



Reaxys

2018.3.9更新

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Elsevier生命科学产品客户顾问

20180309更新主要内容

- 结构面板更新
- Query Builder更新
- 单页显示结果条数更新
- 物质结果界面更新
- 反应结果界面更新
- Synthesis Plan流程更新

Reaxys主界面细看更新内容

20180309更新内容

The screenshot shows the Reaxys homepage. At the top left is the Reaxys logo. A blue callout box labeled 'New Features' with a speech bubble icon points to the 'Synthesis planner' link in the navigation bar, which has a 'new' badge. The navigation bar also includes 'Quick search', 'Query builder', 'Results', 'History', and 'Sign in'. Below the navigation bar is a search bar with the text 'Search substances, reactions, documents and bioactivity data' and a subtext 'in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, LabNetwork and SigmaAldrich'. An 'Import' button is on the left. The search bar contains the query 'Documents, e.g. Tetrahedron, 2014, 70, 2343' and the word 'AND' below it. A dashed box highlights a button that says 'Create Structure or Reaction Drawing' with a pencil icon. The footer contains the Elsevier logo, copyright information '© 2018 RELX Intellectual Properties SA.', links for 'Terms and Conditions', 'Privacy policy', and 'Performance Page', the RELX Group logo, and a 'Feedback' button.

Reaxys New Features

Quick search Query builder Results Synthesis planner **new** History Sign in

Import

Search substances, reactions, documents and bioactivity data
in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, LabNetwork and SigmaAldrich

Q Documents, e.g. Tetrahedron, 2014, 70, 2343

AND

Create Structure or Reaction Drawing

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Feedback

结构面板更新

- 将常用功能，S*，S6，Atom Mapping移动至结构面板显着处
- 移动缩写官能团，通用官能团从下方移动至右侧

The screenshot displays the Marvin JS Structure editor interface. The title bar reads "Structure editor" and includes a "Create structure template from name" button. The main workspace contains the Marvin JS logo and the text "by ChemAxon".

Key updates to the interface are highlighted with callouts:

- Left Toolbar:** The S^{max} and S^{lock} icons are highlighted with a blue box. A callout box explains: "S max : 等同于S6" and "S Lock : 等同于S*".
- Bottom Toolbar:** The $1 \rightarrow 1$ icon is highlighted with a blue box. A callout box explains: "1->1: 等同于Atom Mapping".
- Right Panel:** The R icon is highlighted with a blue box. A callout box explains: " $[\]$: 缩写官能团输入" and "R : Reaxys通用官能团输入".

The right panel also shows a vertical list of element symbols: A, H, C, N, O, S, F, P, Cl, Br, I.

功能解析

- S Max
 - As Drawn检索时起效果
 - 使用后，检索时的意思是该位点处于完全开放状态，等同于S6
- S Lock
 - As Substructure检索时起效果
 - 使用后，在进行Substructure，该位点处于完全封闭状态，等同于S*
- 1->1
 - 手动的Atom Mapping，用于标记反应前后相同的原子
- []
 - 缩写官能团定义，可以通过该功能输入Boc，Fmoc等常见官能团
- R
 - Reaxys通用官能团定义，可以通过该功能输入ALK，ARY，HAR，G等官能团。

Query Builder更新

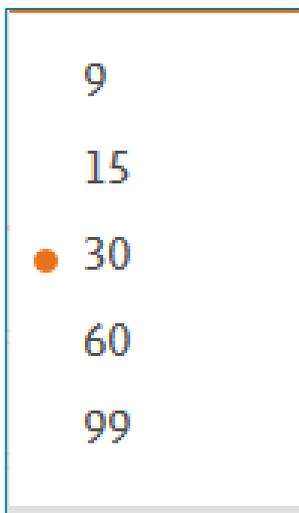
- Query Builder中可以利用2个或多个片段进行组合检索（原先只能1个）
- 如以下案例，寻找糖分子衍生物，但是在衍生物中不能出现苯环结构

Query Builder中可以同时添加多个结构片段，且可以设置这些片段的逻辑关系

The screenshot displays the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, Query builder (selected), Results, Synthesis planner, and History. Below the navigation is a search bar labeled 'Search Substances' and a set of icons for 'Import', 'Save', 'Reset form', and 'Delete all'. The main workspace contains two 'Structure' panels. The top panel shows a sugar molecule (beta-D-glucopyranose) with the text 'On all atoms' below it. The bottom panel shows a benzene ring with the text 'On all atoms' below it. A blue 'NOT' operator is positioned between the two panels. On the right side, there is a sidebar with a search bar 'Find search fields and forms' and a list of search fields including 'Basic Indexes', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'. At the bottom right, there is a 'Feedback' button.

单页结果条目数更新

- 单页结果数可以调整，默认是30条记录，更改无需登录Reaxys账号



物质结果界面更新

- 增强原有界面内容的区分度
- 新增Grid界面浏览物质

The screenshot displays the Reaxys interface with the following components:

- Header:** Reaxys logo, navigation tabs (Quick search, Query builder, Results, Synthesis planner, History), and user profile (Sam Y.).
- Filters and Analysis Panel (Left):** A sidebar with 2,405 items and various filter categories such as 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, and Patent Assignee.
- Main Content Area:** Displays 2,405 Substances out of 777 Documents, containing 2,916 Reactions, 968 Targets. It includes a search bar, selection tools (Limit To, Exclude, Export), and sorting options (Sort by No of References).
- View Selection:** A callout box labeled "Grid浏览" points to the "Grid" view selection button, which is highlighted with a blue box.
- Substance Cards:** Three substance cards are shown, each with a chemical structure, name, formula, and various data points:
 - tyrphostin AG 1478:** C16H14ClN3O2, 315.759, 7437034. Data points include Identification, Bioactivity (All), Spectra - 27, Preparations - 3, Reactions - 5, Targets - 423, and Documents - 224.
 - PD153035:** C16H14BrN3O2, 360.21, 7384032, 153436-54-5. Data points include Identification, Bioactivity (All), Spectra - 16, Preparations - 12, Reactions - 32, Targets - 156, and Documents - 170.
 - WHI-P131:** C16H13N3O3, 297.313, 8154591, 202475-60-3. Data points include Identification, Bioactivity (All), Spectra - 8, Preparations - 6, Reactions - 6, Targets - 68, and Documents - 81.

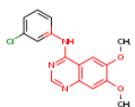
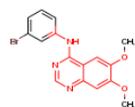
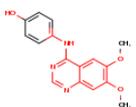
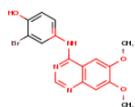
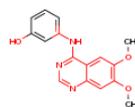
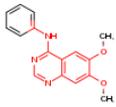
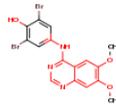
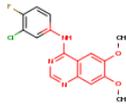
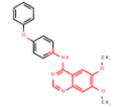
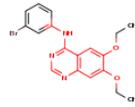
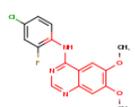
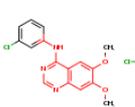
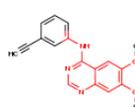
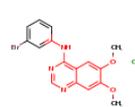
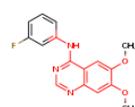
Grid浏览界面

Reaxys® Quick search Query builder Results Synthesis planner History Sam Yu   

2,405 Substances out of 777 Documents, containing 2,916 Reactions, 968 Targets Reaxys - 2,405 

0 selected  Limit To  Exclude  Export

  Sort by No of References  **List**  Heatmap 

 1	 2	 3	 4	 5
 6	 7	 8	 9	 10
 11	 12	 13	 14	 15

[Feedback](#) 

Grid页面物质界面详解

WHI-P131 ×

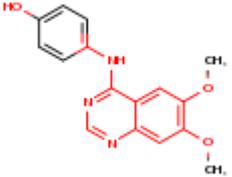
C₁₆H₁₅N₃O₃ 297.313 8154591 202475-60-3

Identification	Physical Data - 3	Preparations - 6
Druglikeness	Spectra - 8	Reactions - 6
Bioactivity (All)	Other Data - 169	Targets - 68
		Documents - 81

View Details >

物质信息概览，无需点击Detail即可查看物质包含信息条数和基本信息，如CAS No，理化性质，谱图，反应，文献数量，如要看具体内容，可点击Detail

3
🔍
📄
☰



🛒
🔗
📄

Options ×

- > Find Similar
- > View related Markush

- > Copy structure to query
- > Use as filter
- > Open in database

放大功能看大结构

物质商业信息

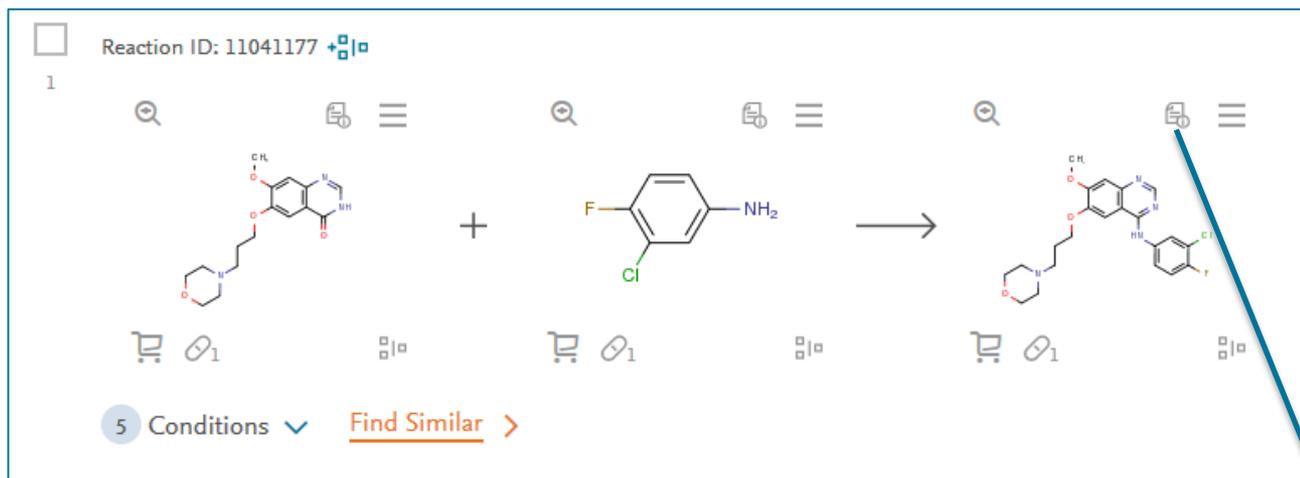
类药性性质

物质合成计划

物质结果的其他选项

反应界面更新

- 反应中的每个物质界面和Grid物质界面相同，可直接查看基本信息



界面呈现形式和Grid物质界面相同，对于每一个物质，可以直接查看基本信息，如物质的分子式，分子量，CAS No，是否有谱图，理化性质等

gefitinib			CAS Number	×
C ₂₂ H ₂₄ ClFN ₄ O ₃	446.909	8949523	184475-35-2	
Identification	Physical Data - 67	Preparations - 65		
Druglikeness	Spectra - 52	Reactions - 101		
Bioactivity (All)	Other Data - 2,552	Targets - 1,040		
		Documents - 3,757		
				View Details >

Synthesis Plan 流程更新

- 手动流程更新
 - 可以直接从反应结果集中添加反应到Synthesis Plan
 - 从Synthesis Plan中继续扩展反应，可以看到条件

126 Reactions out of 49 Documents containing 112 Substances, 1,046 Targets

2 selected Limit To Exclude Export **Syn-Plan**

Reaction ID: 11041177

Reaction ID: 36604056

Step1 :
从反应结果集中
选择反应

Step2 :
利用这两条反应创建
Synthesis Plan

创建好的Synthesis Plan

继续通过反应结果集添加反应

Synthesize

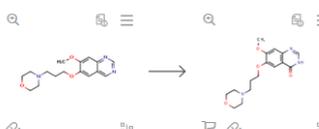
- > Manually
- > Autoplan

33 Reactions out of 18 Documents containing 37 Substances, 0 Targets

2 selected Limit To Exclude Export Syn-Plan

Reaction ID: 29122977

1



2 Conditions Find Similar >

Yield	Conditions	References
87%	Stage #1: 7-methoxy-6-[3'-N-morpholino]propoxyquinazoline With ammonium cerium (IV) nitrate; acetic acid In water Stage #2: With sodium hydroxide In water	Marzaro, Giovanni; Guiotto, Adriano; Pastorini, Giovanni; Chilin, Adriana - Tetrahedron, 2010, vol. 66, # 4, p. 902 - 908 Full Text Cited 21 times Details > Abstract >
85%	With peracetic acid; sulfuric acid In ethanol at 60°C; for 12h;	Jin, Jian-Wen; Zhang, Lin; Meng, Guang-Rong; Zhu, Jian-Hua; Zhang, Qian - Synthetic Communications, 2014, vol. 44, # 3, p. 346 - 351 Full Text Cited 1 times Details > Abstract >

Show Less ^

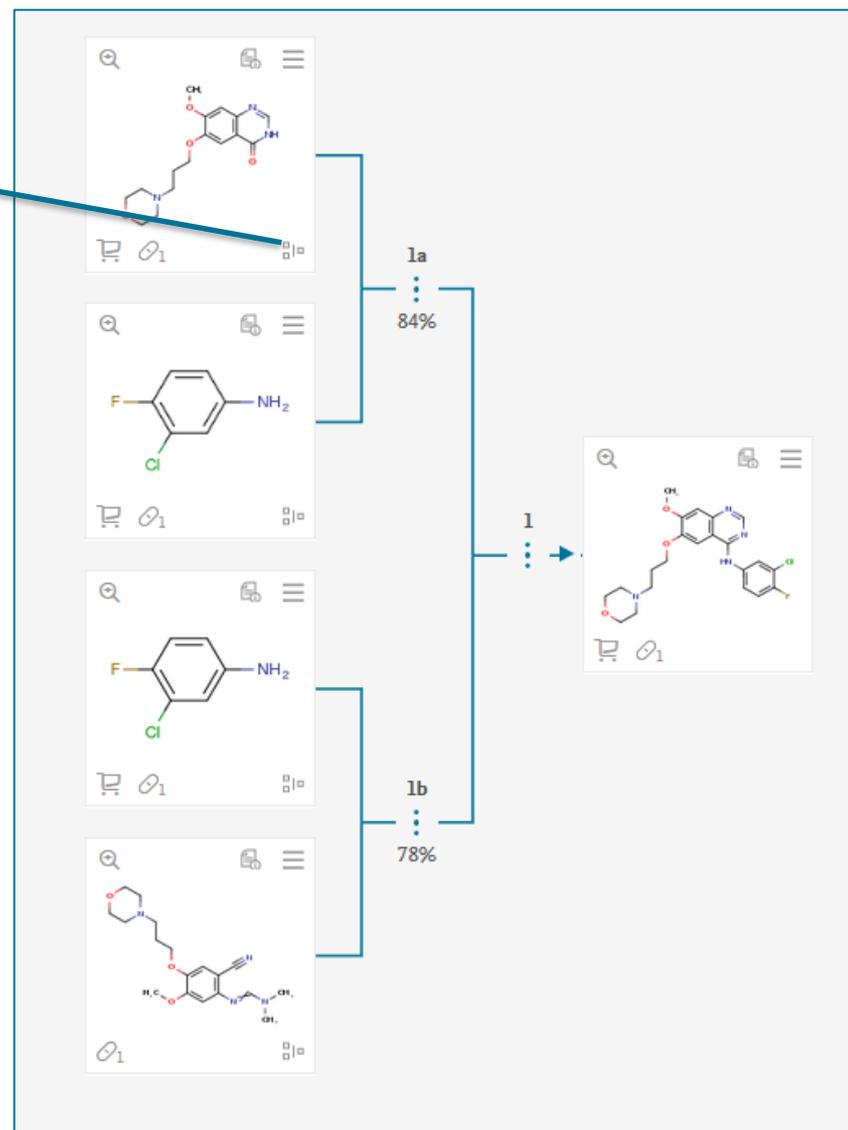
Reaction ID: 43264370

2

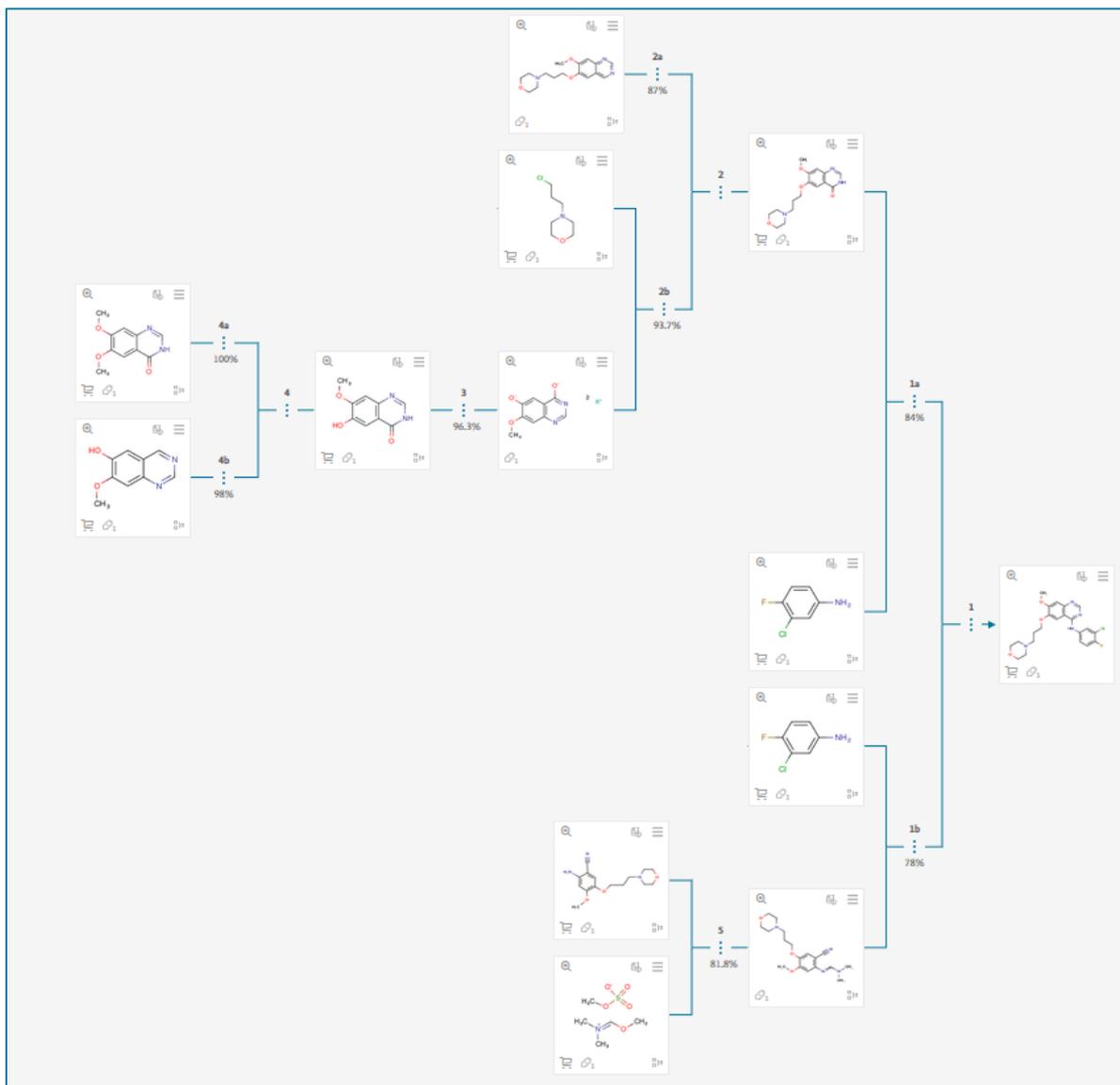


1 Conditions Find Similar >

Yield	Conditions	References
93.7%	With 1-butyl-3-methylimidazolium Tetrafluoroborate In N,N-dimethylformamide at 55 - 60°C; for 5h;	Jiaxing University; Zhang, Yang; Wu, Jiani; Mou, Chengping; Xu, Yongping - CN103910689, 2016, B Location in patent: Paragraph 0041



最后的结果



可以将Synthesis Plan继续导出

**If you have questions feel
free to reach out**

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