New Reaxys 基础培训

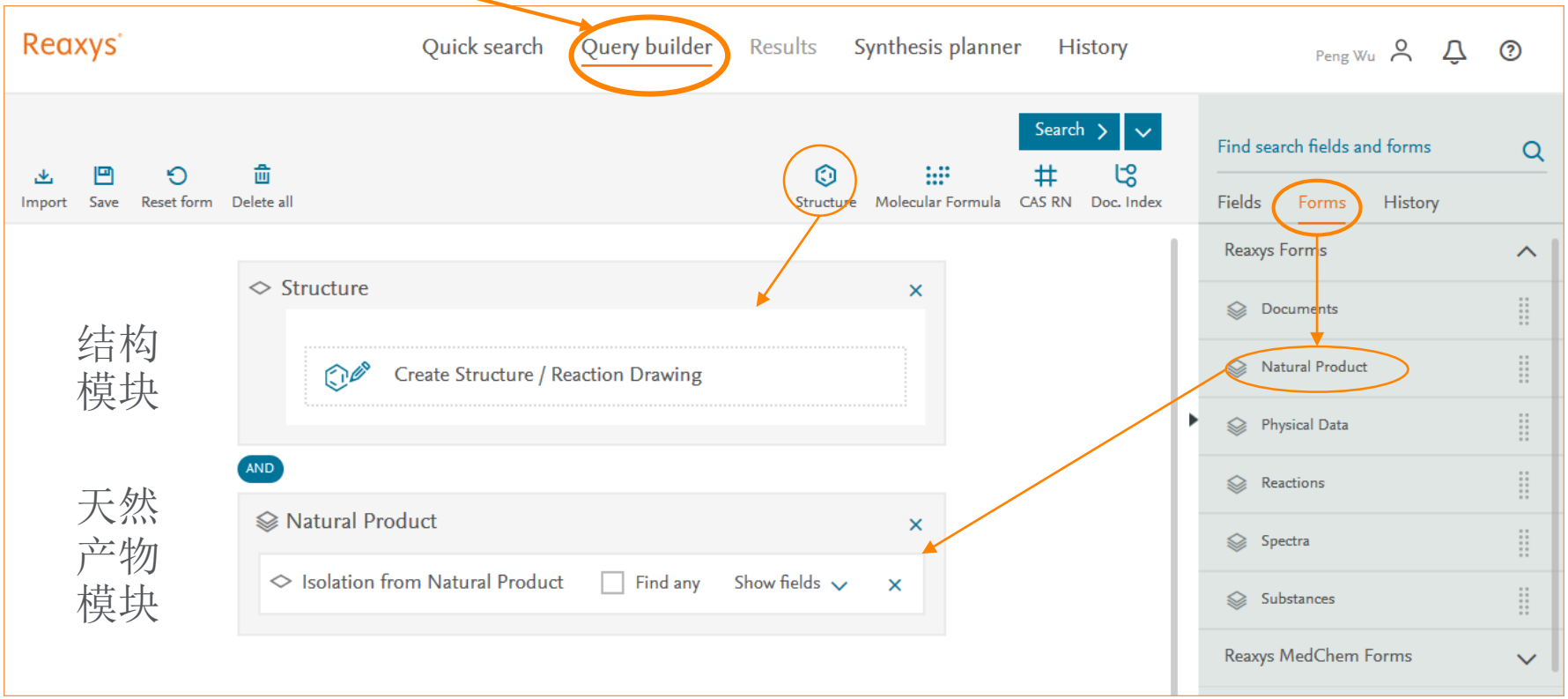
Presented By Markus Bussen

Date

天然提取物的检索

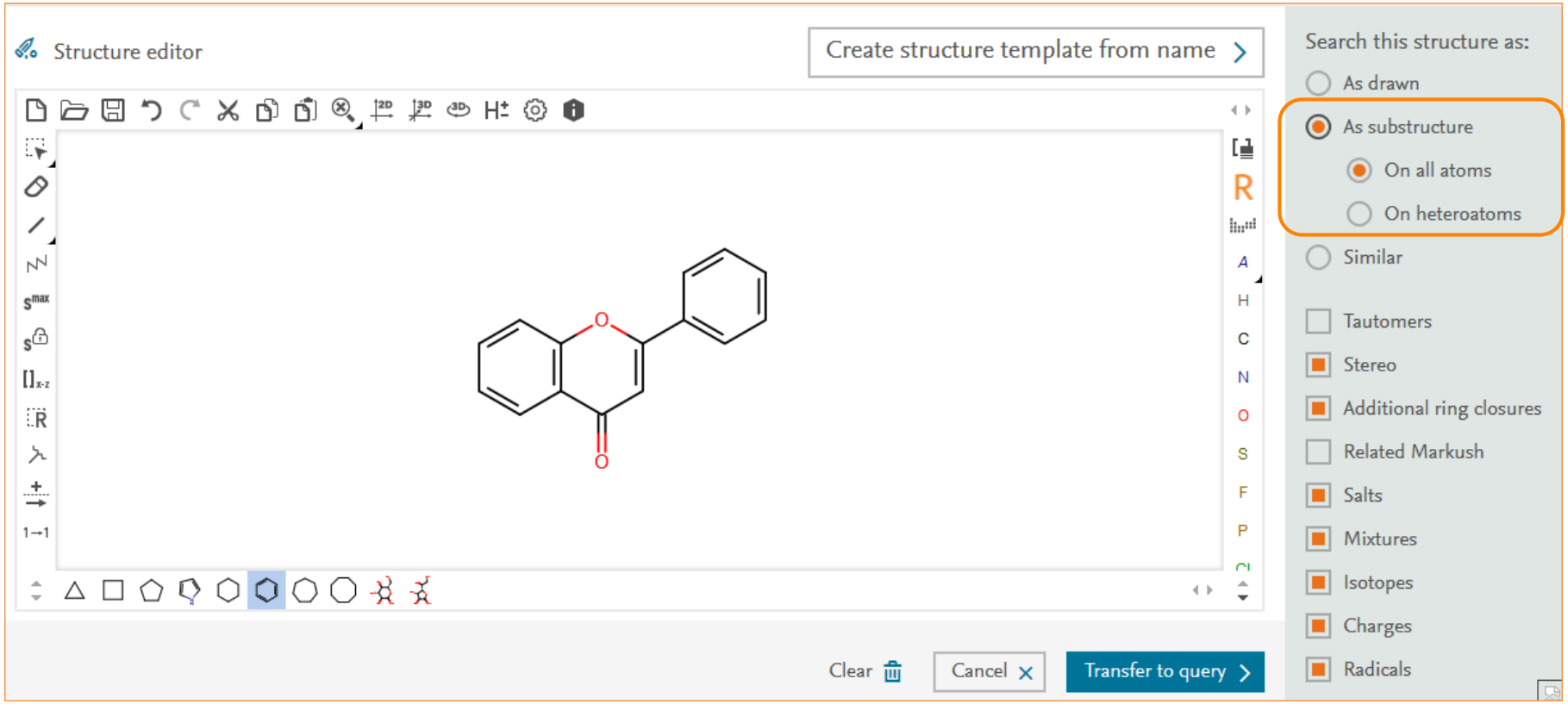
- 无论是什么样的天然提取物，在Reaxys中检索技巧都类似，且也比较方便

在自定义检索界面



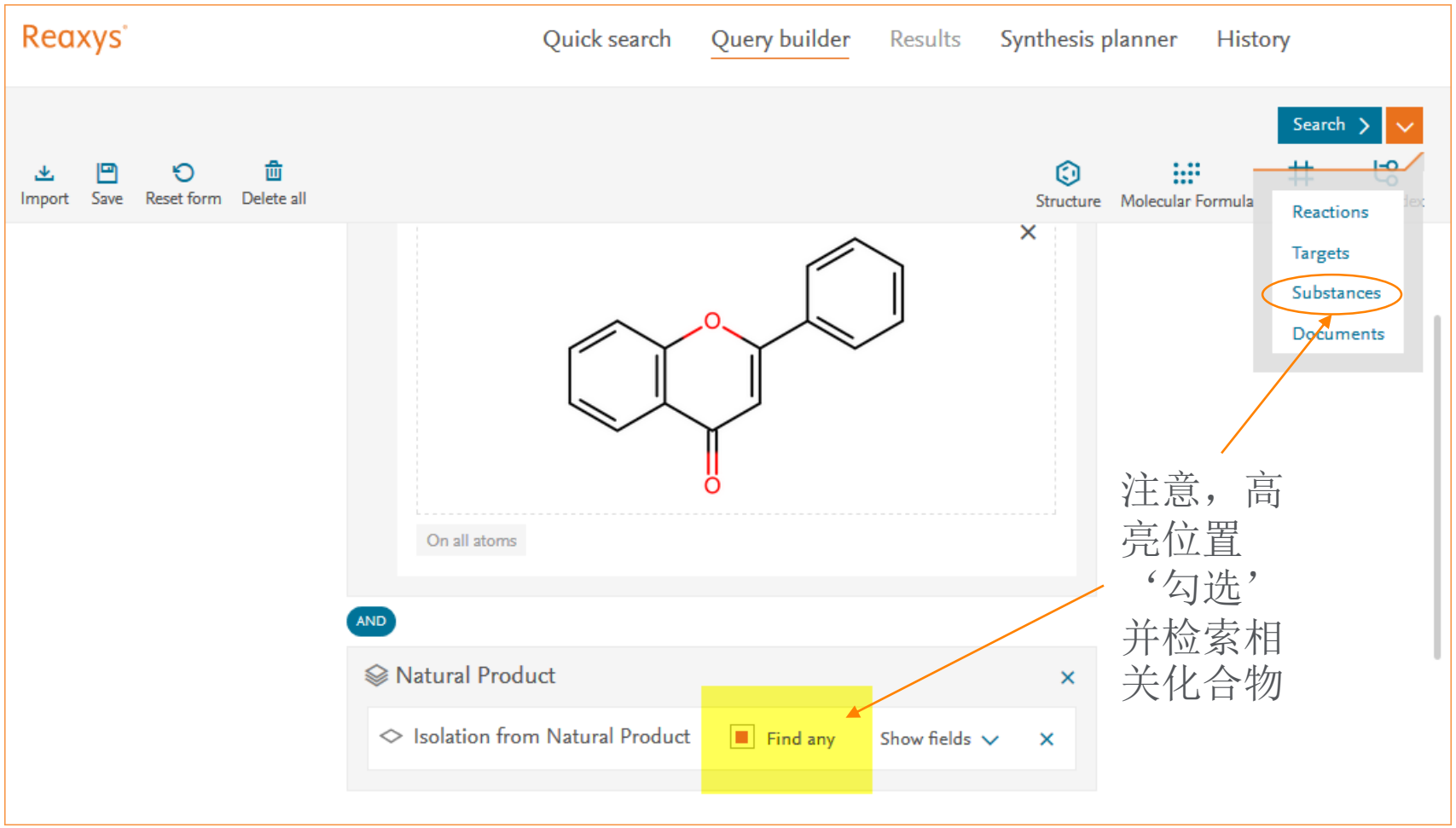
通过母核检索（子结构）

以‘黄酮苷’为例，只需要画入其结构，并作‘子结构’检索其‘碳骨架一样’的所有衍生物



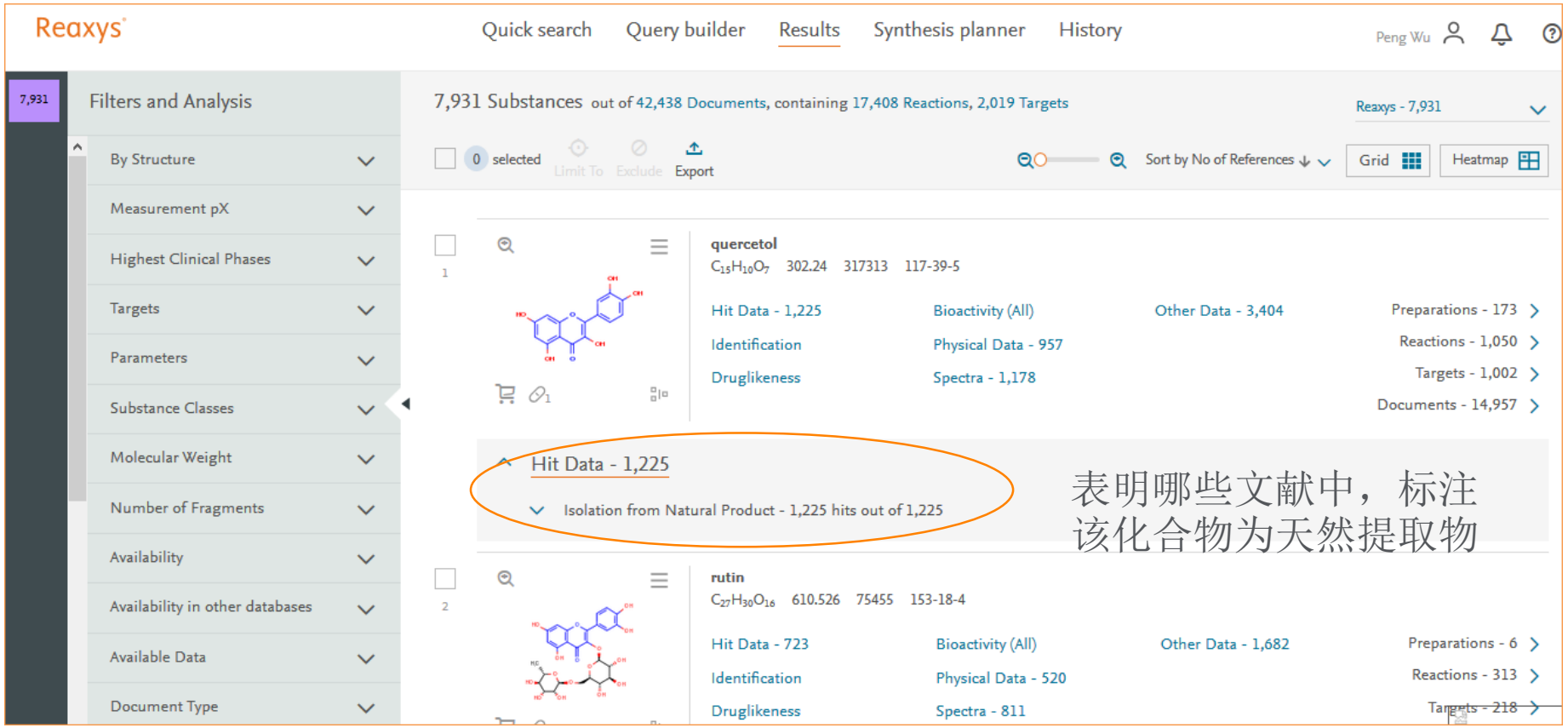
天然提取物标注

- Rx数据库是目前做得比较好的，对文献和专利中记录为‘天然提取物’的化合物进行标注和提炼的数据库

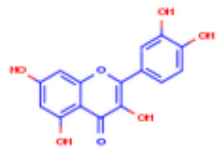


检索结果

- 虽然不是100%全能检索万，但是RX数据库中的1.6万本期刊+7大专利局的专利，至少目前报道80%-90%的数据资料是有的



Rx数据库的数据摘取



quercetol

$C_{15}H_{10}O_7$ 302.24 317313 117-39-5

Hit Data - 1,225 | Bioactivity (All) | Other Data - 3,404

Identification | Physical Data - 957

Druglikeness | Spectra - 1,178

Preparations - 173 >

Reactions - 1,050 >

Targets - 1,002 >

Documents - 14,957 >

Hit Data - 1,225

Isolation from Natural Product - 1,225 hits out of 1,225

Rx尽可能多的把每个化合物的‘具体性质值’给摘录出来

Physical Data - 957

- Melting Point - 235
- Boiling Point - 1
- Density - 2
- Adsorption (MCS) - 18
- Association (MCS) - 123

Spectra - 1,178

- NMR Spectroscopy - 298
- IR Spectroscopy - 36
- Mass Spectrometry - 226
- UV/VIS Spectroscopy - 574
- ESR Spectroscopy - 2

Bioactivity (All)

- In vitro: Efficacy - 7,803
- In vivo: Animal Model - 1,659
- Metabolism - 1,056
- Pharmacokinetic - 403
- Toxicity/Safety Pharmacology - 998

具体数据的摘取

Chemical shifts, Spectrum	13C		dimethylsulfoxide-d6		100	^{13}C NMR (DMSO-d_6, 100 MHz): δ 175.5, 135.4, 163.3, 160.9, 144.7, 146.4, 147.3, 97.8, 93.0, 155.8, 102.6, 121.6, 114.7, 115.2, 119.6	supporting information	175.5, 135.4, 163.3, 160.9, 144.7, 146.4, 147.3, 97.8, 93, 155.8, 102.6, 121.6, 114.7, 115.2, 119.6		Gao, Suyu; Sun, Dejuan; Wang, Guan; Zhang, Jin; Jiang, Yingnan; Li, Guoyu; Zhang, Ke; Wang, Lei; Huang, Jian; Chen, Lixia - Bioorganic Chemistry, **2016**, vol. 69, p. 121 - 128 Full Text Cited 3 times Details Abstract

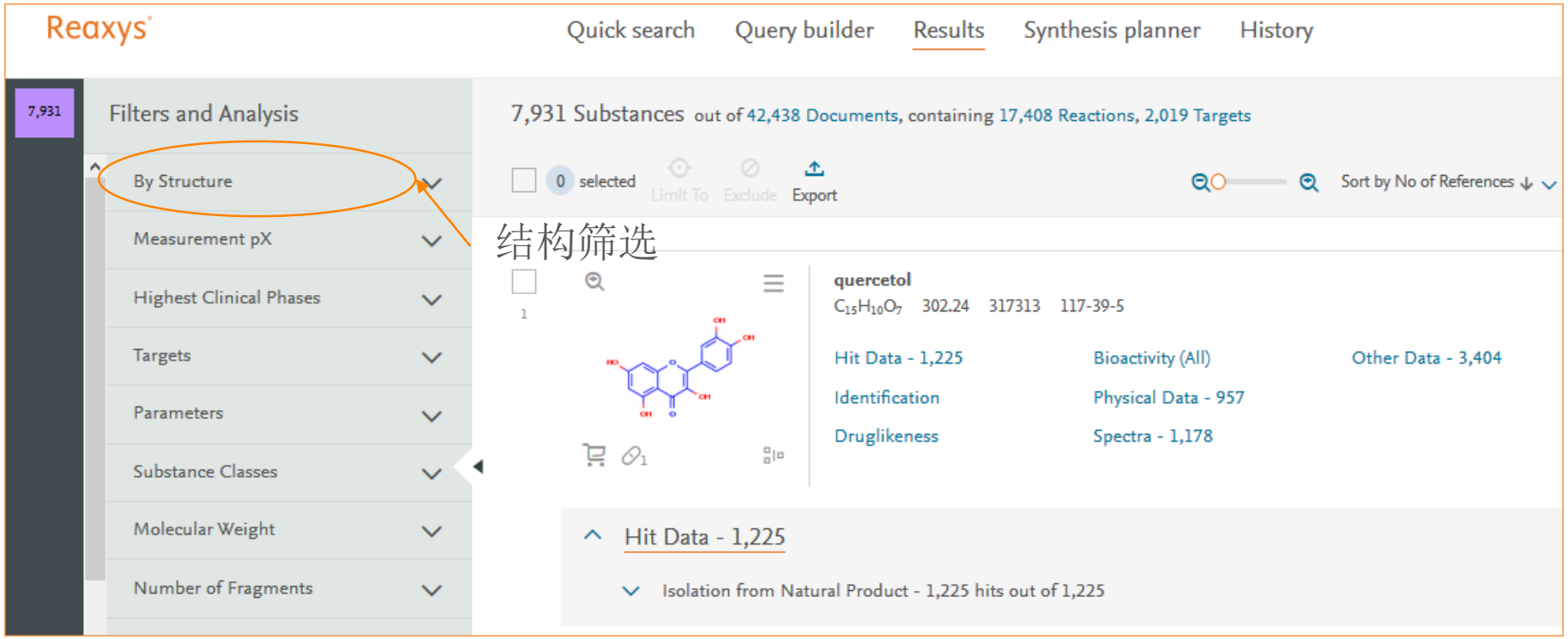
核磁图谱

pX	Parameter	Value (qual)	Value (quant)	Unit	Action on target	Target	Tissue/Organ	Bioassay	Effect	Reference
10.9	IC50	=	12	pM	Inhibitor	Sulfotransferase [human]:Wild	liver			Wang, Li-Quan; James, Margaret O - Current drug metabolism, **2006**, vol. 7, # 1, p. 83 - 104 Full Text Details Abstract
10.8	IC50	=	15	pM	Inhibitor	Sulfotransferase [human]:Wild	duodenum			Wang, Li-Quan; James, Margaret O - Current drug metabolism, **2006**, vol. 7, # 1, p. 83 - 104 Full Text Details Abstract
9.74	Ki		0.00018	μM	Inhibitor	dna gyrase subunit b [escherichia coli]:Wild				Hossion, Abugafar M.L.; Otsuka, Nao; Kandahary, Rafiya K.; Tsuchiya, Tomofusa; Ogawa, Wakano; Iwado, Akimasa; Zamami, Yoshito; Sasaki, Kenji - Bioorganic and Medicinal Chemistry Letters, **2010**, vol. 20, # 17, p. 5349 - 5352 Full Text Cited 18 times Details Abstract

生物活性数据

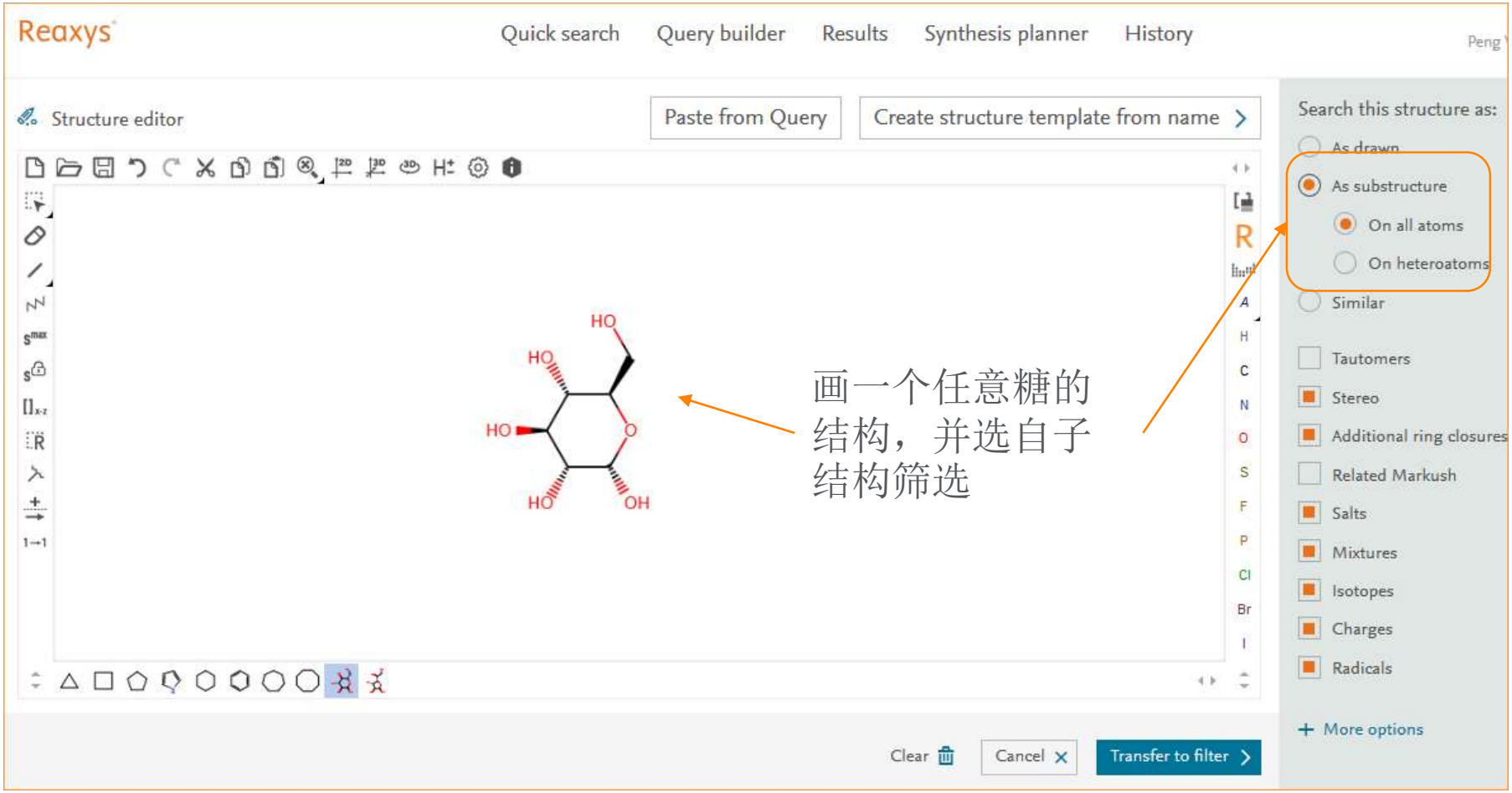
结构筛选

➢ 当要筛选‘黄酮类结构衍生物’中的接了糖苷官能团时，直接筛选即可



点击接够筛选器，会自动跳转到结构别机器界面

结构筛选

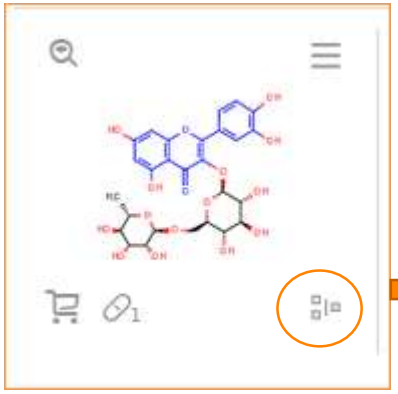

Reaxys
Quick search
Query builder
Results
Synthesis planner
History
Structure editor
Paste from Query
Create structure template from name
Search this structure as:
As drawn
As substructure
On all atoms
On heteroatoms
Similar
Tautomers
Stereo
Additional ring closures
Related Markush
Salts
Mixtures
Isotopes
Charges
Radicals
More options
Clear
Cancel
Transfer to filter
画一个任意糖的结构，并选自子结构筛选

筛选结果

- 在任意位置接了单糖的天然提取物

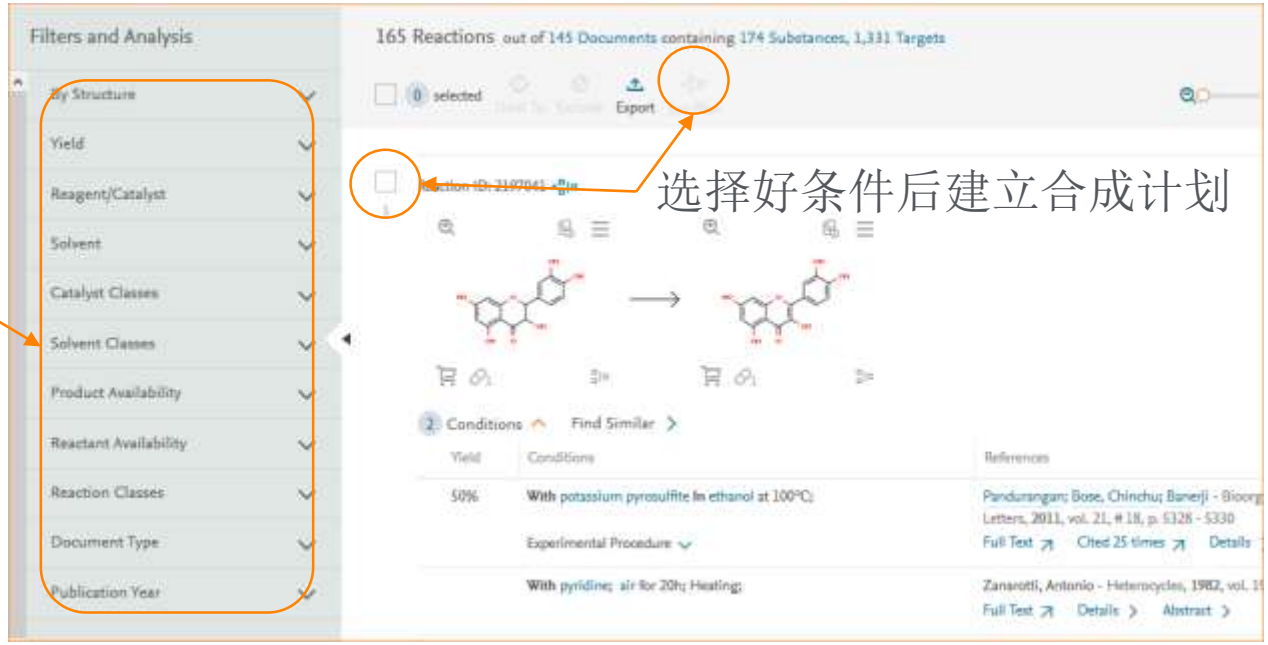
自动设计合成路线

- Rx具有目前市面上最完善的合成路线设计工具



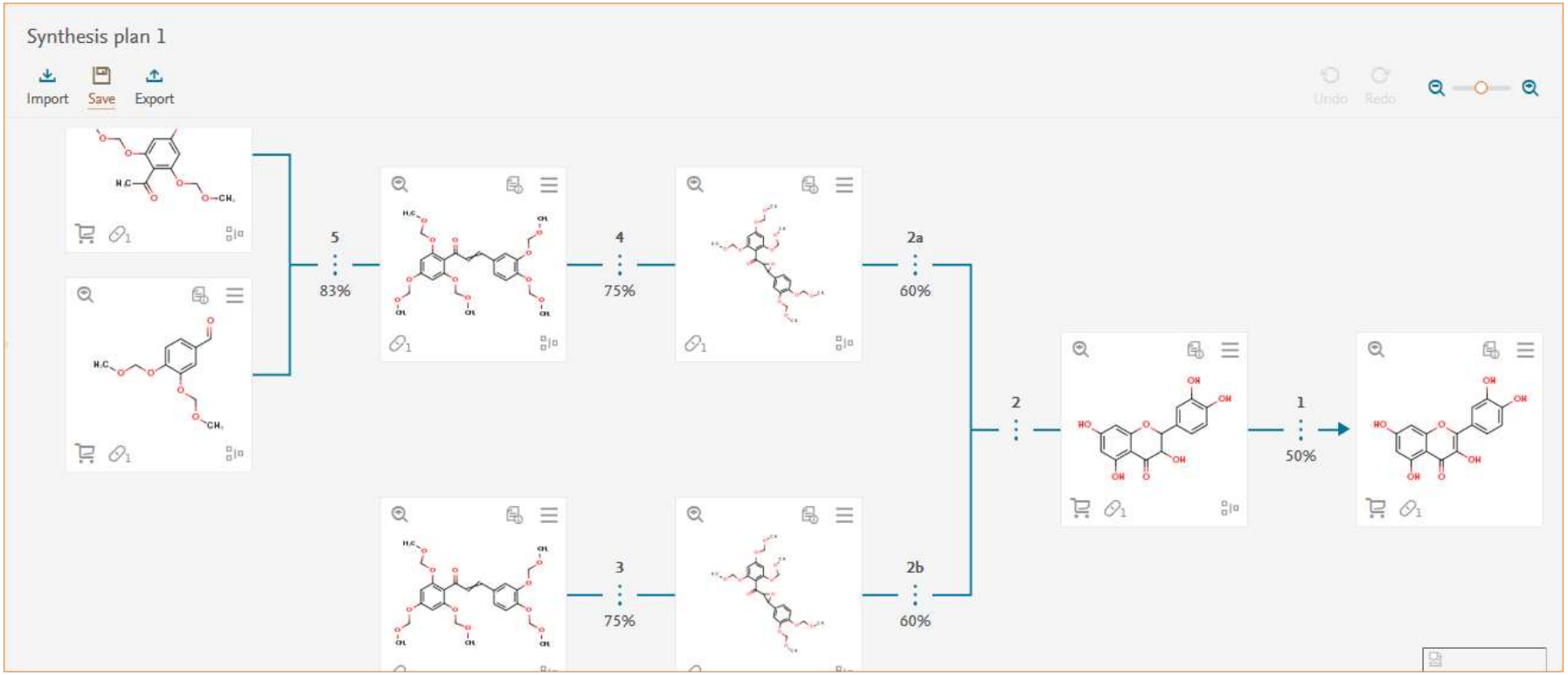
选择‘手动设计’会根据结构把‘最后一步’所有报道的条件罗列出来，可以先筛选条件，再建立合成计划

通过筛选器，筛选条件



合成计划

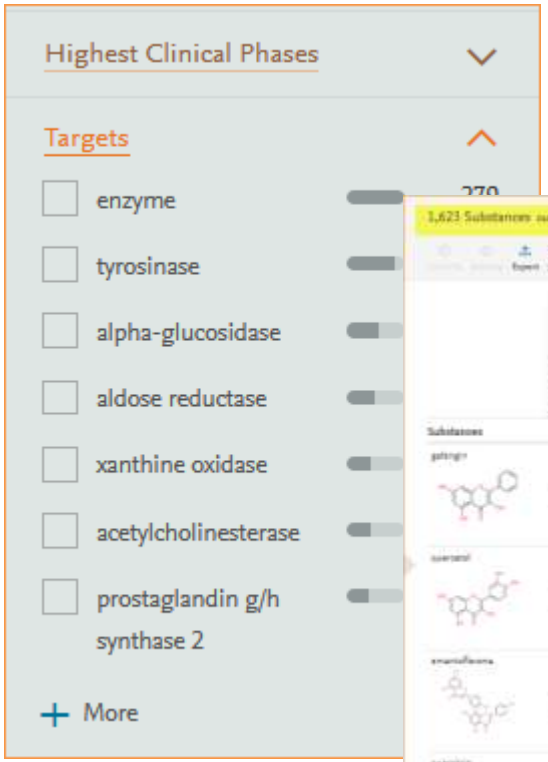
根据需求建立最终计划，该合成计划和条件皆可以导出



更多功能

完整版的Rx（药化模块）具有更多功能

靶点分析



构效关系辅助天然提取物改性，辅助相关小分子药设计等功能