Elsevier
Reaxys中化学信息的获取

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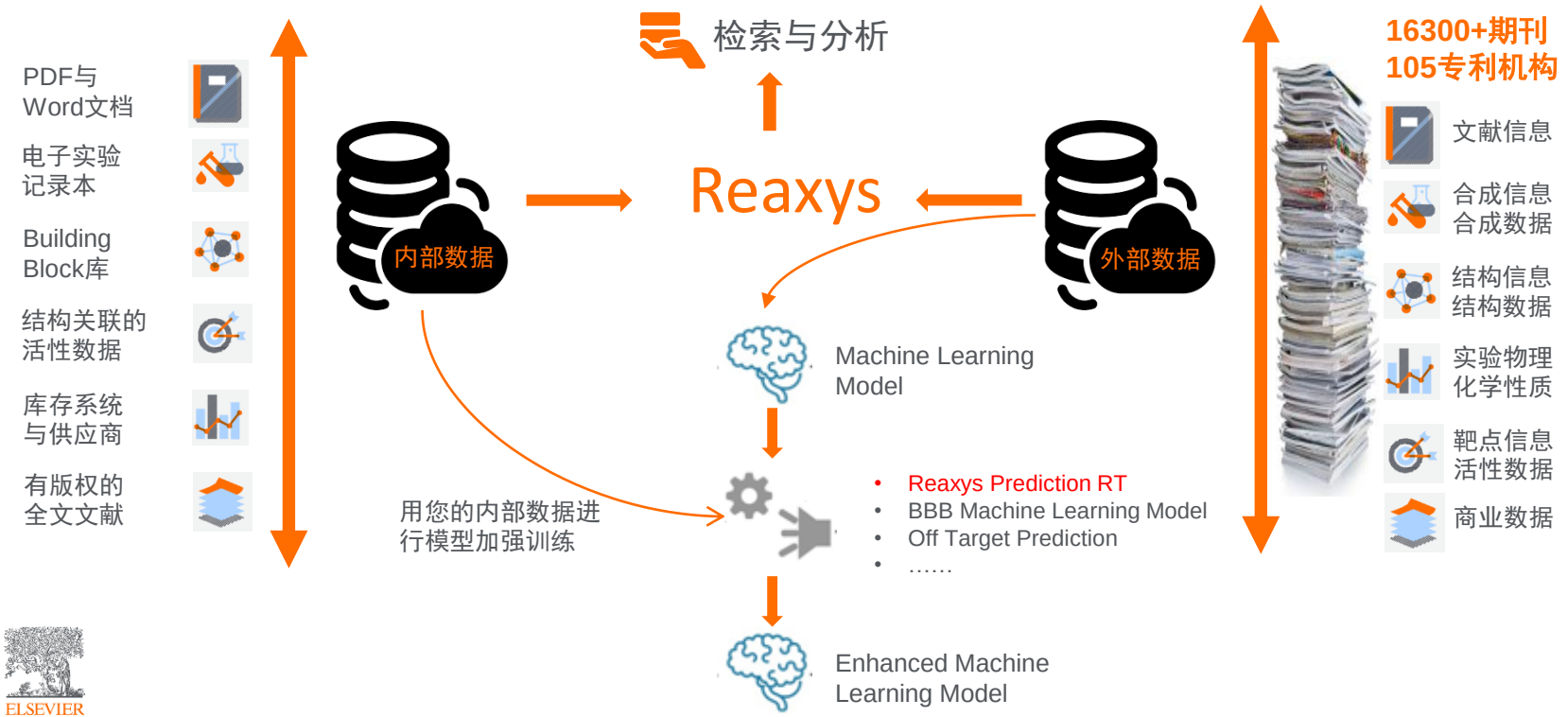
Agenda

- Reaxys介绍与内容
  - Reaxys介绍
  - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
  - Reaxys中的关键词检索
  - Reaxys中物质理化性质数据的查询与反向物质获取
  - Reaxys中结构面板与物质结构和反应数据的获取
  - Reaxys中的实用小案例
- Q&A

Reaxys—从科学数据到数据科学的跨越

Reaxys是Elsevier旗下Life Science产品线中基于数据深度提炼与挖掘，且可以整合内部与外部化学相关学科科学数据的信息检索，分析，数据科学应用平台。



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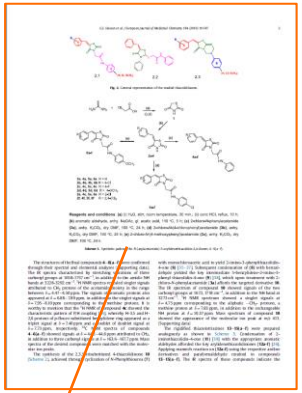
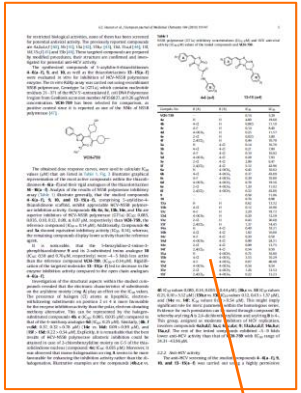
Reaxys对药学与化学文献中的科学数据的提炼


European Journal of Medicinal Chemistry

Anti-hepatitis-C virus activity and QSAR study of certain thiazolidinone and thiazolotriazine derivatives as potential NS5B polymerase inhibitors





实验过程

具体化合物描述

4.1.6. *2-(5-(2-Chlorobenzylidene)-2,4-dioxothiazolidin-3-yl)-N-phenylacetamide (4e)*

Yield: (3.36 g) 90%. m.p. 227–229 °C. R_f: 0.31. IR υ cm^{-1}: 3271 (NH), 1751, 1697, 1666 (C=O), 763 (C–Cl). ^1H NMR δ *ppm*: 4.54 (s, 2H, CH_2), 7.07 (t, 1H, *J* = 7.40 Hz, H-4 phenyl), 7.31 (t, 2H, *J* = 7.94 Hz, H-3,5 phenyl), 7.54–7.58 (m, 4H, H-3,4,5,6 benzylidene), 7.64–7.69 (m, 2H, H-2,6 phenyl), 8.10 (s, 1H, C=CH), 10.41 (s, 1H, NH, exch. D_2O). ^{13}C NMR δ *ppm*: 44.5 (CH_2), 119.6, 124.2, 125.2, 128.6, 129.2, 129.3, 129.5, 130.8, 131.3, 132.6, 134.9, 138.7 (C–Ar, C–S, C=CH), 164.1, 165.3, 167.3 (C=O). MS (*m/z*, %): 372 (M^+, 76), 374 (M^++2, 30), 93 (100). Anal. Calcd. for $C_{18}H_{13}ClN_2O_3S$ (372.83): C, 57.99; H, 3.51; N, 7.51. Found: C, 58.23; H, 3.48; N, 7.37.

4.1.1. 2-(5-Un/substitutedbenzylidene-2,4-dioxothiazolidin-3-yl)-N-un/substitutedphenyl acetamide 4a-f, 5a-f, 6a-f

A solution of the appropriate benzylidene thiazolidindione (**2a-f**) (10 mmol) and anhydrous potassium carbonate (0.69 g, 5 mmol) in dry DMF (20 mL), was stirred at 100 °C for 30 min. The corresponding 2-chloro *N*-un/sub phenyl acetamide (**3a-c**) (10 mmol) was added and stirring was continued at 100 °C for 24 h. The reaction mixture was poured onto crushed ice, the precipitated product was filtered off, dried and crystallized from ethanol.

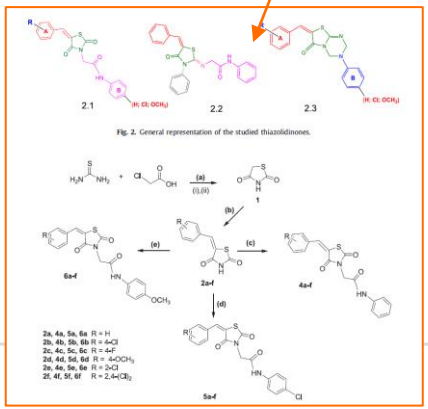
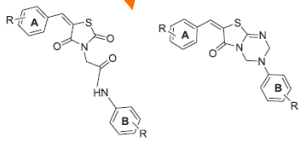

2.1 2.2 2.3

Fig. 2. General representation of the studied thiazolidinones.

2a, 4a, 5a, 6a R = H
2b, 4b, 5b, 6b R = 4-Cl
2c, 4c, 5c, 6c R = 4-F
2d, 4d, 5d, 6d R = 4-OCH_3
2e, 4e, 5e, 6e R = 2-Cl
2f, 4f, 5f, 6f R = 2,4-Cl_2

Table 1
NS5B polymerase (GT1a) inhibitory concentrations (IC_{50} μM) and HCV anti-viral activity (EC_{50} μM) values of the tested compounds and **VCH-759**.


4-6 (a-f)

13-15 (a-f)

Compds. No	R (A)	R (B)	IC_{50}	EC_{50}
VCH-759	–	–	0.14	5.29
4a	H	H	4.80	19.60
4b	4-Cl	H	0.085	11.10
4c	4-F	H	0.14	8.40
4d	4-OCH_3	H	0.25	11.57
4e	2-Cl	H	0.035	3.80
4f	2,4(Cl_2)	H	0.44	10.78
5a	H	4-Cl	0.14	16.70
5b	4-Cl	4-Cl	0.21	7.80

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。

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Reaxys对科学数据的提炼—题录，摘要，结构，反应

1

Anti-hepatitis-C virus activity and QSAR study of certain thiazolidinone and thiazolotriazine derivatives as potential NS5B polymerase inhibitors

Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [**European Journal of Medicinal Chemistry**, **2019**, vol. 184, art. no. 111747]

Abstract ^ Index Terms ^ Substances 71 v Reactions 59 v Targets v Full Text ↗

Abstract

The present study reports on evaluation of anti-HCV activity and QSAR of certain arylidenethiazolidinone derivatives as potential inhibitors of HCV-NS5B polymerase. The pursued compounds involving, 5-aryliden-3-arylacetamidothiazolidin-2,4-diones 4–6(a–f), 5-arylidine-2-(N-arylacetamido)-iminothiazolidin-4-one (10) and their rigid counterparts 5-arylidinethiazolotriazines 13–15(a–f), were synthesized and their structures confirmed by spectral and elemental analyses. The results of NS5B polymerase inhibition assay revealed compound 4e, as the most active inhibitor (IC_{50} = 0.035 μM), which is four folds greater than that of the reference agent, VCH-759, (IC_{50} = 0.14 μM). Meanwhile, compounds 4b, 4c, 5a, and 5c, and 13b, 14e and 15c displayed equipotency to 2 folds higher activity than VCH-759 (IC_{50} values: 0.085, 0.14, 0.14, 0.10, 0.12, 0.09 and 0.07 μM, respectively). Assessment of the anti-HCV activity (GT1a) using human hepatoma cell line (Huh-7.5) illustrates superior activity of 4e (EC_{50} = 3.80 μM) relative to VCH-759 (EC_{50} = 5.29 μM). Cytotoxicity evaluation on, Transformed normal cell lines (Human Liver Epithelial-2, THLE-2 and Proximal Tubular Epithelial, RPTEC/TERT1), demonstrate enhanced safety profile of 4e (CC_{50} = 102.77, 161.37 μM, respectively) compared to VCH-759 (CC_{50} = 61.83, 81.28 μM, respectively). Molecular docking of the synthesized derivatives to NS5B polymerase allosteric site (PDB: 2HWH) showed similar binding modes to that of the co-crystallized ligand. Moreover, QSAR models were established for the studied thiazolidinones and thiazolotriazines to investigate the molecular characteristics contributing to the observed NS5B polymerase inhibition activity. The obtained results inspire further investigations of thiazolidinones and thiazolotriazine aiming at affording more potent, safe and orally active non-nucleoside NS5B polymerase inhibitors as anti-HCV drug candidates.

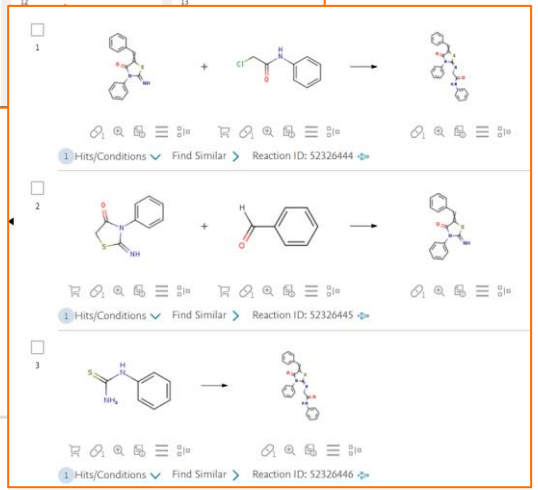
Index Terms

Author keyword: 2D QSAR, Anti-HCV, HCV-NS5B polymerase, Molecular docking, Thiazolidinones, Thiazolotriazines

EMTREE drug term: 2 (5 benzylidene 2,4 dioxothiazolidin 3 yl) n phenylacetamide, 2 (5 benzylidene 2,4 dioxothiazolidin 3 yl) n (4 chlorophenyl)acetamide, 2 (5 benzylidene 2,4 dioxothiazolidin 3 yl) n (4 methoxyphenyl)acetamide, 2 (5 benzylidene 4 oxo 3 phenylthiazolidin 2 ylideneimino) n phenylacetamide, 2 [5 (2 chlorobenzylidene) 2,4 dioxothiazolidin 3 yl] n (4methoxyphenyl)acetamide, 2 [5 (2 chlorobenzylidene) 2,4 dioxothiazolidin 3 yl] n phenylacetamide, 2 [5 (2 chlorobenzylidene) 2,4 dioxothiazolidin 3yl] n (4 chlorophenyl)acetamide, 2 [5 (2,4 dichlorobenzylidene) 2,4 dioxothiazolidin 3 yl) n (4 chlorophenyl)acetamide, 2 [5 (2,4 dichlorobenzylidene) 2,4 dioxothiazolidin 3 yl) n (4 methoxyphenyl)acetamide, 2 [5 (2,4 dichlorobenzylidene) 2,4 dioxothiazolidin 3 yl) n (4 methoxyphenyl)acetamide, 2 [5 (2,4 dichlorobenzylidene) 2,4 dioxothiazolidin 3 yl) n phenylacetamide, 2 [5 (4 chlorobenzylidene) 2,4 dioxothiazolidin 3 yl) n (4 chlorophenyl)acetamide, 2 [5 (4 chlorobenzylidene) 2,4 dioxothiazolidin 3 yl] n (4 methoxyphenyl)acetamide, 2 [5 (4 fluorobenzylidene) 2,4 dioxothiazolidin 3 yl) n (4 chlorophenyl)acetamide, 2 [5 (4 fluorobenzylidene) 2,4 dioxothiazolidin 3 yl) n (4 methoxyphenyl)acetamide, 2 [5 (4 fluorobenzylidene) 2,4 dioxothiazolidin 3 yl] n (4 chlorophenyl)acetamide, 2 [5 (4 fluorobenzylidene) 2,4 dioxothiazolidin 3 yl] n phenylacetamide, 2 [5 (4 methoxybenzylidene) 2,4 dioxothiazolidin 3 yl) n (4 methoxyphenyl)acetamide, 2 [5 (4 methoxybenzylidene) 2,4 dioxothiazolidin 3 yl] n (4 chlorophenyl)acetamide, 2 [5 (4 methoxybenzylidene) 2,4 dioxothiazolidin 3 yl] n phenylacetamide, 2,4 thiazolidinedione derivative, 7 (4 chorobenzylidene) 3,4 dihydro 3 phenyl 2h thiazolo[3,2 a][1,3,5]triazin 6(7h) one, 7 (4 fluorobenzylidene) 3,4 dihydro 3 phenyl 2h thiazolo[3,2 a][1,3,5]tliazin 6(7h) one, 7 benzylidene 3,4 dihydro 3 phenyl 2h thiazolo[3,2a][1,3,5]triazin 6(7h) one, antivirus agent, nonstructural protein 5B, RNA directed RNA polymerase inhibitor, thiazole derivative, triazine derivative, unclassified drug, unindexed drug, vch 759, [5 (4 chlorobenzylidene) 2,4 dioxothiazolidin 3 yl] n phenylacetamide

EMTREE medical term: allosteric site, antiviral activity, Article, cell viability, controlled study, crystal structure, drug cytotoxicity, drug protein binding, drug synthesis, EC50, enzyme inhibition, hepatitis C, Hepatitis C virus, Huh-7.5 cell line, human, human cell, IC50, in vitro study, molecular docking, nonhuman, selectivity index, two dimensional quantitative structure activity relationship

Reaxys Index Terms: percent inhibition, 1,3-cycloaddition, Katritzky reaction, Mannich reaction, Molecular modeling, QSAR study, Scintillation, aminomethylation, crystal structure, crystallization, enzyme inhibition, halogenation, hydrophobic surface, lipophilicity, luminiscence type, radial distribution function, surface area, tautomerization



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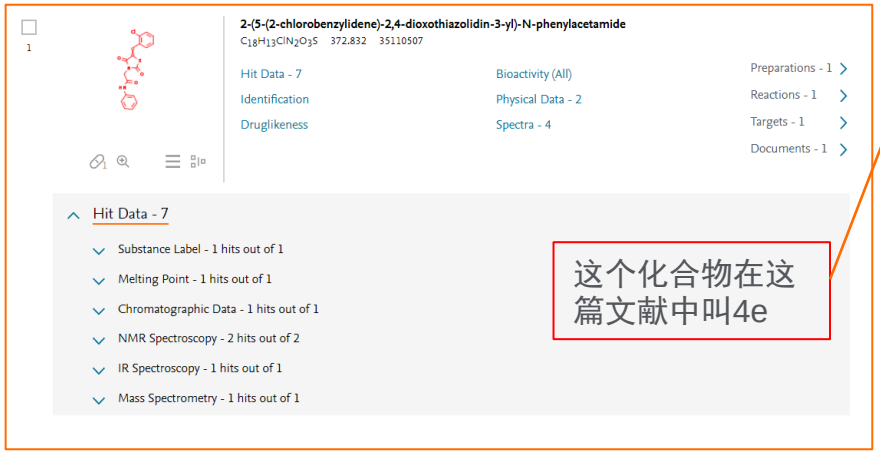
Reaxys对科学数据的提炼—化合物标签，理化性质



这个化合物在这篇文献中叫4e

Label	Reference
4e	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[**European Journal of Medicinal Chemistry, 2019**, vol. 184, art. no. 111747] Full Text Cited 1 times Details Abstract

Melting Point, °C	Solvent (Melting Point)	Reference
227 - 229	ethanol	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[**European Journal of Medicinal Chemistry, 2019**, vol. 184, art. no. 111747] Full Text Cited 1 times Details Abstract

NMR Spectroscopy - 2 hits out of 2

Show/Hide columns

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Temperature (NMR Spectroscopy), °C	Frequency (NMR Spectroscopy), MHz	Location	Reference
Chemical shifts, Spectrum	1H	dimethylsulfoxide-d6	24.94	400.2	supporting information	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[**European Journal of Medicinal Chemistry, 2019**, vol. 184, art. r 111747] Full Text Cited 1 times Details Abstra
Chemical shifts	13C	dimethylsulfoxide-d6	24.84	100	supporting information	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[**European Journal of Medicinal Chemistry, 2019**, vol. 184, art. r 111747] Full Text Cited 1 times Details Abstra

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。

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Reaxys对科学数据的提炼—活性数据(所有活性数据在RMC模块中）

Compds. No	R (A)	R (B)	IC_{50}	EC_{50}
VCH-759	–	–	0.14	5.29
4a	H	H	4.80	19.60
4b	4-Cl	H	0.085	11.10
4c	4-F	H	0.14	8.40
4d	4-OCH_3	H	0.25	11.57
4e	2-Cl	H	0.035	3.80
4f	2,4$(Cl)_2$	H	0.44	10.78

In vitro: Efficacy - 2

Quantitative Results

Show/Hide columns

pX	Parameter	Value (quant)	Unit	Biological Species	Action on target	Target	Cell	Effect	Reference
7.46	IC50	0.035	µM	Hepatitis C virus subtype 1a	Inhibitor	NS5B RNA dependent RNA polymerase, hepatitis C virus [Hepatitis C virus]:Wild		anti-HCV	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[**European Journal of Medicinal Chemistry, 2019**, vol. 184, art. no. 111747] Full Text Cited 1 times Details Abstract
5.42	EC50	3.8	µM		Inhibitor	NS5B RNA dependent RNA polymerase, hepatitis C virus [Hepatitis C virus]:Wild	Huh-7.5 cell line	anti-HCV	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[**European Journal of Medicinal Chemistry, 2019**, vol. 184, art. no. 111747] Full Text Cited 1 times Details Abstract

Table 2
Cytotoxicity (CC_{50}, µM)[a] and Selectivity index (SI)[b] values of the tested compound and **VCH-759**.

Code	THLE-2 cell line		RPTEC/TERT1 cell line	
	CC_{50}	SI	CC_{50}	SI
VCH-759	61.83	11.69	81.28	15.36
4e	102.77	27.04	161.37	42.47

[a] **CC_{50}** is the concentration of compounds that reduce the cell viability by 50%.
[b] **SI:** is the ratio of CC_{50} values on normal cells to EC_{50} on hepatoma infected cell lines (Huh7.5).

Toxicity/Safety Pharmacology - 2

Quantitative Results

Show/Hide columns

pX	Parameter	Value (quant)	Unit	Cell	Effect	Reference
3.99	CC50 (cytotoxic concentration)	102.77	µM	THLE-2 cell line	Cytotoxic	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[**European Journal of Medicinal Chemistry, 2019**, vol. 184, art. no. 111747] Full Text Cited 1 times Details Abstract
3.79	CC50 (cytotoxic concentration)	161.37	µM	RPTEC/TERT1 cell line	Cytotoxic	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A.[**European Journal of Medicinal Chemistry, 2019**, vol. 184, art. no. 111747] Full Text Cited 1 times Details Abstract

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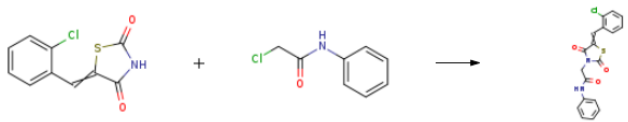
Reaxys对科学数据的提炼—实验过程



1 Hits/Conditions | Find Similar | Reaction ID: 52326456

Conditions	Yield	Reference
Stage #1: 5-(2-chlorobenzylidene)-2,4-thiazolidinedione **With** potassium carbonate **In** N,N-dimethyl-formamide at 100°C; for 0.5h; **Stage #2:** N-chloroacetyl-aniline **In** N,N-dimethyl-formamide at 100°C; for 24h; Experimental Procedure	90%	Hassan, Ghaneya S.; Georgey, Hanan H.; Mohammed, Esraa Z.; Omar, Farghaly A. [**European Journal of Medicinal Chemistry, 2019**, vol. 184, art. no. 111747] Full Text ↗ Cited 1 times ↗ Details › Abstract ›

4.1.1. 2-(5-Un/substitutedbenzylidene-2,4-dioxothiazolidin-3-yl)-N-un/substitutedphenyl acetamide 4a-f, 5a-f, 6a-f

General procedure: A solution of the appropriate benzylidene thiazolidindione (2af)(10 mmol) and anhydrous potassium carbonate (0.69 g, 5 mmol)in dry DMF (20 mL), was stirred at 100 °C for 30 min. The corresponding2-chloro N-un/sub phenyl acetamide (3a-c) (10 mmol)was added and stirring was continued at 100 °C for 24 h. The reaction mixture was poured onto crushed ice, the precipitated product was filtered off, dried and crystallized from ethanol.

4.1.1. 2-(5-Un/substitutedbenzylidene-2,4-dioxothiazolidin-3-yl)-N-un/substitutedphenyl acetamide 4a-f, 5a-f, 6a-f

A solution of the appropriate benzylidene thiazolidindione (**2a-f**) (10 mmol) and anhydrous potassium carbonate (0.69 g, 5 mmol) in dry DMF (20 mL), was stirred at 100 °C for 30 min. The corresponding 2-chloro *N*-un/sub phenyl acetamide (**3a-c**) (10 mmol) was added and stirring was continued at 100 °C for 24 h. The reaction mixture was poured onto crushed ice, the precipitated product was filtered off, dried and crystallized from ethanol.

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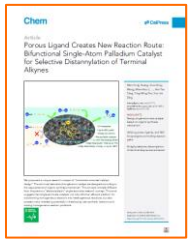
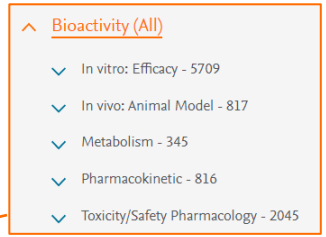
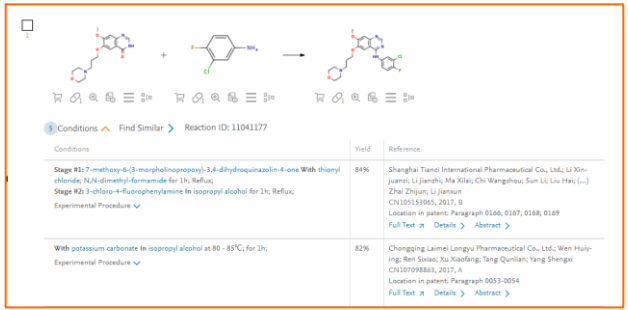
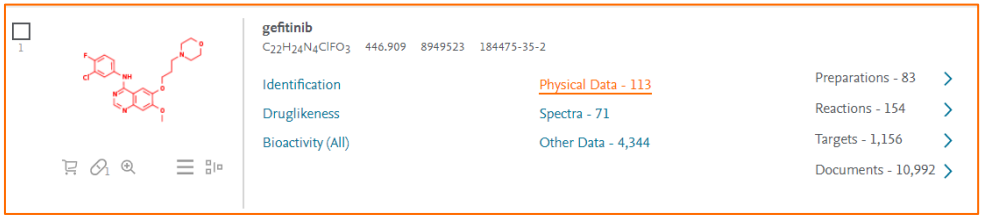
Reaxys将文献中报道的科学数据进行了抽提，归纳，标准化









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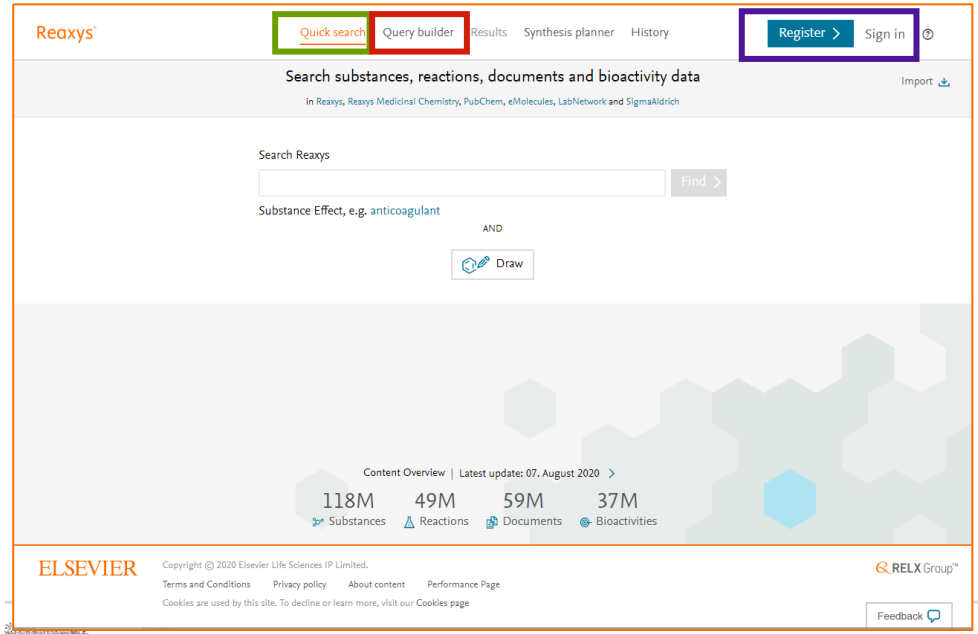
Reaxys的登录界面

- 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

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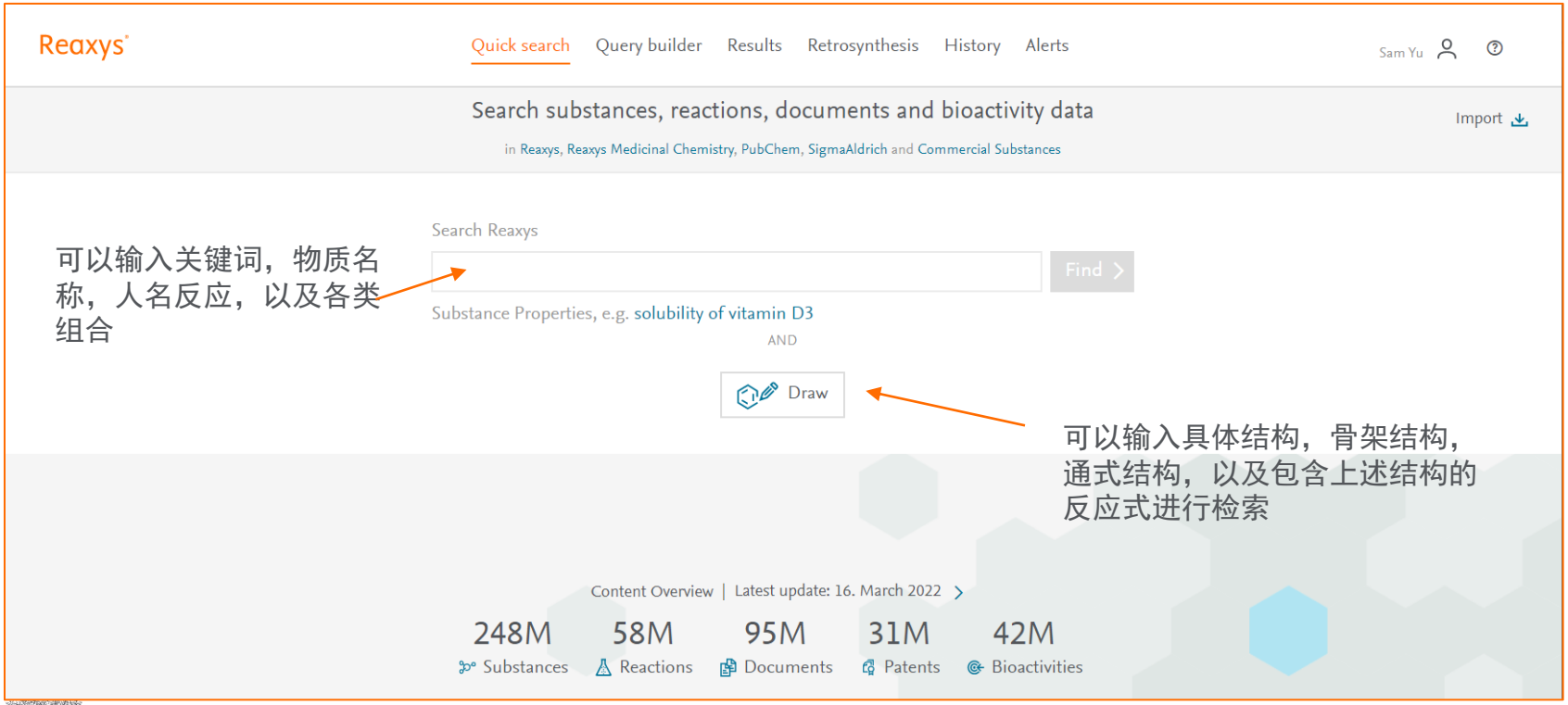
Quick Search界面



可以输入关键词，物质名称，人名反应，以及各类组合

可以输入具体结构，骨架结构，通式结构，以及包含上述结构的反应式进行检索

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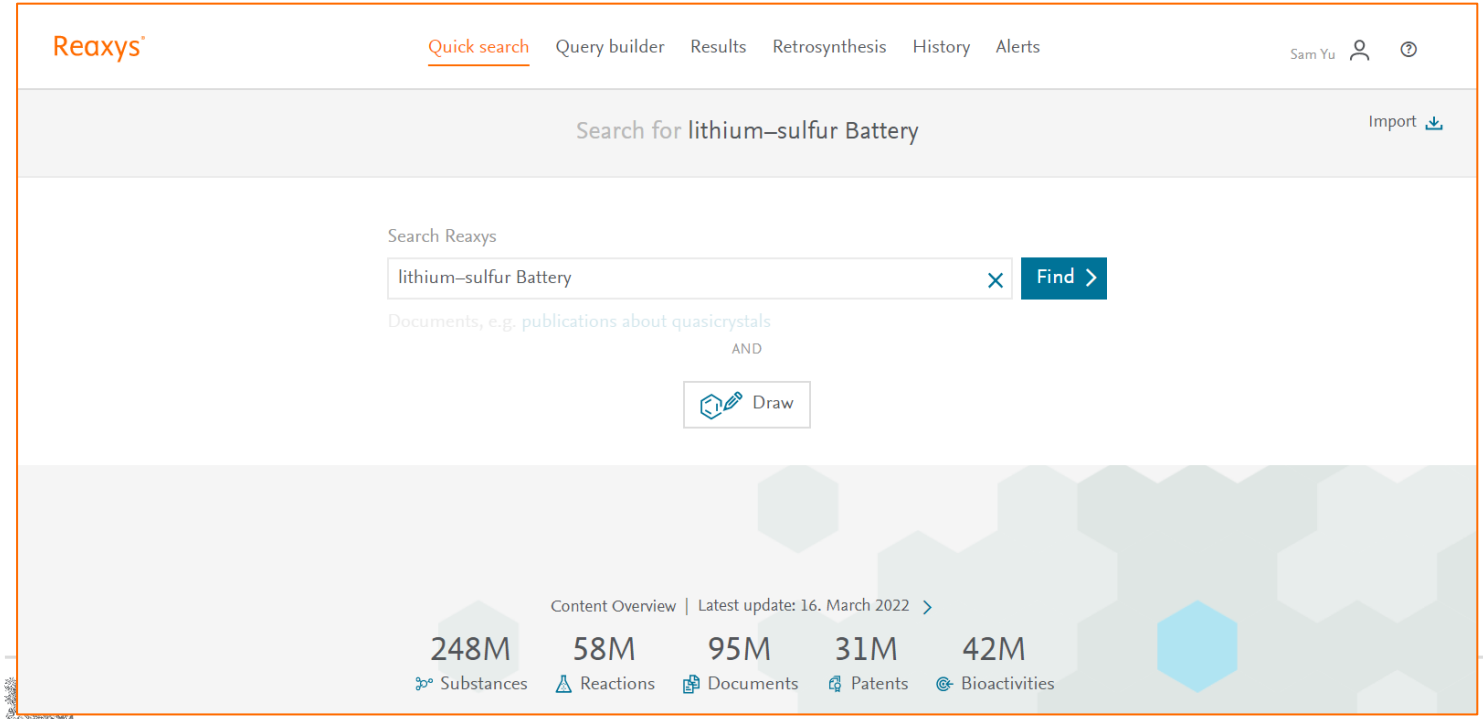
  - Reaxys中的实用小案例
- Q&A

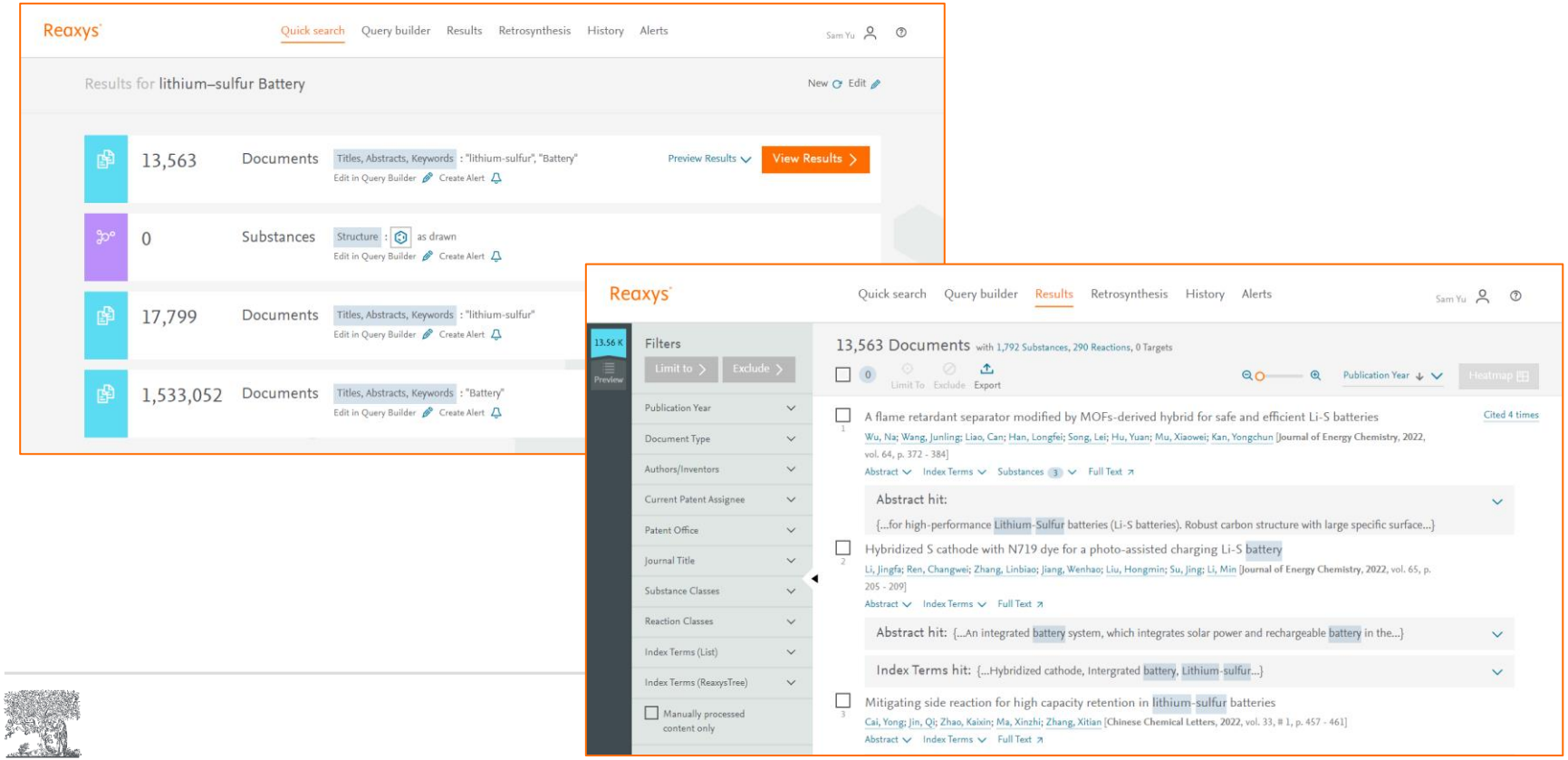
Case 1：关键词检索—锂硫电池

- Lithium–Sulfur Battery



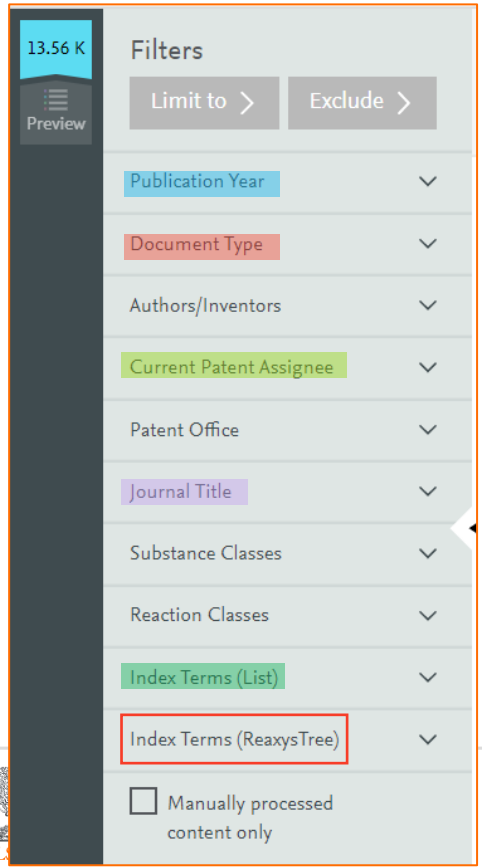
ELSEVIER

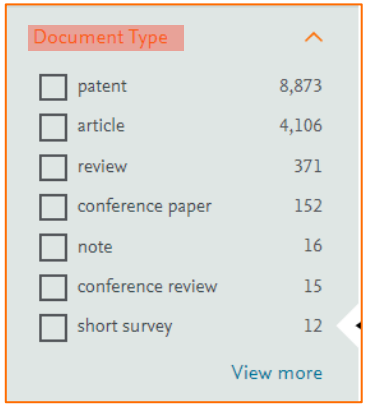
Reaxys中的检索结果

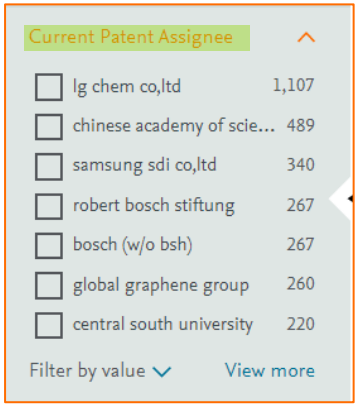


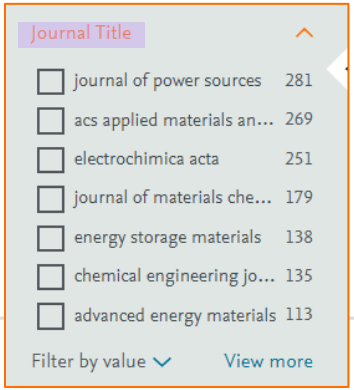
ELSEVIER

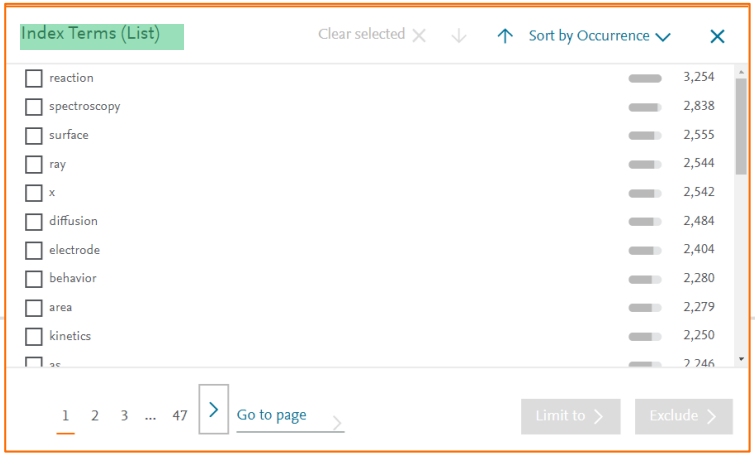
Reaxys中对于文献检索结果的分析



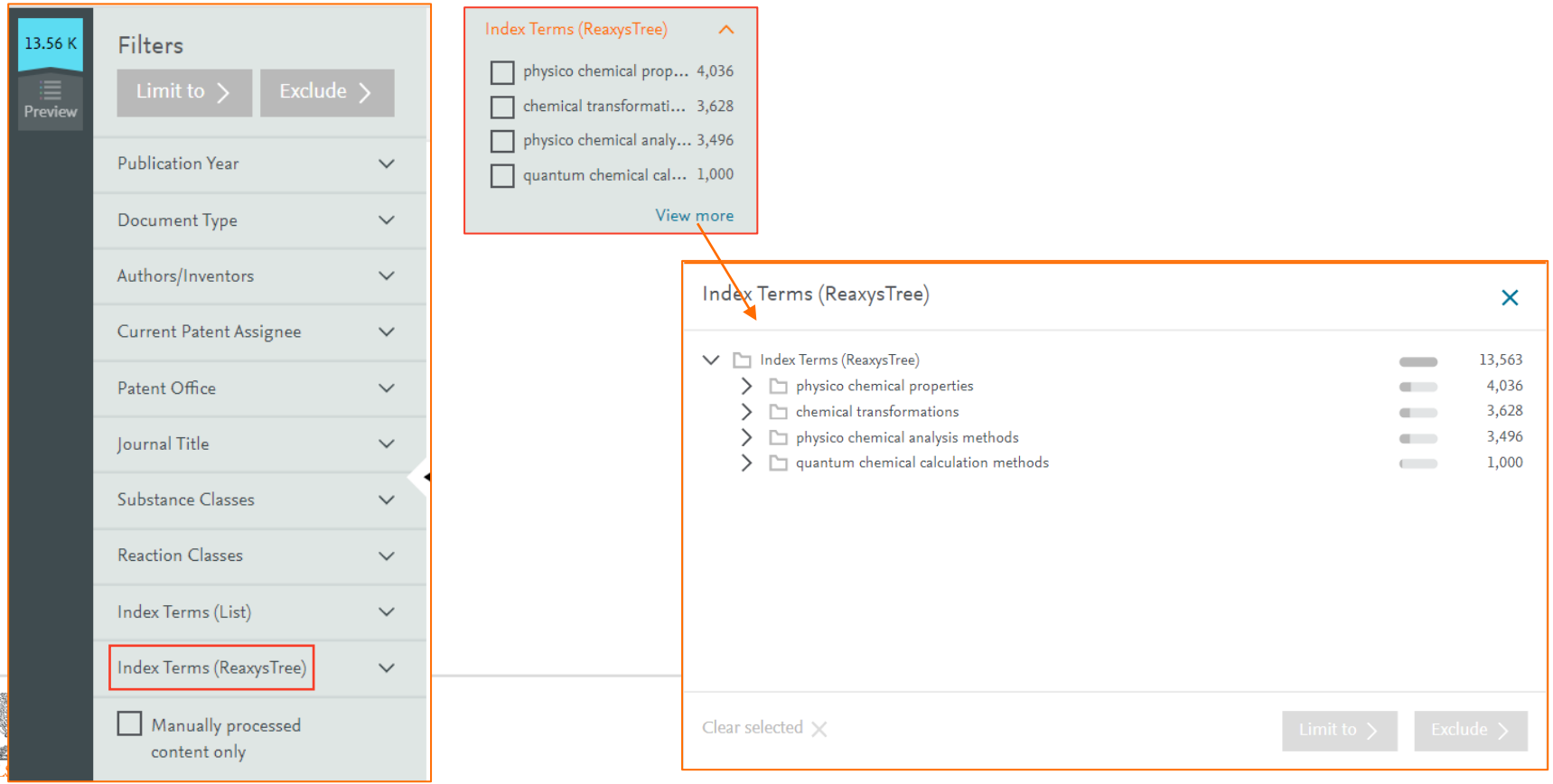




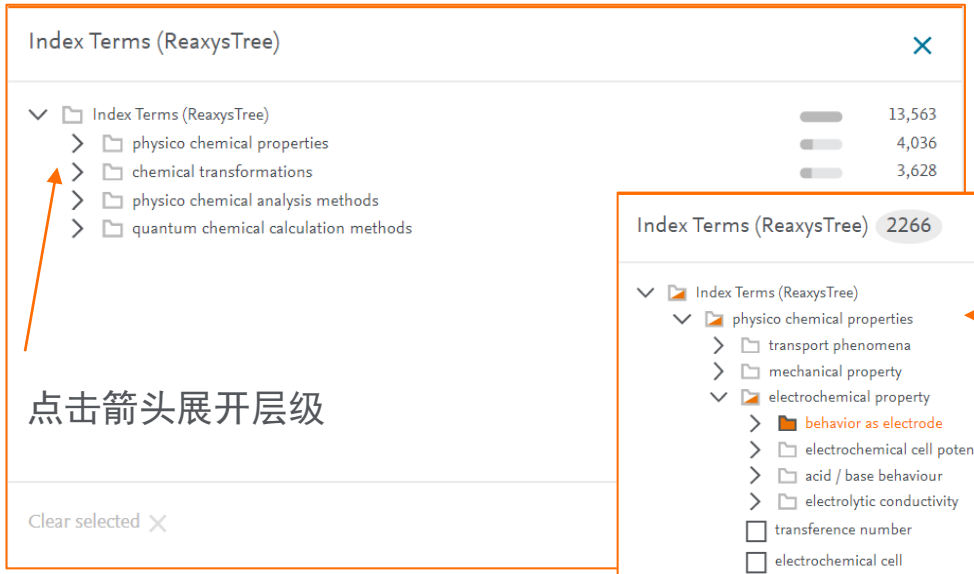


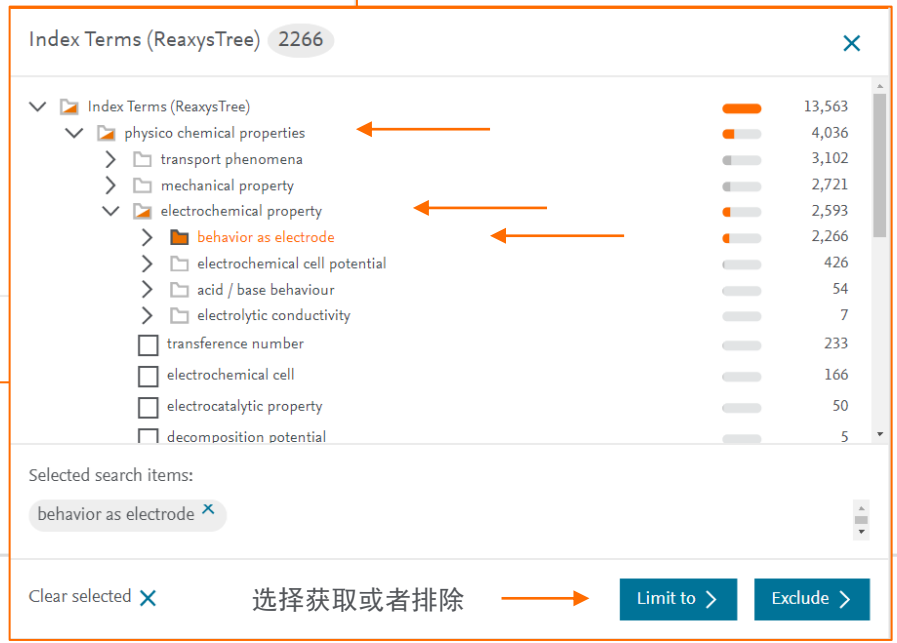


Reaxys中的Index Terms（Reaxys Tree）学科分类



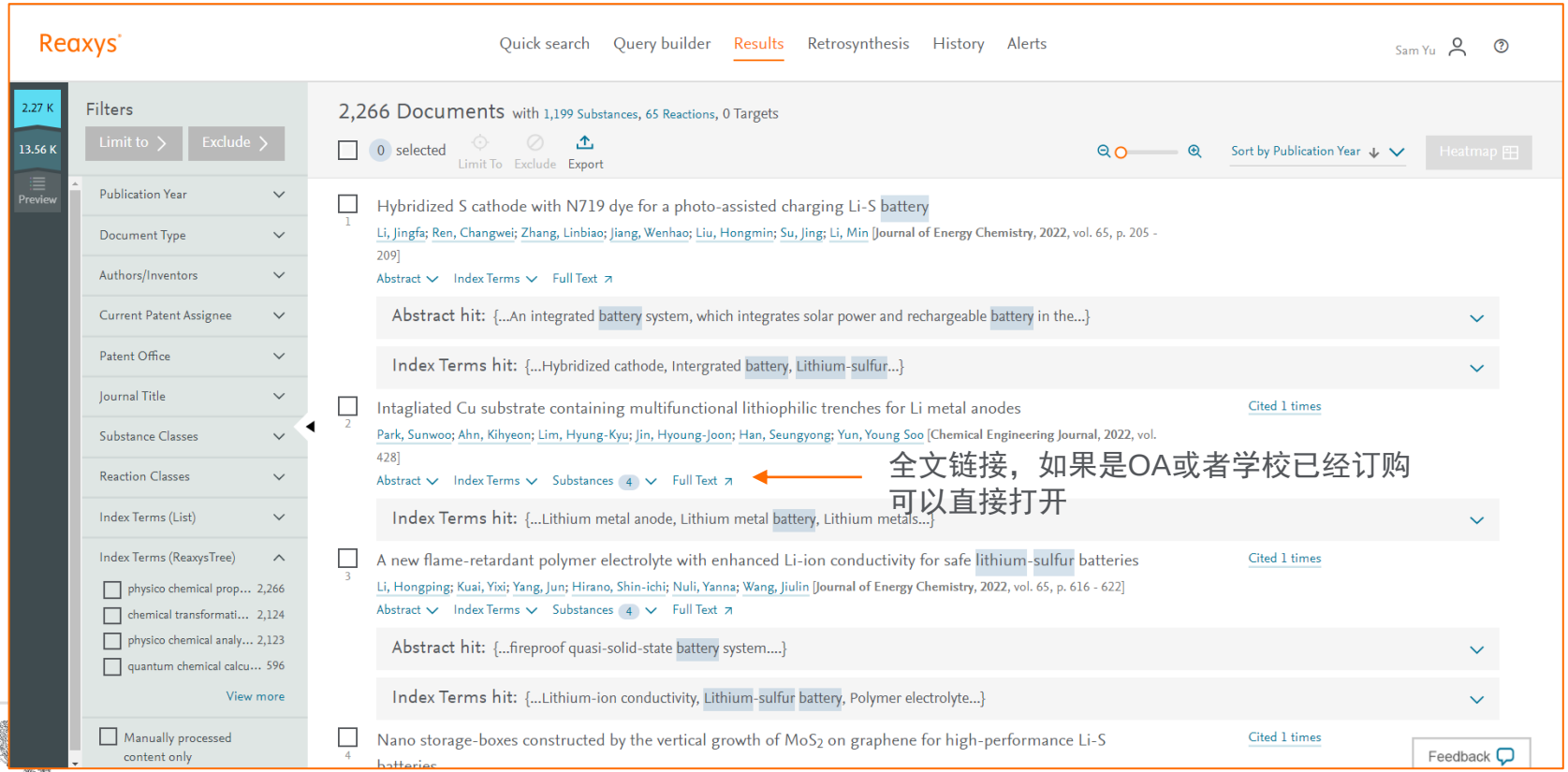
利用树状图进行学科分类





ELSEVIER

最后的检索结果

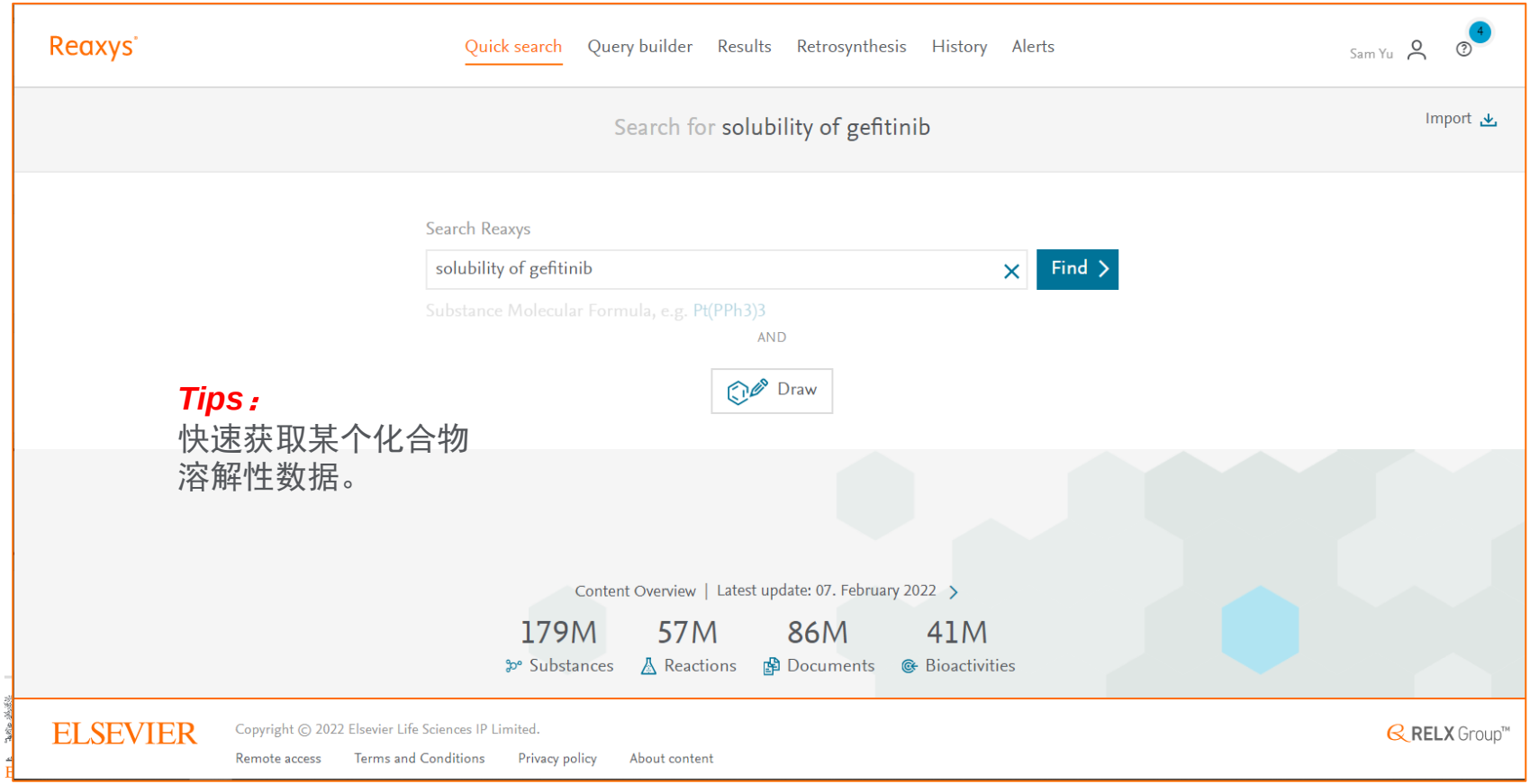


ELSEVIER

Agenda

- Reaxys介绍与内容
  - Reaxys介绍
  - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
  - Reaxys中的关键词检索
  - Reaxys中物质理化性质数据的查询与反向物质获取
  - Reaxys中结构面板与物质结构和反应数据的获取
  - Reaxys中的实用小案例
- Q&A

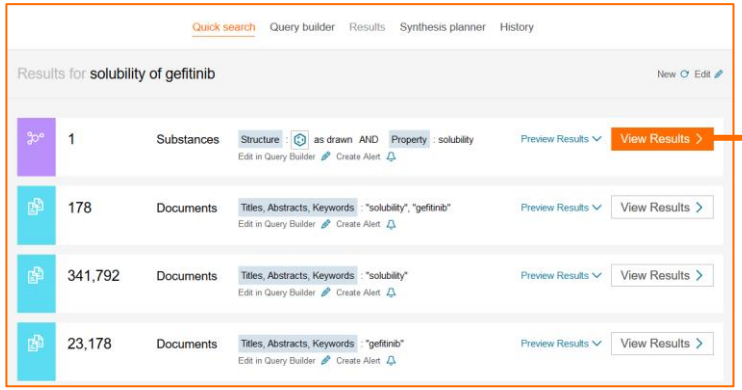
Case 2：快速获取化合物的理化性质

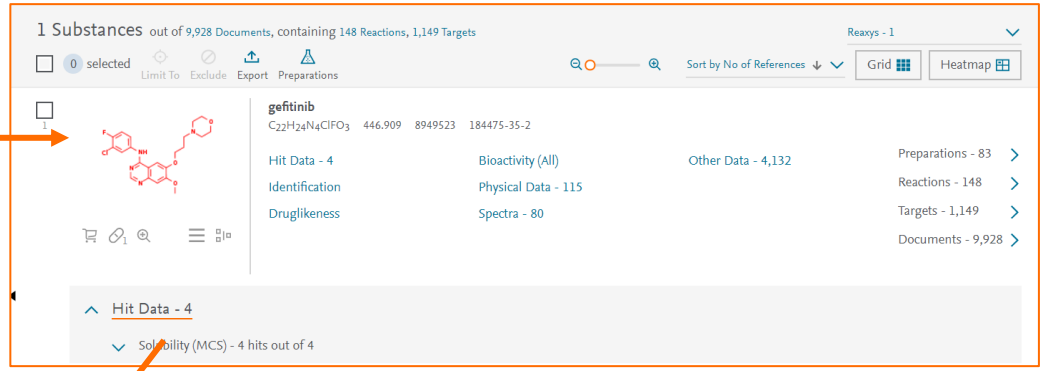


Tips：

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

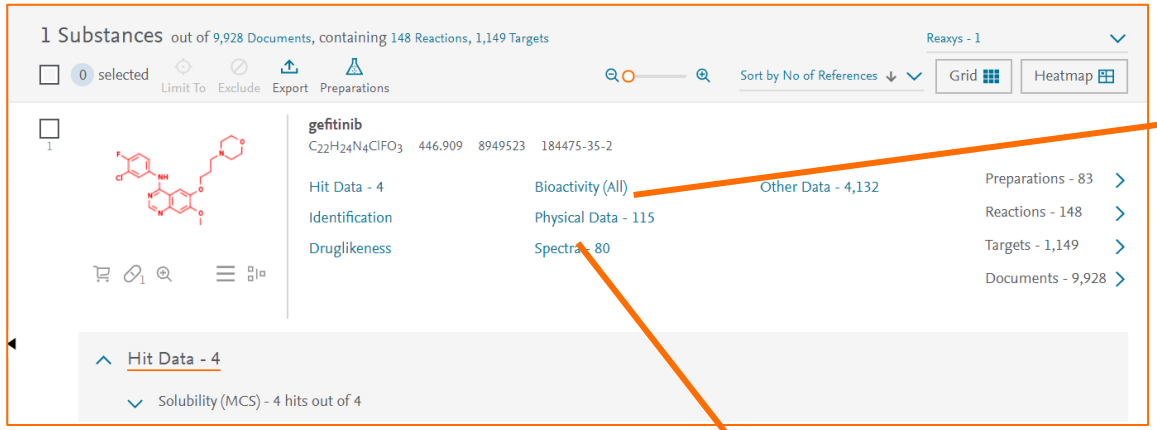
Solubility (MCS) - 4 hits out of 4

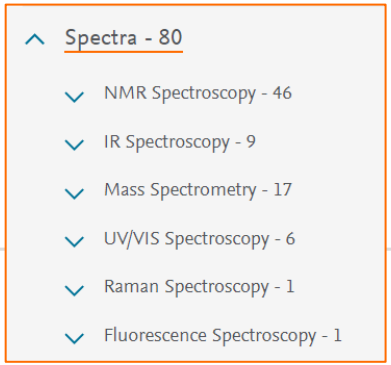
Show/Hide columns

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

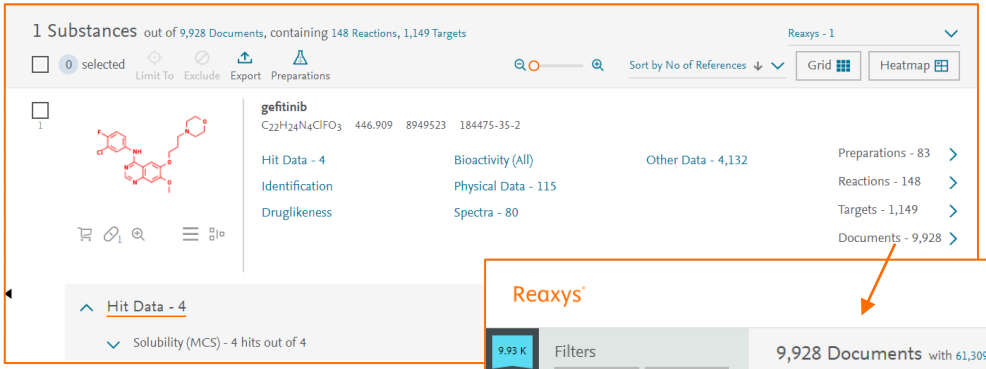


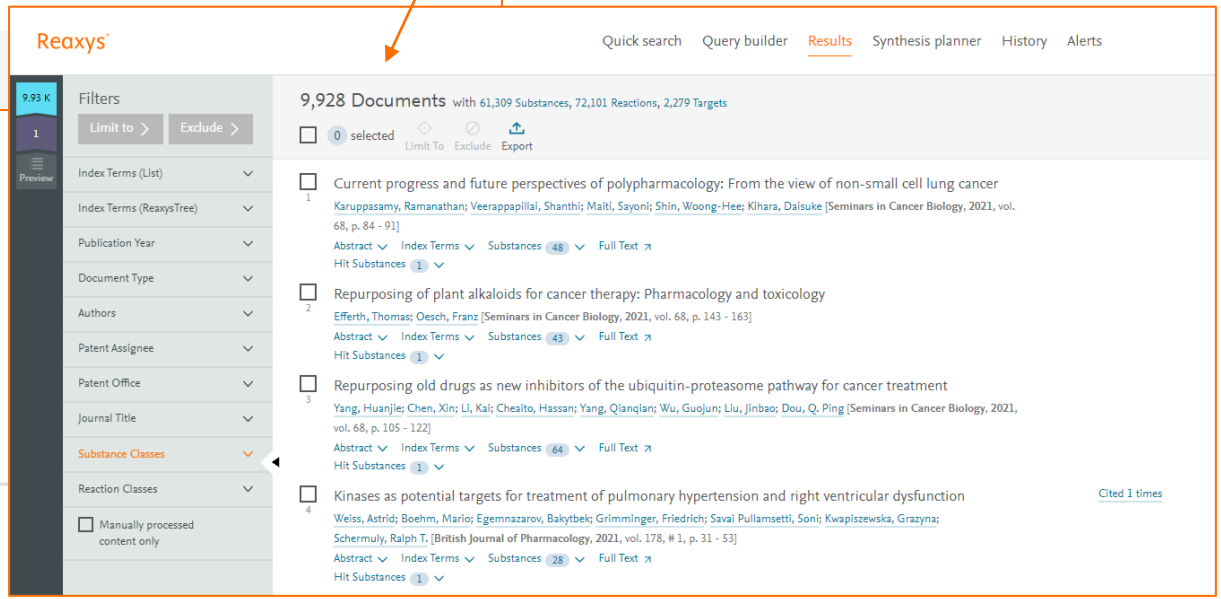


直接获取化合物的理化性质或者谱图数据

ELSEVIER

Reaxys中与化合物分析有关文献的获取

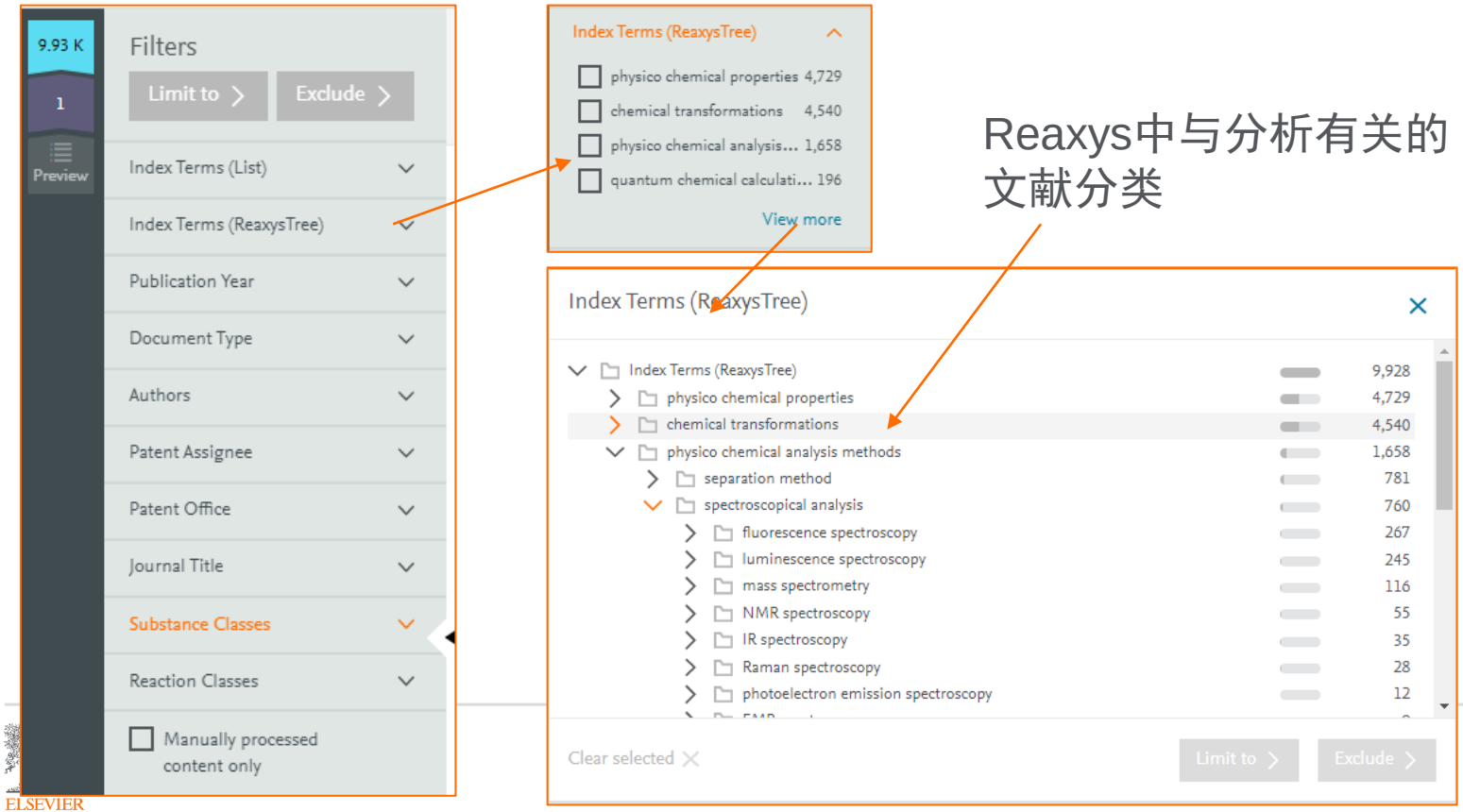




可以一次性获取与该化合物有关的文献

ELSEVIER

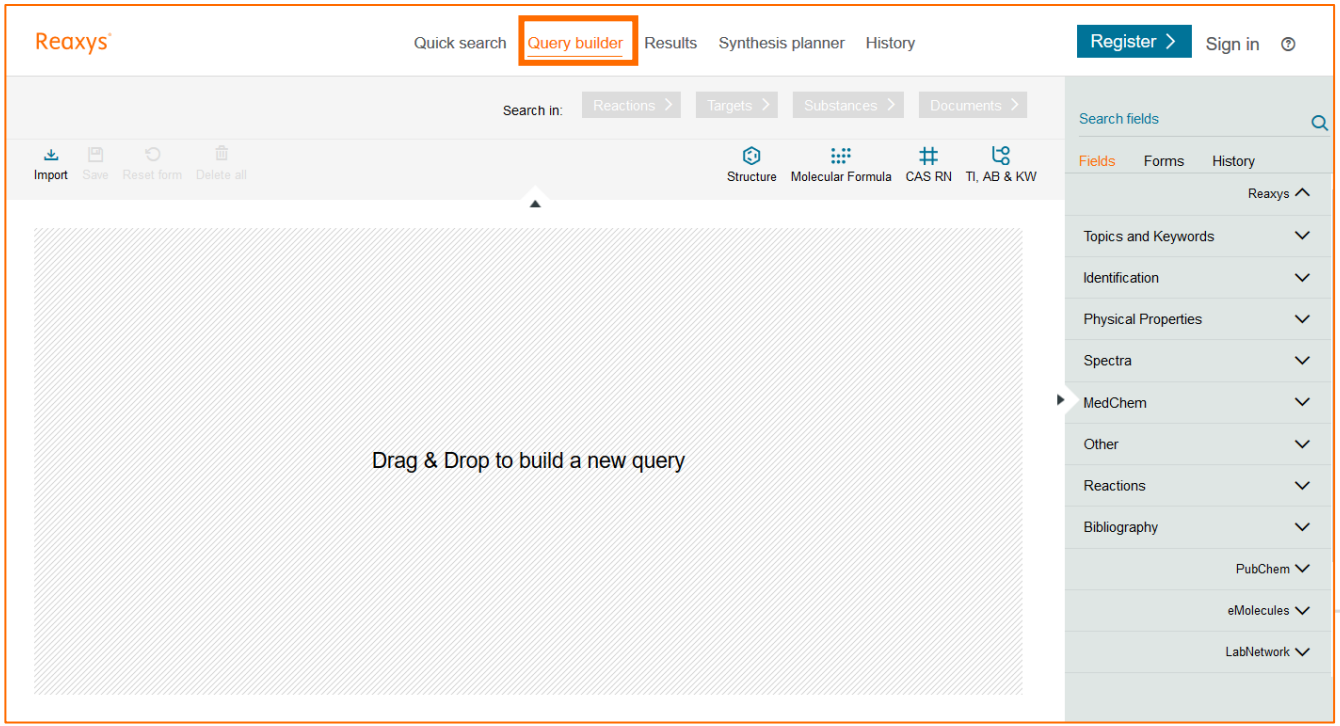
Reaxys中的文献分析工具



Reaxys中与分析有关的文献分类

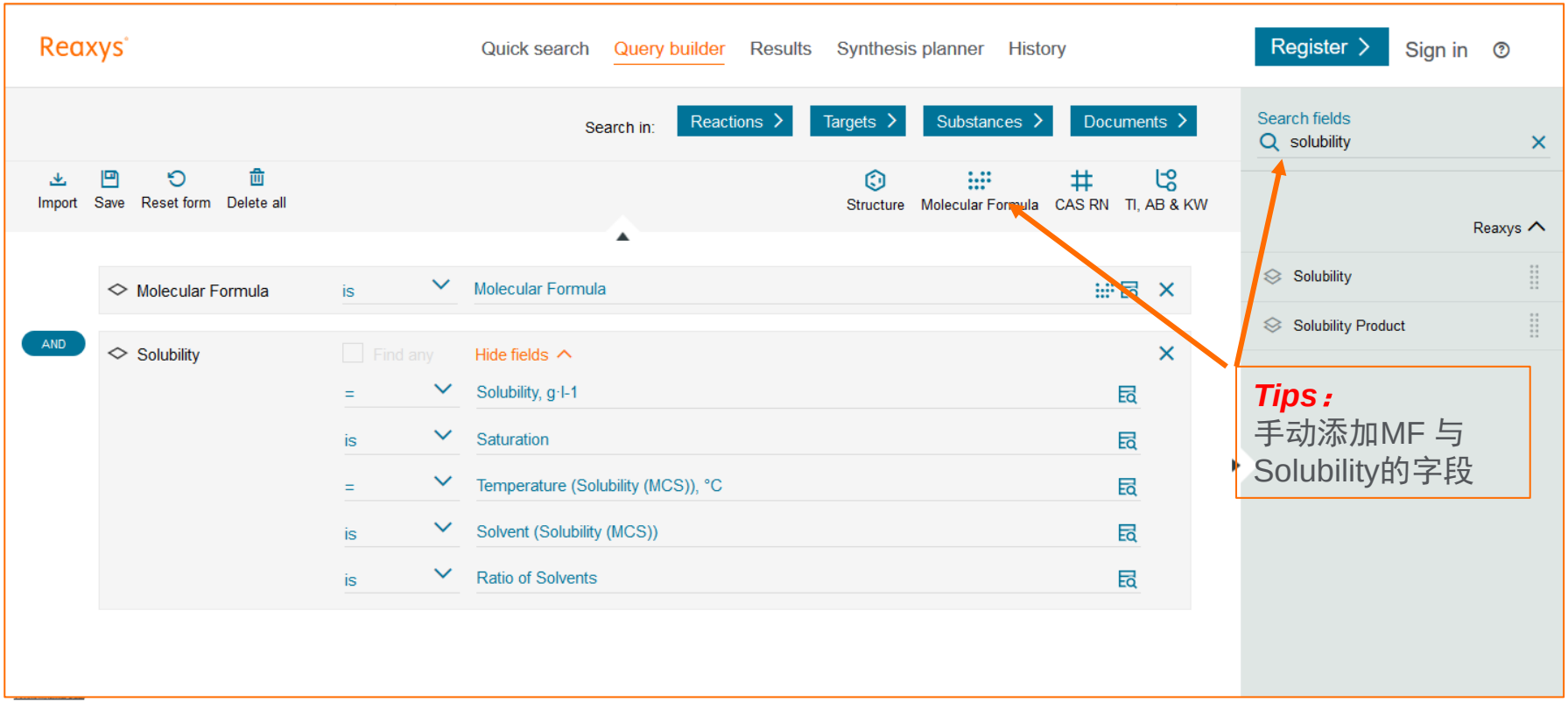
Case 3：理化性质的高级应用

- 获取KCl在乙醇中的溶解度

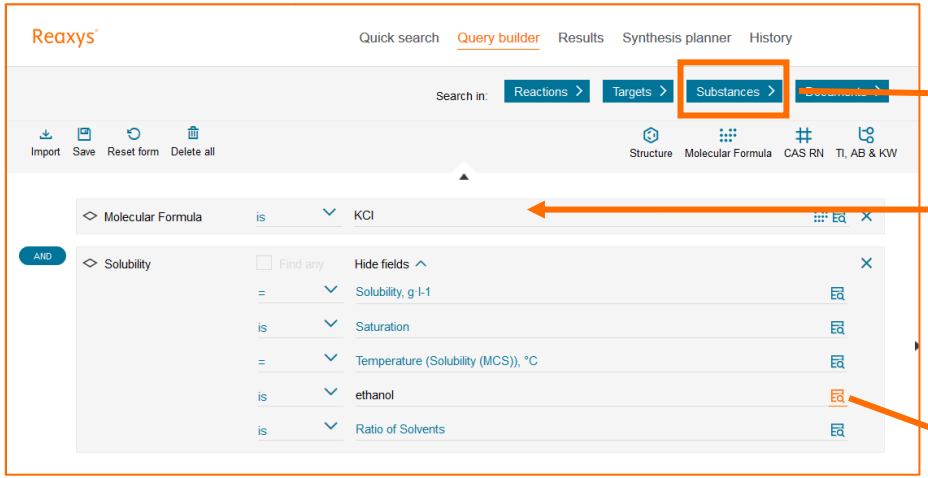


Reaxys中的Query Builder可以按照一定的规则构建检索式，Reaxys一共提供180+字段和字段组，科研人员可以自由的对这些字段和字段组进行组合，同时Reaxys也根据一些常见的需求，内置了多种检索策略模板，如“天然产物”，“hERG”等

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

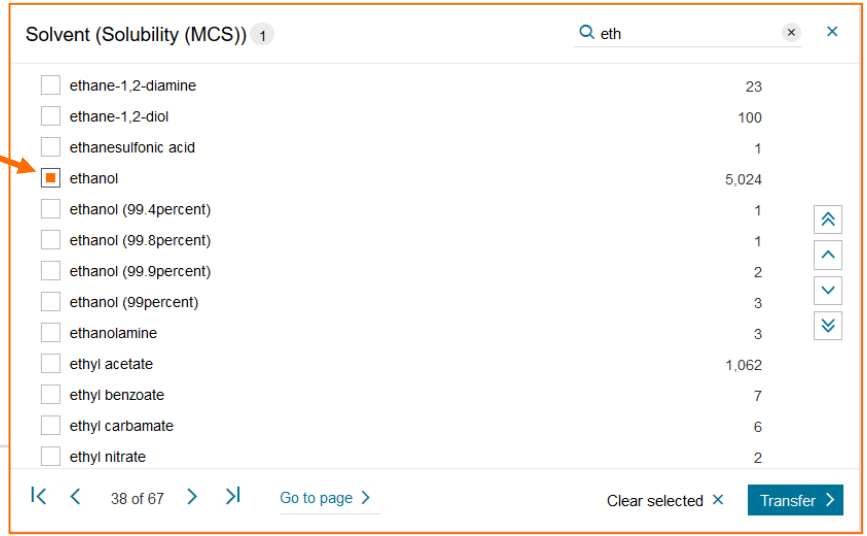
条件的输入



Step3：进行物质检索

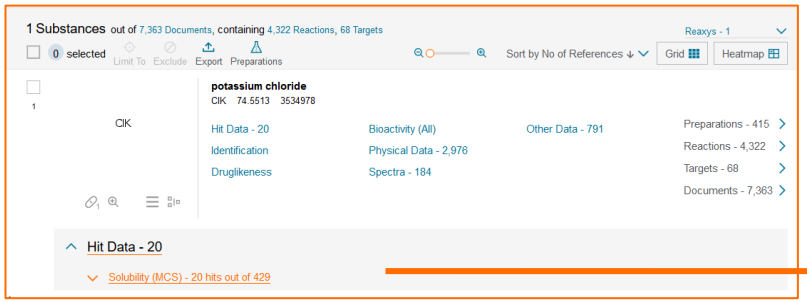
Step1：输入分子式KCl

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

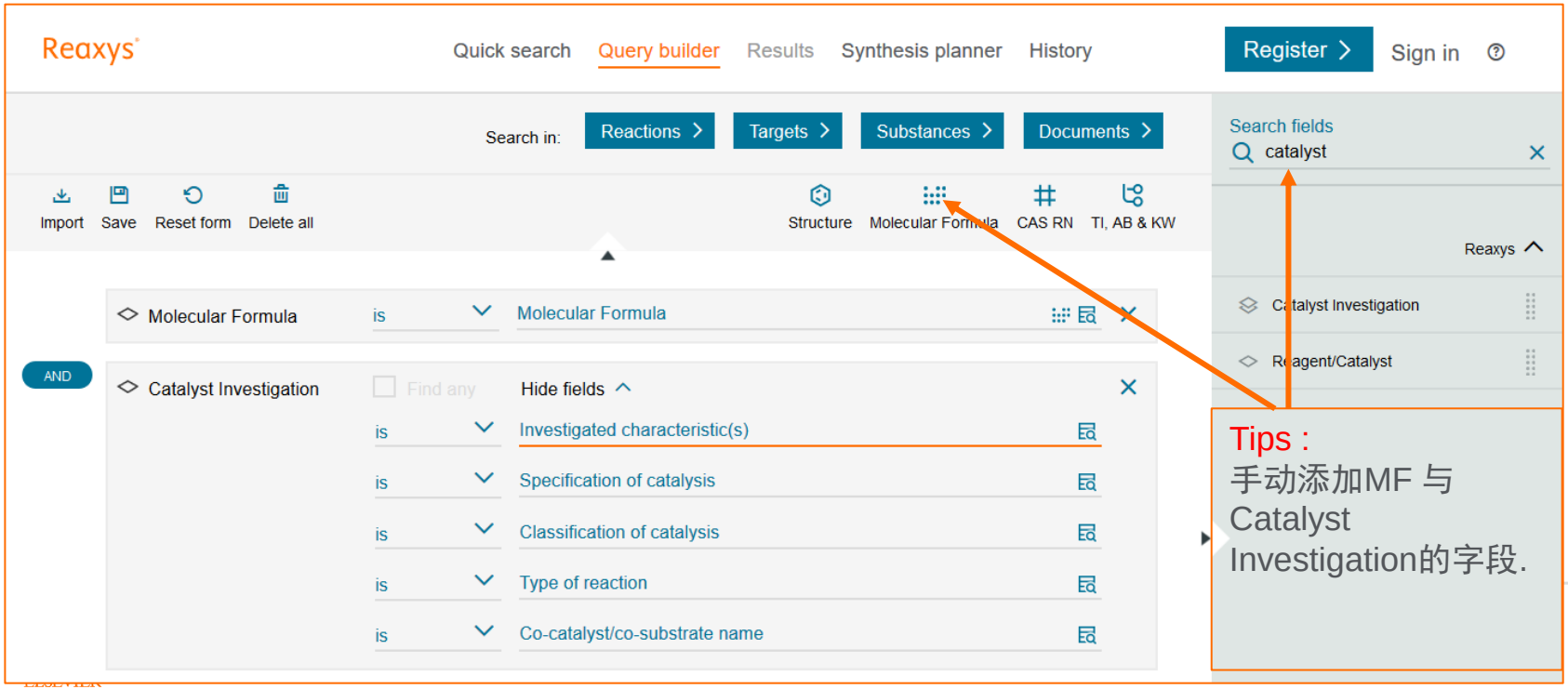
Show/Hide columns

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

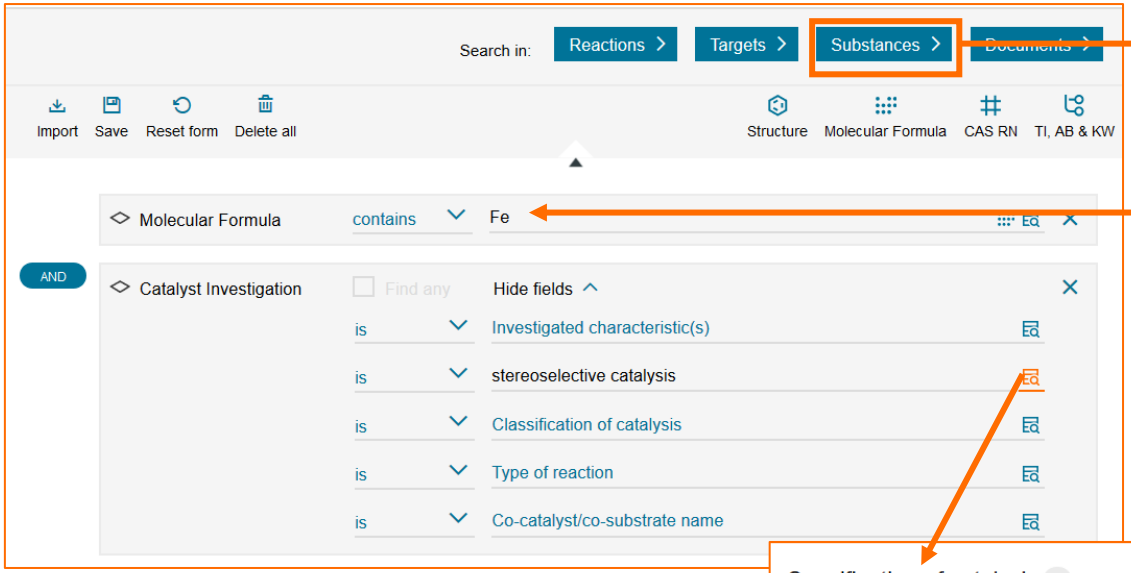
ELSEVIER

Case 4：“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

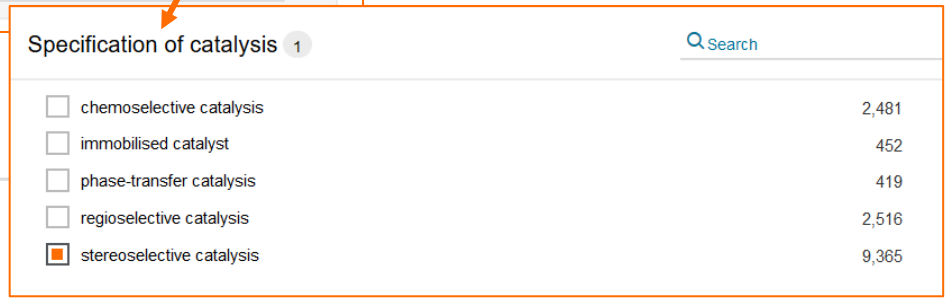


条件的输入



Step3：进行物质检索

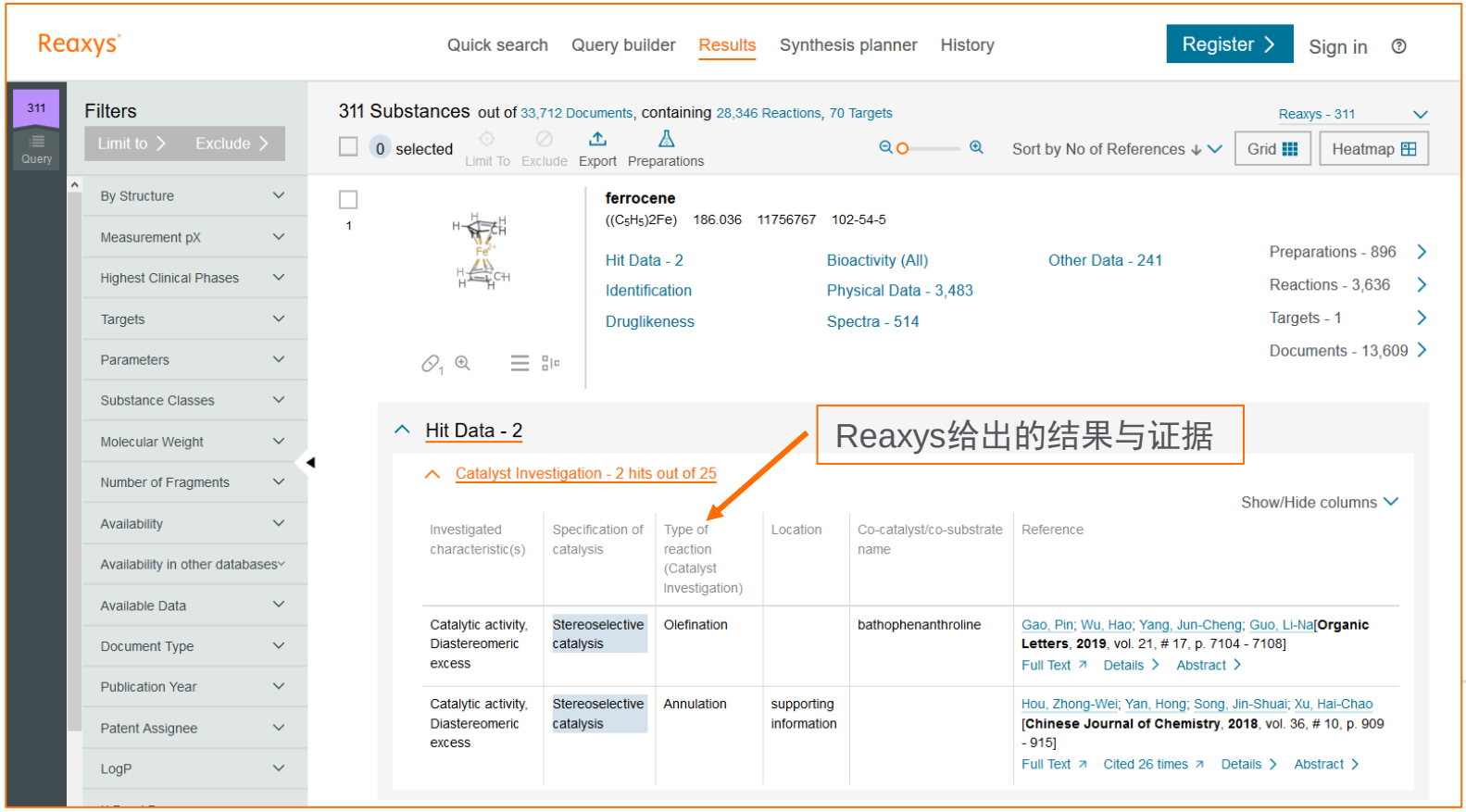
Step1：输入分子式Fe，并将逻辑关系改成“Contains”，即只要分子式中包含Fe，就检索出来



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

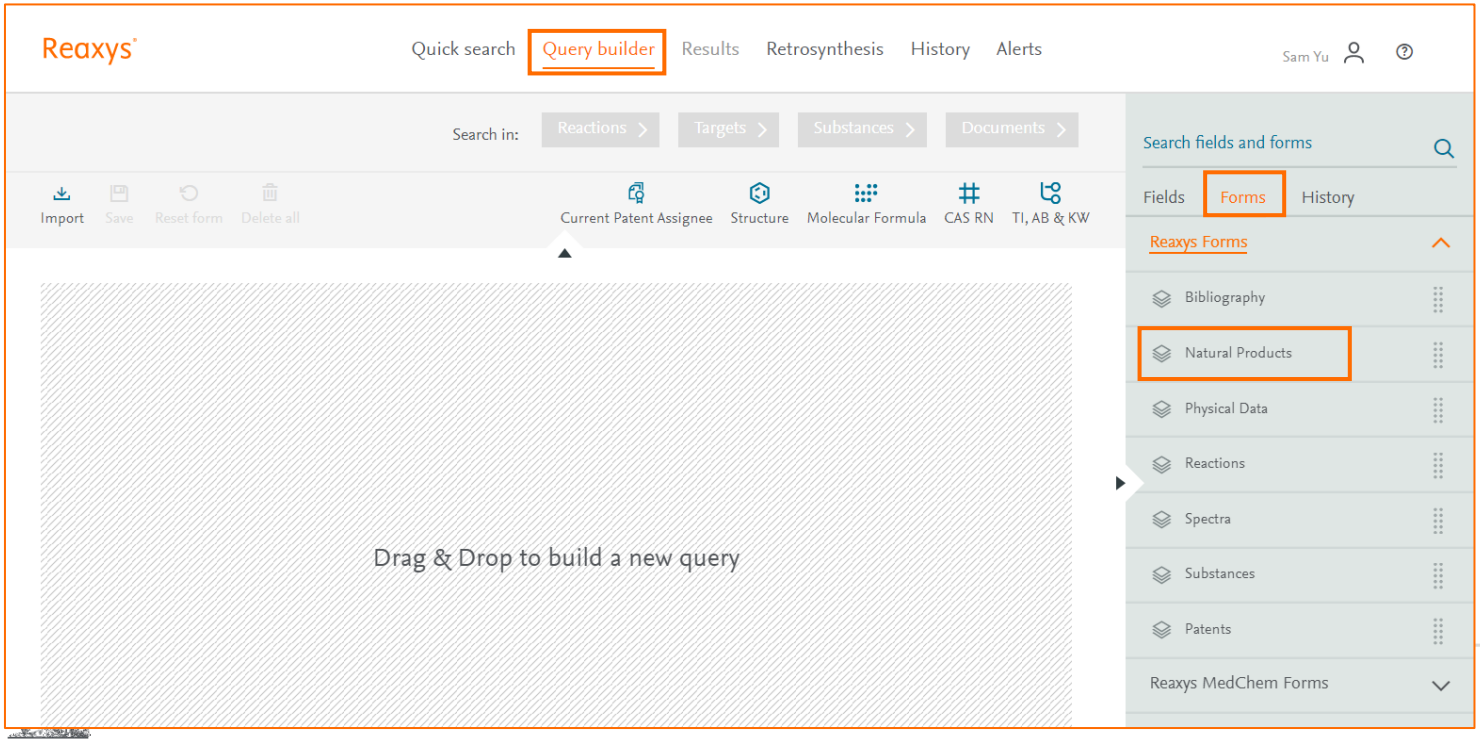
ELSEVIER

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

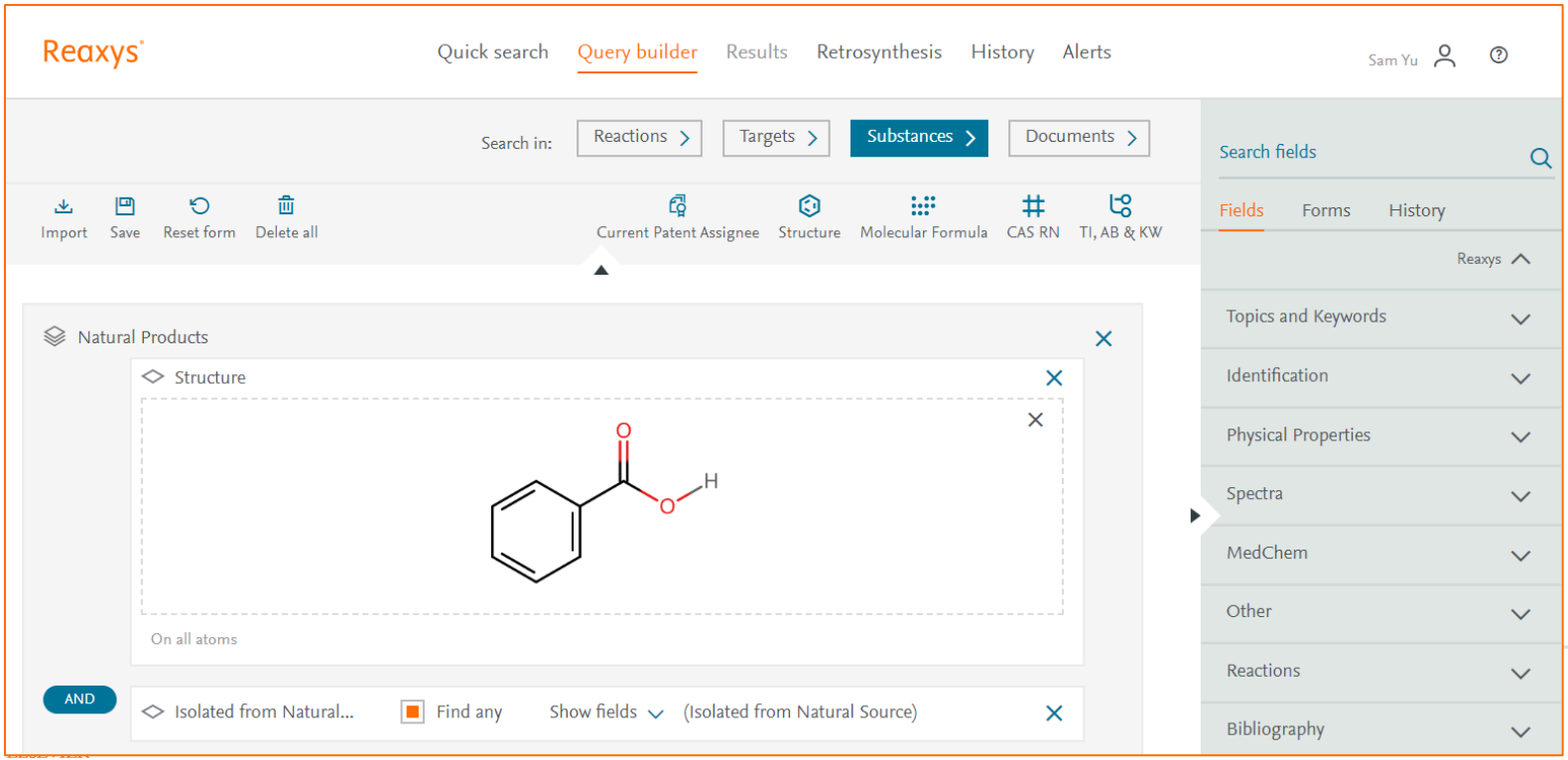
Case 5：活性天然产物的获取

- 检索包含特定结构的天然产物，并做活性分析

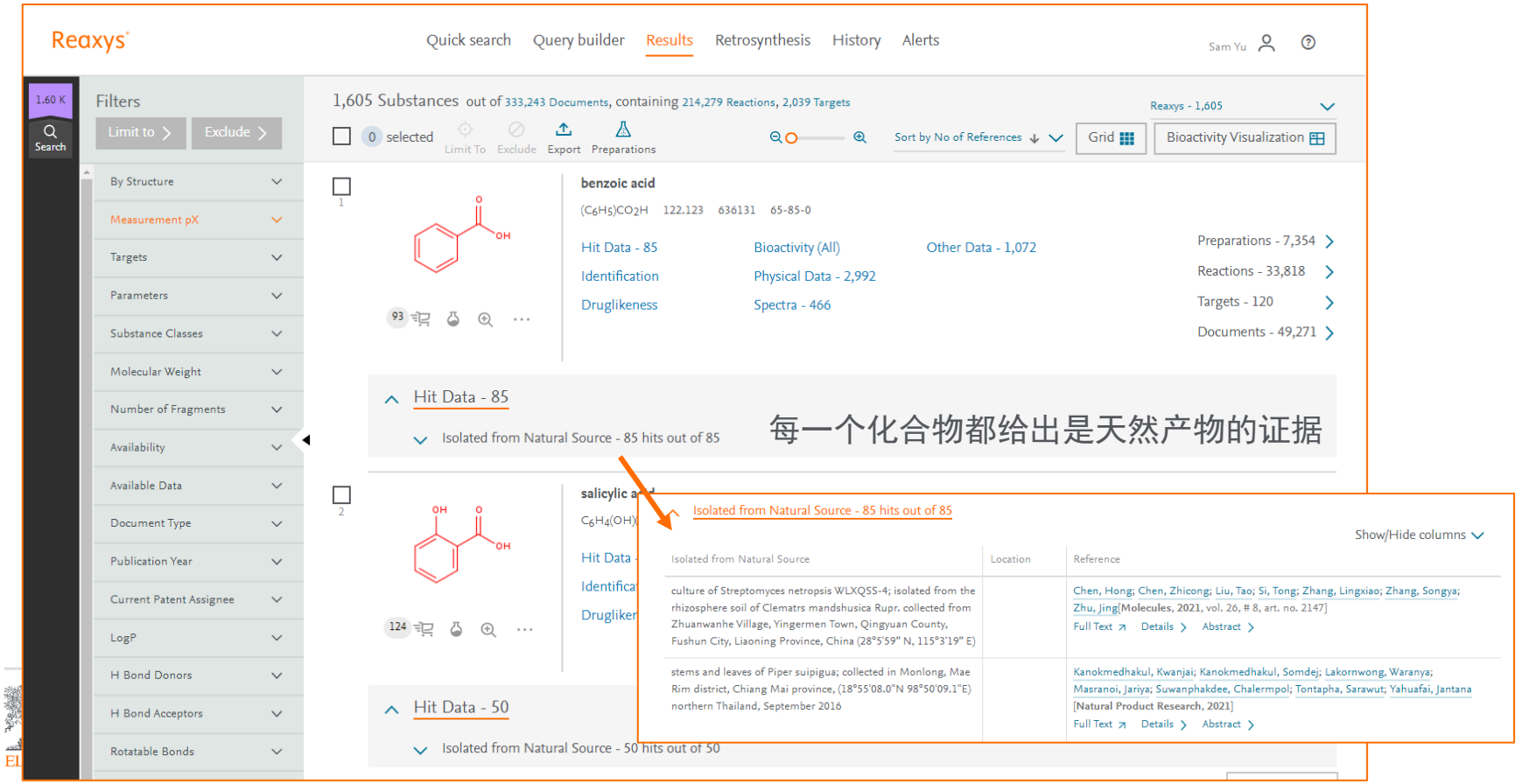


添加天然产物模块

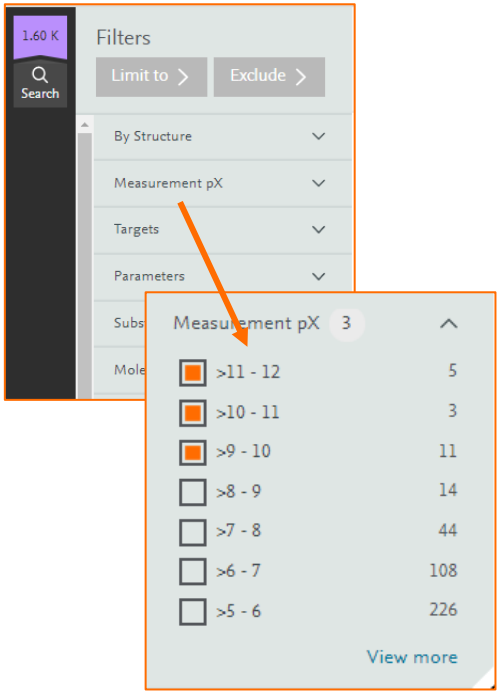
- 添加结构和勾选天然产物

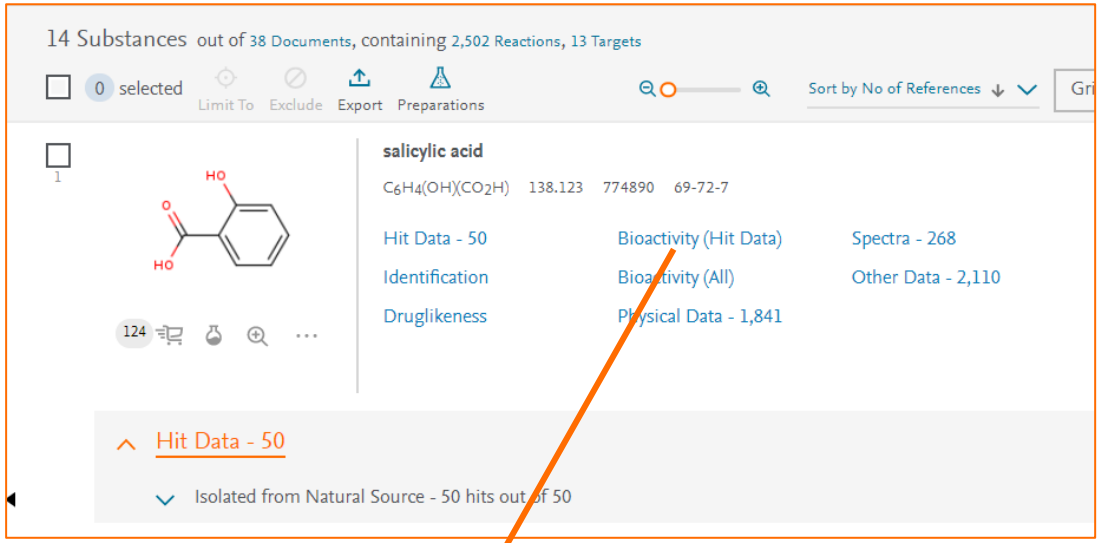


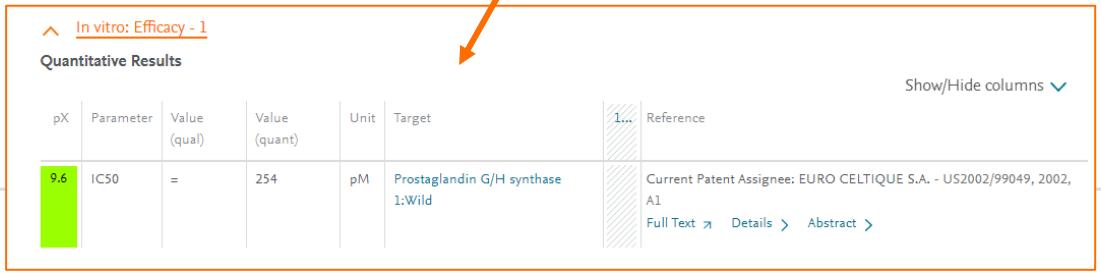
最后的结果


Reaxys
Quick search
Query builder
Results
Retrosynthesis
History
Alerts
Sam Yu
1.60 K
Search
Filters
Limit to
Exclude
By Structure
Measurement pX
Targets
Parameters
Substance Classes
Molecular Weight
Number of Fragments
Availability
Available Data
Document Type
Publication Year
Current Patent Assignee
LogP
H Bond Donors
H Bond Acceptors
Rotatable Bonds
1,605 Substances out of 333,243 Documents, containing 214,279 Reactions, 2,039 Targets
0 selected
Limit To
Exclude
Export
Preparations
Sort by No of References
Grid
Bioactivity Visualization
Reaxys - 1,605
benzoic acid
(C6H5)CO2H 122.123 636131 65-85-0
Hit Data - 85
Bioactivity (All)
Other Data - 1,072
Identification
Physical Data - 2,992
Druglikeness
Spectra - 466
Preparations - 7,354
Reactions - 33,818
Targets - 120
Documents - 49,271
Hit Data - 85
Isolated from Natural Source - 85 hits out of 85
每一个化合物都给出是天然产物的证据
Isolated from Natural Source - 85 hits out of 85
Show/Hide columns
Isolated from Natural Source
Location
Reference
culture of Streptomyces netropsis WLXQSS-4; isolated from the rhizosphere soil of Clematrs mandshusica Rupr. collected from Zhuanwanhe Village, Yingermen Town, Qingyuan County, Fushun City, Liaoning Province, China (28°5'59" N, 115°3'19" E)
Chen, Hong; Chen, Zhicong; Liu, Tao; Si, Tong; Zhang, Lingxiao; Zhang, Songya; Zhu, Jing[Molecules, 2021, vol. 26, # 8, art. no. 2147]
Full Text
Details
Abstract
stems and leaves of Piper suipigua; collected in Monlong, Mae Rim district, Chiang Mai province, (18°55'08.0"N 98°50'09.1"E) northern Thailand, September 2016
Kanokmedhakul, Kwanjai; Kanokmedhakul, Somdej; Lakornwong, Waranya; Masranoi, Jariya; Suwanphakdee, Chalermpol; Tontapha, Sarawut; Yahuafai, Jantana [Natural Product Research, 2021]
Full Text
Details
Abstract
Hit Data - 50
Isolated from Natural Source - 50 hits out of 50

活性的分析





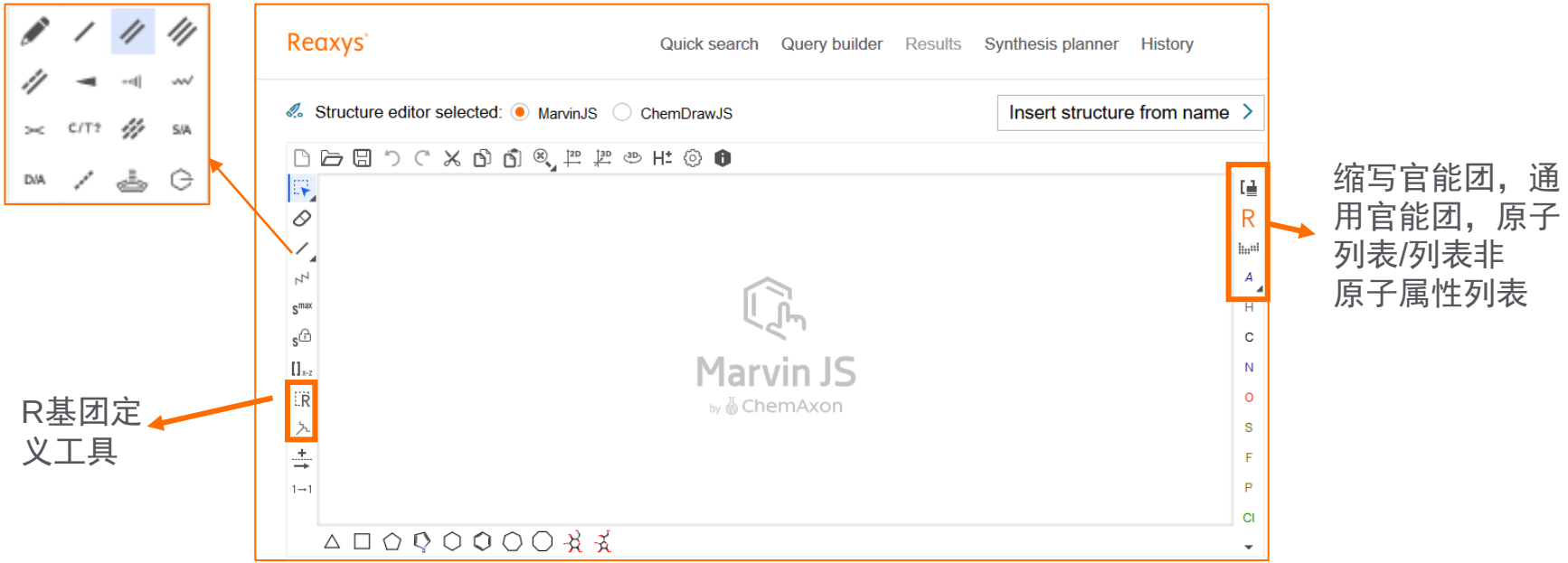


ELSEVIER

Agenda

- Reaxys介绍与内容
  - Reaxys介绍
  - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
  - Reaxys中的关键词检索
  - Reaxys中物质理化性质数据的查询与反向物质获取
  - Reaxys中结构面板与物质结构和反应数据的获取
  - Reaxys中的实用小案例
- Q&A

Reaxys中的结构面板

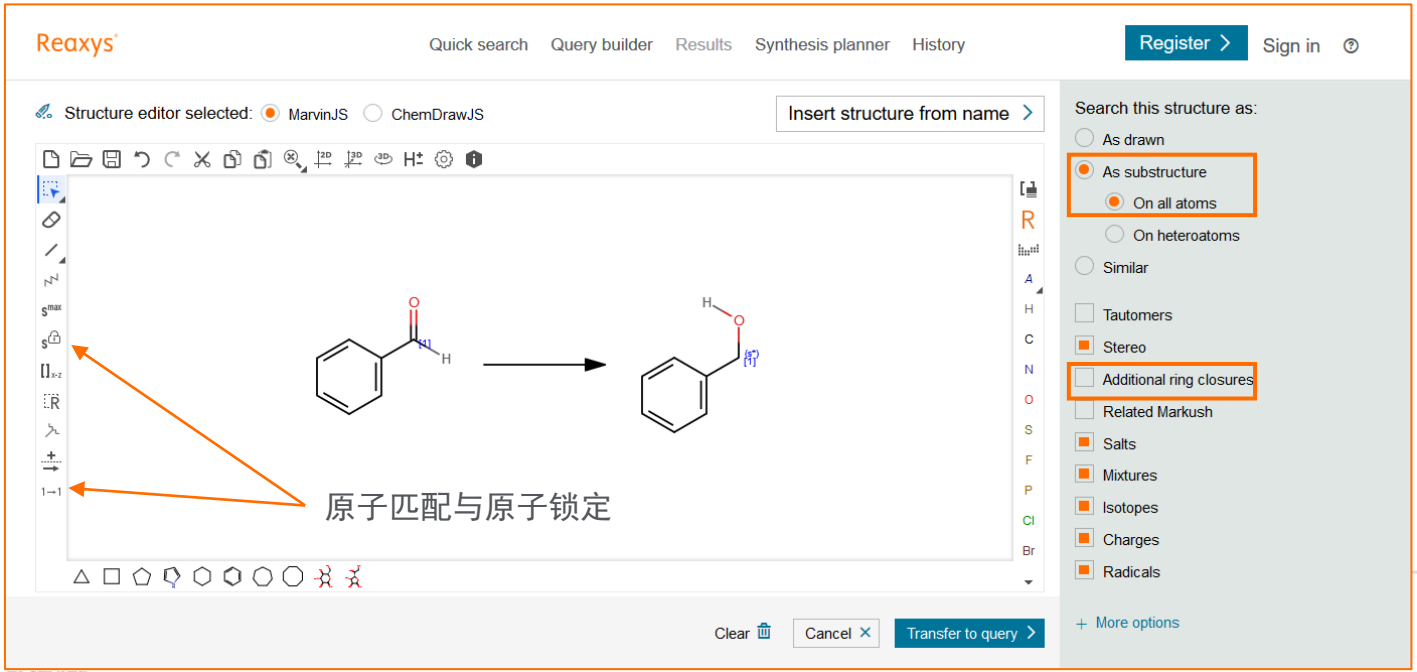


一些常见的功能使用视频

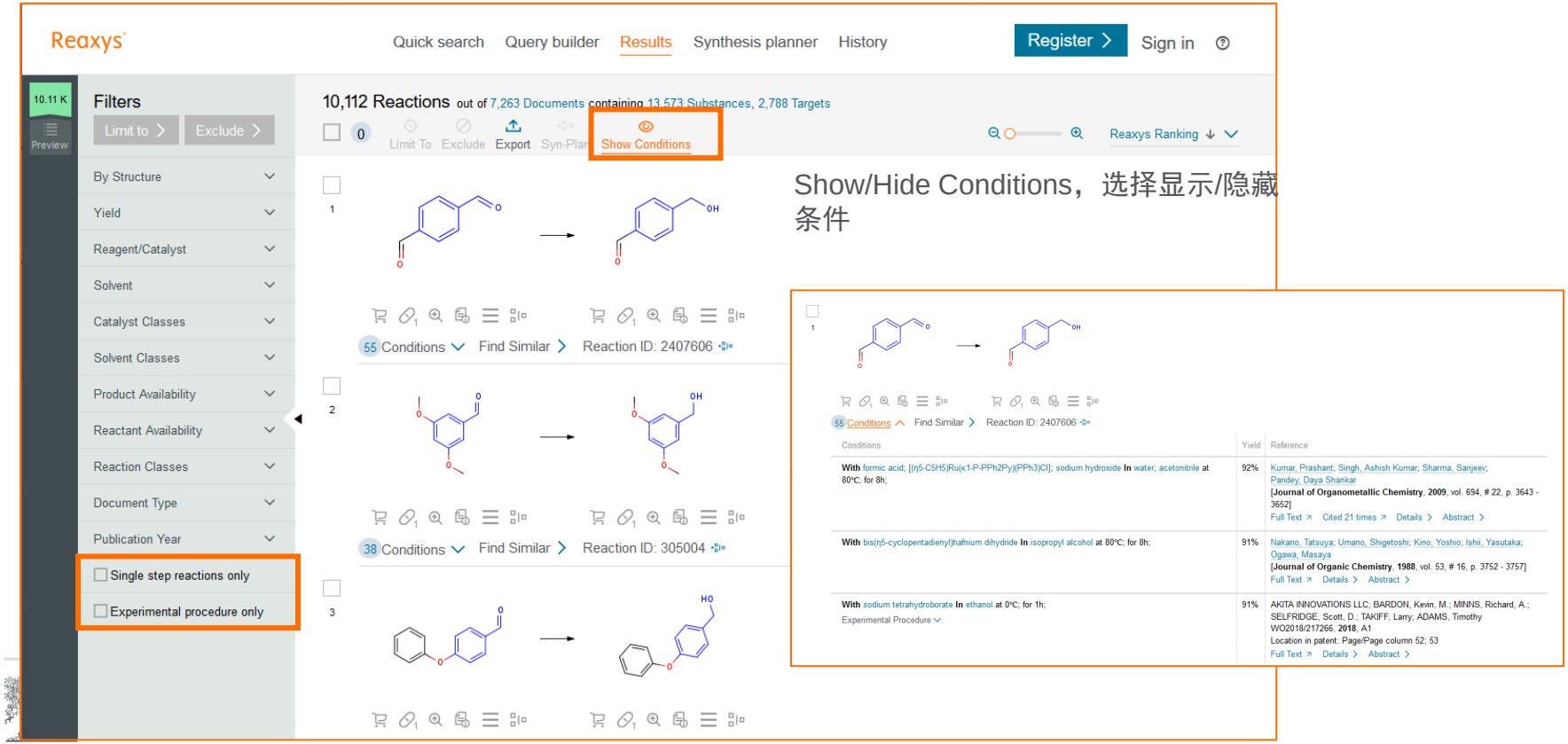
2022新版结构面板	视频链接		
1-最基本功能	https://www.bilibili.com/video/BV1Jm4y1F7hG		
2-不定位键	https://www.bilibili.com/video/BV1xP4y127G9		
3-缩写写官能团	https://www.bilibili.com/video/BV16K411o72c		
4-通用官能团与G	https://www.bilibili.com/video/BV16P4y1y7QA		
5-原子列表与列表非	https://www.bilibili.com/video/BV1w84y117yD		
	R基团与Linker：	关于R基团的讨论	
6,7-R基团的使用与讨论	https://www.bilibili.com/video/BV1Ze4y1p7hx	https://www.bilibili.com/video/BV1w14y1n7dD	
	讨论1：基本使用方法和逻辑	讨论2：取代基的控制	讨论3：As Draw的控制
8,9,10-检索模式的讨论	https://www.bilibili.com/video/BV1rG4y1V7Hw	https://www.bilibili.com/video/BV1aG4y1G7cb	https://www.bilibili.com/video/BV1k14y1n76d
11-反应的基本定义	https://www.bilibili.com/video/BV17W4y1p7p1		
12-配位化合物同位素盐	https://www.bilibili.com/video/BV15v4y1R7xb		
	属性列表讨论（上）	属性列表讨论（下）	
13,14-原子属性列表	https://www.bilibili.com/video/BV1UM411B7rQ	https://www.bilibili.com/video/BV1KW4y1T7Pv	
15-键的控制	https://www.bilibili.com/video/BV1LD4y1h79d		
16-More Option	https://www.bilibili.com/video/BV1U84y147ao		

Case 6：Reaxys中最简单的反应定义与筛选

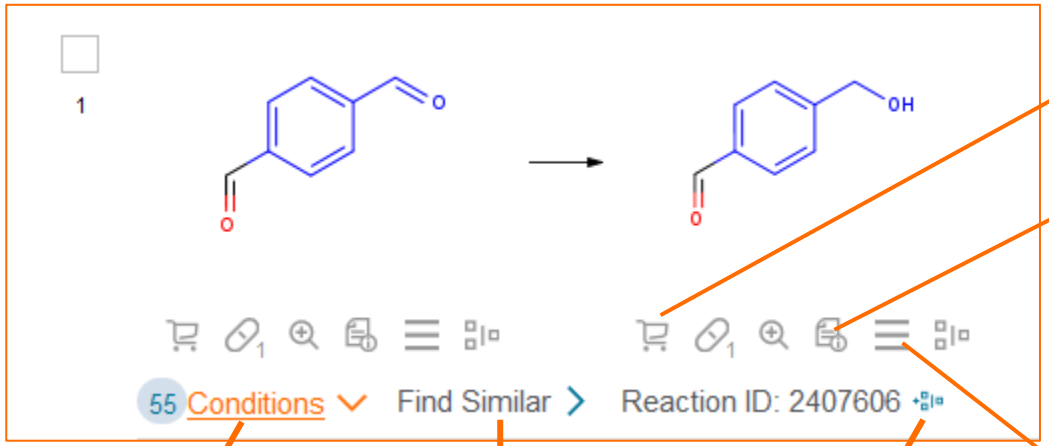
- 检索以下核心结构反应并进行反应筛选操作
- 视频操作过程
  - https://www.bilibili.com/video/BV1BT4y1F7vT



Reaxys中的结果

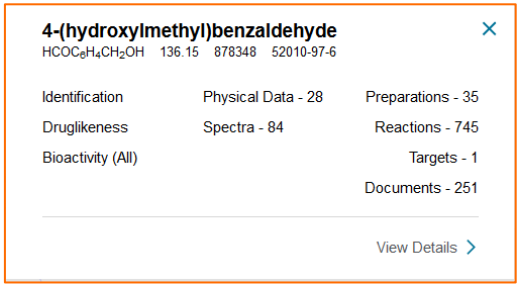

Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Register
Sign in
10.11 K
Preview
Filters
Limit to
Exclude
10,112 Reactions out of 7,263 Documents containing 13,573 Substances, 2,788 Targets
Limit To
Exclude
Export
Syn-Plan
Show Conditions
Reaxys Ranking
By Structure
Yield
Reagent/Catalyst
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

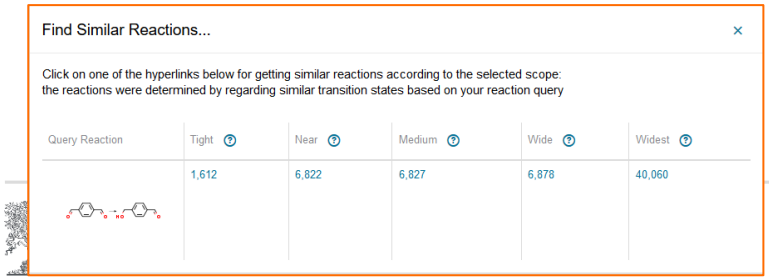


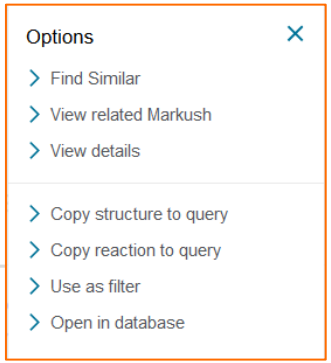
查看条件

寻找相似反应

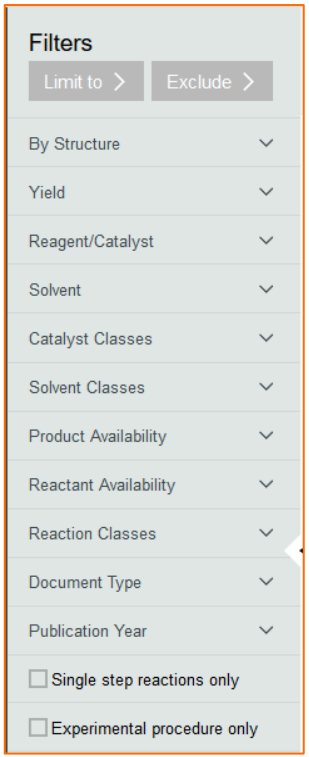
合成计划按钮

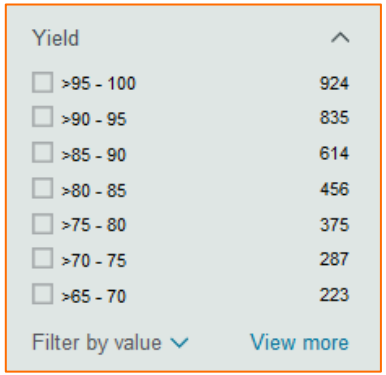
更多与物质相关操作

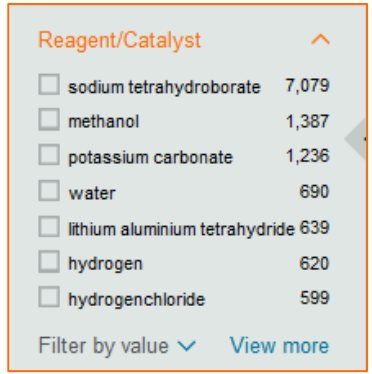


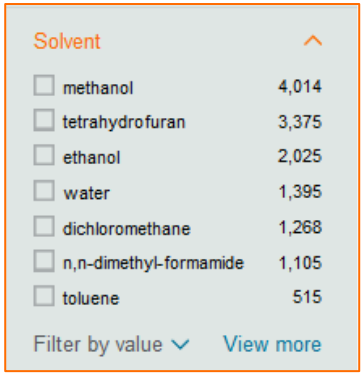


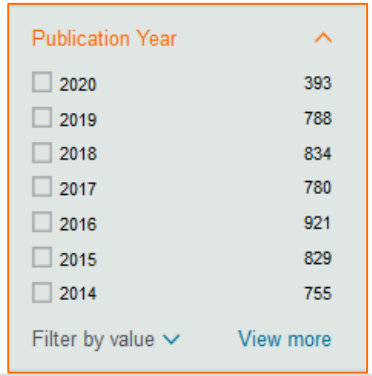
Reaxys的筛选操作











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

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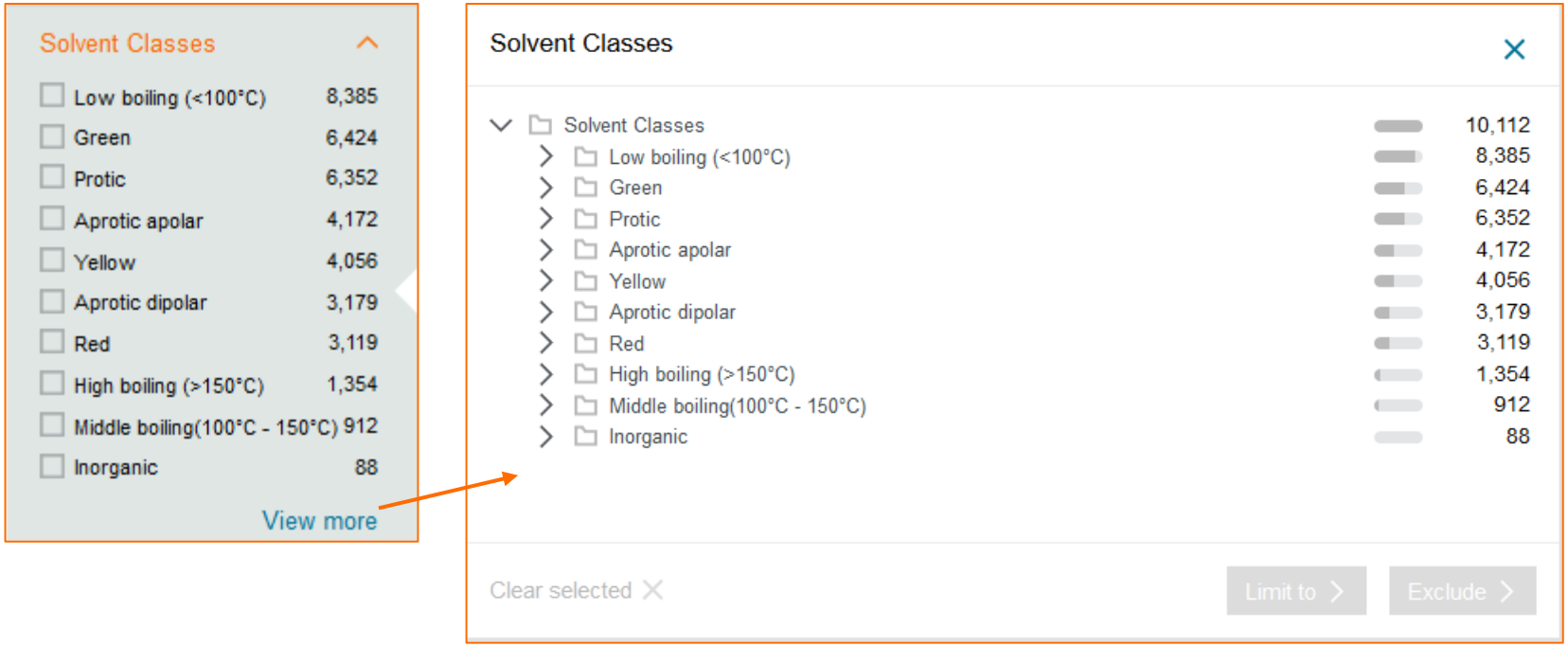
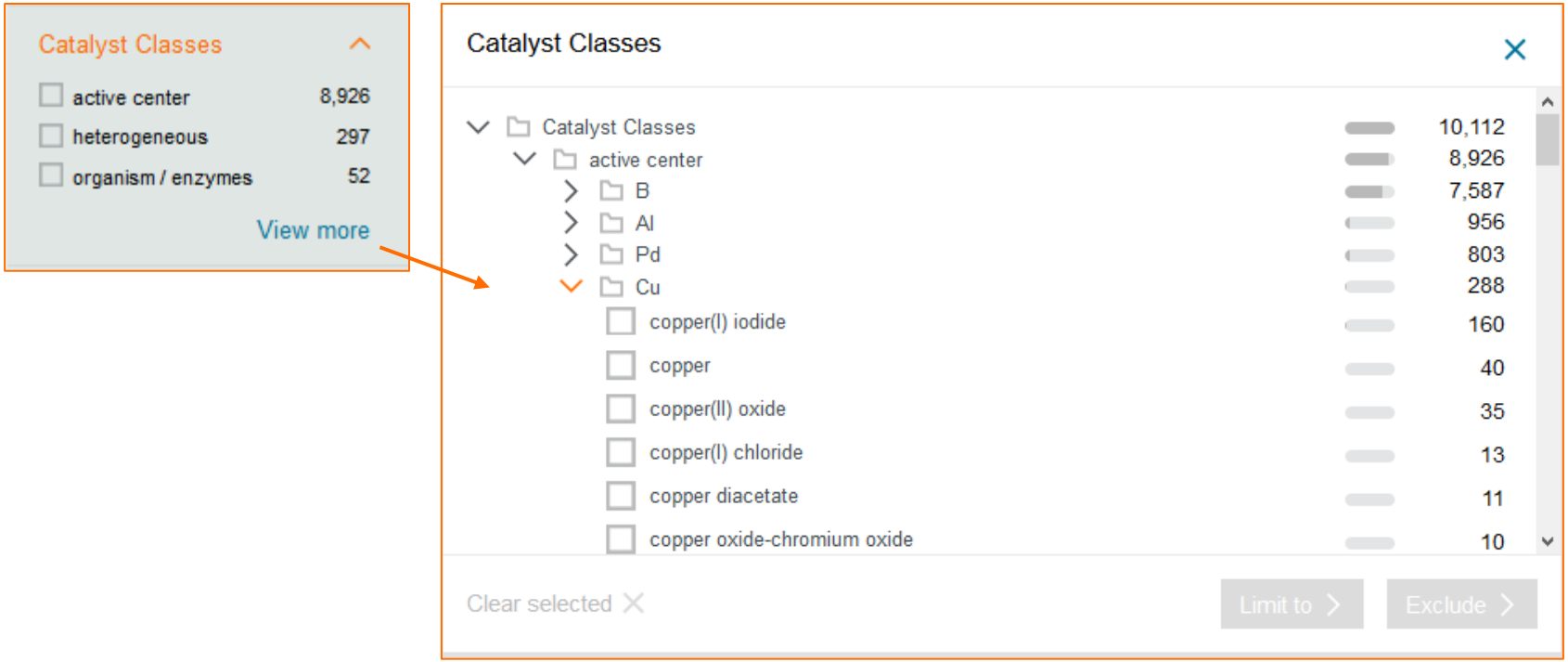
Reaxys中的一些特殊筛选工具—溶剂分类



Reaxys中的一些特殊筛选工具—催化剂分类



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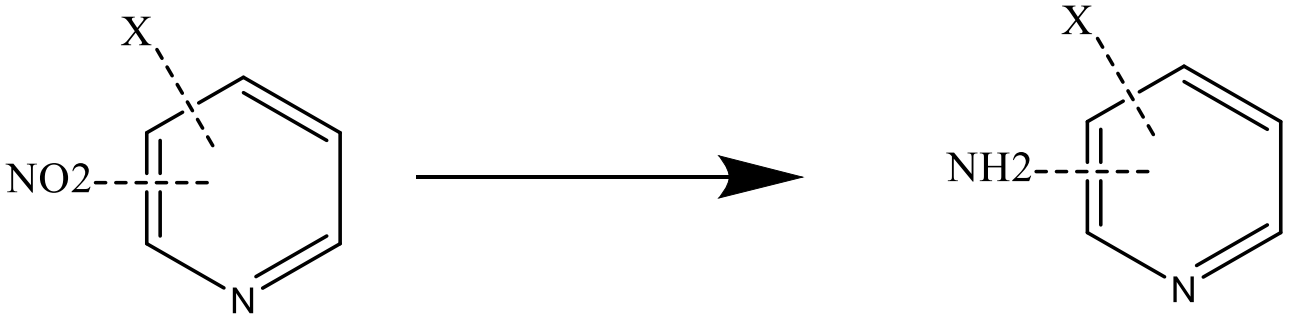
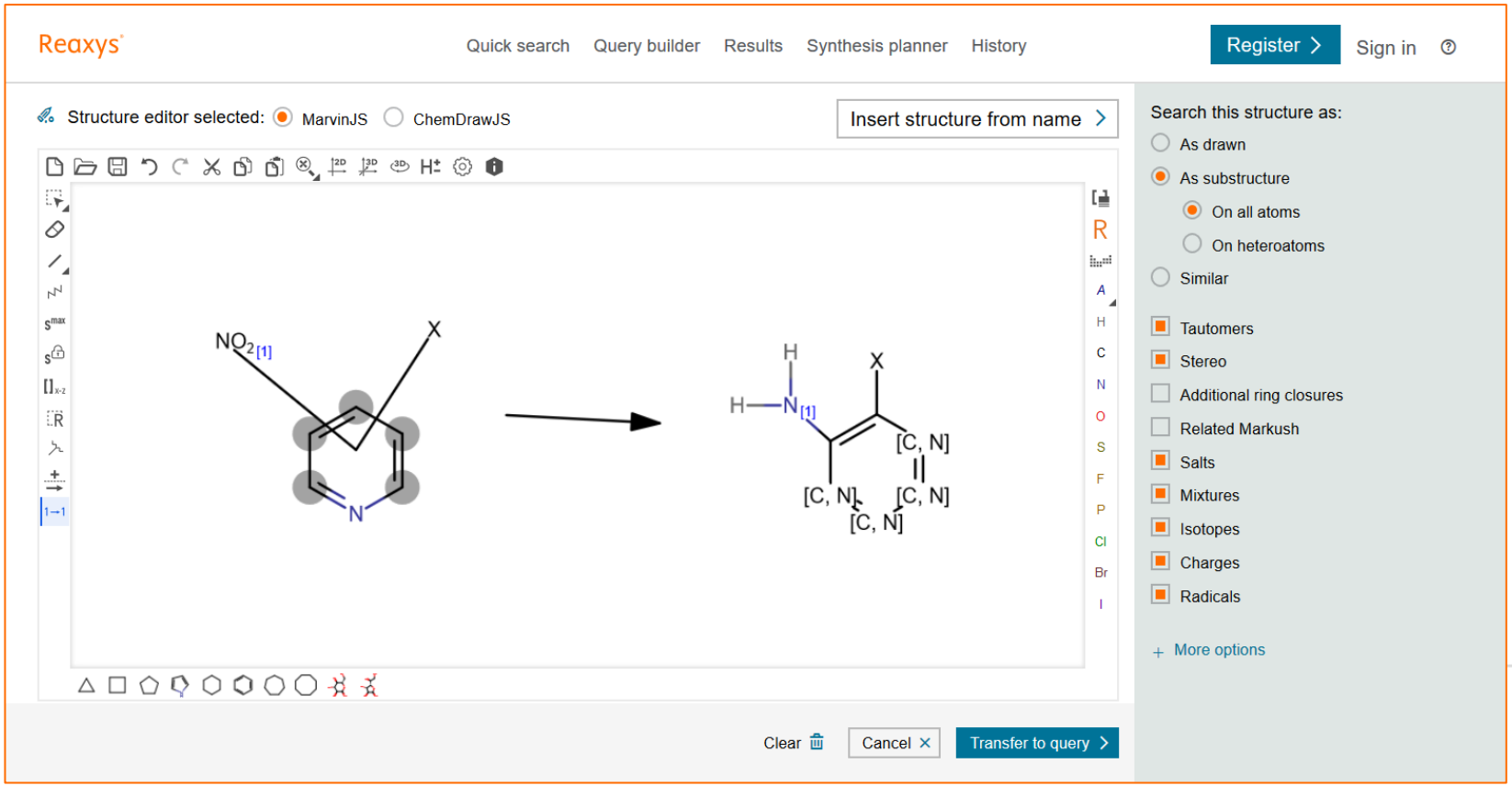
Case 7：结构中有特殊需求的反应定义

- 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

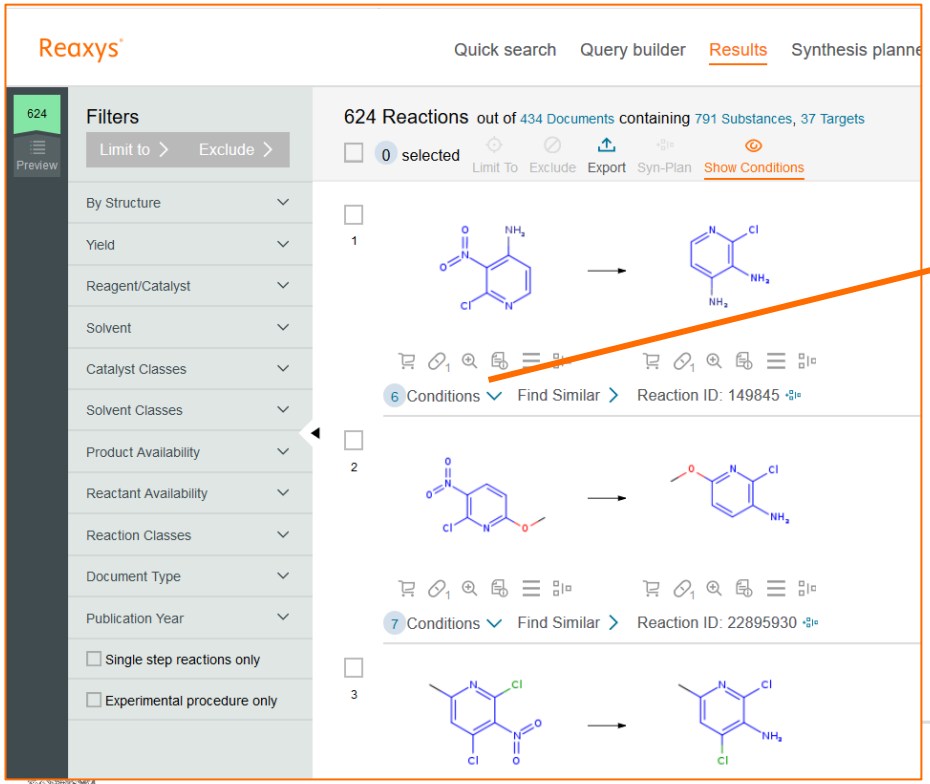


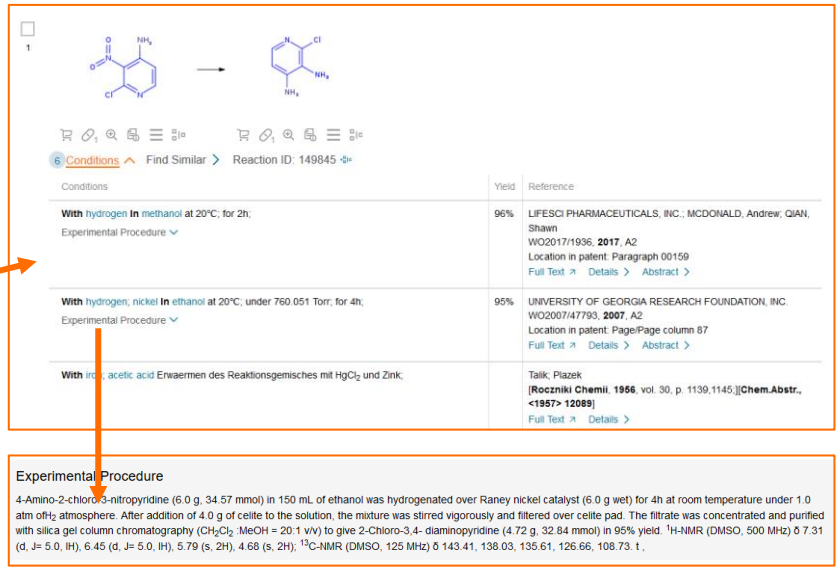
视频操作过程：
https://www.bilibili.com/video/BV1si4y177as

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。

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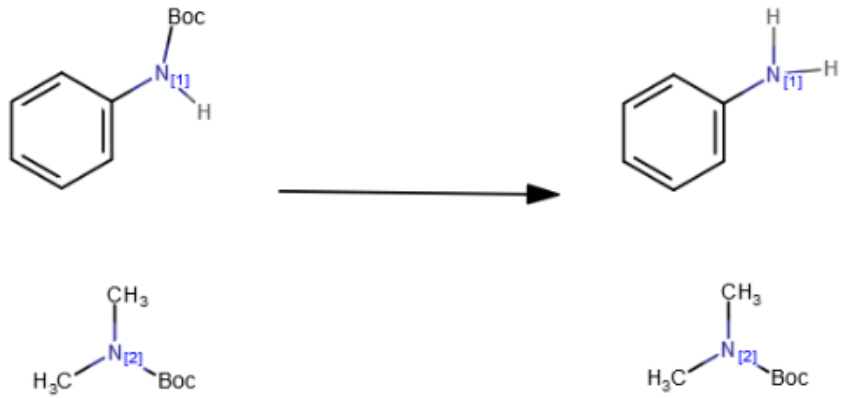
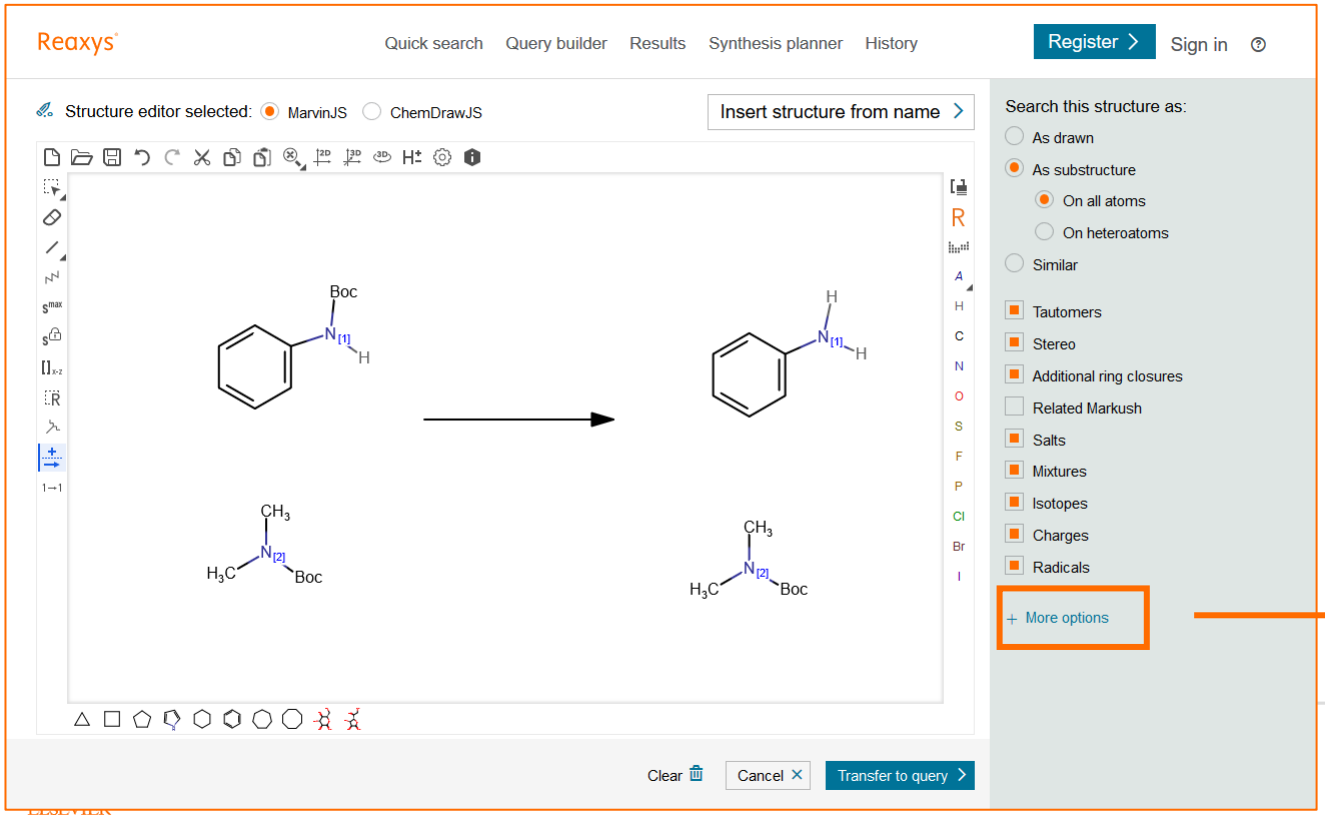
Case 8：选择性氧化还原脱保护反应的定义

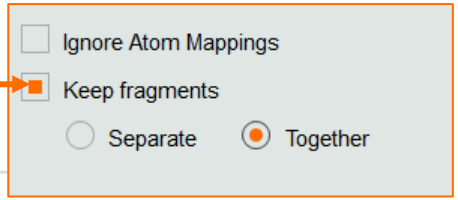
- 结构中两个带Boc的片段，两个片段以任意的形式相接在一个分子中
- 反应过后把其中一个片段的Boc脱掉，但是另外一个Boc不变



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

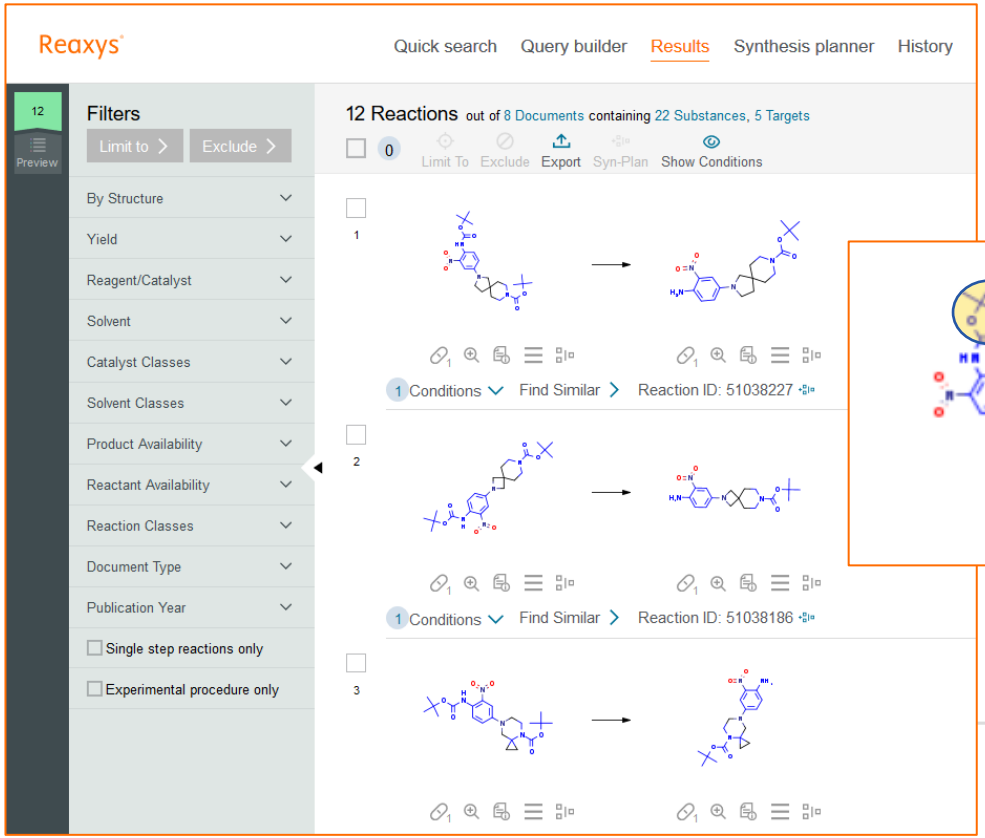
Reaxys中的结构定义

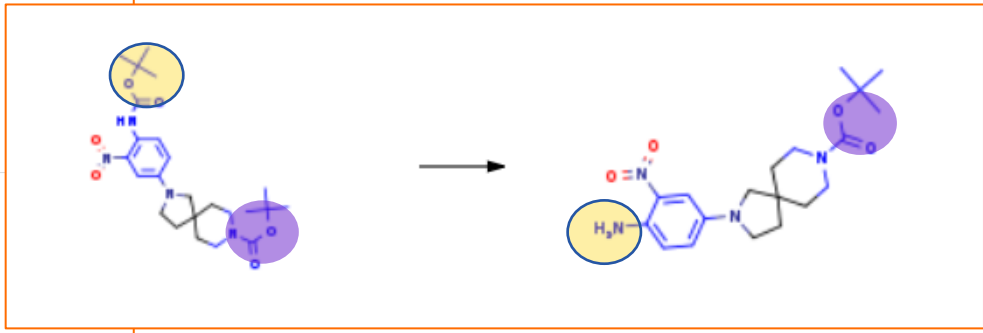




Reaxys可以直接设定这些片段在一个结构中

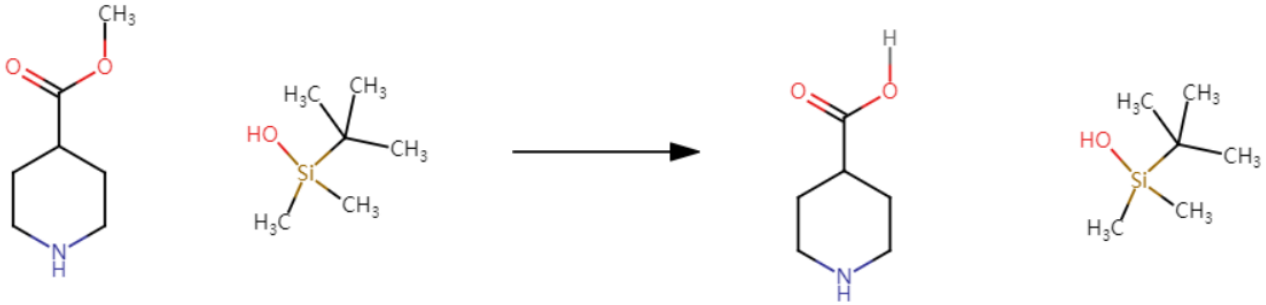
Reaxys中结果


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



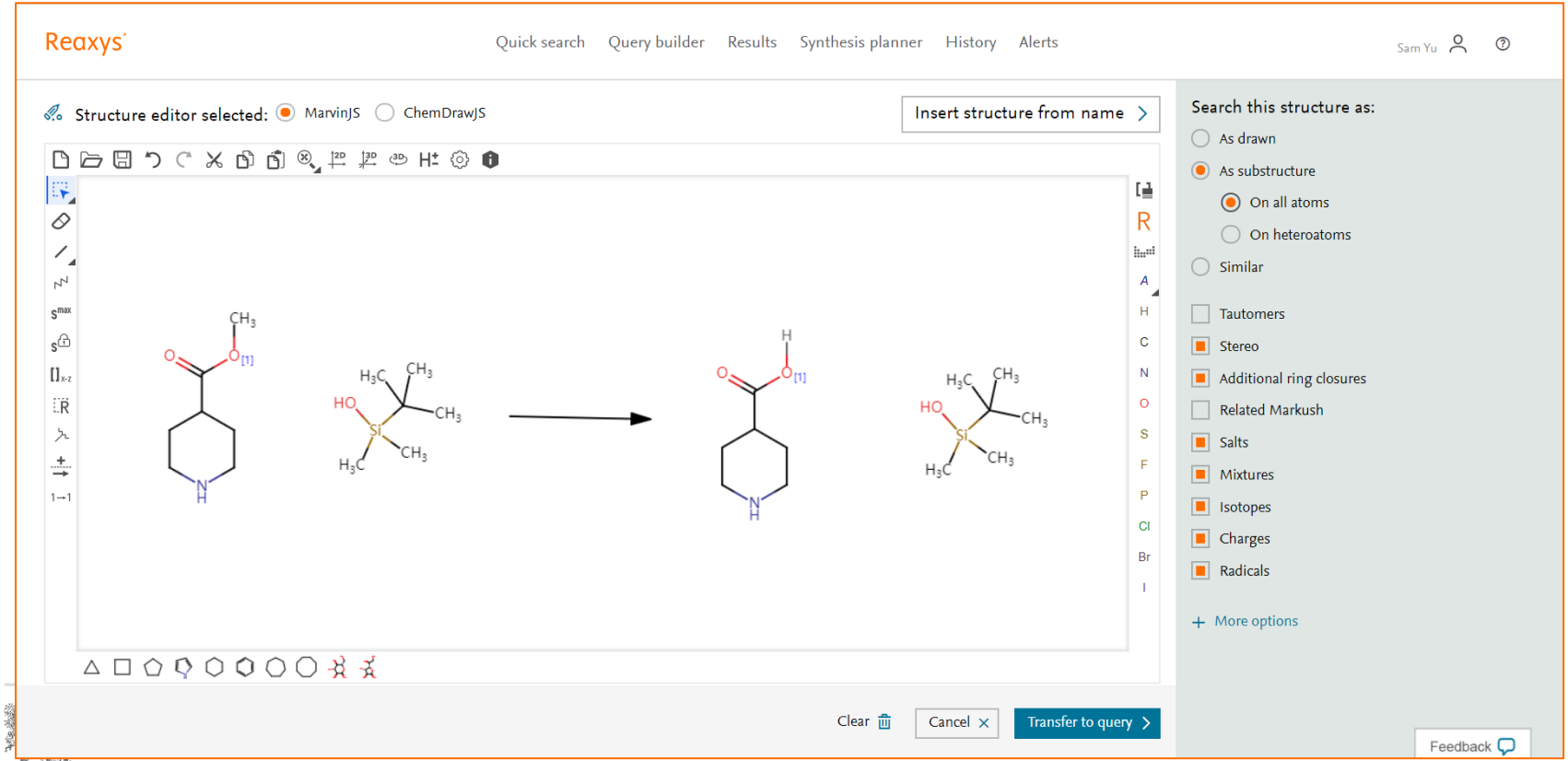
Case 9：检索结果不理性时的拓展策略

- 在硅基存在的情况下，水解脂基
- 检索结果不太好，如何扩展结果

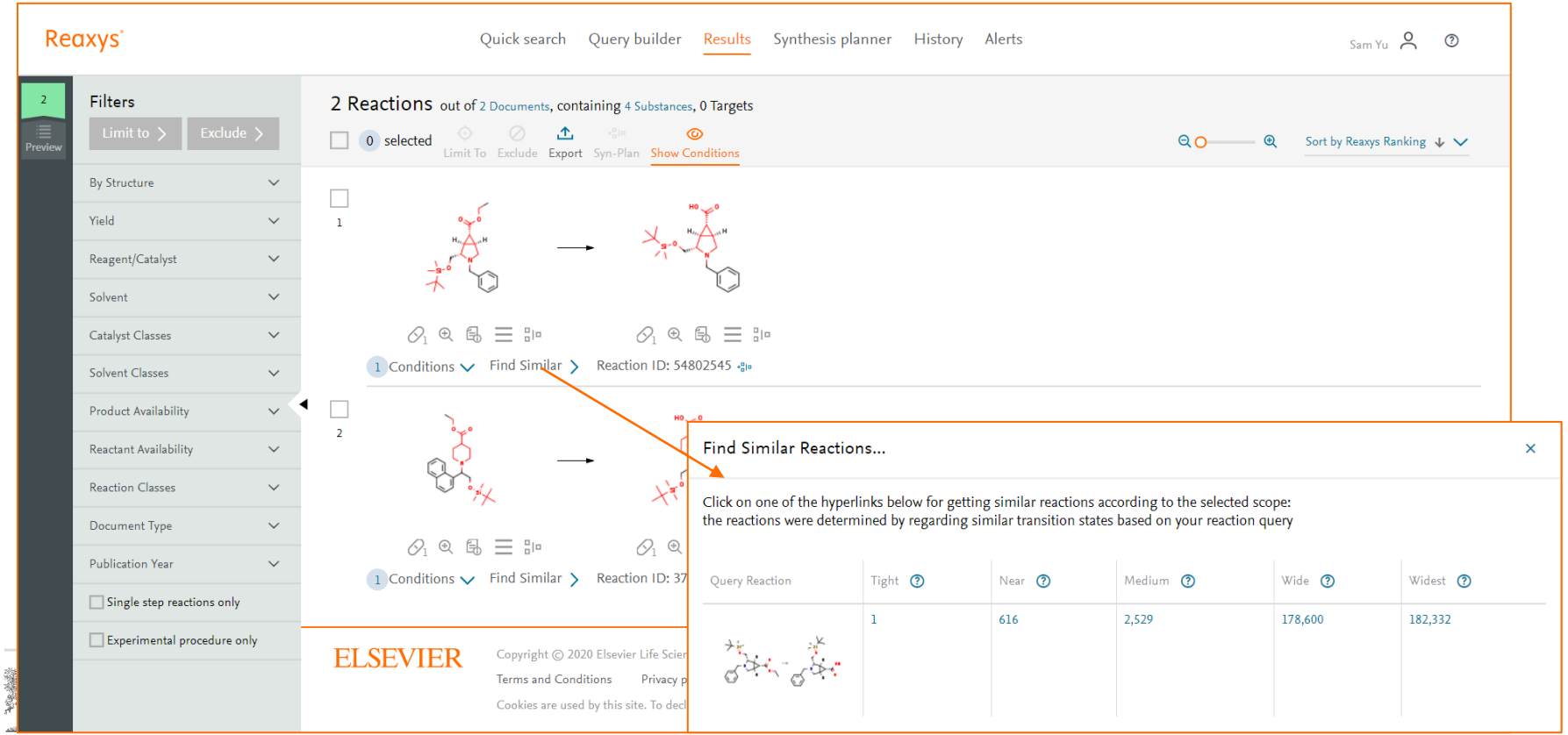


视频操作: https://www.bilibili.com/video/BV14A41147gL

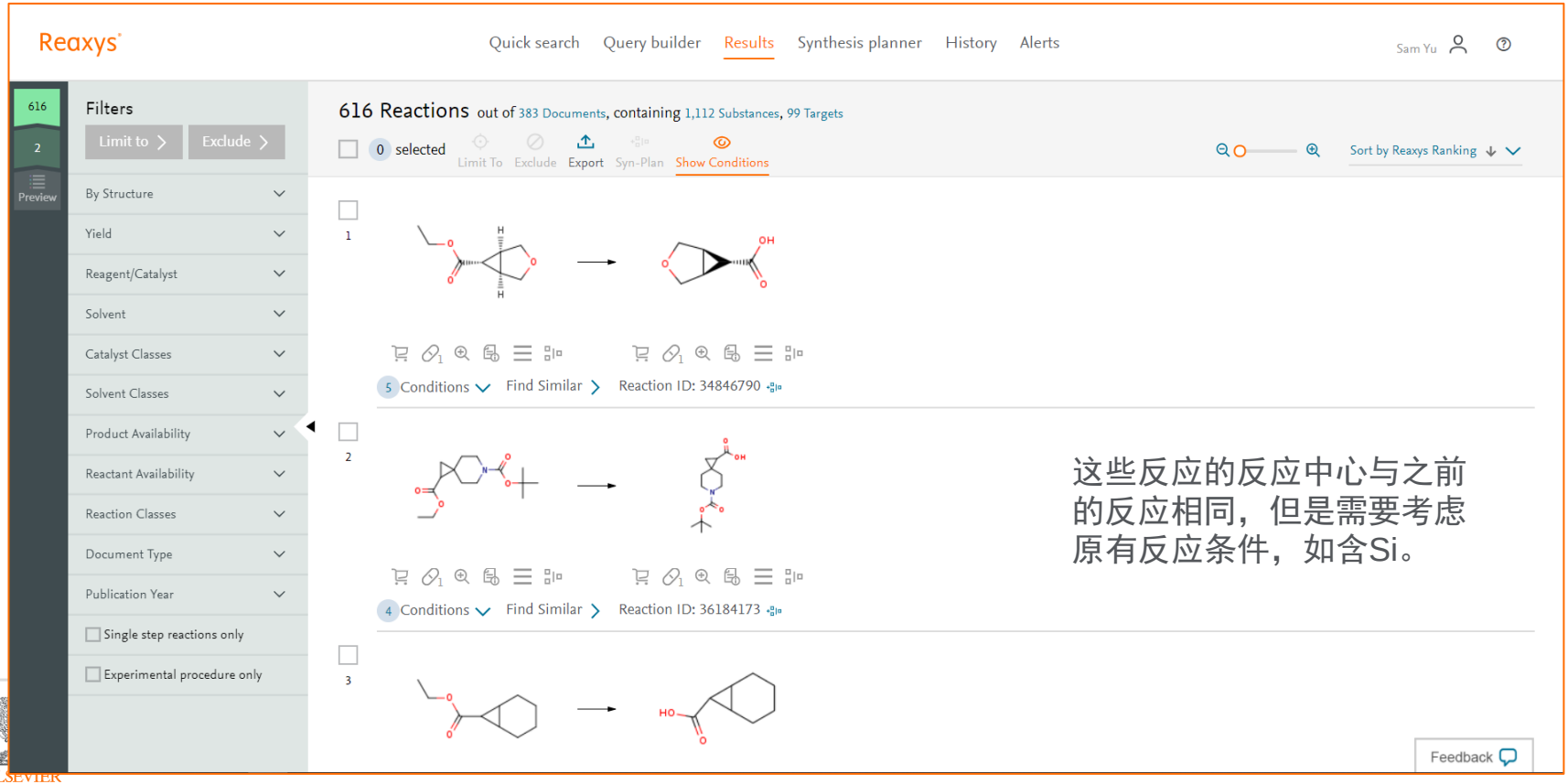
利用Reaxys的碎片反应检索策略



最后的结果

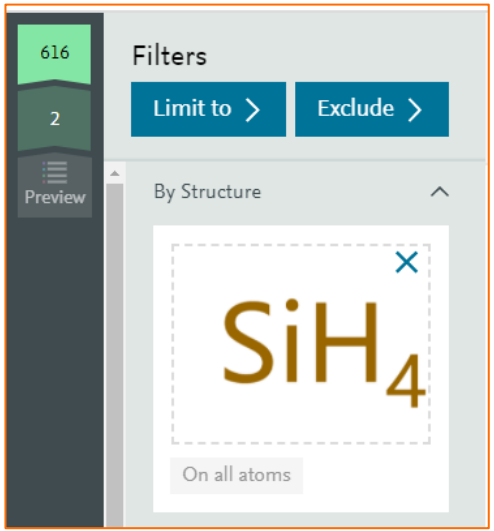

Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Sam Yu
Filters
Limit to
Exclude
Preview
By Structure
Yield
Reagent/Catalyst
Solvent
Catalyst Classes
Solvent Classes
Product Availability
Reactant Availability
Reaction Classes
Document Type
Publication Year
Single step reactions only
Experimental procedure only
2 Reactions out of 2 Documents, containing 4 Substances, 0 Targets
0 selected
Limit To
Exclude
Export
Syn-Plan
Show Conditions
Sort by Reaxys Ranking
1
1 Conditions
Find Similar
Reaction ID: 54802545
2
1 Conditions
Find Similar
Reaction ID: 37
Find Similar Reactions...
Click on one of the hyperlinks below for getting similar reactions according to the selected scope:
the reactions were determined by regarding similar transition states based on your reaction query
Query Reaction
Tight
Near
Medium
Wide
Widest
1
616
2,529
178,600
182,332
ELSEVIER
Copyright © 2020 Elsevier Life Scier
Terms and Conditions
Privacy p
Cookies are used by this site. To decl

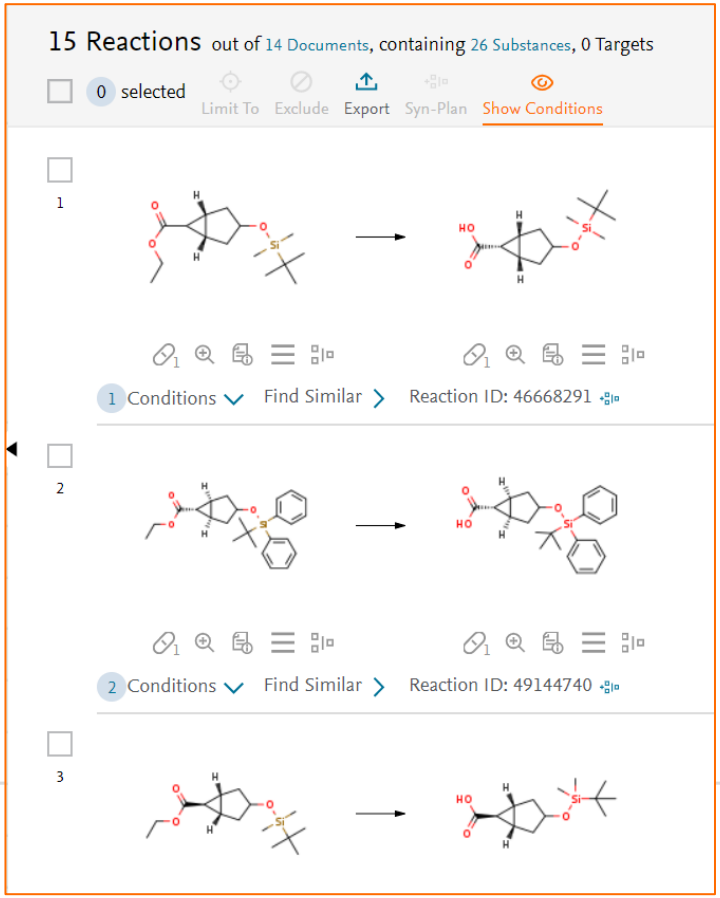
发现检索到的结果中并没有Si



这些反应的反应中心与之前的反应相同，但是需要考虑原有反应条件，如含Si。

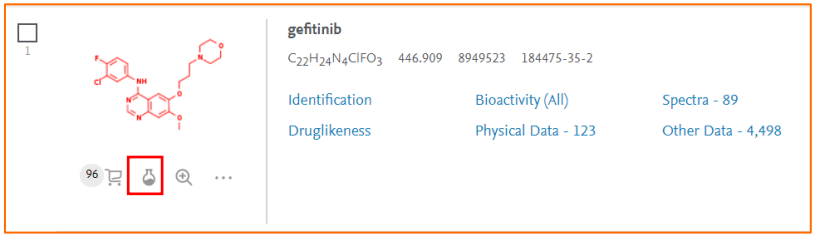
限定Si

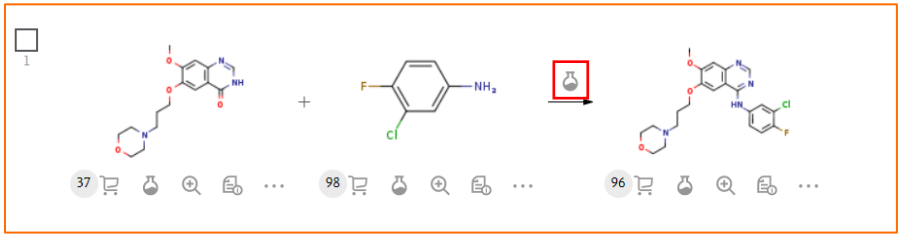


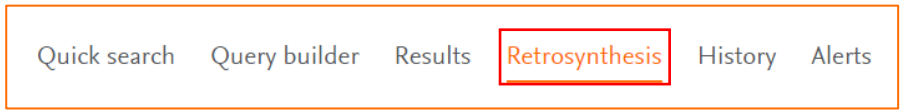


Case 10：Reaxys中合成计划的制作

- 针对具体的化合物进行合成计划制作
  - 需要自行注册账号才可以用这个功能
  - 可以直接从物质界面，或者反应界面直接进入，也可以通过Retrosynthesis功能进入

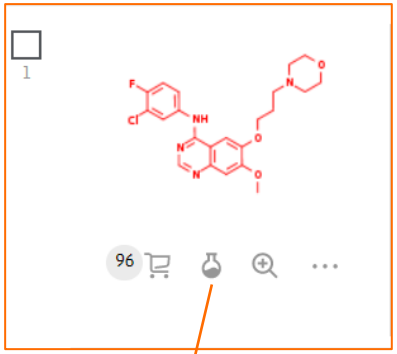


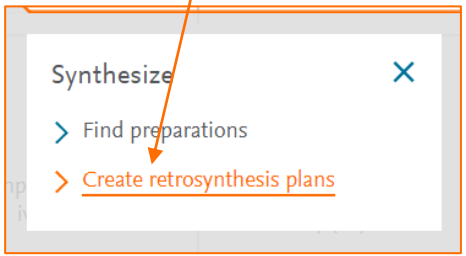


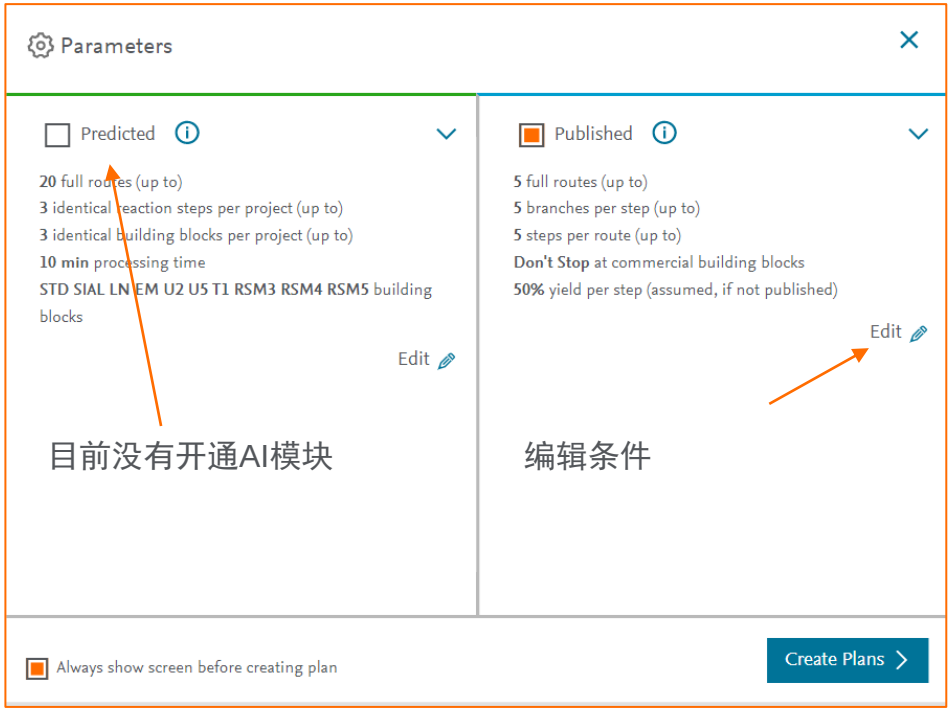


视频操作过程：
https://www.bilibili.com/video/BV1oL411u7yP

从具体物质出发的合成计划制作







条件的编辑及结果

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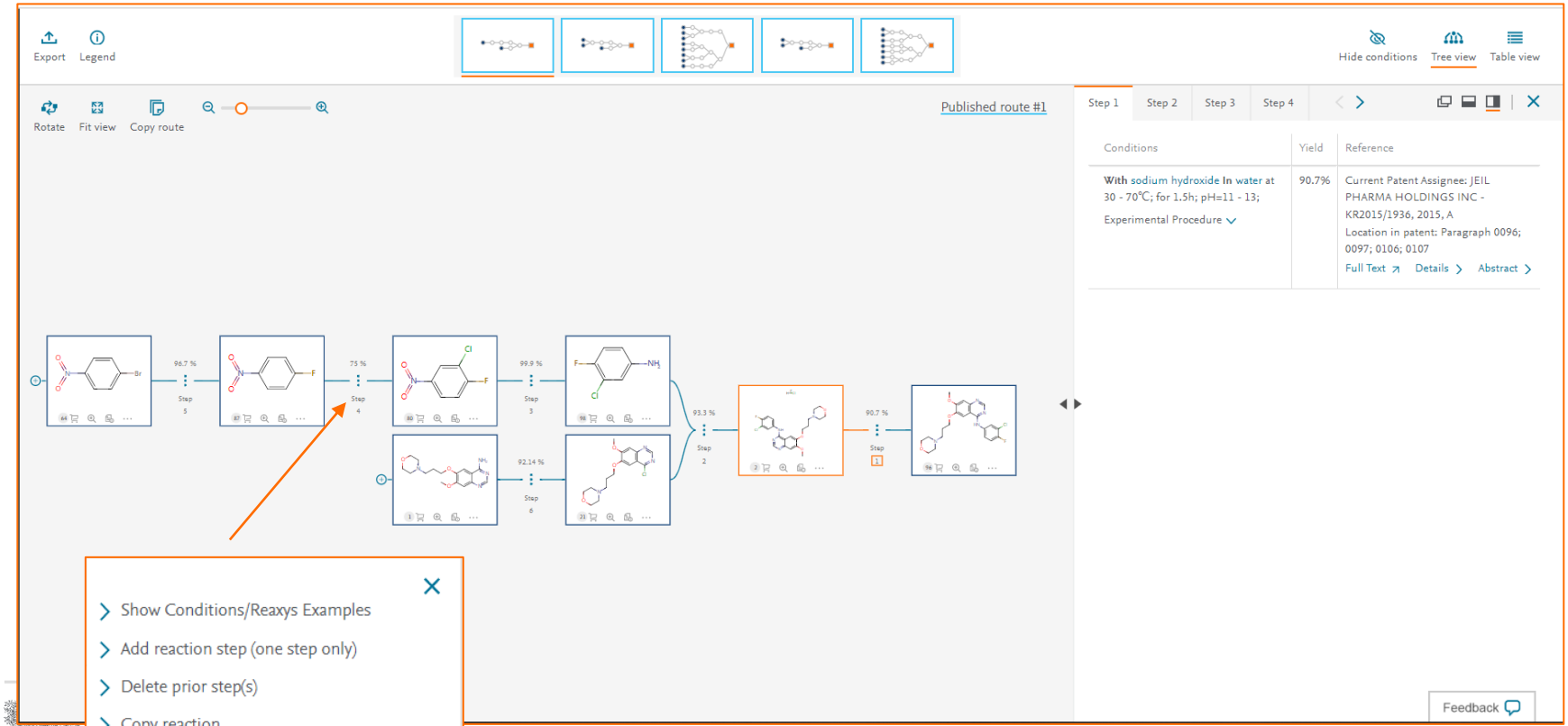
结果的呈现



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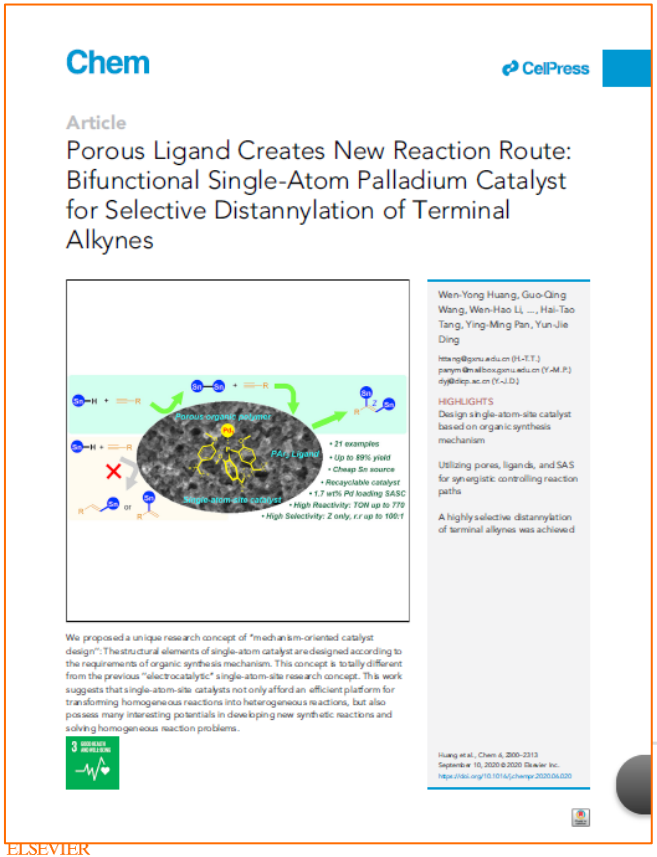
Agenda

- Reaxys介绍与内容
  - Reaxys介绍
  - Reaxys对于科技文献的提炼
- Reaxys中的化学科学数据获取
  - Reaxys中的关键词检索
  - Reaxys中物质理化性质数据的查询与反向物质获取
  - Reaxys中结构面板与物质结构和反应数据的获取
  - Reaxys中的实用小案例
- Q&A

Case 11：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

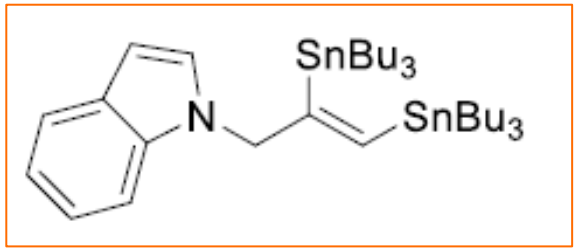
A highly selective distannylation of terminal alkynes was achieved

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？

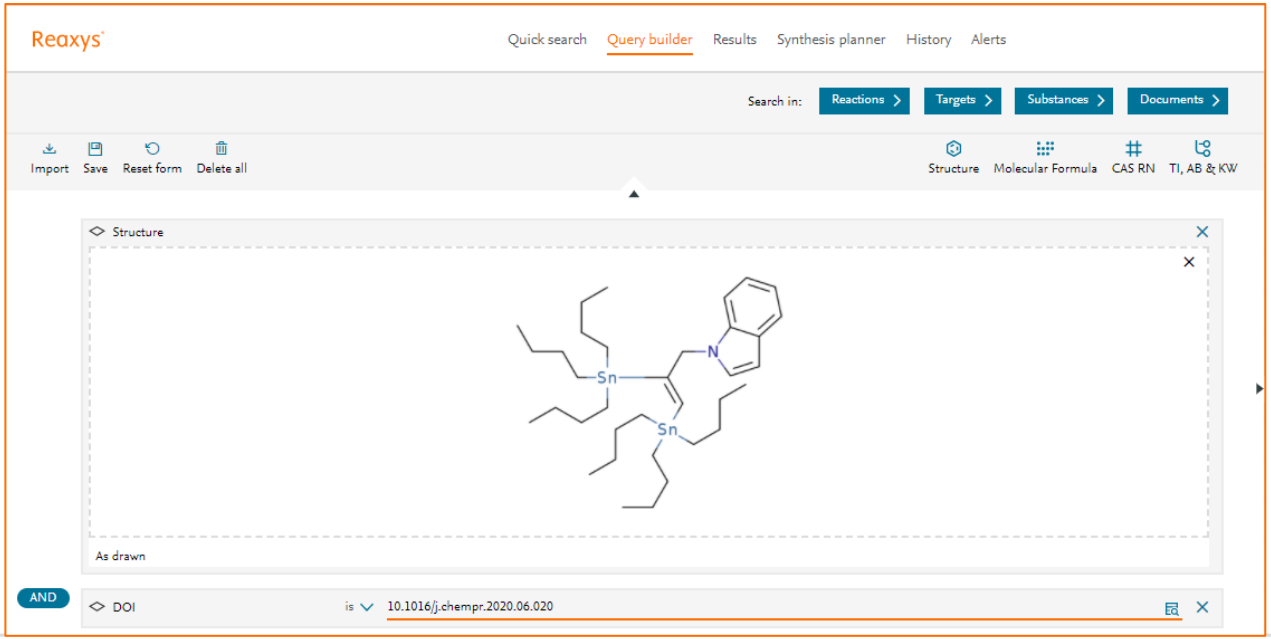


视频操作过程：

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



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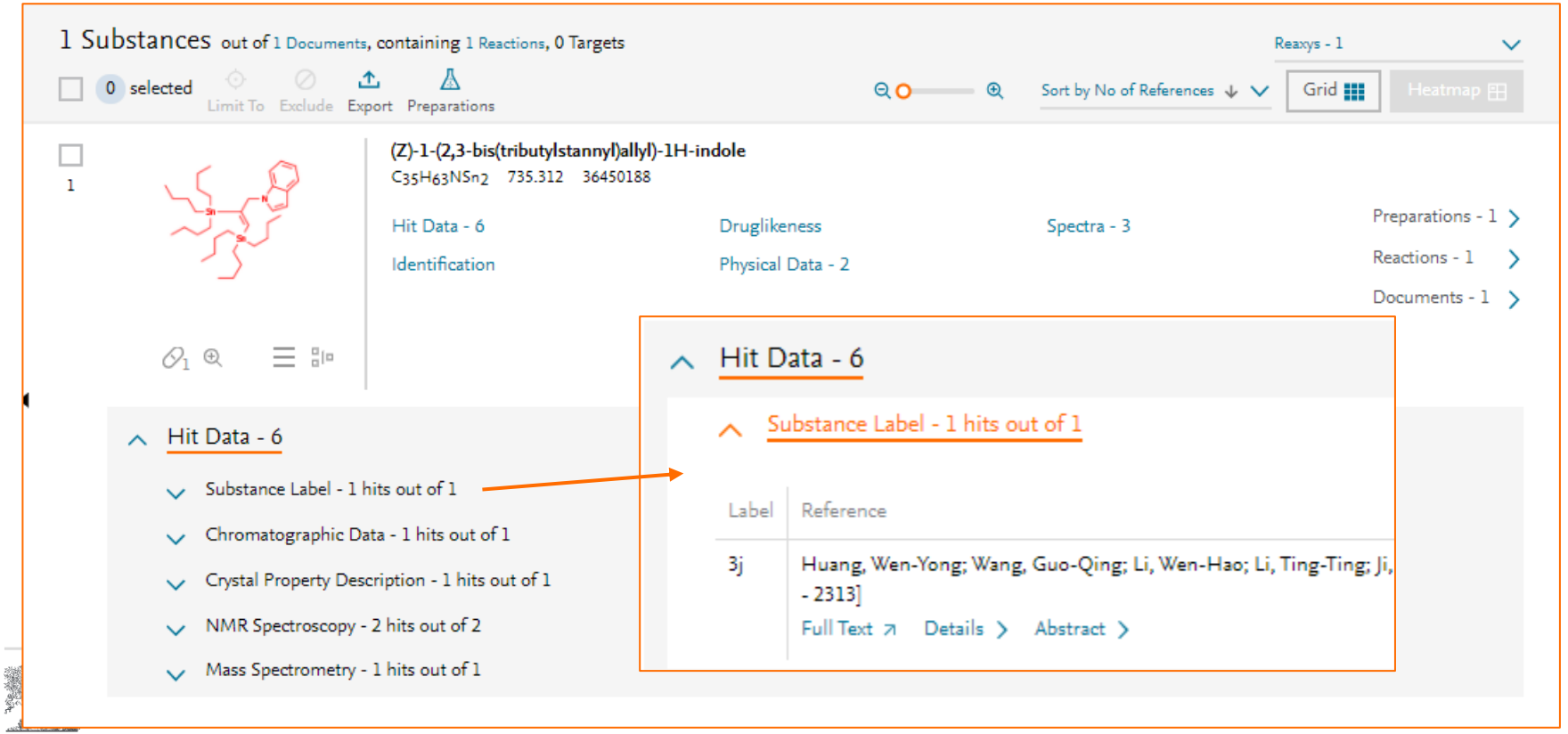
Reaxys中的结果



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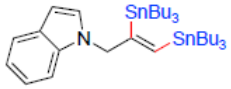
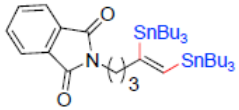
全文检索3J定位化合物

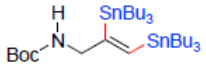
N-containing terminal alkynes



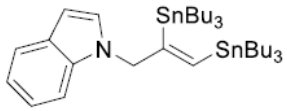
3j 89% (100:1)



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,

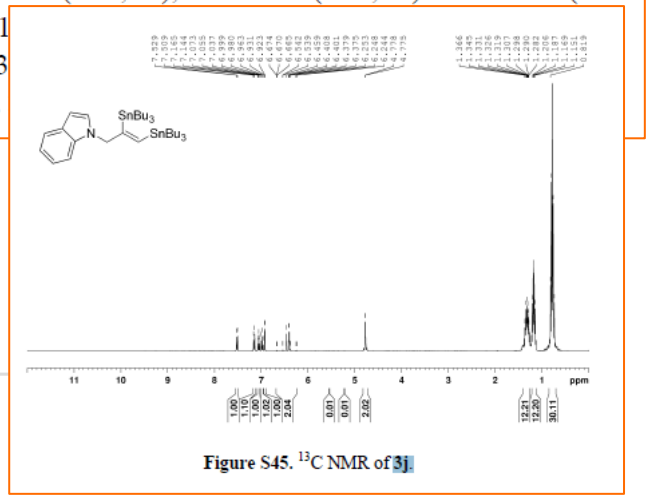
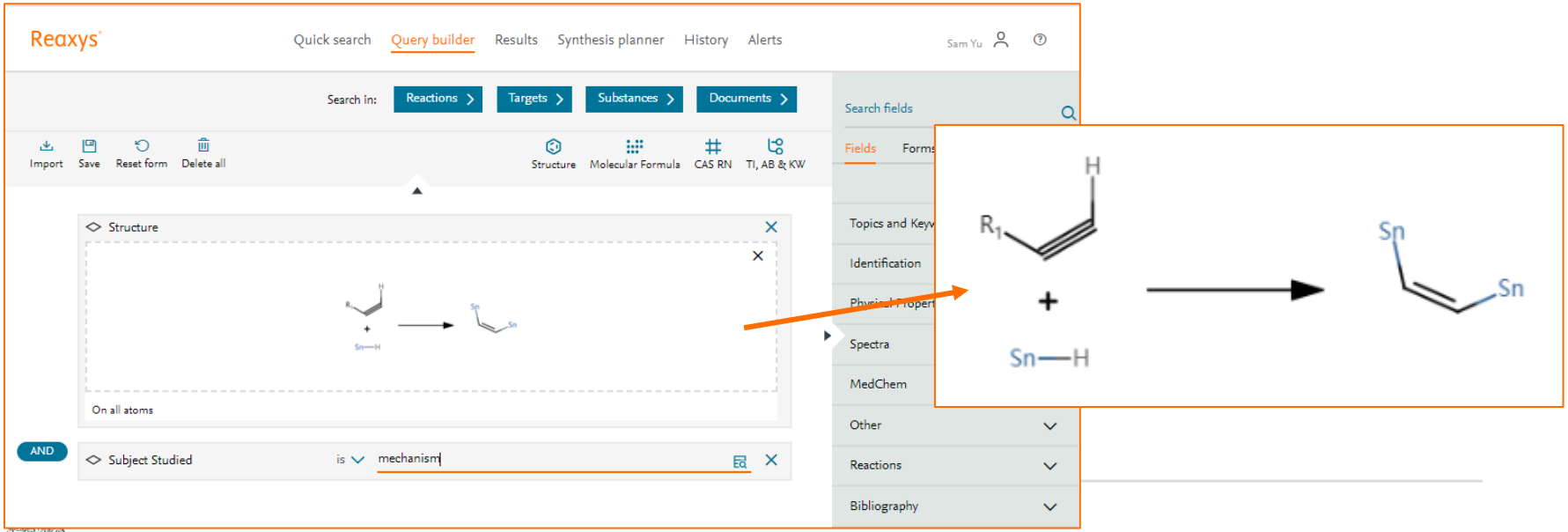


Figure S45. ^{13}C NMR of **3j**.

用于文献中化合物信息的快速定位。

Case 12：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



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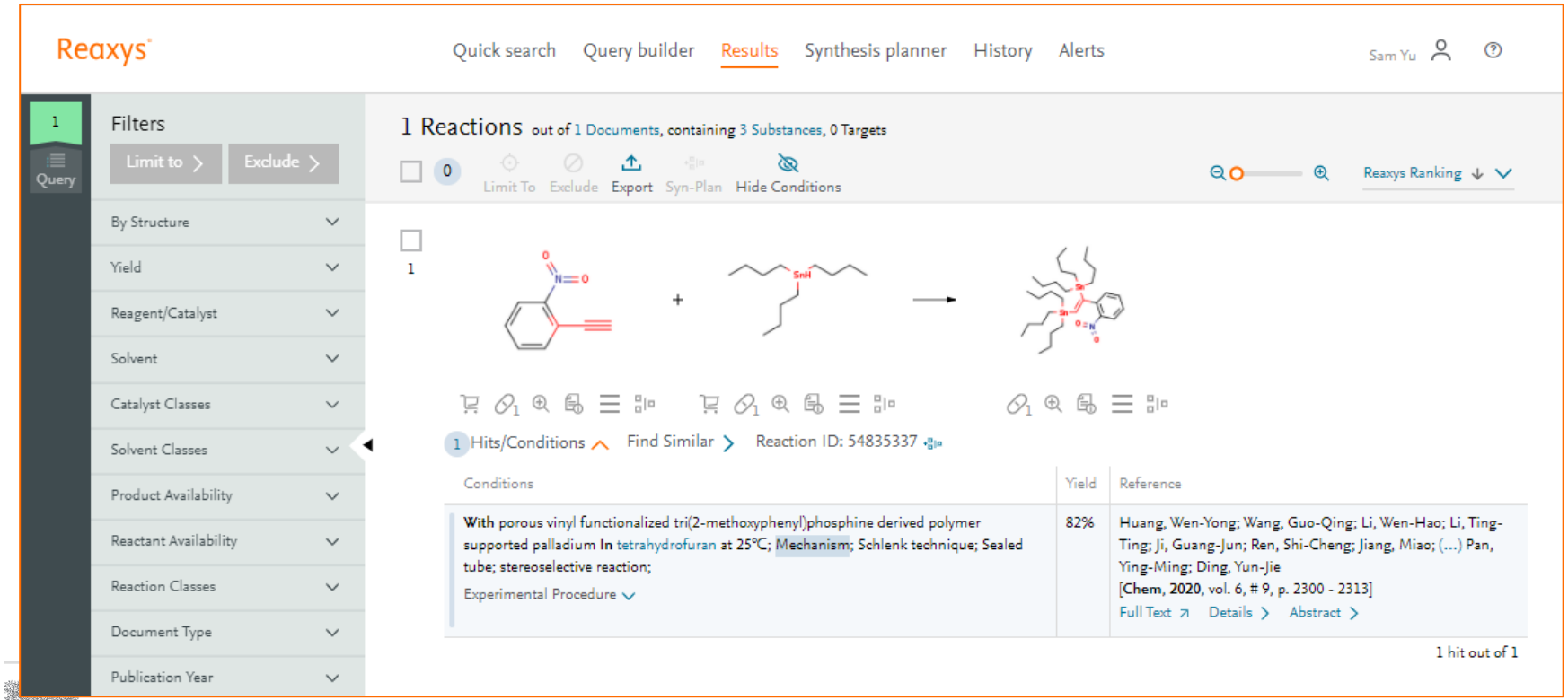
最后的结果



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Reaxys小结

- Reaxys拥有便捷的使用方式，IP范围内授权，不限制同时登录人数，可以自由注册ID。
- 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：
  - 添加微信小助手ELS-LSS邀请进用户群：获取最新的咨询以及Q&A
  - 关注B站Up主（非官方）：ELS生命科学，获取所有Elsevier Life Science数据库的使用视频
  - 微信公众号（非官方）：闲谈化学药学数据获取，检索原理与检索心得分享

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Thank you