Reaxys
使用介绍

俞靓
爱思唯尔生命科学客户顾问
s.yu.2@elsevier.com

今天的内容

- Reaxys基本介绍
- Reaxys的使用
  - Reaxys中化合物理化性质的检索
  - Reaxys中的结构面板与反应检索
  - Reaxys中的反应设计与筛选
- Reaxys小结与未来展望

Reaxys—基于数据深度提炼的科研信息平台

16.000 期刊
(journals, books and patents)

- **6000万文献**
- (Elsevier, ACS, Nature-Springer, Blackwell, Taylor and Francis,etc)

- **150万专利**
- WPO, USPO, EPO [≈ mid 70´s >]
- PO: JP, KR, CN, TW [2015 >]
- **2020年将扩展到100家专利机构**

- **38万书的章节**
- Beilstein, Gmelin,….

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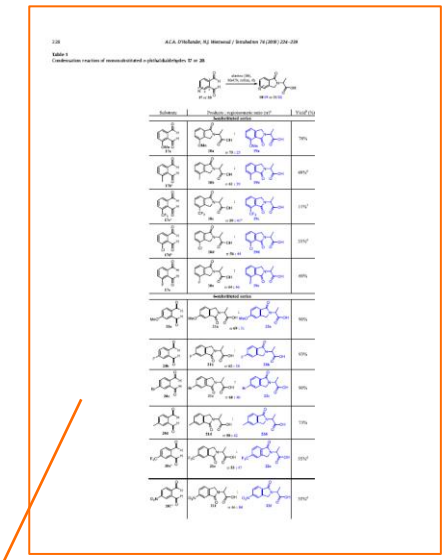
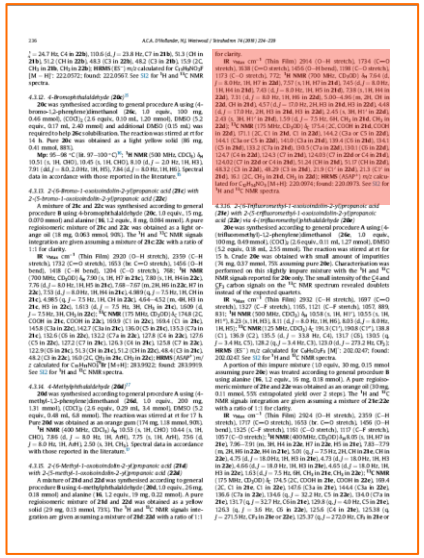
一篇常见的化学相关文献的构成

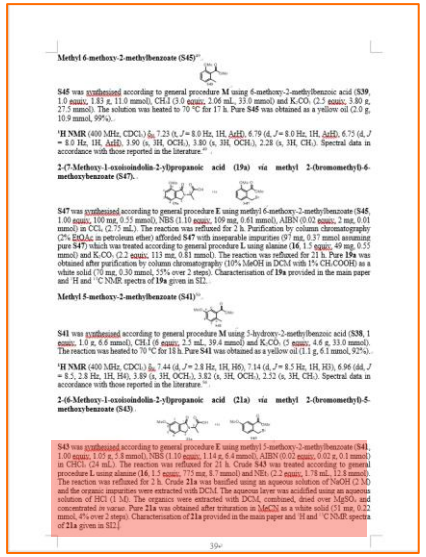

Tetrahedron

Assessment of the regioselectivity in the condensation reaction of unsymmetrical *o*-phthaldialdehydes with alanine

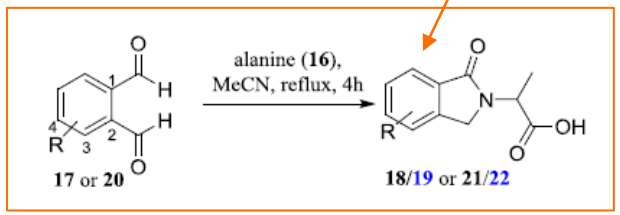
Agathe CA. D'Hollander, Nicholas J. Westwood*

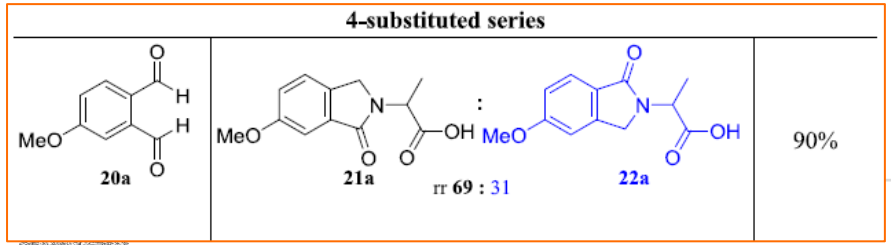






一篇全文以及Support Information中有大量的数据，科研人员如果要获取，需要花费多的时间去阅读全文。

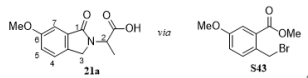




21a: **Mp:** 194–196 °C; **IR** ν_{max} cm^{-1} (thin film) 3370 (O–H stretch), 1730 (C=O stretch), 1636 (C=O stretch), 1493 (C=C stretch), 1456 (C–H bend), 1447 (C–H bend), 1196 (C–O stretch), 1022, 770; **^{1}H NMR** (500 MHz, CD_3OD) δ_H 7.48 (d, J = 8.5 Hz, 1H, H4), 7.29 (d, J = 2.5 Hz, 1H, H7), 7.19 (dd, J = 8.5, 2.5 Hz, 1H, H5), 5.00 (q, J = 7.5 Hz, 1H, CH), 4.54 (d, J = 17.0 Hz, 1H, H3), 4.48 (d, J = 17.0 Hz, 1H, H3), 3.86 (s, 3H, OCH_3), 1.61 (d, J = 7.5 Hz, 3H, CH_3); **^{13}C NMR** (125 MHz, CD_3OD) δ_C 174.8 (COOH), 171.0 (C1), 161.6 (C6), 135.8 (C3a), 134.3 (C7a), 125.2 (C4), 121.0 (C5), 107.4 (C7), 56.1 (OCH_3), 51.2 (CH), 48.1 (C3), 15.9 (CH_3); **HRMS** (ES^+) *m/z* calculated for $C_{12}H_{14}NO_4$ $[M+H]^+$: 236.0917; found: 236.0921. See SI1 part IX for experimental procedure and SI2 for ^{1}H and ^{13}C NMR spectra.

22a: **Mp:** 191–193 °C; **IR** ν_{max} cm^{-1} (thin film) 3229 (O–H stretch), 1717 (C=O stretch), 1628 (C=O stretch), 1611 (C=C stretch), 1558 (C=C stretch), 1506 (C=C stretch), 1447 (C–H bend), 1435 (C–H bend), 1298 (C–N stretch), 1206 (C–O stretch), 1086, 1026, 845, 775; **^{1}H NMR** (500 MHz, CD_3OD) δ_H 7.68 (d, J = 8.5 Hz, 1H, H7), 7.13 (d, J = 2.0 Hz, 1H, H4), 7.04 (dd, J = 8.5, 2.2 Hz, 1H, H6), 4.98 (q, J = 7.5 Hz, 1H, CH), 4.57 (d, J = 17.0 Hz, 1H, H3), 4.50 (d, J = 17.0 Hz, 1H, H3), 3.88 (s, 3H, OCH_3), 1.60 (d, J = 7.5 Hz, 3H, CH_3); **^{13}C NMR** (125 MHz, CD_3OD) δ_C 174.8 (COOH), 171.0 (C1),164.9 (C5), 146.2 (C3a), 125.6 (C7), 125.4 (C7a), 116.3 (C6), 108.8 (C4), 56.2 (OCH_3), 50.9 (CH), 48.4 (C3), 15.9 (CH_3); **HRMS** (ES^+) *m/z* calculated for $C_{12}H_{14}NO_4$ $[M+H]^+$: 236.0917; found: 236.0921. See SI1 part IX for experimental procedure and SI2 for ^{1}H and ^{13}C NMR spectra.

2-(6-Methoxy-1-oxoisoindolin-2-yl)propanoic acid (21a) *via* methyl 2-(bromomethyl)-5-methoxybenzoate (S43)



S43 was synthesised according to general procedure **E** using methyl 5-methoxy-2-methylbenzoate (**S41**, 1.00 equiv, 1.05 g, 5.8 mmol), NBS (1.10 equiv, 1.14 g, 6.4 mmol), AIBN (0.02 equiv, 0.02 g, 0.1 mmol) in $CHCl_3$ (24 mL). The reaction was refluxed for 21 h. Crude **S43** was treated according to general procedure **L** using alanine (**16**, 1.5 equiv, 775 mg, 8.7 mmol) and NEt_3 (2.2 equiv, 1.78 mL, 12.8 mmol). The reaction was refluxed for 2 h. Crude **21a** was basified using an aqueous solution of NaOH (2 M) and the organic impurities were extracted with DCM. The aqueous layer was acidified using an aqueous solution of HCl (1 M). The organics were extracted with DCM, combined, dried over $MgSO_4$ and concentrated *in vacuo*. Pure **21a** was obtained after trituration in MeCN as a white solid (51 mg, 0.22 mmol, 4% over 2 steps). Characterisation of **21a** provided in the main paper and ^{1}H and ^{13}C NMR spectra of **21a** given in SI2.

Reaxys对这篇全文的提炼

1 Assessment of the regioselectivity in the condensation reaction of unsymmetrical o-phthaldialdehydes with alanine

D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, **2018**, vol. 74, # 2, p. 224 - 239]

Abstract ^ Index Terms ^ Substances 103 v Reactions 236 v Full Text ↗

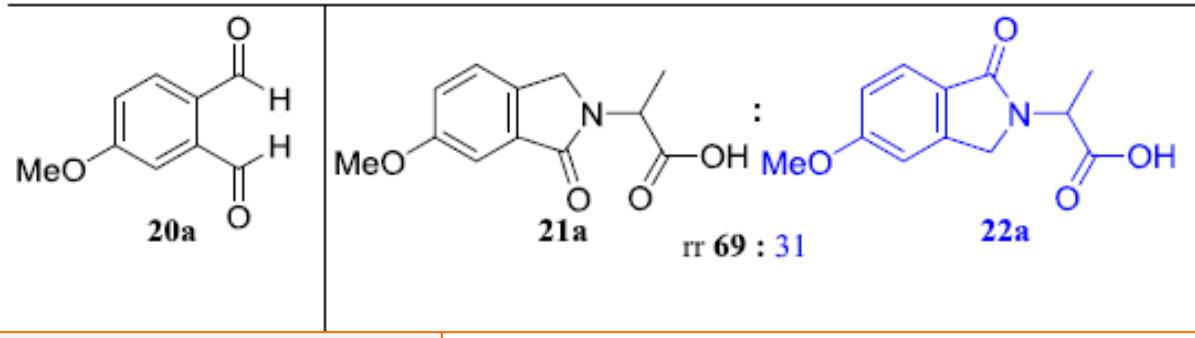
Abstract

One approach for the synthesis of isoindolinones, a privileged bioactive heterocyclic core structure, involves a conden-
sation reaction of o-phthaldialdehydes with a suitable nitrogen-containing nucleophile. This fascinating re
visited here in the context of the use of o-phthaldialdehydes that contain additional substituents in the aro
leading to a detailed analysis of the regioselectivity of the reaction. Eleven monosubstituted o-phthaldialde
synthesised and reacted with alanine. The regioselectivity observed across the eleven substrates led to the
disubstituted substrate that reacted with very high control. A gram-scale reaction followed by esterification
major regioisomer in high yield. In addition, the regioselectivity observed on reaction of two novel monod
substrates led to an increased mechanistic understanding.

Index terms

Author keyword: Condensation reaction, Mechanistic understanding, o-phthaldialdehyde, Regioselectivity
EMTREE drug term: alanine, phthalaldehyde
EMTREE medical term: Article, esterification, polymerization, priority journal, regioselectivity, synthesis
Reaxys Index Terms: Swern oxidation, condensation reaction, esterification, pure, reactivity, regioselectivity, separation method, tautomerization

4-substituted series



1 Assessment of the regioselectivity in the condensation reaction of unsymmetrical o-phthaldialdehydes with alanine

D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, **2018**, vol. 74, # 2, p. 224 - 239]

Abstract v Index Terms v Substances 103 v Reactions 236 v Full Text ↗

Reaxys对于文献中的结构与反应都做了提炼

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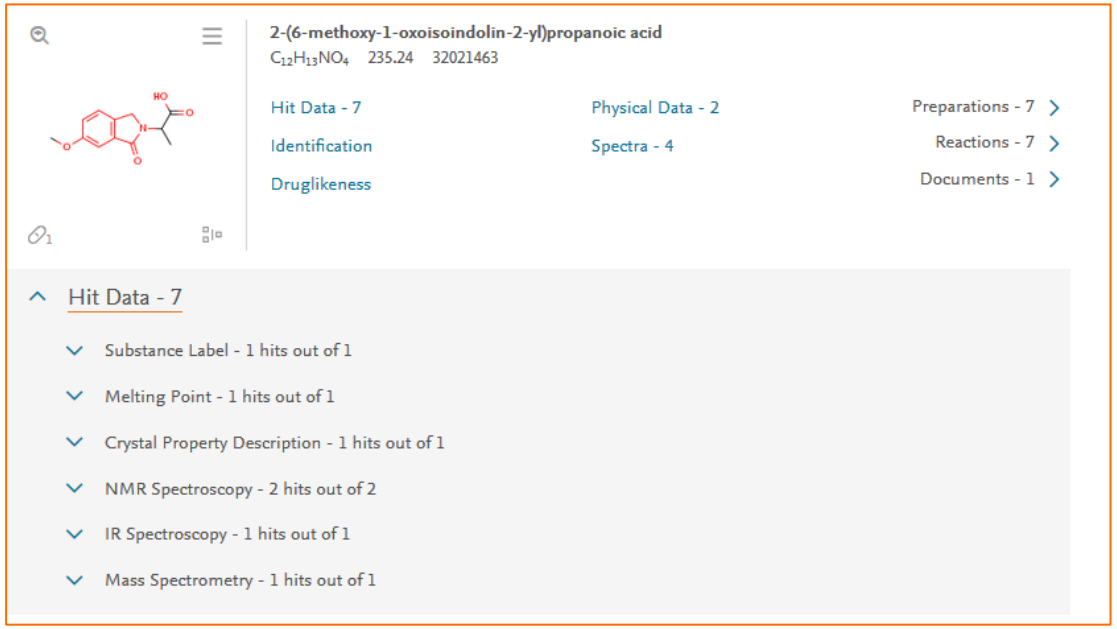
Reaxys对文献中的化合物的结构化数据提炼



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。

Label	Reference
21a	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, **2018**, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract

Melting Point, °C	Reference
194 - 196	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, **2018**, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract

Colour & Other Properties	Location	Reference
white	supporting information	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, **2018**, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Frequency (NMR Spectroscopy), MHz	Location	Reference
Chemical shifts, Spectrum	1H	d(4)-methanol	500	supporting information	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, **2018**, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract
Chemical shifts, Spectrum	13C	d(4)-methanol	125.8	supporting information	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, **2018**, vol. 74, # 2, p. 224 - 239] Full Text Details Abstract

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Reaxys对原文反应的提炼（21a)

Reaction ID: 47133770

1 Conditions Find Similar

Yield	Conditions	Reference
	In acetonitrile for 4h; Reflux; Inert atmosphere; Overall yield = 90 percent; Overall yield = 38 mg; regioselective reaction;	D'Hollander, Agathe C.A.; Westwood, Nicholas J. - [Tetrahedron, 2018, vol. 74, # 2, p. 224 - 239]

Full Text Details Abstract

Experimental Procedure

General procedure: Alanine (16, 1.2 equiv.) was added to a solution of unsymmetrical o-phthaldialdehyde (1.0 equiv.) in anhydrous MeCN (3.8 mL per mmol of o-phthaldialdehyde). The reaction mixture was heated at reflux for 4 h under a nitrogen atmosphere. The solution was then cooled to rt before being concentrated in vacuo to afford the crude mixture of regioisomers.

*4.3.9. 2-(6-Methoxy-1-oxoisoindolin-2-yl)propanoic acid (**21a**) with 2-(5-methoxy-1-oxoisoindolin-2-yl)propanoic acid (**22a**)*

A mixture of **21a** and **22a** was synthesised according to general procedure **B** using 4-methoxyphthalaldehyde (**20a**, 1.0 equiv., 30 mg, 0.18 mmol) and alanine (**16**, 1.2 equiv., 19 mg, 0.22 mmol). A

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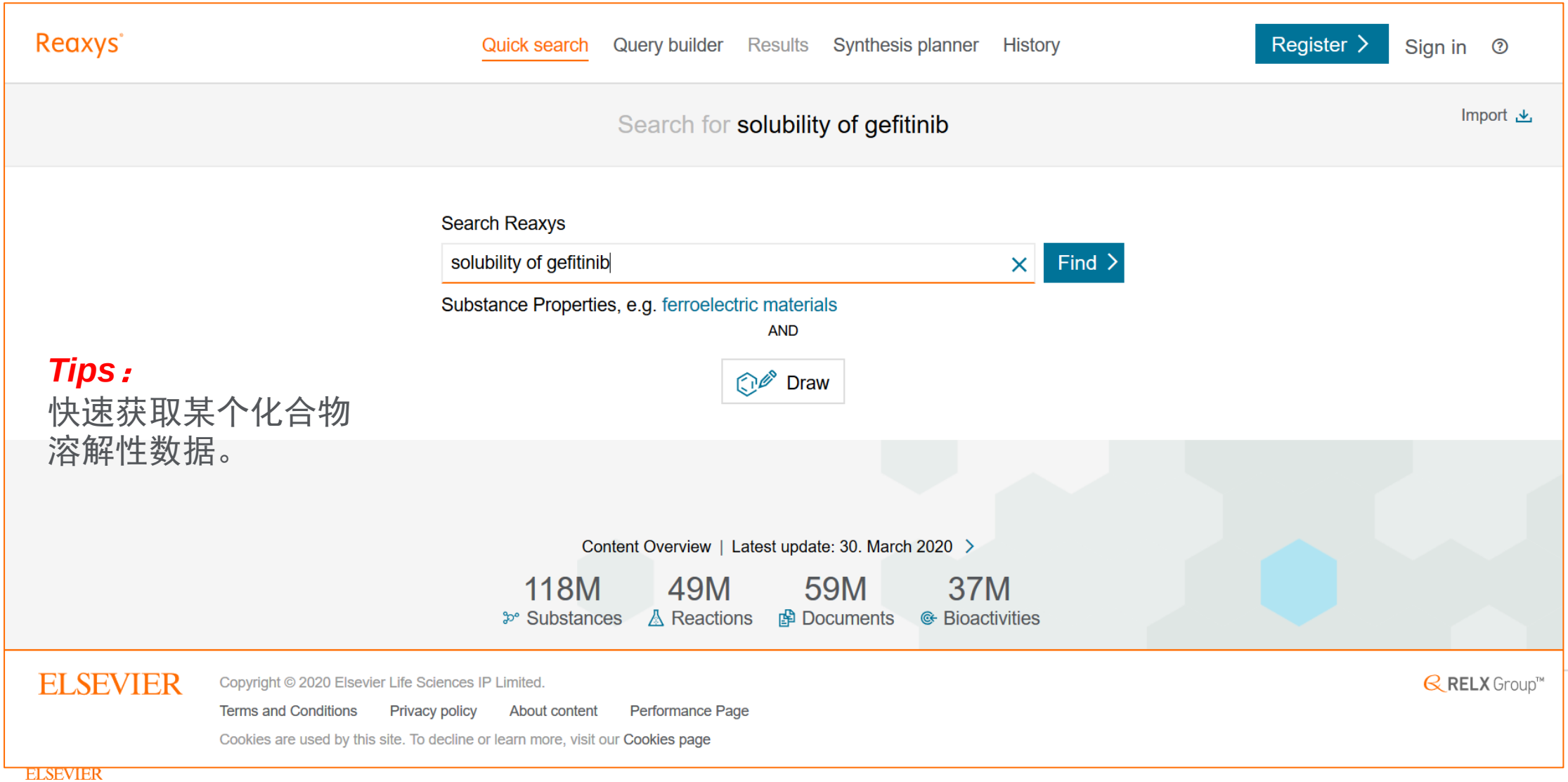
  - Reaxys中的反应设计与筛选
- Reaxys小结与未来展望

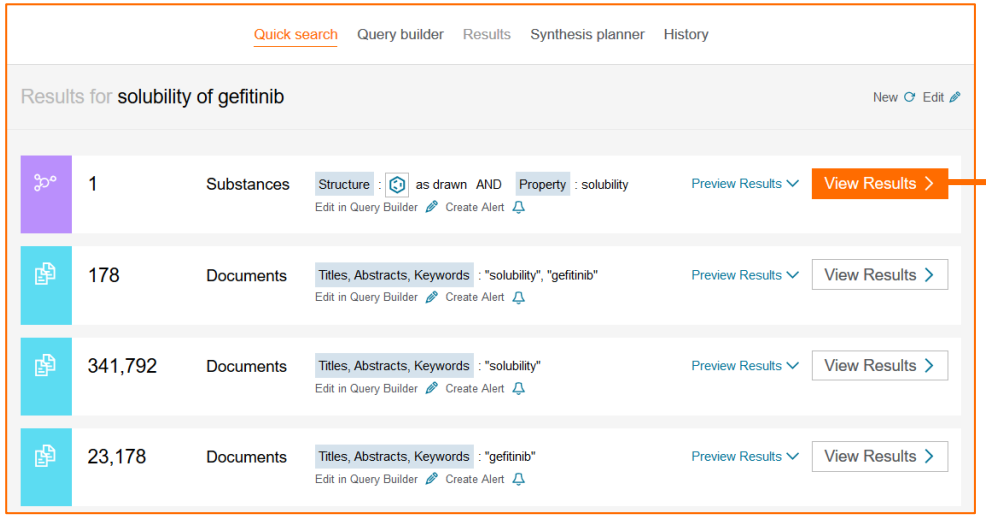
Case 1：快速获取化合物的理化性质

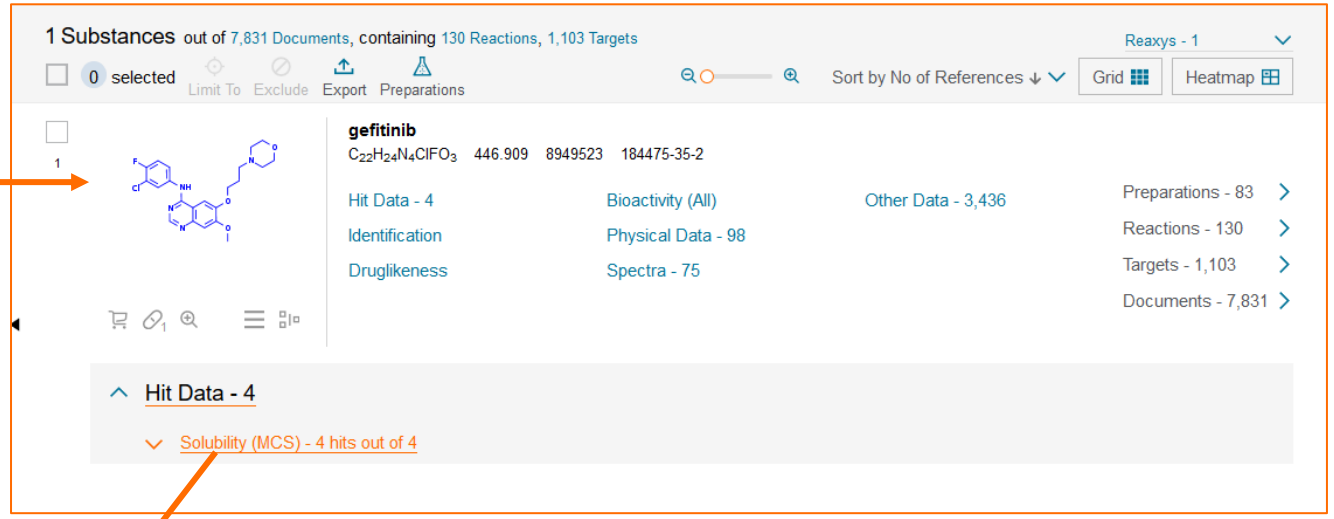


Tips：

快速获取某个化合物溶解性数据。

Reaxys中的结果





抽提的数据包括具体的数值，或者相关的文字性描述

Solubility, 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 ›

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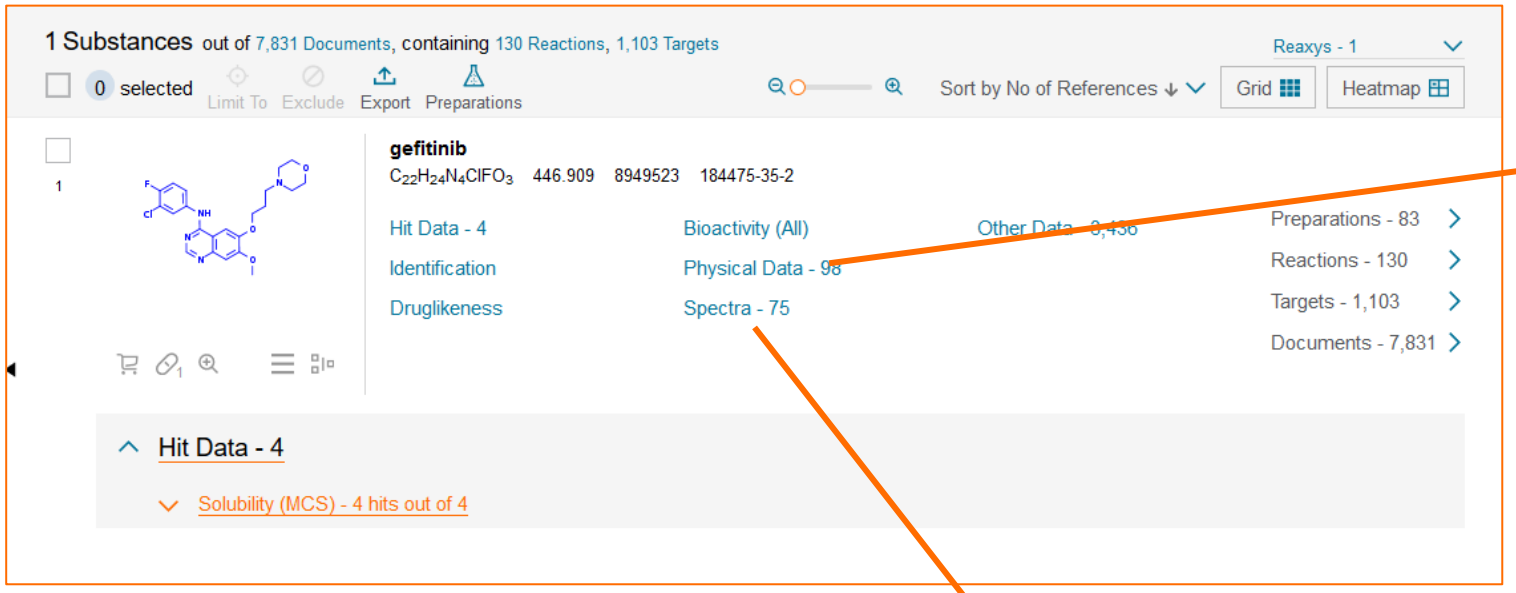
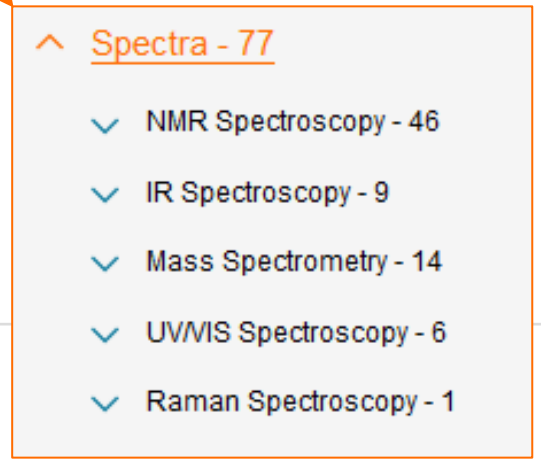
Reaxys中化合物更多的理化性质





直接获取化合物的理化性质或者谱图数据

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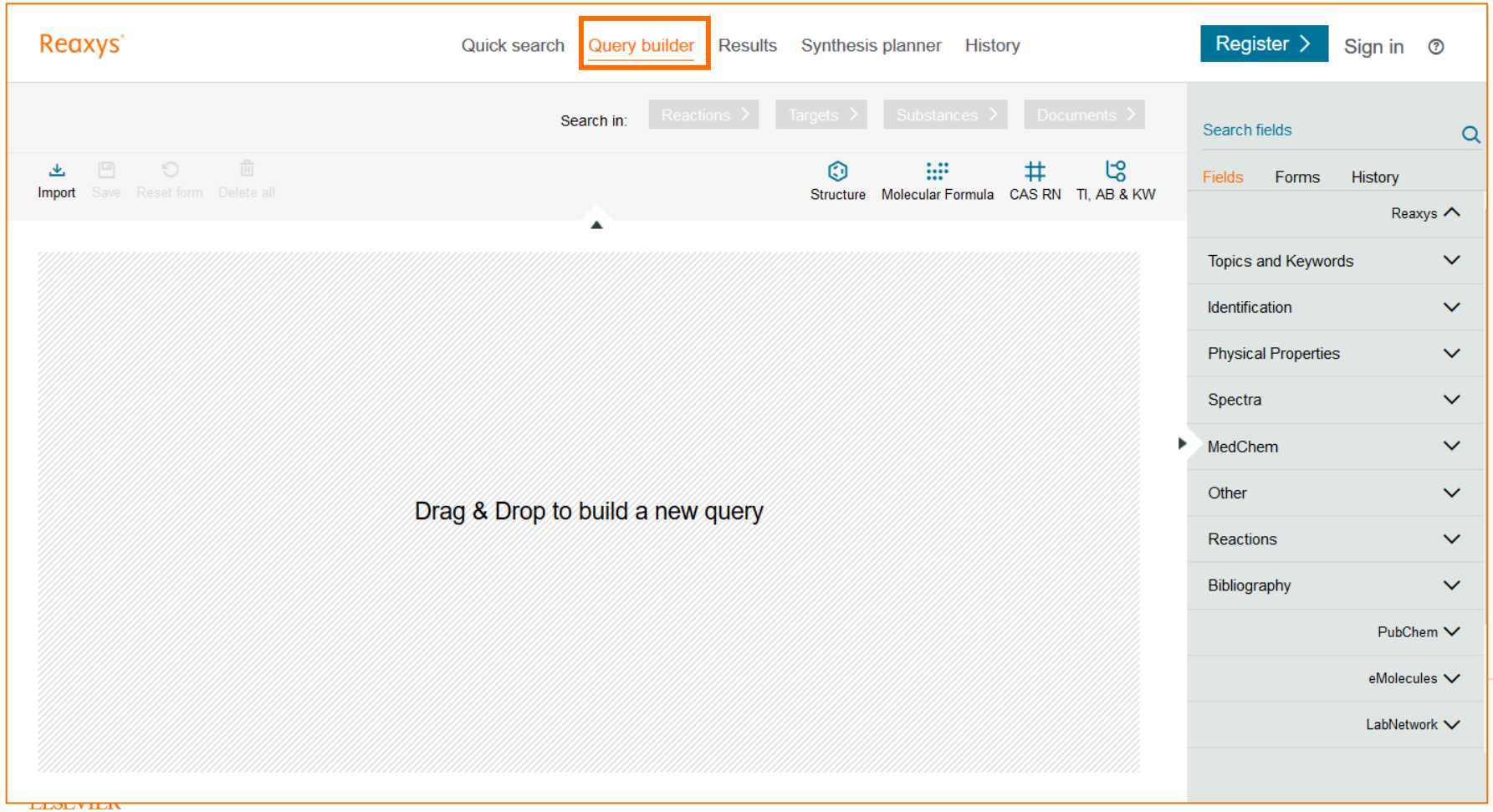
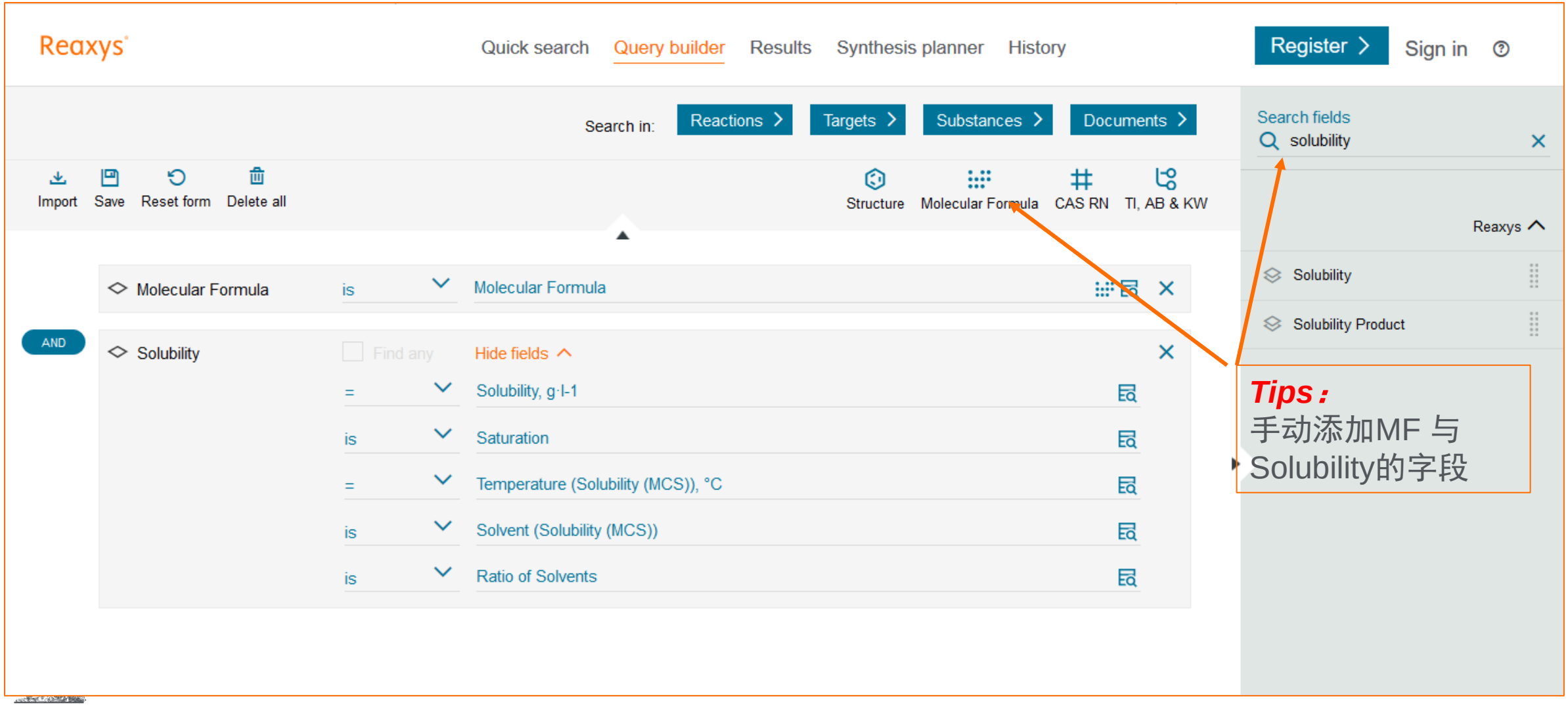
Case 2：理化性质的高级应用

- 获取KCl在乙醇中的溶解度

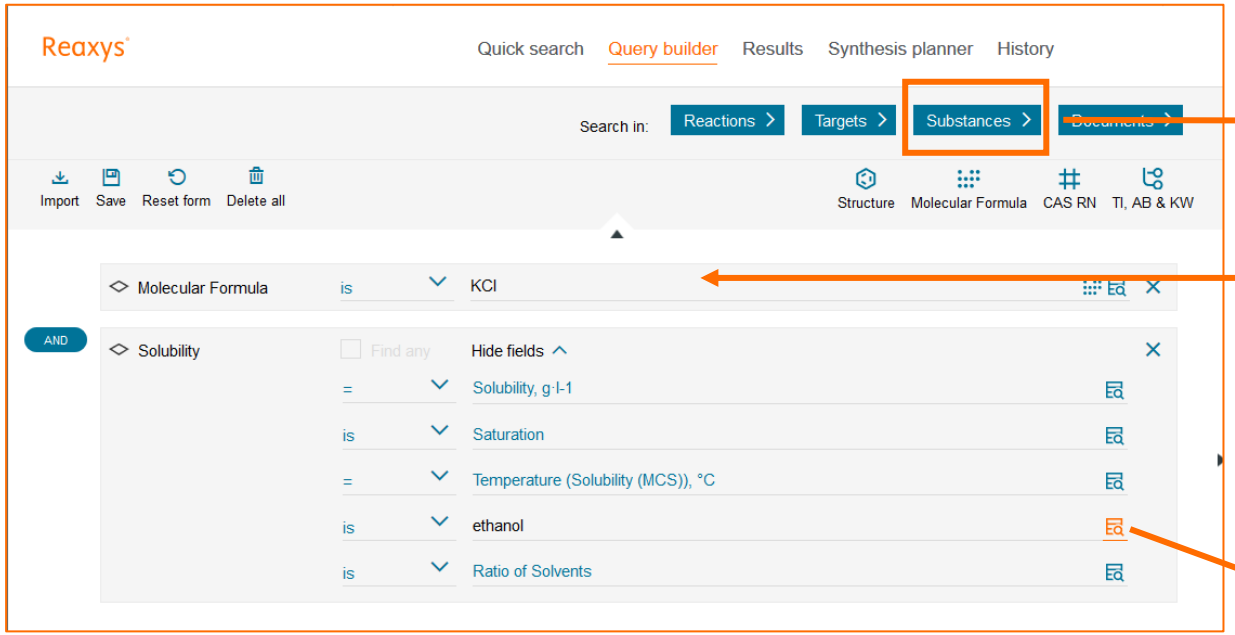


Reaxys中的Query Builder可以按照一定的规则构建检索式，Reaxys一共提供180+字段和字段组，科研人员可以自由的对这些字段和字段组进行组合，同时Reaxys也根据一些常见的需求，内置了多种检索策略模板，如“天然产物”，“hERG”等

检索策略的构建


Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Register
Sign in
Search in:
Reactions
Targets
Substances
Documents
Import
Save
Reset form
Delete all
Structure
Molecular Formula
CAS RN
TI, AB & KW
Search fields
solubility
Reaxys
Solubility
Solubility Product
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
Tips：
手动添加MF 与
Solubility的字段

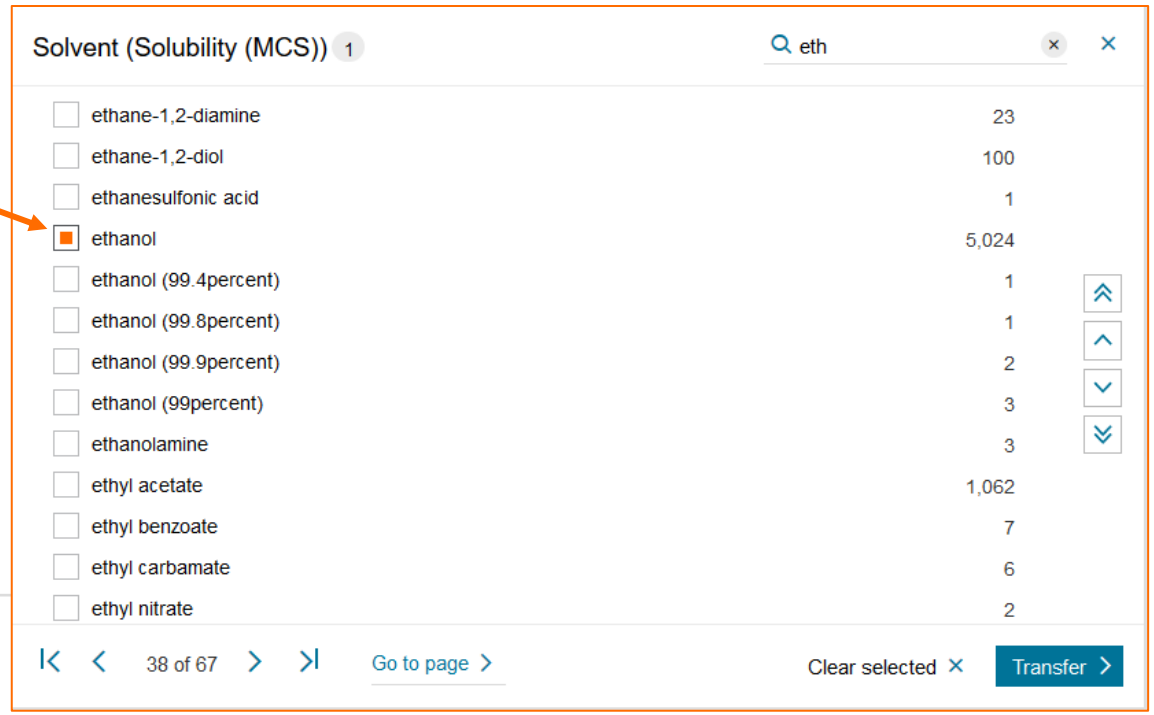
条件的输入



Step3：进行物质检索

Step1：输入分子式KCl

Step2：在溶剂一块选择乙醇



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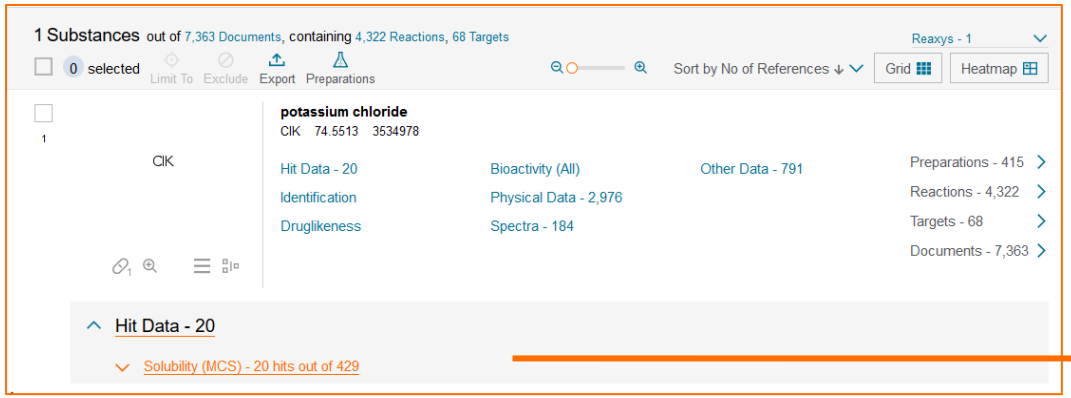
最后的结果



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, $g \cdot l^{-1}$	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

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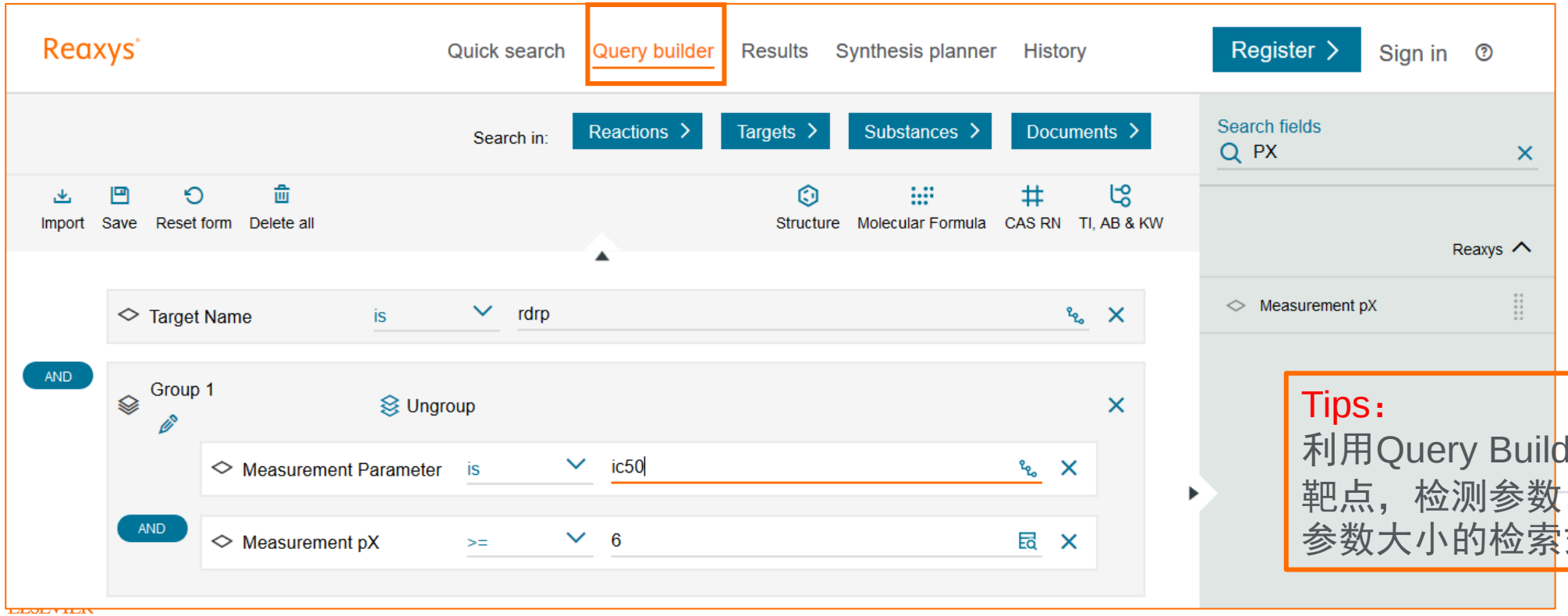
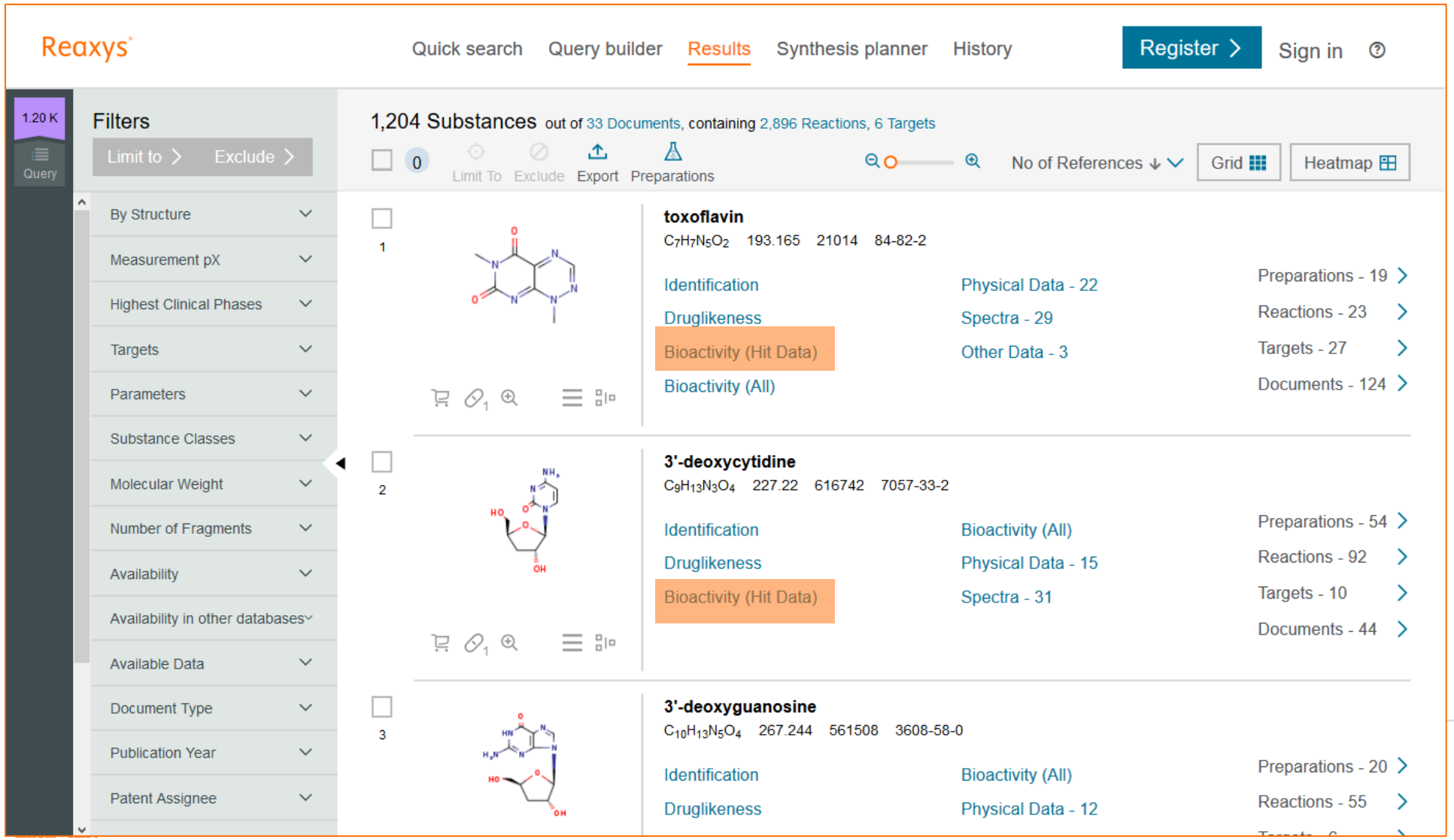
Case 3：如何用Reaxys快速筛选对“冠状病毒”有活性的化合物

- 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
- 视频操作：https://www.bilibili.com/video/BV13A411b73P （2分10秒开始）



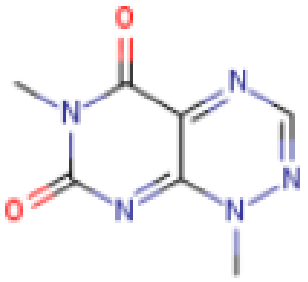
Tips：
利用Query Builder构建靶点，检测参数，以及参数大小的检索式

Reaxys中的结果

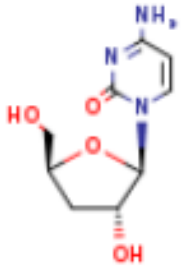


Reaxys直接给出符合条件的化合物，大量节省了科研人员阅读文献，并查找数据的时间，可以通过各自的Hit Data查看具体数据

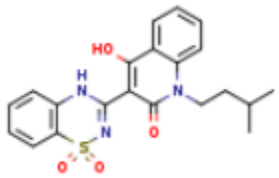
Reaxys中的结果



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Concomitants	Reference
6.22	IC50	=	0.6	μM	Hepatitis C virus	Inhibitor	RNA-dependent RNA polymerase [Hepatitis C virus]:Wild	Other compound: ATP; Radioligand: [3H]UTP;	Middleton; Lim; Montgomery; Rockway; Liu; Klein; Qin; Harlan; Kati; Molla[**Letters in drug design and discovery**, **2007**, vol. 4, # 1, p. 1 - 8] Full Text ↗ Cited 3 times ↗ Details > Abstract >



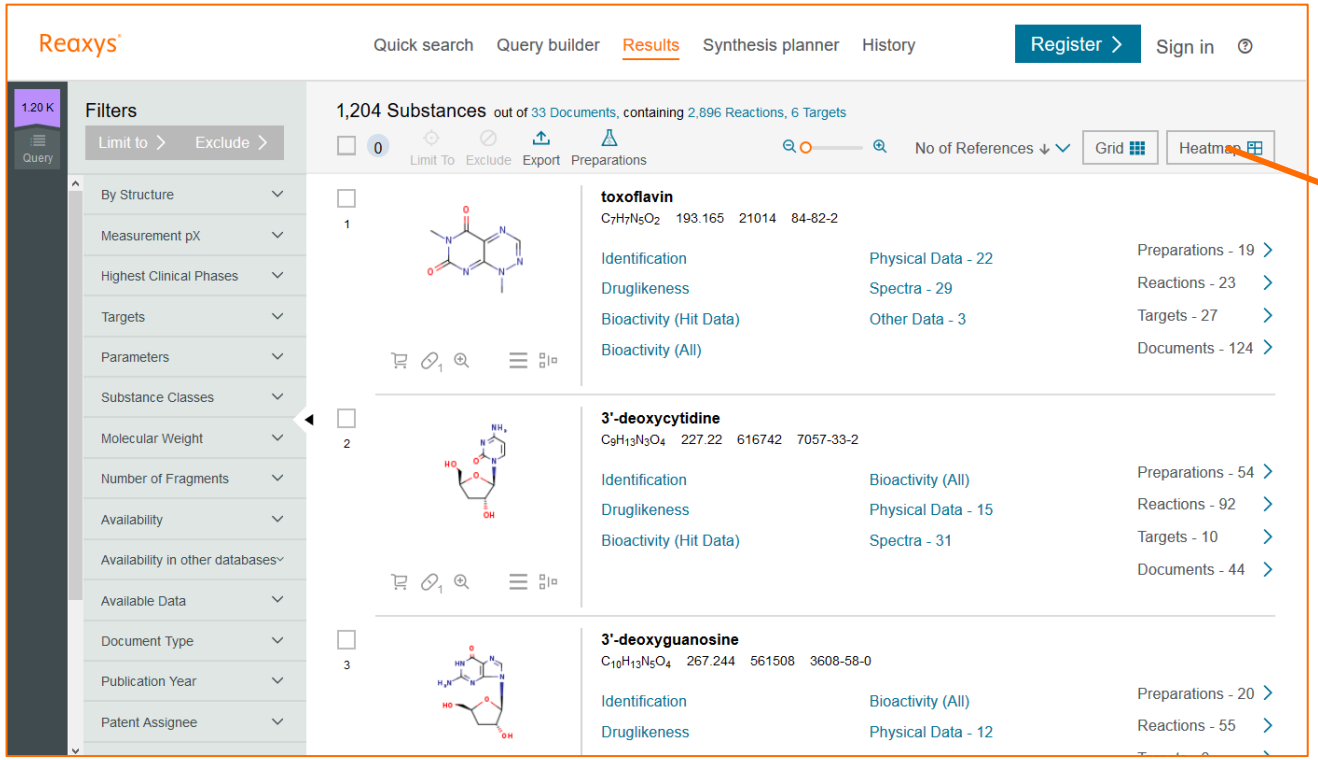
pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Concomitants	Reference
7.1	IC50		0.08 - 1.2	μM	Hepatitis C virus		RNA-dependent RNA polymerase [Hepatitis C virus]:Wild		Mayhoub, Abdelrahman S.[**Bioorganic and Medicinal Chemistry**, **2012**, vol. 20, # 10, p. 3150 - 3161] Full Text ↗ Cited 35 times ↗ Details > Abstract >

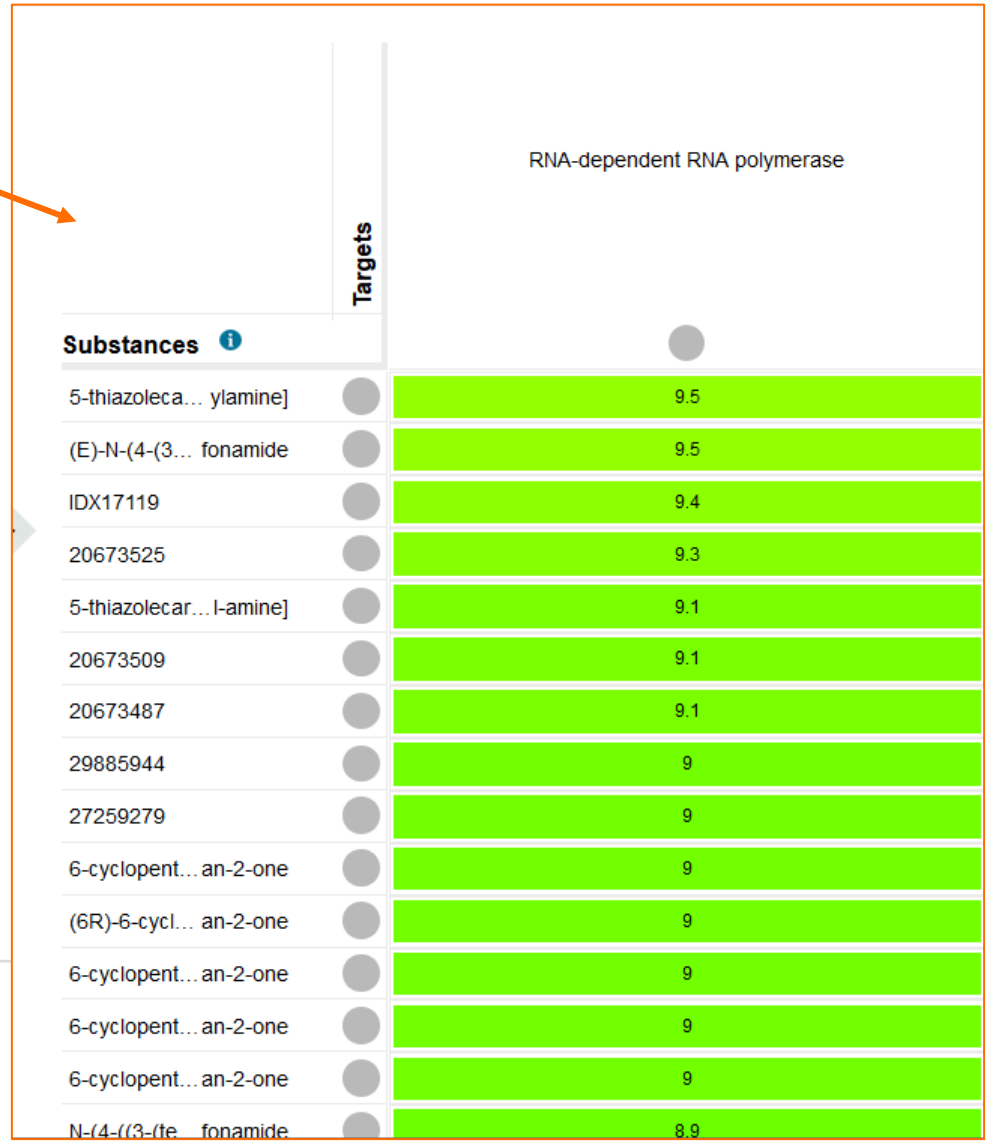


pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Concomitants	Reference
7.1	IC50	=	0.08	μM	Hepatitis C virus (strain DELTA 21)	Inhibitor	RNA-dependent RNA polymerase [Hepatitis C virus]:Wild		Dhanak, Dashyant; Duffy, Kevin J.; Johnston, Victor K.; Lin-Goerke, Juili; Darcy, Michael; Shaw, Antony N.; Gu, Baohua; (…) Keenan, Richard M.; Sarisky, Robert T. [**Journal of Biological Chemistry**, **2002**, vol. 277, # 41 p. 38322 - 38327] Full Text ↗ Cited 172 times ↗ Details > Abstract

ELSEVIER

利用HeatMap看结构与靶点关系



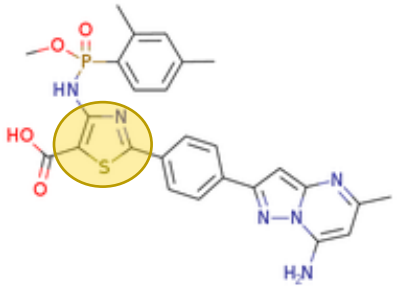


利用Reaxys中的Heat Map，直接进行查看，靶点，结构，活性数据之间的关系，并可将活性从高到低进行排序。

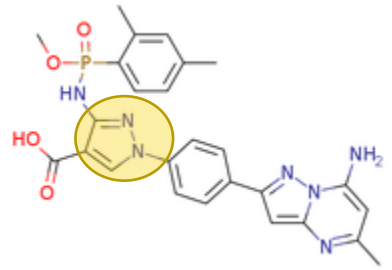
ELSEVIER

一些非常有意思的结构

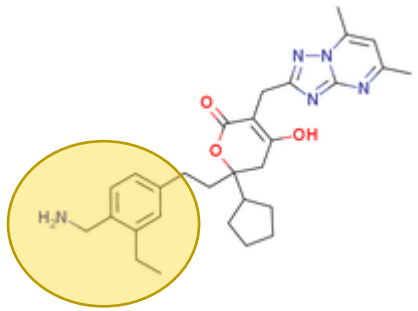
Substances	Targets: RNA-dependent RNA polymerase
5-thiazolec… ylamine]	9.5
(E)-N-(4-(… fonamide	9.5
IDX17119	9.4
20673525	9.3
5-thiazolec… l-amine]	9.1
20673509	9.1
20673487	9.1
29885944	9
27259279	9
6-cyclope… an-2-one	9
(6R)-6-cy… an-2-one	9
6-cyclope… an-2-one	9
6-cyclope… an-2-one	9
6-cyclope… an-2-one	9
N-(4-((3-(t… fonamide	8.9
5-[2-(4-flu…boxamide	8.7
(1aR,12b… boxamide	8.7
20673500	8.7
N-[4-(2-[2-…cetamide	8.7
6-cyclope… an-2-one	8.7
6-cyclope… an-2-one	8.7
N-[2-[4-(2-…cetamide	8.7
6-cyclope… an-2-one	8.7



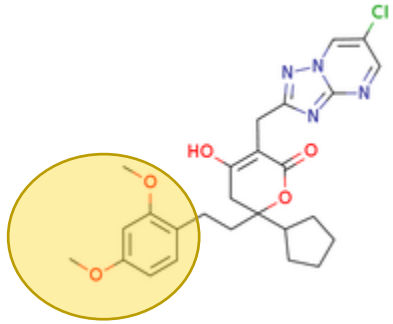
PX=9.5



PX=9.4



PX=8.0



PX=7.7

今天的内容

- Reaxys基本介绍
- Reaxys的使用
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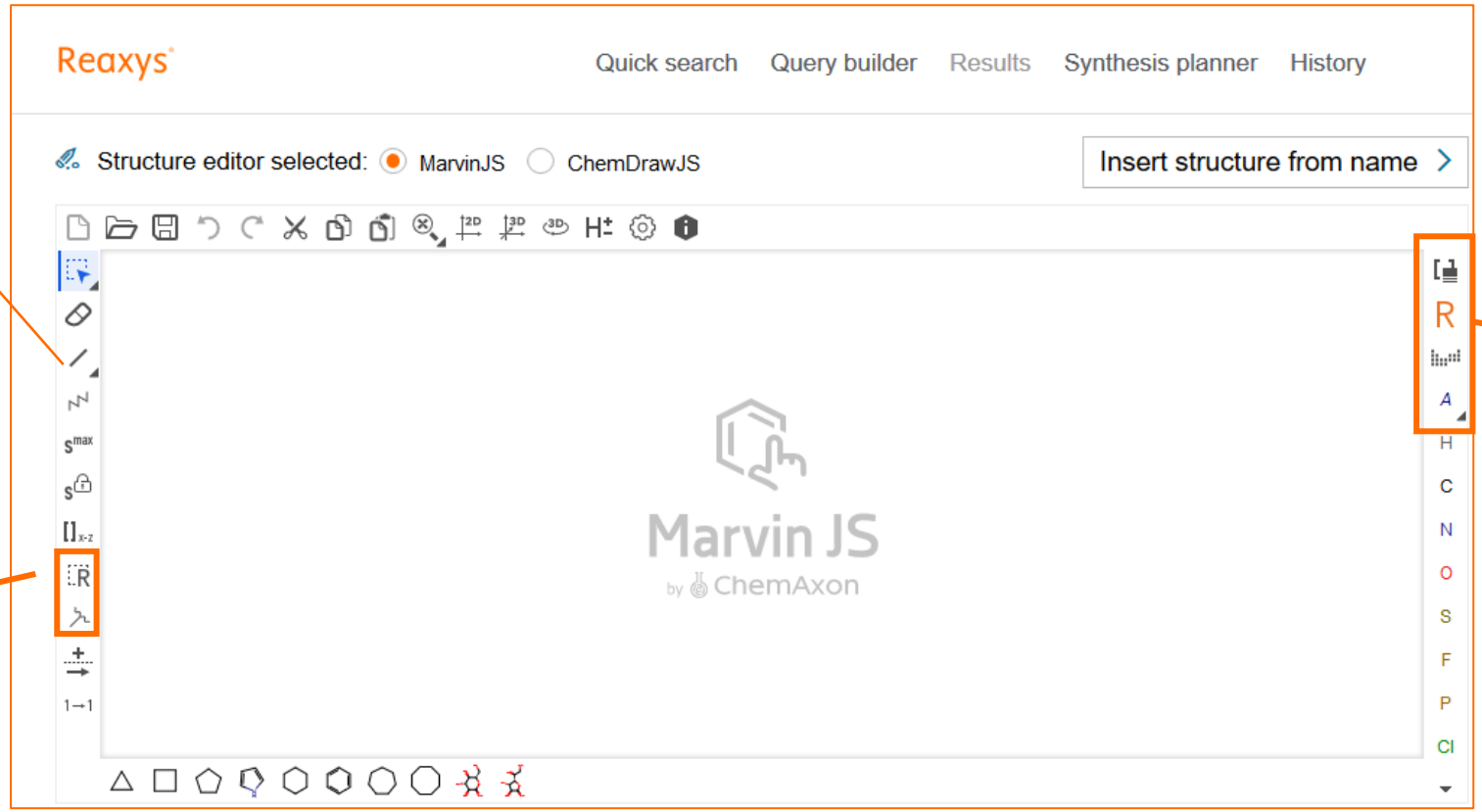
  - Reaxys中的结构面板与反应检索
  - Reaxys中的反应设计与筛选
- Reaxys小结与未来展望

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

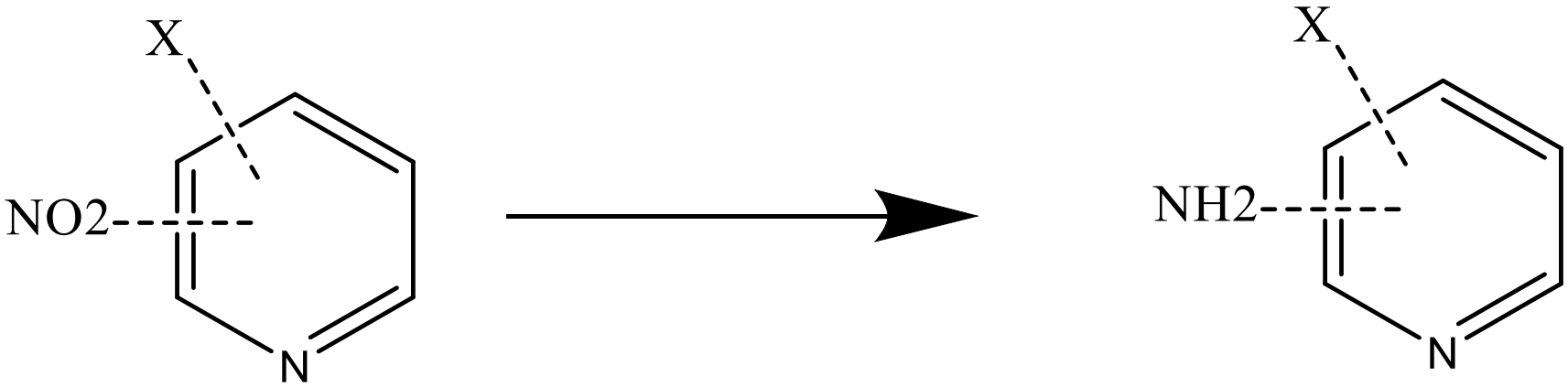
R基团定义工具

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/av92474230
不定位键	https://www.bilibili.com/video/av92568326
通用/缩写官能团	https://www.bilibili.com/video/av92474816
原子列表与列表非	https://www.bilibili.com/video/av92571129
R基团定义	https://www.bilibili.com/video/av92569854
原子锁定与环锁定	https://www.bilibili.com/video/av92833557
G Group与通用原子	https://www.bilibili.com/video/BV1Tp4y1y7SS
原子属性列表	https://www.bilibili.com/video/BV1B54y197G6
盐，自由基，同位素	https://www.bilibili.com/video/BV1pg4y1z7AB

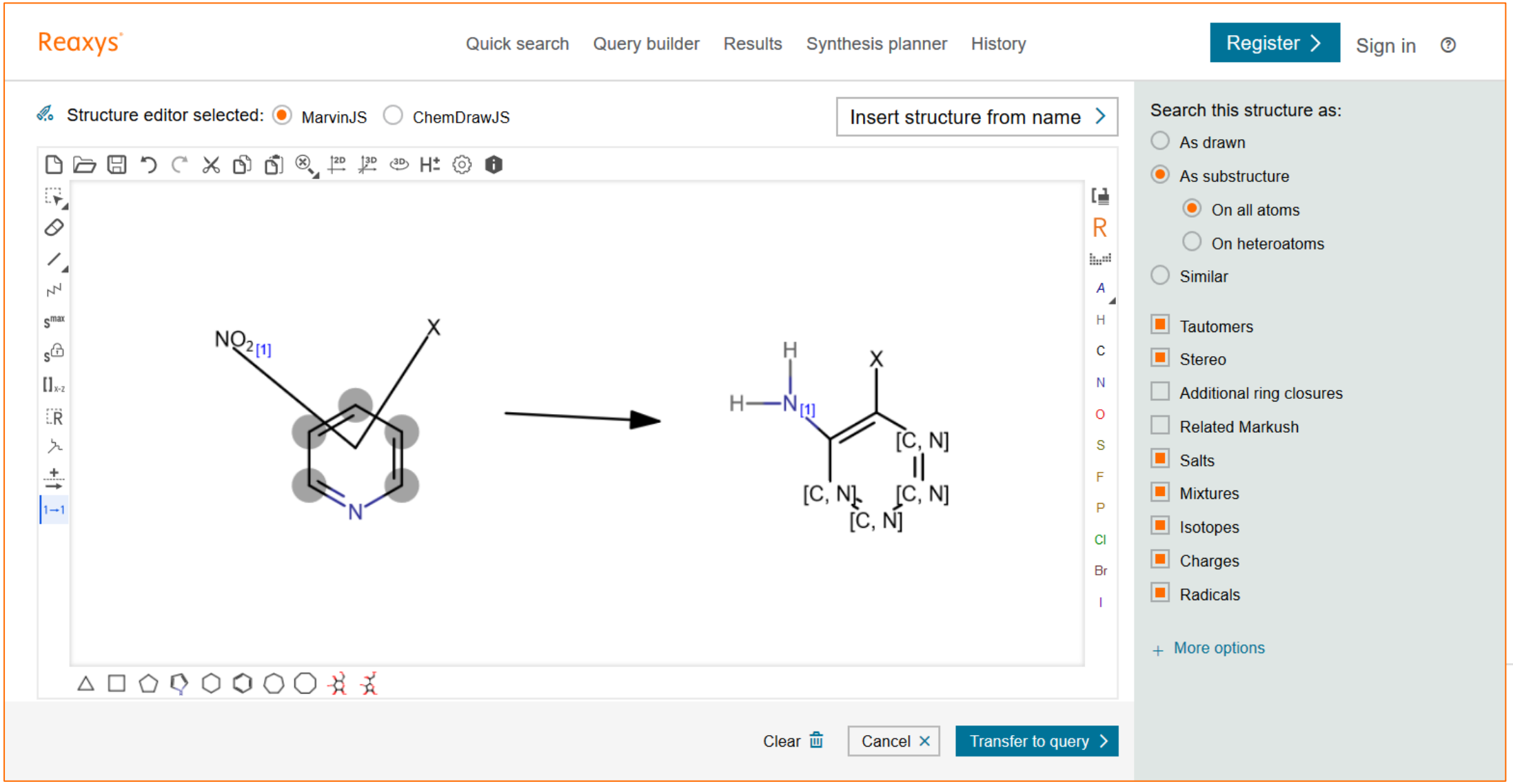
Case 4：结构中有特殊需求的反应定义

- 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

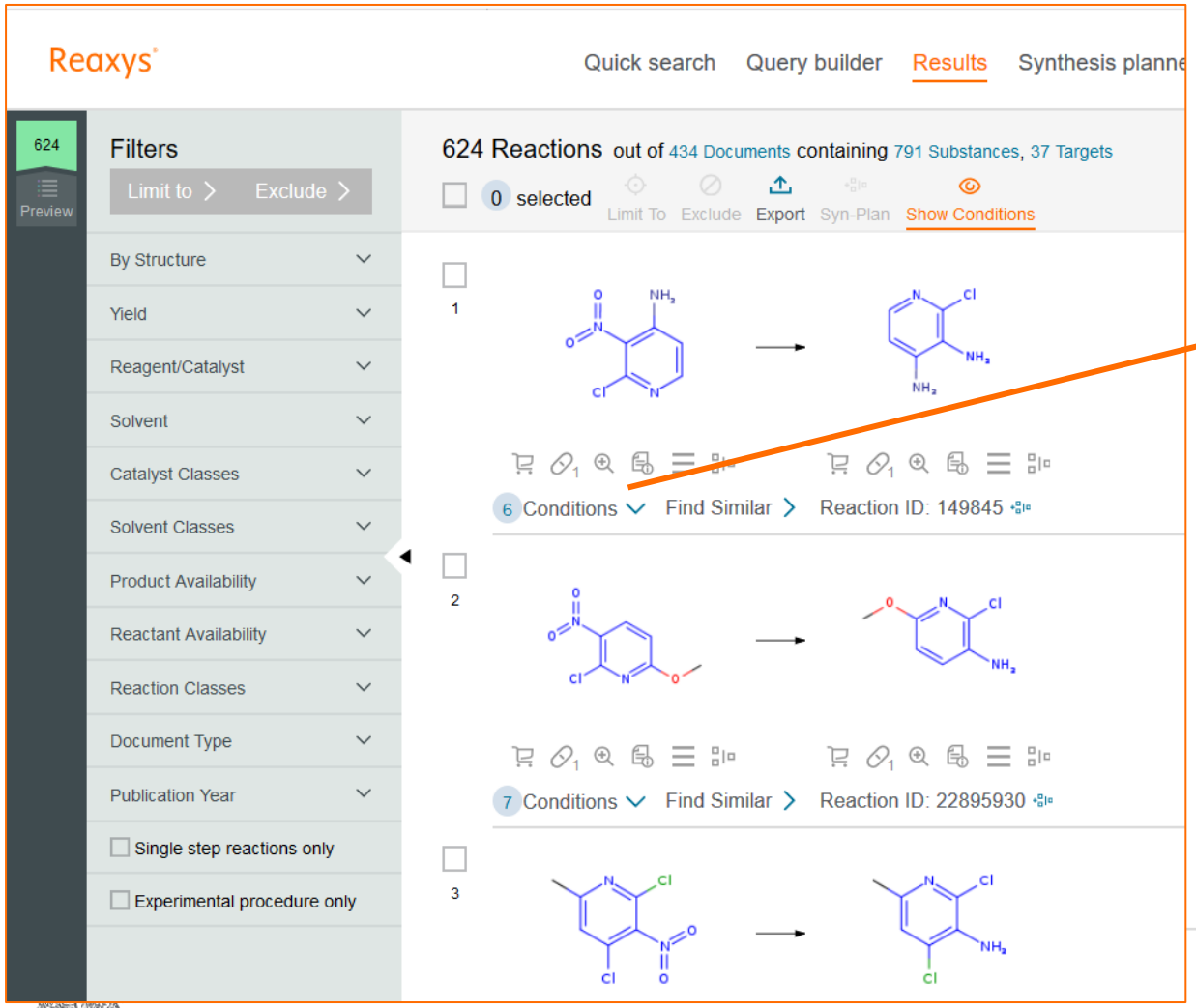


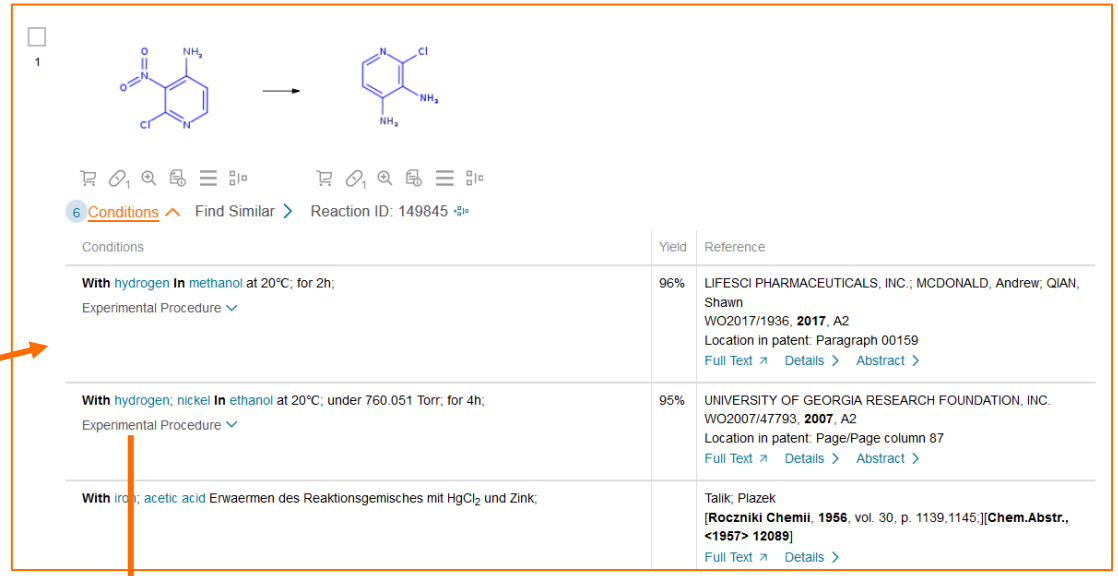
视频操作过程：
https://www.bilibili.com/video/BV1ua4y147q2

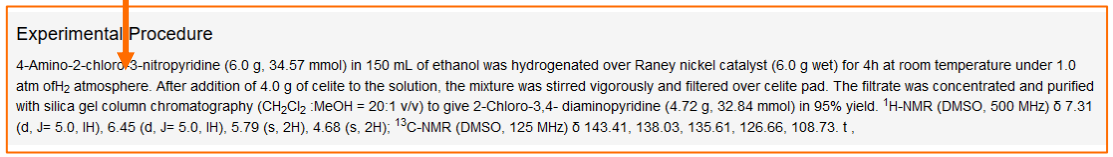
Reaxys中的结构定义



最后的结果



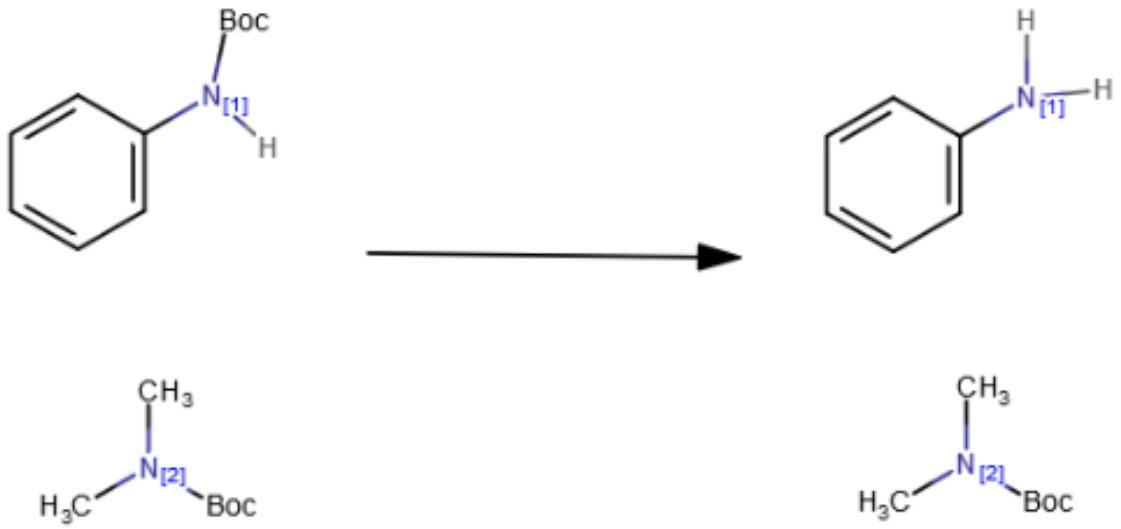




Reaxys将相同scheme的反应全部整合成1条反应，在同样的反应下列举不同的反应条件。

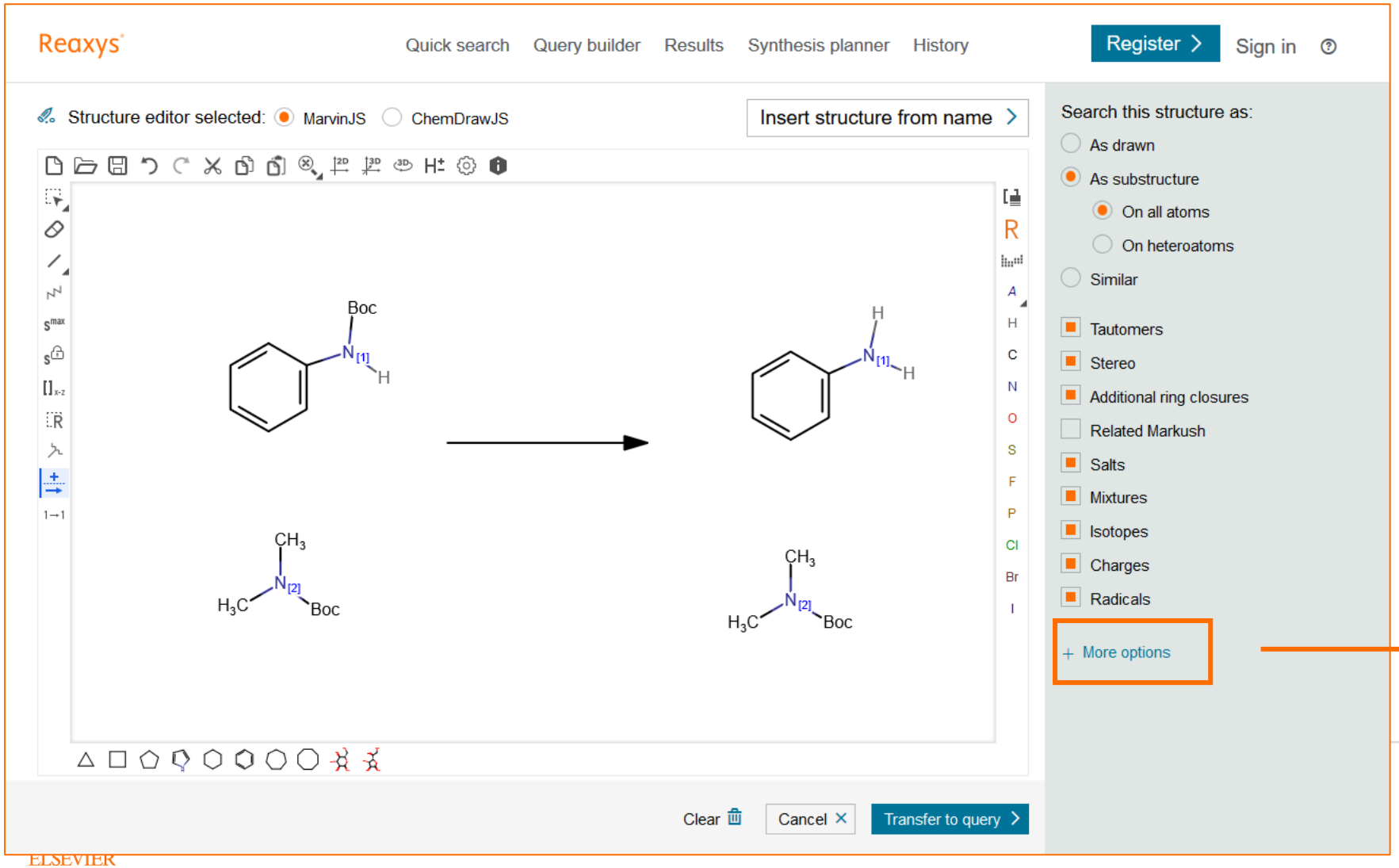
Case 5：选择性氧化还原脱保护反应的定义

- 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

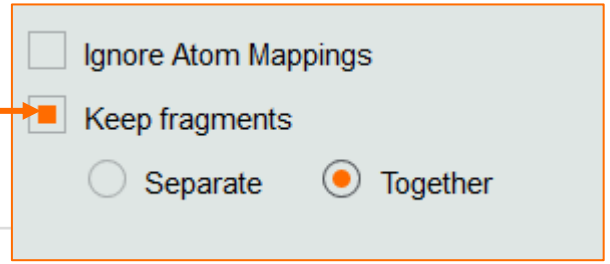


视频操作过程：
https://www.bilibili.com/video/av92577868

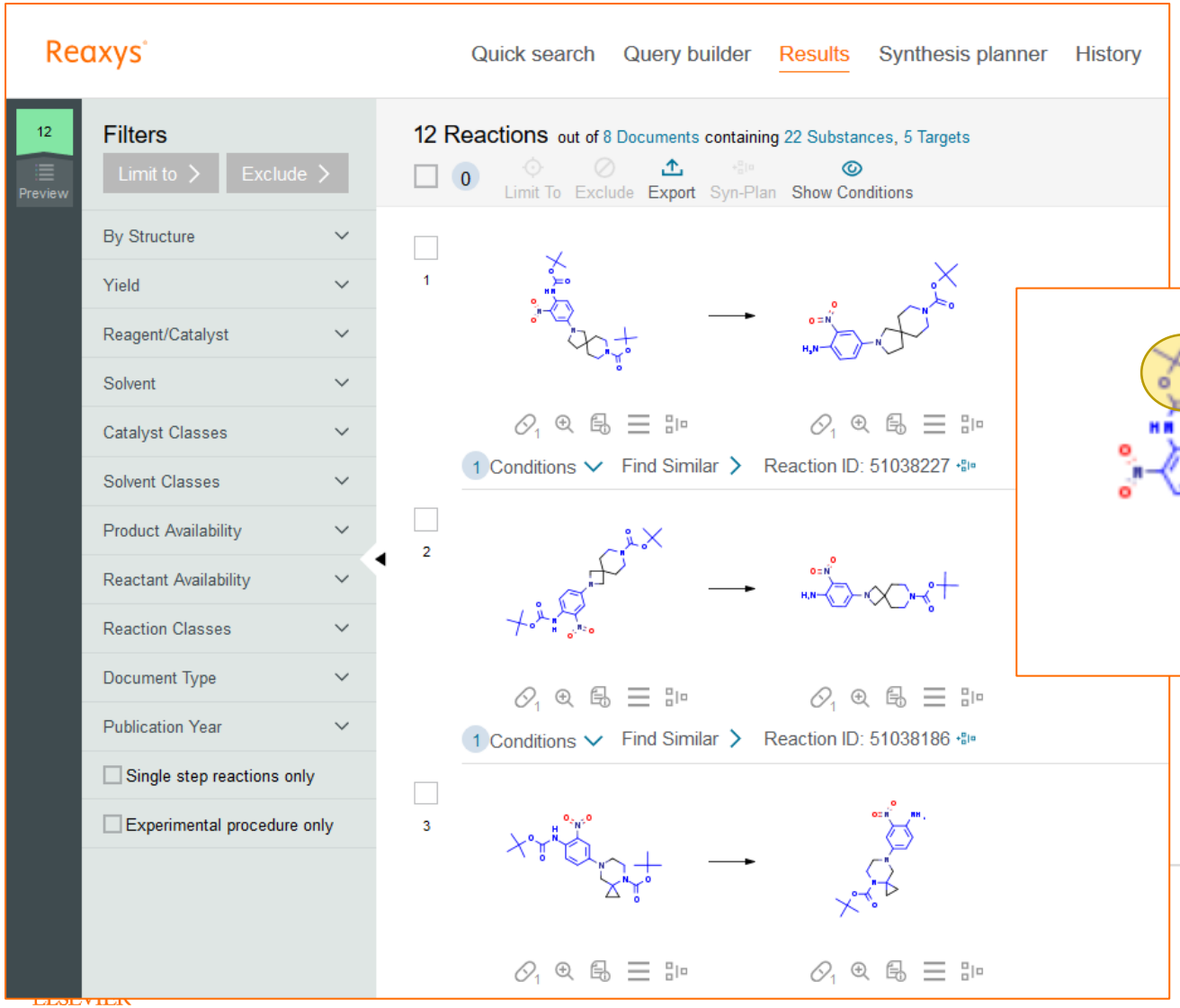
Reaxys中的结构定义

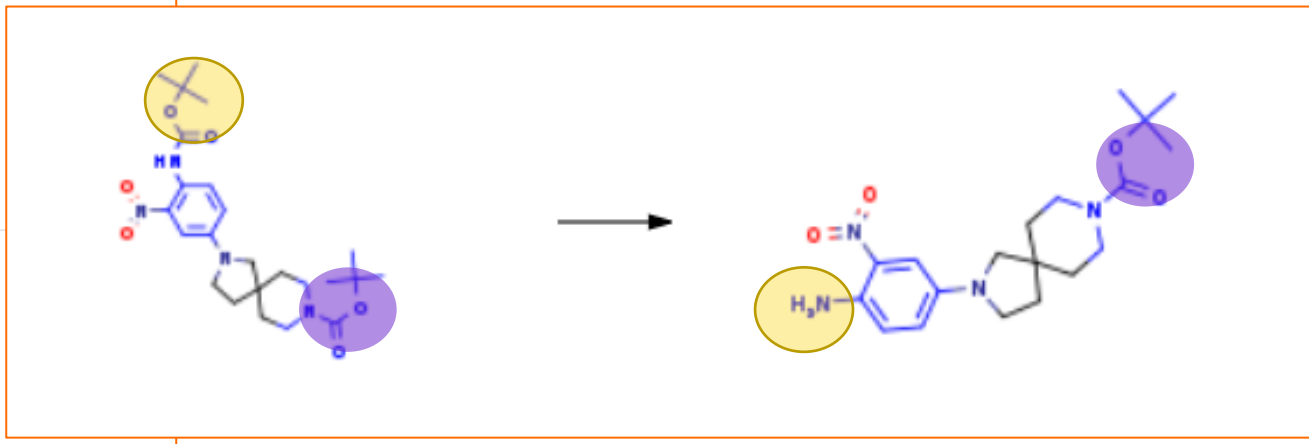


Reaxys可以直接设定这些片段在一个结构中



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
2
3
1 Conditions
Find Similar
Reaction ID: 51038227
1 Conditions
Find Similar
Reaction ID: 51038186



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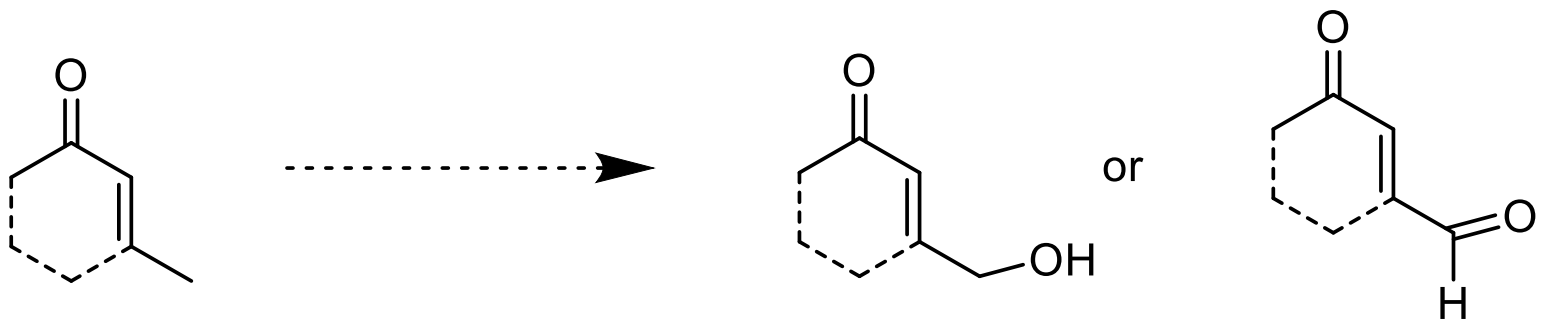
  - Reaxys中的反应设计与筛选
- Reaxys小结与未来展望

Case Study 6：

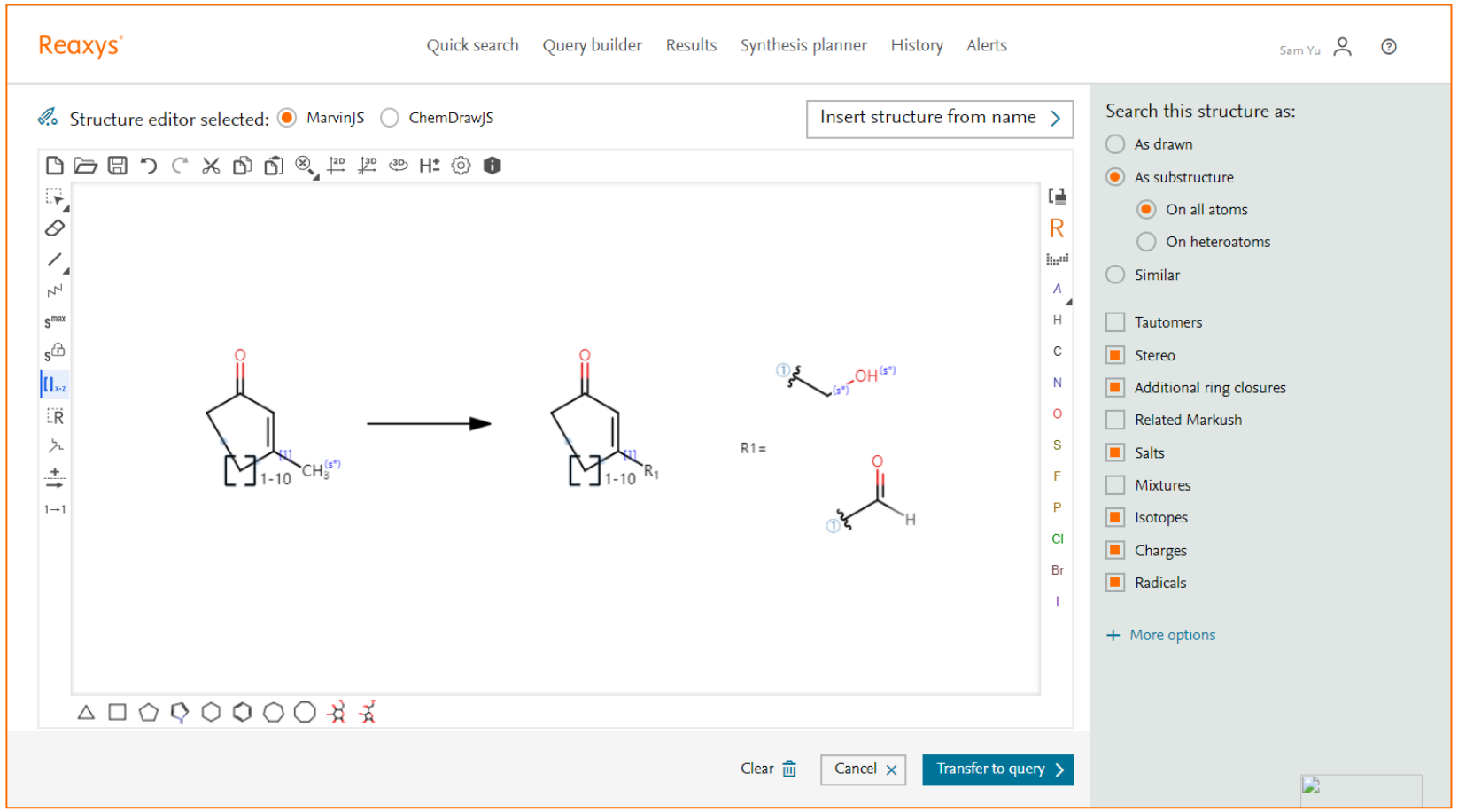
- 获取以下反应



Requirement:

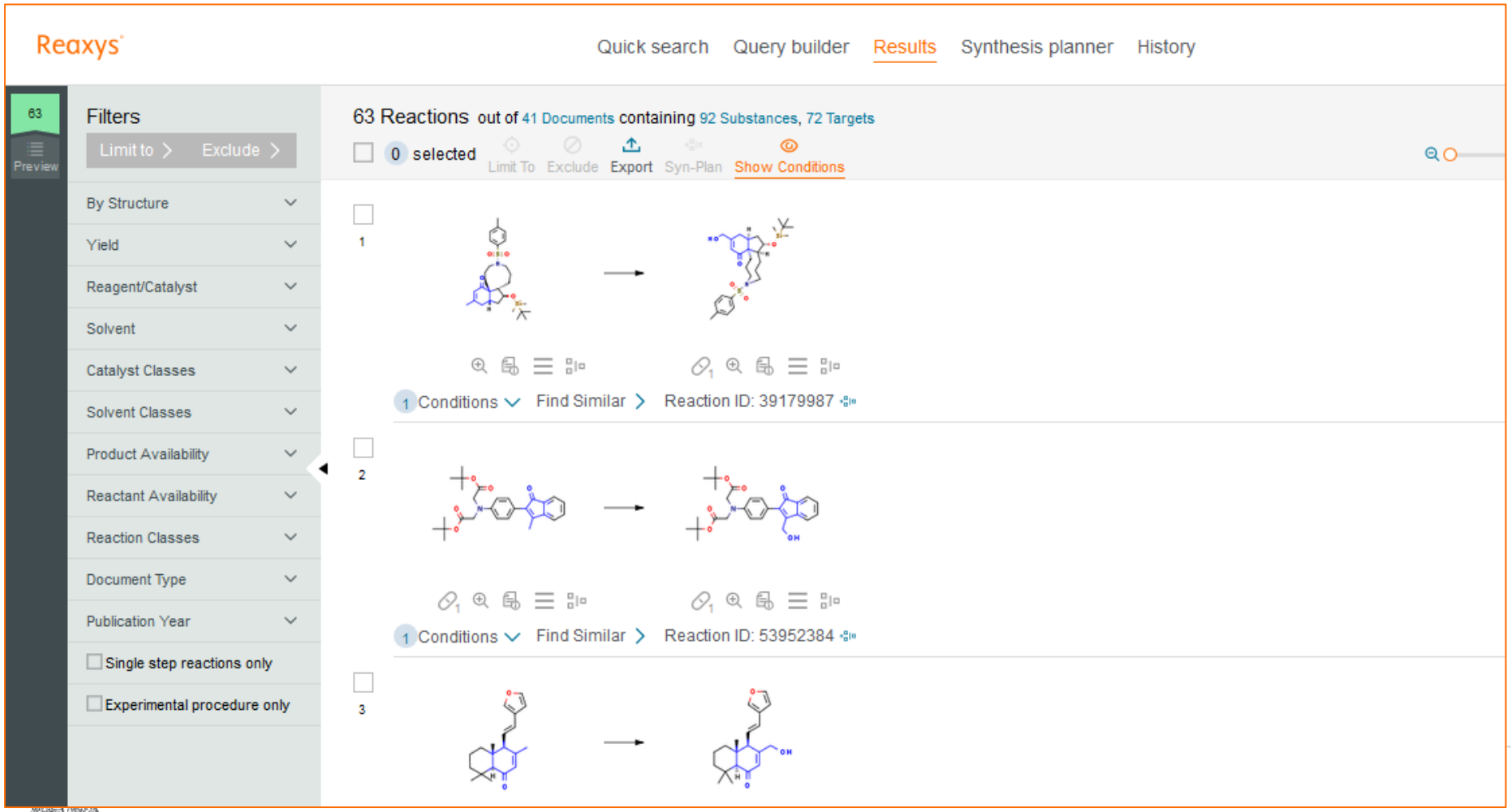
- 虚线部分是大于5个C原子的环
- 结构中不能发生互变异构
- 产物的CH2OH，CHO是有底物的CH3变化过来

Reaxys中的结构绘制



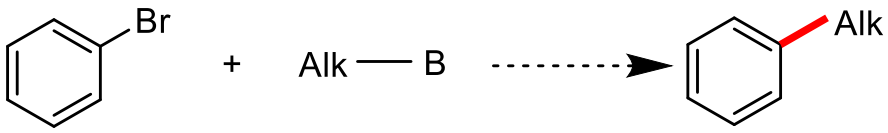
- R基团定义工具，定义侧链
- S*定义侧链CH2OH，以及底物CH3无取代
- 重复基团定义工具，定义环的大小
- 无互变异构

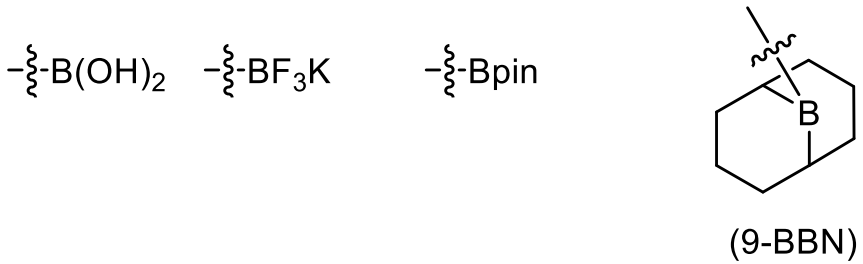
最后的结果



Case Study 7：

- 获取以下反应性对比的文献（收率）

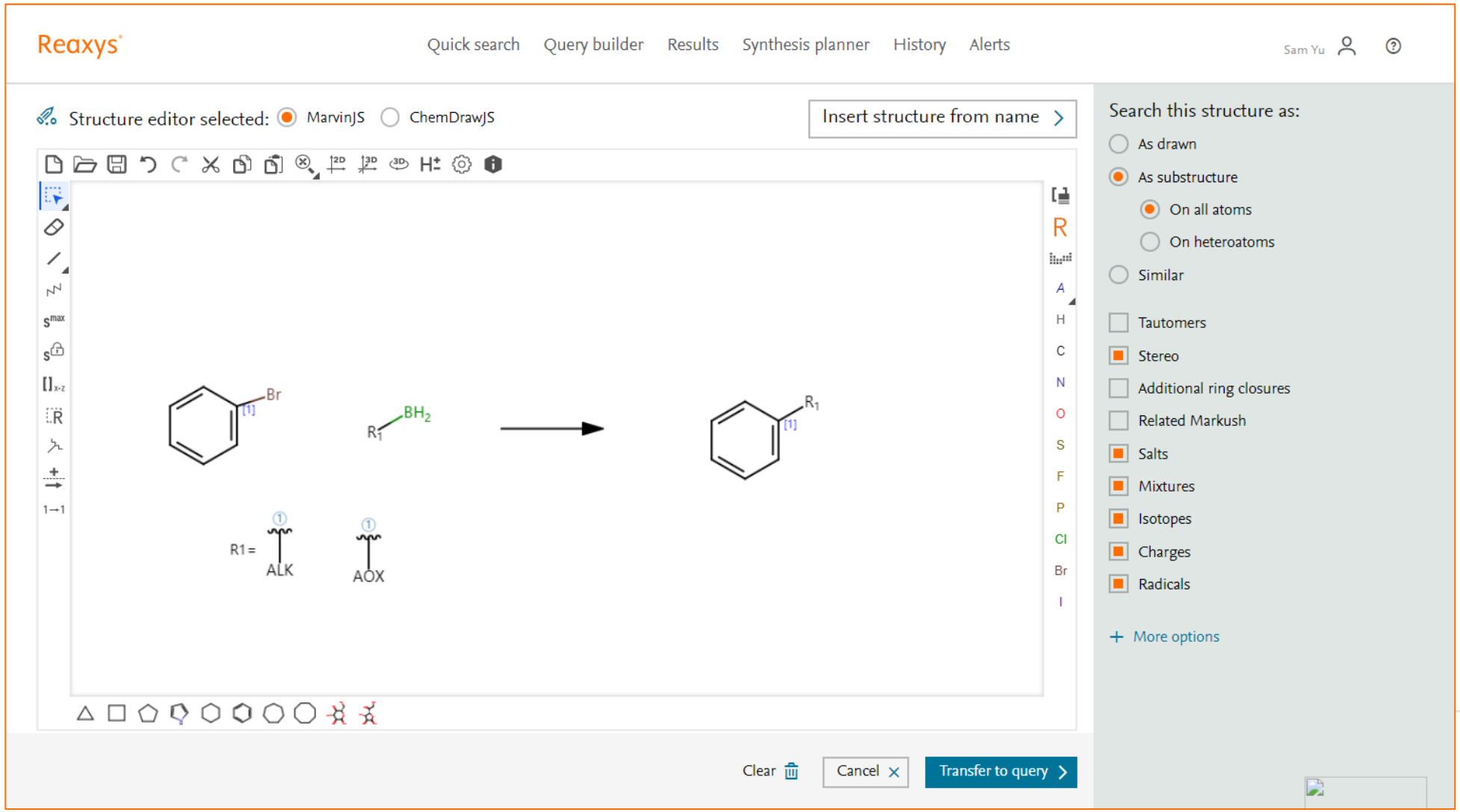




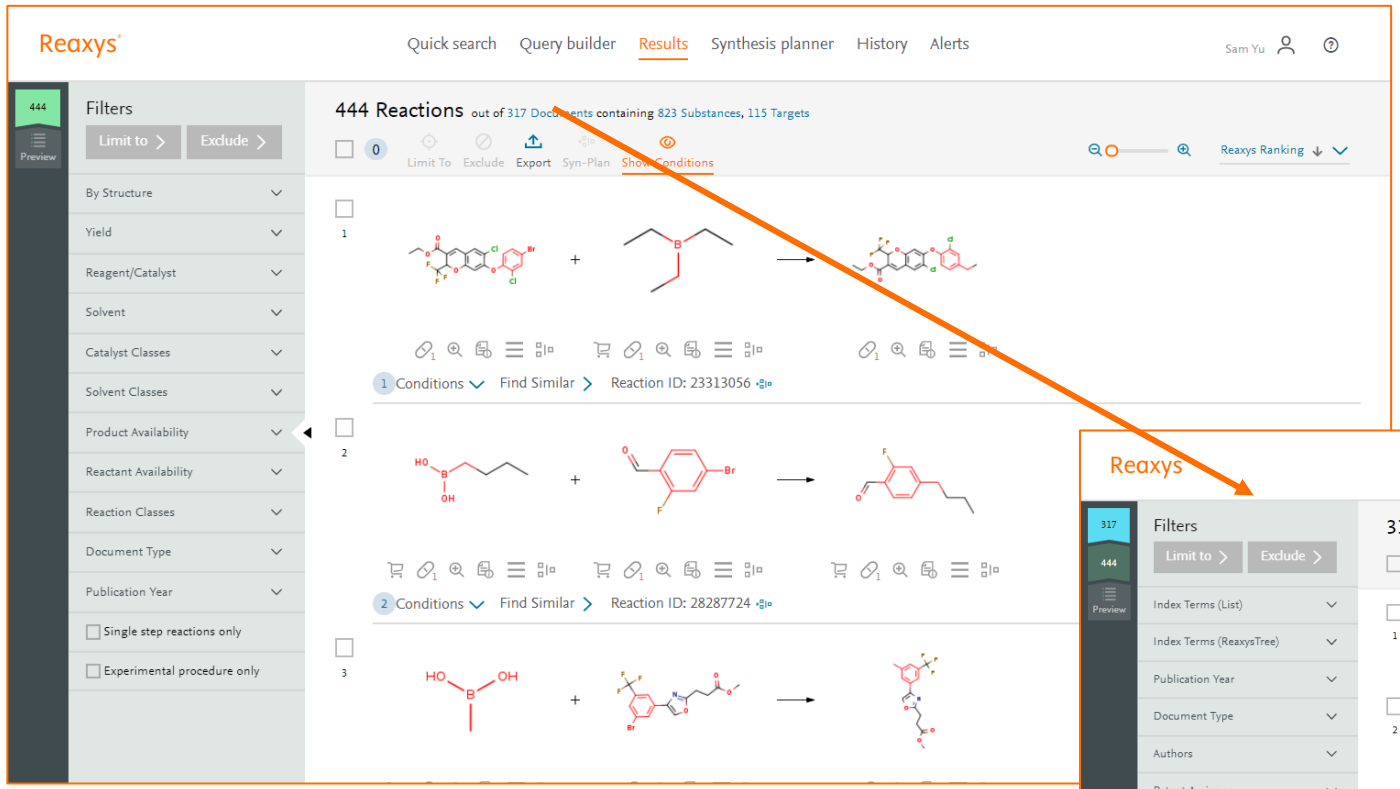
Requirement:

- 希望获得在一篇文献中讨论过同一个B试剂和不同底物反应的对比
- ALK也可以是醚

Reaxys中的解决方案



Reaxys中的结果



直接获取这些反应的文献

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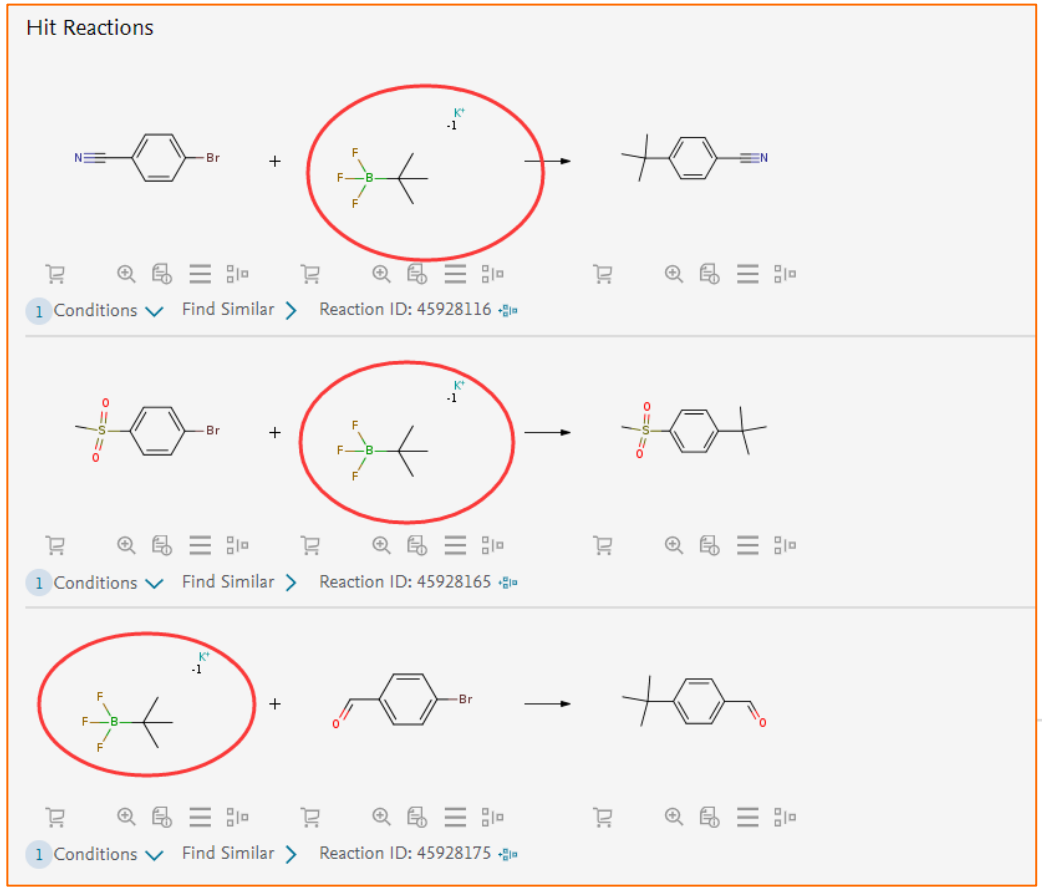
Reaxys中的结果

Enabling the Cross-Coupling of Tertiary Organoboron Nucleophiles through Radical-Mediated Alkyl Transfer

Primer, David N.; Molander, Gary A. [**Journal of the American Chemical Society, 2017**, vol. 139, # 29, p. 9847 - 9850]

Abstract | Index Terms | Substances 88 | Reactions 58 | Full Text

Hit Reactions 8



专门找Hit Reaction >1的文献，先进行预览，看是否存在相同硼试剂，不同底物的。

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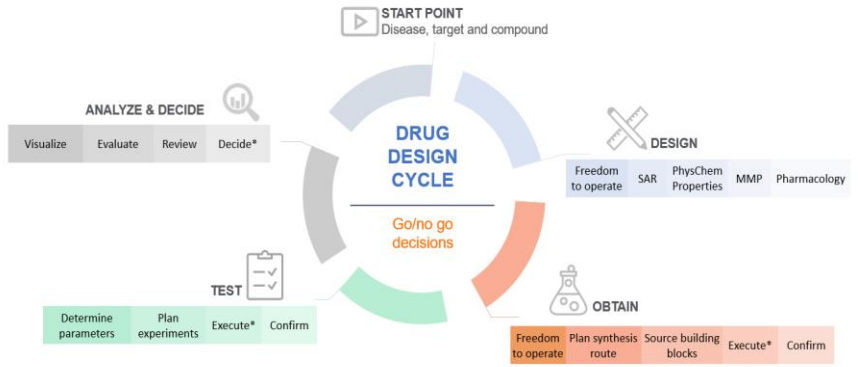
Reaxys已经开始嵌入药物研发流程的中信息的获取，分析，预测

“Workflow Solution”

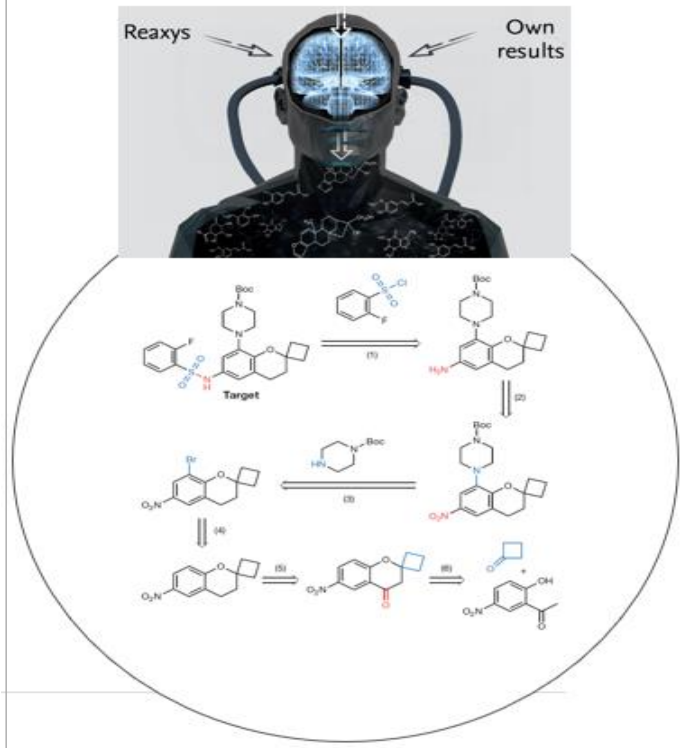
面向早期药物发现和开发的,以客户为中心的工作流解决方案



现在的Reaxys可以提供从传统数据库，AI模型预测，专业数据服务等多种服务类型，以满足药物研发全流程中的信息需求。

“Predictive Retrosynthesis ”

基于深度神经网络算法的全新化合物合成路线设计



“MMP Analysis and Target Prediction”

将MMP与深度学习相结合，预测药物可能毒性与毒性

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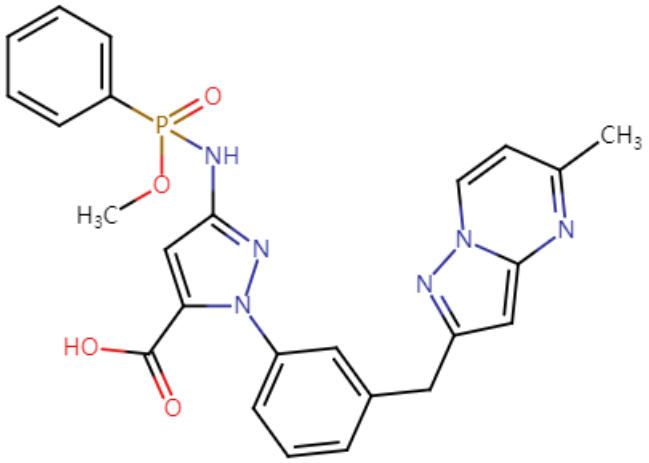
Reaxys逆合成模块



该结构是Case 3中根据现有活性化合物设计出来的全新结构，无文献报道，无合成线路报道。

Show 10 entries

Route no.	Buildingblocks to target	Route confidence score	No. of steps	View route
1		0.78	10	Table View / Tree View
2		0.758	10	Table View / Tree View
3		0.75	12	Table View / Tree View

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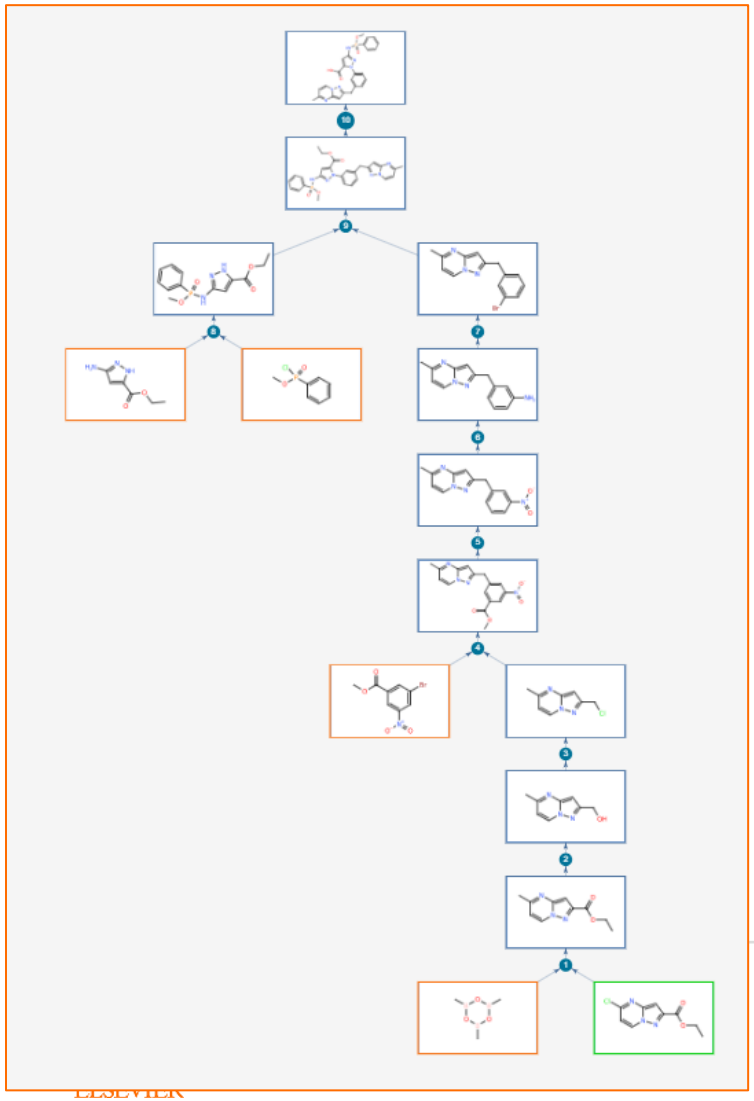
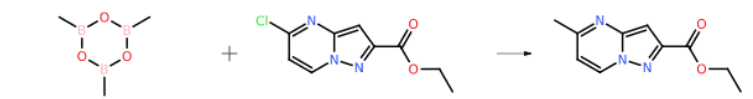
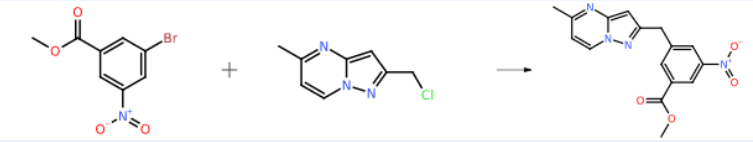
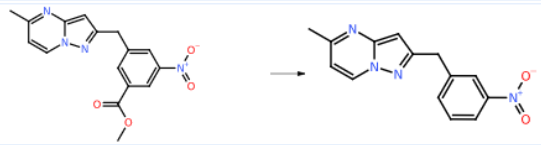
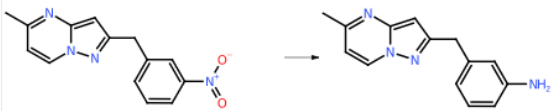
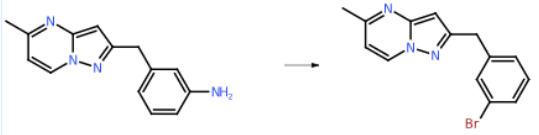
Reaxys逆合成模块结果呈现—所有起始原料都可以购买的到



Step no.	Reaction	Step confidence score	
1		0.93	Show Reaxys Examples
2		1	Show Reaxys Examples
3		1	Show Reaxys Examples
4		0.96	Show Reaxys Examples
5		1	Show Reaxys Examples
6		1	Show Reaxys Examples
7		0.99	Show Reaxys Examples

2020年Reaxys变化之—扩大专利覆盖范围与数据提炼范围

- 7 个专利机构(US, EP, WO, JP, CH, KR; TW)
- 选择性收入专利族(覆盖90%化学相关专利)
- 自动与手动的数据提炼(基于全文)
- 药物化学数据仅源自US, EP and WO
- 录入时间:
  - 自动: 5-10 days
  - 手动:
    - 30 days Reaxys
    - 45 days RMC

~2019Q4

- 100 专利机构(from TotalPatents)
- 所有专利族
- 选择更多的专利范围，用于手动数据提炼，(10% of additional patents expected)
- 录入时间:
  - 自动: 1-2 days
  - 手动:
    - 20 days Reaxys
    - 30 days RMC

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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
- Reaxys培训中心网址：

https://www.elsevier.com/zh-cn/rd-solutions/pharma-and-life-sciences-solutions/life-sciences-online-training-center

Thank you

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