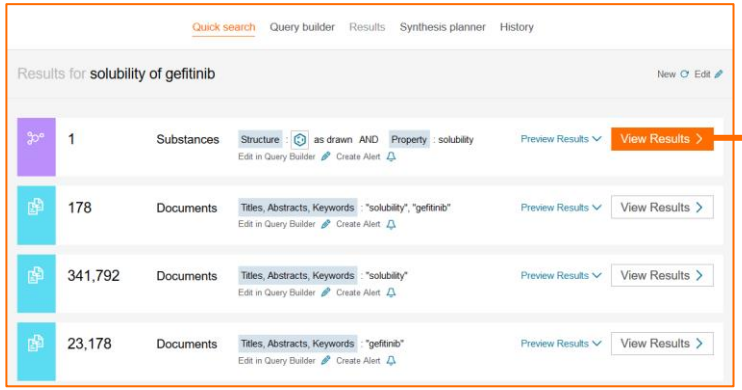
Case 1：快速获取化合物的理化性质

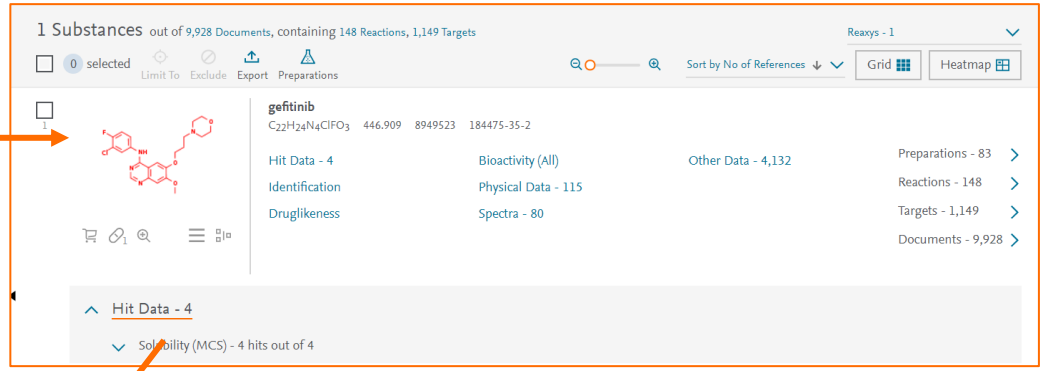


Tips：

快速获取某个化合物溶解性数据。

Reaxys中的结果





抽提的数据包括具体的数值，或者相关的文字性描述

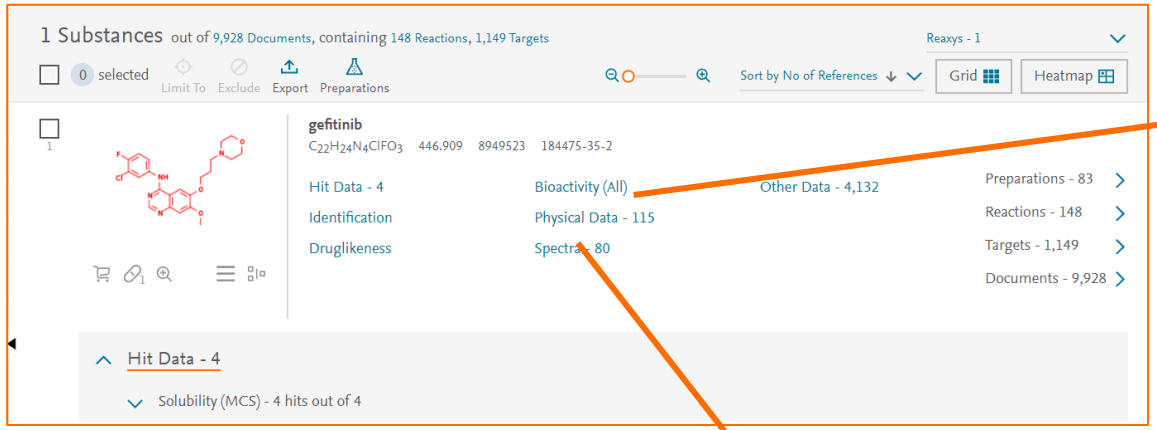
Solubility (MCS) - 4 hits out of 4

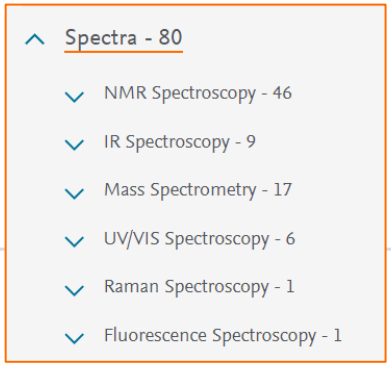
Show/Hide columns

Solubility, g·l-1	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Location	Comment (Solubility (MCS))	Reference
					freely soluble in DMSO,THP and PEG-400, sparingly soluble in 2-butanol and slightly soluble in 1-butanol, IPA, ethanol,methanol, EG and PG	Alanazi, Abdullah; Alshehri, Sultan; Altamimi, Mohammad; Shakeel, Faiyaz[**Journal of Molecular Liquids**, **2020**, vol. 299, art. no. 112211] Full Text ↗ Details › Abstract ›
					soluble in water and 1-octanol	Wu, Kuen-Da; Chen, Grace Shiahuy; Liu, Jia-Rong; Hsieh, Chen-En; Chern, Ji-Wang[**ACS Medicinal Chemistry Letters**, **2019**, vol. 10, # 1, p. 22 - 26] Full Text ↗ Cited 1 times ↗ Details › Abstract ›
0.009832	in pure solvent	25	water	supporting information		Wang, Xin-Xin; Tian, Fei-Yang; Liu, Ming; Chen, Kai; Zhang, Yun-Qian; Zhu, Qian-Jiang; Tao, Zhu[**Tetrahedron**, **2019**, vol. 75, # 37, art. no. 130488] Full Text ↗ Details › Abstract ›
0.0021	in pure solvent	20	water			Zhao, Feng; Lin, Zhaohu; Wang, Feng; Zhao, Weili; Dong, Xiaochun[**Bioorganic and Medicinal Chemistry Letters**, **2013**, vol. 23, # 19, p. 5385 - 5388] Full Text ↗ Cited 22 times ↗ Details › Abstract ›

ELSEVIER

Reaxys中化合物更多的理化性质

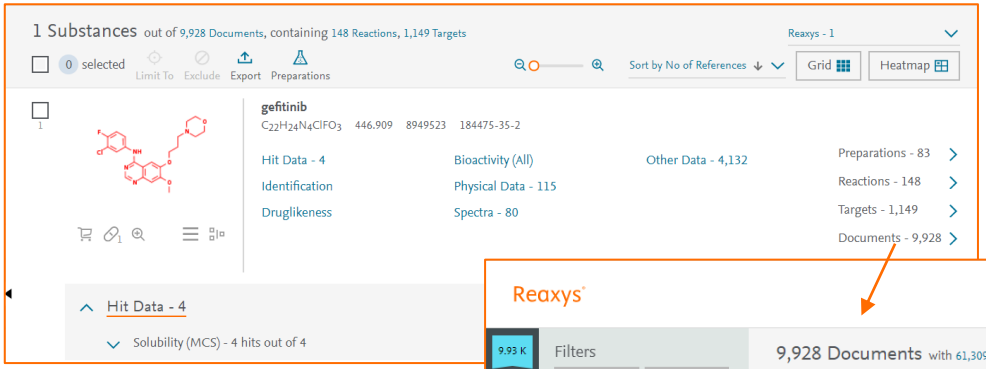


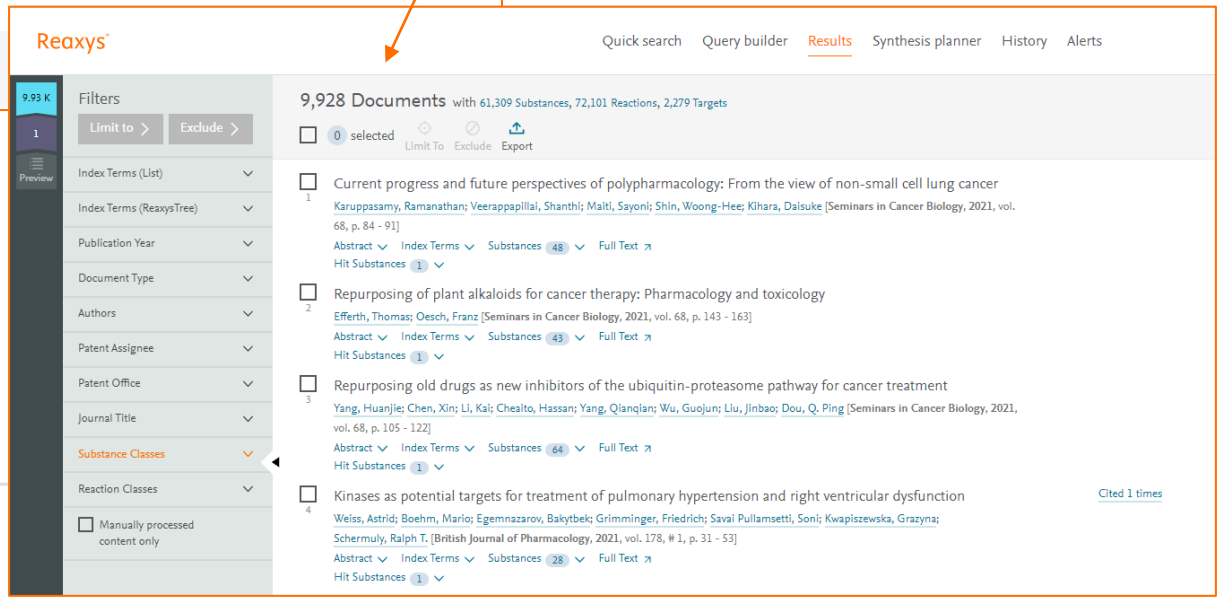


直接获取化合物的理化性质或者谱图数据

ELSEVIER

Reaxys中与化合物分析有关文献的获取

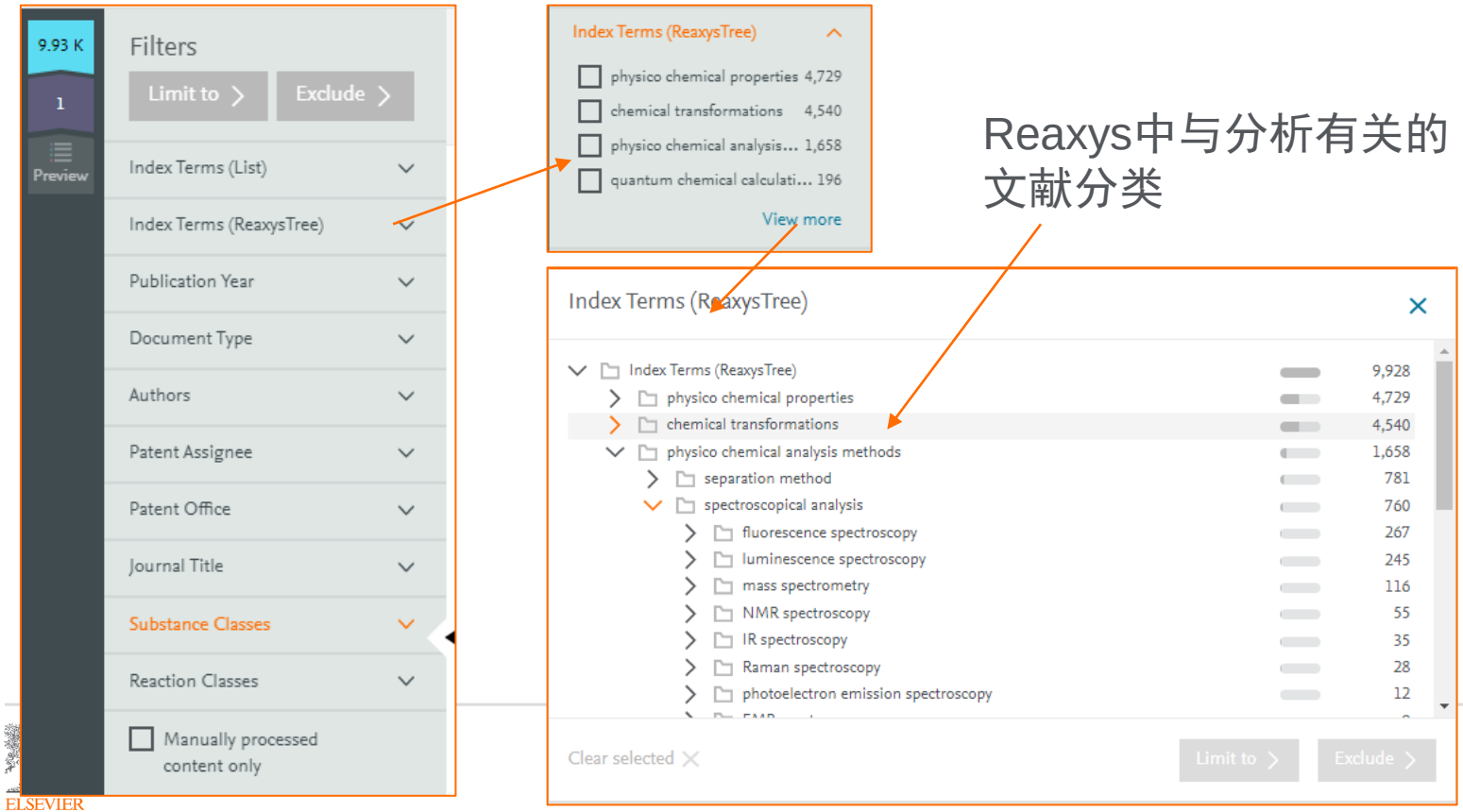




可以一次性获取与该化合物有关的文献

ELSEVIER

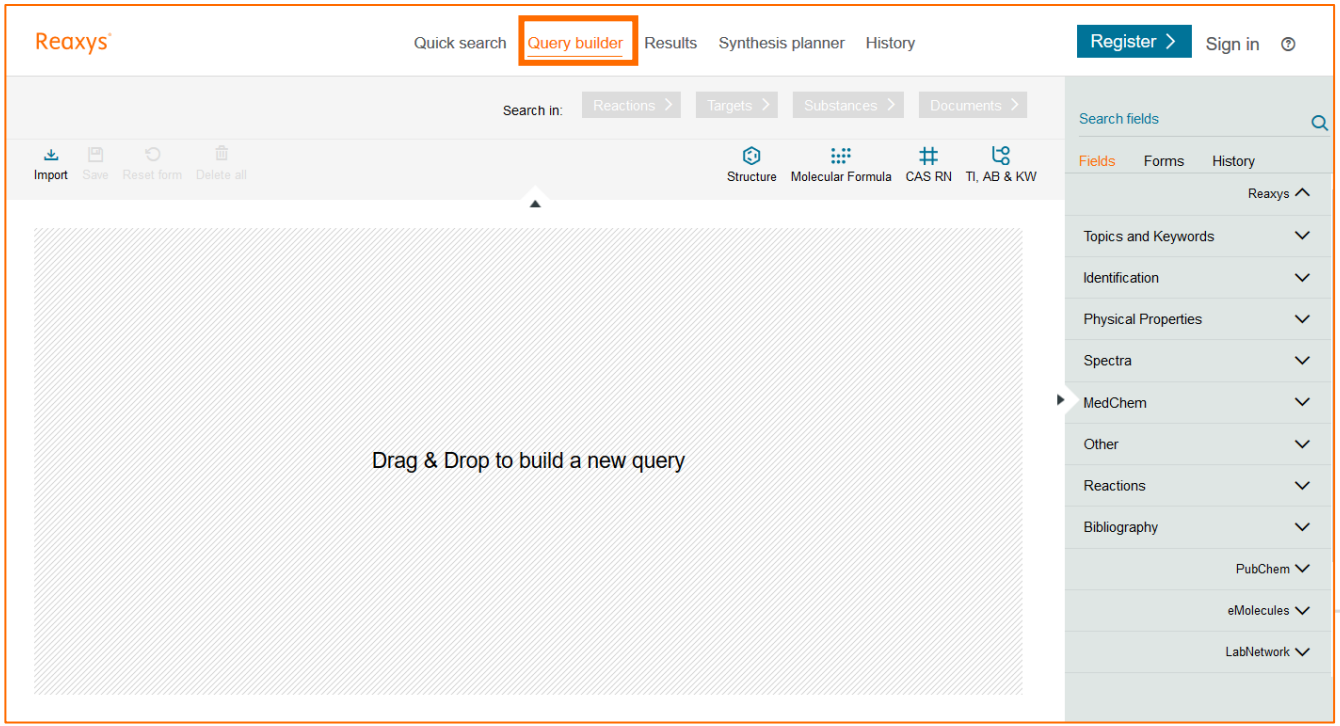
Reaxys中的文献分析工具



Reaxys中与分析有关的文献分类

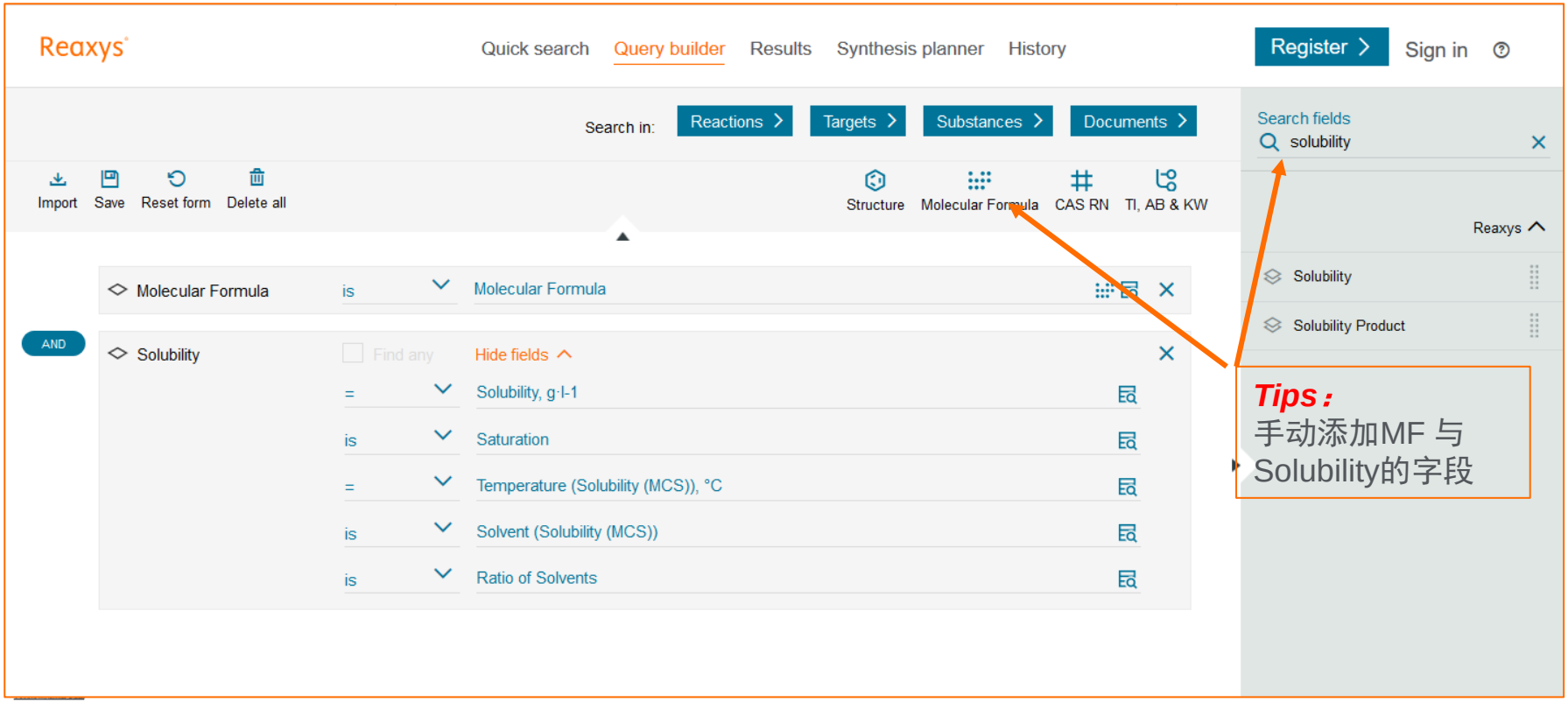
Case 2：理化性质的高级应用

- 获取KCl在乙醇中的溶解度

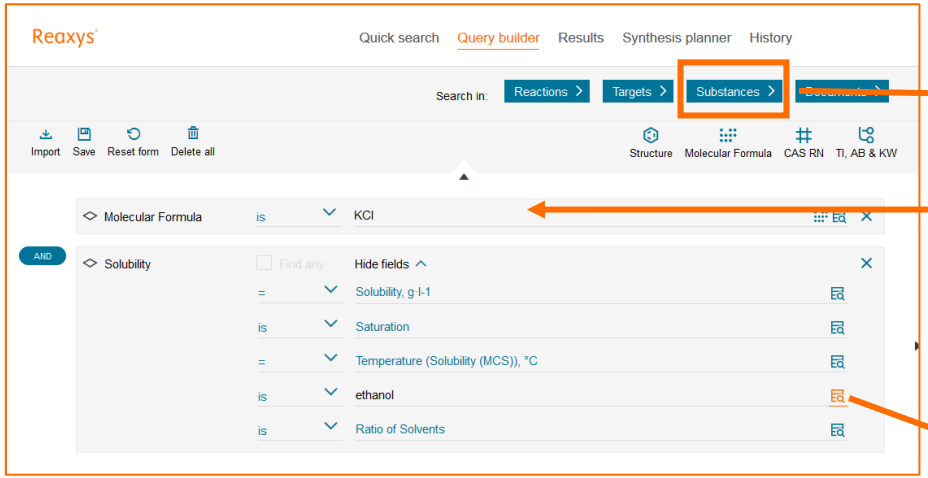


Reaxys中的Query Builder可以按照一定的规则构建检索式，Reaxys一共提供180+字段和字段组，科研人员可以自由的对这些字段和字段组进行组合，同时Reaxys也根据一些常见的需求，内置了多种检索策略模板，如“天然产物”，“hERG”等

检索策略的构建


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Register
Sign in
Search in:
Reactions
Targets
Substances
Documents
Import
Save
Reset form
Delete all
Structure
Molecular Formula
CAS RN
TI, AB & KW
Molecular Formula
is
Molecular Formula
AND
Solubility
Find any
Hide fields
=
Solubility, g·l-1
is
Saturation
=
Temperature (Solubility (MCS)), °C
is
Solvent (Solubility (MCS))
is
Ratio of Solvents
Search fields
solubility
Reaxys
Solubility
Solubility Product
Tips：
手动添加MF 与
Solubility的字段

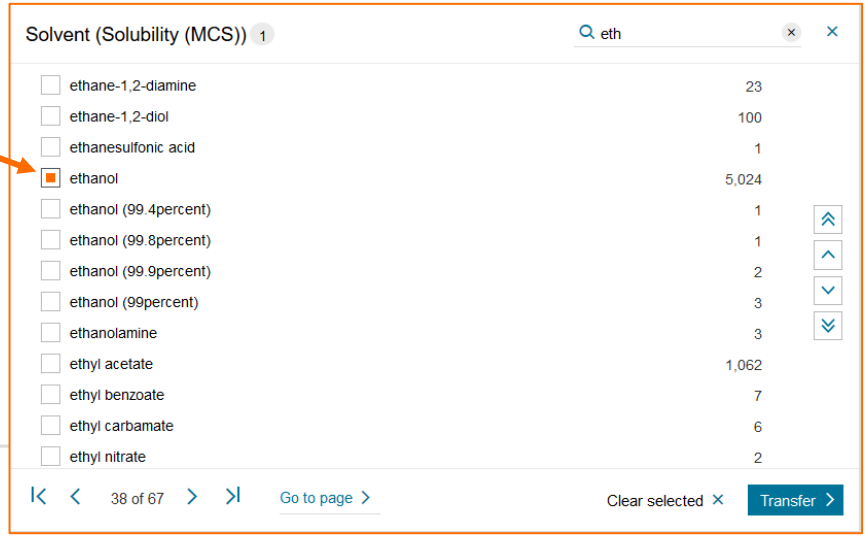
条件的输入



Step3：进行物质检索

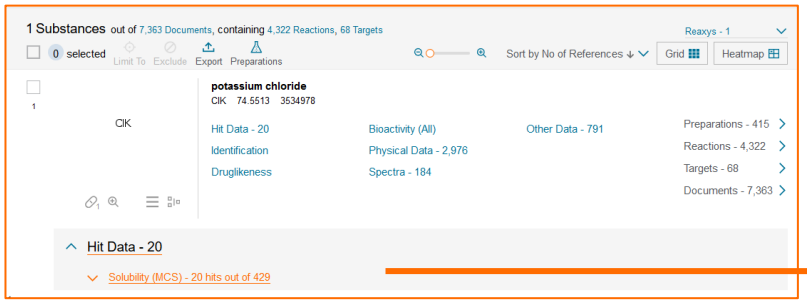
Step1：输入分子式KCl

Step2：在溶剂一块选择乙醇



ELSEVIER

最后的结果



Reaxys直接给出具体的数据和数据的文献出处，其实也可以设定更多的条件，如温度.....

Solubility (MCS) - 20 hits out of 429

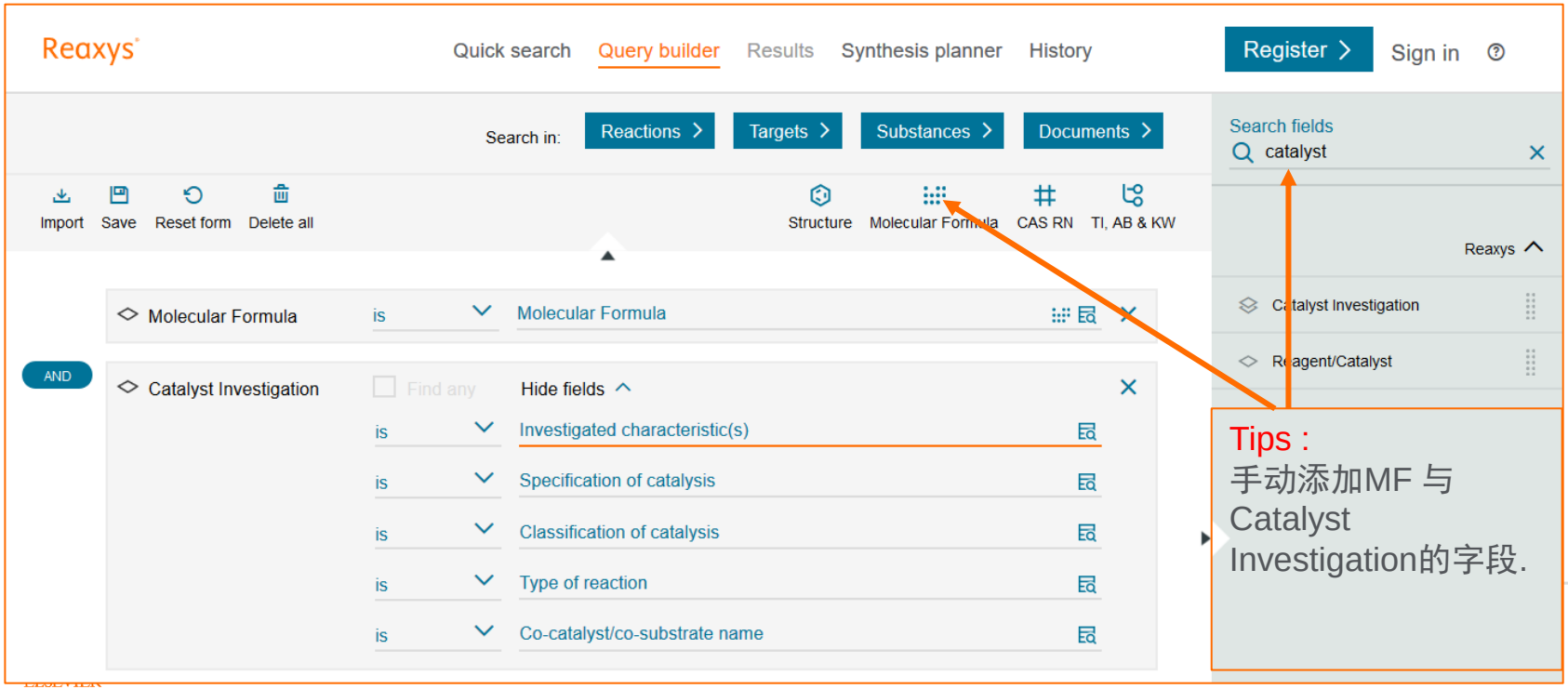
Show/Hide columns

Solubility, g·l-1	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Comment (Solubility (MCS))	Reference
	20	ethanol	Solubility: 0.012 mol/kg solvent	El-Dossoki[**Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical**, **2005**, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
	25	ethanol	Solubility: 0.025 mol/kg solvent	El-Dossoki[**Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical**, **2005**, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
	30	ethanol	Solubility: 0.037 mol/kg solvent	El-Dossoki[**Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical**, **2005**, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
	35	ethanol	Solubility: 0.043 mol/kg solvent	El-Dossoki[**Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical**, **2005**, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
0.320571		ethanol		Abakshin, V. A.; Eliseeva, O. V.; Krasnoperova, A. P.; Lebedeva, L. T.; Krestov, G. A.[**Doklady Physical Chemistry**, **1991**, vol. 317, p. 303 - 306][**Dokl. Phys. Chem. (Transl. of Dokl. Akad. Nauk.)**, **1991**, vol. 317, p. 1140 - 1143] Full Text Details
	20	ethanol	Solubility: 1.270E0 mol/1000mol solvent	Kirn; Dunlap[**Journal of the American Chemical Society**, **1931**, vol. 53, p. 393] Full Text Details
	45	ethanol	Solubility: 1.277E0 mol/1000mol solvent	Kirn; Dunlap[**Journal of the American Chemical Society**, **1931**, vol. 53, p. 393] Full Text Details

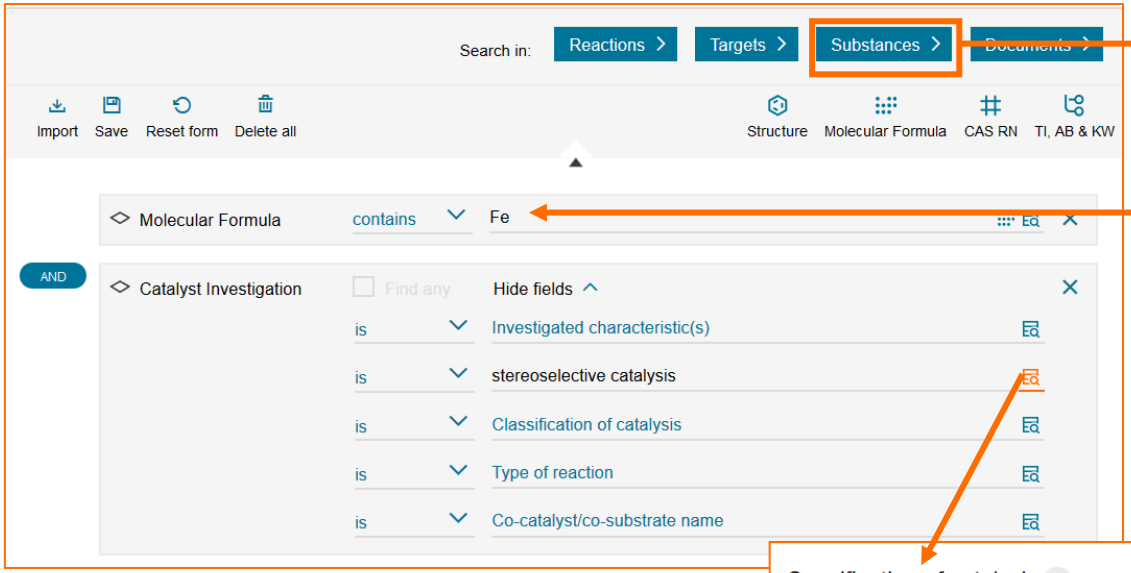
ELSEVIER

Case 3：“特定研究领域”的催化剂选择

- 检索可用于立体选择性催化的含Fe的催化剂

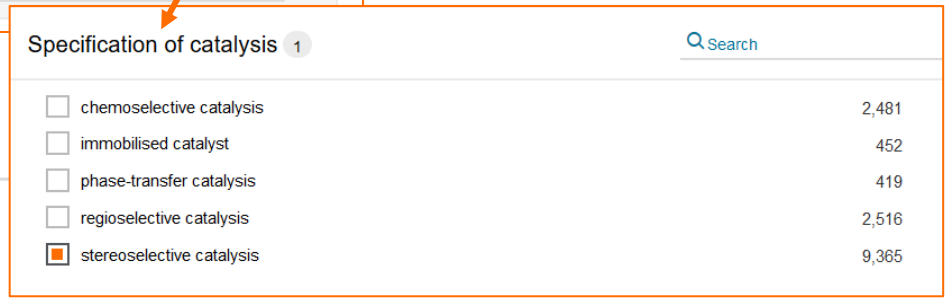


条件的输入



Step3：进行物质检索

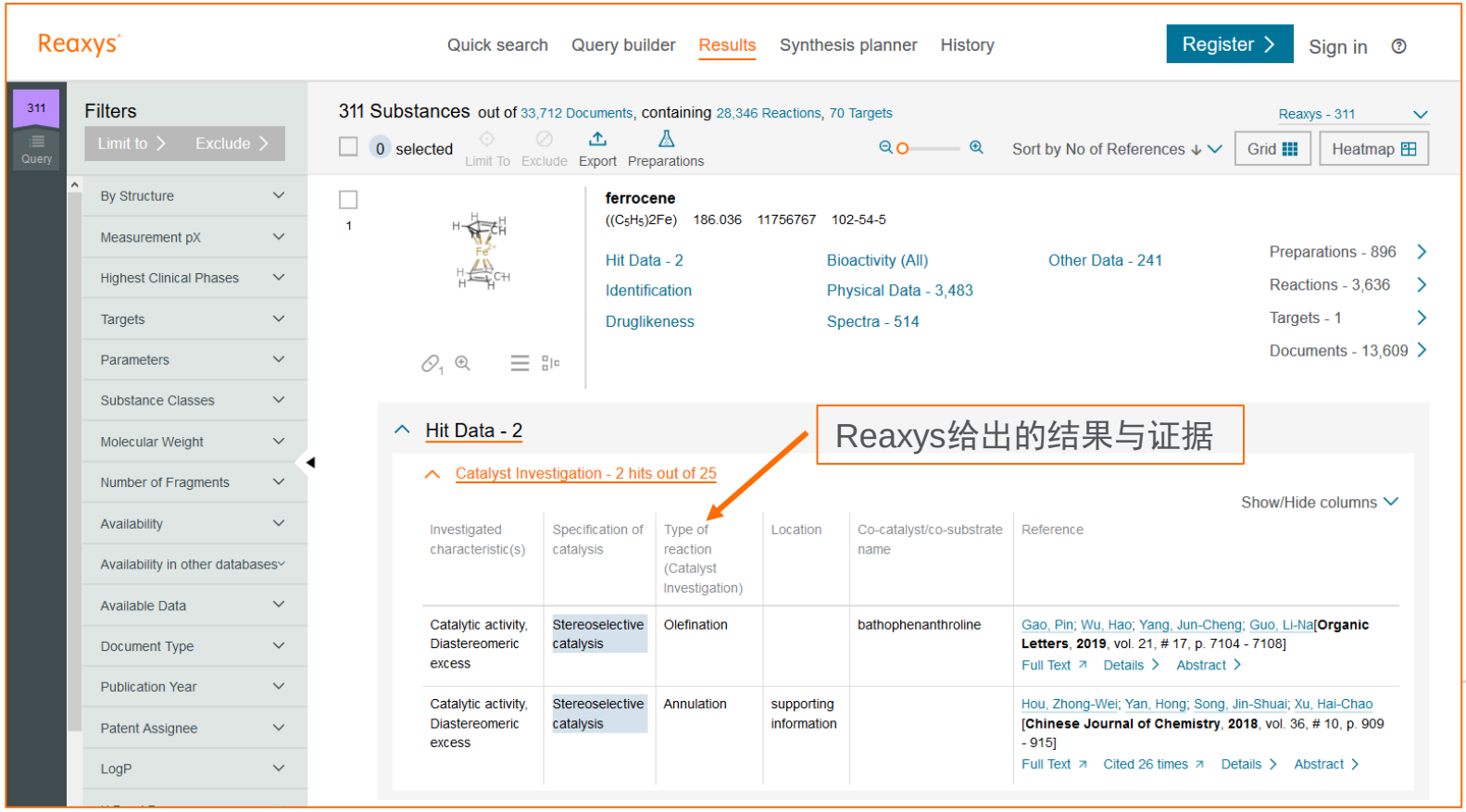
Step1：输入分子式Fe，并将逻辑关系改成“Contains”，即只要分子式中包含Fe，就检索出来



Step2：Specification of Catalysis部分选择
立体选择性催化

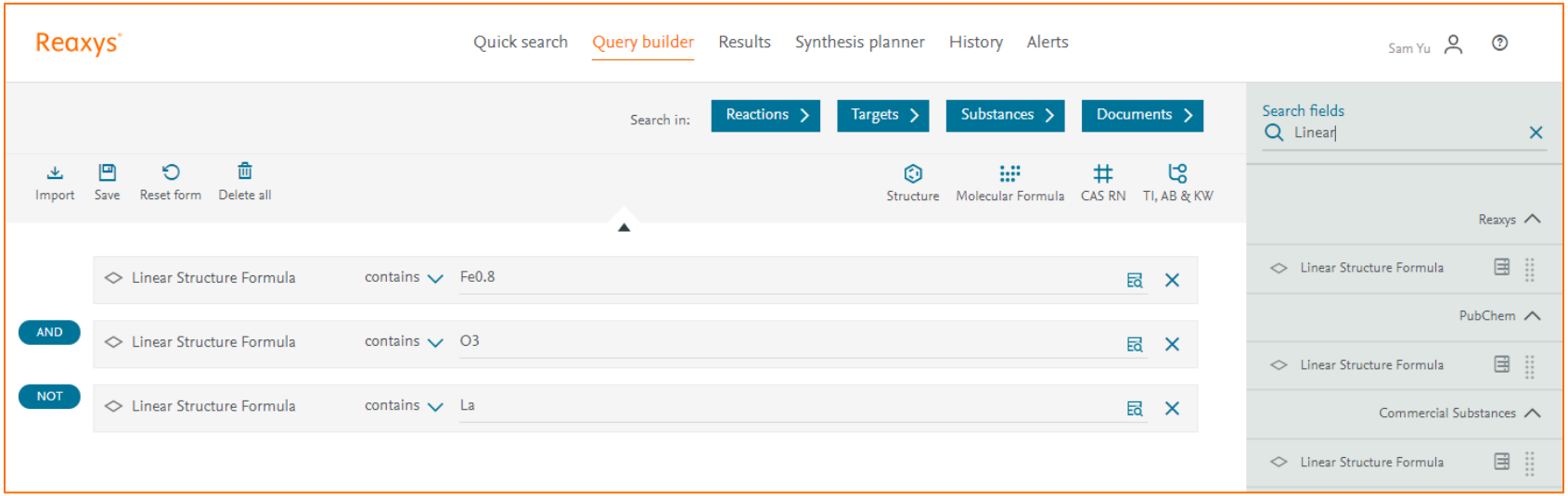
ELSEVIER

最后的结果


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Register
Sign in
311
Query
Filters
Limit to
Exclude
By Structure
Measurement pX
Highest Clinical Phases
Targets
Parameters
Substance Classes
Molecular Weight
Number of Fragments
Availability
Availability in other databases
Available Data
Document Type
Publication Year
Patent Assignee
LogP
311 Substances out of 33,712 Documents, containing 28,346 Reactions, 70 Targets
Reaxys - 311
0 selected
Limit To
Exclude
Export
Preparations
Sort by No of References
Grid
Heatmap
1
ferrocene
((C5H5)2Fe) 186.036 11756767 102-54-5
Hit Data - 2
Bioactivity (All)
Other Data - 241
Identification
Physical Data - 3,483
Druglikeness
Spectra - 514
Preparations - 896
Reactions - 3,636
Targets - 1
Documents - 13,609
Hit Data - 2
Reaxys给出的结果与证据
Catalyst Investigation - 2 hits out of 25
Show/Hide columns
Investigated characteristic(s)
Specification of catalysis
Type of reaction (Catalyst Investigation)
Location
Co-catalyst/co-substrate name
Reference
Catalytic activity, Diastereomeric excess
Stereoselective catalysis
Olefination
bathophenanthroline
Gao, Pin; Wu, Hao; Yang, Jun-Cheng; Guo, Li-Na[Organic Letters, 2019, vol. 21, # 17, p. 7104 - 7108]
Full Text
Details
Abstract
Catalytic activity, Diastereomeric excess
Stereoselective catalysis
Annulation
supporting information
Hou, Zhong-Wei; Yan, Hong; Song, Jin-Shuai; Xu, Hai-Chao [Chinese Journal of Chemistry, 2018, vol. 36, # 10, p. 909 - 915]
Full Text
Cited 26 times
Details
Abstract

Case 4：钙钛矿类化合物的获取

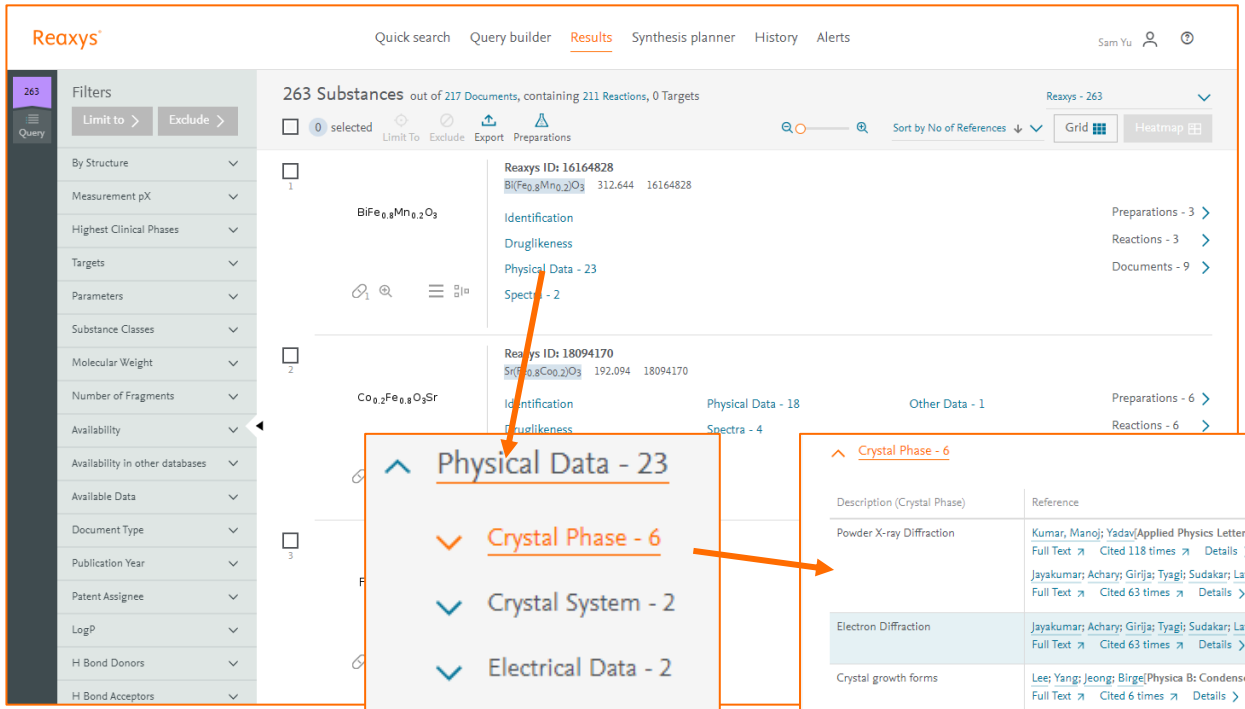
- 检索含特定组分的“钙钛矿”类化合物如必须含Fe0.8，O3，但是一定不含 La



全部选择Contains，并且根据逻辑关系定义Fe0.8 and O3 not La

ELSEVIER

Reaxys中的检索结果

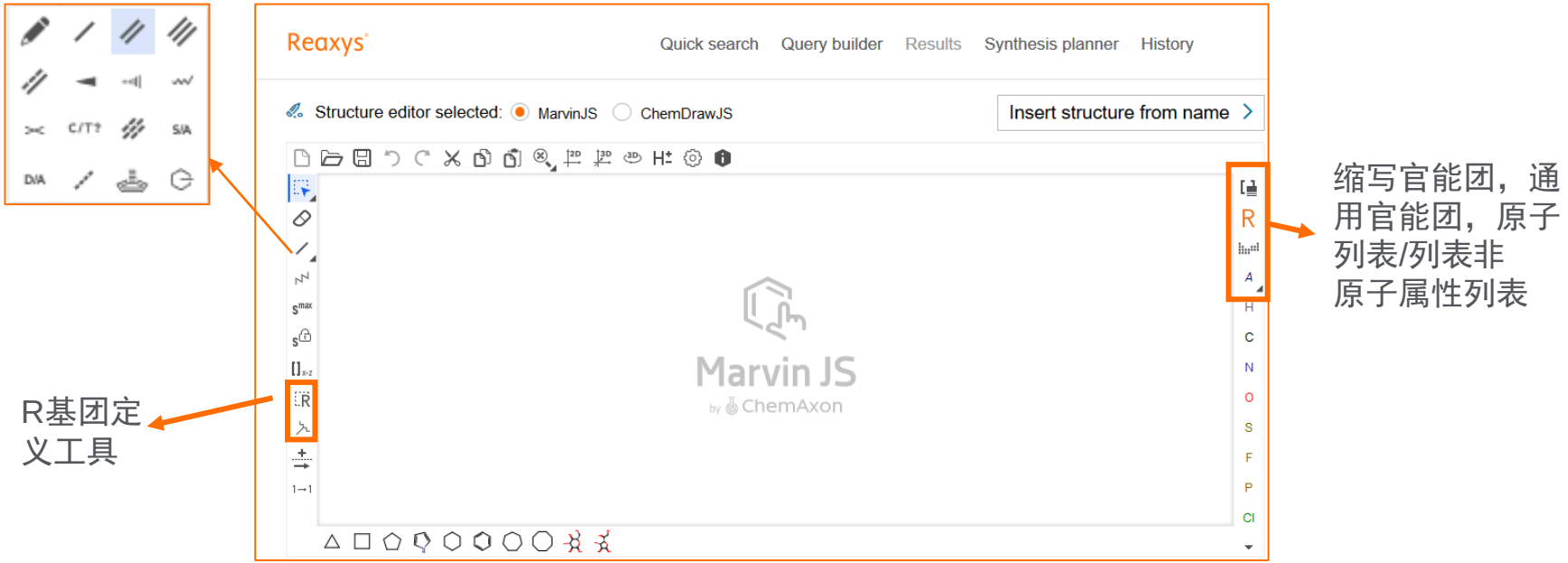


与该物质有关的XRD有关的报道

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
  - Reaxys对文献的提炼
  - Reaxys中物质与物性数据获取反向检索
  - Reaxys中结构面板与反应数据获取
  - Reaxys中的实用小案例
- Q&A

Reaxys中的结构面板



一些常见的功能使用视频

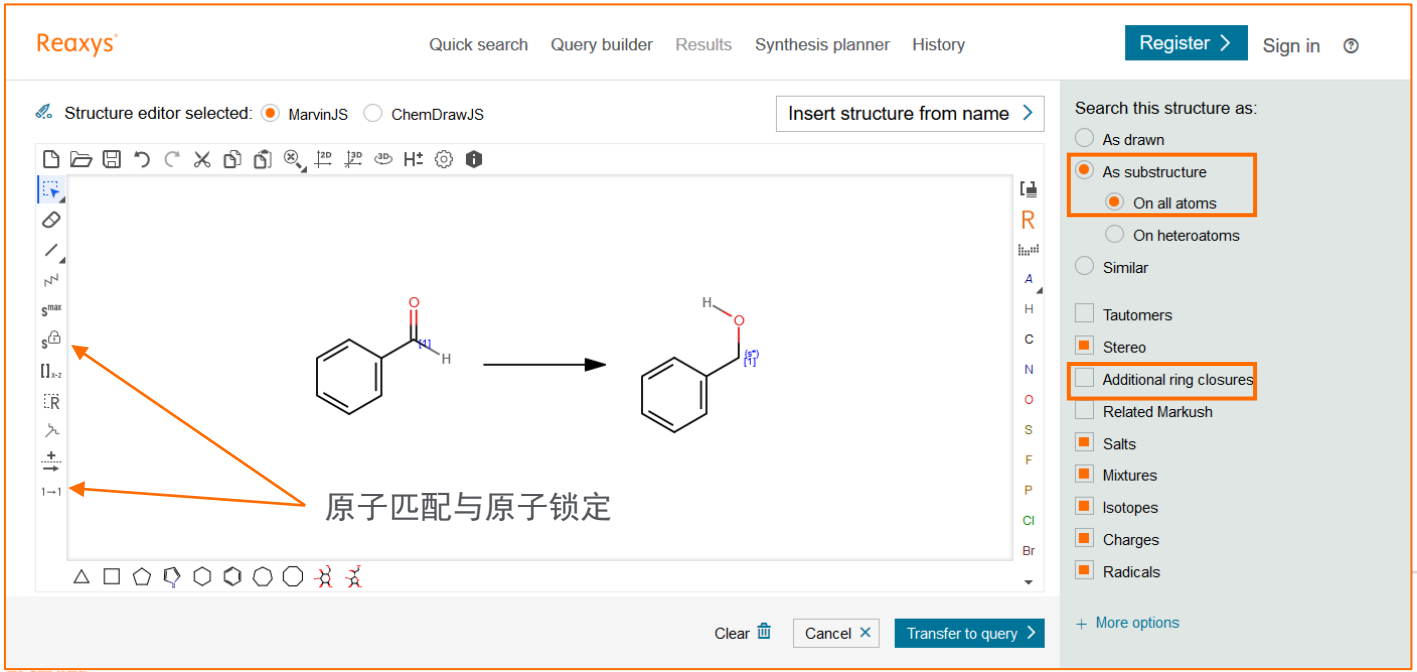
常用功能	视频链接
最基本功能	https://www.bilibili.com/video/BV13i4y177wV
不定位键	https://www.bilibili.com/video/BV1LK411P7nW
通用/缩写官能团	https://www.bilibili.com/video/BV1PV41117J6
原子列表与列表非	https://www.bilibili.com/video/BV1Ay4y1z7a5
R基团定义	https://www.bilibili.com/video/BV1654y1r7be
原子锁定与环锁定	https://www.bilibili.com/video/BV175411V77h
G Group与通用原子	https://www.bilibili.com/video/BV1fy4y1B7LU
原子属性列表	https://www.bilibili.com/video/BV1uD4y1R7K2
盐，自由基，同位素	https://www.bilibili.com/video/BV1Rr4y1c7AL

一些简单案例视频

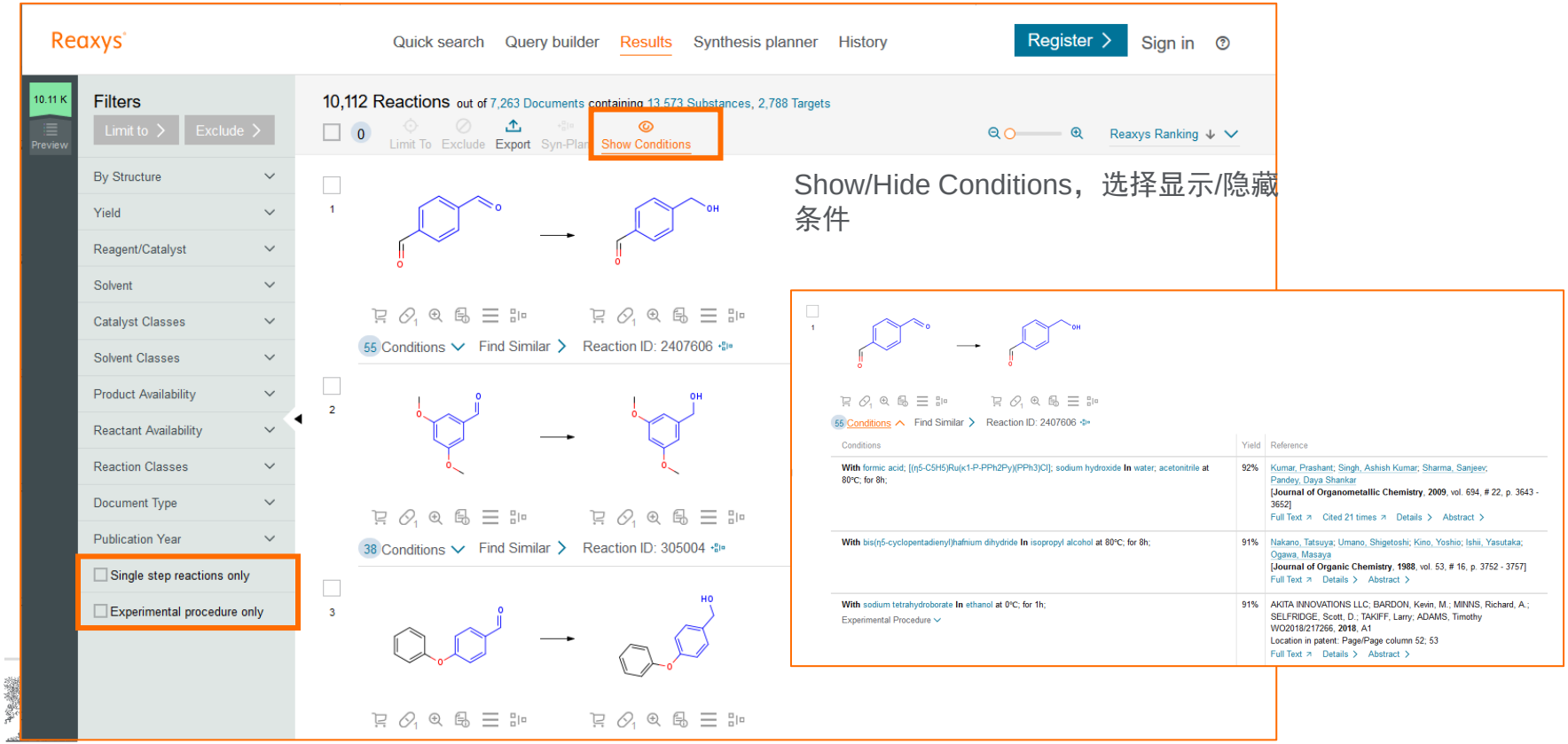
常用功能	视频链接
合成计划的制作	https://www.bilibili.com/video/BV1Ni4y1L7Lt
机理性文献查询	https://www.bilibili.com/video/BV1pK4y1E7Qx
反应定义基本操作	https://www.bilibili.com/video/BV19r4y1w7Z5
反应条件的定义	https://www.bilibili.com/video/BV1Af4y1q7xk

Case 5：Reaxys中最简单的反应定义与筛选

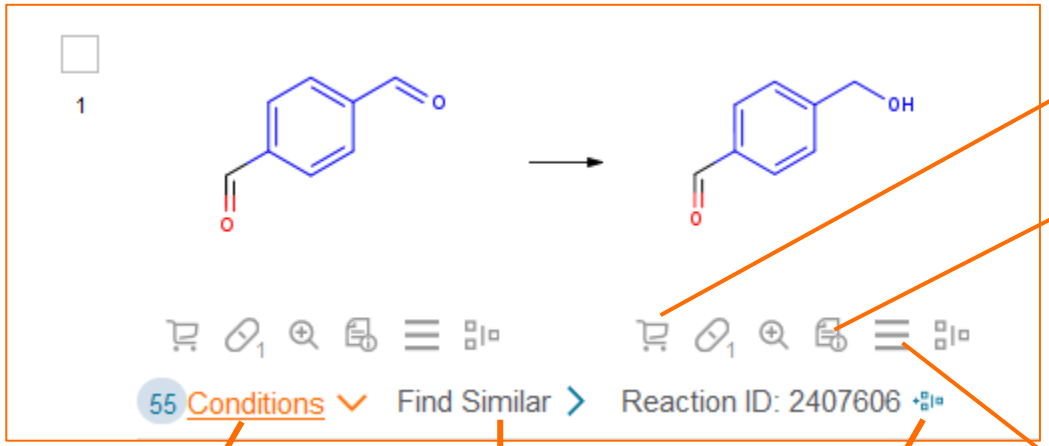
- 检索以下核心结构反应并进行反应筛选操作
- 视频操作过程
  - https://www.bilibili.com/video/BV1BT4y1F7vT



Reaxys中的结果

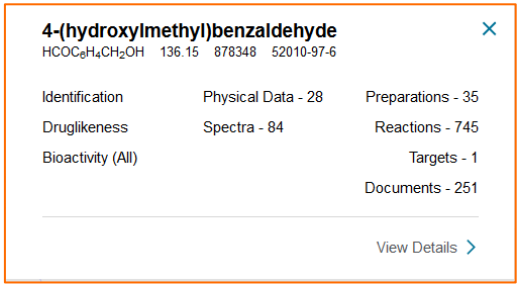

Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Register
Sign in
10.11 K
Preview
Filters
Limit to
Exclude
10,112 Reactions out of 7,263 Documents containing 13,573 Substances, 2,788 Targets
Limit To
Exclude
Export
Syn-Plan
Show Conditions
Reaxys Ranking
By Structure
Yield
Reagent/Catalyst
Solvent
Catalyst Classes
Solvent Classes
Product Availability
Reactant Availability
Reaction Classes
Document Type
Publication Year
Single step reactions only
Experimental procedure only
55 Conditions
Find Similar
Reaction ID: 2407606
38 Conditions
Reaction ID: 305004
Show/Hide Conditions，选择显示/隐藏条件
Conditions
Yield
Reference
With formic acid; [(η5-C5H5)Ru(κ1-P-PPh2Py)(PPh3)Cl]; sodium hydroxide In water; acetonitrile at 80°C; for 8h;
92%
Kumar, Prashant; Singh, Ashish Kumar; Sharma, Sanjeev; Pandey, Daya Shankar
[Journal of Organometallic Chemistry, 2009, vol. 694, # 22, p. 3643 - 3652]
Full Text
Cited 21 times
Details
Abstract
With bis(η5-cyclopentadienyl)hafnium dihydride In isopropyl alcohol at 80°C; for 8h;
91%
Nakano, Tatsuya; Umano, Shigetoshi; Kino, Yoshio; Ishii, Yasutaka; Ogawa, Masaya
[Journal of Organic Chemistry, 1988, vol. 53, # 16, p. 3752 - 3757]
With sodium tetrahydroborate In ethanol at 0°C; for 1h;
Experimental Procedure
91%
AKITA INNOVATIONS LLC; BARDON, Kevin, M.; MINNS, Richard, A.; SELFRIDGE, Scott, D.; TAKIFF, Larry; ADAMS, Timothy
WO2018/217266, 2018, A1
Location in patent: Page/Page column 52; 53

Reaxys的一条反应的界面



查看商业来源

查看物质详情

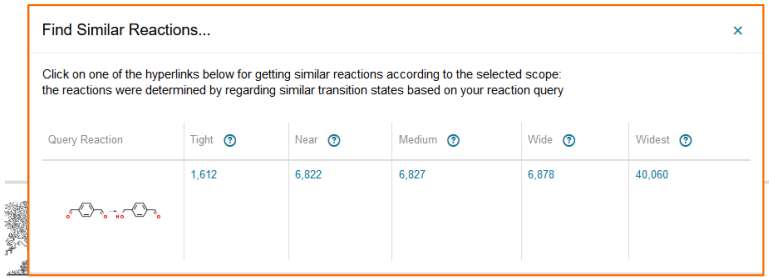


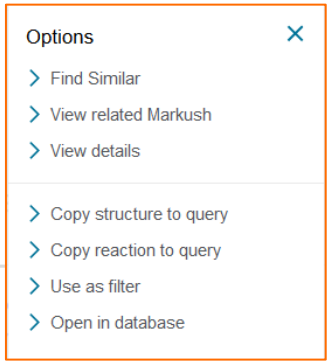
查看条件

寻找相似反应

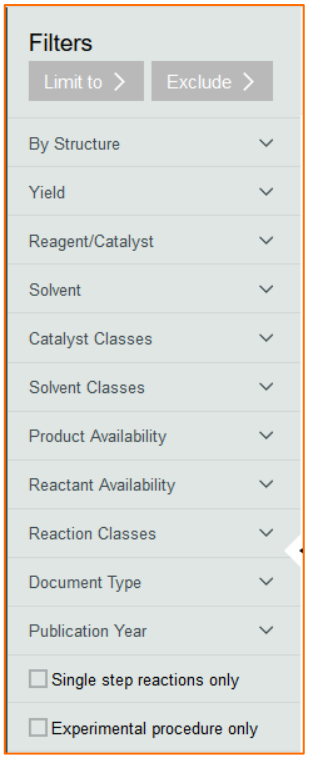
合成计划按钮

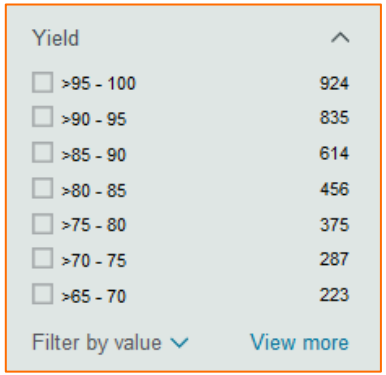
更多与物质相关操作

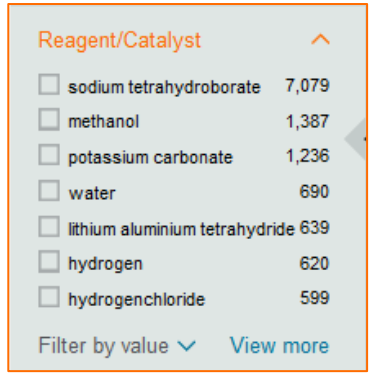


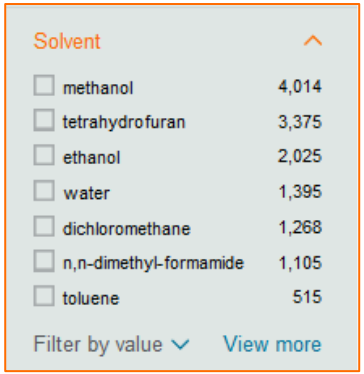


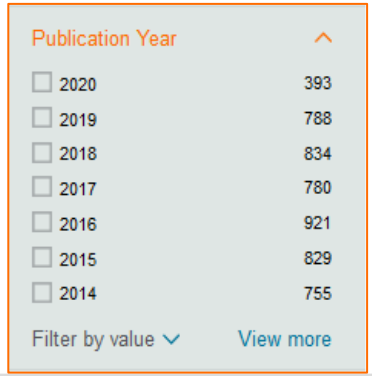
Reaxys的筛选操作









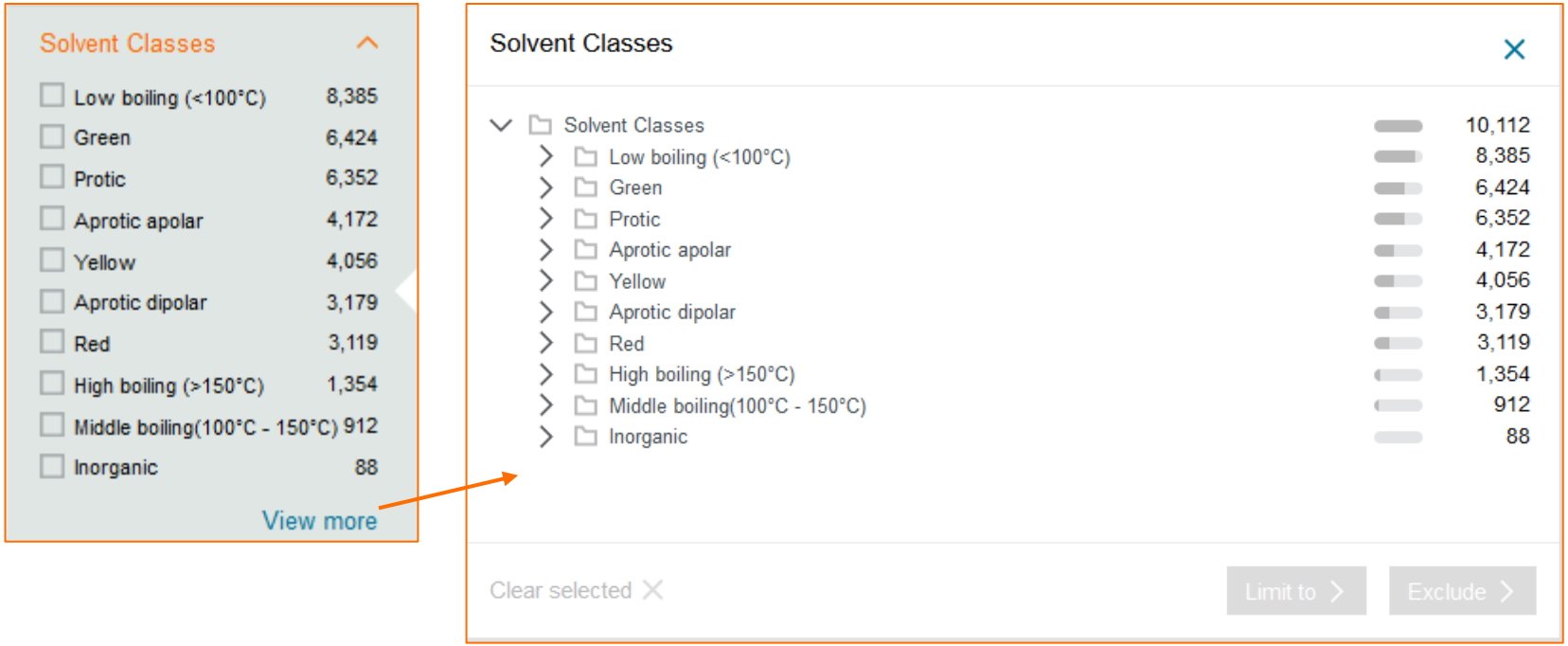


Tips:

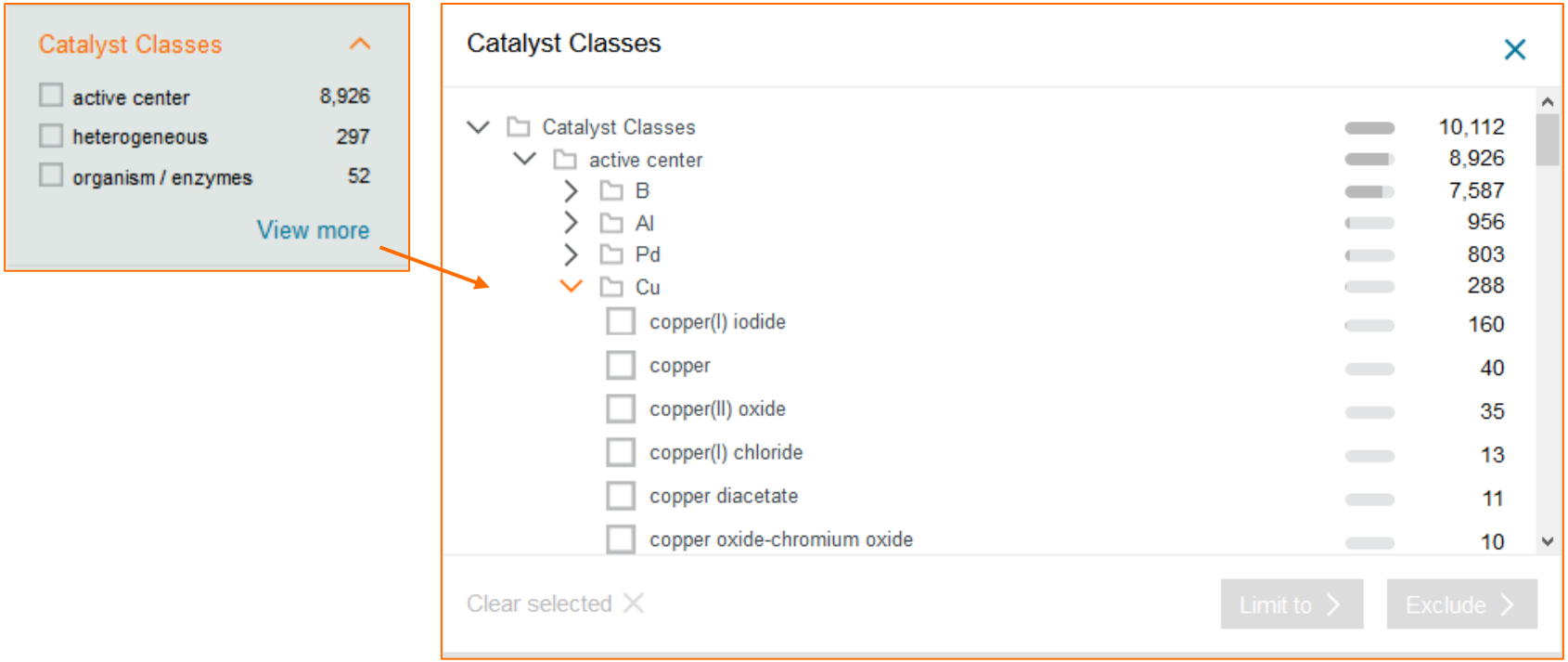
常见的一些反应筛选工具，如:收率，催化剂/试剂，溶剂，文献类型，出版年限等

ELSEVIER

Reaxys中的一些特殊筛选工具—溶剂分类



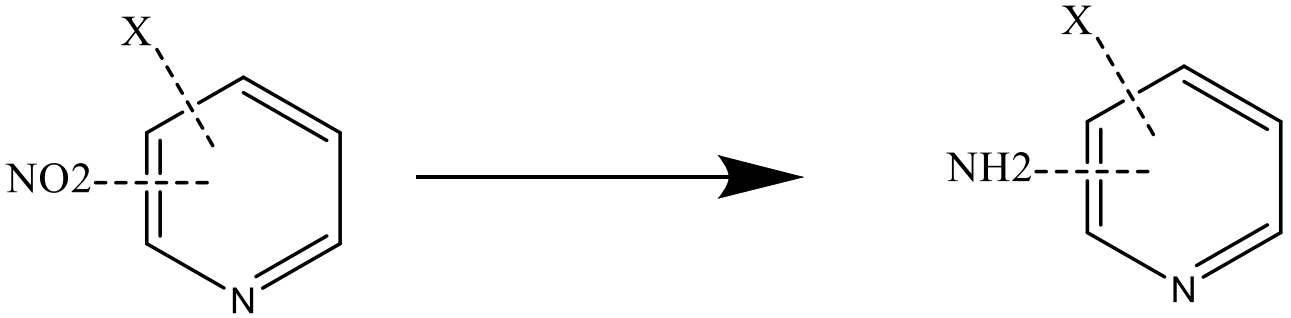
Reaxys中的一些特殊筛选工具—催化剂分类



ELSEVIER

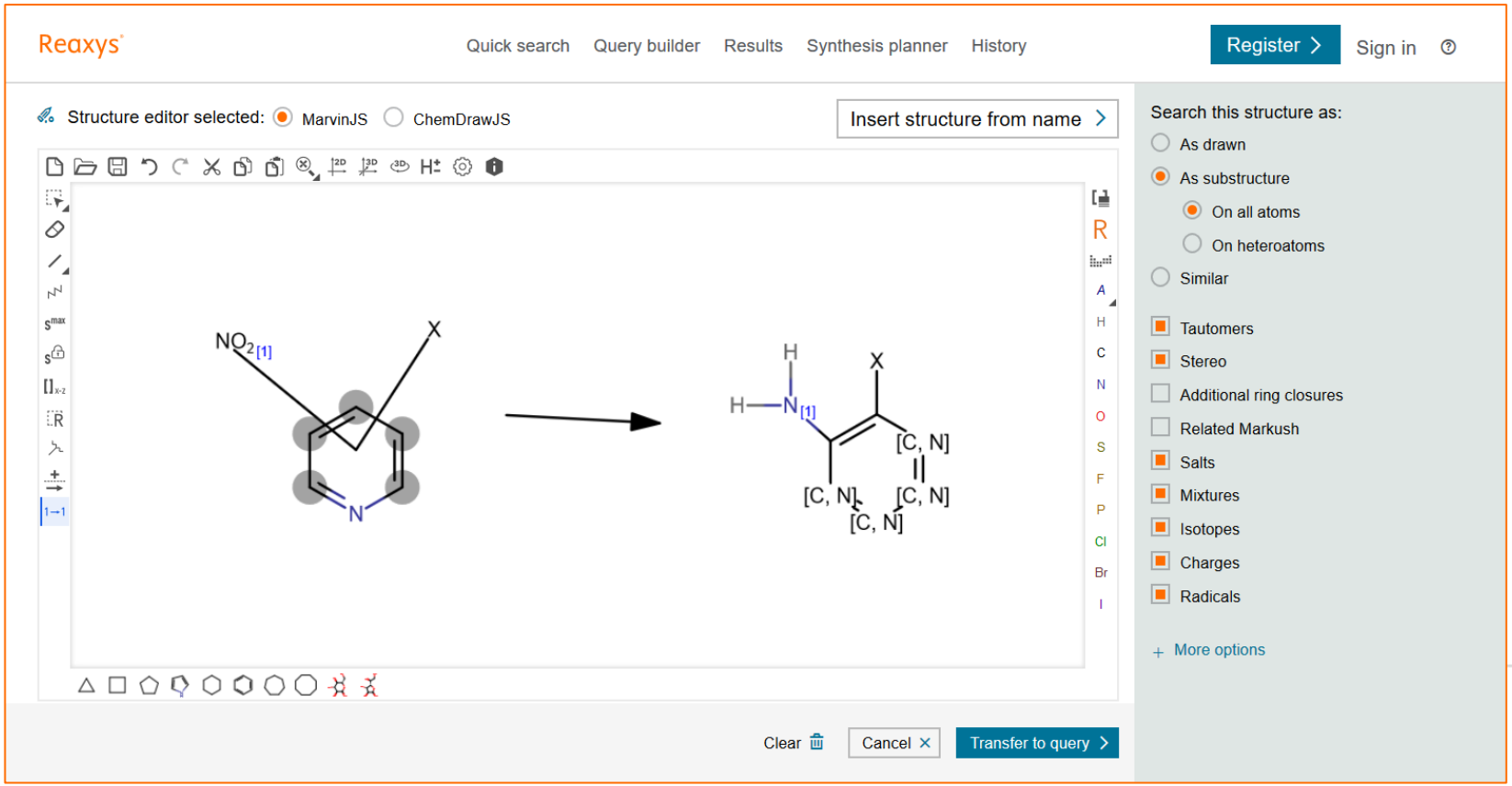
Case 6：结构中有特殊需求的反应定义

- 检索以下反应
  - 吡啶环上存在一个硝基，一个卤素，且这两个官能团处于邻位
  - 反应过后硝基还原成氨基
  - 定义难点：如果确保NO2和卤素处于邻位

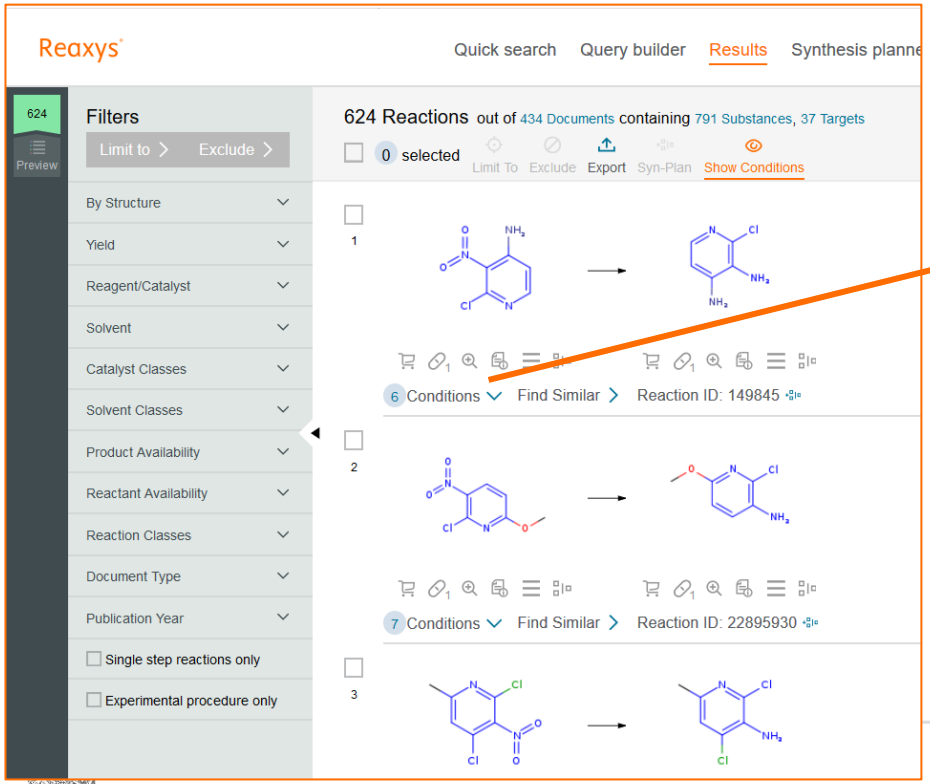


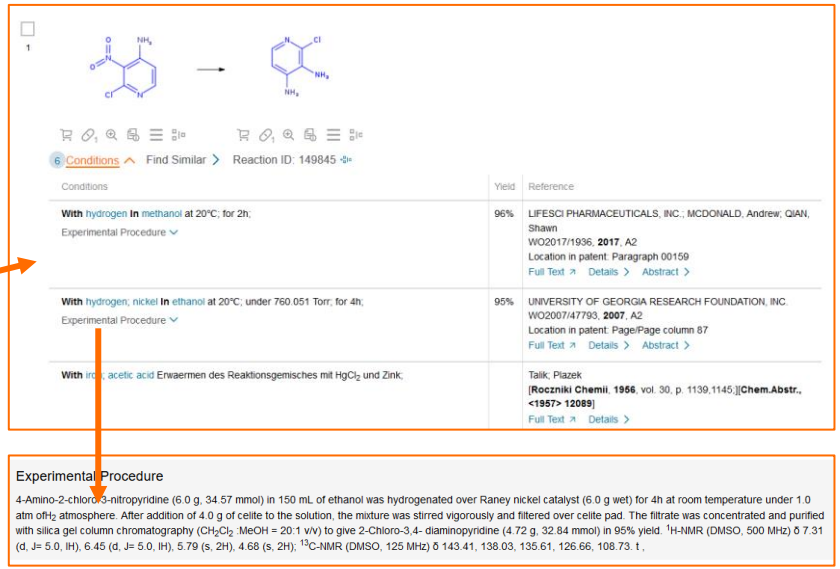
视频操作过程：
https://www.bilibili.com/video/BV1si4y177as

Reaxys中的结构定义



最后的结果



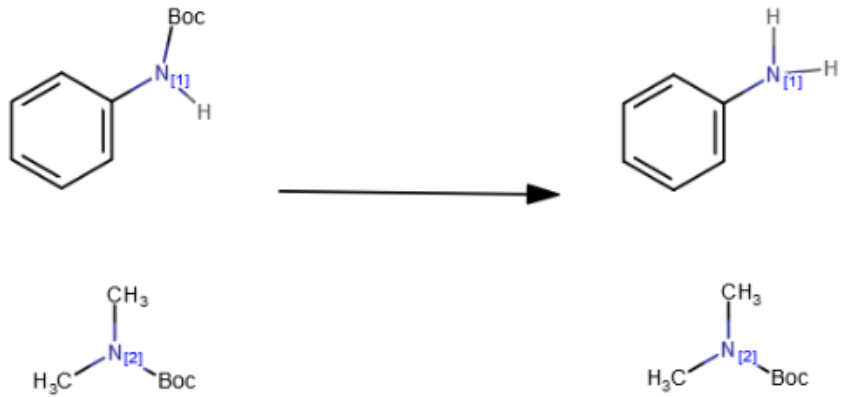


Reaxys将相同scheme的反应全部整合成1条反应，在同样的反应下列举不同的反应条件。

ELSEVIER

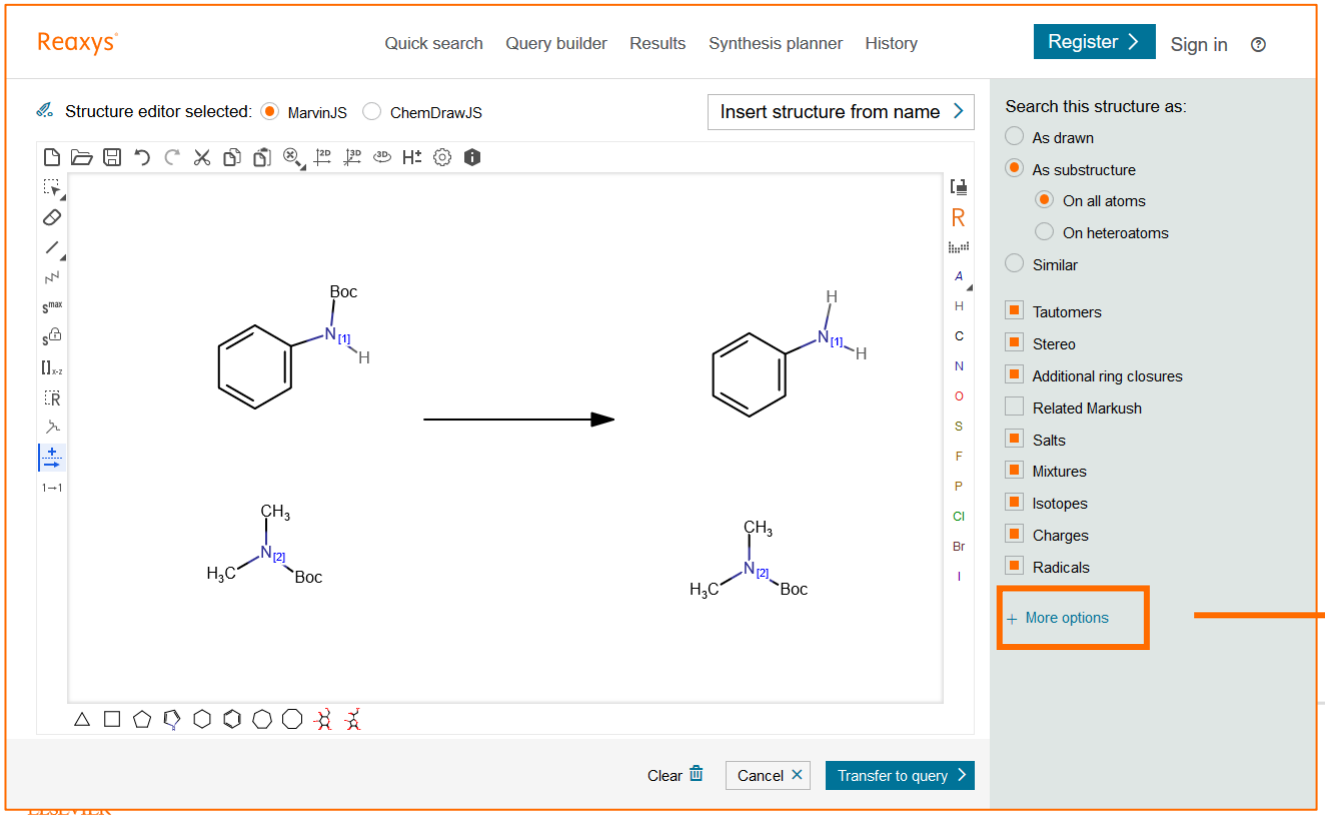
Case 7：选择性氧化还原脱保护反应的定义

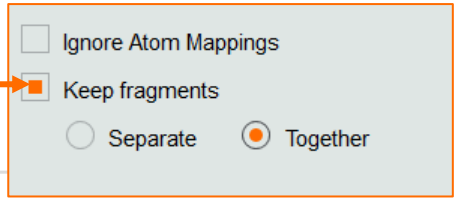
- 结构中两个带Boc的片段，两个片段以任意的形式相接在一个分子中
- 反应过后把其中一个片段的Boc脱掉，但是另外一个Boc不变



视频操作过程：
https://www.bilibili.com/video/BV1Vv411r7Bc

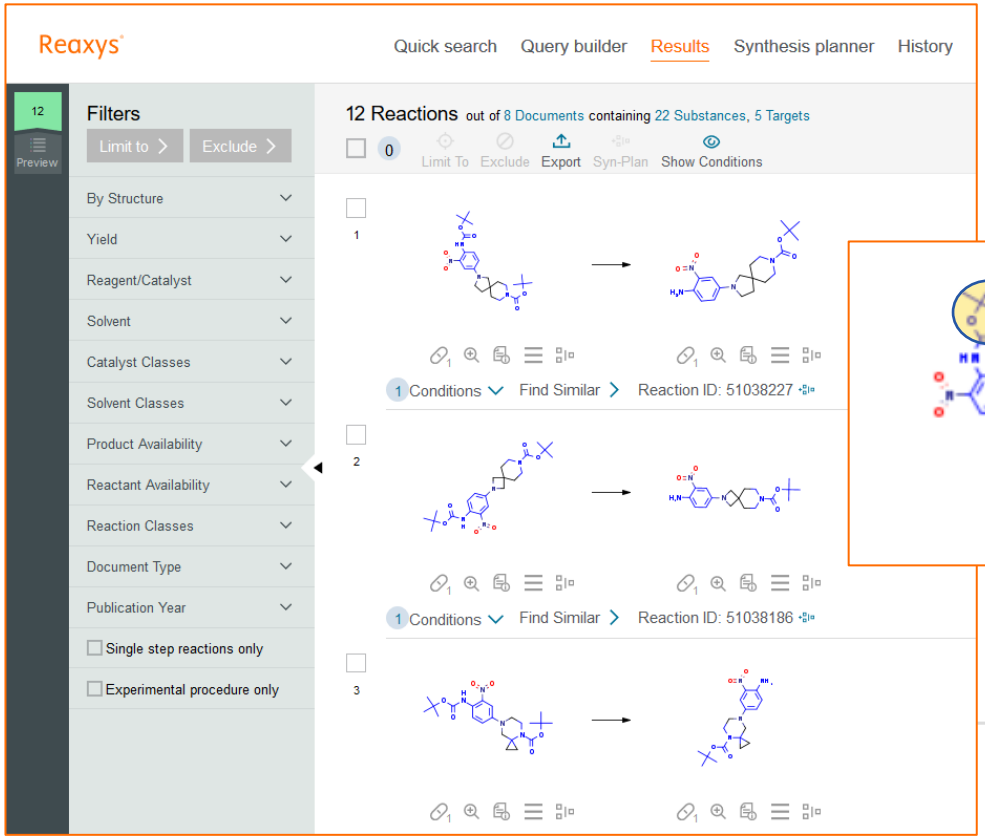
Reaxys中的结构定义

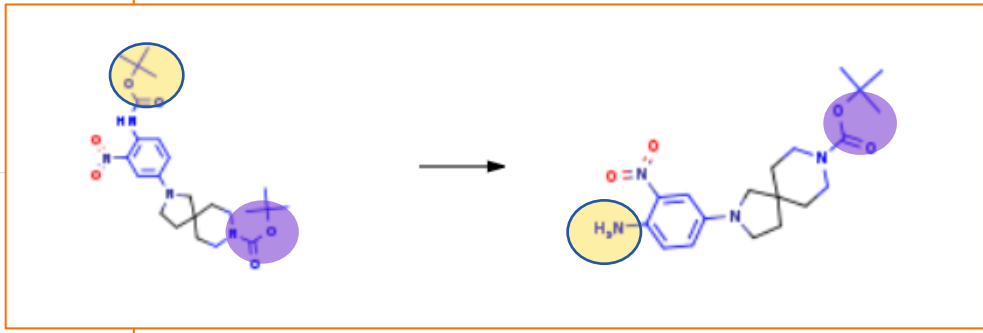




Reaxys可以直接设定这些片段在一个结构中

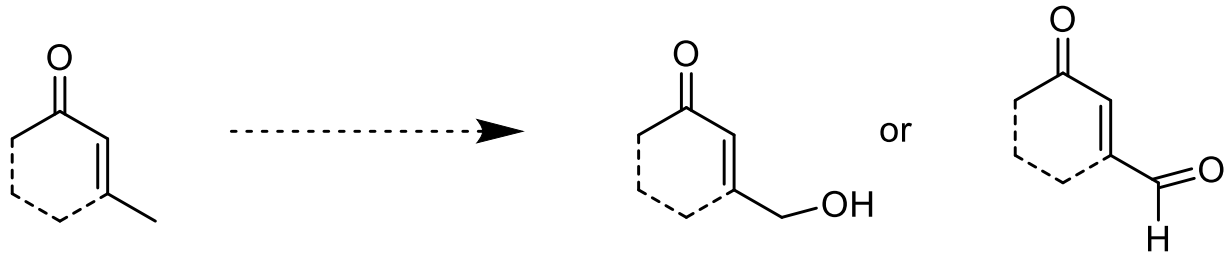
Reaxys中结果


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
12
Preview
Filters
Limit to
Exclude
By Structure
Yield
Reagent/Catalyst
Solvent
Catalyst Classes
Solvent Classes
Product Availability
Reactant Availability
Reaction Classes
Document Type
Publication Year
Single step reactions only
Experimental procedure only
12 Reactions out of 8 Documents containing 22 Substances, 5 Targets
0
Limit To
Exclude
Export
Syn-Plan
Show Conditions
1
1 Conditions
Find Similar
Reaction ID: 51038227
2
1 Conditions
Find Similar
Reaction ID: 51038186
3



Case 8：涉及环系变化的反应定义

- 获取以下反应

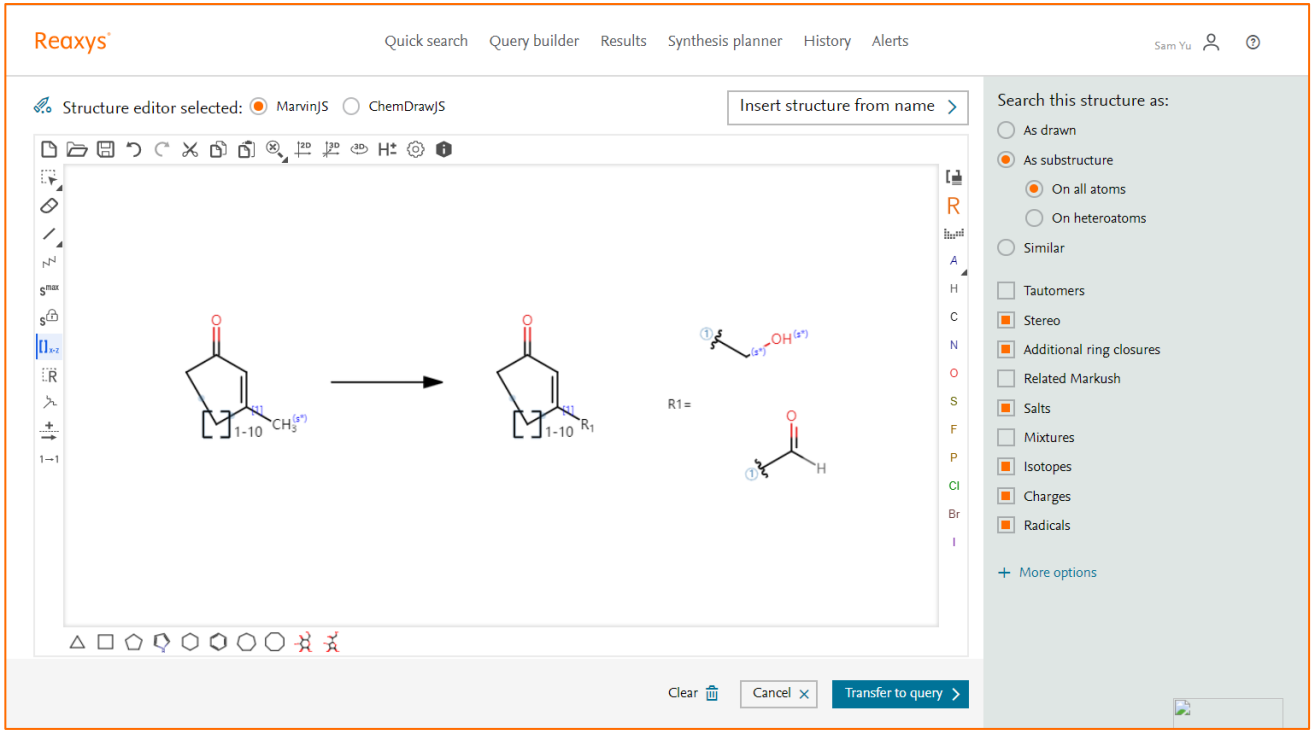


Requirement:

- 虚线部分是大于5个C原子的环
- 结构中不能发生互变异构
- 产物的CH2OH，CHO是有底物的CH3变化过来
- 视频操作（结构类似）：

https://www.bilibili.com/video/BV1gv411r7oc

Reaxys中的定义

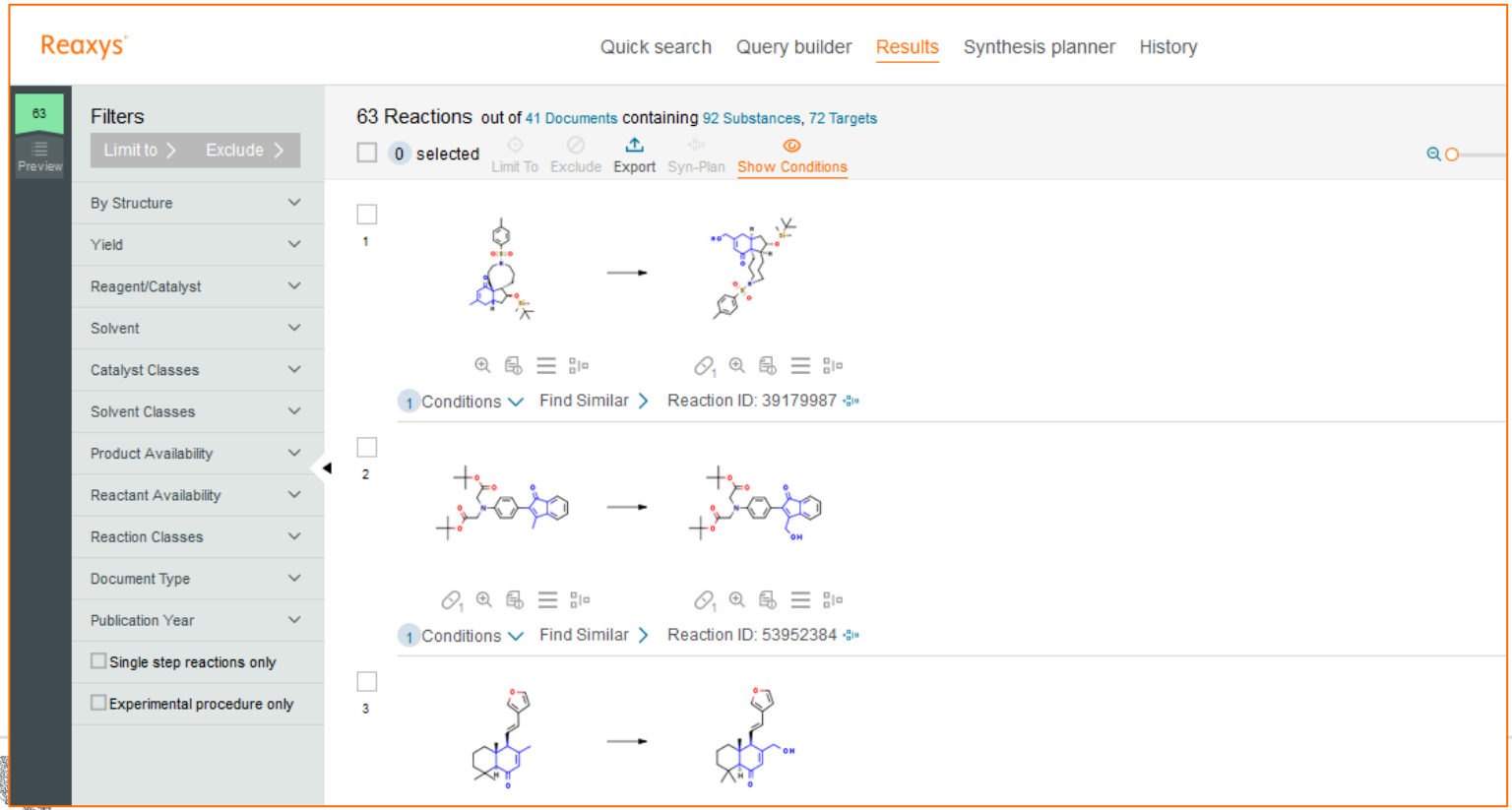


定义方法：

- R基团定义工具，定义侧链
- S*定义侧链CH2OH，以及底物CH3无取代
- 重复基团定义工具，定义环的大小
- 无互变异构

ELSEVIER

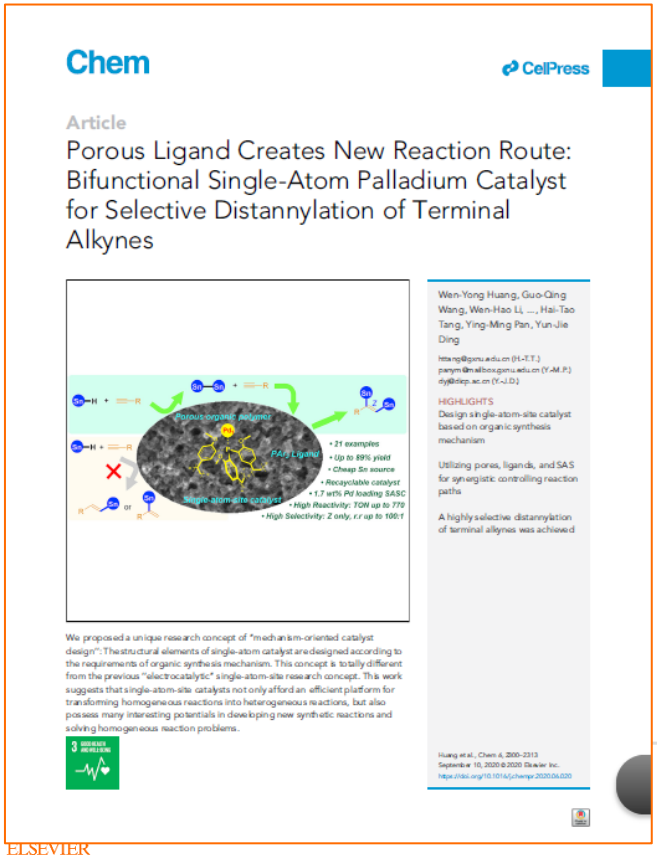
最后的结果



Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
  - Reaxys对文献的提炼
  - Reaxys中物质与物性数据获取反向检索
  - Reaxys中结构面板与反应数据获取
  - Reaxys中的实用小案例
- Q&A

Case 9：化合物的文献定位


Chem

CellPress

Article

Porous Ligand Creates New Reaction Route: Bifunctional Single-Atom Palladium Catalyst for Selective Distannylation of Terminal Alkynes

Wen-Yong Huang, Guo-Qing Wang, Wen-Hao Li, ..., Hai-Tao Tang, Ying-Ming Pan, Yun-Jie Ding

HIGHLIGHTS

Design single-atom-site catalyst based on organic synthesis mechanism

Utilizing pores, ligands, and SAS for synergistic controlling reaction paths

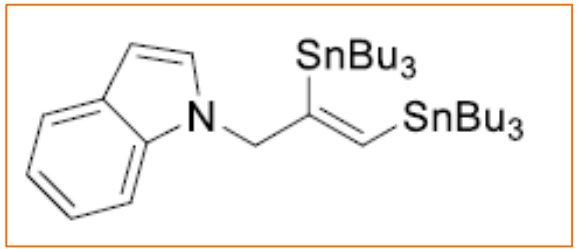
A highly selective distannylation of terminal alkynes was achieved

We proposed a unique research concept of "mechanism-oriented catalyst design": The structural elements of single-atom catalyst are designed according to the requirements of organic synthesis mechanism. This concept is totally different from the previous "electrocatalytic" single-atom-site research concept. This work suggests that single-atom-site catalysts not only afford an efficient platform for transforming homogeneous reactions into heterogeneous reactions, but also possess many interesting potentials in developing new synthetic reactions and solving homogeneous reaction problems.

这是一篇常见的化学文献，包含：

1. 15页PDF全文
2. 52页Support Information文档

已知文献中报道了这个化合物，如何在上述的67页文档中找到有关这个化合物的描述？

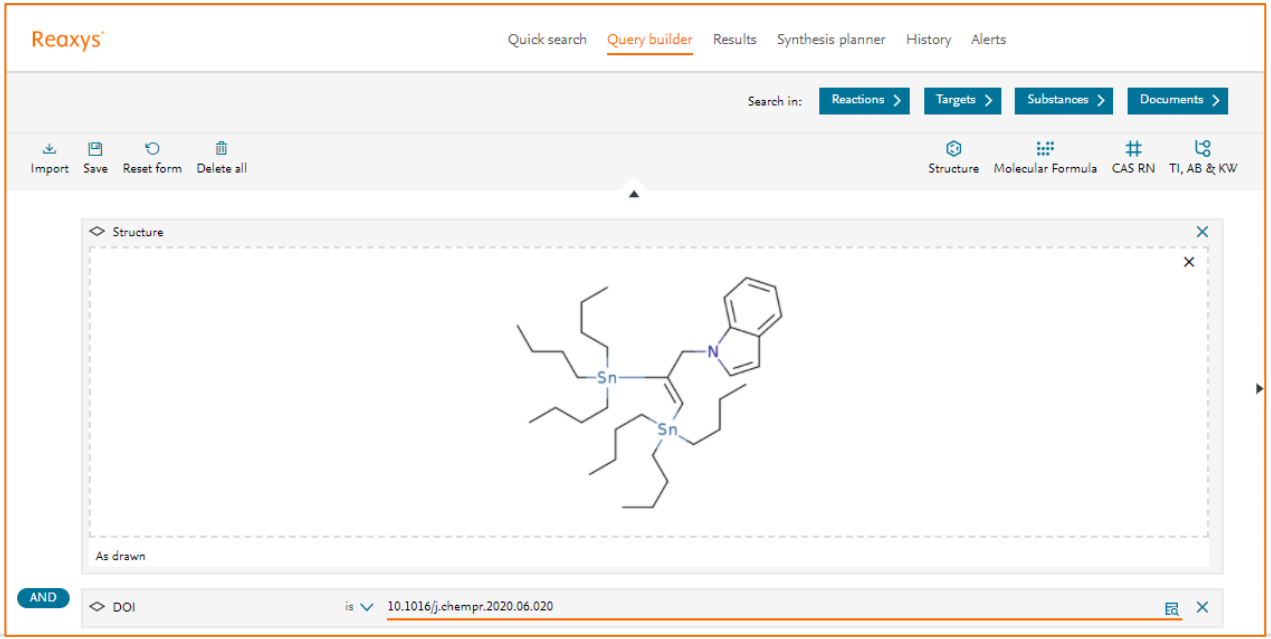


视频操作过程：

https://www.bilibili.com/video/BV1gA411x7KE

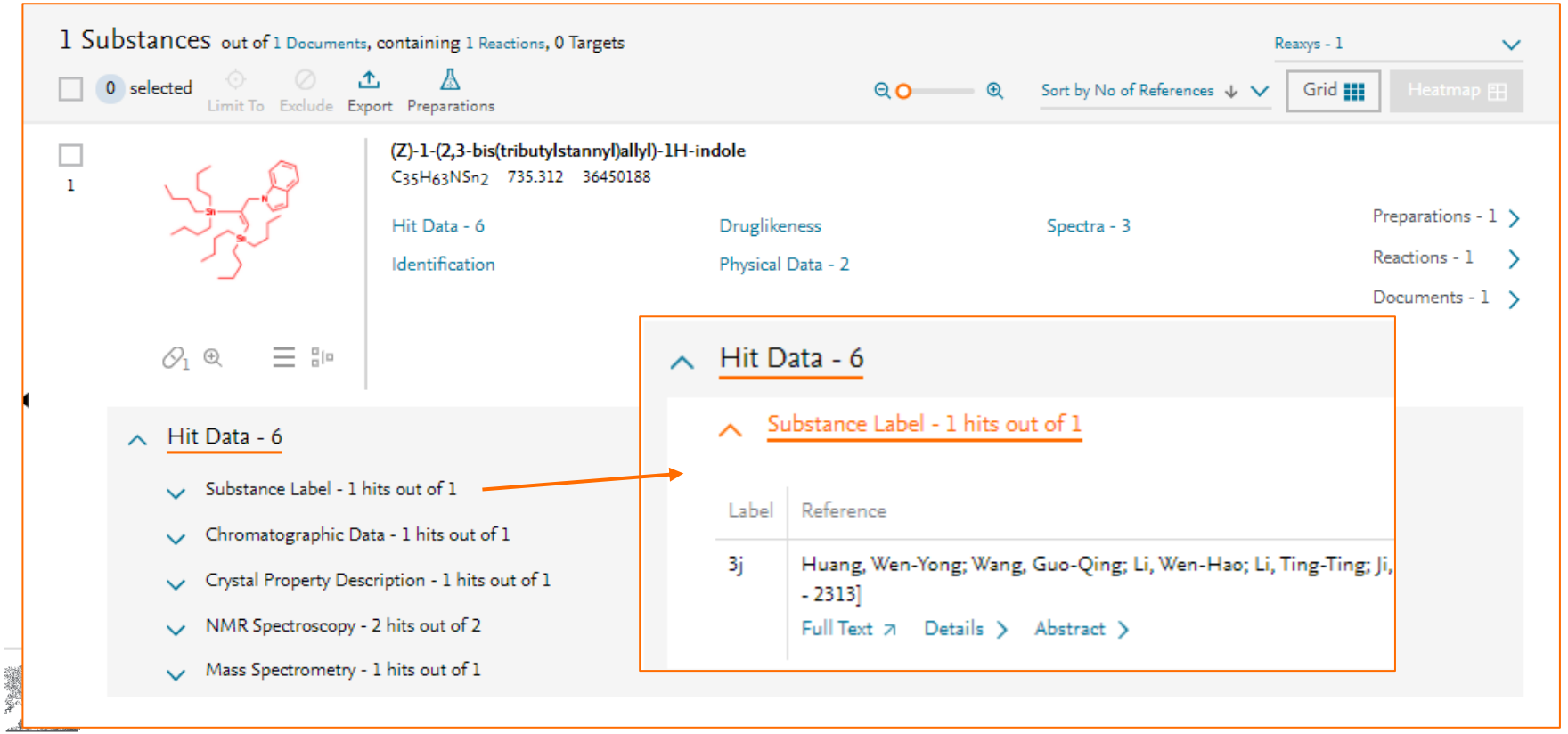
Reaxys中的检索

- Query Builder联合化合物结构与文献DOI号



ELSEVIER

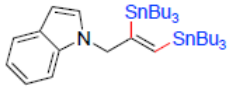
Reaxys中的结果



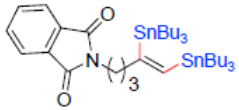
ELSEVIER

全文检索3J定位化合物

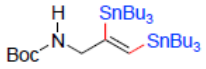
N-containing terminal alkynes



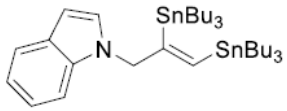
3j 89% (100:1)



3k 58% (25:1)



3n 81% (100:1)



(*Z*)-1-(2,3-bis(tributylstannyl)allyl)-*1H*-indole 3j: colorless oil. Petroleum ether as eluent for column chromatography (**3j**, R_f = 0.75; **2j**, R_f = 0.4, 42% of alkyne was isolated and recovered); ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.52 (1H, d, *J* = 7.8 Hz), 7.15 (1H, d, *J* = 8.2 Hz), 7.08-7.03 (1H, m), 7.01-6.95 (1H, m), 6.93 (1H, d, *J* = 3.1 Hz), 6.46 (1H, s, *J* = 168.4 Hz, 65.5 Hz), 6.40 (1H, d, *J* = 3.1 Hz), 4.78 (2H, d, *J* = 1.3 Hz), 1.40-1.25 (12H, m), 1.22-1.14 (12H, m), 0.88-0.72 (30H, m). ^{13}C NMR (400 MHz, $CDCl_3$) δ = 160.6, 144.4, 1
60.1, 29.2, 29.1, 27.4, 27.3, 13
$C_{35}H_{63}KNSn_2[M+K]^+$ 774.2630,

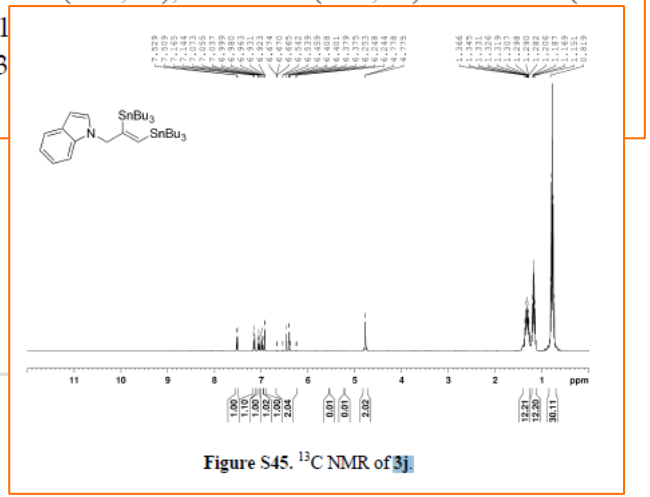
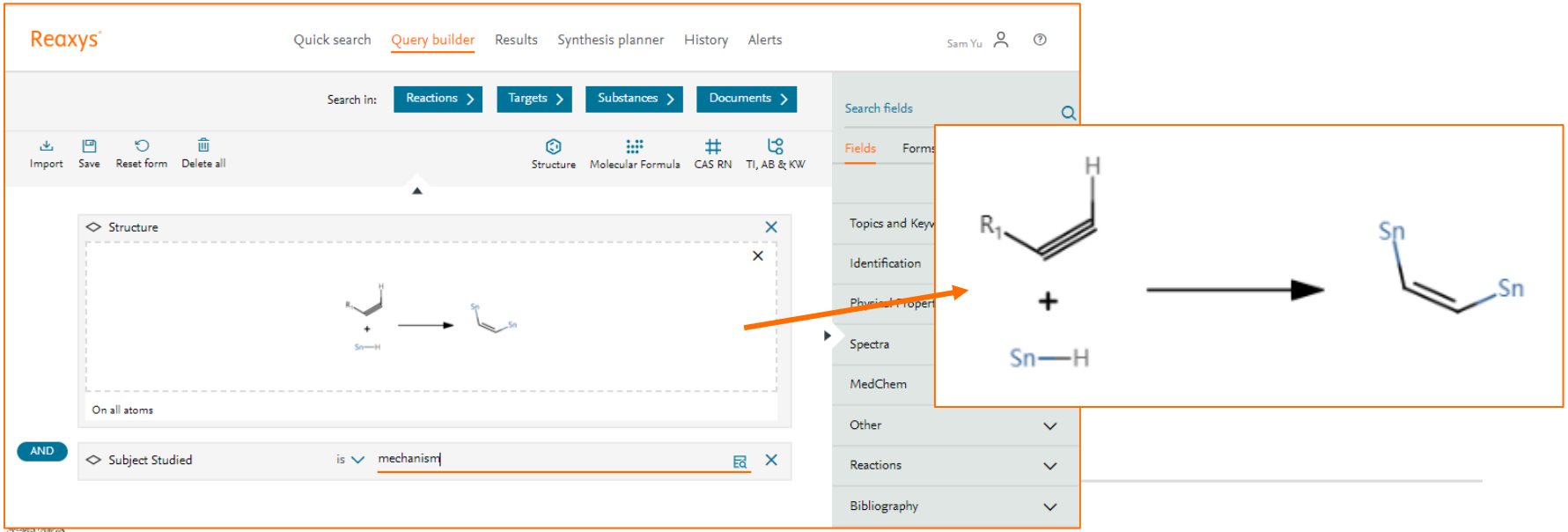


Figure S45. ^{13}C NMR of **3j**.

用于文献中化合物信息的快速定位。

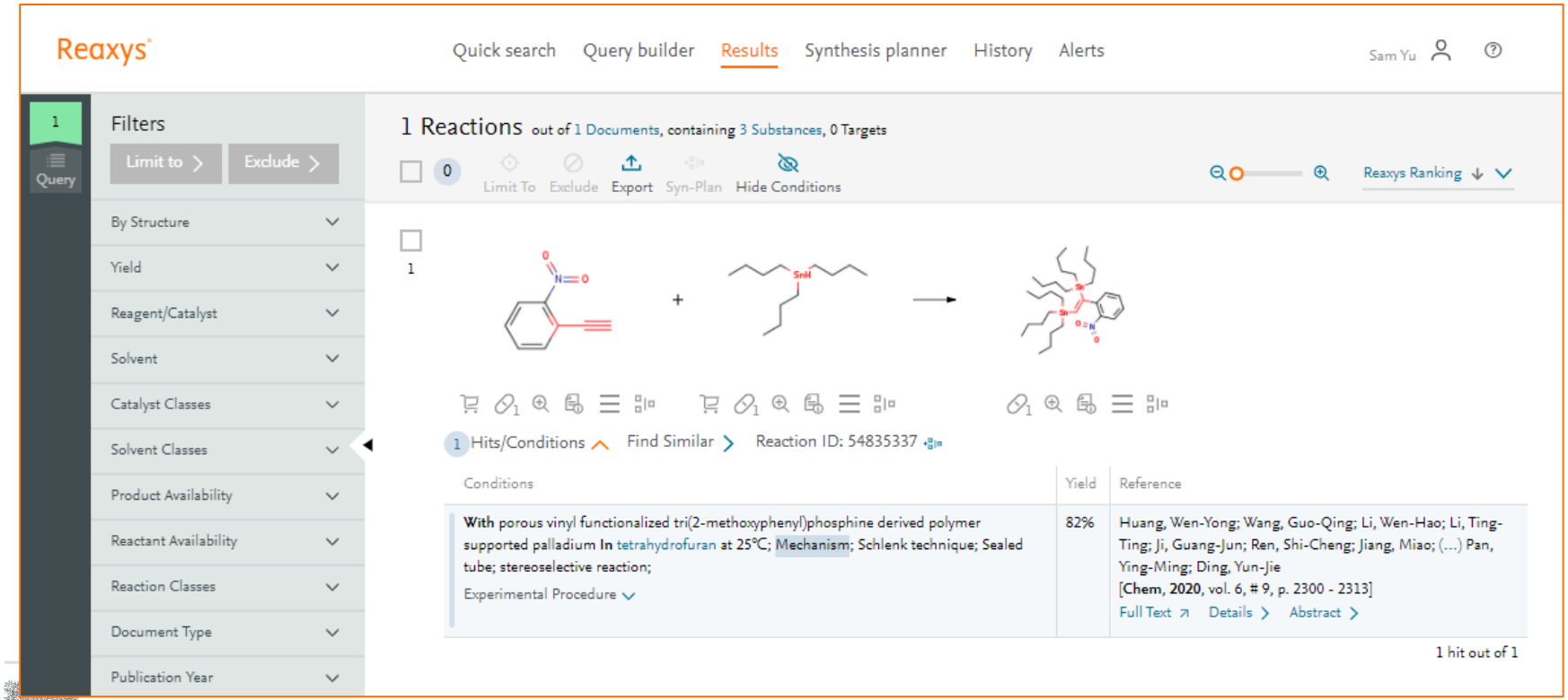
Case 10：机理性文献的检索

- Query Builder中结构与Subject Study联合检索
- 视频操作：https://www.bilibili.com/video/BV1pK4y1E7Qx



ELSEVIER

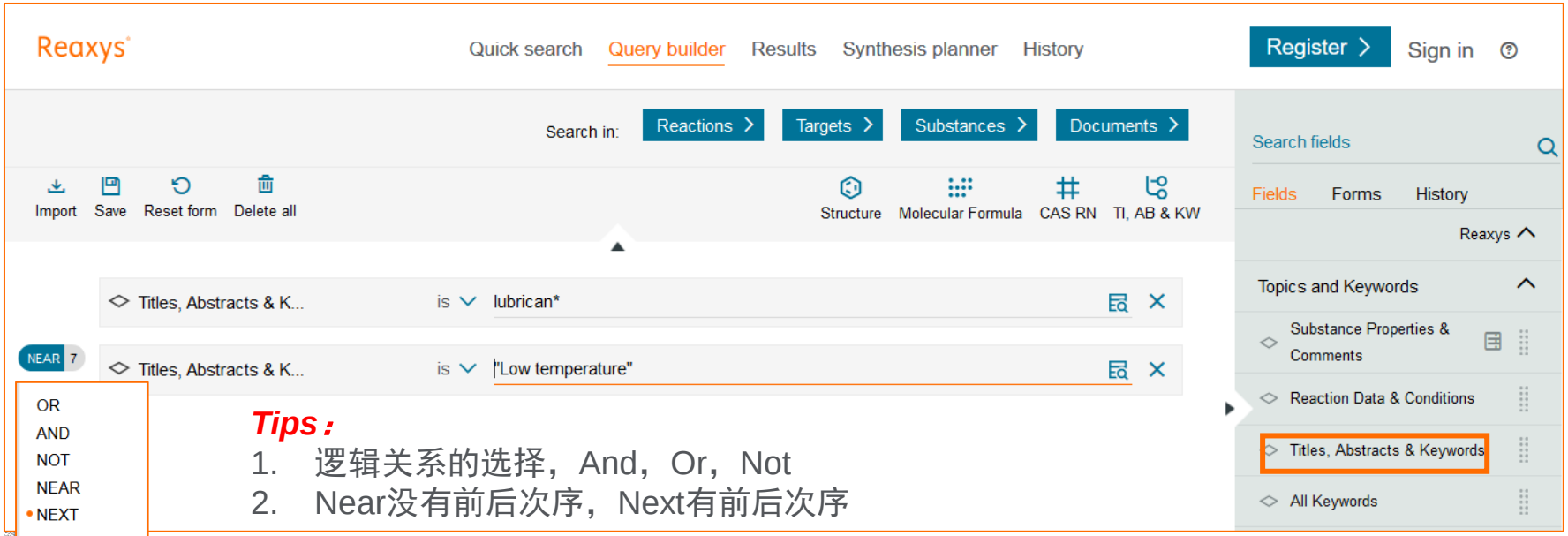
最后的结果



ELSEVIER

Case 11：文献关键词检索时词语之间距离的设定

- 希望在主题，摘要，关键词中进行检索低温润滑剂的文献
- Low temperature与lubricant两单词之间距离小于7

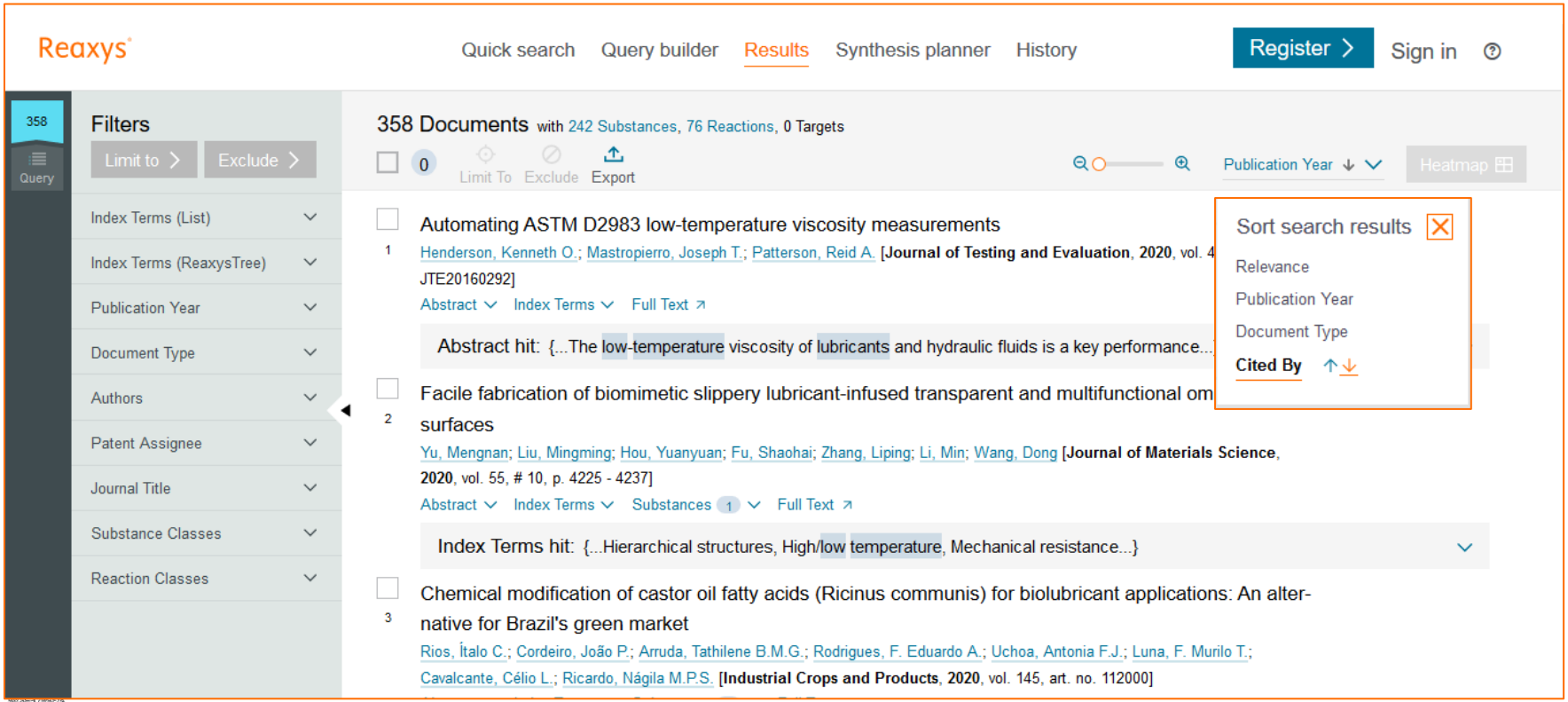


Tips：

1. 逻辑关系的选择，And，Or，Not
2. Near没有前后次序，Next有前后次序

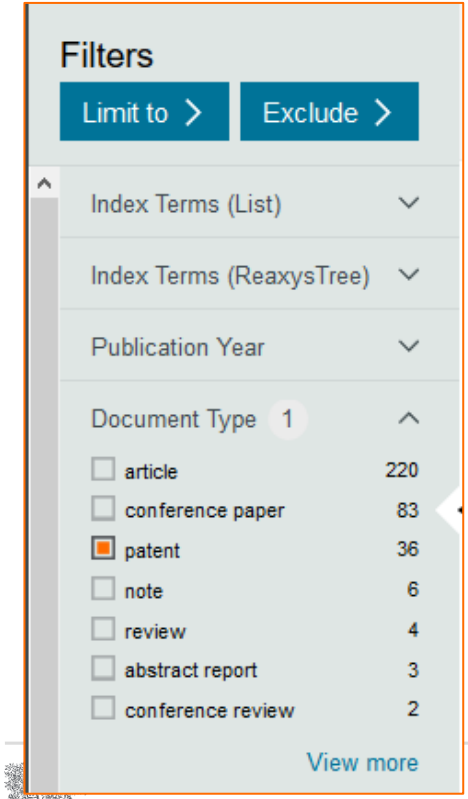
ELSEVIER

Reaxys中的结果



ELSEVIER

Reaxys中的专利的筛选



ELSEVIER

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
  - Reaxys对文献的提炼
  - Reaxys中物质与物性数据获取反向检索
  - Reaxys中结构面板与反应数据获取
  - Reaxys中的实用小案例
- Q&A

Reaxys小结

- 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
- 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
- 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
- Elsevier Life Science线上服务：
  - 关注B站Up主：ELS生命科学，获取所有Elsevier Life Science数据库的使用视频
  - 添加Elsevier Life Science小助手微信号：ELS-LSS，邀请进Elsevier Life Science用户群，获取最新资料分享以及使用Q&A

请就今天的培训
进行问卷调查

ELSEVIER

ELSEVIER

Thank you