Elsevier
Reaxys中化学信息的获取

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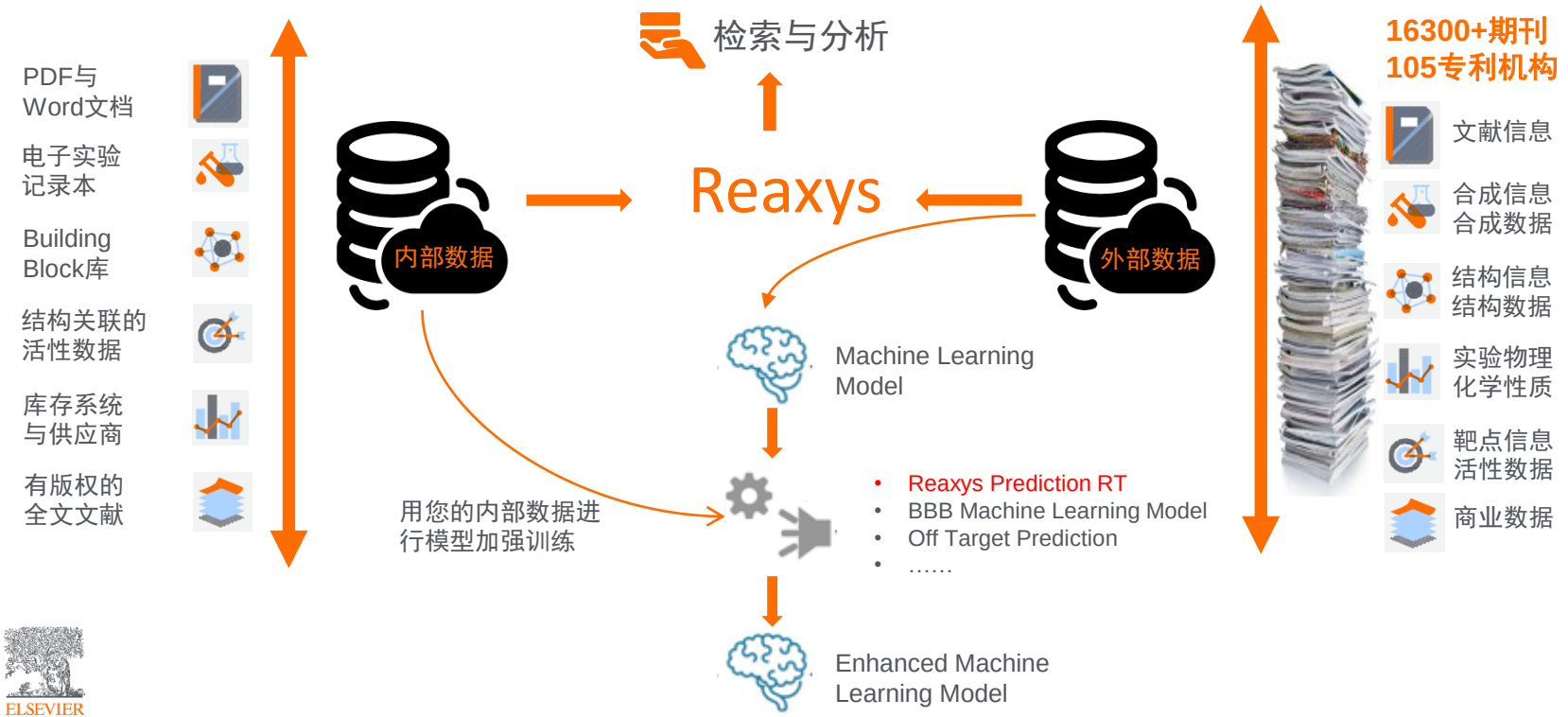
Agenda

- 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中的科技文献检索与分析
  - 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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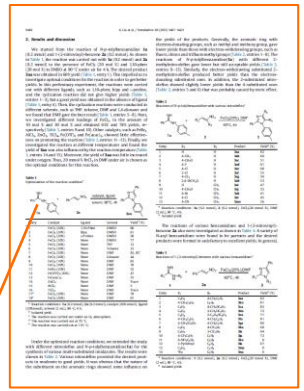
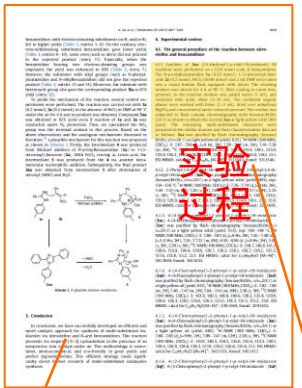
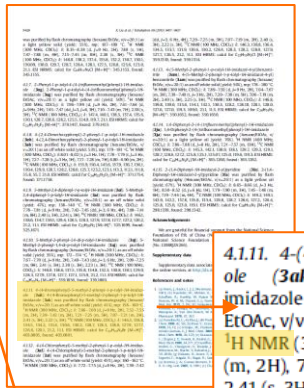
一篇常见的化学相关文献的构成





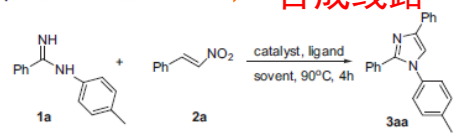


实验过程

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。

Table 1
Optimization of the reaction condition[a]

合成线路



结论

*4.1.11. 4-(4-Bromophenyl)-5-methyl-2-phenyl-1-p-tolyl-1H-imidazole (**3ak**).* 4-(4-Bromophenyl)-5-methyl-2-phenyl-1-*p*-tolyl-1*H*-imidazole (**3ak**) was purified by flash chromatography (hexane/EtOAc, v/v=20:1) as an off white solid (yield: 41%), mp: 158–160 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ: 7.66–7.69 (d, *J*=9 Hz, 2H), 7.52–7.55 (m, 2H), 7.39–7.42 (m, 2H), 7.21–7.25 (m, 5H), 7.07–7.21 (m, 2H), 2.41 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ: 146.3, 138.8, 134.5, 134.2, 131.4, 130.6, 130.2, 128.7, 128.3, 128.0, 127.9, 127.7, 126.6, 120.1, 21.2, 11.1. ESI HRMS: calcd for $C_{22}H_{19}N_2Br$ [M+H]$^+$: 403.0805, found: 403.0801.

- 新的催化剂
- 3+2环化加成
- 区域选择性
- 环保

3. Conclusion

In conclusion, we have successfully developed an efficient and novel catalytic approach for synthesis of multi-substituted imidazoles via nitroolefins and *N*-aryl benzamidines. This reaction proceeds via stepwise [3+2] cycloaddition in the presence of an inexpensive iron catalyst under air. This methodology is convenient, atom-economical, and eco-friendly in good yields and prefect regioselectivities. This efficient strategy could significantly direct further research of multi-substituted imidazoles synthesis.

4.1. The general procedure of the reaction between nitroolefins and benzamidines

*4.1.1. Synthesis of **3aa** (2,4-diphenyl-1-p-tolyl-1H-imidazole).* All reactions were performed on a 0.20 mmol scale of benzamidine. The *N*-*p*-tolylbenzamidine **1a** (0.20 mmol), 1-(2-nitrovinyl)-benzene **2a** (0.2 mmol), $FeCl_3$ (0.040 mmol) and 2 mL DMF were taken into a round bottom flask equipped with stirrer. The resulting mixture was stirred for 4 h at 90 °C. After cooling to room temperature, to the reaction mixture was added water (2 mL), and extracted with acetic ether (3×10 mL). The combined organic phases were washed with brine (2×5 mL), dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The residue was subjected to flash column chromatography with hexanes/EtOAc (20:1) as eluent to obtain the desired **3aa** as light yellow solid (90% yield). The remaining multi-substituted imidazoles were

化合物性质数据

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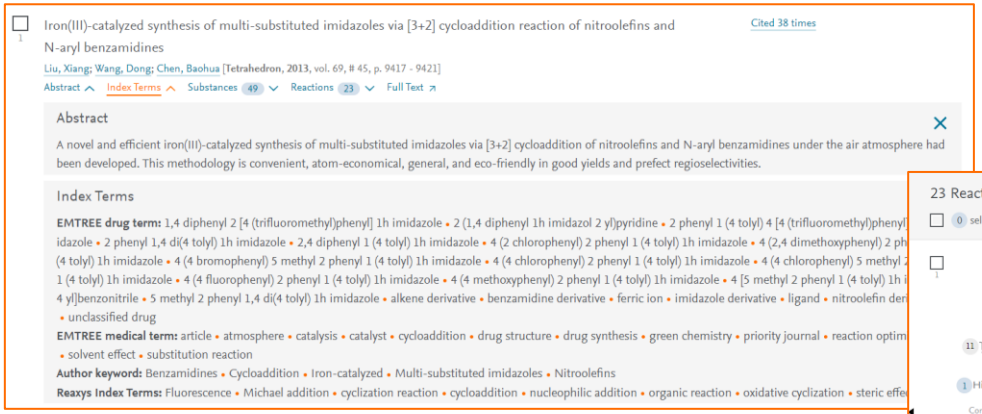
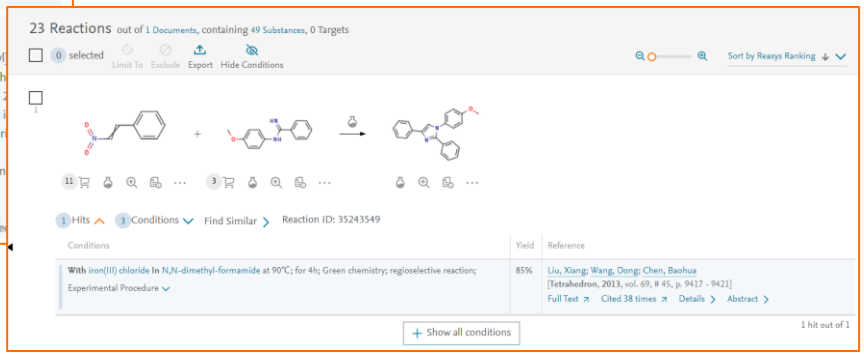
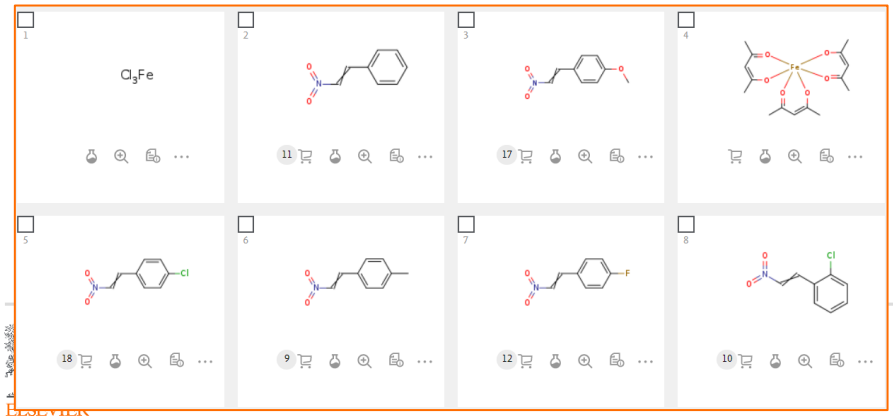
Reaxys对这篇全文的提炼—概览







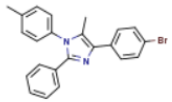
Reaxys提炼全文中的：

- 题录，摘要，关键词
- 物质结构，
- 反应Scheme

Reaxys对全文中的化合物（产物）的相关数据提炼

*4.1.11. 4-(4-Bromophenyl)-5-methyl-2-phenyl-1-p-tolyl-1H-imidazole (**3ak**).* 4-(4-Bromophenyl)-5-methyl-2-phenyl-1-*p*-tolyl-1*H*-imidazole (**3ak**) was purified by flash chromatography (hexane/EtOAc, v/v=20:1) as an off white solid (yield: 41%), mp: 158–160 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ: 7.66–7.69 (d, *J*=9 Hz, 2H), 7.52–7.55 (m, 2H), 7.39–7.42 (m, 2H), 7.21–7.25 (m, 5H), 7.07–7.21 (m, 2H), 2.41 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ: 146.3, 138.8, 134.5, 134.2, 131.4, 130.6, 130.2, 128.7, 128.3, 128.0, 127.9, 127.7, 126.6, 120.1, 21.2, 11.1. ESI HRMS: calcd for $C_{22}H_{19}N_2Br$ $[M+H]^+$: 403.0805, found: 403.0801.

46



4-(4-bromophenyl)-5-methyl-2-phenyl-1-(p-tolyl)-1H-imidazole

$C_{23}H_{19}BrN_2$ 403.321 24040362 1462876-22-7

Hit Data - 6 | Druglikeness | Spectra - 3

Identification | Physical Data - 2

NMR Spectroscopy - 2 hits out of 2

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Frequency (NMR Spectroscopy), MHz	Original Text (NMR Spectroscopy)
Chemical shifts, Spectrum	1H	chloroform-d1	300	^{1}H NMR (300 MHz, $CDCl_3$): δ: 7.66-7.69 (d, J=9 Hz, 2H), 7.52-7.55 (m, 2H), 7.39-7.42 (m, 2H), 7.21-7.25 (m, 5H), 7.07-7.21 (m, 2H), 2.41 (s, 3H), 2.22 (s, 3H)
Chemical shifts, Spectrum	13C	chloroform-d1	100	^{13}C NMR (100 MHz, $CDCl_3$): δ: 146.3, 138.8, 134.5, 134.2, 131.4, 130.6, 130.2, 128.7, 128.3, 128.0, 127.9, 127.7, 126.6, 120.1, 21.2, 11.1

Hit Data - 6

- Substance Label - 1 hits out of 1
- Melting Point - 1 hits out of 1
- Crystal Property Description - 1 hits out of 1
- NMR Spectroscopy - 2 hits out of 2
- Mass Spectrometry - 1 hits out of 1

Label: 3ak

Melting Point, °C: 158 - 160

Colour & Other Properties: white

Description (Mass Spectrometry)

high resolution mass spectrometry (HRMS), electrospray ionisation (ESI), spectrum

Peak

403.0801 m/z

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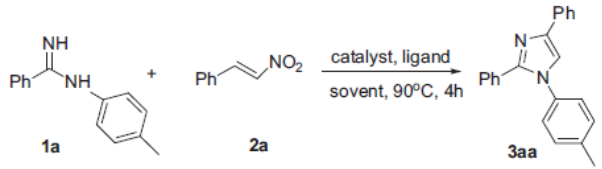
Reaxys对全文中的化合物（催化剂）的相关数据提炼

Table 1
Optimization of the reaction condition[a]



Entry	Catalyst	Ligand	Solvent	Yield[b] (%)
1	$FeCl_3$ (20%)	1,10-Phen	DMSO	60
2	$FeCl_3$ (20%)	Bipy	DMSO	61
3	$FeCl_3$ (20%)	L-Proline	DMSO	58
4	$FeCl_3$ (20%)	None	DMSO	77
5	$FeCl_3$ (20%)	None	THF	12
6	$FeCl_3$ (20%)	None	Toluene	23
7	$FeCl_3$ (20%)	None	DMF	82, 82[c]
8	$FeCl_3$ (20%)	None	Dioxane	44
9	$FeCl_3$ (10%)	None	DMF	65
10	$FeCl_3$ (30%)	None	DMF	78
11	$FeBr_3$ (20%)	None	DMF	53
12	$Fe(OTf)_3$ (20%)	None	DMF	47
13	$Fe(acac)_3$	None	DMF	55
14	$ZnCl_2$	None	DMF	Trace
15	$AlCl_3$	None	DMF	5
16	$TiCl_4$	None	DMF	Trace
17[d]	$FeCl_3$ (20%)	None	DMF	79
18[e]	$FeCl_3$ (20%)	None	DMF	67

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.2 mmol), catalyst (20% mmol), ligand (20%mmol), solvent (2 mL), 90 °C, 4 h.
[b] Isolated yield.
[c] The reaction was carried out under an O_2 atmosphere.
[d] The reaction was carried out at 70 °C.
[e] The reaction was carried out at 110 °C.

iron(III) chloride

Cl_3Fe 162.206 11323458 Retrieve CAS RN

Hit Data - 4 | Physical Data - 26
Identification | Spectra - 58
Druglikeness | Other Data - 128
Bioactivity (All)

Hit Data - 4

Catalyst Investigation - 4 hits out of 303

Show/Hide columns

Investigated characteristic(s)	Specification of catalysis	Type of reaction (Catalyst Investigation)	Co-catalyst/co-substrate name	Reference
Catalytic activity	Regioselective catalysis	Cycloaddition		Liu, Xiang; Wang, Dong; Chen, Baohua[Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract
Catalytic activity	Regioselective catalysis	Cycloaddition	[2,2]bipyridinyl	Liu, Xiang; Wang, Dong; Chen, Baohua[Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract
Catalytic activity	Regioselective catalysis	Cycloaddition	1,10-Phenanthroline	Liu, Xiang; Wang, Dong; Chen, Baohua[Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract
Catalytic activity	Regioselective catalysis	Cycloaddition	L-proline	Liu, Xiang; Wang, Dong; Chen, Baohua[Tetrahedron, 2013, vol. 69, # 45, p. 9417 - 9421] Full Text Cited 38 times Details Abstract

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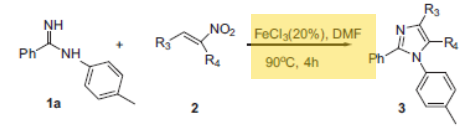
Reaxys对全文中的合成线路的相关数据提炼

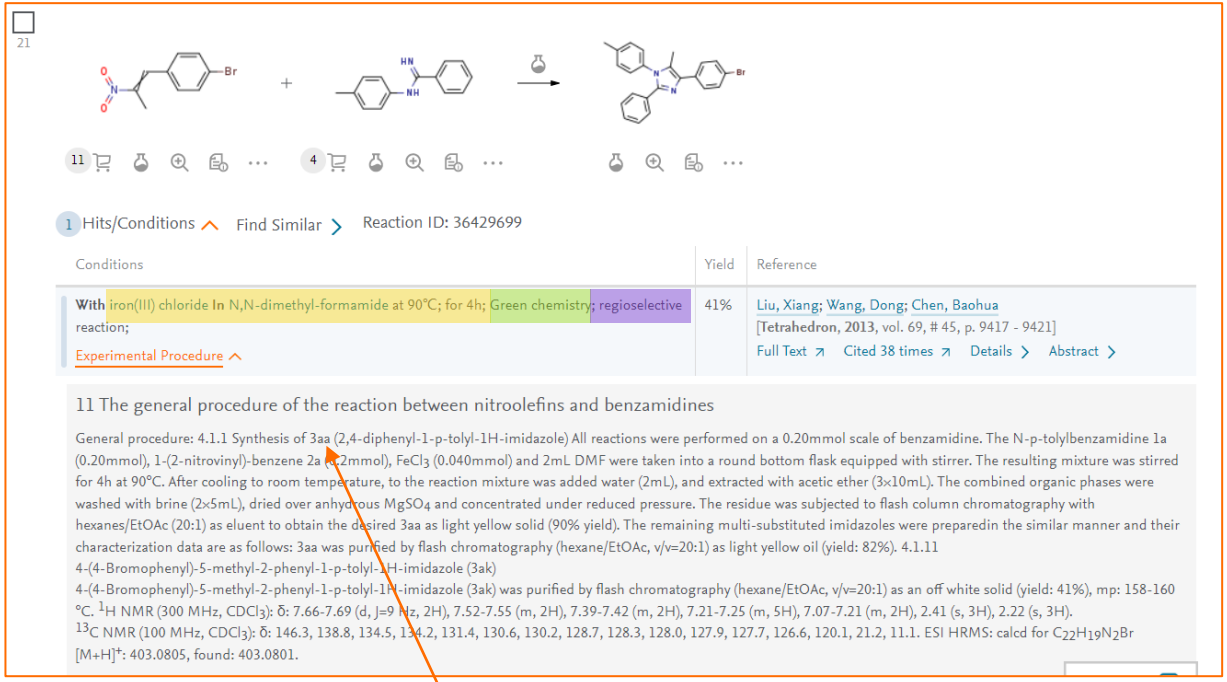
Table 2
Reactions of *N*-*p*-tolylbenzamidine with various nitroolefins[a]



Entry	R_3	R_4	Product	Yield[b] (%)
1	H	H	**3aa**	82
2	4-CH_3	H	**3ab**	60
3	4-CH_3O	H	**3ac**	51
4	4-F	H	**3ad**	61
5	4-Cl	H	**3ae**	68
6	2-Cl	H	**3af**	55
7	4-CF_3	H	**3ag**	50
8	2,4-$DiCH_3O$	H	**3ah**	53
9	H	CH_3	**3ai**	47
10	4-CH_3O	CH_3	**3aj**	35
11	4-Br	CH_3	**3ak**	41
12	4-Cl	CH_3	**3al**	45
13	4-CN	CH_3	**3am**	56

3. Conclusion

In conclusion, we have successfully developed an efficient and novel catalytic approach for synthesis of multi-substituted imidazoles via nitroolefins and *N*-aryl benzamidines. This reaction proceeds via stepwise [3+2] cycloaddition in the presence of an inexpensive iron catalyst under air. This methodology is convenient, atom-economical, and eco-friendly in good yields and prefect regioselectivities. This efficient strategy could significantly direct further research of multi-substituted imidazoles synthesis.



实验过程与条件

Reaxys从文献中提炼出来的内容

文献记录：
>94.7 million
16300+期刊
105专利机构的专利
38万书的章节

化合物记录：
>170 million
期刊，专利，商品
2022年中前完成105家专利机构中专利物质的回溯

化学反应记录：
>57.8 million
单步多步反应，同时提炼文献与专利中的实验过程

实验性质记录：
> 500 million
化合物实验数据，并提炼实验数据检测条件

生物活性记录：
> 41.9 million数据
> 35,000靶点
> 7.9 million化合物
化合物在不同生物体内活性数据

数据更新时间：2022/2/7

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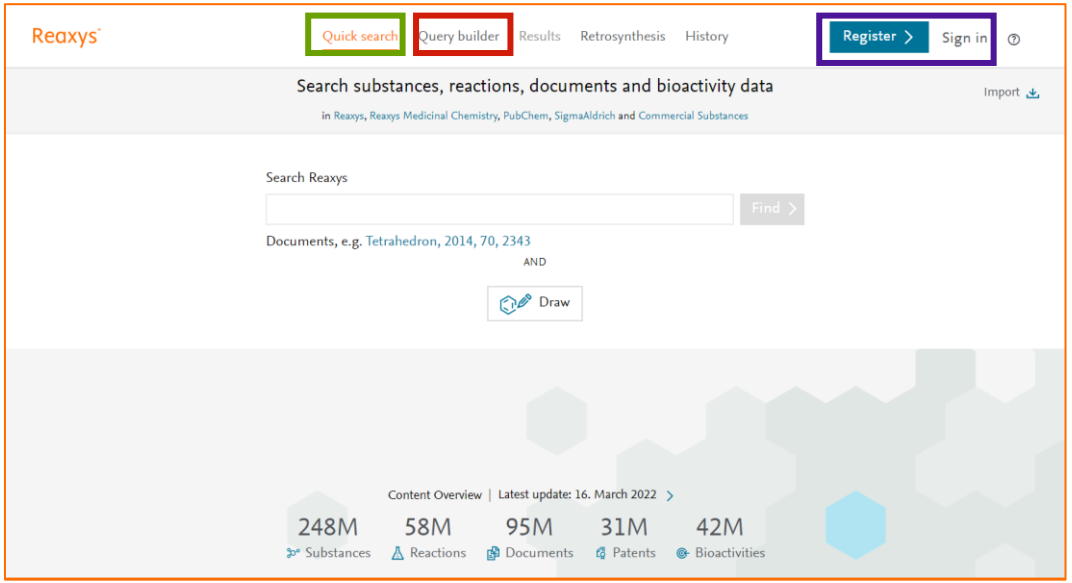
Reaxys的登录界面

- 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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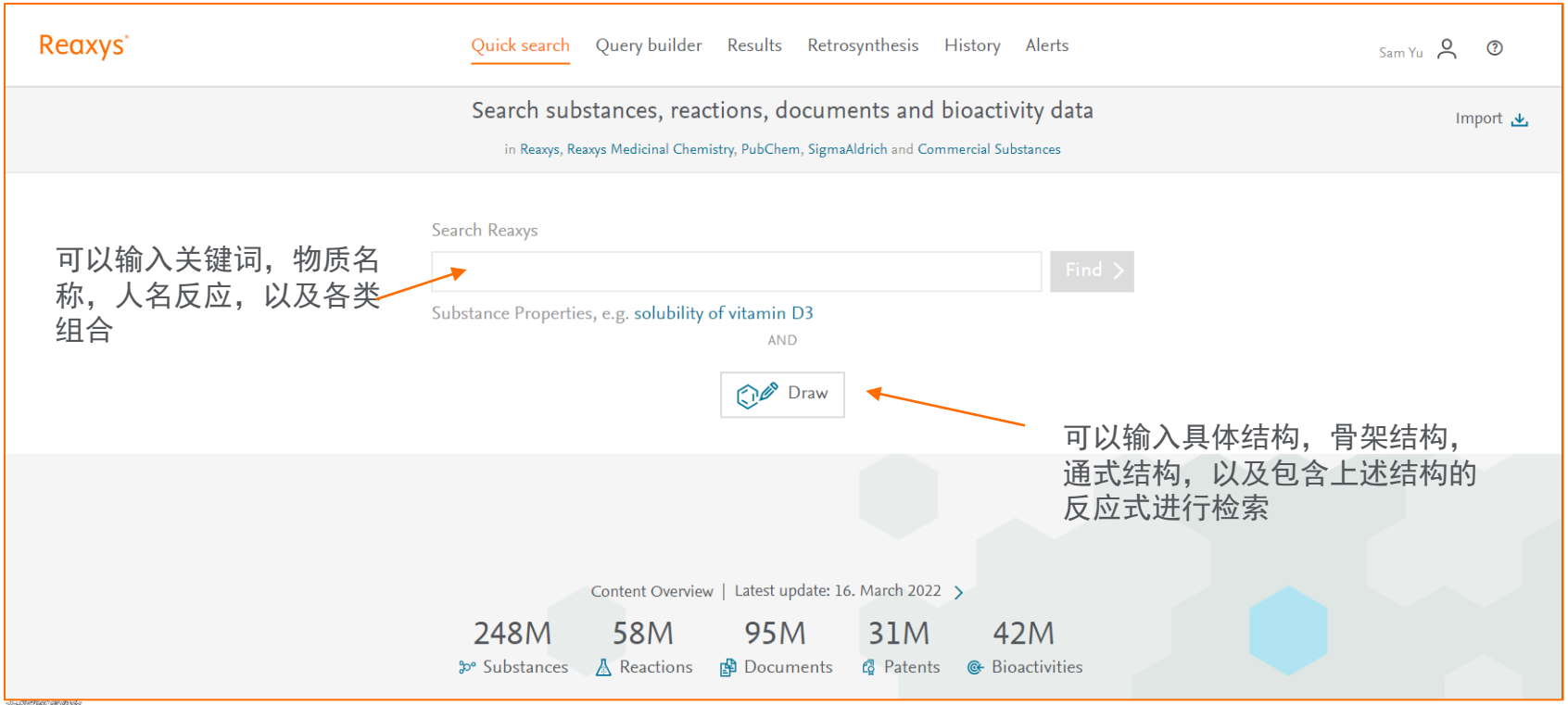
Quick Search界面



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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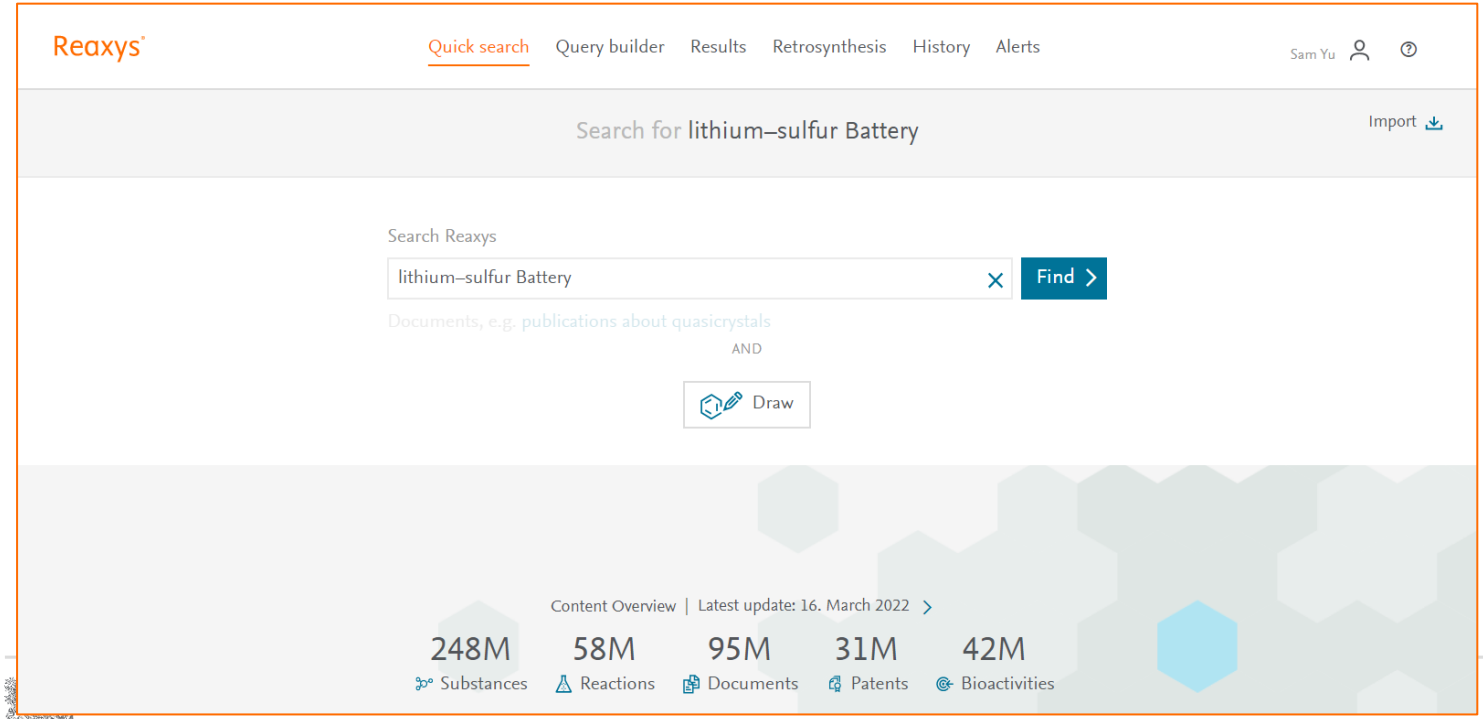
- Reaxys中的化学科学数据获取
  - Reaxys中的科技文献检索与分析
  - Reaxys中物质理化性质数据的查询与反向物质获取
  - Reaxys中结构面板与物质结构和反应数据的获取
  - Reaxys中的实用小案例
- Q&A

Case 1：关键词检索—锂硫电池

- Lithium–Sulfur Battery



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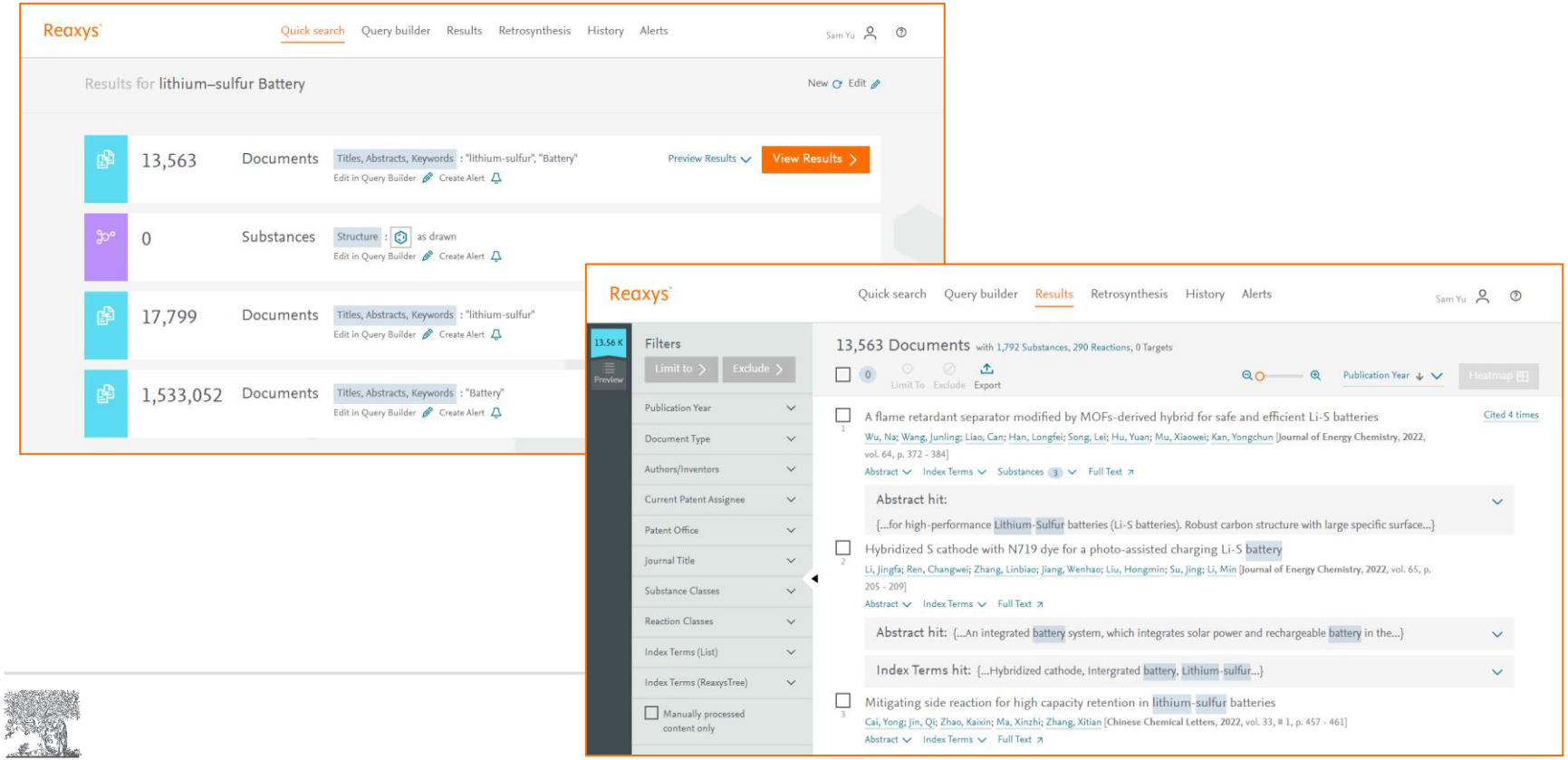
Reaxys中的检索结果



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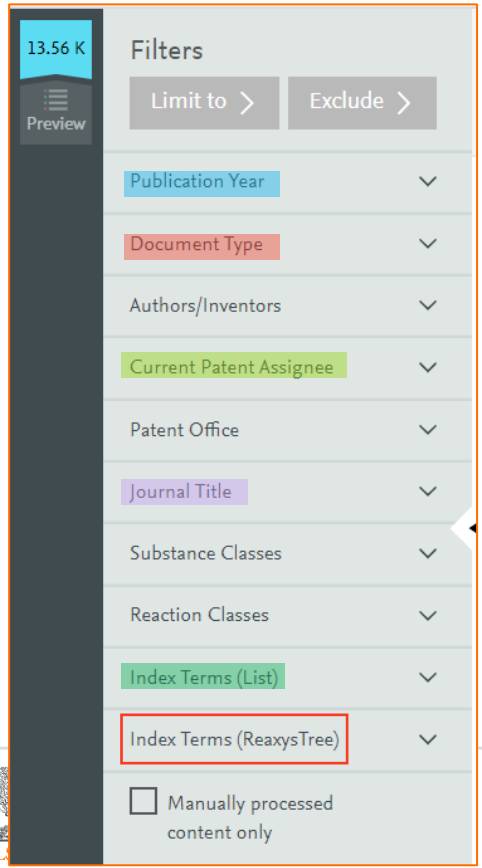
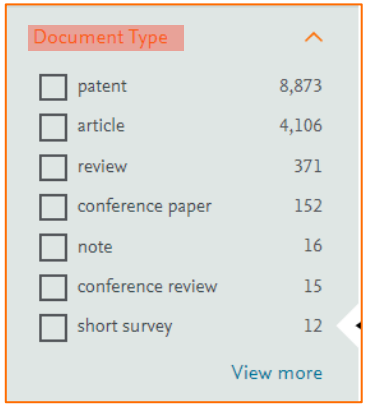
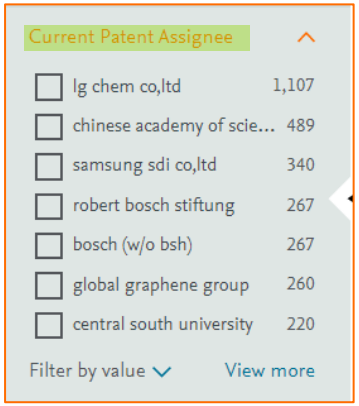
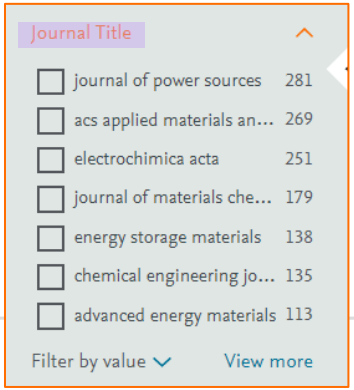
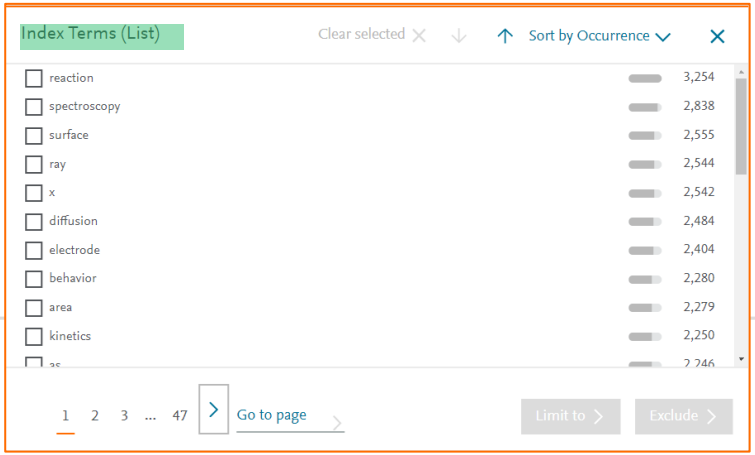
Reaxys中对于文献检索结果的分析



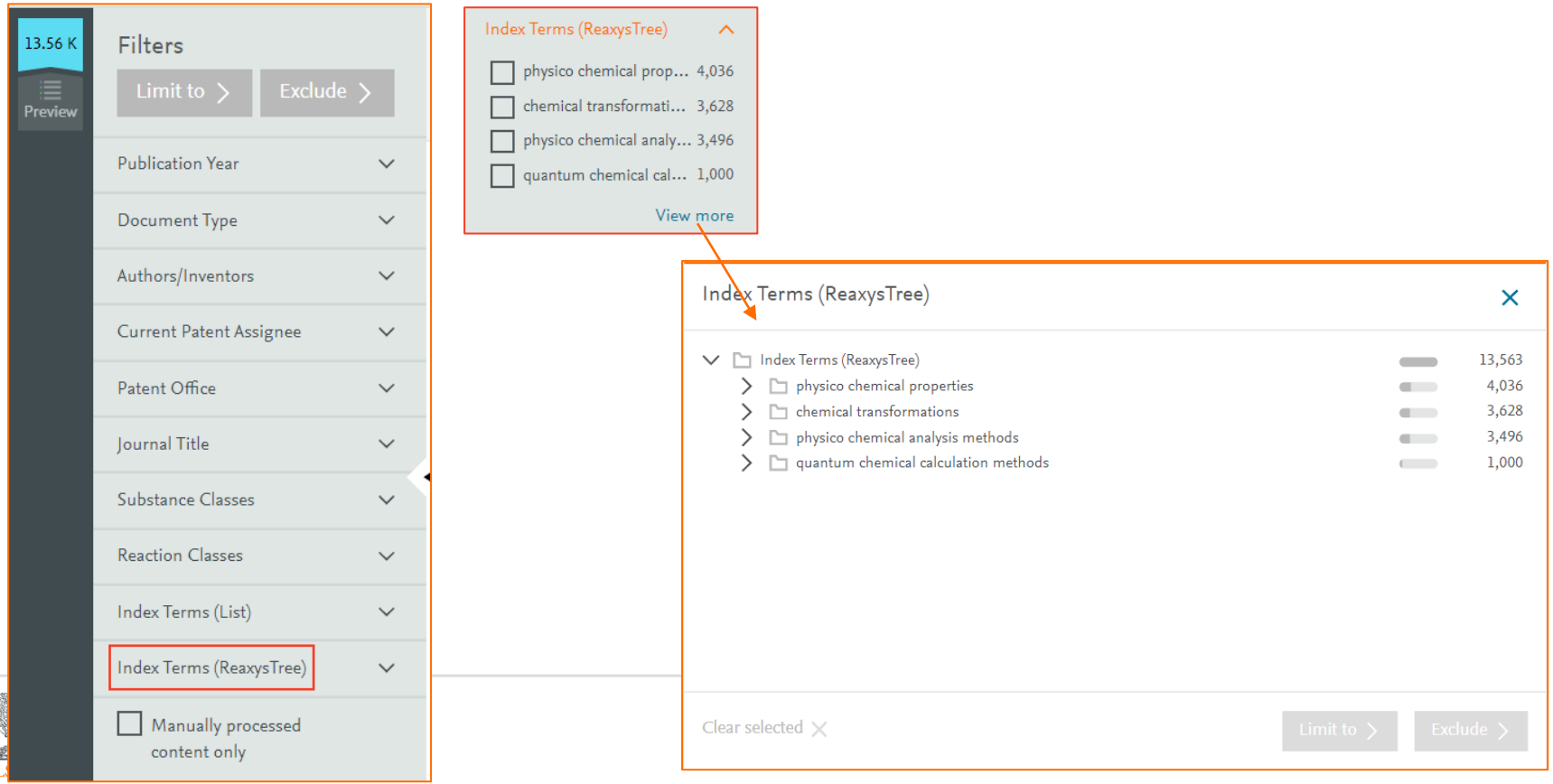




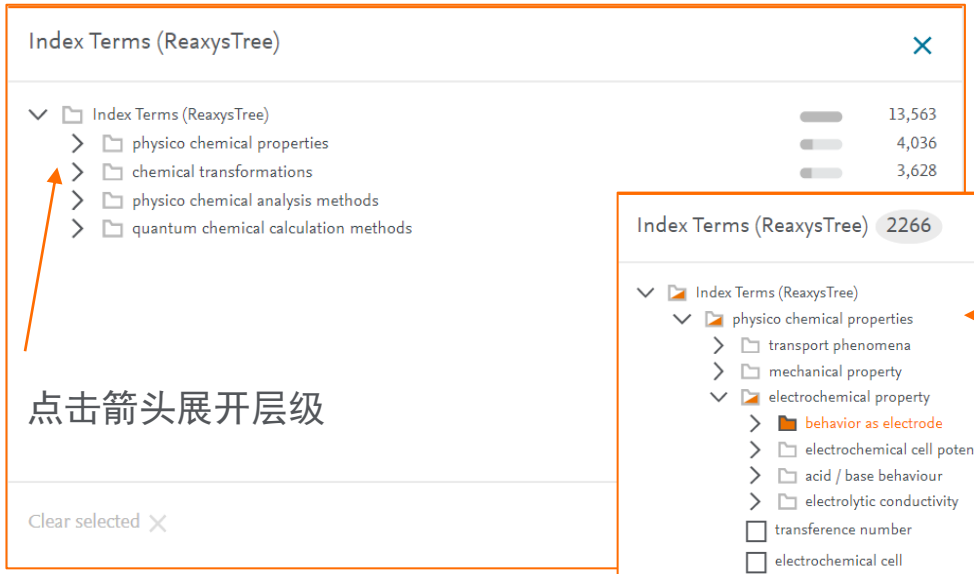


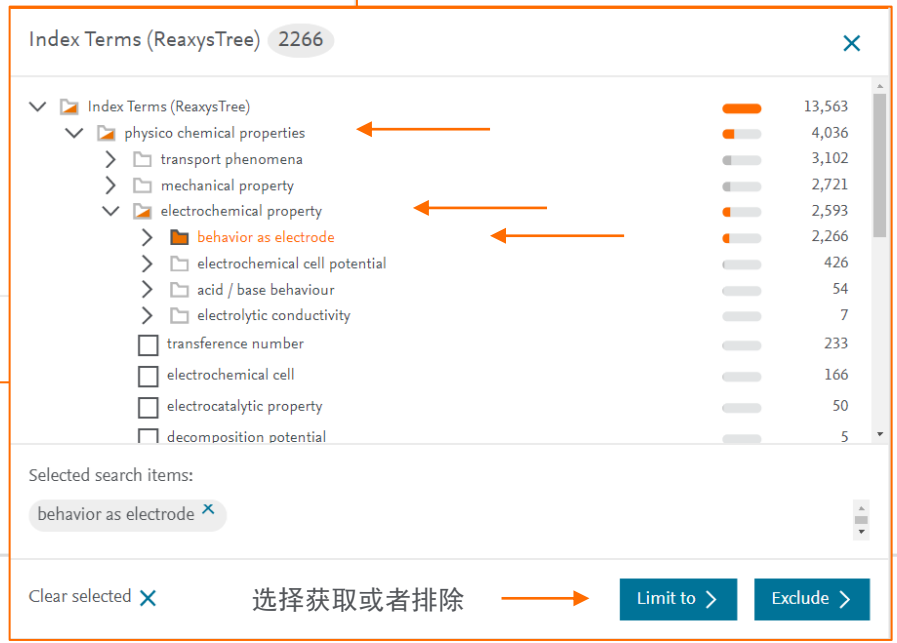


Reaxys中的Index Terms（Reaxys Tree）学科分类



利用树状图进行学科分类





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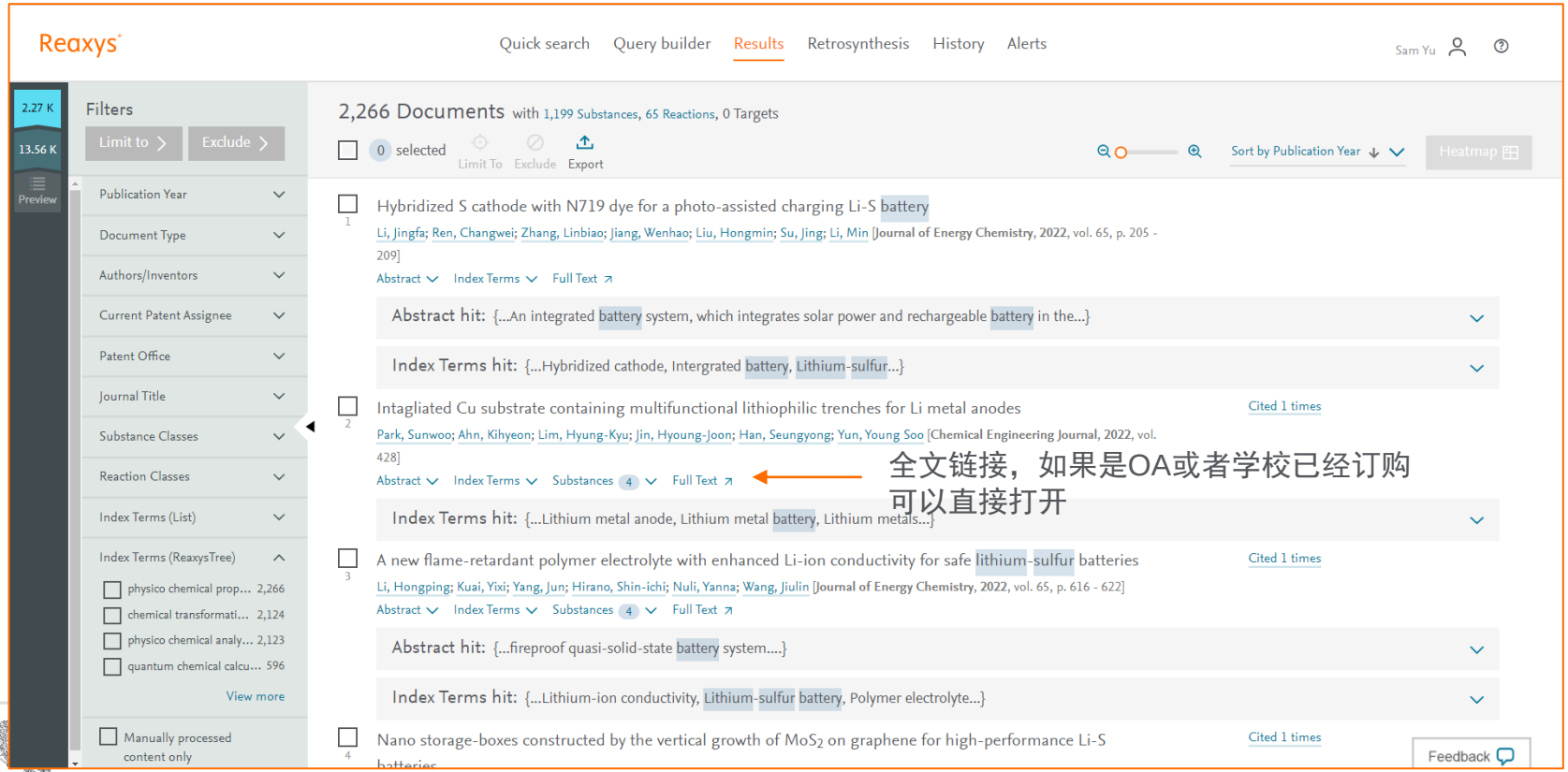
最后的检索结果



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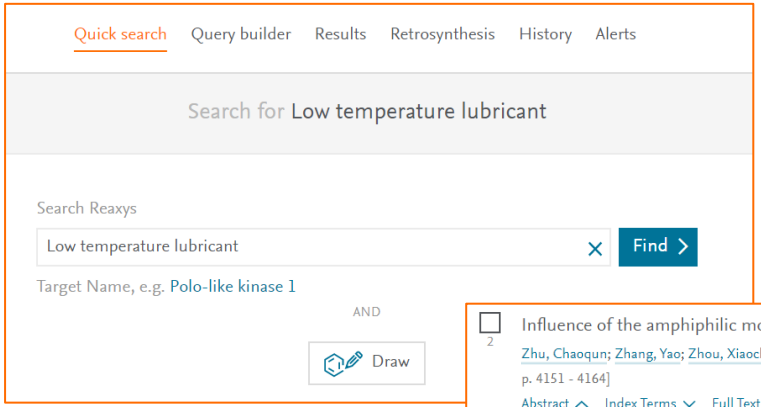
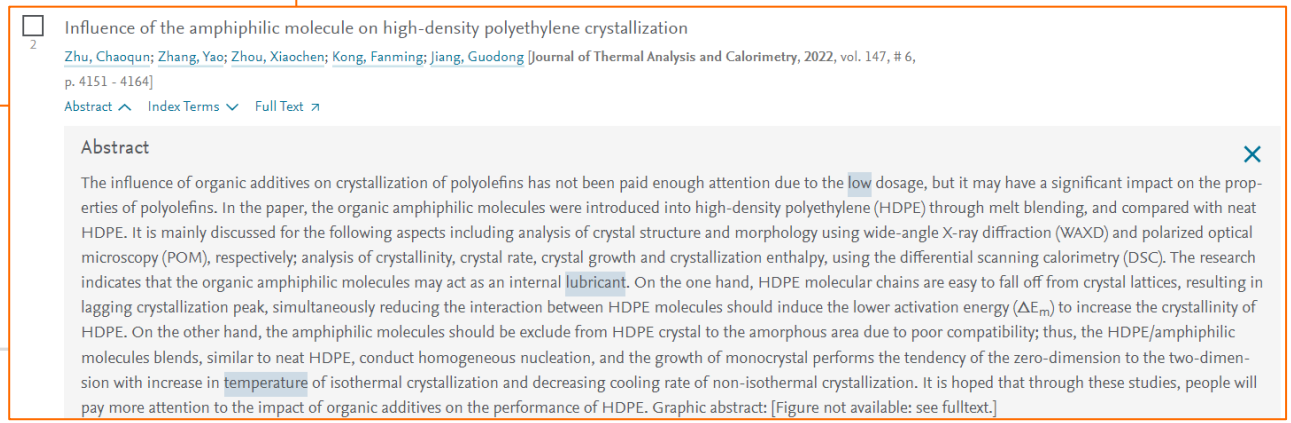
关键词检索时的麻烦问题

- 获取与低温润滑剂相关的文献“Low temperature lubricant”



因为对输入的关键词不做任何控制，所以给出来的结果会存在一定程度上的不准确。



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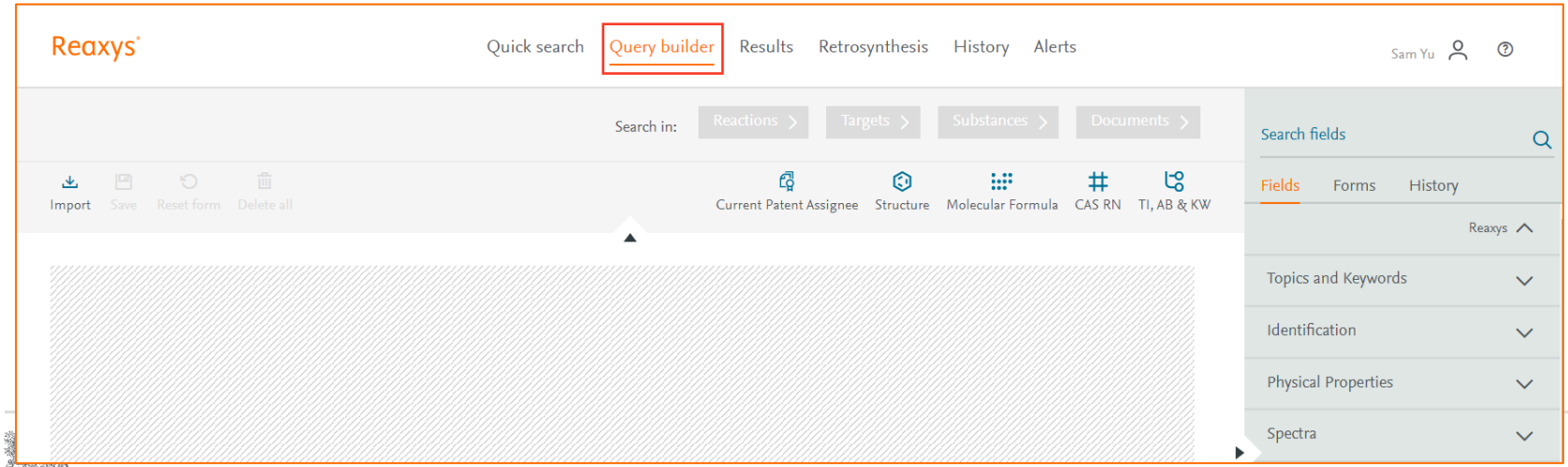
Case 2：关键词检索时词语的控制

- 获取与低温润滑剂相关的文献“Low temperature lubricant”
  - Low Temperature以词组的形式存在，Reaxys中用引号解决
  - Lubricant可能存在多种形式的词根，Reaxys中用通配符解决
  - Low Temperature与Lubricant之间的距离在一定数量的单词内（好比<7)，Reaxys中用Query Builder解决



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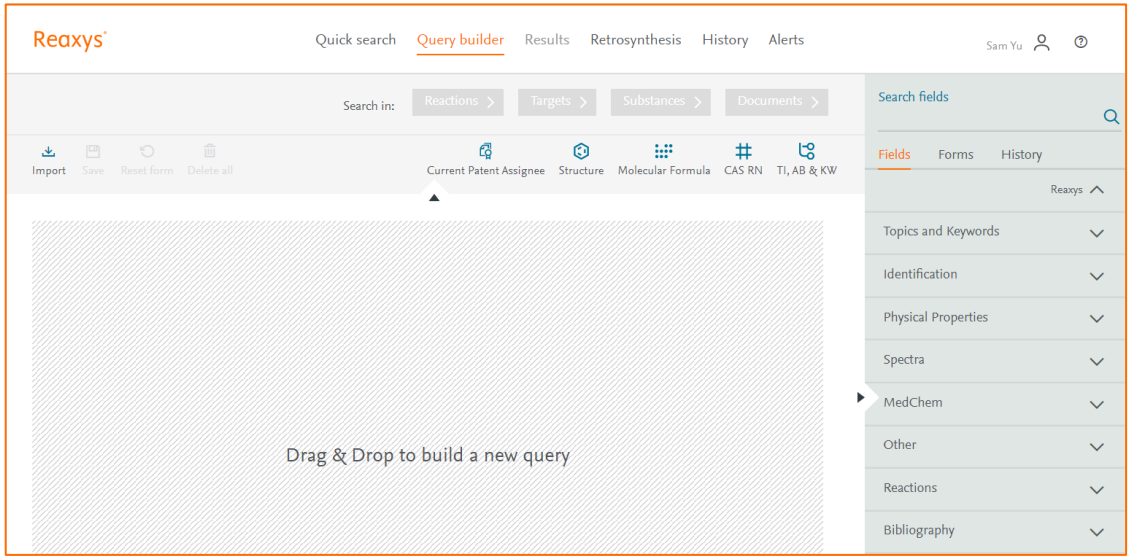
Reaxys中的Query Builder是一种高级的组合检索模式



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

Query Builder的使用步骤，第一步是选择字段，第二步是输入条件，第三步是确定不同字段之间的逻辑关系

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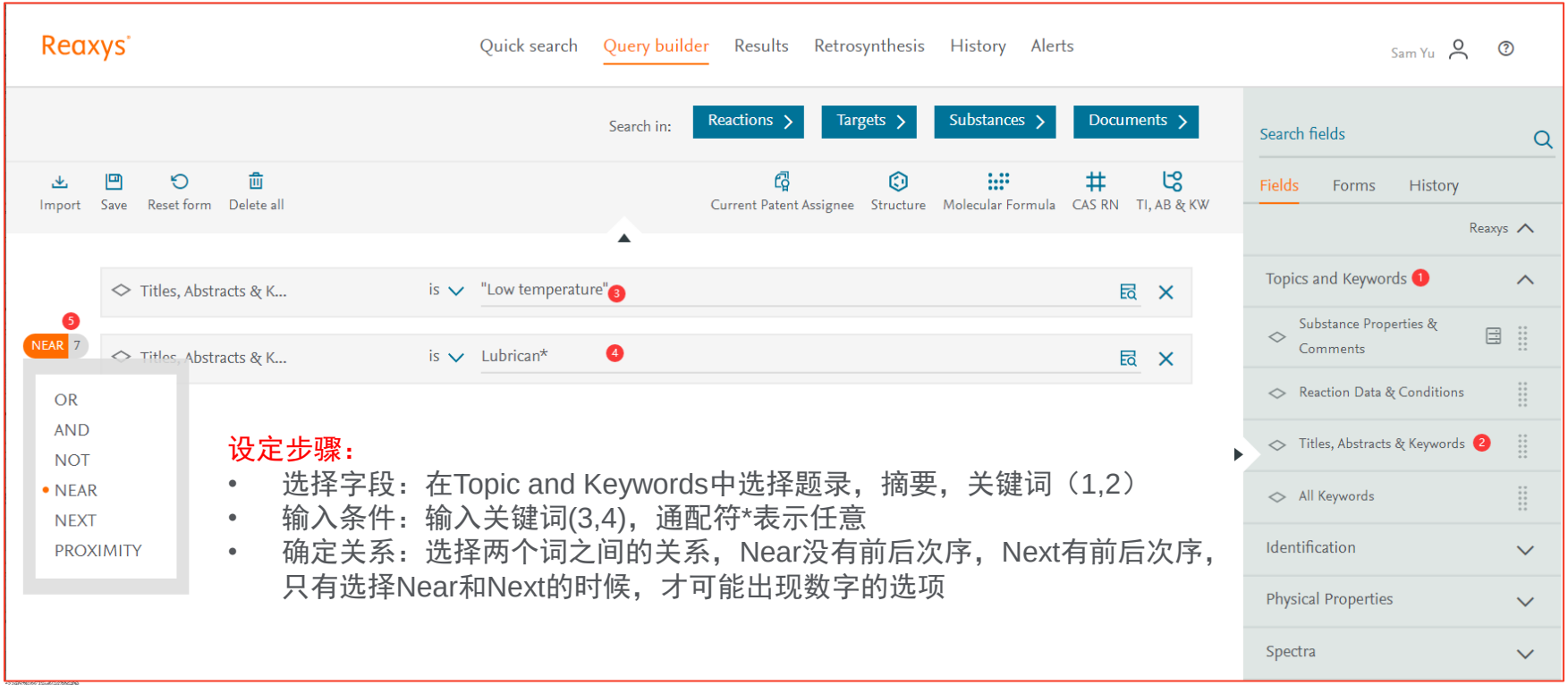
Reaxys中检索策略



设定步骤：

- 选择字段：在Topic and Keywords中选择题录，摘要，关键词（1,2）
- 输入条件：输入关键词(3,4)，通配符*表示任意
- 确定关系：选择两个词之间的关系，Near没有前后次序，Next有前后次序，只有选择Near和Next的时候，才可能出现数字的选项

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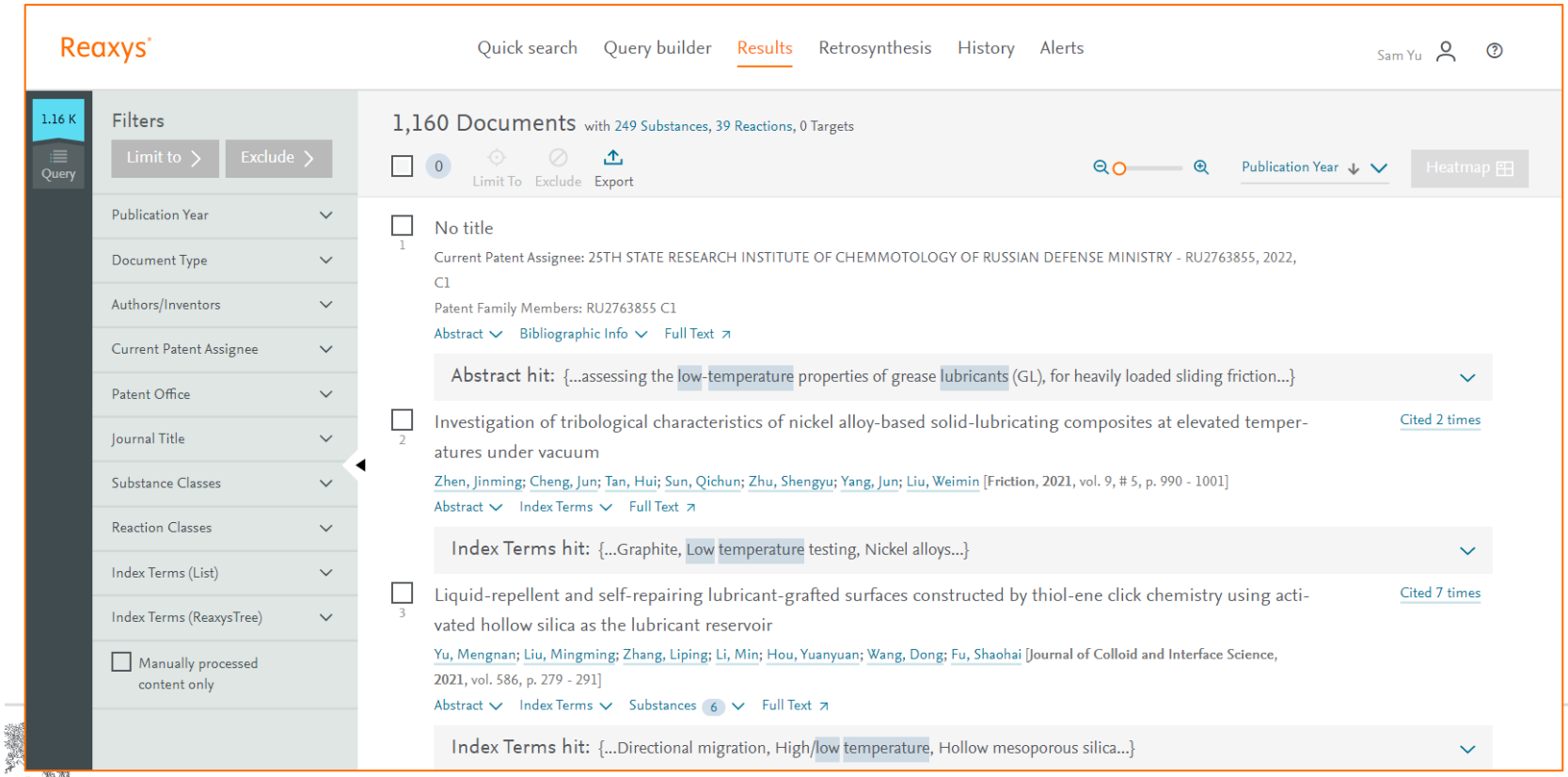
文献检索的结果



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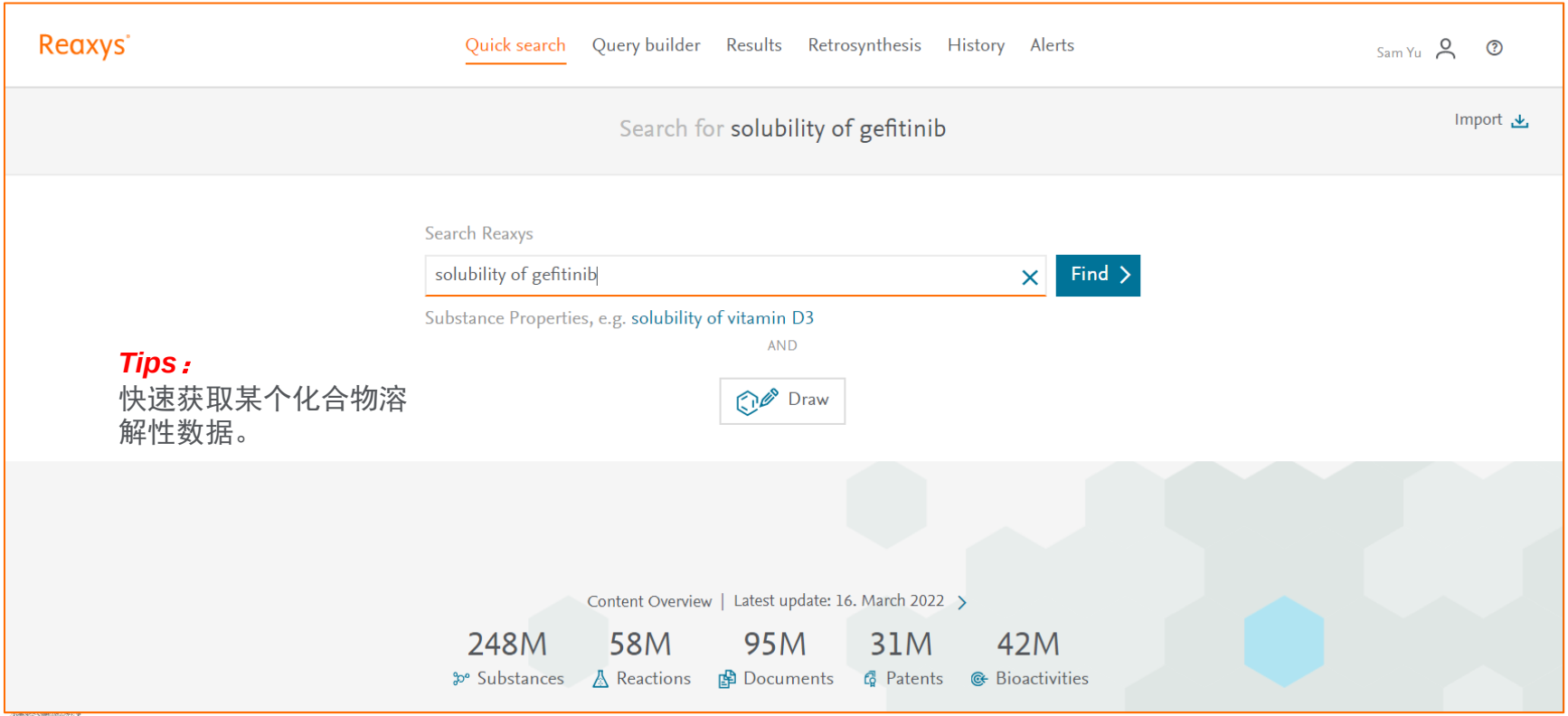
Agenda

- 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中的科技文献检索与分析
  - 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 3：Reaxys中化合物理化性质的快速获取



Tips：

快速获取某个化合物溶解性数据。

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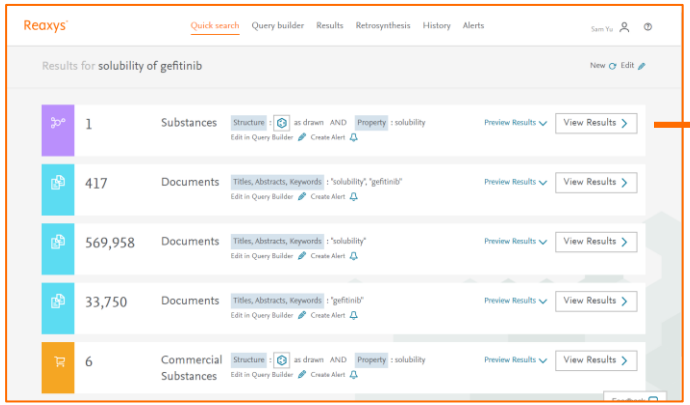
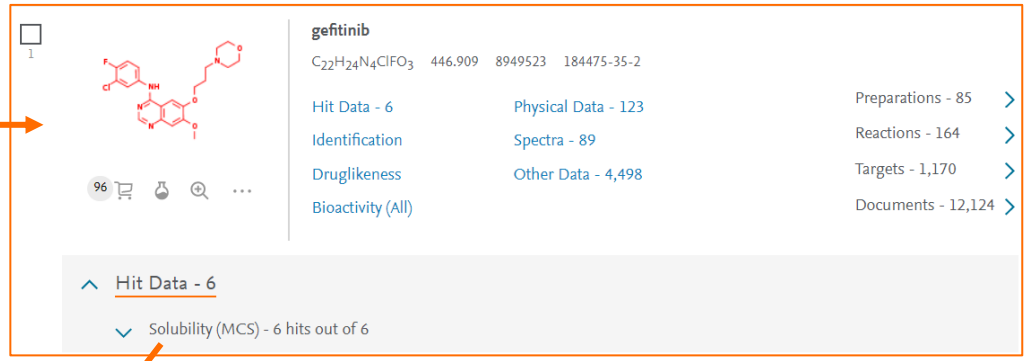
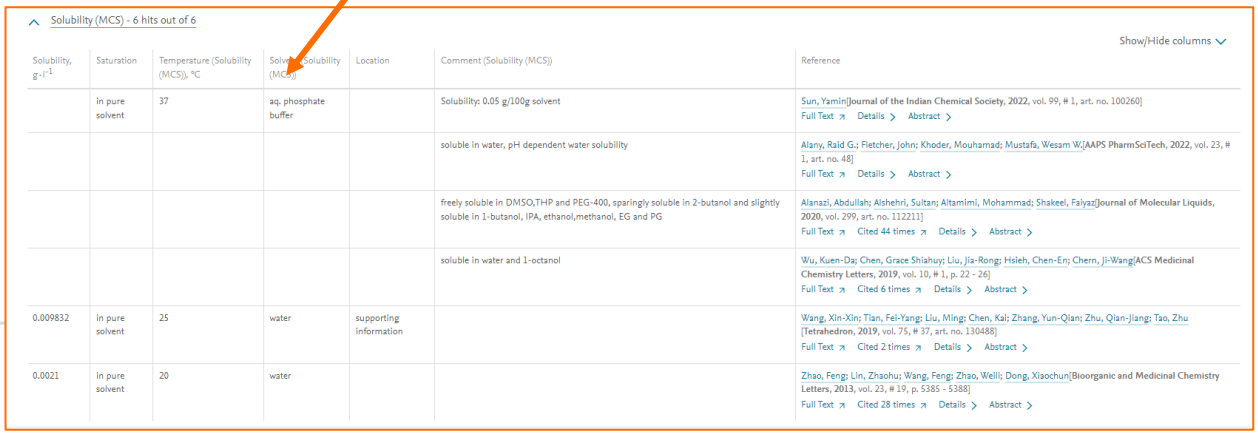
Reaxys中的结果





抽提的数据包括具体的数值，
或者相关的文字性描述



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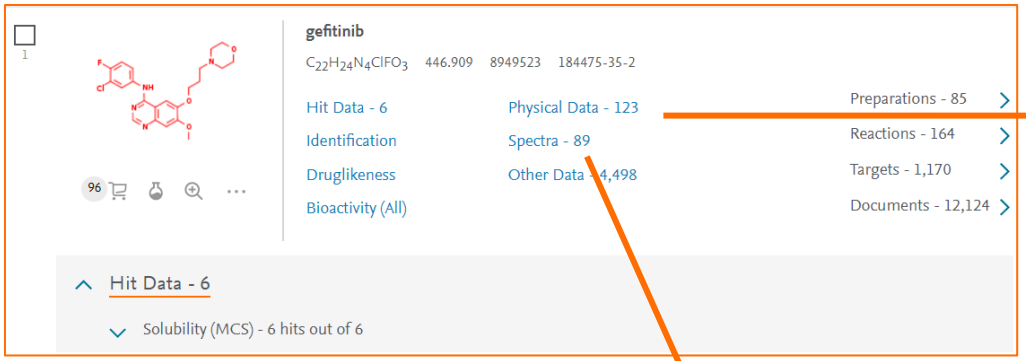
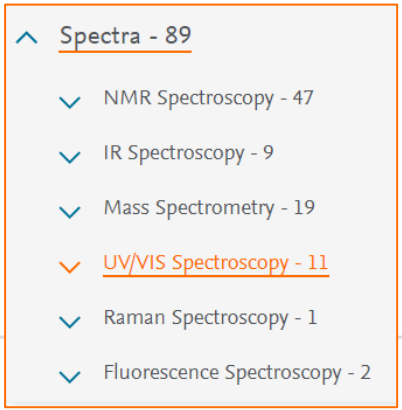
Reaxys中化合物更多的理化性质





直接获取化合物的理化性质或者谱图数据

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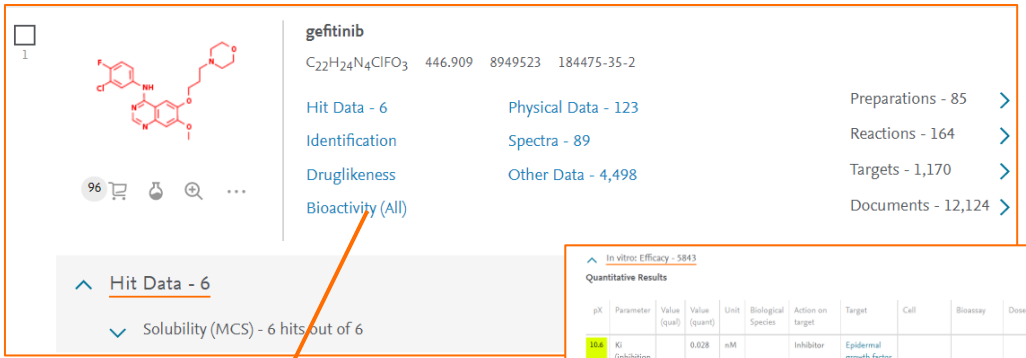
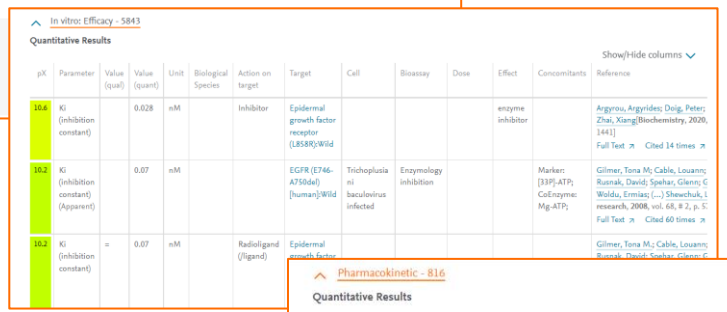
Reaxys中化合物的生物活性数据（需要RMC模块）





RMC是Reaxys药物化学模块，文献与专利中的活性数据全部收录在其中。

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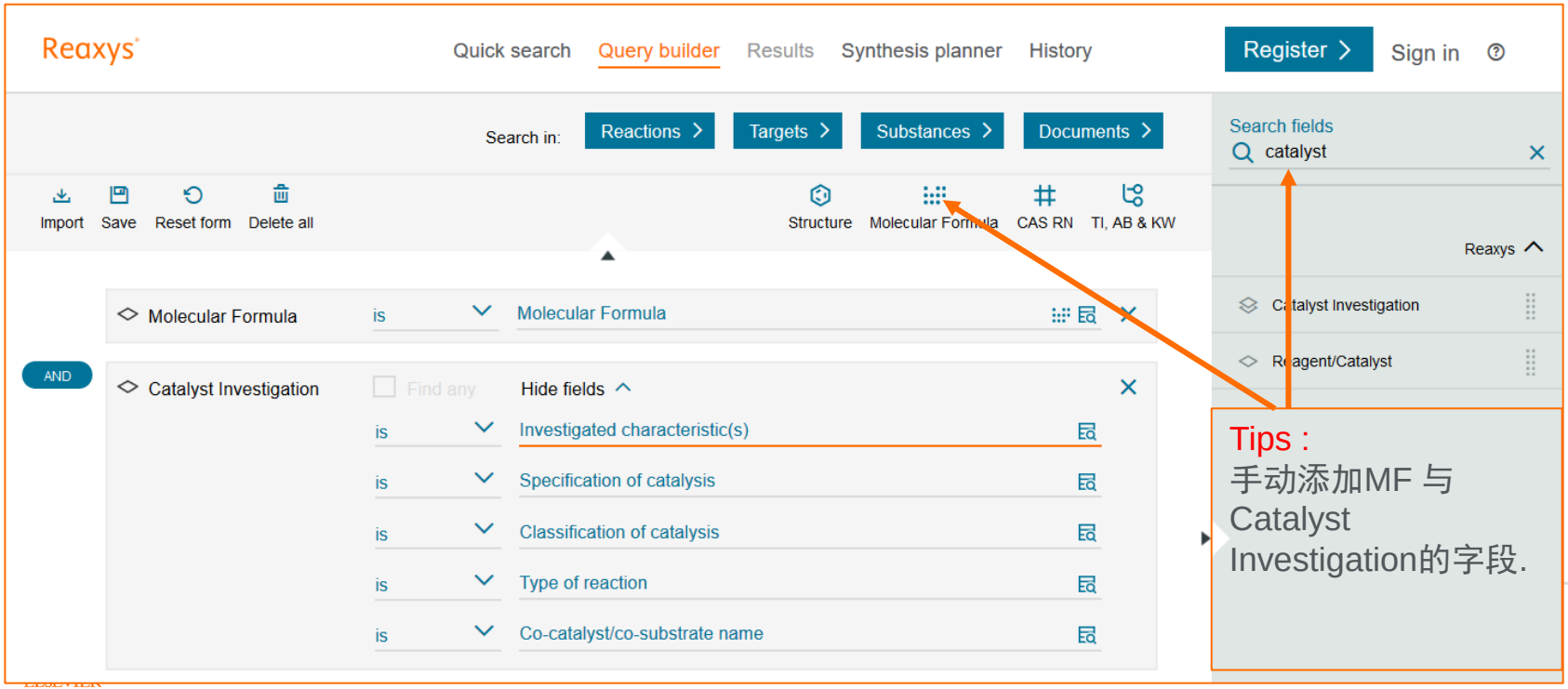
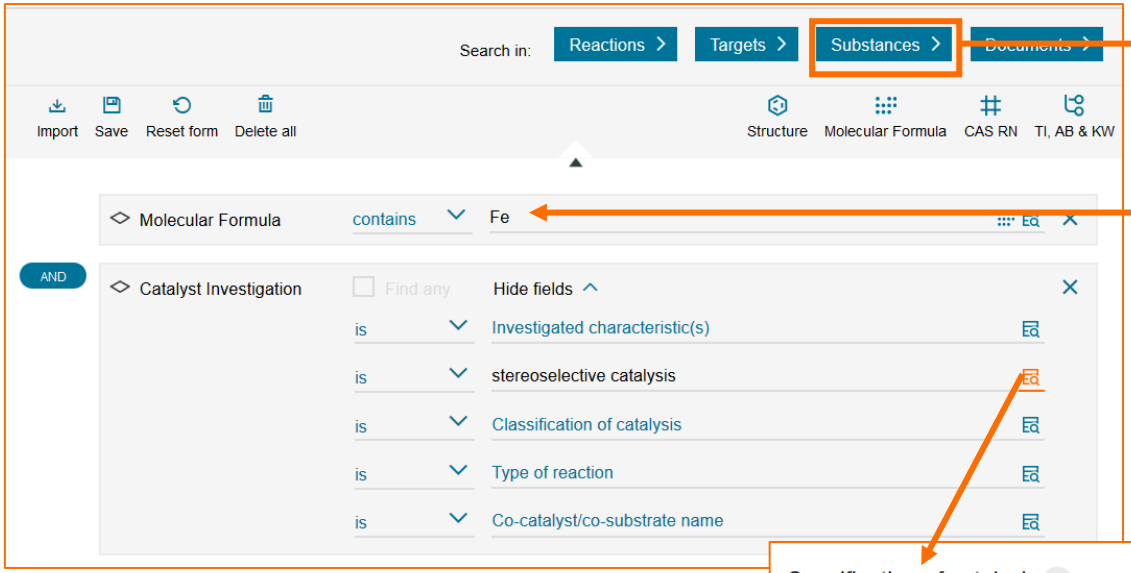
Case 4：“特定研究领域”的催化剂选择

- 检索可用于立体选择性催化的含Fe的催化剂

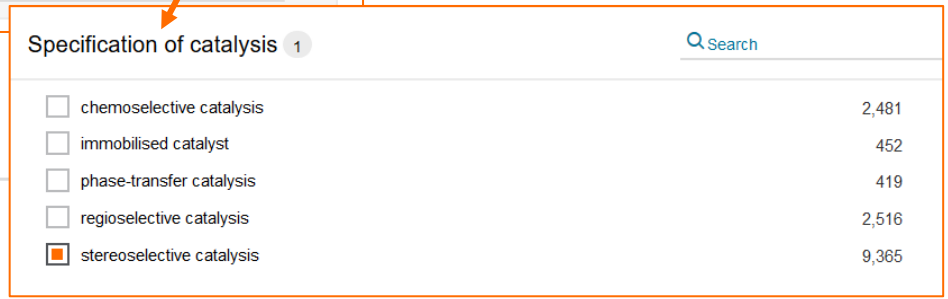


条件的输入



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

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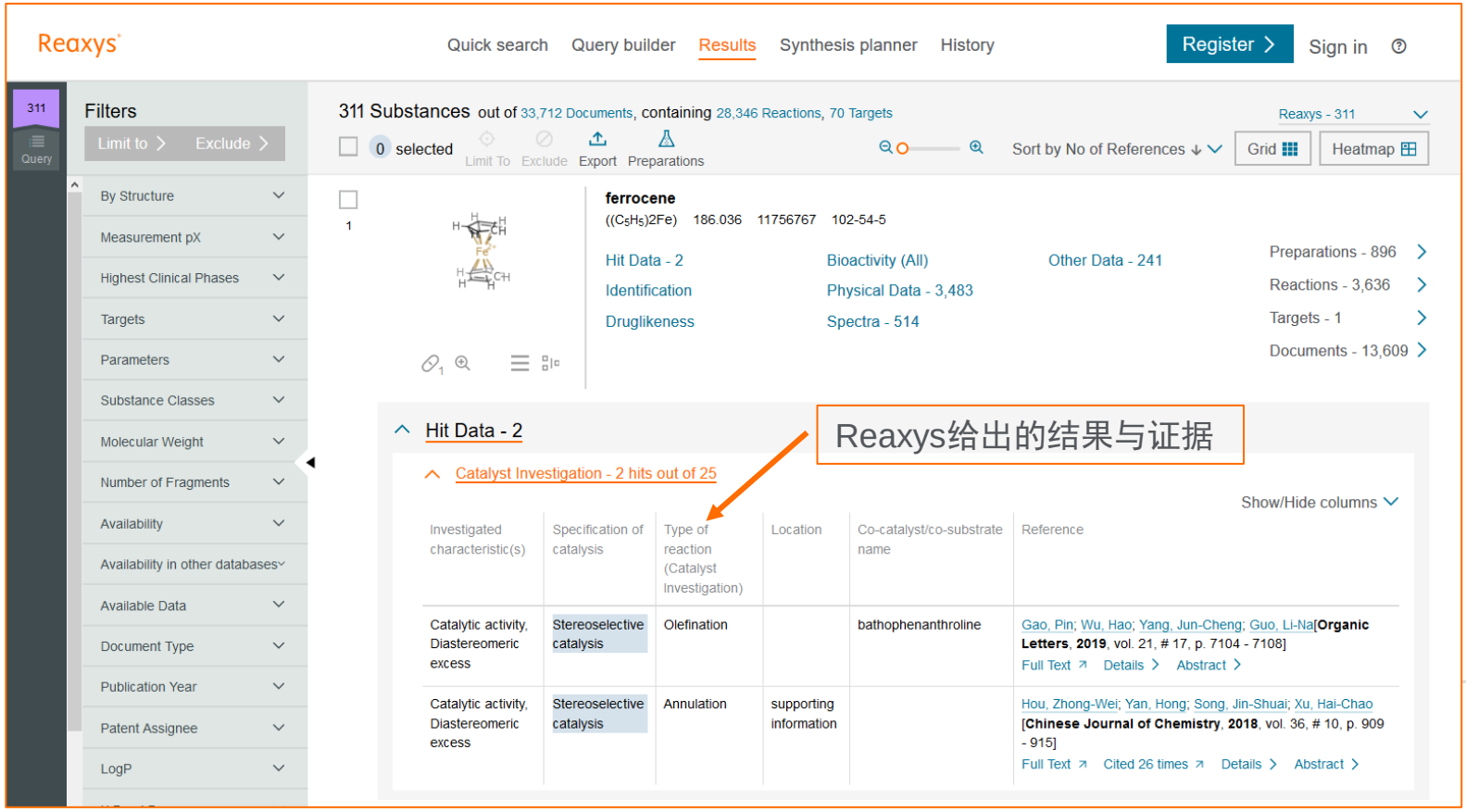
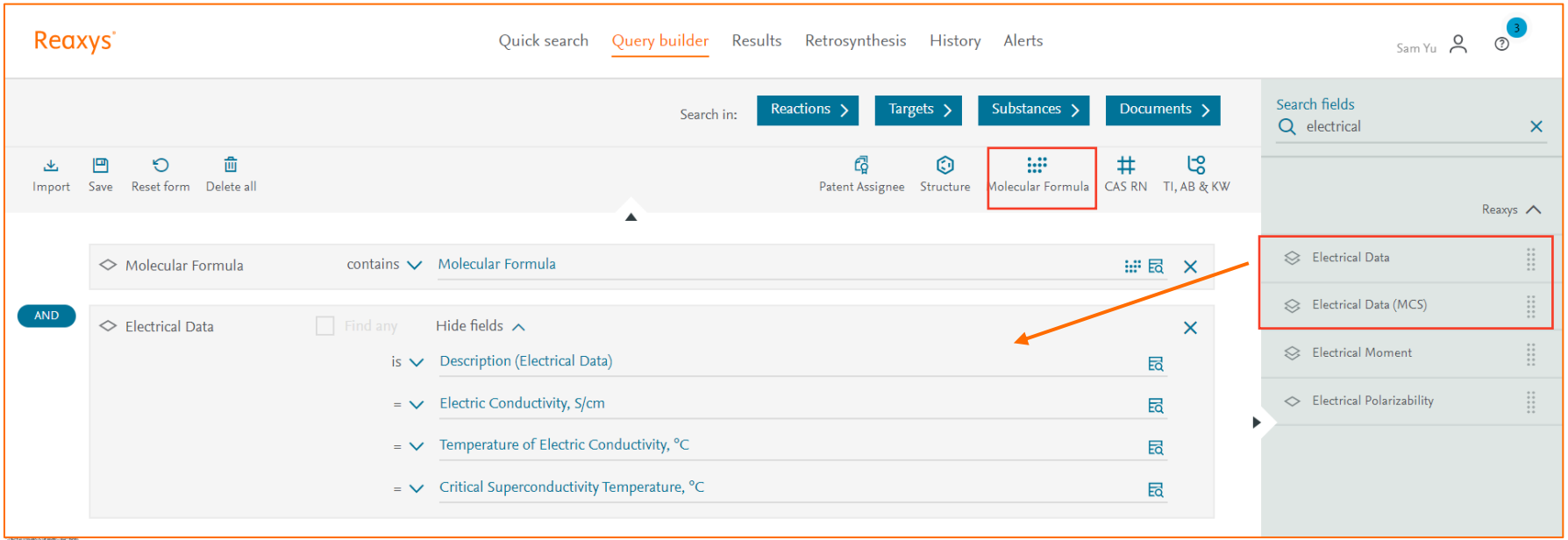
最后的结果


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：获取含C的在低温具有导电性能的化合物

- 获取在零下250摄氏度下，含有C的，且电导率>10000s/cm的化合物
- Query Builder下联合Electrical Data与分子式进行检索



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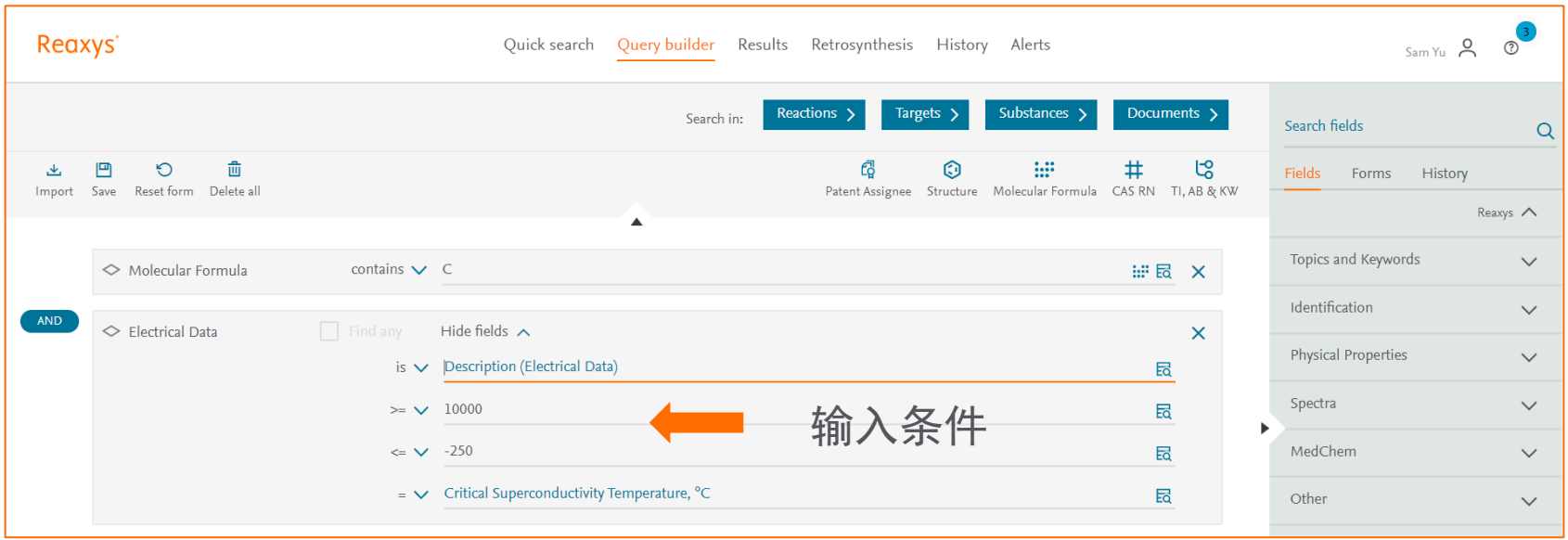
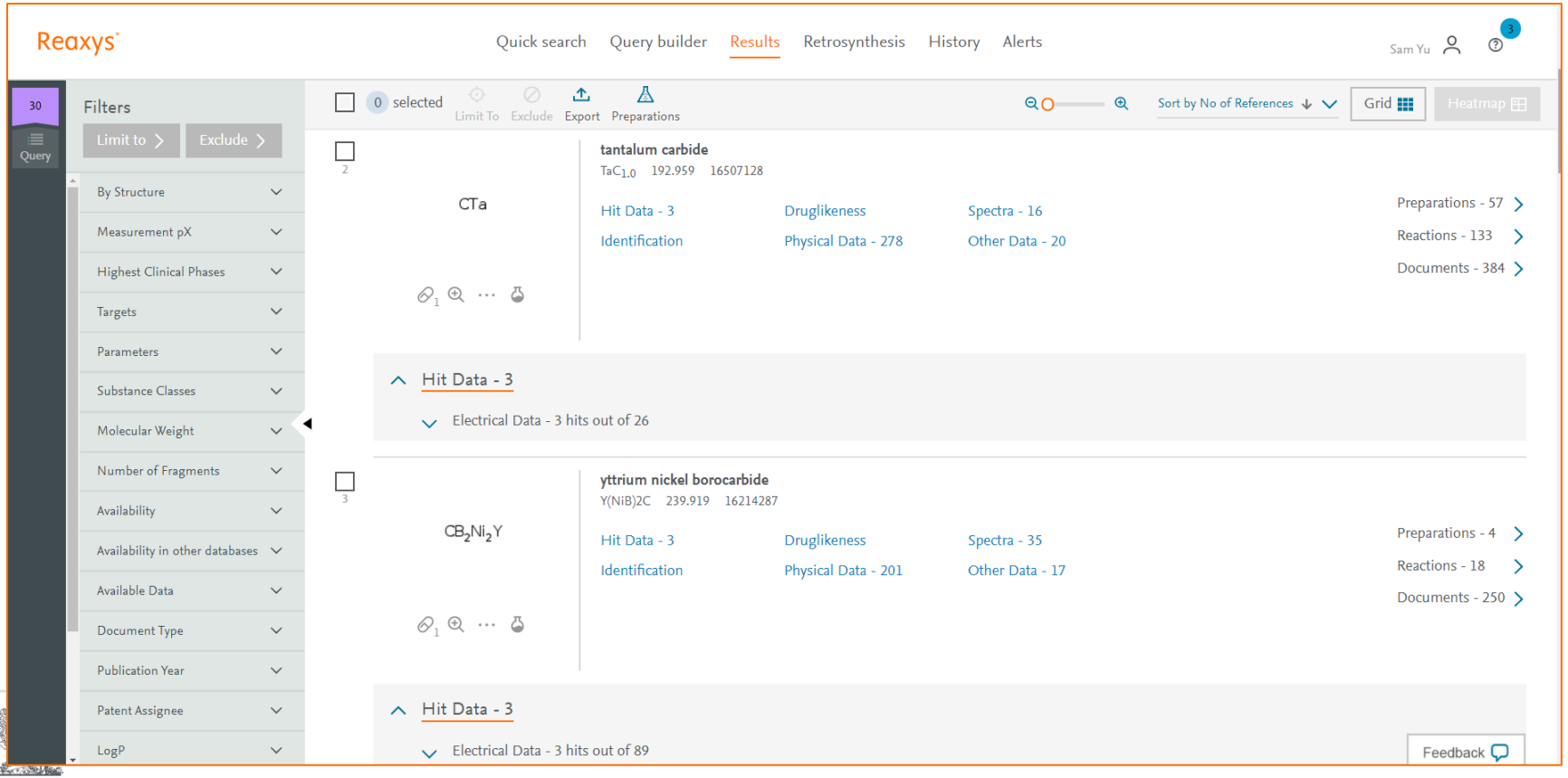
设定条件

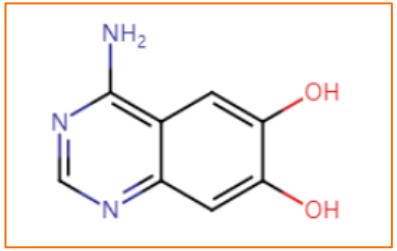

Reaxys
Quick search
Query builder
Results
Retrosynthesis
History
Alerts
Sam Yu
3
Search in:
Reactions
Targets
Substances
Documents
Import
Save
Reset form
Delete all
Patent Assignee
Structure
Molecular Formula
CAS RN
TI, AB & KW
Molecular Formula
contains
C
AND
Electrical Data
Find any
Hide fields
is
Description (Electrical Data)
>=
10000
<=
-250
=
Critical Superconductivity Temperature, °C
输入条件
Search fields
Fields
Forms
History
Reaxys
Topics and Keywords
Identification
Physical Properties
Spectra
MedChem
Other

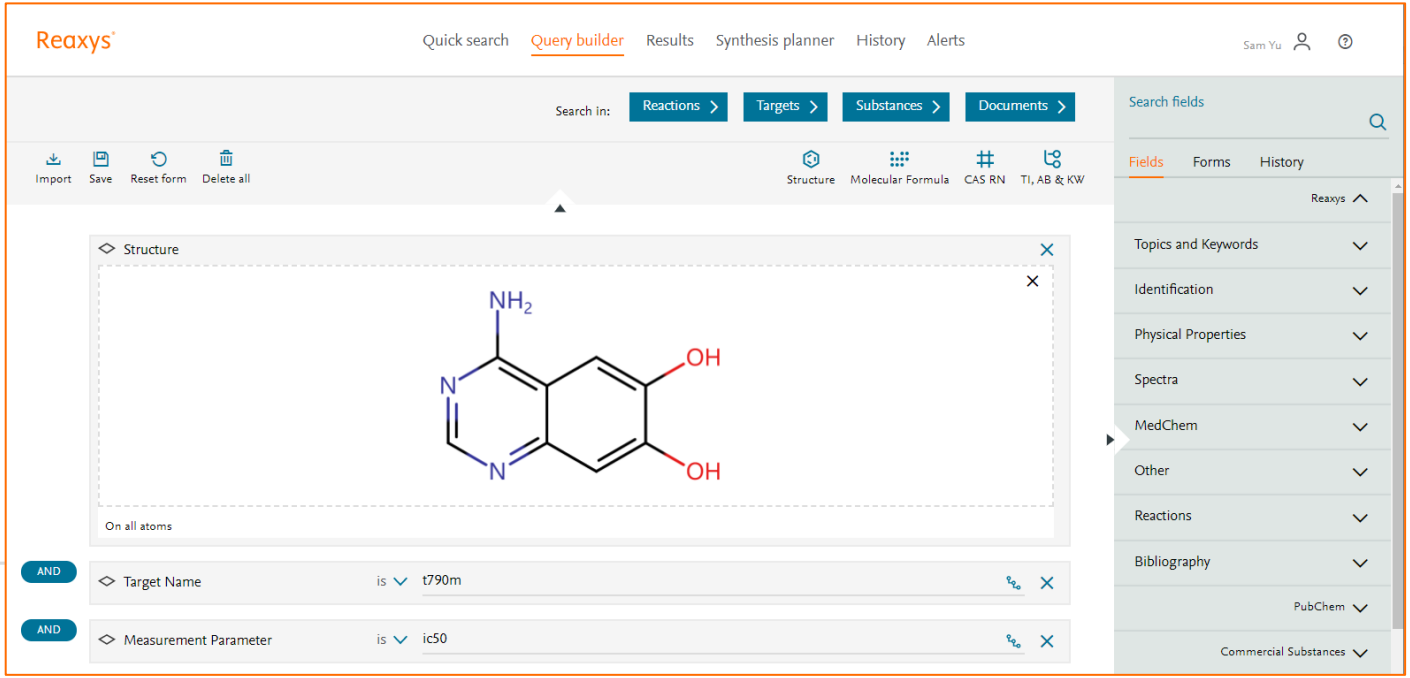
最后的结果



Case 6：骨架化合物活性获取（需要RMC模块）

- 获取包含下面骨架，且在EGFR-T790M上有活性，且有ic50报道的化合物
- 类似视频操作：https://www.bilibili.com/video/bv1pK411G7rX





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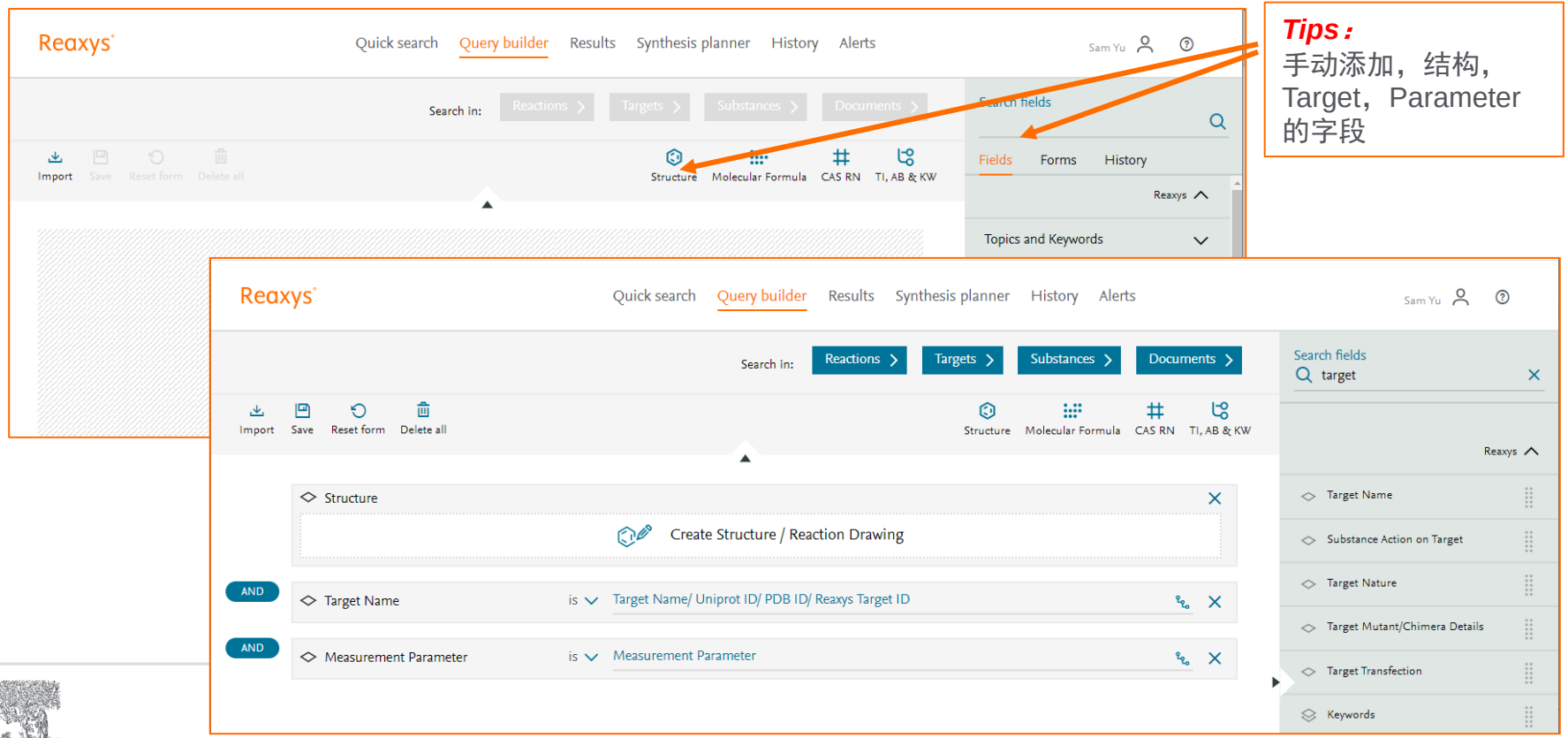
检索策略的构建



Tips：
手动添加，结构，Target，Parameter的字段

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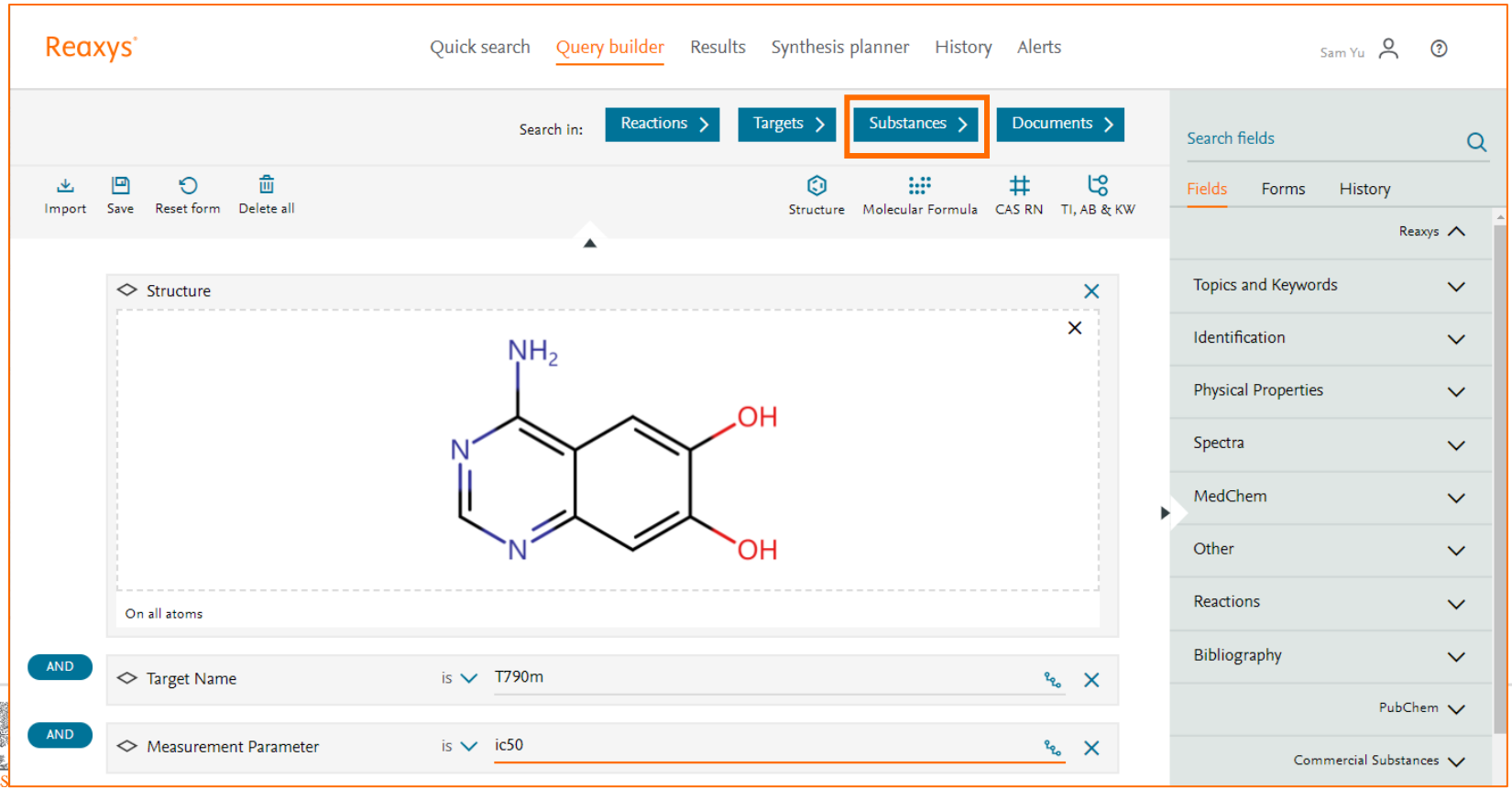
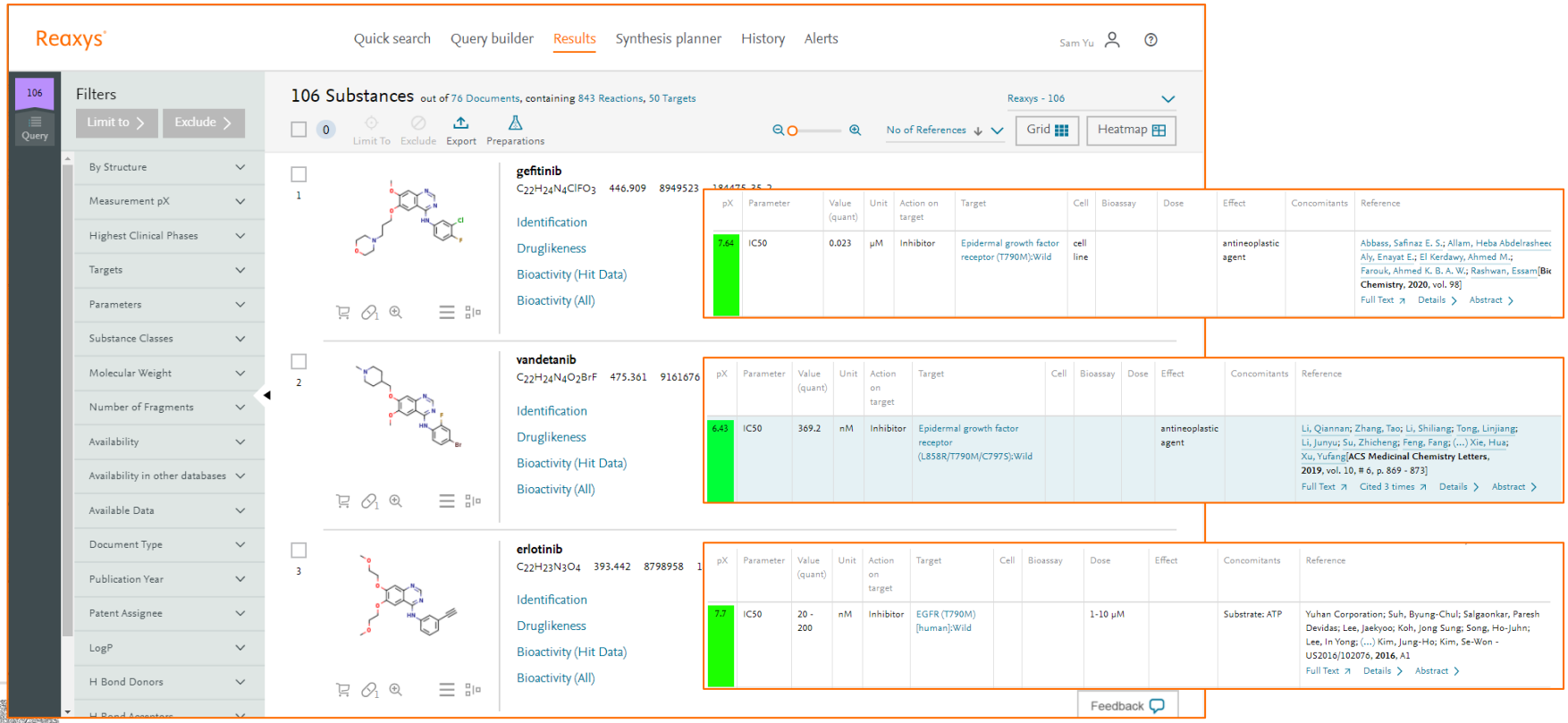
条件的输入


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Alerts
Sam Yu
Search in:
Reactions
Targets
Substances
Documents
Import
Save
Reset form
Delete all
Structure
Molecular Formula
CAS RN
TI, AB & KW
Structure
NH2
OH
N
N
OH
On all atoms
AND
Target Name
is
T790m
AND
Measurement Parameter
is
ic50
Search fields
Fields
Forms
History
Reaxys
Topics and Keywords
Identification
Physical Properties
Spectra
MedChem
Other
Reactions
Bibliography
PubChem
Commercial Substances

最后的结果



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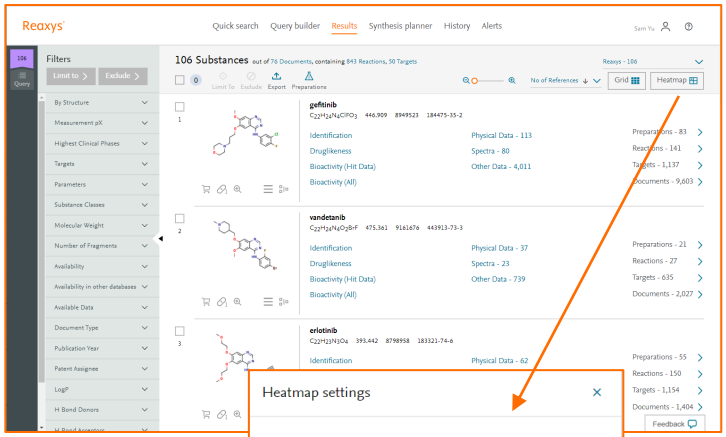
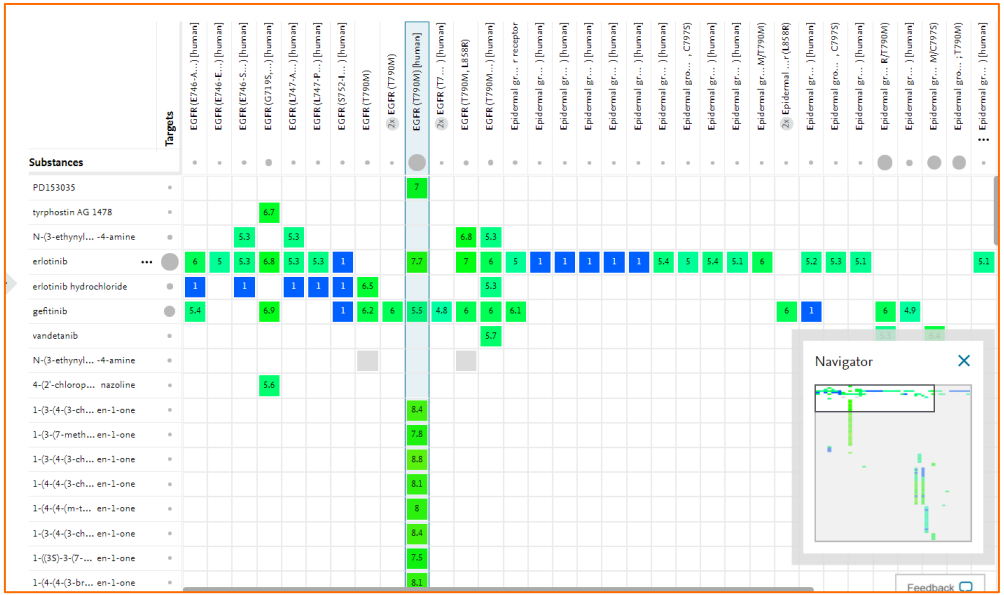
查看活性热图关系





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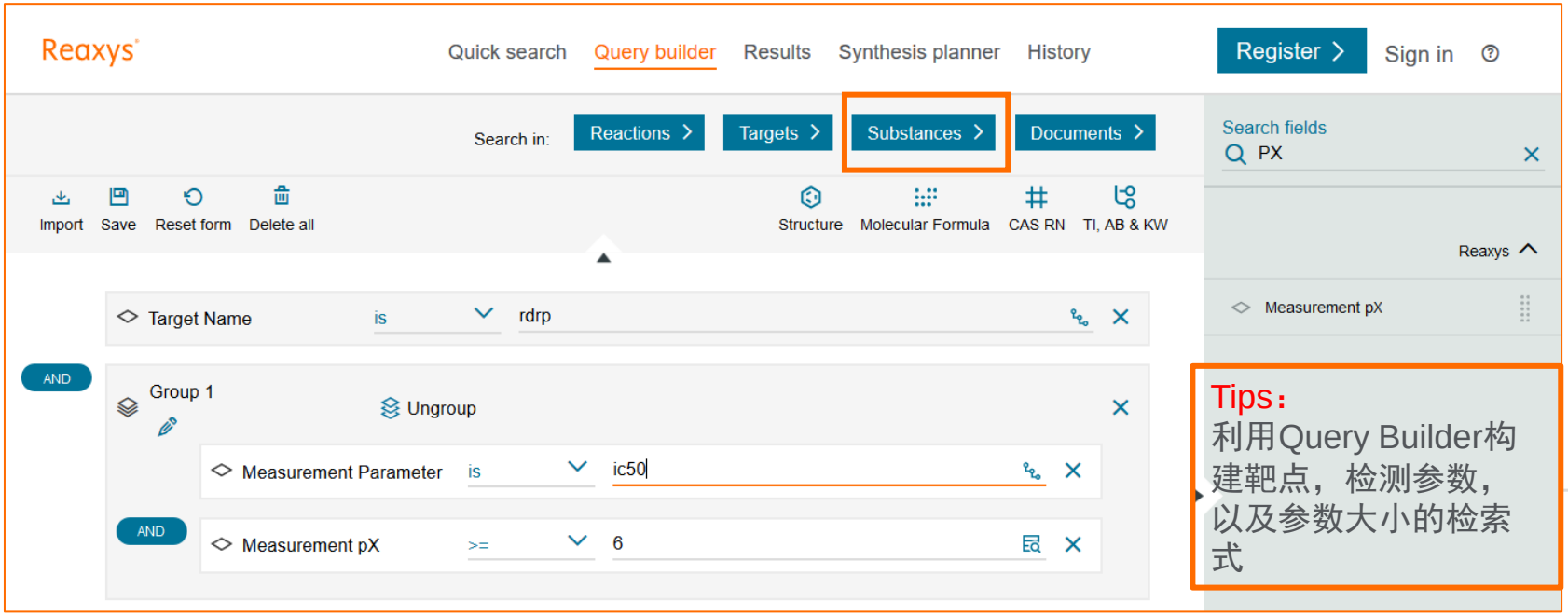
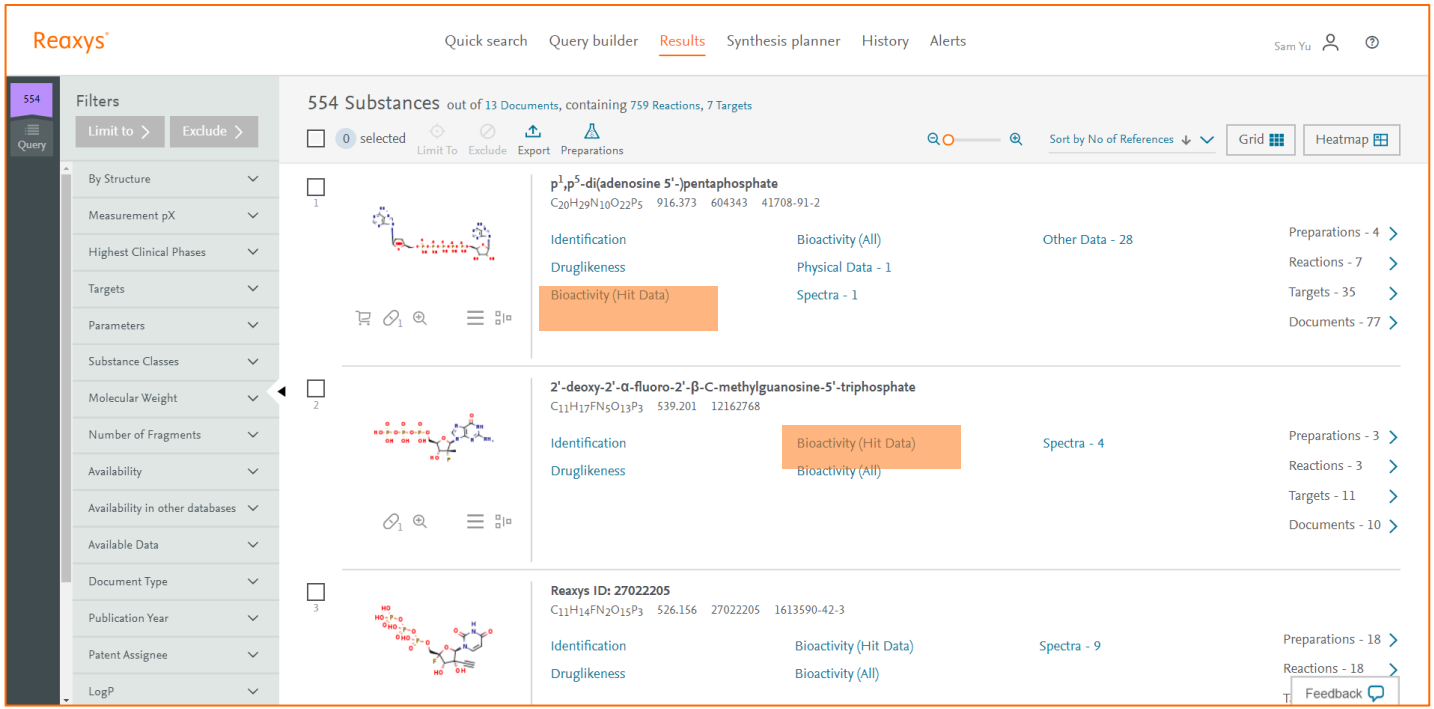
Case 7：快速筛选对特定靶点有活性的化合物（需要RMC模块）

- 获取文献中报道的对“RNA依赖的RNA聚合酶（RdRp）”有活性报道的化合物
- 希望这些化合物的IC50在um级别



Reaxys中的结果



Reaxys直接给出符合条件的化合物，大量节省了科研人员阅读文献，并查找数据的时间，可以通过各自的Hit Data查看具体数据

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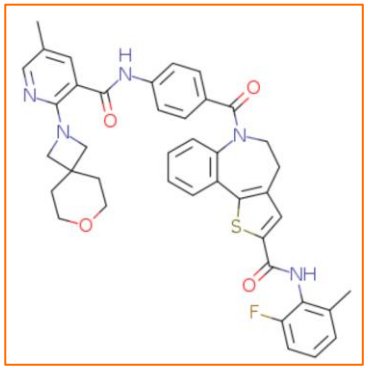
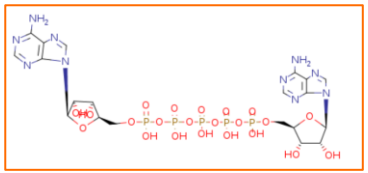
Reaxys中的结果



pX	Parameter	Value (quant)	Unit	Biological Species	Action on target	Target	(Clinical) findings / disease	Cell	Dose	Effect	Reference
6.97	IC50 (AUC viral load (Log,PFU/ml *Day))	108	nM	human	Inhibitor	RNA-directed RNA polymerase L:Wild	lung cancer	Small airway epithelial cell	28-700 nM	antivirus agent	Brookes, Daniel W; Coates, Matthew; Allen, Heather; Daly, Leah; Constant, Samuel; Huang, Song; Hows, Mark; (...) Rapeport, Garth; Ito, Kazuhiro[**British Journal of Pharmacology, 2018**, vol. 175, # 12, p. 2520 - 2534] Full Text ↗ Cited 13 times ↗ Details › Abstract ›
6.81	IC50 (AUC viral load (Log,PFU/ml *Day))	154	nM	human	Inhibitor	RNA-directed RNA polymerase L:Wild	lung cancer	Bronchial airway epithelial cell	28-700 nM	antivirus agent	Brookes, Daniel W; Coates, Matthew; Allen, Heather; Daly, Leah; Constant, Samuel; Huang, Song; Hows, Mark; (...) Rapeport, Garth; Ito, Kazuhiro[**British Journal of Pharmacology, 2018**, vol. 175, # 12, p. 2520 - 2534] Full Text ↗ Cited 13 times ↗ Details › Abstract ›



Reaxys将全文中的活性数据提炼出来，并进行标准化处理。

pX	Parameter	Value (quant)	Unit	Biological Species	Action on target	Target	Effect	Reference
7.05	IC50 (with extended primer)	0.09	μM	Influenza A virus (A/Puerto Rico/8/1934(H1N1))	Inhibitor	RNA-directed RNA polymerase [Influenza A virus]:Wild + No given title	anti-influenza virus agent	Bhat, Rakesh; Kumar D, Jagadeesh; Landi, Abdolamir; Pagadala, Nataraj Sekhar[**Medicinal Chemistry Research, 2020**] Full Text ↗ Details › Abstract ›

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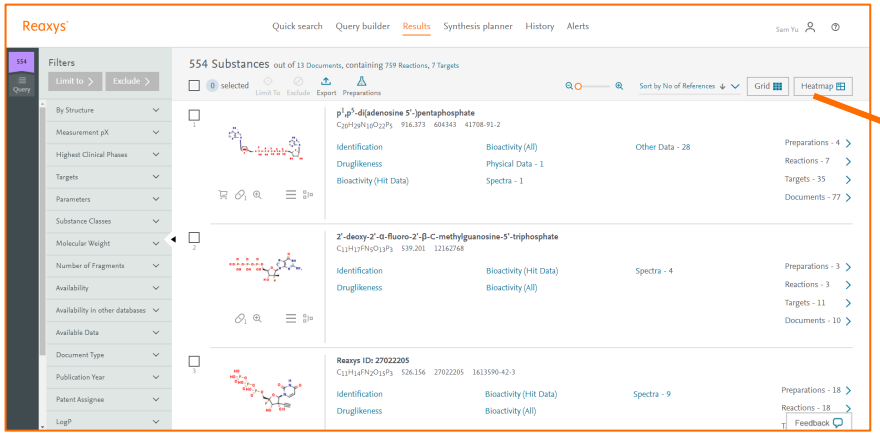
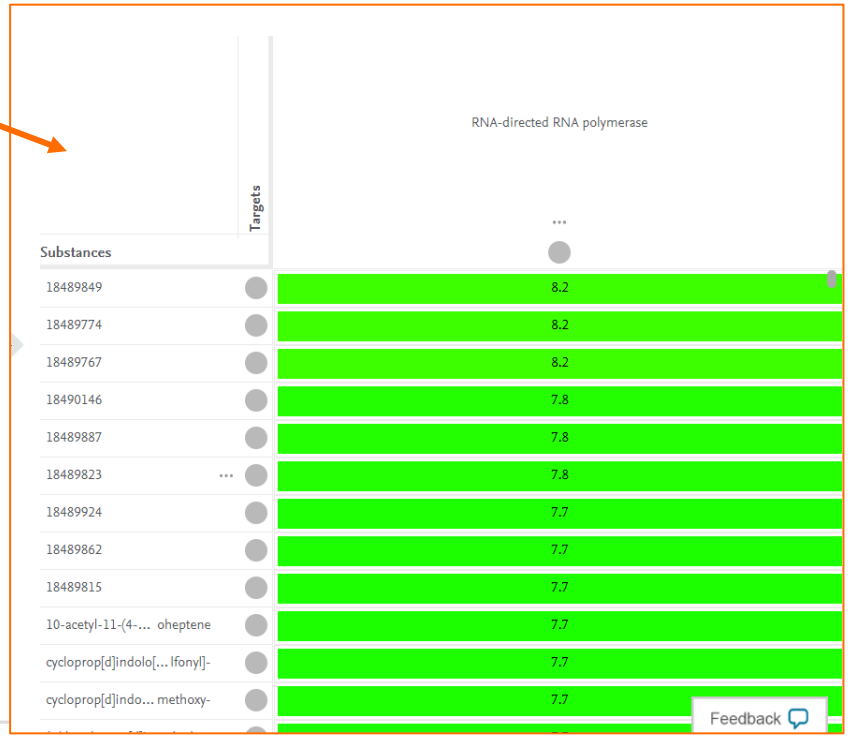
利用HeatMap看结构与靶点关系





利用Reaxys中的Heat Map，直接进行查看，靶点，结构，活性数据之间的关系，并可将活性从高到低进行排序。

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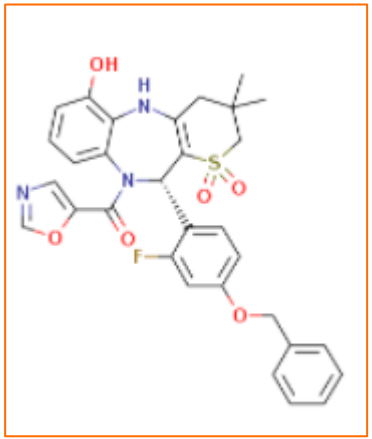
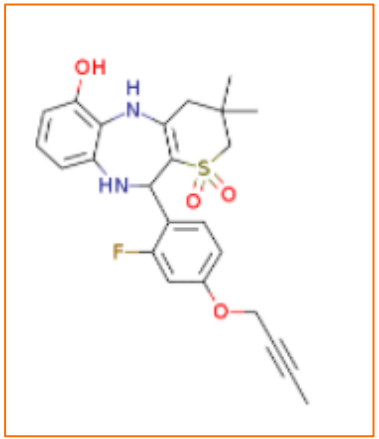
一些非常有意思的结构



PX=8.2



PX=6.9

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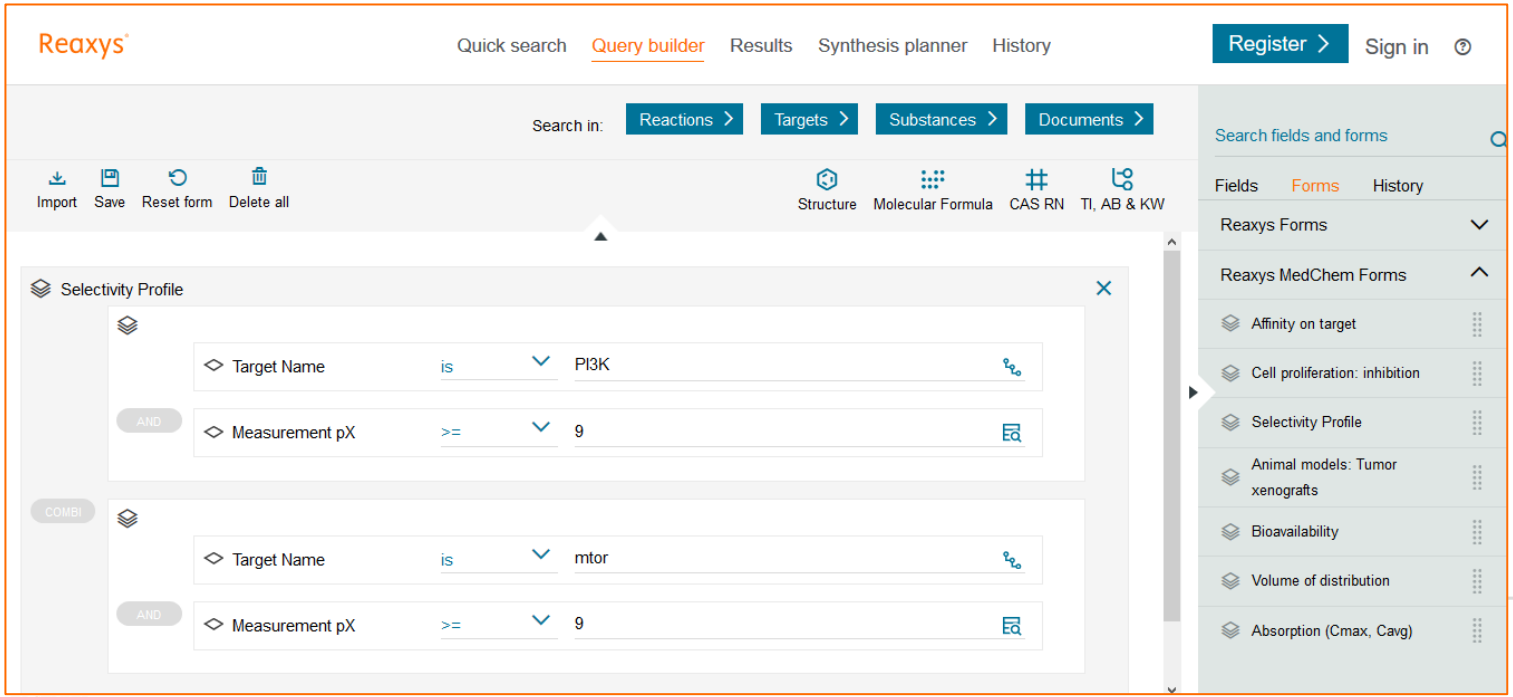
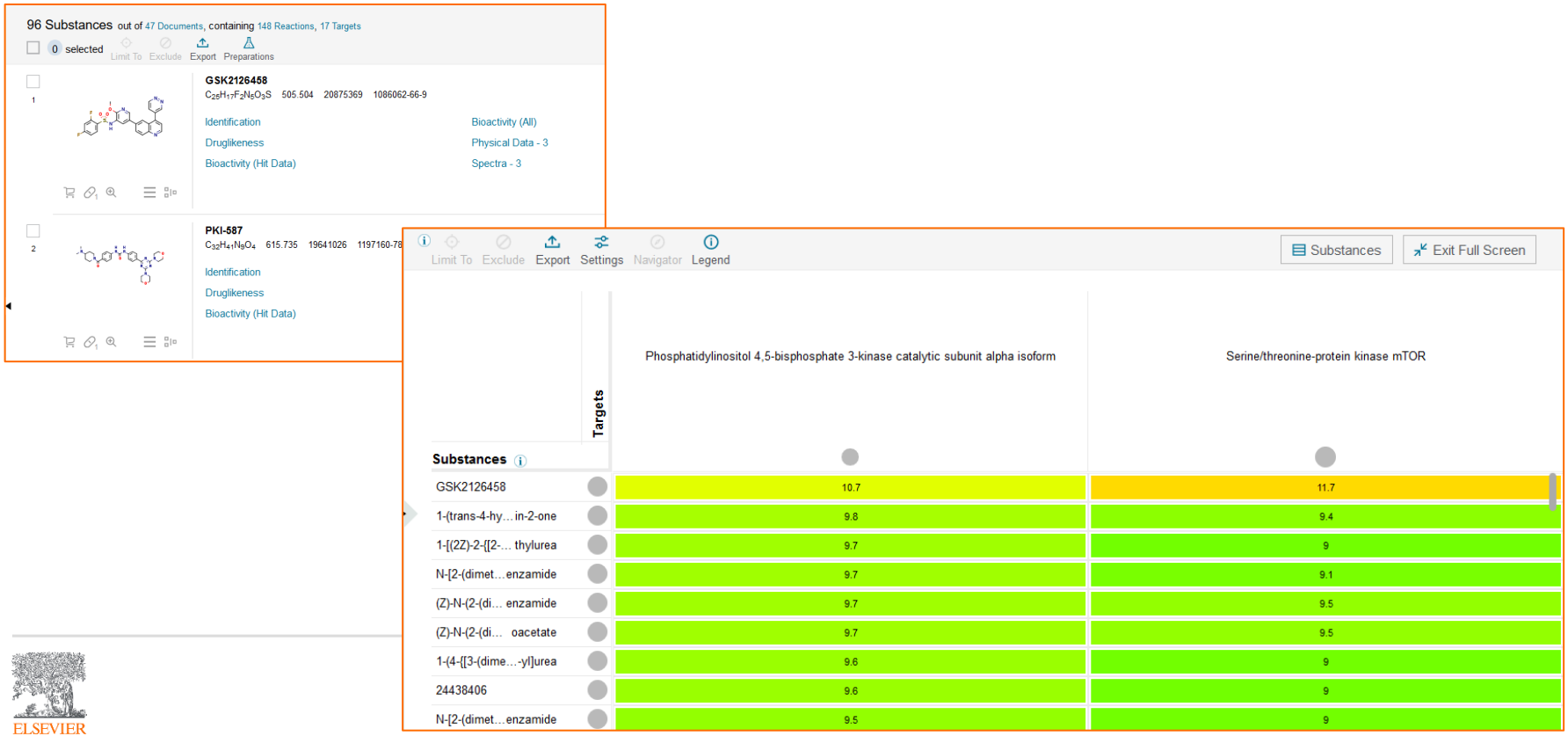
Case 8：双靶点活性化合物的获取（需要RMC模块）

- PI3K和mTOR双抑制剂，且活性都在nM级别化合物

  视频操作链接：https://www.bilibili.com/video/BV1vK4y1Z7fr



双靶点活性化合物



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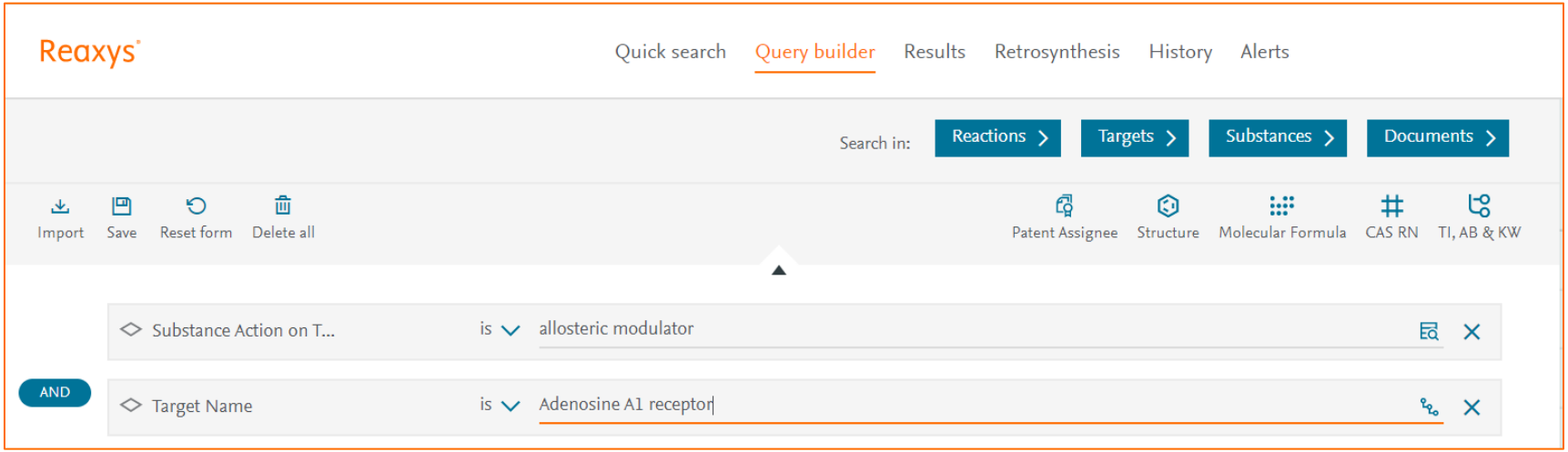
Case 9：寻找在特定靶点上存在变构调节的分子

- 传统Adenosine A1 receptor激动剂由于正构位点保守性造成选择性差而无法进入临床，因此，在具有特异性的A1R变构位点上发现激动剂就存在巨大的潜力



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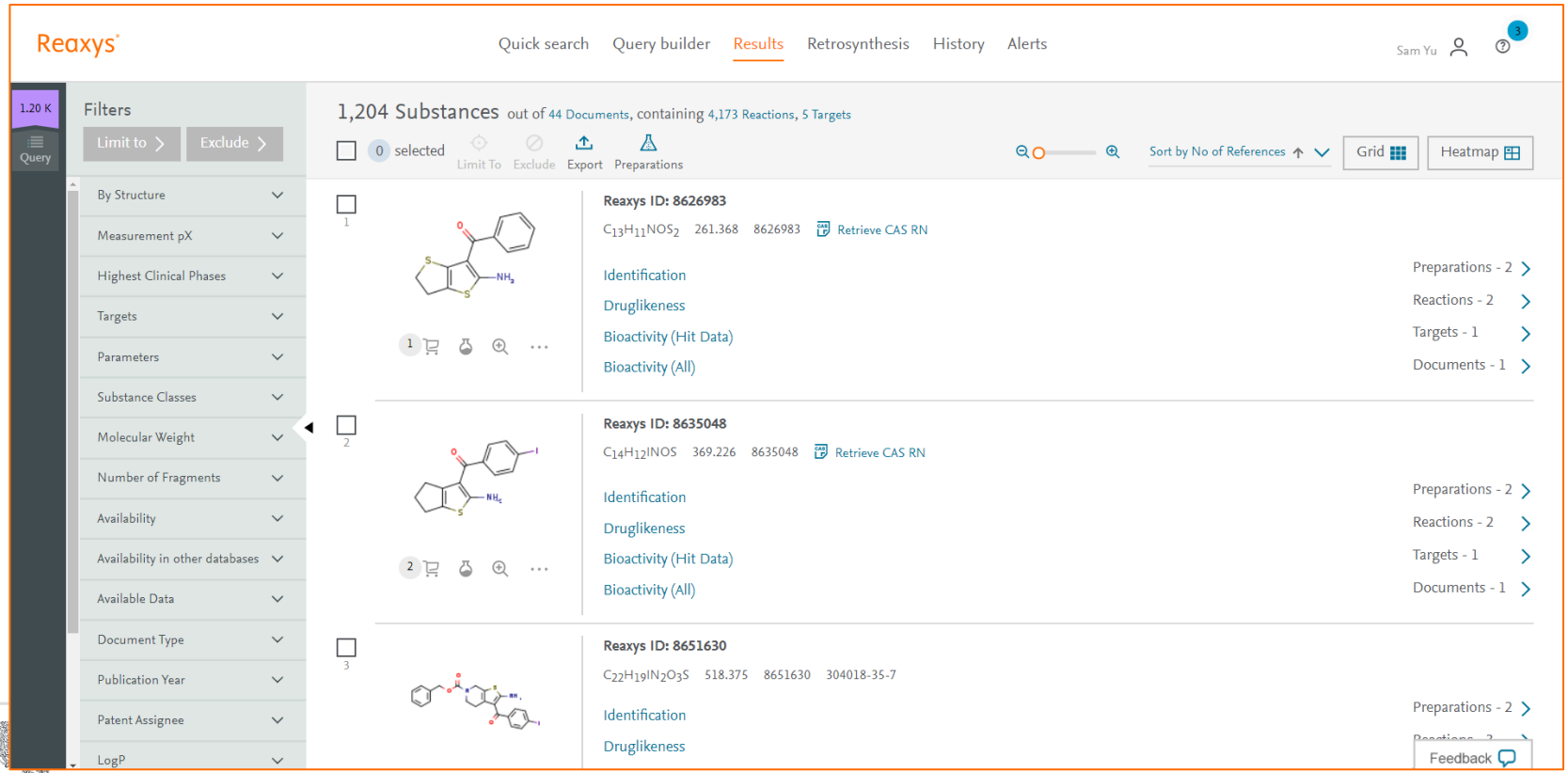
有变构调节研究的化合物



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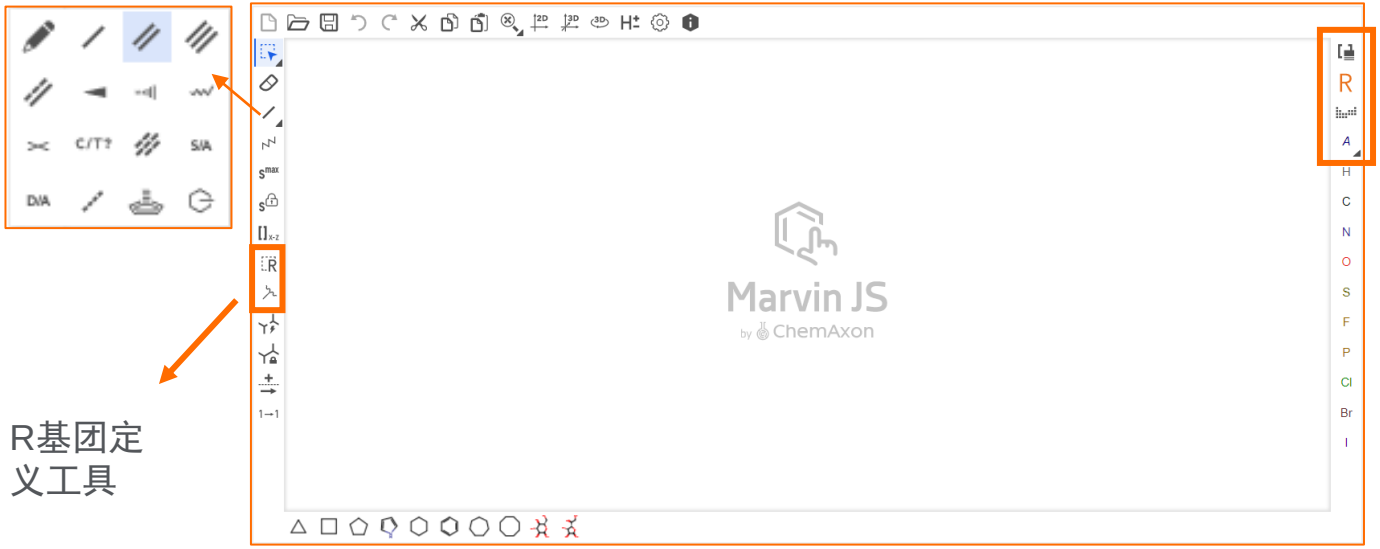
Agenda

- 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中的科技文献检索与分析
  - 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



缩写官能团，通用官能团，原子列表/列表非原子属性列表

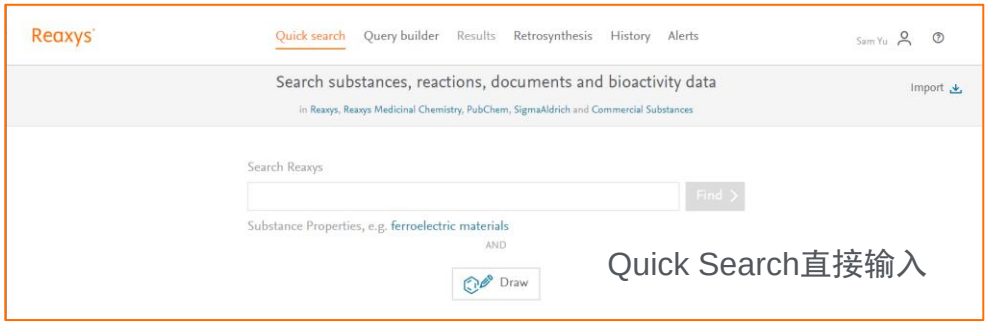
R基团定义工具

一些常见的功能使用视频

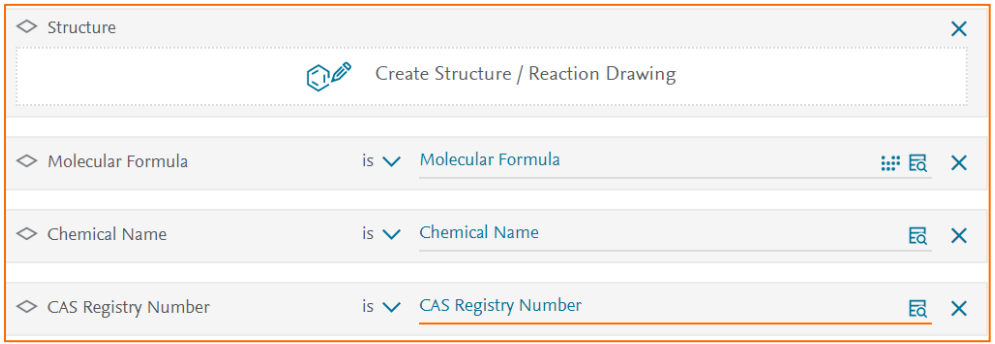
常用功能	视频链接	
最基本功能	https://www.bilibili.com/video/BV13i4y177wV	基础结构面板使用
不定位键	https://www.bilibili.com/video/BV1LK411P7nW	
通用/缩写官能团	https://www.bilibili.com/video/BV1PV41117J6	
原子列表与列表非	https://www.bilibili.com/video/BV1Ay4y1z7a5	
R基团定义	https://www.bilibili.com/video/BV1654y1r7be	
原子锁定与环锁定	https://www.bilibili.com/video/BV175411V77h	
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	
反应定义基本操作	https://www.bilibili.com/video/BV19r4y1w7Z5	基础反应功能使用
反应条件的定义	https://www.bilibili.com/video/BV1Af4y1q7xk	
合成计划的制作	https://www.bilibili.com/video/BV1oL411u7yP	
机理性文献查询	https://www.bilibili.com/video/BV1pK4y1E7Qx	

Reaxys中的结构获取物质的常用方法小结

- Reaxys中获取物质的方法
  - 物质名称
  - 物质分子式
  - 物质结构式
  - CAS No



Quick Search直接输入



Query Builder选择不同字段

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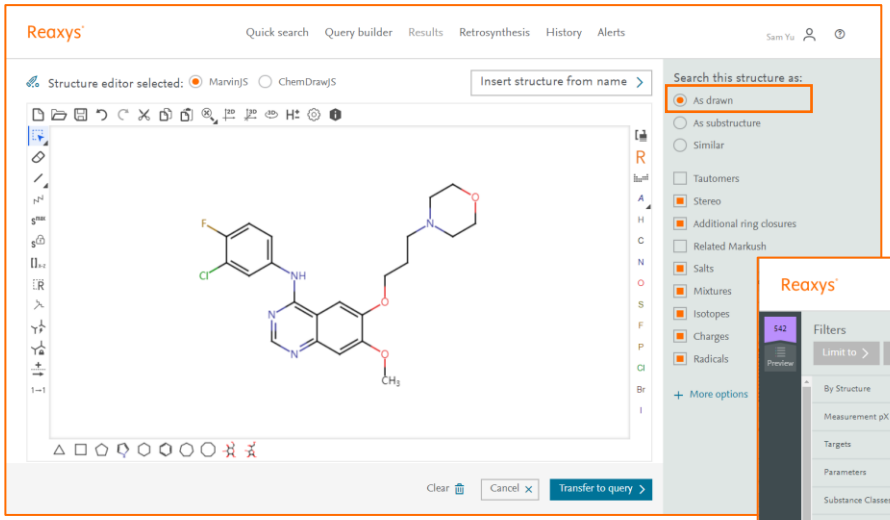
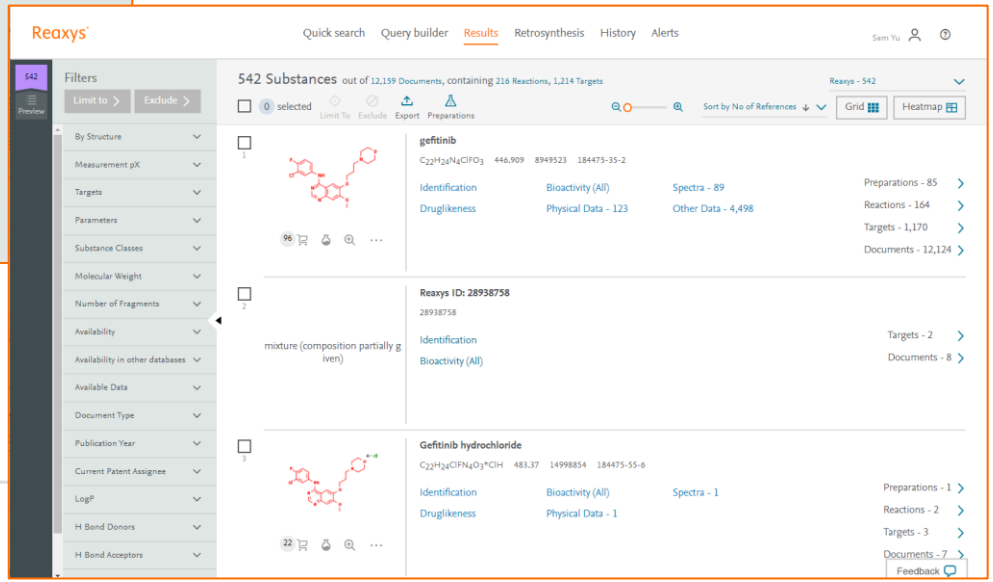
CASE 10：Reaxys中具体化合物的获取



结构面板中绘制具体化合物，同时使用As Drawn进行检索，即可获取具体化合物，包括盐，同位素，配合物，混合物等



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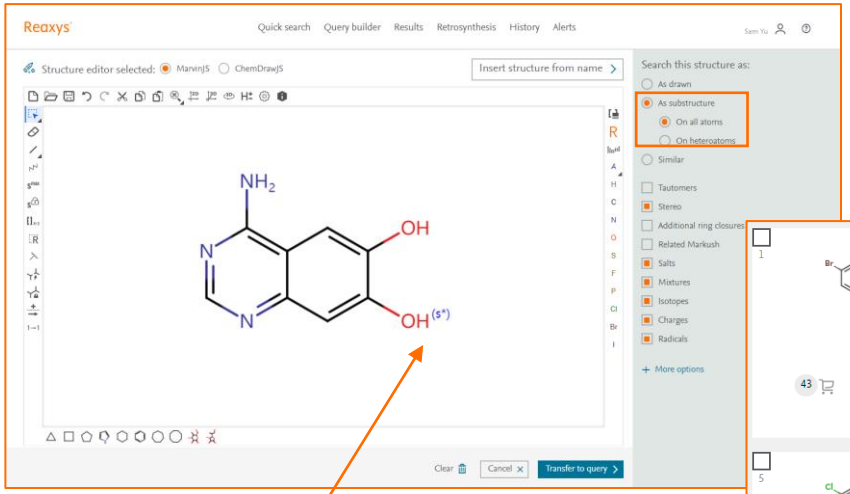
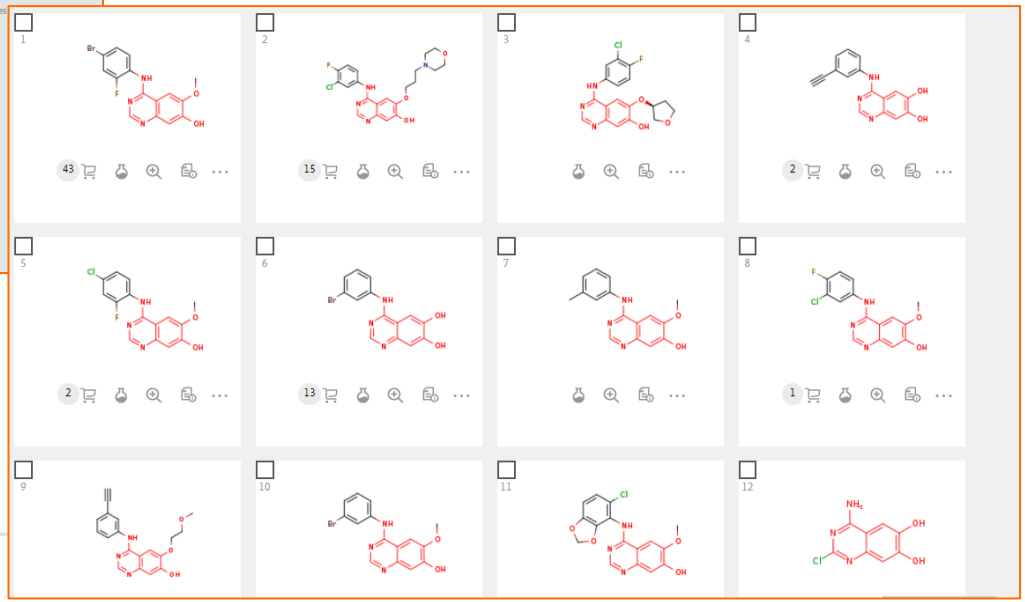
CASE 11：Reaxys中骨架化合物的获取



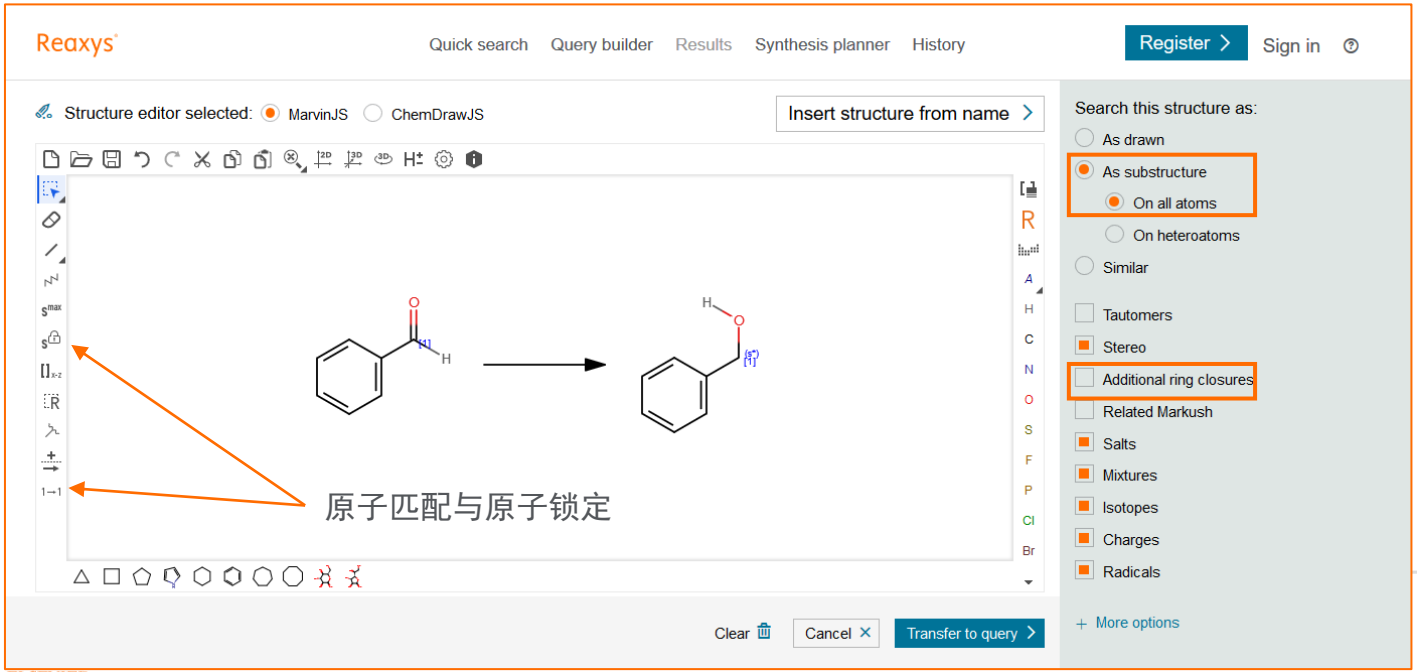
结构面板中绘制具体或通式结构，同时使用As Substructure进行检索，即可获得包含这个骨架的化合物。



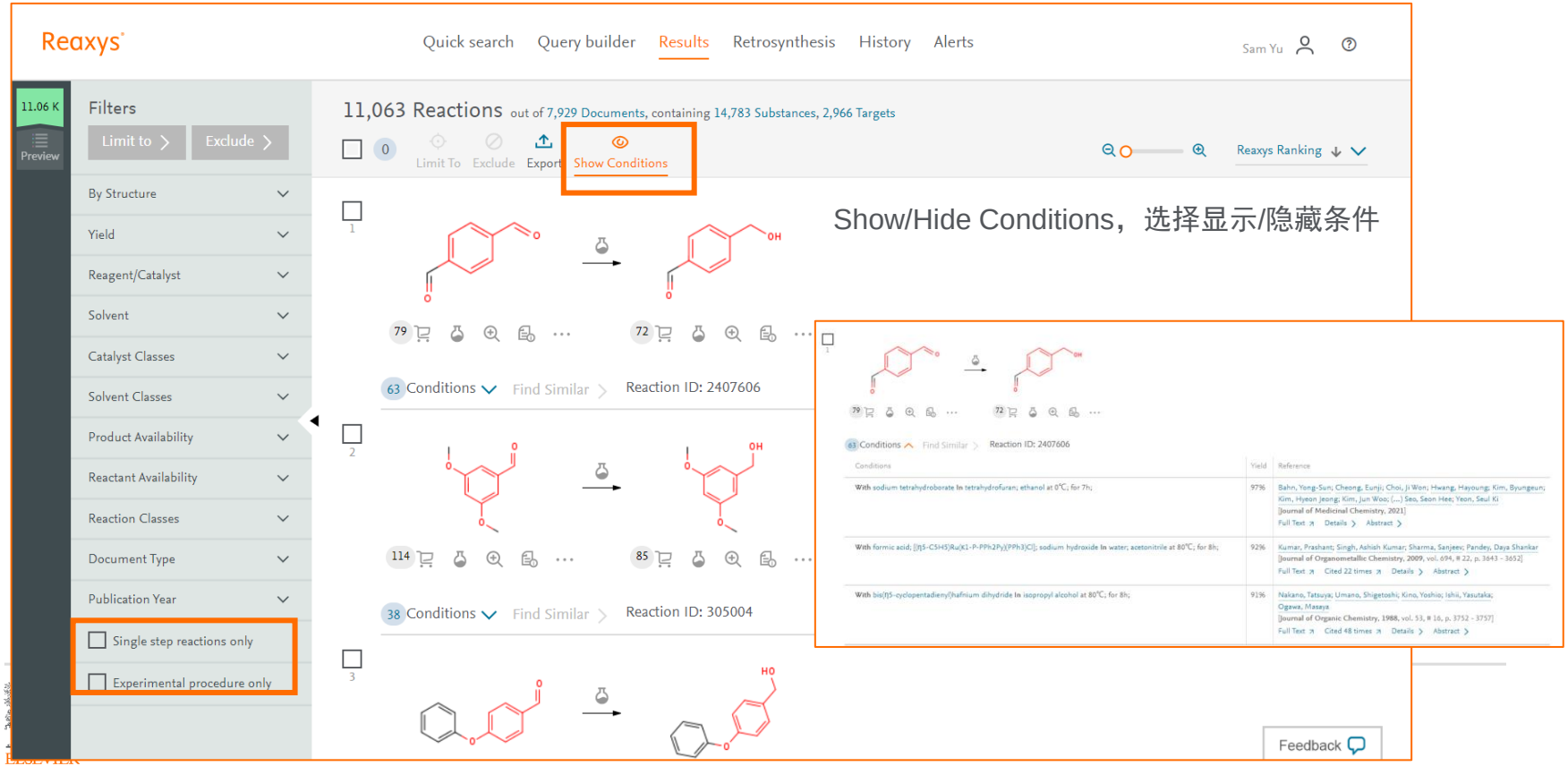
标记这个位点上不允许有取代

Case 12：Reaxys中最简单的反应定义与筛选

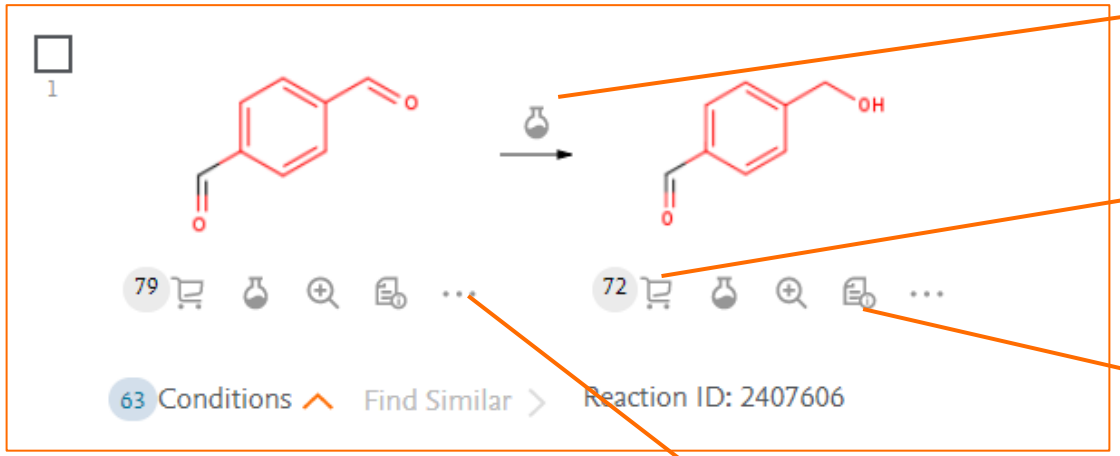
- 检索以下核心结构反应并进行反应筛选操作
- 视频操作过程
  - https://www.bilibili.com/video/BV1BT4y1F7vT



Reaxys中的结果

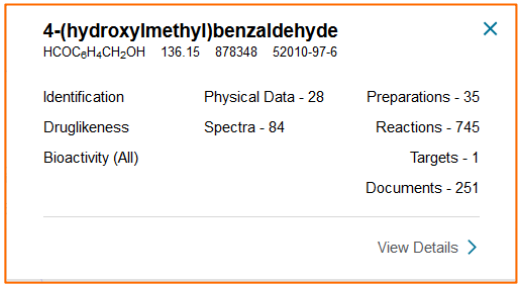

Reaxys
Quick search
Query builder
Results
Retrosynthesis
History
Alerts
Sam Yu
11.06 K
Preview
Filters
Limit to
Exclude
By Structure
Yield
Reagent/Catalyst
Solvent
Catalyst Classes
Solvent Classes
Product Availability
Reactant Availability
Reaction Classes
Document Type
Publication Year
Single step reactions only
Experimental procedure only
11,063 Reactions out of 7,929 Documents, containing 14,783 Substances, 2,966 Targets
Limit To
Exclude
Export
Show Conditions
Reaxys Ranking
63 Conditions
Find Similar
Reaction ID: 2407606
114 Conditions
Reaction ID: 305004
Feedback
Show/Hide Conditions，选择显示/隐藏条件

Reaxys的一条反应的界面



进行合成计划

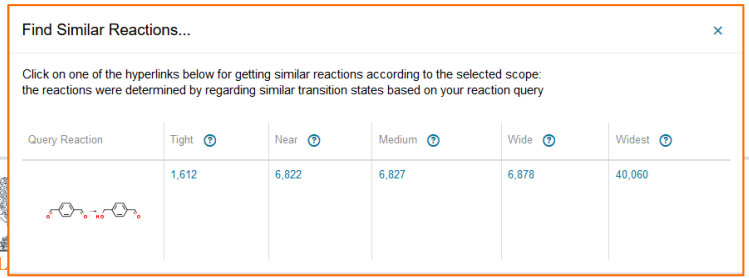
查看商业来源

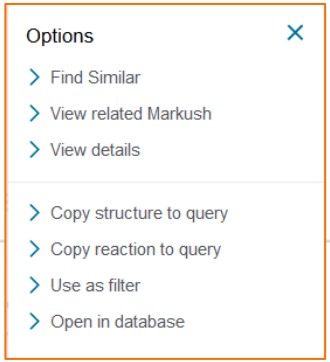


查看物质详情

查看条件

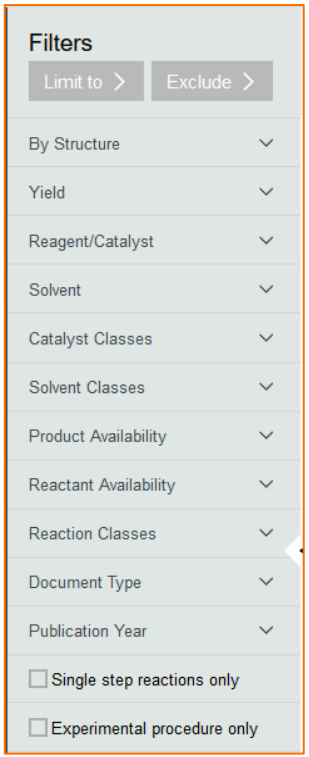
寻找相似反应

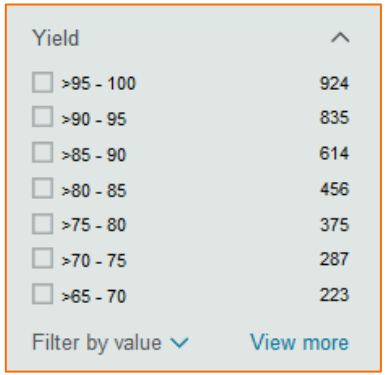


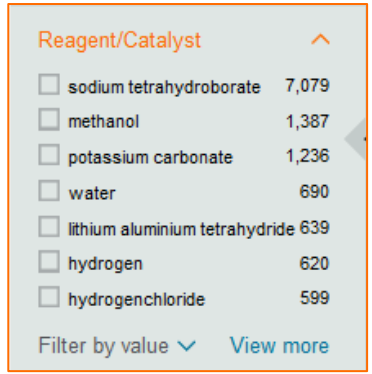


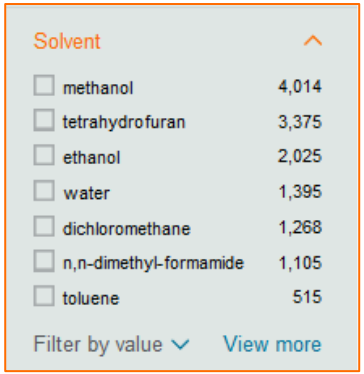
更多与物质相关操作

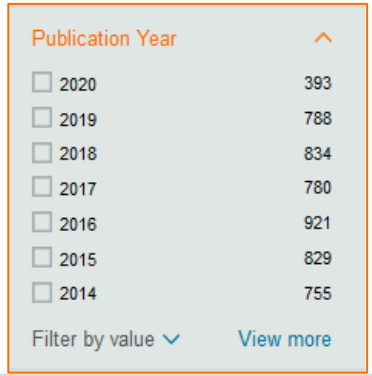
Reaxys的筛选操作











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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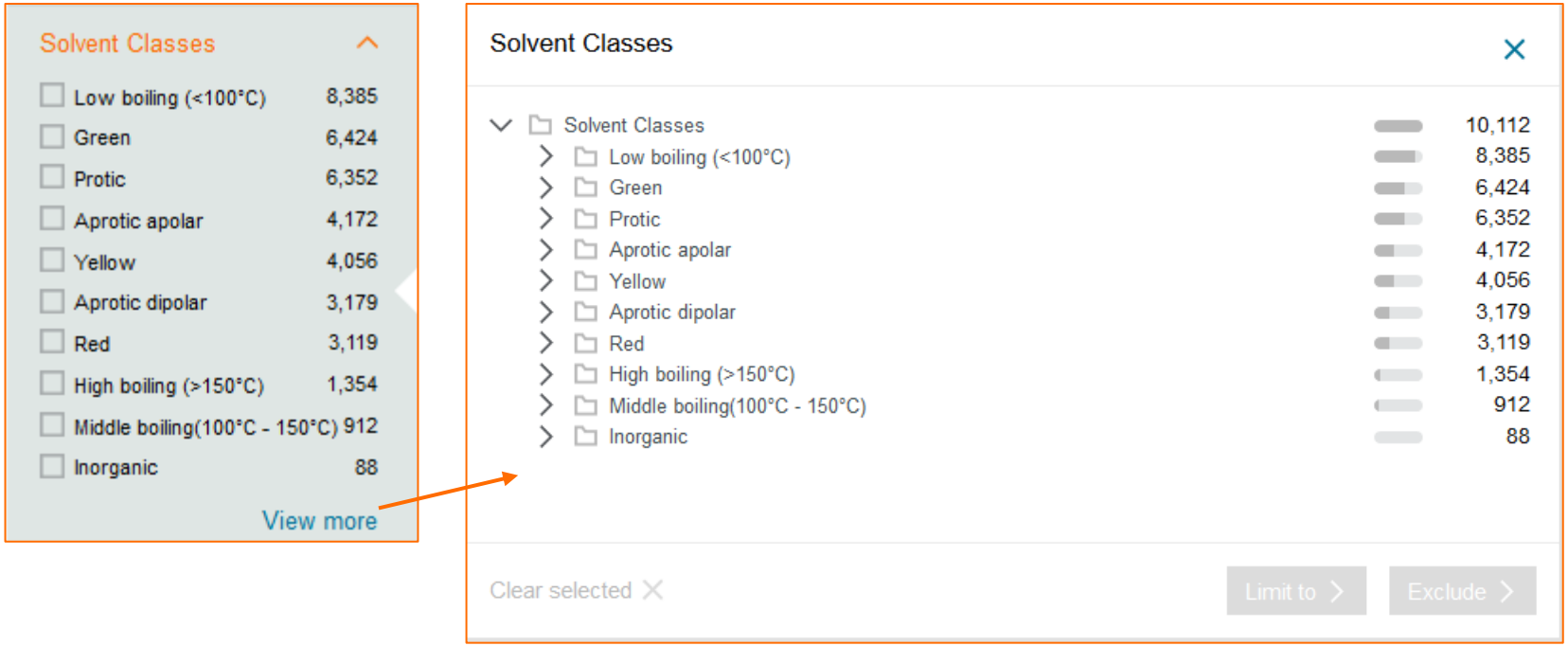
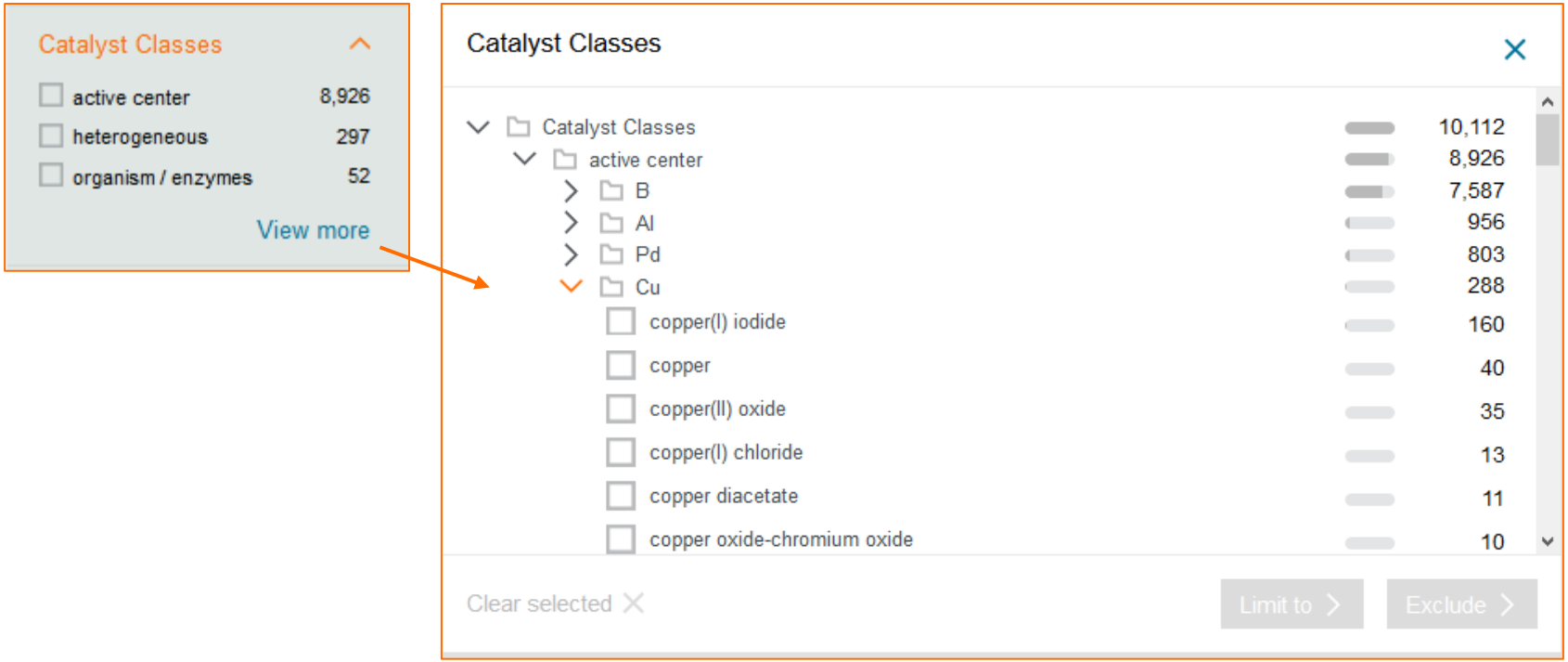
Reaxys中的一些特殊筛选工具—溶剂分类



Reaxys中的一些特殊筛选工具—催化剂分类



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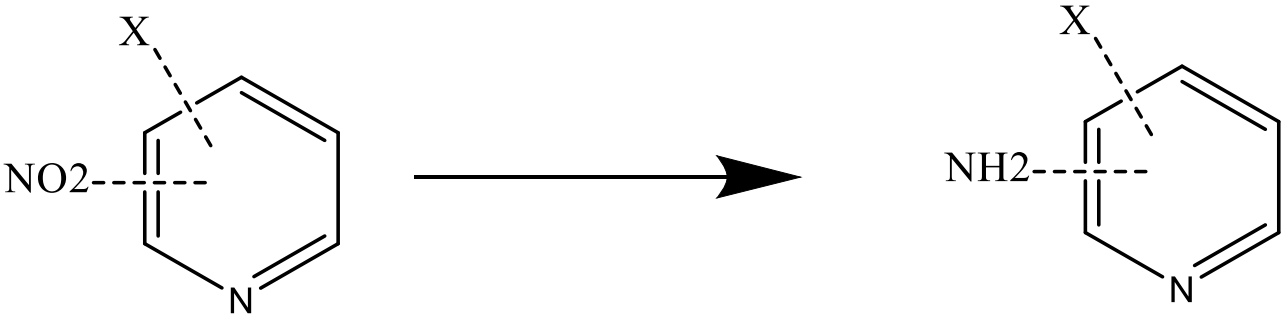
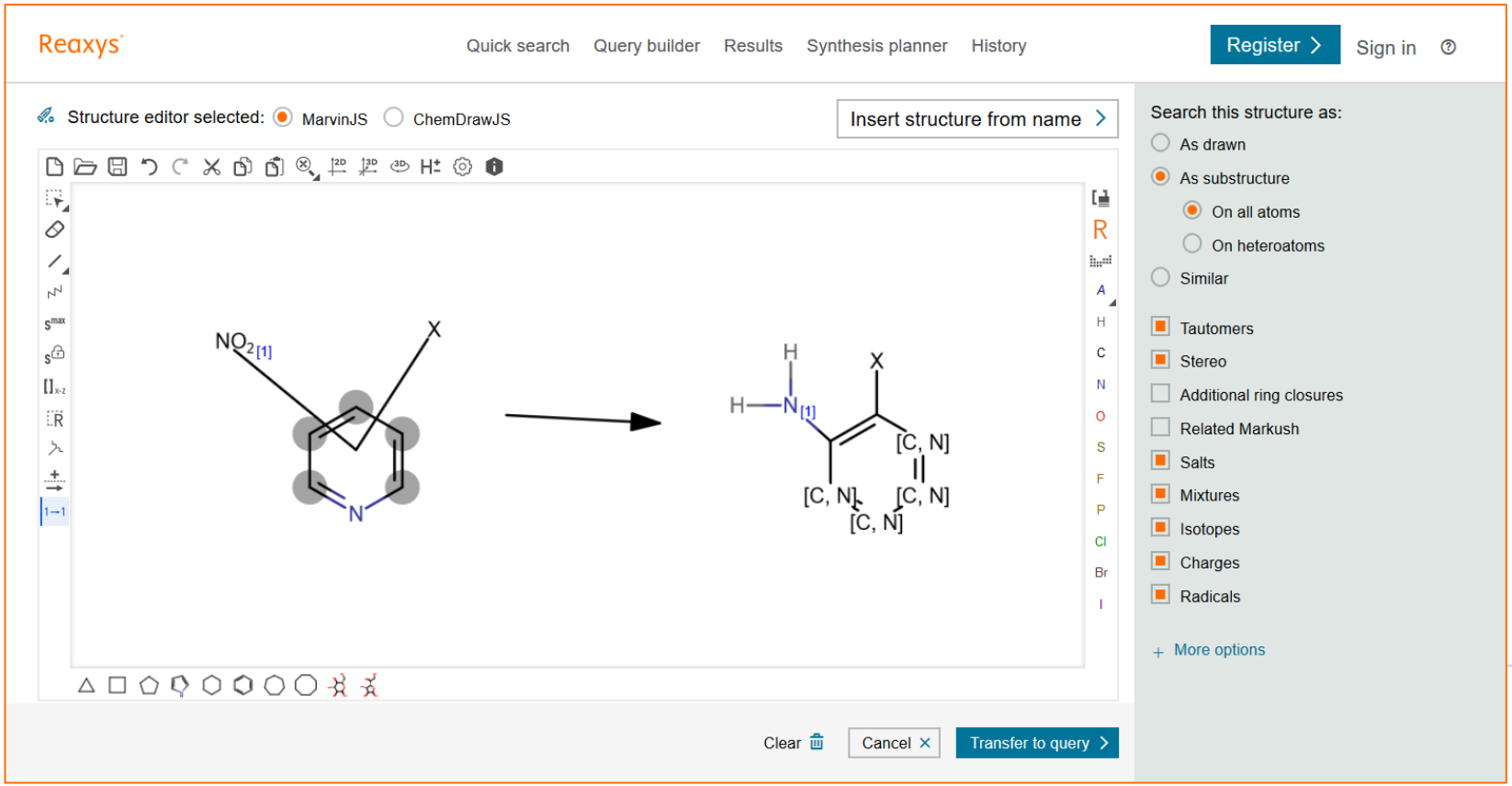
Case 13：结构中有特殊需求的反应定义

- 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

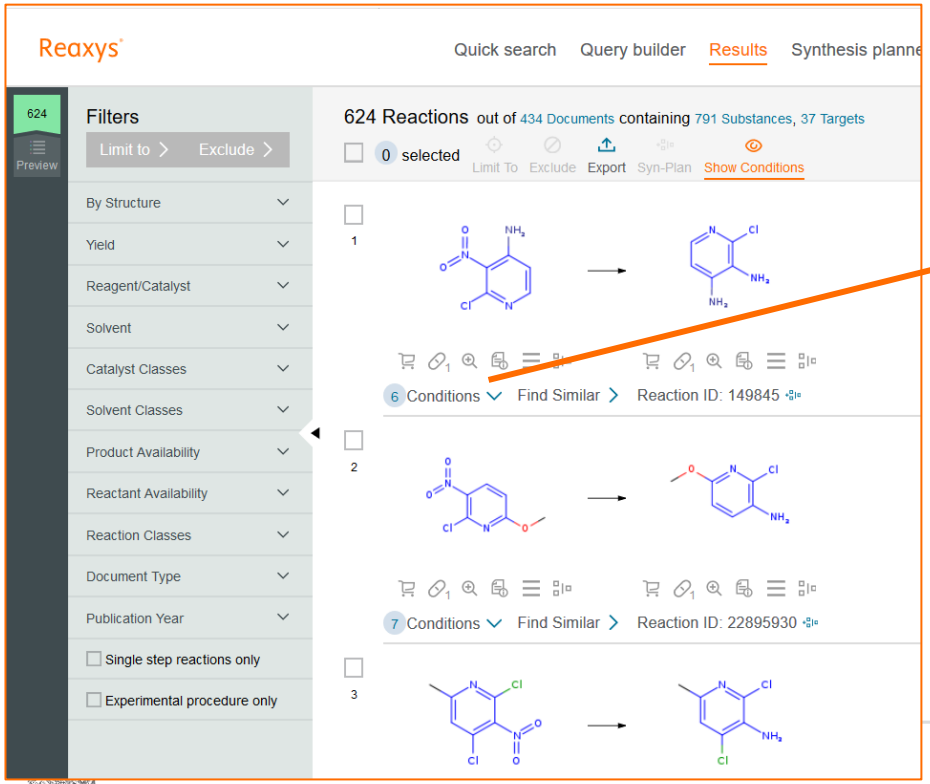


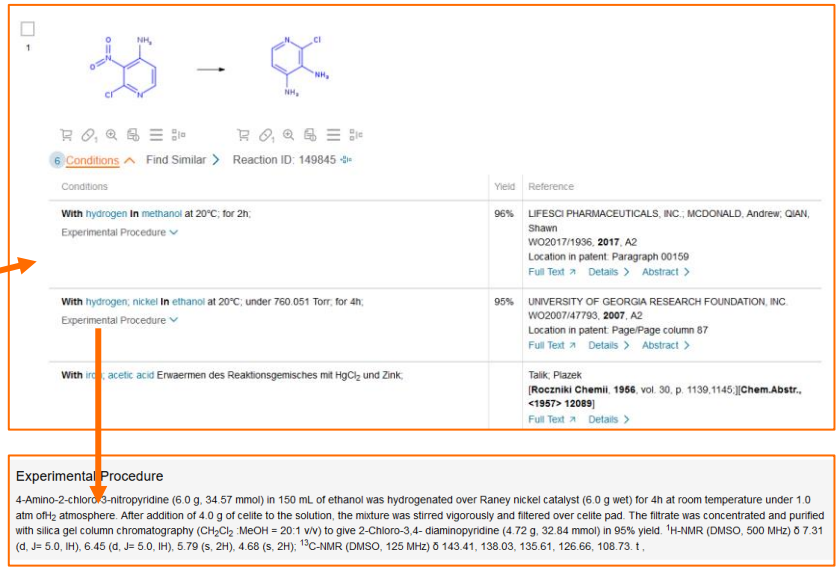
视频操作过程：
https://www.bilibili.com/video/BV1si4y177as

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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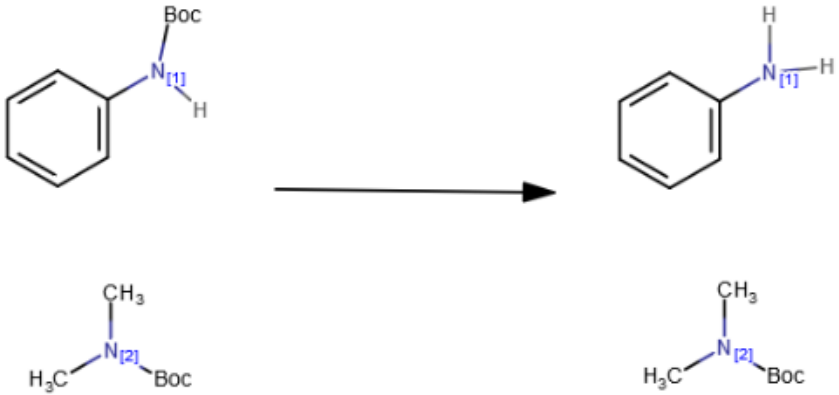
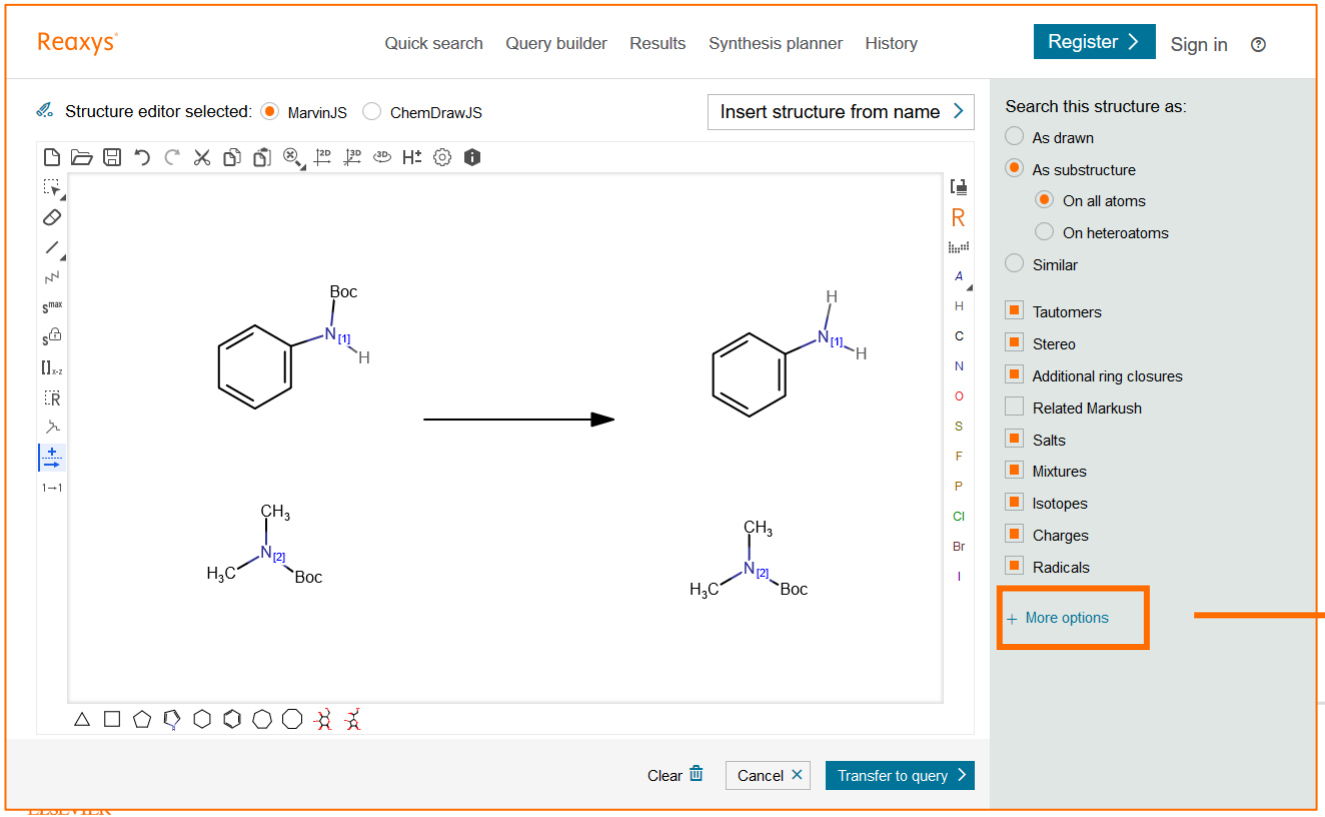
Case 14：选择性氧化还原脱保护反应的定义

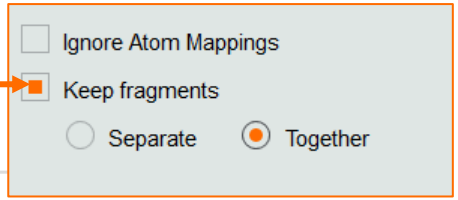
- 结构中两个带Boc的片段，两个片段以任意的形式相接在一个分子中
- 反应过后把其中一个片段的Boc脱掉，但是另外一个Boc不变



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

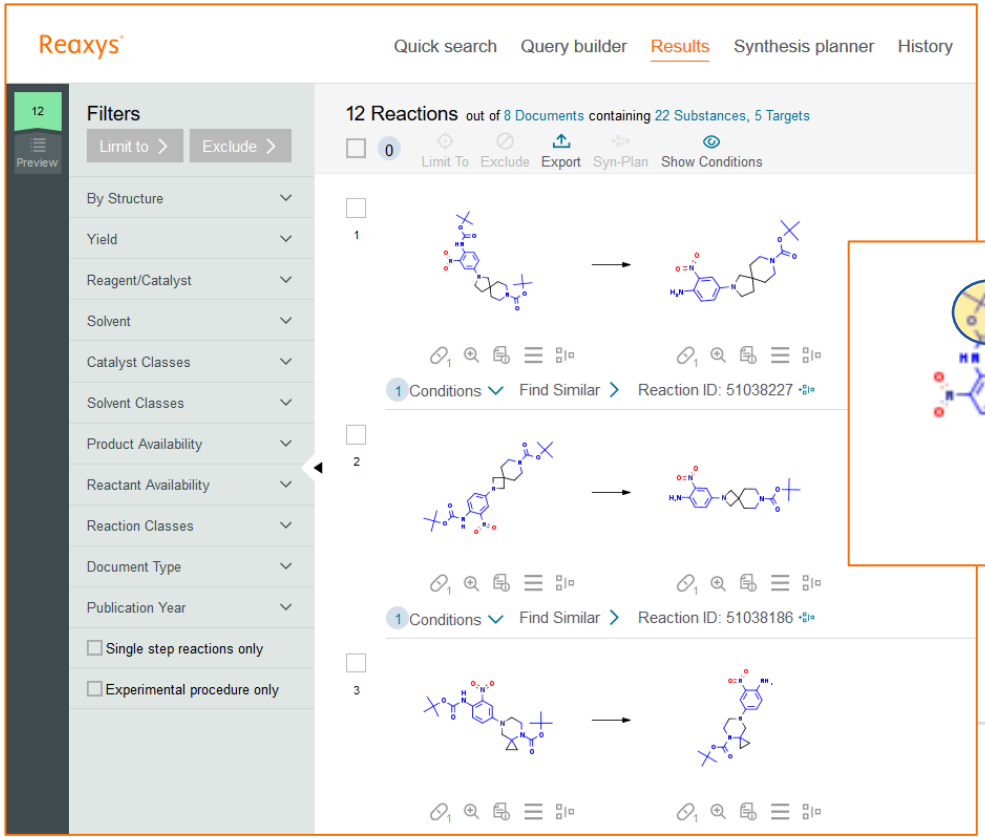
Reaxys中的结构定义

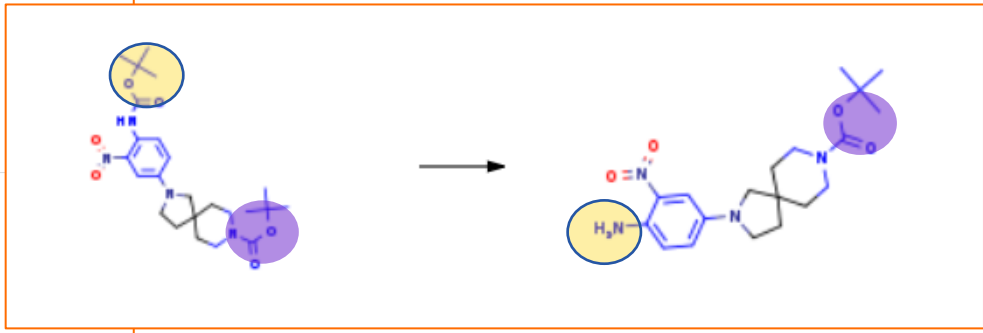




Reaxys可以直接设定这些片段在一个结构中

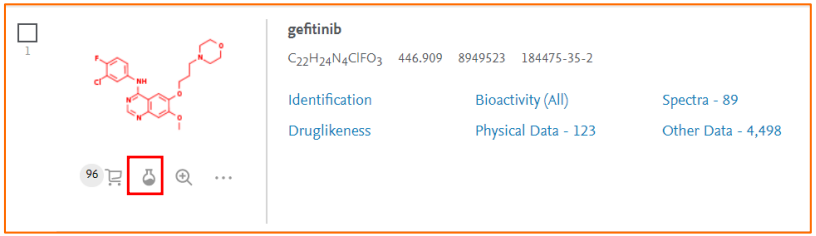
Reaxys中结果

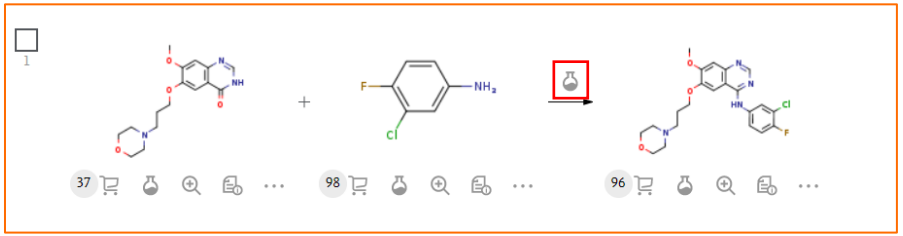

Reaxys
Quick search
Query builder
Results
Synthesis planner
History
12
Preview
Filters
Limit to
Exclude
By Structure
Yield
Reagent/Catalyst
Solvent
Catalyst Classes
Solvent Classes
Product Availability
Reactant Availability
Reaction Classes
Document Type
Publication Year
Single step reactions only
Experimental 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

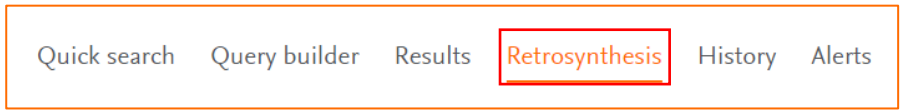


Case 15：Reaxys中合成计划的制作

- 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

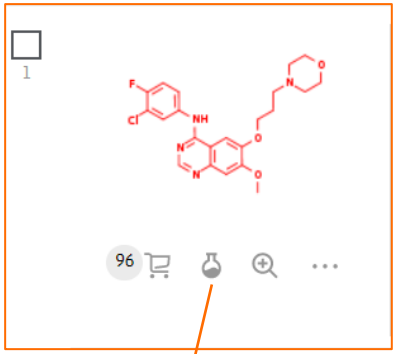


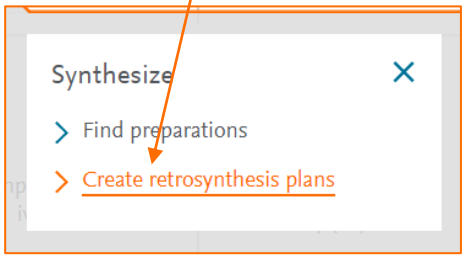


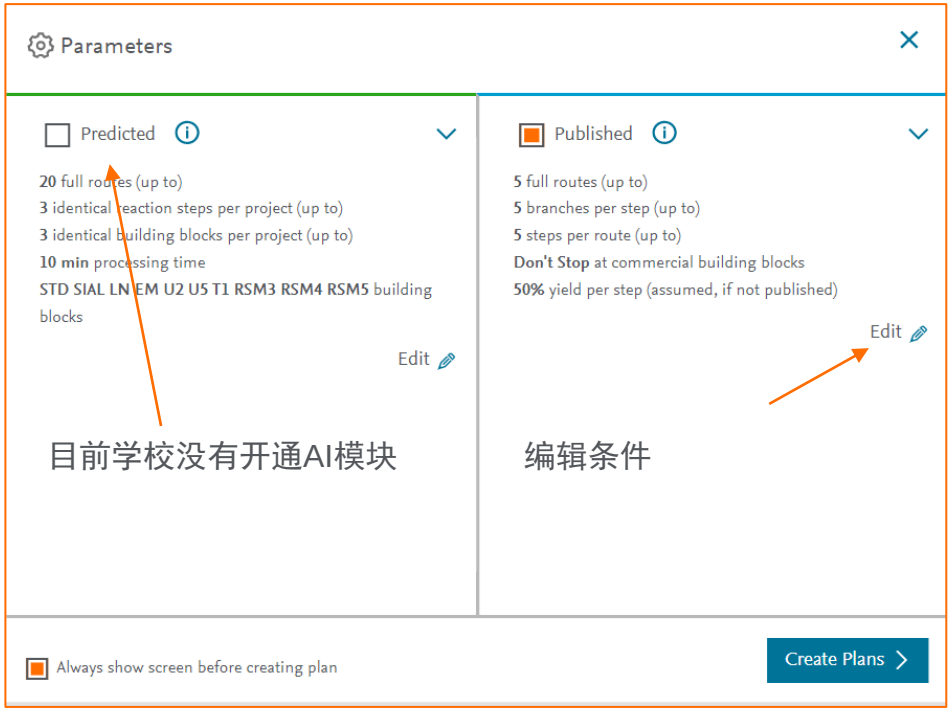


视频操作过程：
https://www.bilibili.com/video/BV1oL411u7yP

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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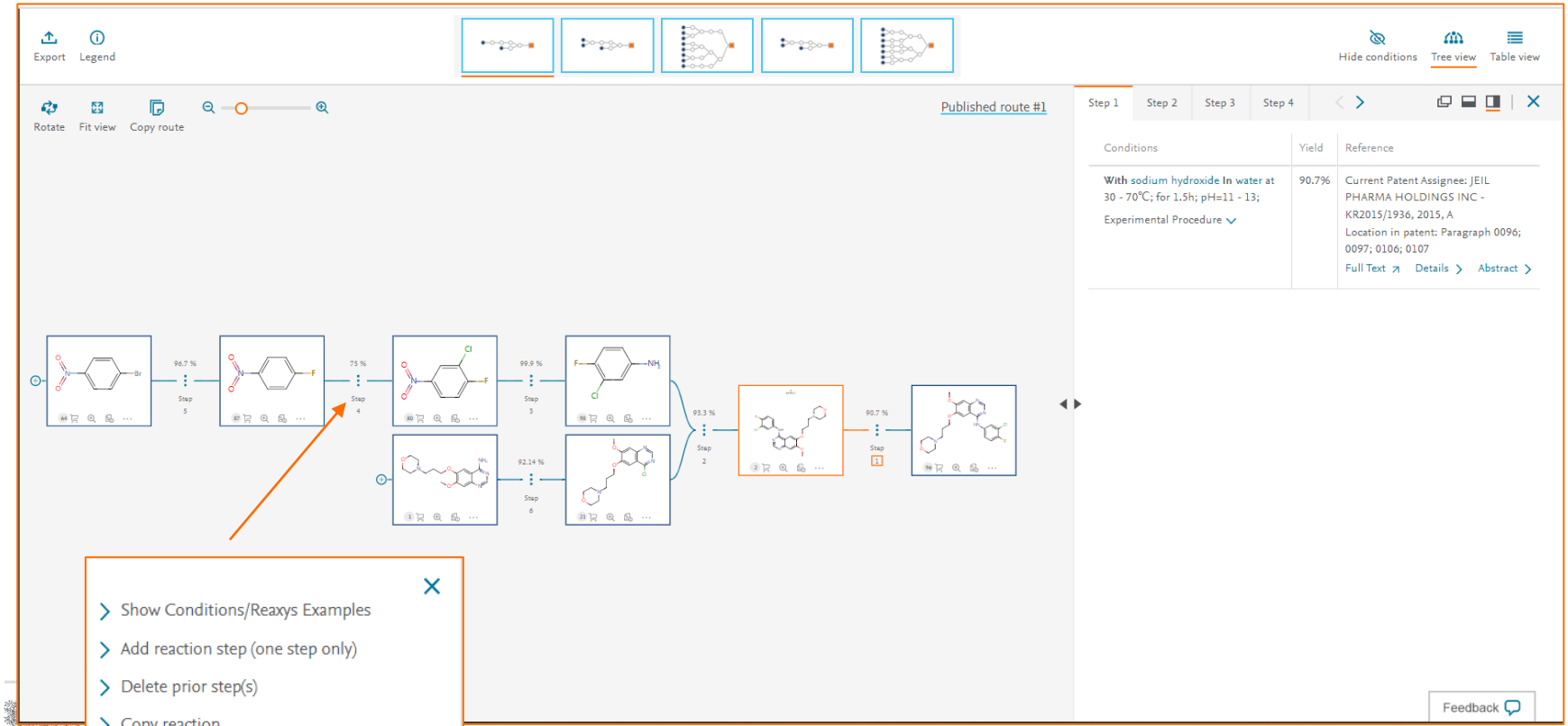
结果的呈现



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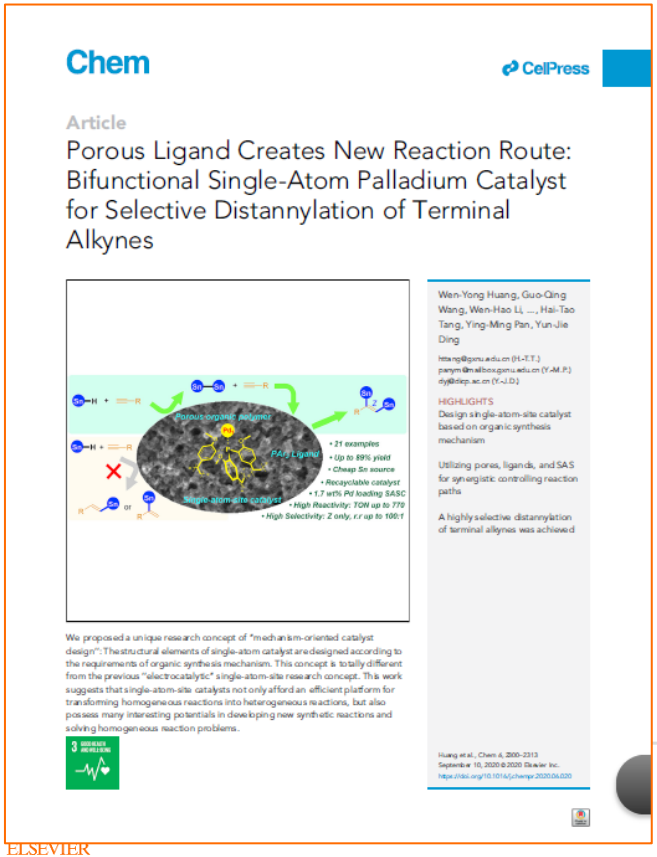
  - Reaxys中的科技文献检索与分析
  - Reaxys中物质理化性质数据的查询与反向物质获取
  - Reaxys中结构面板与物质结构和反应数据的获取
  - Reaxys中的实用小案例
- Q&A

Case 16：化合物的文献定位



Chem

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Article

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

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.

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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 allynes was achieved

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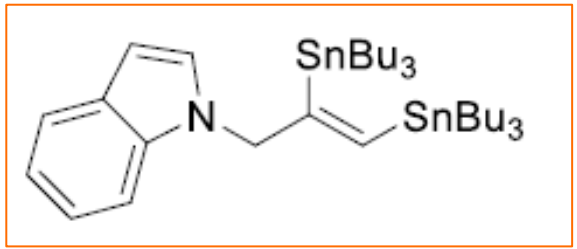
这是一篇常见的化学文献，包含：

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

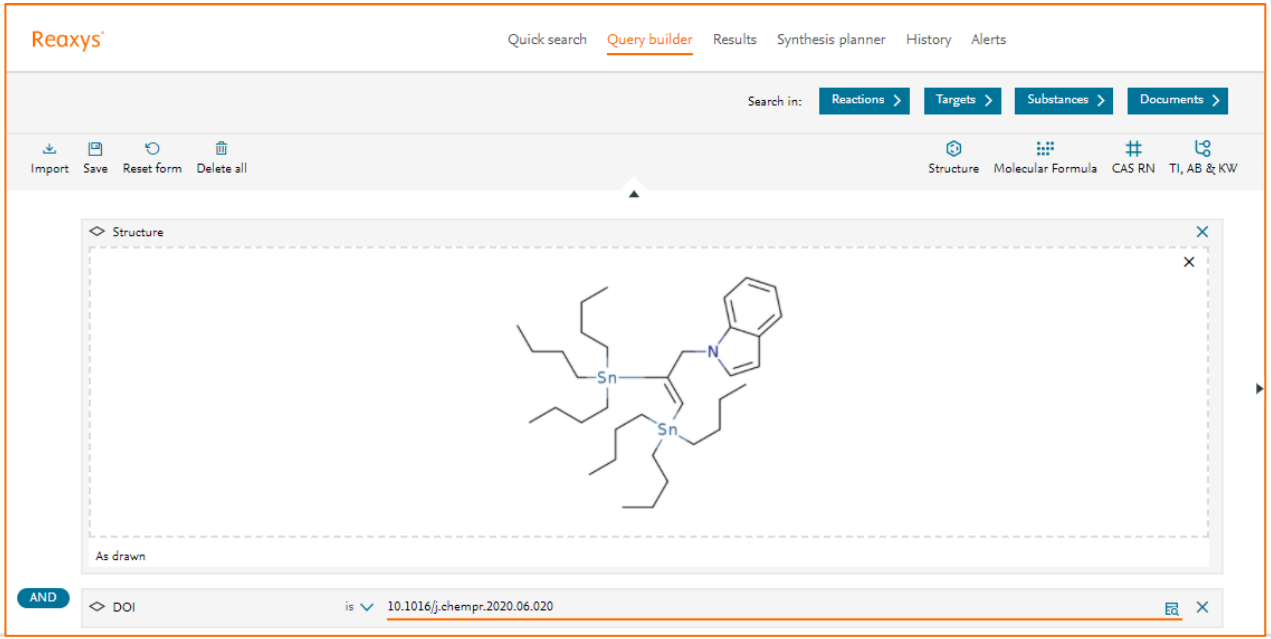
已知文献中报道了这个化合物，如何在上述的67页文档中找到有关这个化合物的描述？



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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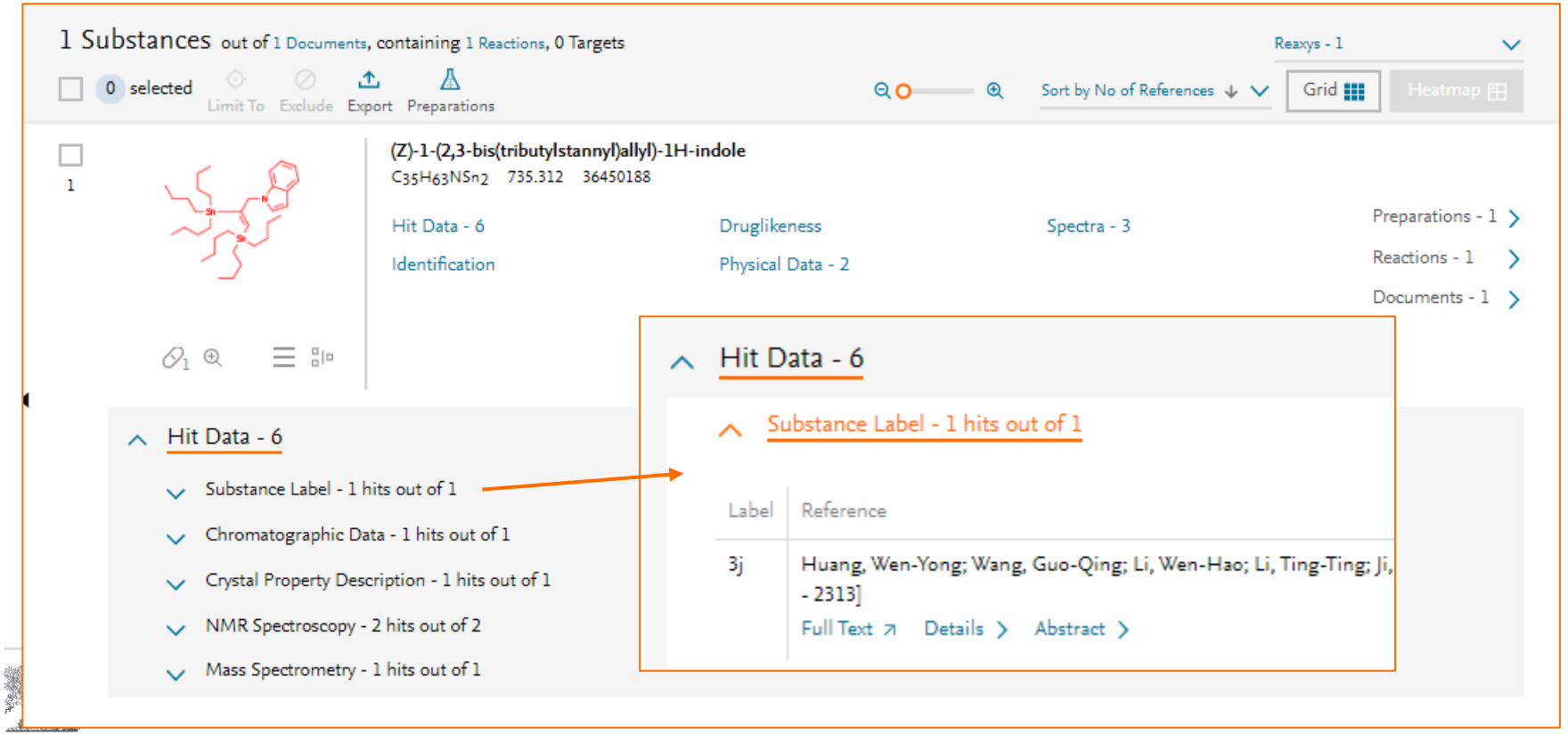
Reaxys中的结果



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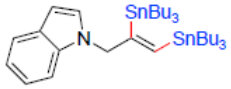
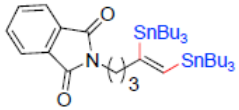
全文检索3J定位化合物

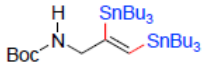
N-containing terminal alkynes



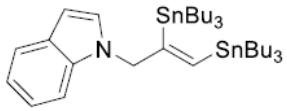
3j 89% (100:1)



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,

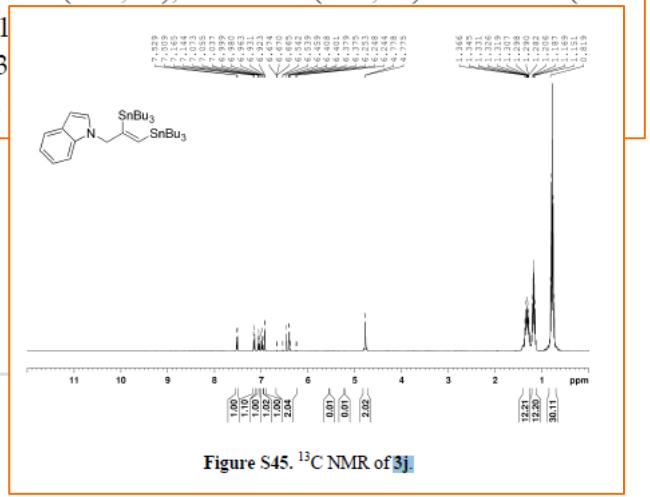
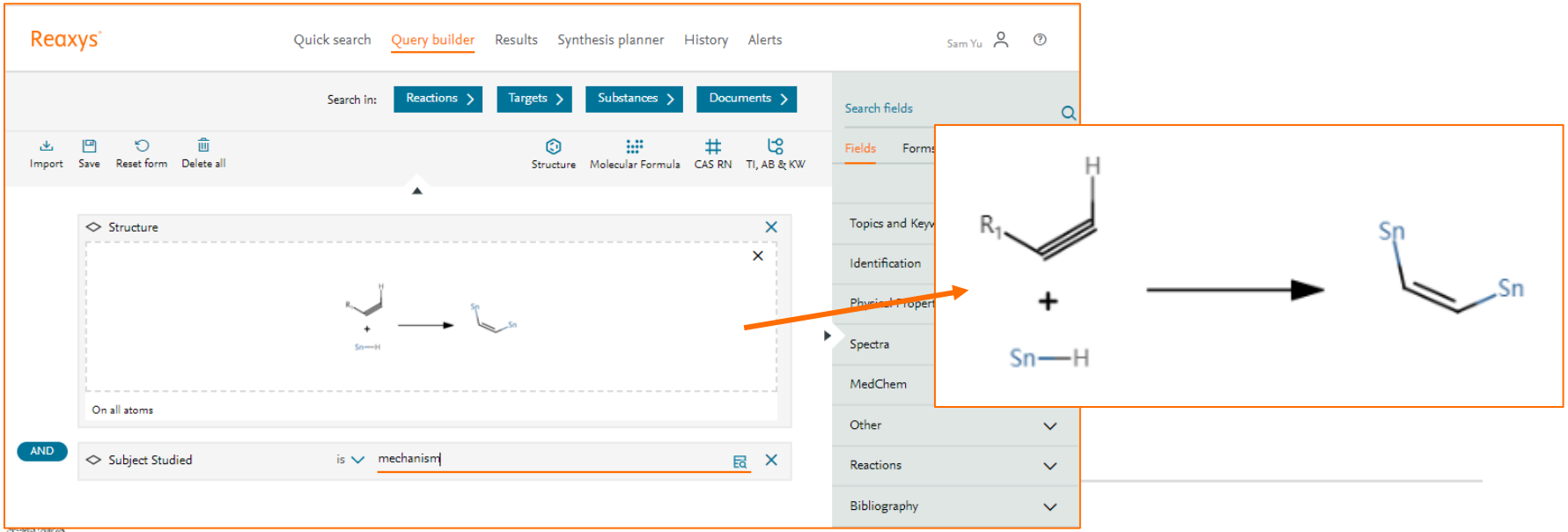


Figure S45. ^{13}C NMR of **3j**.

用于文献中化合物信息的快速定位。

Case 17：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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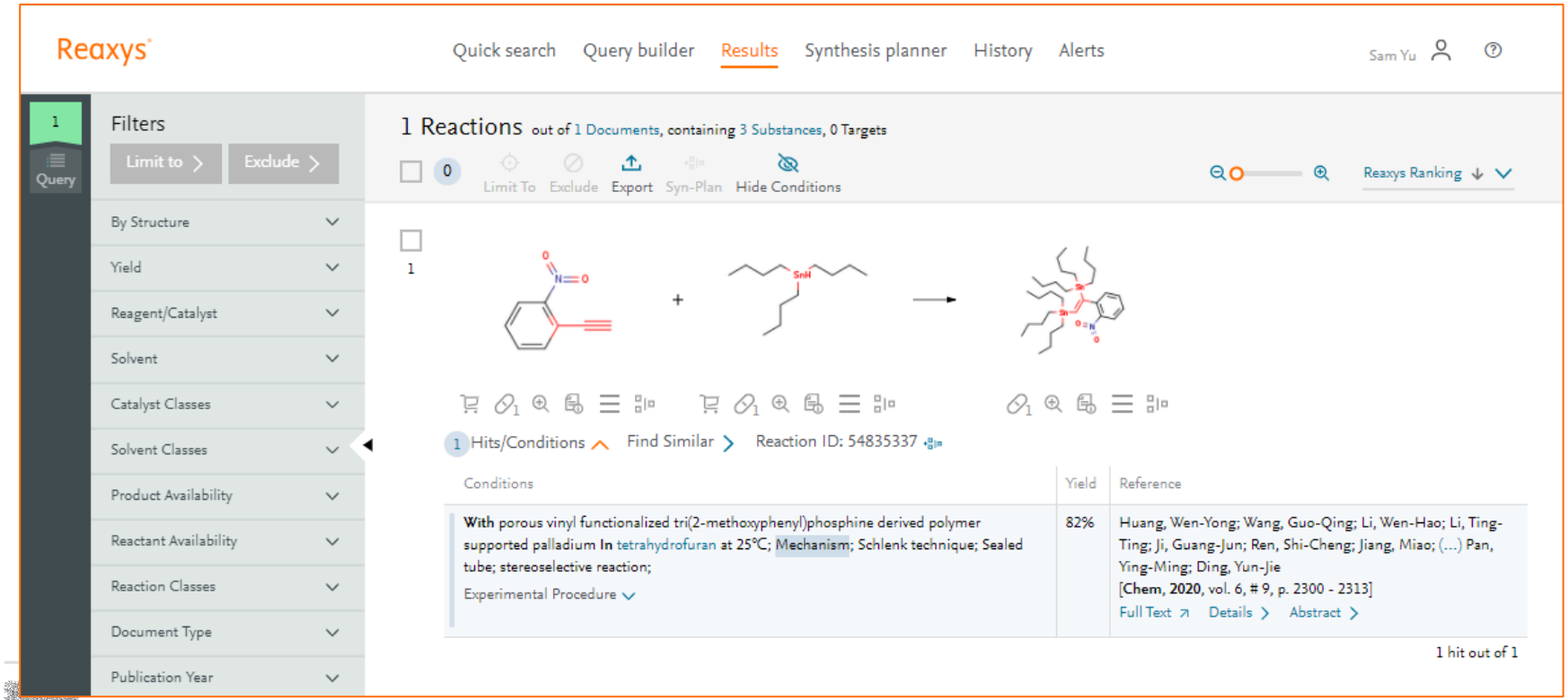
最后的结果



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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中的科技文献检索与分析
  - 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
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请就今天的培训
进行问卷调查

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Thank you