

# New Reaxys 基础培训

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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

The screenshot displays the Reaxys Query Builder interface. At the top, the 'Query builder' tab is selected and circled in orange. Below the navigation bar, there are icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index', with the 'Structure' icon also circled in orange. The main workspace contains two search modules: 'Structure' and 'Natural Product'. The 'Structure' module has a 'Create Structure / Reaction Drawing' button. The 'Natural Product' module is expanded to show the 'Isolation from Natural Product' search field, which includes a 'Find any' checkbox and a 'Show fields' dropdown. On the right side, a sidebar titled 'Find search fields and forms' lists various search categories, with 'Forms' circled in orange and an arrow pointing to the 'Natural Product' entry in the main workspace.

Reaxys<sup>®</sup> Quick search **Query builder** Results Synthesis planner History Peng Wu

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

Structure

Create Structure / Reaction Drawing

AND

Natural Product

Isolation from Natural Product  Find any Show fields

Find search fields and forms

Fields **Forms** History

Reaxys Forms

Documents

Natural Product

Physical Data

Reactions

Spectra

Substances

Reaxys MedChem Forms

结构模块

天然产物模块

## 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

The screenshot displays a chemical structure editor window. The central canvas shows the chemical structure of a flavone derivative, specifically a 2-phenylchromone. The structure consists of a benzopyrone core with a phenyl group attached to the 2-position. The oxygen atom and the carbonyl oxygen are highlighted in red.

The interface includes a toolbar at the top left with various editing tools. At the top right, there is a button labeled "Create structure template from name >". On the right side, a search options panel is visible, titled "Search this structure as:". The options are:

- As drawn
- As substructure
  - On all atoms
  - On heteroatoms
- Similar

Below these options, there are several checkboxes for additional search criteria: Tautomers, Stereo, Additional ring closures, Related Markush, Salts, Mixtures, Isotopes, Charges, and Radicals. At the bottom of the editor, there are buttons for "Clear", "Cancel", and "Transfer to query".

## 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

The screenshot displays the Reaxys web interface. At the top, there are navigation tabs: "Quick search", "Query builder" (which is underlined), "Results", "Synthesis planner", and "History". Below these are utility icons for "Import", "Save", "Reset form", and "Delete all". The main workspace shows a chemical structure of a benzofuran derivative with a phenyl group. Below the structure, there is a search filter section. A dropdown menu is open, showing options: "Reactions", "Targets", "Substances" (which is circled in orange), and "Documents". An orange arrow points from this menu to the "Substances" option. Below the filter section, there is a filter for "Natural Product" with a sub-filter "Isolation from Natural Product" and a checkbox labeled "Find any" (which is highlighted in yellow). Another orange arrow points from the Chinese text to this checkbox. The text "On all atoms" is visible below the structure.

注意，高亮位置‘勾选’并检索相关化合物

## 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

Reaxys® Quick search Query builder Results Synthesis planner History Peng Wu

7,931 Substances out of 42,438 Documents, containing 17,408 Reactions, 2,019 Targets Reaxys - 7,931

0 selected Limit To Exclude Export Sort by No of References ↓ Grid Heatmap

**quercetol**  
C<sub>15</sub>H<sub>10</sub>O<sub>7</sub> 302.24 317313 117-39-5

Hit Data - 1,225 Bioactivity (All) Other Data - 3,404 Preparations - 173 >  
Identification Physical Data - 957 Reactions - 1,050 >  
Druglikeness Spectra - 1,178 Targets - 1,002 >  
Documents - 14,957 >

**Hit Data - 1,225**  
Isolation from Natural Product - 1,225 hits out of 1,225

**rutin**  
C<sub>27</sub>H<sub>30</sub>O<sub>16</sub> 610.526 75455 153-18-4

Hit Data - 723 Bioactivity (All) Other Data - 1,682 Preparations - 6 >  
Identification Physical Data - 520 Reactions - 313 >  
Druglikeness Spectra - 811 Targets - 218 >

表明哪些文献中，标注该化合物为天然提取物

# Rx数据库的数据摘取

quercetol  
C<sub>15</sub>H<sub>10</sub>O<sub>7</sub> 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  
v 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

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

## ^ Spectra - 1,178

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

## ^ Bioactivity (All)

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

## 具体数据的摘取

Chemical shifts, Spectrum	<sup>13</sup> C		dimethylsulfoxide-d <sub>6</sub>	100	<sup>13</sup> C NMR (DMSO-d <sub>6</sub> , 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	<a href="#">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</a> <a href="#">Full Text ↗</a> <a href="#">Cited 3 times ↗</a> <a href="#">Details &gt;</a> <a href="#">Abstract &gt;</a>
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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			<a href="#">Wang, Li-Quan; James, Margaret O - Current drug metabolism, 2006, vol. 7, # 1, p. 83 - 104</a> <a href="#">Full Text ↗</a> <a href="#">Details &gt;</a> <a href="#">Abstract &gt;</a>
10.8	IC50	=	15	pM	Inhibitor	Sulfotransferase [human]:Wild	duodenum			<a href="#">Wang, Li-Quan; James, Margaret O - Current drug metabolism, 2006, vol. 7, # 1, p. 83 - 104</a> <a href="#">Full Text ↗</a> <a href="#">Details &gt;</a> <a href="#">Abstract &gt;</a>
9.74	Ki		0.00018	μM	Inhibitor	dna gyrase subunit b [escherichia coli]:Wild				<a href="#">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</a> <a href="#">Full Text ↗</a> <a href="#">Cited 18 times ↗</a> <a href="#">Details &gt;</a> <a href="#">Abstract &gt;</a>

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

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History

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0 selected Limit To Exclude Export Sort by No of References ↓

**结构筛选**

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Identification Physical Data - 957  
Druglikeness Spectra - 1,178

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

点击接够筛选器，会自动跳转到结构别机器界面

By Structure

Create Structure Drawing



# 结构筛选

Reaxys® Quick search Query builder Results Synthesis planner History Peng

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

画一个任意糖的结构，并选自子结构筛选

Clear  Transfer to filter >

# 筛选结果

➤ 在任意位置接了单糖的天然提取物

79 Substances out of 96 Documents, containing 30 Reactions, 9 Targets

Reaxys - 79

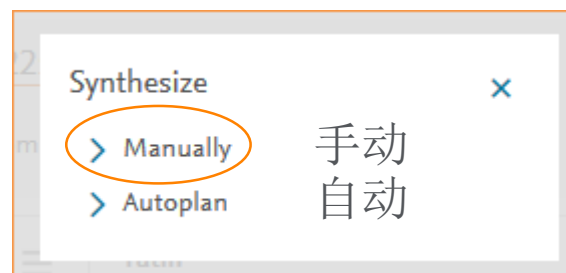
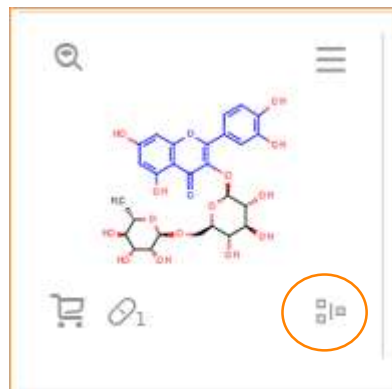
0 selected    Limit To    Exclude    Export

Sort by No of References ↓    List    Heatmap

The screenshot displays a grid of 15 chemical structures, numbered 1 through 15. Each structure is presented in a card format with a search icon, a zoom icon, and a list icon. The structures are complex organic molecules, many of which feature sugar moieties (glucopyranosides) attached to various aglycone cores. The interface includes a search bar at the top with the text '79 Substances out of 96 Documents, containing 30 Reactions, 9 Targets' and a dropdown menu for 'Reaxys - 79'. Below the search bar are buttons for 'Limit To', 'Exclude', and 'Export'. On the right side, there are buttons for 'Sort by No of References ↓', 'List', and 'Heatmap'. The grid shows the first 15 results, with the 15th result partially cut off on the right edge.

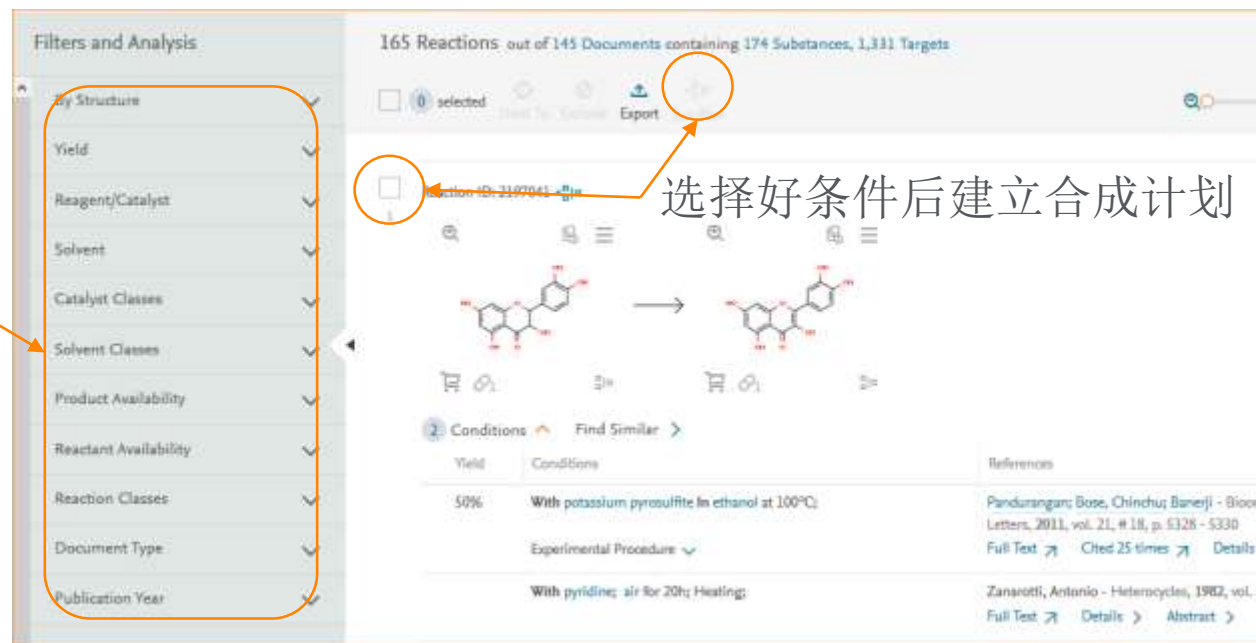
# 自动设计合成路线

➤ 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



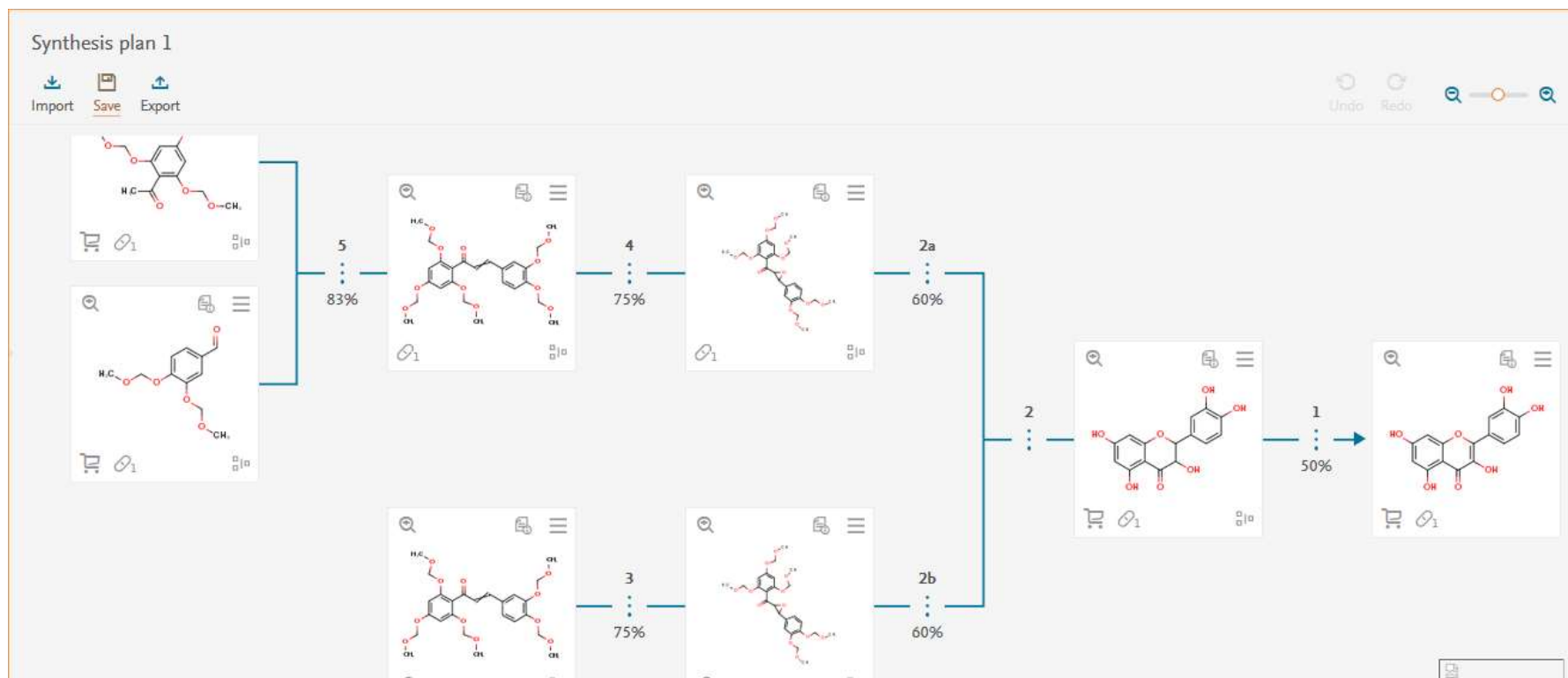
A screenshot of the 'Filters and Analysis' panel and the reaction results. The left panel shows a list of filters: Structure, Yield, Reagent/Catalyst, Solvent, Catalyst Classes, Solvent Classes, Product Availability, Reactant Availability, Reaction Classes, Document Type, and Publication Year. The right panel shows '165 Reactions: out of 145 Documents containing 174 Substances, 1,331 Targets'. There is a search bar, an 'Export' button, and a list of reactions. One reaction is selected, showing a chemical structure and conditions: '50% With potassium pyrosulfite in ethanol at 100°C'. Below this, there is a table with columns for 'Yield', 'Conditions', and 'References'. The table lists two conditions: 'With potassium pyrosulfite in ethanol at 100°C' and 'With pyridine; air for 20h; Heating:'. The 'References' column lists 'Pandurangam; Bose, Chinchu; Banerji - Bioorg Letters, 2011, vol. 21, # 18, p. 5328 - 5330' and 'Zanarotti, Antonio - Heterocycles, 1982, vol. 11'. A red circle highlights the 'Export' button, and an arrow points to the selected reaction.

Yield	Conditions	References
50%	With potassium pyrosulfite in ethanol at 100°C	Pandurangam; Bose, Chinchu; Banerji - Bioorg Letters, 2011, vol. 21, # 18, p. 5328 - 5330 Full Text <a href="#">↗</a> Cited 25 times <a href="#">↗</a> Details <a href="#">↗</a>
	With pyridine; air for 20h; Heating:	Zanarotti, Antonio - Heterocycles, 1982, vol. 11 Full Text <a href="#">↗</a> Details <a href="#">↗</a> Abstract <a href="#">↗</a>

选择好条件后建立合成计划

# 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

The screenshot displays a software interface for target analysis. On the left, a sidebar lists various targets with checkboxes and sliders:

- enzyme (slider: 270)
- tyrosinase (slider: 270)
- alpha-glucosidase (slider: 270)
- aldose reductase (slider: 270)
- xanthine oxidase (slider: 270)
- acetylcholinesterase (slider: 270)
- prostaglandin g/h synthase 2 (slider: 270)
- + More

The main window shows a table of substances with their chemical structures and associated data:

Substances	Count
gallagin	111
curcumin	49
emodinone	111
quercetin	111

The table header indicates: 1,623 Substances out of 1,847 Documents containing 4,142 Reactions, 1,032 Targets. The interface also includes a search bar, a 'Name' dropdown, and buttons for 'Substances' and 'Full Screen'.