



Reaxys系列之

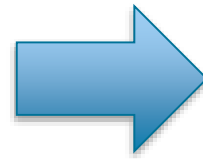
事实型实验数据的运用与物质检索

提纲

- 常见的与物质物质检索有关的困难案例
- Reaxys中的解决方案
 - Reaxys中的Query Builder检索模式
 - Reaxys中的困难案例解决方案
 - Reaxys中的更多与性质检索有关技巧
- Reaxys物质检索小结

Case Study 1: “特定溶剂”下物质溶解度的查询

- 检索要求：
 - 如何快速获得物质的溶解度
 - 氯化钾在乙醇中的，20 °C，25 °C，30 °C 下的溶解度

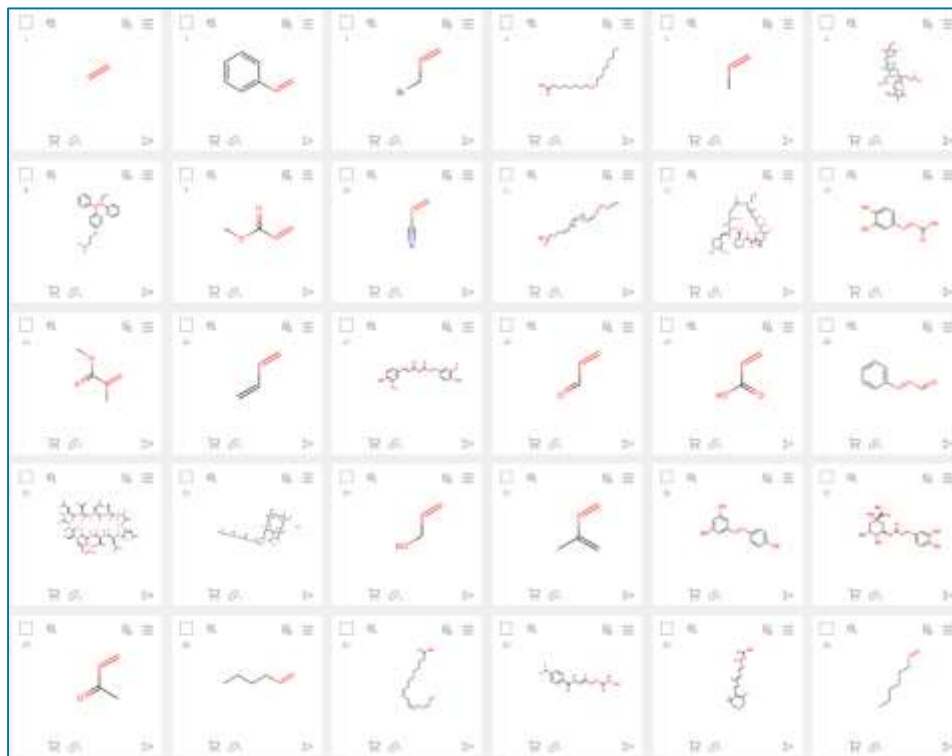


H₂O

Ethanol

Case Study 2: 具备“特殊性能”的物质检索

- 检索要求
 - 乙烯衍生物，不能成环
 - 具备机械性能报道，尤其是涉及“弹性性能”报道的化合物



Case Study 3: “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，或者含镧系金属的催化剂

Chemoselectivity

Stereoselective

Regioselectivity

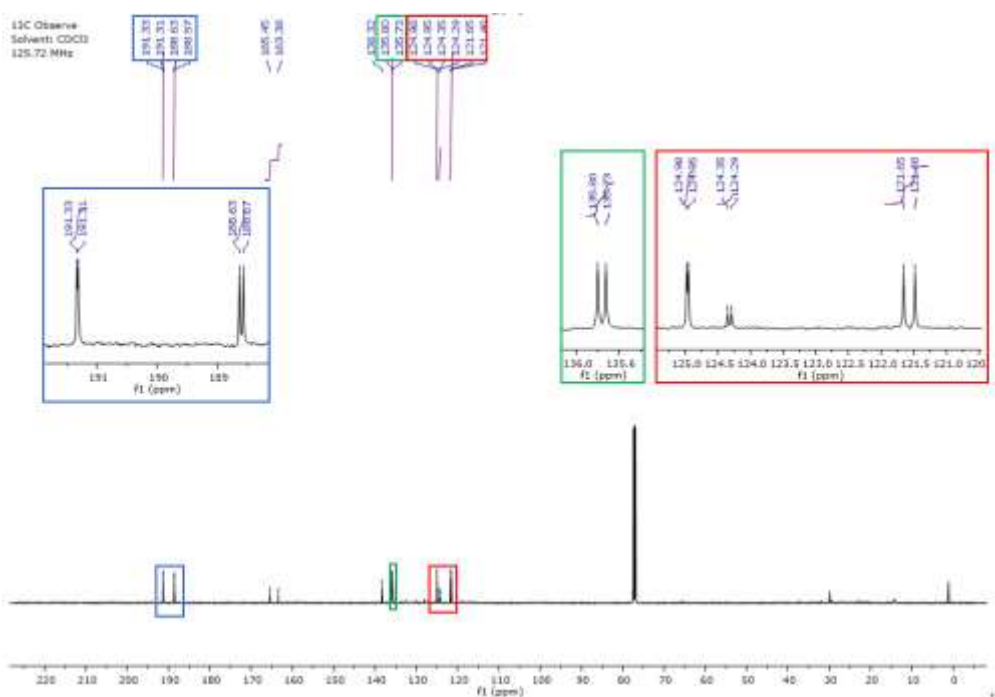
Fe

A periodic table of elements with columns numbered 1 to 18. The lanthanide series (La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) is circled in red. The lanthanide series is shown below the main table, starting from element 57 (La) to 71 (Lu).

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H																	2 He
2 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6 Cs	56 Ba	57-71 La-Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7 Fr	88 Ra	89-103 Ac-Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
			57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
			89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Case Study 4: 如何利用数据进行化合物解谱

- 常见的情况
 - 知道是天然产物
 - 分子量348.456
 - 从谱图上可以看到一些明显的片段结构
 - 有多组谱图的数据



提纲

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Reaxys的界面

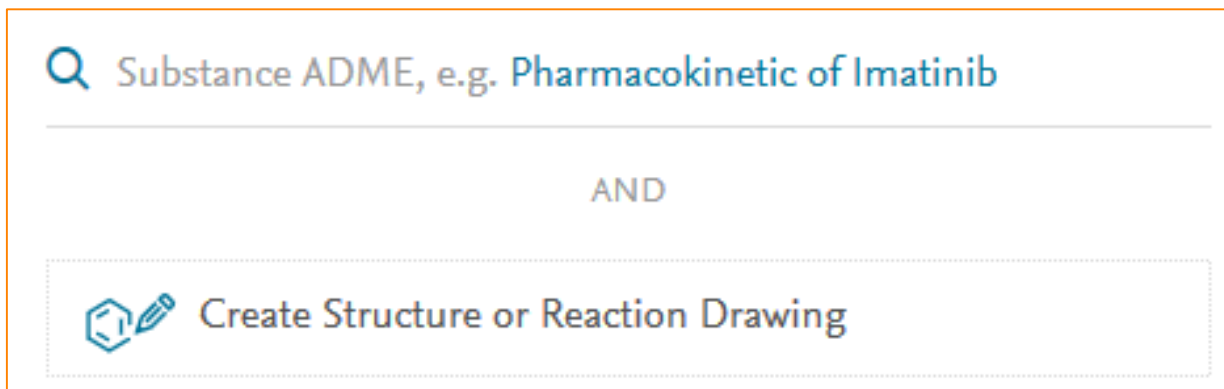
- www.reaxys.com

Quick Search

Query Builder


The screenshot displays the Reaxys website interface. At the top left is the Reaxys logo. The navigation bar includes 'Quick search' (highlighted), 'Query builder' (highlighted), 'Results', 'Synthesis planner', and 'History'. On the right side of the navigation bar, there is a user profile 'Sam Yu' and icons for a person, a bell, and a question mark. Below the navigation bar is a search area with the text 'Search substances, reactions, documents and bioactivity data' and a subtext 'in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, LabNetwork and SigmaAldrich'. There is an 'Import' button with a download icon. The main search area contains a search bar with the text 'Reactions, e.g. phosphorylation'. Below the search bar is an 'AND' operator. At the bottom of the search area is a dashed box containing a pencil icon and the text 'Create Structure or Reaction Drawing'.

Reaxys的检索方式—Quick Search



Q Substance ADME, e.g. Pharmacokinetic of Imatinib

AND

 Create Structure or Reaction Drawing

Quick Search中可以使用的的方式：

1. 物质名称, Gefitinib
2. 反应名称, Wittig Reaction
3. 物质理化性质, Solubility of Gefitinib
4. 物质的谱图, NMR of Gefitinib
5. 分子式, C₂₂H₂₄ClFN₄O₃
6. 反应类型, Substitution
7. 关键词, Immunology Oncology
8. 反应结构, 物质结构

Reaxys的检索方式—Query Builder

Reaxys[®] Quick search Query builder Results Synthesis planner History Sign in ?

Search > ▾

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

Find search fields and forms 🔍

Fields Forms History

Reaxys ^

- Basic Indexes ▾
- Identification ▾
- Physical Properties ▾
- Spectra ▾
- MedChem ▾
- Other ▾
- Reactions ▾
- Bibliography ▾

Drag & Drop to build a new query

Query Builder模块下，Fields中可以选择不同类型的字段进行自由组合检索

Reaxys中的字段检索

Tips:

Reaxys提供8种不同的分类，每种分类中拥有和这种分类相关的多种字段，可以依据这些字段自由组合进行检索

Basic Indexes		^
◇	Substance Basic Index	☰ ⋮
◇	Reaction Basic Index	⋮
◇	Document Basic Index	⋮

Identification		^
◇	Chemical Name	☰ ⋮
◇	Element Symbols	☰ ⋮
◇	Molecular Formula	☰ ⋮
◇	Molecular Weight	☰ ⋮
◇	Preferred CAS Registry Number	⋮
◇	CAS Registry Number	☰ ⋮
◇	Bioactivity Presence	⋮
◇	Catalyst Investigation	⋮
◇	Charge	☰ ⋮
◇	Chemical Name Segment	☰ ⋮
◇	Derivative	⋮
◇	Druglikeness	⋮
◇	Element Counts	☰ ⋮

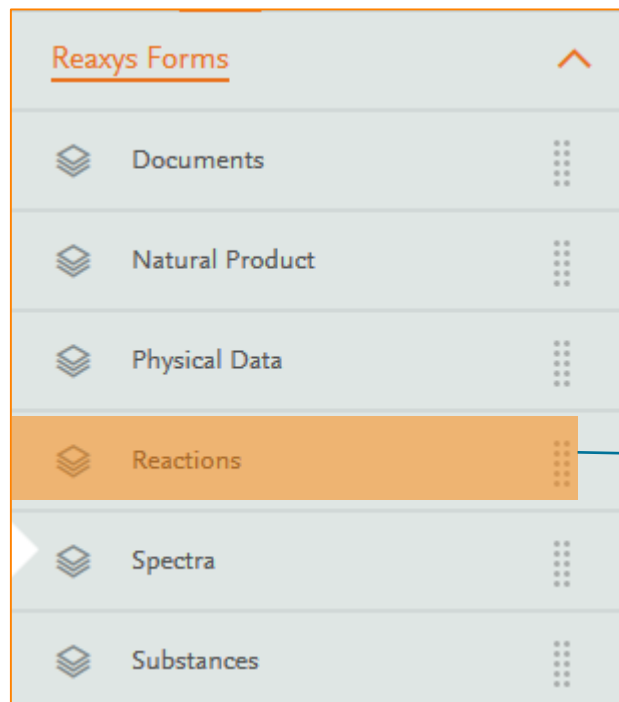
Physical Properties		^
◇	Melting Point	⋮
◇	Boiling Point	⋮
◇	Sublimation	⋮
◇	Refractive Index	⋮
◇	Density	⋮
◇	Adsorption	⋮
◇	Association	⋮
◇	Autoignition	⋮
◇	Azeotropes	⋮
◇	Boundary Surface Phenomena	⋮
◇	Chromatographic Data	⋮
◇	Bulk Viscosity	⋮
◇	Circular Dichroism	⋮

Reaxys检索方式—Query Builder Forms

The screenshot displays the Reaxys Query Builder interface. At the top, the Reaxys logo is on the left, and navigation tabs for 'Quick search', 'Query builder' (which is underlined), 'Results', 'Synthesis planner', and 'History' are in the center. On the far right, there are 'Sign in' and a help icon. Below the navigation, a toolbar contains icons for 'Import', 'Save', 'Reset forms', and 'Delete all'. To the right of these are icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'. A search bar with a dropdown arrow is also present. The main workspace is a large grey area with a diagonal grid pattern and the text 'Drag & Drop to build a new query'. On the right side, there is a sidebar with a search bar labeled 'Find search fields and forms'. Below this, there are two tabs: 'Fields' and 'Forms' (which is highlighted with an orange border). Under the 'Forms' tab, there are two items: 'Reaxys Forms' and 'Reaxys MedChem Forms', each with a downward arrow.

Query Builder模块下，Forms中Reaxys和RMC的预设模块检索

Reaxys Form中的预设模块



A screenshot of the Reactions form in Reaxys. The form is titled "Reactions" and contains several sections, each with a dropdown menu and a search field. The sections are: Structure (with a "Create Structure / Reaction Drawing" button), Yield (with a dropdown set to "Yield"), Solvent (with a dropdown set to "Solvent"), Reagent/Catalyst (with a dropdown set to "Reagent/Catalyst"), Time (Reaction Details) (with a dropdown set to "Time (Reaction Details)"), Temperature (Reaction Details) (with a dropdown set to "Temperature (Reaction Details)"), Pressure (Reaction Details), Torr (with a dropdown set to "Pressure (Reaction Details), Torr"), and Reaction Type (with a dropdown set to "Reaction Type"). Each section is separated by an "AND" connector.

反应结构

反应收率

反应溶剂

试剂催化剂

反应时间

反应温度

反应压力

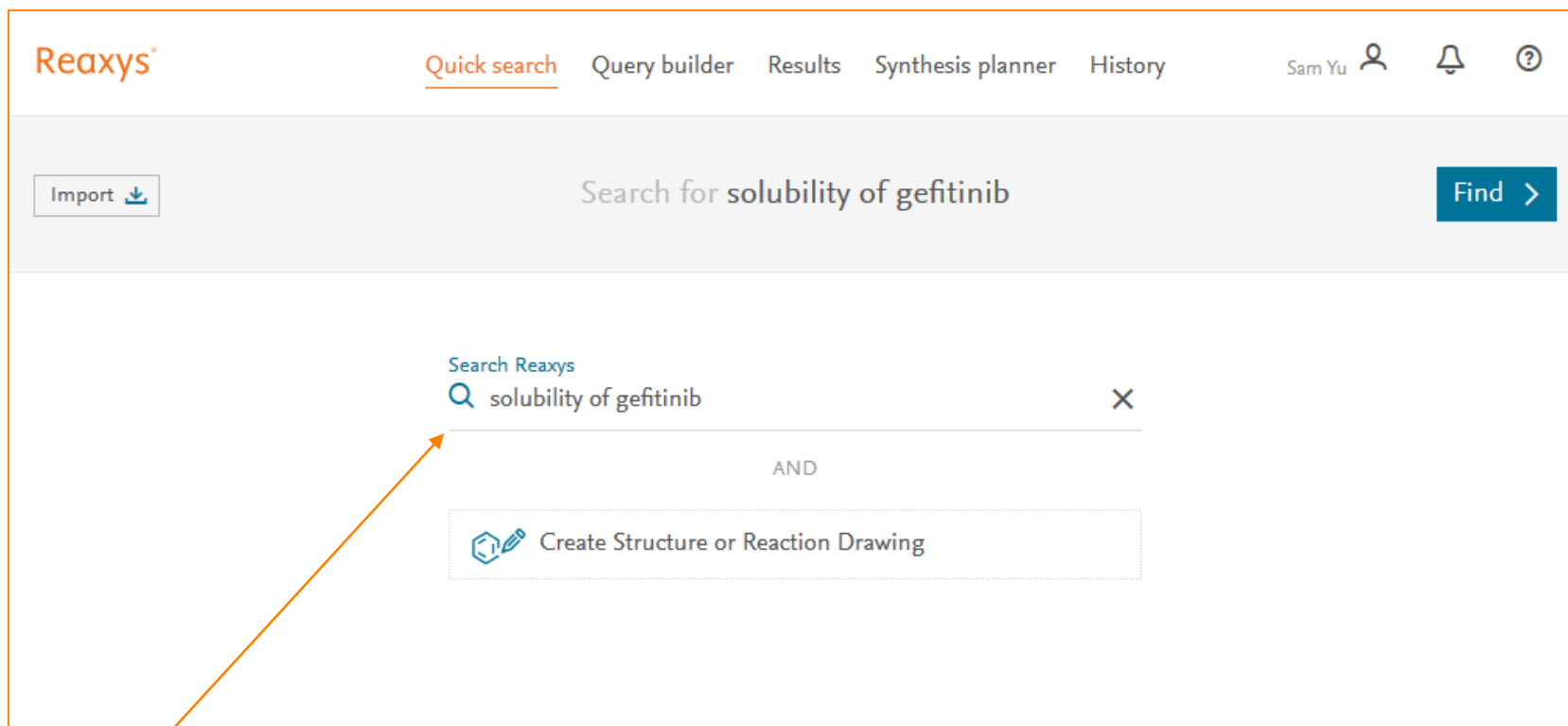
反应类型

提纲

- 常见的与物质物质检索有关的困难案例
- Reaxys中的解决方案
 - Reaxys中的Query Builder检索模式
 - Reaxys中的困难案例解决方案
 - Reaxys中的更多与性质检索有关技巧
- Reaxys物质检索小结

Case Study 1: 快速获得物质的理化性质

- 快速的案例
- 检索具体化合物的溶解性数据（Gefitinib）



The screenshot displays the Reaxys web interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History' are in the center. On the right, there is a user profile for 'Sam Yu' and notification icons. Below the navigation bar, there is a search bar with the text 'Search for solubility of gefitinib' and a 'Find >' button. An 'Import' button is also visible on the left. Below the search bar, a search input field contains the text 'solubility of gefitinib'. Below this field, the word 'AND' is displayed. At the bottom of the search area, there is a button labeled 'Create Structure or Reaction Drawing' with a pencil icon. An orange arrow points from the bottom left towards the search input field.

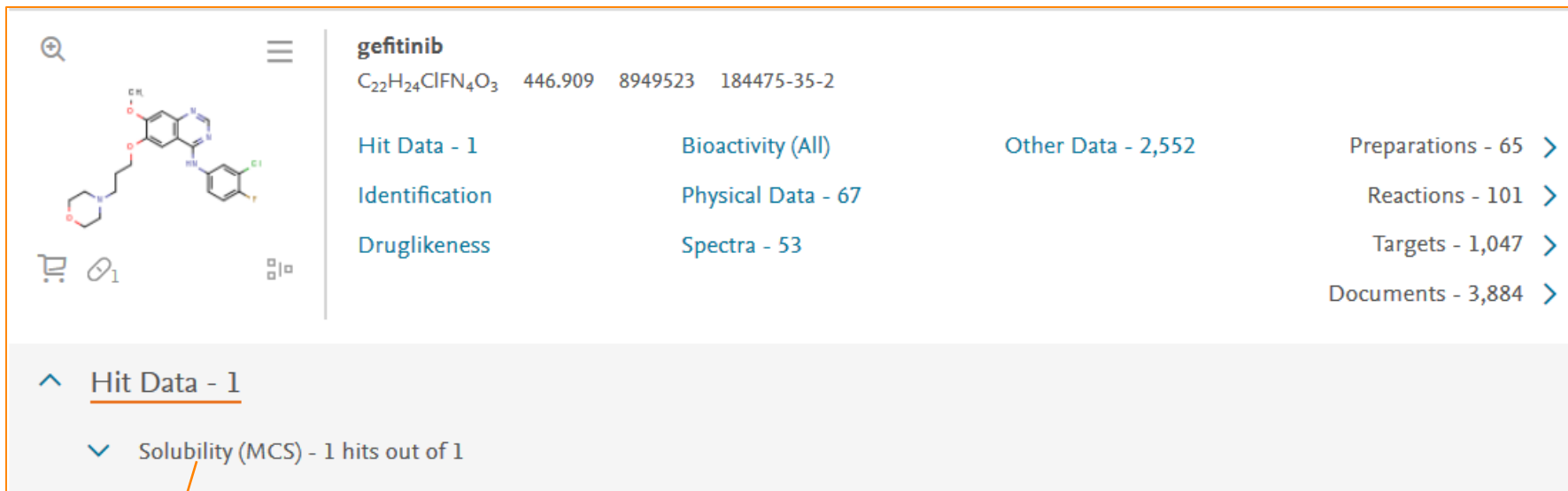
直接用自然语言在输入，solubility of gefitinib，检索

Reaxys直接给出结果

The screenshot shows the Reaxys search results page. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The user 'Sam Yu' is logged in. The search results are for 'solubility of gefitinib'. The first result is highlighted with a purple icon and a 'View Results' button circled in orange.

Icon	Count	Category	Search Criteria	Actions
	1	Substances	Structure : as drawn AND Property : solubility	Preview Results View Results >
	110	Documents	Titles, Abstracts, Keywords : solubility, gefitinib	Preview Results View Results >
	301,491	Documents	Titles, Abstracts, Keywords : solubility	Preview Results View Results >
	20,075	Documents	Titles, Abstracts, Keywords : gefitinib	Preview Results View Results >

最后的结果



gefitinib
C₂₂H₂₄ClFN₄O₃ 446.909 8949523 184475-35-2

Hit Data - 1 Bioactivity (All) Other Data - 2,552 Preparations - 65 >

Identification Physical Data - 67 Reactions - 101 >

Druglikeness Spectra - 53 Targets - 1,047 >

Documents - 3,884 >

^ Hit Data - 1

▼ Solubility (MCS) - 1 hits out of 1

^ Solubility (MCS) - 1 hits out of 1 Show/Hide columns ▼

Solubility, g·l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Reference
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 16 times ↗ Details > Abstract >

Hit Data直接给出具体的实验数据，以及检测条件和全文链接

Reaxys中的物质理化性质

gefitinib
 $C_{22}H_{24}ClFN_4O_3$ 446.909 8949523 184475-35-2

Hit Data - 1
 Identification
 Druglikeness

Bioactivity (All)
 Physical Data - 67
 Spectra - 53

Other Data - 2,552
 Preparations - 65 >
 Reactions - 101 >
 Targets - 1,047 >
 Documents - 3,884 >

Physical Data - 67

- ✓ Melting Point - 21
- ✓ Association (MCS) - 1
- ✓ Chromatographic Data - 4
- ✓ Conformation - 1
- ✓ Crystal Phase - 7
- ✓ Crystal Property Description - 14
- ✓ Crystal System - 1
- ✓ Dissociation Exponent - 2
- ✓ Further Information - 1
- ✓ Interatomic Distances and Angles - 2

Colour & Other Properties	Location	Reference
white	Paragraph 0037	CSPC Zhongqi Pharmaceutical Technology(Shijiazhuang)Corporation Limited; CSPC Ouyi Pharmaceutical Co., Ltd; Zhang, Yanqiao; Li, Xiaofang; Sun, Wentao; Zhang, Sujuan; Geng, Jia - CN103319422, 2016, B Full Text Details Abstract No author - CN106854184, 2017, A Full Text Details Abstract
white	Paragraph 0037; 0047	No author - CN106854185, 2017, A Full Text Details Abstract
white	Paragraph 0065	Chongqing Laimel Longyu Pharmaceutical Co., Ltd.; Wen Huiying; Ren Sixiao; Xu Xiaofang; Tang Qunlian; Yang Shengxi - CN107098863, 2017, A Full Text Details Abstract
white	Paragraph 0015	Zhengzhou University The First Affiliated Hospital; Cheng Weiyang; Zhang Xiaojian; Tian Xin - CN106432202, 2017, A Full Text Details Abstract
yellow	supporting information	Kang, Sung Kwon; Lee, Seung Wook; Woo, Daekoo; Sim, Jaehoon; Suh, Young-Ger - Synthetic Communications, 2017, vol. 47, # 21, p. 1990 - 1998 Full Text Details Abstract
white	Paragraph 0126; 0133	shanghai tianci shengwu gu Biological Engineering Co., Ltd.; Li, Han Pu; Li, Jianzhi; Liu, Hai; Hu, Xu Hua; Zheng, Xiaoli; Sun, Li; Xie, Lin - CN105218476, 2016, A Full Text Details Abstract

Reaxys中的谱图

gefitinib
 $C_{22}H_{24}ClFN_4O_3$ 446.909 8949523 184475-35-2

Hit Data - 1
 Identification
 Druglikeness

Bioactivity (All)
 Physical Data - 67
 Spectra - 53

Other

Spectra - 53

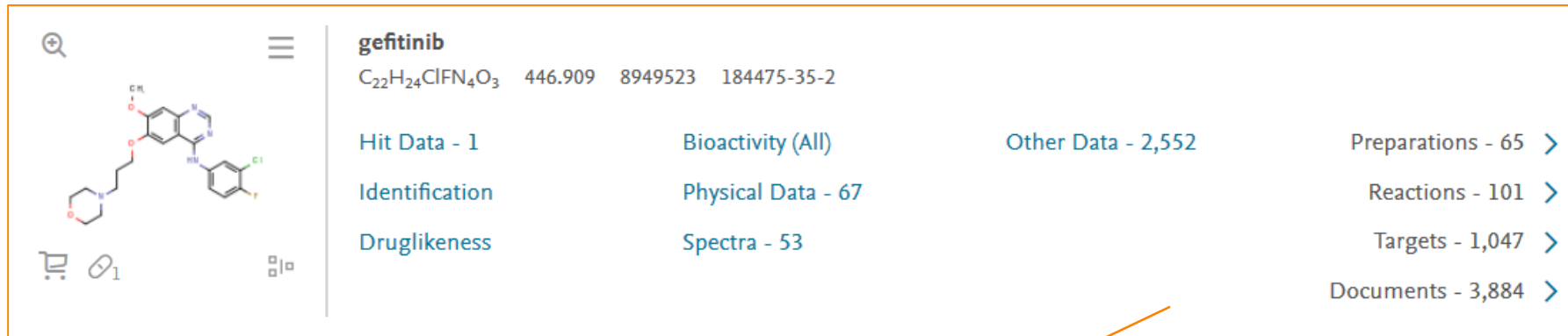
- NMR Spectroscopy - 31
- IR Spectroscopy - 6
- Mass Spectrometry - 11
- UV/VIS Spectroscopy - 4
- Raman Spectroscopy - 1

Tips:

Reaxys直接摘录原文中的NMR谱图描述，并提供原文中的位置

<p>¹H NMR (400 MHz, d₆-DMSO) 0 9.44 (5, 1H), 8.50 (5, 1H), 8.12 (dd, J = 6.9, 2.7 Hz, 1H), 7.80 (m, 2H), 7.44 (t, 1H), 7.20 (5, 1H), 4.18 (t, J = 6.7 Hz, 2H), 3.94 (5, 3H), 3.59 (t, J = 4.4 Hz, 4H), 2.49 (t, J = 6.9 Hz, 2H), 2.41 (bs, 4H), 2.00 (m, 2H).</p>	Paragraph 0035	<p>SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou - WO2015/188318, 2015, A1</p> <p>Full Text ↗ Show details ></p>
<p>¹³C NMR (100 MHz, d₆-DMSO) 0 156.48, 154.94, 153.57 (J = 241 Hz), 153.05, 148.74, 147.43, 137.33 (J = 3 Hz), 123.91, 122.77 (J = 7 Hz), 119.19 (J = 19 Hz), 116.90 (J = 21 Hz), 109.26, 107.72, 103.14, 67.59, 66.43, 56.31, 55.35, 53.73, 26.13.</p>	Paragraph 0035	<p>SCINOPHARM (CHANGSHU) PHARMACEUTICALS, LTD.; ZHANG, Xiao-heng; LV, Xizhou - WO2015/188318, 2015, A1</p> <p>Full Text ↗ Show details ></p>

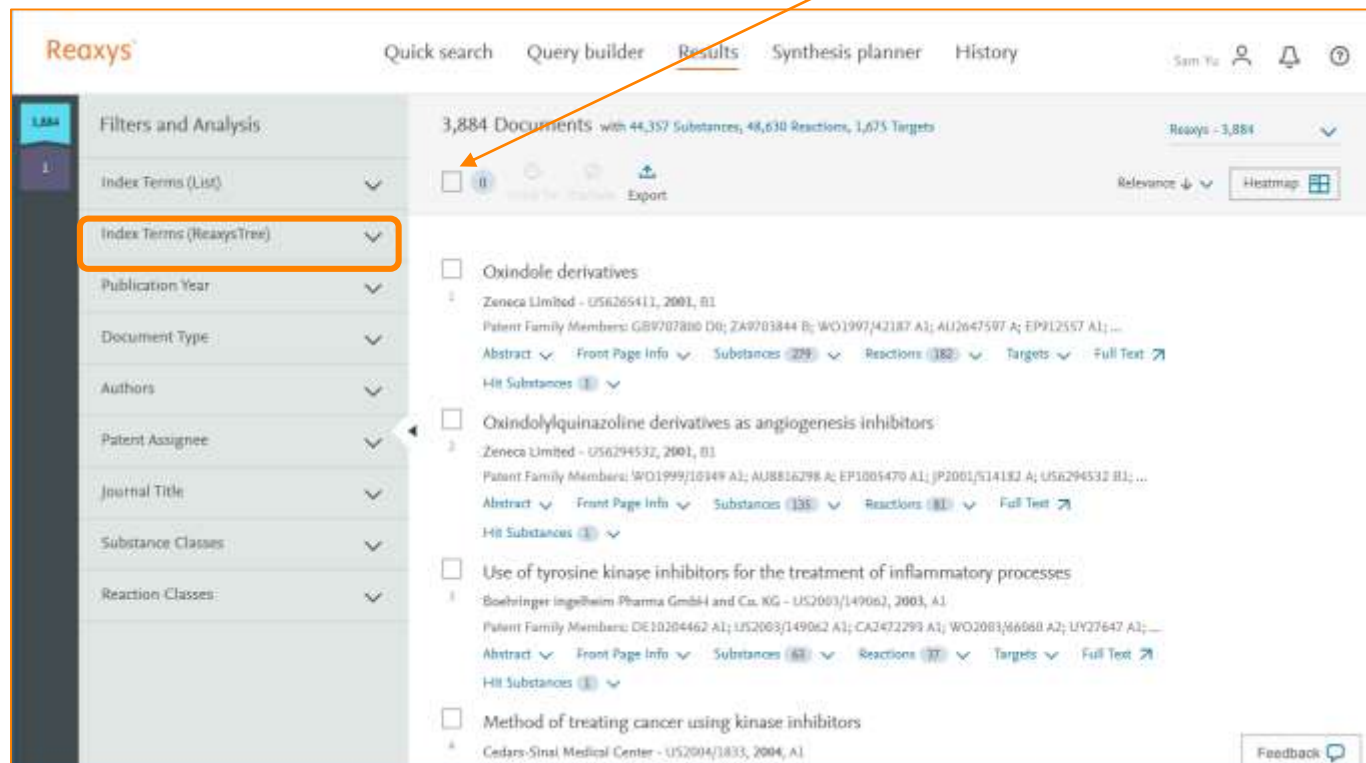
Reaxys中的分析文献的获取



The screenshot shows the Reaxys search results for the query "gefatinib". On the left, there is a chemical structure of gefitinib and a shopping cart icon. The main content area displays the search results for "gefatinib" with the molecular formula $C_{22}H_{24}ClFN_4O_3$ and CAS numbers 446.909, 8949523, and 184475-35-2. Below the search results, there are several categories and their corresponding counts: Hit Data - 1, Identification, Druglikeness, Bioactivity (All), Physical Data - 67, Spectra - 53, Other Data - 2,552, Preparations - 65, Reactions - 101, Targets - 1,047, and Documents - 3,884. An orange arrow points from the "Documents - 3,884" link to the "3,884 Documents" link in the screenshot below.

Tips:

获得文献后，
可以通过
Reaxys的文
献过滤工具
对文献进行
后处理



The screenshot shows the Reaxys search results page for "gefatinib". The top navigation bar includes "Quick search", "Query builder", "Results", "Synthesis planner", and "History". The search results are displayed as a list of documents. The "Index Terms (ReaxysTree)" filter is highlighted with an orange box. The search results show 3,884 Documents with 44,357 Substances, 48,630 Reactions, and 1,675 Targets. The results are sorted by Relevance. The first three results are:

- Oxindole derivatives
Zeneca Limited - US6265411, 2001, B1
Patent Family Members: GB9707800 D0; ZA9703844 B; WO199742187 A1; AU2647507 A; EP912557 A1; ...
Abstract Front Page Info Substances (29) Reactions (182) Targets Full Text
Hit Substances
- Oxindolyquinazoline derivatives as angiogenesis inhibitors
Zeneca Limited - US6294532, 2001, B1
Patent Family Members: WO199910149 A1; AU8816298 A; EP1005470 A1; JP2001514182 A; US6294532 B1; ...
Abstract Front Page Info Substances (135) Reactions (81) Full Text
Hit Substances
- Use of tyrosine kinase inhibitors for the treatment of inflammatory processes
Boehringer Ingelheim Pharma GmbH and Co. KG - US2003149062, 2003, A1
Patent Family Members: DE10204462 A1; US2003149062 A1; CA2422293 A1; WO200306698 A2; UY27647 A1; ...
Abstract Front Page Info Substances (63) Reactions (37) Targets Full Text
Hit Substances

The "Index Terms (ReaxysTree)" filter is highlighted with an orange box. The search results show 3,884 Documents with 44,357 Substances, 48,630 Reactions, and 1,675 Targets. The results are sorted by Relevance. The first three results are:

Index Term Reaxys Tree的应用

Reaxys通过Index Term Reaxys Tree的方式，将文献进行精确分类，帮助大家快速定位所需分析文献。

Index Terms (List) ∨

Index Terms (ReaxysTree) ∧

- physico chemical properties 1,065
- chemical transformations 1,042
- physico chemical analysis methods 350
- quantum chemical calculation methods

+ More

Index Terms (ReaxysTree) ×

- Index Terms (ReaxysTree) 3,004
 - physico chemical properties 1,129
 - chemical transformations 1,105
 - 物理化学分析方法** 374
 - quantum chemical calculation methods 31

Clear selected × Limit To > Exclude >

物理化学分析方法中的细节性分类

Index Terms (ReaxysTree)			
✓	Index Terms (ReaxysTree)	<input type="checkbox"/>	3,345
>	physico chemical properties	<input type="checkbox"/>	1,306
>	chemical transformations	<input type="checkbox"/>	1,290
✓	physico chemical analysis methods	<input type="checkbox"/>	431
>	spectroscopical analysis	<input type="checkbox"/>	206
>	separation method	<input type="checkbox"/>	188
>	microscopy	<input type="checkbox"/>	86
>	quantitative analysis	<input type="checkbox"/>	22
>	elemental analysis	<input type="checkbox"/>	21
>	crystal structure determination	<input type="checkbox"/>	17
>	thermal analysis	<input type="checkbox"/>	16
>	electro analytical method	<input type="checkbox"/>	3

Clear selected ×

Limit To > Exclude >

谱图分析方法下面的细节分类

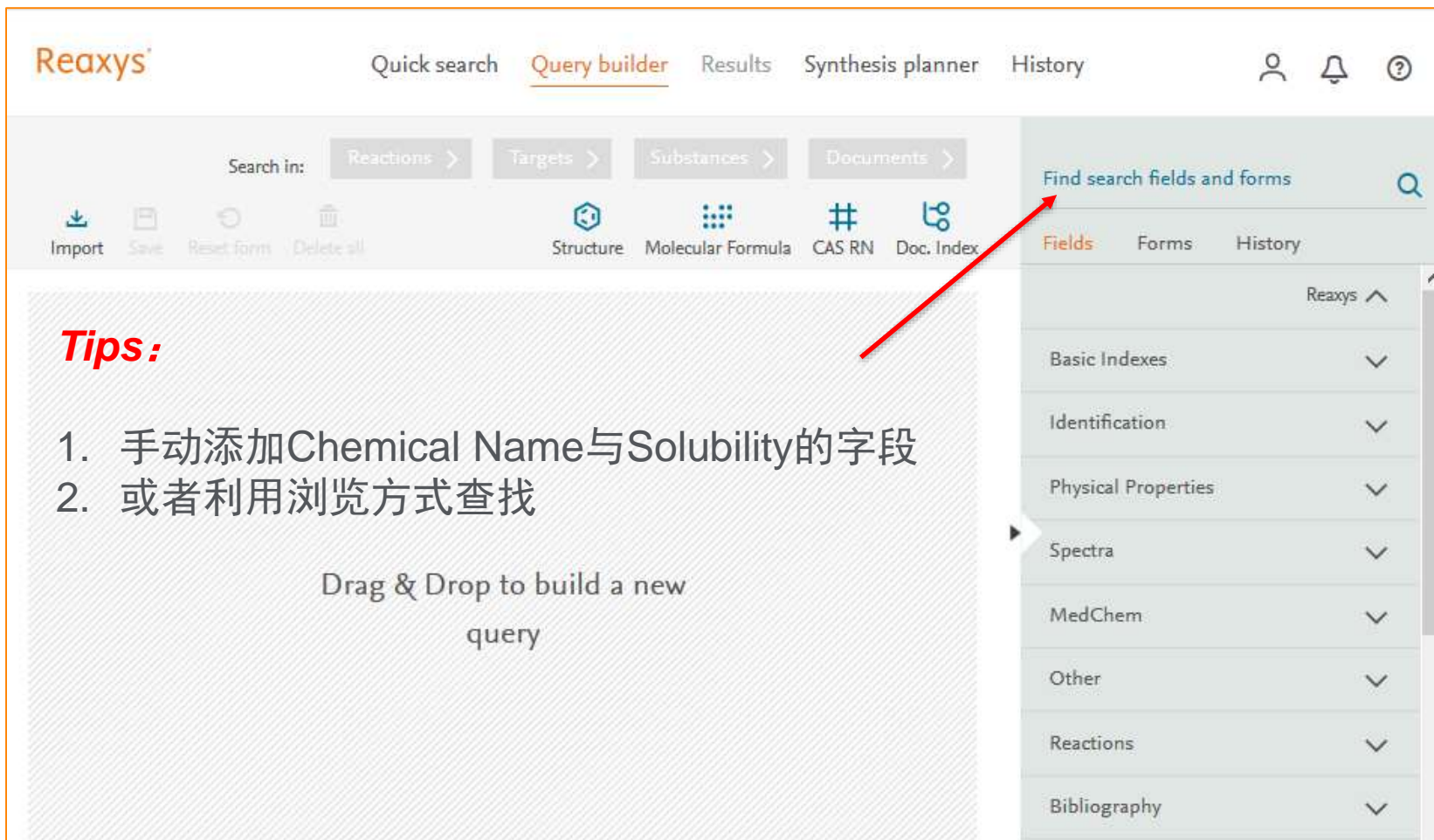
Index Terms (ReaxysTree) ×

✓ <input type="checkbox"/> physico chemical analysis methods		<input type="checkbox"/>	431
✓ <input checked="" type="checkbox"/> spectroscopical analysis	谱图分析方法	<input type="checkbox"/>	206
> <input type="checkbox"/> luminescence spectroscopy		<input type="checkbox"/>	70
> <input type="checkbox"/> fluorescence spectroscopy		<input type="checkbox"/>	62
> <input checked="" type="checkbox"/> mass spectrometry	Mass	<input type="checkbox"/>	39
✓ <input checked="" type="checkbox"/> NMR spectroscopy	NMR	<input type="checkbox"/>	23
✓ <input type="checkbox"/> NMR spectroscopy type		<input type="checkbox"/>	17
> <input checked="" type="checkbox"/> ¹³ C-NMR spectroscopy	¹³ C NMR	<input type="checkbox"/>	3
> <input type="checkbox"/> 2D-nuclear magnetic resonance		<input type="checkbox"/>	2
> <input checked="" type="checkbox"/> ¹⁵ N NMR spectroscopy	¹⁵ N NMR	<input type="checkbox"/>	1
> <input type="checkbox"/> ¹⁹ F NMR spectroscopy		<input type="checkbox"/>	1
<input type="checkbox"/> ¹ H-NMR spectroscopy		<input type="checkbox"/>	13

Clear selected × Limit To > Exclude >

案例的衍生：理化性质的高级应用

- 检索检索氯化钾在乙醇中的溶解度



Reaxys Quick search Query builder Results Synthesis planner History

Search in: Reactions > Targets > Substances > Documents >

Find search fields and forms

Fields Forms History

Reaxys ^

Basic Indexes v

Identification v

Physical Properties v

Spectra v

MedChem v

Other v

Reactions v

Bibliography v

Tips:

1. 手动添加Chemical Name与Solubility的字段
2. 或者利用浏览方式查找

Drag & Drop to build a new query

利用Query Builder创建检索式

- Reaxys中的检索策略

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. On the right, there are buttons for Register and Sign in. Below the navigation, there is a search bar with 'Substances' selected. A sidebar on the right lists search fields and forms, including Reaxys, Basic Indexes, Identification, Physical Properties, Spectra, MedChem, Other, Reactions, and Bibliography. The main area shows a query builder with two sections: 'Solubility' and 'Chemical Name'. The 'Solubility' section has a dropdown menu with options: Solubility, g·l⁻¹; Saturation; Temperature (Solubility (MCS)), °C; Solvent (Solubility (MCS)) ethanol; and Ratio of Solvents. The 'Chemical Name' section has a dropdown menu with the option: Chemical Name potassium chloride. Red arrows point to the 'Solvent (Solubility (MCS)) ethanol' and 'Chemical Name potassium chloride' options. A text box on the left explains that the solvent is entered in the Solubility field and the substance name is entered in the Chemical Name field.

Solubility字段中输入溶剂，Chemical Name中输入物质名称即可

Reaxys直接给出结果

1 Substances out of 7,118 Documents, containing 4,141 Reactions, 60 Targets Reaxys - 1

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

1

1

1

potassium chloride
CIK 74.5513 3534978

Hit Data - 20 Bioactivity (All) Other Data - 784 Preparations - 414 >

Identification Physical Data - 2,972 Reactions - 4,141 >

Druglikeness Spectra - 182 Targets - 60 >

Documents - 7,118 >

Hit Data - 20

Solubility (MCS) - 20 hits out of 429 Show/Hide columns

Solubility, g·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 Chemistry, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 4 times Details Abstract
	25	ethanol	Solubility: 0.025 mol/kg solvent	El-Dossoki - [Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 4 times Details Abstract
	30	ethanol	Solubility: 0.037 mol/kg solvent	El-Dossoki - [Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 4 times Details Abstract
	35	ethanol	Solubility: 0.043 mol/kg solvent	El-Dossoki - [Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 4 times Details Abstract

Case Study 2: 具备“特殊性能”的物质检索

- 检索要求

- 乙烯衍生物，不能成环
- 具备“机械性能”报道的化合物
- 按照以下的标签顺序进行“理化性质”反推的检索
- “弹性性能”在案例衍生中解决

The screenshot displays the Reaxys Query builder interface. The top navigation bar includes 'Quick search', 'Query builder' (highlighted with a red box and labeled '1'), 'Results', 'Synthesis planner', and 'History'. Below the navigation bar, there are search filters for 'Reactions', 'Targets', 'Substances', and 'Documents'. A search input field is labeled 'Search in:'. On the left side, there are icons for 'Import', 'Save', 'Reset form', and 'Delete all'. On the right side, there is a 'Find search fields and forms' dropdown menu with options: 'Fields' (highlighted with a red box and labeled '2'), 'Forms', and 'History'. The 'Fields' dropdown is expanded, showing a list of search categories: 'Basic Indexes', 'Identification', 'Physical Properties' (highlighted with a red box and labeled '3'), 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'. The main area of the interface contains the text 'Drag & Drop to build a new query'.

Reaxys的理化性质列表

The image shows a screenshot of the Reaxys interface displaying a list of physical properties. The 'Mechanical Properties' option is highlighted with an orange border.

Physical Properties (Expanded)

- Melting Point
- Boiling Point
- Sublimation
- Refractive Index
- Density
- Adsorption
- Association
- Autoignition
- Critical Temperature
- Critical Volume
- Crystal Phase
- Crystal Property Description
- Crystal System
- Decomposition
- Dielectric Constant
- Dissociation Energy
- Dissociation Exponent

Electrochemical & Energy Data (Expanded)

- Electrical Moment
- Electrical Polarizability
- Electrochemical Behaviour
- Electrochemical Characteristics
- Electrochemistry Data
- Electrolytic Conductivity
- Electron Binding
- Energy Barriers
- Energy Data

Mechanical & Physical Properties (Expanded)

- Liquid/Vapour Systems
- Magnetic Data
- Magnetic Susceptibility
- Mechanical & Physical Properties
- Mechanical Properties**
- Molecular Deformation
- Mutarotation
- Optical Data
- Optical Rotatory Dispersion

添加“机械属性”列表与结构属性

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 these are search filters for 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar includes 'Import', 'Save', 'Reset form', and 'Delete all' buttons, along with icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'. The main query area shows two conditions: 'Mechanical Properties' and 'Structure', connected by an 'AND' operator. The 'Mechanical Properties' condition has a 'Find any' button highlighted with an orange box. An orange arrow points from this button to the 'Structure' condition's input field, which contains the text 'Create Structure / Reaction Drawing'. On the right side, a sidebar titled 'Find search fields and forms' lists various fields such as 'Ionization Potential', 'Isoelectric Point pH', 'Kinematic Viscosity', 'Liquid Phase', 'Liquid/Liquid Systems', 'Liquid/Solid Systems', and 'Liquid/Vapour Systems'.

Tips:

通过Query Builder将结构和“机械属性”联合起来，点击结构添加“乙烯”

结构的绘制

The screenshot displays the Reaxys software interface for structure editing. At the top, navigation options include 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The main workspace shows the chemical structure of ethylene ($\text{H}_2\text{C}=\text{CH}_2$) drawn in the center. To the right, a search configuration panel is visible, with several options highlighted by orange boxes: 'As substructure', 'On all atoms', and 'Additional ring closure'. The 'Additional ring closure' option is currently unchecked.

Tips:

亚结构检索确保是乙烯衍生物，Additional Ring Closure去掉确保不成环。

最后的检索式

The screenshot displays the Reaxys Query Builder interface. At the top, the navigation bar includes "Quick search", "Query builder" (which is underlined), "Results", "Synthesis planner", and "History". On the right side of the navigation bar are icons for a user profile, a notification bell, and a help icon.

Below the navigation bar, the "Search in:" section contains four dropdown menus: "Reactions", "Targets", "Substances" (which is highlighted with an orange box), and "Documents". Below these are icons for "Structure", "Molecular Formula", "CAS RN", and "Doc. Index".

The main search area shows a query builder with two conditions:

- Condition 1: "Mechanical Properties" with a "Find any" checkbox and a "Show fields" dropdown.
- Condition 2: "Structure" with a chemical structure of ethylene ($\text{H}_2\text{C}=\text{CH}_2$) drawn in a dashed box. Below the structure is a button labeled "As drawn".

The conditions are connected by an "AND" operator. On the right side, a sidebar titled "Find search fields and forms" contains a search bar and a list of search fields under the "Fields" tab:

- Reaxys (expanded)
- Basic Indexes
- Identification
- Physical Properties (expanded)
- Melting Point
- Boiling Point
- Sublimation
- Refractive Index
- Density

最后的结果—乙烯的数据

ethene
H₂CCH₂ 28.0538 1730731 74-85-1

Hit Data - 12 Bioactivity (All) Other Data - 121 Preparations - 4,591 >

Identification Physical Data - 2,344 Reactions - 20,397 >

Druglikeness Spectra - 266 Documents - 30,028 >

Hit Data - 12

Mechanical Properties - 12 hits out of 12

不同文献中报道的关于“乙烯”的“机械属性”

Mechanical Properties - 12 hits out of 12		
Description (Mechanical Properties)	Comment (Mechanical Properties)	Reference
Elastic properties	弹性属性	Maksimkin, Aleksey; Kaloshkin, Sergey; Zadorozhnyy, Mikhail; Tcherdyntsev, Victor - [Journal of Alloys and Compounds, 2014, vol. 586, # SUPPL 1, p. S214-S217] Full Text ↗ Cited 15 times ↗ Details > Abstract >
Virial coefficients of the equation of state	状态方程 维里系数	Sweet; Steele - [Journal of Chemical Physics, 1967, vol. 47, p. 3029,3033] Full Text ↗ Details > Gainar et al. - [Berichte der Bunsen-Gesellschaft, 1973, vol. 77, p. 372,373, 375] Full Text ↗ Details > Orcutt - [Journal of Chemical Physics, 1963, vol. 39, p. 605] Full Text ↗ Cited 33 times ↗ Details > Das Gupta et al. - [Journal of Chemical Physics, 1973, vol. 59, p. 1999] Full Text ↗ Cited 14 times ↗ Details >

最后的结果—衍生物的数据



styrene
CH₂CH(C₆H₅) 104.152 1071236 292638-84-7

Hit Data - 5 Bioactivity (All) Other Data - 289 Preparations - 1,662 >

Identification Physical Data - 876 Reactions - 30,403 >

Druglikeness Spectra - 253 Targets - 8 >

Documents - 25,350 >

Hit Data - 5

▼ **Mechanical Properties - 5 hits out of 5**

涉及到“苯乙烯”的摩尔体积，可压缩性，维里系数，粘性方面的报道

Description (Mechanical Properties)	Reference
Molar volume	<p>Berberi; Decroocq - [Journal de Chimie Physique et de Physico-Chimie Biologique, 1974, vol. 71, p. 673,678] Full Text ↗ Details ></p> <p>Miller et al. - [Journal of Chemical and Engineering Data, 1975, vol. 20, p. 417,418, 419] Full Text ↗ Details ></p> <p>Ghosal, Saswati; Samoc, Marek; Prasad, Paras N.; Tufariello, Joseph J. - [Journal of Physical Chemistry, 1990, vol. 94, # 7, p. 2847 - 2851] Full Text ↗ Cited 101 times ↗ Details > Abstract ></p> <p>Hayduk, Walter; Minhas, Bhupender S. - [Journal of Chemical & Engineering Data, 1987, vol. 32, # 3, p. 285 - 290] Full Text ↗ Details > Abstract ></p>
Virial coefficients of the equation of state	<p>Balashova, I. M.; Mokrushina, L. V.; Morachevskii, A. G. - [J. Appl. Chem. USSR (Engl. Transl.), 1989, vol. 62, # 12, p. 2744 - 2750,2546 - 2551] Full Text ↗ Details > Abstract ></p>
PVT Relationship	<p>Sasuga et al. - [Journal of Physical Chemistry, 1979, vol. 83, p. 3290] Full Text ↗ Cited 6 times ↗ Details ></p>
Compressibility	<p>Yakusheva et al. - [Russian Journal of Physical Chemistry, 1977, vol. 51, p. 973] [p. 1657] Full Text ↗ Details ></p>
Viscosity	<p>Olaj - [Monatshefte fuer Chemie, 1971, vol. 102, p. 648] Full Text ↗ Cited 3 times ↗ Details ></p>

案例衍生—如果特指与“弹性”有关的性能报道

- 对于以下的检索，该如何修改

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. On the right, there are icons for user profile, notifications, and help. Below the navigation, there are search filters: Reactions, Targets, Substances, and Documents. A search bar contains the text "Search in:". Below the search bar, there are icons for Import, Save, Reset form, and Delete all. In the center, there are icons for Structure, Molecular Formula, CAS RN, and Doc. Index. On the right side, there is a sidebar with the text "Find search fields and forms" and a search icon. Below this, there are tabs for Fields, Forms, and History. The main search area shows two criteria: "Mechanical Properties" with a "Find any" checkbox and a "Show fields" dropdown menu (highlighted with an orange box), and "Structure" with a chemical structure of ethene ($\text{H}_2\text{C}=\text{CH}_2$) and an "As drawn" label. The sidebar on the right lists various search fields: Reaxys, Basic Indexes, Identification, Physical Properties, Melting Point, Boiling Point, Sublimation, Refractive Index, and Density.

修改检索条件

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 these are search filters: Reactions, Targets, Substances, and Documents. A toolbar includes icons for Import, Save, Reset form, and Delete all, along with icons for Structure, Molecular Formula, CAS RN, and Doc. Index. The main search area shows two conditions:

- Mechanical Properties**: A dropdown menu is set to "contains" and the search term is "elastic".
- Structure**: A chemical structure of ethene (H2C=CH2) is shown in a dashed box.

An orange arrow points from the Chinese text below to the "contains" dropdown menu in the Mechanical Properties condition.

On the right side, there is a sidebar titled "Find search fields and forms" with a search icon. It lists various search fields and forms, including Basic Indexes, Identification, Physical Properties, Melting Point, Boiling Point, Sublimation, Refractive Index, Density, and Adsorption.


注意修改成Contains, 并添加为“弹性”词条。

最后的结果

111 Substances out of 53,348 Documents, containing 25,663 Reactions, 275 Targets Reaxys - 111

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

1



ethene
H₂CCH₂ 28.0538 1730731 74-85-1

Hit Data - 1 Bioactivity (All) Other Data - 121 Preparations - 4,591 >

Identification Physical Data - 2,344 Reactions - 20,397 >

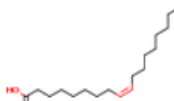
Druglikeness Spectra - 266 Documents - 30,028 >

Hit Data - 1

▼ Mechanical Properties - 1 hits out of 12

Description (Mechanical Properties)	Reference
Elastic properties	Maksimkin, Aleksey; Kaloshkin, Sergey; Zadorozhnyy, Mikhail; Tcherdy S214-S217]
	Full Text > Cited 15 times > Details > Abstract >

2



cis-Octadecenoic acid
C₈H₁₇CHCH(CH₂)₇COOH 282.467 17265

Hit Data - 1 Bioactivity (All) Other Data - 1,028 Preparations - 134 >

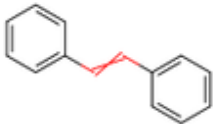
Identification Druglikeness

Hit Data - 1

▼ Mechanical Properties - 1 hits out of 6

Description (Mechanical Properties)	Reference
Elasticity constants	Bazaron et al. - [Sov. Phys. Dokl. (Engl. Transl.), 1973, vol. 17, p. 1324,769]
	Full Text > Details >
	Bazaron et al. - [Sov. Phys. Dokl. (Engl. Transl.), 1973, vol. 17, p. 1325,997]
	Full Text > Details >
	Bazaron et al. - [Sov. Phys. Dokl. (Engl. Transl.), 1965, vol. 10, p. 799,134]
	Full Text > Details >

其中一个化合物—理化性质



stilbene
 $C_6H_5CH=CHC_6H_5$ 180.249 1904445 588-59-0

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)

Physical Data - 157

Spectra - 139

Other Data - 56

Preparations - 638 >

Reactions - 1,022 >

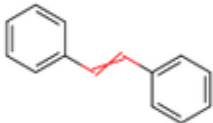
Documents - 1,588 >

^ Physical Data - 157

- ✓ Melting Point - 38
- ✓ Boiling Point - 8
- ✓ Density - 1
- ✓ Adsorption (MCS) - 1
- ✓ Association (MCS) - 15
- ✓ Chromatographic Data - 3
- ✓ Conformation - 1
- ✓ Crystal Phase - 1
- ✓ Crystal Property Description - 7
- ✓ Decomposition - 1

Colour & Other Properties	Location	Reference
colourless		Potier, Jonathan; Manuel, Stephane; Rousseau, Jolanta; Tumkevicius, Sigitas; Hapiot, Frederic; Monflier, Eric - [Applied Catalysis A: General, 2014, vol. 479, p. 1 - 8] Full Text Cited 11 times Details Abstract >
yellow		Kireenko, Marina M.; Zaitsev, Kirill V.; Oprunenko, Yuri F.; Churakov, Andrei V.; Tafeenko, Viktor A.; Karlov, Sergey S.; Zaitseva, Galina S. - [Dalton Transactions, 2013, vol. 42, # 22, p. 7901 - 7912] Full Text Cited 18 times Details Abstract >
white	supporting information	Yang, Fu-Lai; Ma, Xian-Tao; Tian, Shi-Kai - [Chemistry - A European Journal, 2012, vol. 18, # 6, p. 1582 - 1585] Full Text Cited 92 times Details Abstract >
white		Ren, Gerui; Cui, Xiuling; Yang, Erbing; Yang, Fan; Wu, Yangjie - [Tetrahedron, 2010, vol. 66, # 23, p. 4022 - 4028] Full Text Cited 48 times Details Abstract >
		Lu, Jian-Mei; Ma, Hui; Li, Sha-Sha; Ma, Dan; Shao, Li-Xiong - [Tetrahedron, 2010, vol. 66, # 27-28, p. 5185 - 5189] Full Text Cited 32 times Details Abstract >
		Tang, Yi-Qiang; Chu, Chun-Yan; Zhu, Lei; Qian, Bin; Shao, Li-Xiong - [Tetrahedron, 2011, vol. 67, # 49, p. 9479 - 9483] Full Text Cited 28 times Details Abstract >

其中一个化合物—理化性质



stilbene
 $C_6H_5CH=CHC_6H_5$ 180.249 1904445 588-59-0

Hit Data - 1 Bioactivity (All) Other Data -

Identification Physical Data - 157

Druglikeness Spectra - 139

^ Spectra - 139

- ∨ [NMR Spectroscopy - 67](#)
- ∨ [IR Spectroscopy - 8](#)
- ∨ [Mass Spectrometry - 17](#)
- ∨ [UV/VIS Spectroscopy - 17](#)
- ∨ [ESR Spectroscopy - 2](#)

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Coupling Nuclei	Solvents (NMR Spectroscopy)	Temperature (NMR Spectroscopy), °C	Frequency (NMR Spectroscopy), MHz	Original Text (NMR Spectroscopy)	Location	Comment (NMR Spectroscopy)	Signals, ppm	Kind of signal	Reference
shifts, Spectrum						MHz, CDCl ₃) δ: 7.12 (s, 2H), 7.27 (t, J = 7.4 Hz, 2H), 7.37 (t, J = 7.4 Hz, 4H), 7.53 (dd, J = 1.4 and 8.4 Hz, 3H)	information				- [Tetrahedron, 2017, vol. 73, # 27-28, p. Full Text ↗ Details > Abstract :
Chemical shifts, Spectrum	¹³ C		chloroform-d1		125	¹³ C NMR (125 MHz, CDCl ₃) δ: 127.4, 128.5, 129.5, 138.22	supporting information		127.4, 128.5, 129.5, 138.22		Tanaka, Chihiro; Nakamura, Kimiaki; Ni; - [Tetrahedron, 2017, vol. 73, # 27-28, p. Full Text ↗ Details > Abstract :

Case Study 3: “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

The screenshot displays the Reaxys Query Builder interface. At the top, the 'Query builder' tab is selected and highlighted with a red box and the number '1'. Below this, the 'Search in:' section shows 'Substances' selected, with 'Molecular Formula' also highlighted by a red box and the number '4'. The main search area contains two criteria: 'Catalyst Investigation' and 'Molecular Formula'. The 'Molecular Formula' criterion is set to 'is' and has a search field containing 'Molecular Formula'. On the right side, a 'Find search fields and forms' panel shows 'catalyst' entered in the search box, highlighted with a red box and the number '2'. Below this, 'Catalyst Investigation' is selected in the list, highlighted with a red box and the number '3'. The interface also includes navigation buttons like 'Import', 'Save', 'Reset form', and 'Delete all', and a 'Feedback' button at the bottom right.

Tips:

- Query Builder是Reaxys中的组合检索模式，该模式可以自由组合检索条件，实现数据，结构，Key Word的联合检索
- 按照1，2，3，4的步骤，添加检索条件
- 通过分子式和催化研究模块进行组合检索

条件的逐渐添加—Catalyst Investigation

◇ Catalyst Investigation Find any Show fields ▾ ×

◇ Catalyst Investigation Find any Hide fields ▲ ×

- is ▾ Investigated characteristic(s) 🔍
- is ▾ Specification of catalysis 🔍
- is ▾ Classification of catalysis 🔍
- is ▾ Type of reaction 🔍
- is ▾ Co-catalyst/co-substrate 🔍

逐渐添加Catalyst Investigation中的参数

Specification of catalysis 1 🔍 Search ×

<input type="checkbox"/> chemoselective catalysis	2,058	⬆️
<input type="checkbox"/> immobilised catalyst	382	⬆️
<input type="checkbox"/> phase-transfer catalysis	381	⬇️
<input type="checkbox"/> regioselective catalysis	2,074	⬇️
<input checked="" type="checkbox"/> stereoselective catalysis	7,864	⬇️

Clear selected × Transfer >

条件的逐渐添加—MF的添加

◇ Molecular Formula

is Molecular Formula

ends with

is

● contains

starts with

Molecular formula: Fe

Use this formula >

Special group:

Me Et Ph

	1A	2A	3B	4B	5B	6B	7B	8B	9B	10B	1B	2B	3A	4A	5A	6A	7A	8A
n1	H																	He
n2	Li	Be											B	C	N	O	F	Ne
n3	Na	Mg											Al	Si	P	S	Cl	Ar
n4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
n5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
n6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
n7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt									
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Nonmetals: Metalloids, Other Nonmetals, Halogens, Noble Gases

Metals: Alkali Metals, Alkaline Earth Metals, Lanthanoids, Actinoids, Transition Metals, Post Transition Metals

可以按照种类进行选择，过渡态金属，镧系金属等

完成的检索式

The screenshot displays the Reaxys Query Builder interface. At the top, there are navigation tabs: 'Quick search', 'Query builder' (which is underlined), 'Results', 'Synthesis planner', and 'History'. Below these, a 'Search in:' section has four buttons: 'Reactions >', 'Targets >', 'Substances >', and 'Documents >'. An orange arrow points from the 'Substances >' button to the right. Below the search in section, there are icons for 'Import', 'Save', 'Reset form', and 'Delete all'. To the right of these are icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'. The main area shows two query blocks. The first block is titled 'Catalyst Investigation' and has a 'Find any' checkbox. It contains five rows, each starting with 'is' and a dropdown arrow, followed by a search criterion and a magnifying glass icon. The criteria are: 'Investigated characteristic(s)', 'Specification of catalysis stereoselective catalysis', 'Classification of catalysis', 'Type of reaction', and 'Co-catalyst/co-substrate name'. Below this block is a blue 'AND' button. The second block is titled 'Molecular Formula' and contains one row starting with 'contains' and a dropdown arrow, followed by the search criterion 'Molecular Formula Fe' and a magnifying glass icon.

物质检索

最后的结果

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

269 Substances out of 15,957 Documents, containing 18,678 Reactions, 49 Targets Reaxys - 269

0 selected Limit To Exclude Export Sort by No of References

1 **iron(II) chloride**
FeCl2 126.753 8135986

Cl₂Fe

Hit Data - 8 Bioactivity (All) Other Data - 56 Preparations - 225 >
Identification Physical Data - 392 Reactions - 5,255 >
Druglikeness Spectra - 41 Targets - 22 >
Documents - 4,426 >

Hit Data - 8 ← **Hit Data是命中的关键**
Catalyst Investigation - 8 hits out of 83

2 **ferrous(II) sulfate heptahydrate**
Fe(2+)*SO4(2-)*7H2O=FeSO4*7H2O 278.018 11322534

Hit Data - 1 Bioactivity (All) Other Data - 18 Preparations - 24 >
Identification Physical Data - 191 Reactions - 2,442 >
Druglikeness Spectra - 29 Targets - 1 >
Documents - 2,454 >

Hit Data - 1
Catalyst Investigation - 1 hits out of 19

其中一个化合物中的命中记录

269 Substances out of 15,957 Documents, containing 38,678 Reactions, 49 Targets

iron(II) chloride
FeCl₂ 126.753 8135966

Cl₂Fe

Hit Data - 8

Identification
Druglikenss

Bioactivity (All)
Physical Data - 392
Spectra - 41

Other Data - 56

Preparations - 225 >
Reactions - 5,255 >
Targets - 22 >
Documents - 4,426 >

Hit Data - 8

Catalyst Investigation - 8 hits out of 88

Investigated characteristic(s)	Specification of catalyst	Type of reaction (Catalyst Investigation)	Location	Co-catalyst(s)-substrate name	References
Catalytic activity, Diastereomeric excess	Stereoselective catalysis	Cross-coupling reaction			Hoffmayer, Maximilian S.; Harmann, Jeffrey M.; Cahiez, Gérard; Knöchel, Paul. (Synlett, 2018, vol. 29, # 1, p. 65 - 70) Full Text > Details > Abstract >
Catalytic activity	Stereoselective catalysis	Silylation			Xu, Rui; Cai, Chun. (Catalysis Communications, 2018, vol. 107, p. 5 - 8) Full Text > Details > Abstract >
Catalytic activity	Stereoselective catalysis	Silylation	supporting information		Lu, Shenglin; Tian, Tian; Xu, Rui; Li, Zhiping. (Tetrahedron Letters, 2018, vol. 59, # 26, p. 2604 - 2606) Full Text > Details > Abstract >
Catalytic activity, Enantiomeric excess	Stereoselective catalysis			4,6'-bis(3)-4-isopropylazocin-2-yl]-2,2'-bipyridine	Jélu, Angèle; Rogier, Noémie; Ollivier, Thierry. (European Journal of Organic Chemistry, 2017, vol. 2017, # 12, p. 1628 - 1637) Full Text > Cited 5 times > Details > Abstract >
Catalytic activity	Stereoselective catalysis, Regioselective catalysis				Linga, Hugo; Vibert, François; Mouysset, Dominique; Sirl, Didier; Bertrand, Michèle R.; Ferry, Laurence. (Tetrahedron, 2017, vol. 73, # 25, p. 3415 - 3422) Full Text > Details > Abstract >

Reaxys给出结果的逻辑是，先给答案，再给出支持答案的文献出处。

Case Study 4: 如何利用数据进行化合物解谱

- 常见的情况
 - 知道是天然产物
 - 分子量348.456
 - 从谱图上可以看到一些明显的片段结构
 - 有一组NMR的数据
- 检索策略
 - Query Builder, 添加天然产物选项
 - 分子量设定为 ≥ 348 , 且 ≤ 349 , 避免一些误差
 - 有明确结构的时候, 可以同时添加结构片段, 或在后期进行筛选
 - 有谱图数据的话, 可以直接添加谱图数据 (案例衍生中涉及)
 - Reaxys中Substance Class分析结构

Query Builder检索式的创建

- 首先添加天然产物模块

The screenshot displays the Reaxys Query Builder interface. The top navigation bar includes 'Quick search', 'Query builder' (highlighted with a red box and labeled '1'), 'Results', 'Synthesis planner', and 'History'. Below the navigation bar, there are icons for 'Import', 'Save', 'Reset form', and 'Delete all'. The main search area features a 'Search Substances' button and a dropdown menu. The right sidebar contains a search bar and a list of search fields: 'Fields', 'Forms' (highlighted with a red box and labeled '2'), and 'History'. The 'Forms' section is expanded, showing 'Reaxys Forms' (highlighted with a red box and labeled '3') and 'Natural Product' (highlighted with a red box and labeled '4'). The 'Natural Product' section is further expanded, showing 'Isolation from Natural Product' (highlighted with a red box and labeled '5') and a 'Find any' checkbox (highlighted with a red box and labeled '5').

Tips:

- 按照1, 2, 3, 4, 5的步骤, 添加天然产物的检索条件
- 这种模式下检索的化合物, 一定是天然产物

Query Builder检索式的创建

- 分子量条件的添加，在1的地方输入分子量，点击两下2，可以看到3

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. The user's name, Sam Yu, and notification icons are visible in the top right. Below the navigation, there are action buttons: Import, Save, Reset form, and Delete all. A search bar labeled 'Search Substances' is present. The main workspace shows a query builder with several conditions. A red box labeled '3' highlights two conditions, both set to 'Molecular Weight = Molecular Weight'. A red box labeled '2' highlights the 'Molecular Weight' field in the search fields list on the right. A red box labeled '1' highlights the search input field in the search fields list, which contains 'Molecular Weight'. The search fields list on the right includes sources like Reaxys, PubChem, eMolecules, LabNetwork, and SigmaAldrich, each with a 'Molecular Weight' field.

条件的组合

The screenshot shows 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, there are utility icons: "Import", "Save", "Reset form", and "Delete all". On the right, there are search options: "Search Substances" (selected), "Structure", "Molecular Formula", "CAS RN", and "Doc. Index".

The main query area contains three conditions:

- Natural Product**: Isolation from Natural Product. Find any. Show fields \downarrow .
- AND** (connector)
- Group** (containing two conditions):
 - Molecular Weight**: \geq 348
 - Molecular Weight**: \leq 349

Red arrows point from the text on the left to the "Group" button and the "AND" connector. On the right, a dropdown menu is open, showing "Reactions", "Targets", "Substances" (highlighted in orange), and "Documents". A red arrow points from the "Search Substances" button to the "Substances" option in the dropdown.




检索物质

将两者拖至重叠，形成一个Group，且关系是And，输入条件一个是 ≥ 348 ，一个是 ≤ 349

Reaxys的初步检索结果

Reaxys




Quick search Query builder **Results** Synthesis planner History


Sam Yu   

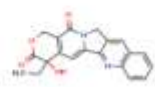
1,397 **Filters and Analysis**

1,397 Substances out of 7,052 Documents, containing 3,546 Reactions, 347 Targets

Reaxys - 1,397

0 selected    Export

Sort by No of References ↓ 

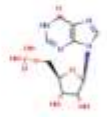
1 

camptothecin
C₂₀H₁₈N₂O₆ [348,358](#) 6075662 7689-03-4

Hit Data - 30 Bioactivity (All) Other Data - 1,813 Preparations - 236 >
Identification Physical Data - 136 Reactions - 1,207 >
Druglikeness Spectra - 147 Targets - 145 >
Documents - 4,164 >

Hit Data - 30


Isolation from Natural Product - 30 hits out of 30

2 

5'-inosine monophosphate
C₁₀H₁₂N₄O₉P [348,209](#) 630517 131-99-7

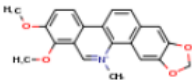
Hit Data - 3 Bioactivity (All) Other Data - 6 Preparations - 15 >
Identification Physical Data - 63 Reactions - 66 >
Druglikeness Spectra - 27 Targets - 10 >
Documents - 212 >

Hit Data - 3

Feedback 

其中的一个物质

3



🛒 1

chelerythrinium

C₂₁H₁₈NO₄ 348.378 3915260 34316-15-9

Hit Data - 23 Bioactivity (All) Other Data - 48

Identification Physical Data - 42

Druglikeness Spectra - 23

Preparations - 15 >

Reactions - 27 >

Targets - 57 >

Documents - 197 >

^
Hit Data - 23

^
Isolation from Natural Product - 23 hits out of 23

Isolation from Natural Product	Reference
roots of <i>Toddalia asiatica</i> (Linn.) Lam.; collected from Khon Kaen Province	Hirunwong, Chayanis; Sukieum, Sanwat; Phatchana, Ratchanee; Yenjai, Chavi - <i>Phytochemistry Letters</i> , 2016, vol. 17, p. 242 - 246 Full Text ↗ Cited 1 times ↗ Details > Abstract >
aerial part and roots of <i>Stylophorum lasiocarpum</i> (Oliv.) Fedde (Papaveraceae) cultivated in the Medicinal Herbs Centre of the Faculty of Medicine of Masaryk University, Brno, Czech Republic	Šebrlová, Kristýna; Peš, Ondřej; Slaninová, Iva; Vymazal, Ondřej; Kantorová, Jana; Táborská, Eva - <i>Chemical Papers</i> , 2015, vol. 69, # 5, p. 698 - 708 Full Text ↗ Cited 4 times ↗ Details > Abstract >
roots of <i>Zanthoxylum atchoum</i> ; collected by Prof. Ake Assi in Yapo (Agboville), Ivory Coast, April 2003	Akoua Yao-Kouassi, Philomne; Caron, Catherine; Ramiarantsoa, Harisololo; Prost, Ise; Harakat, Dominique; Le Magrex-Debar, Iisabeth; Gangloff, Sophie C.; Coffy, Antoine Ahibo; Zches-Hanrot, Monique - <i>Comptes Rendus Chimie</i> , 2015, vol. 18, # 8, p. 891 - 897 Full Text ↗ Cited 2 times ↗ Details > Abstract >
extract of <i>Chelidonium herba</i> ; was deposited at the Institute of Pharmaceutical Biology, University of Bonn	Orland; Knapp; König; Ulrich-Merzenich; KnöB - <i>Phytomedicine</i> , 2014, vol. 21, # 12, p. 1587 - 1596 Full Text ↗ Cited 2 times ↗ Details > Abstract >

取自泰国坤敬府，飞龙掌血的根部

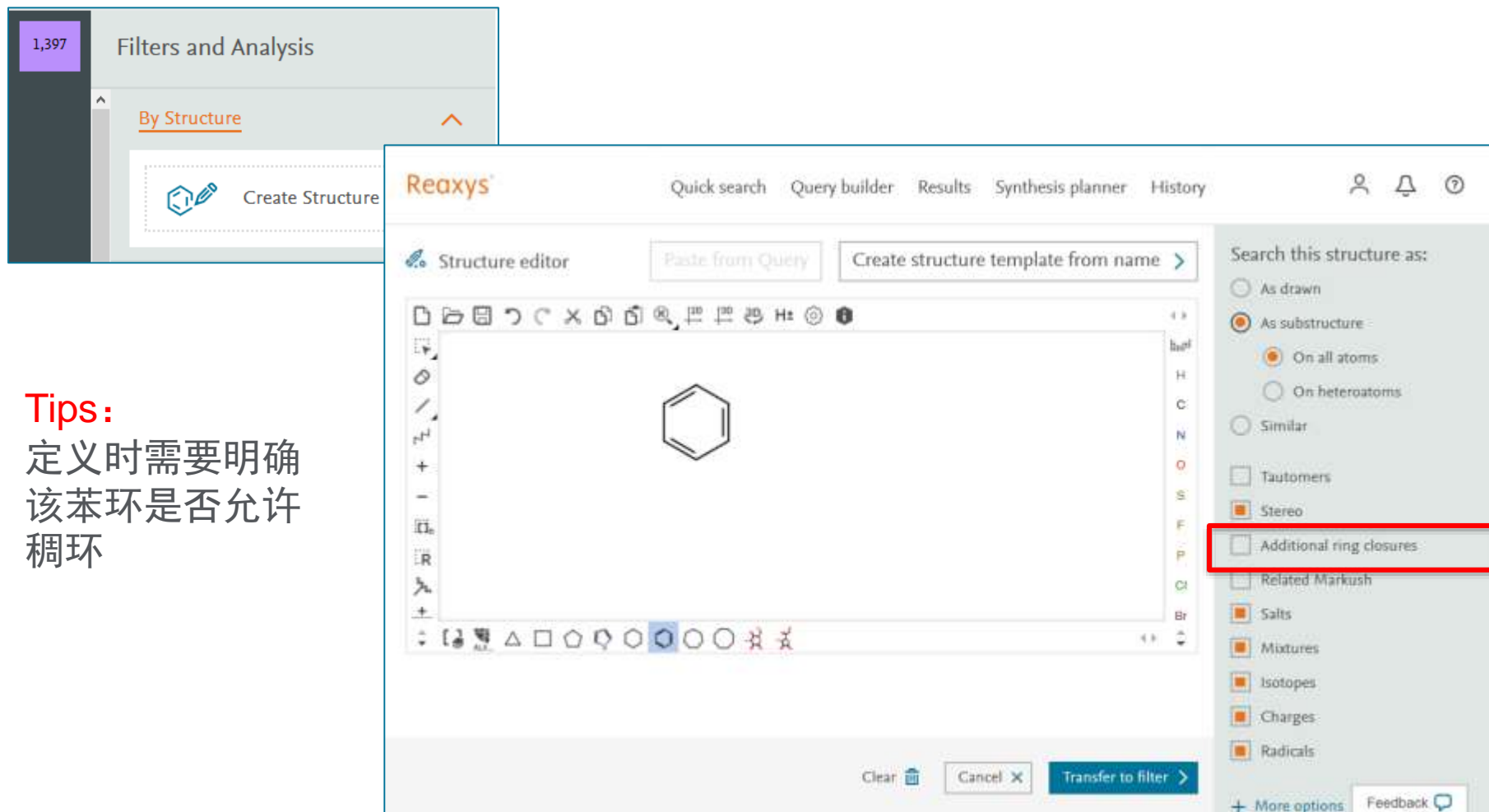
Show/Hide columns ▾

罂粟科植物人血草的地上部分和根部

Feedback

如何筛选—利用碎片结构进行筛选

- 如果已经知道结构中是否存在，或者不存在的片段，可以添加结构定义



The screenshot displays the Reaxys software interface. On the left, a 'Filters and Analysis' panel shows '1,397' results and a 'By Structure' filter. The main 'Structure editor' window contains a benzene ring structure. The right-hand panel, 'Search this structure as:', lists various search options. The 'Additional ring closures' option is highlighted with a red box, indicating its selection for the filter.

Tips:
定义时需要明确
该苯环是否允许
稠环

如何筛选—添加的时候可以进行Limit/Exclude操作

The screenshot displays the Reaxys web interface. On the left, a sidebar titled 'Filters and Analysis' is highlighted with a red box. It contains two buttons: 'Limit to >' and 'Exclude >'. Below these buttons, there is a section 'By Structure' with a chemical structure of benzene and a 'Limit to' button. The main area shows search results for '1,397 Substances'. The first result is 'camptothecin' (C₂₀H₁₀N₂O₄, 348,358) with various data links. The second result is '5'-inosine monophosphate' (C₁₀H₁₃N₄O₈P, 348,209) with similar data links. The interface includes navigation tabs like 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'.

Reaxys

Quick search Query builder Results Synthesis planner History

Sam Yu

1,397 Filters and Analysis

Limit to > Exclude >

By Structure

On all atoms

Measurement pX

Highest Clinical Phases

Targets

Parameters

Substance Classes

Molecular Weight

1,397 Substances out of 7,052 Documents, containing 3,546 Reactions, 347 Targets

Reaxys - 1,397

0

Export

No of References

Heatmap

1

camptothecin

C₂₀H₁₀N₂O₄ 348,358 6075662 7689-03-4

Hit Data - 30

Identification

Druglikeness

Bioactivity (All)

Physical Data - 136

Spectra - 147

Other Data - 1,813

Preparations - 236

Reactions - 1,207

Targets - 145

Documents - 4,164

Hit Data - 30

Isolation from Natural Product - 30 hits out of 30

2

5'-inosine monophosphate

C₁₀H₁₃N₄O₈P 348,209 630517 131-99-7

Hit Data - 3

Identification

Druglikeness

Bioactivity (All)

Physical Data - 63

Spectra - 27

Other Data - 6

Preparations - 15

Reactions - 66

Targets - 10

Documents - 212

Feedback

更多结构上的筛选工具

- 在不知道结构的情况下，Reaxys可以帮助分析这些结构中的共性

1,397 Filters and Analysis

- By Structure ▾
- Measurement pX ▾
- Highest Clinical Phases ▾
- Targets ▾
- Parameters ▾
- Substance Classes** ▾
- Molecular Weight ▾
- Number of Fragments ▾
- Availability ▾
- Availability in other databases ▾
- Available Data ▾

Substance Classes ▲

- Functional Group Classification 1,389
- Ring Classification 1,358
- Richter Classification 1,338
- + More**

Substance Class树状图

Substance Classes		✕	
✓	Substance Classes	1,397	
>	Functional Group Classification	1,389	官能团分类
>	Ring Classification	1,358	环系分类
>	Richter Classification	1,338	Richter分类

Clear selected ✕

Limit To > Exclude >

Functional Group分类

Substance Classes ×

✓	Substance Classes	1,397
✓	Functional Group Classification	1,389
>	O in Functional Group	1,384
>	C=C in Functional Group	1,293
>	N in Functional Group	42
>	X in Functional Group	20
>	C#C in Functional Group	10
>	S in Functional Group	9
>	P in Functional Group	2
>	Ring Classification	1,358
>	Richter Classification	1,338

Clear selected × Limit To > Exclude >

已有结构中的一些官能团分类

Ring Classification

Substance Classes ×

✓	Substance Classes	<input type="checkbox"/>	1,397
>	Functional Group Classification	<input type="checkbox"/>	1,389
✓	Ring Classification	<input type="checkbox"/>	1,358
>	9-18-membered rings	<input type="checkbox"/>	1,161
>	6-membered rings	<input type="checkbox"/>	1,105
>	5-membered rings	<input type="checkbox"/>	869
>	7-membered rings	<input type="checkbox"/>	326
>	bridged ring systems	<input type="checkbox"/>	225
>	3-membered rings	<input type="checkbox"/>	173
>	8-membered rings	<input type="checkbox"/>	88
>	macrocycles (18+ ring atoms)	<input type="checkbox"/>	32

Clear selected × Limit To > Exclude >

已有结构中的一些环系分类

案例的衍生1—如何一开始就加入结构片段

The screenshot displays the Reaxys 'Query builder' interface. At the top, navigation tabs include 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The 'Query builder' tab is active, showing a search query with several fragments:

- Natural Product**: Isolation from Natural Product
- Group: Ungroup**: Molecular Weight (348)
- Molecular Weight**: Molecular Weight (349)
- Structure**: Create Structure / Reaction Drawing

The 'Structure' fragment is highlighted with a red box, and a red arrow points from this box to the 'Structure' fragment in the query list. The right sidebar shows search fields and forms, with 'Structure' selected. The bottom left corner contains the text 'javascript:void(0)' and the bottom right corner has a 'Feedback' button.

案例的衍生2—如果有NMR的数据

- 分子量348.456
- 天然产物
- NMR的数据： ^{13}C NMR (DMSO- d_6 , 150 MHz) δ 173.5, 157.8, 153.4, 150.1, 148.1, 145.9, 131.6, 130.4, 130.2, 129.2, 128.7, 128.1, 127.8, 120.1, 96.9, 73.6, 65.6, 50.8, 30.2, 7.8
- 想法：
 - 既然Reaxys中包含大量的谱图数据，那么能否利用谱图数据直接给出结构？
- 问题：
 - 如何解决数据的容差
- 解决方案
 - 节选部分数据的整数，且小数部分在0.5左右

案例的衍生2—如果有NMR的数据

- 数据的节选
- ^{13}C NMR (DMSO-d₆, 150 MHz) δ 173.5, 157.8, 153.4, 150.1, 148.1, 145.9, 131.6, 130.4, 130.2, 129.2, 128.7, 128.1, 127.8, 120.1, 96.9, 73.6, 65.6, 50.8, 30.2, 7.8

Tips:

1. 设定谱图数据中，包含，173，153，130，可以将上述的谱图找到，这样就可以解决容差问题，其实是在寻找包含173.0-173.9的谱图
2. 由于容差问题，不太建议加太多的数据上去
3. 常见做法，选择一个数据，然后检索该数据 ± 1 的范围，如选择173.5.那么可以考虑检索，172，173，174，这样会有更大的容差范围

案例的衍生2—如果有NMR的数据，如何做

- Query Builder, 添加如之前的检索条件如下

The screenshot displays the Reaxys Query Builder interface. The main search area contains three conditions:

- Natural Product**: Isolation from Natural Product (Find any, Show fields)
- AND**
- Group**: Molecular Weight \geq 348
- AND**
- Group**: Molecular Weight \leq 349

On the right sidebar, the search bar "Find search fields and forms" contains the text "NMR". A red box highlights this search bar, and a red arrow points to the "NMR Spectroscopy" category in the sidebar. A text label "添加NMR的条件" (Add NMR conditions) is positioned next to the sidebar.

NMR条件的设定

◇ NMR Spectroscopy Find any **Show fields** ▾ ×

◇ NMR Spectroscopy Find any Hide fields ▲ ×

is	▾	Description (NMR Spectroscopy)	🔍
is	▾	Nucleus (NMR Spectroscopy)	🔍
is	▾	Coupling Nuclei	🔍
is	▾	Solvents (NMR Spectroscopy)	🔍
=	▾	Temperature (NMR Spectroscopy), °C	🔍
=	▾	Frequency (NMR Spectroscopy), MHz	🔍
contains	▾	Original Text (NMR Spectroscopy) 173	🔍

Tips:

Original Text中选择Contains，可以解决容差问题，

最后完成的Query Builder

The screenshot shows a Query Builder interface with three main conditions connected by AND operators:

- Condition 1:** Natural Product (Isolation from Natural Product) with options "Find any" and "Show fields".
- Condition 2:** Molecular Weight (Molecular Weight) with operator \geq and value 348.
- Condition 3:** Molecular Weight (Molecular Weight) with operator \leq and value 349.
- Condition 4:** NMR Spectroscopy (NMR Spectroscopy) with options "Find any" and "Hide fields".

The NMR Spectroscopy condition is expanded to show the following fields and operators:

Operator	Field
is	Description (NMR Spectroscopy)
is	Nucleus (NMR Spectroscopy)
is	Coupling Nuclei
is	Solvents (NMR Spectroscopy)
=	Temperature (NMR Spectroscopy), °C
=	Frequency (NMR Spectroscopy), MHz
contains	Original Text (NMR Spectroscopy)

条件1：检索天然产物

条件2：分子量组合， $348 \leq MW \leq 349$

条件3：NMR数据中包含173，即检索173.0-173.9的数据

物质检索的结果

camptothecin
 $C_{20}H_{16}N_2O_4$ **348.358** 6075662 7689-03-4



Hit Data - 31
 Identification
 Druglikeness

Bioactivity (All)
 Physical Data - 136
 Spectra - 147

Other Data - 1,813

Preparations - 236 >
 Reactions - 1,207 >
 Targets - 145 >
 Documents - 4,164 >

Hit Data - 31

- NMR Spectroscopy - 1 hits out of 59
- Isolation from Natural Product - 30 hits out of 30

^ NMR Spectroscopy - 1 hits out of 59

Show/Hide columns

Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Frequency (NMR Spectroscopy), MHz	Original Text (NMR Spectroscopy)	Comment (NMR Spectroscopy)	Reference
13C	dimethylsulfoxide-d6	150	13C NMR (DMSO-d6, 150 MHz) δ 173.6 (C, C-21), 157.6 (C, C-22), 153.5 (C, C-2), 150.1 (C, C-15), 148.1 (C, C-13), 145.9 (C, C-3), 131.5 (CH, C-7), 130.6 (C, C-6), 130.2 (CH, C-11), 129.2 (CH, C-12), 128.7 (CH, C-9), 128.1 (C, C-8), 127.8 (CH, C-10), 120.1 (C, C-16), 96.9 (CH, C-14), 73.6 (C, C-20), 65.6 (CH2, C-17), 50.8 (CH2, C-5), 30.2 (CH2, C-19), 7.8 (CH3, C-18).	Signals given	Stephen F. Austin State University - US2007/134282, 2007, A1 Full Text Details Abstract

提纲

- 常见的与物质物质检索有关的困难案例
- Reaxys中的解决方案
 - Reaxys中的Query Builder检索模式
 - Reaxys中的困难案例解决方案
 - Reaxys中的更多与性质检索有关技巧
- Reaxys物质检索小结

化合物的文献定位

Tetrahedron 74 (2008) 224–238

Contents lists available at ScienceDirect

Tetrahedron

journal homepage: www.elsevier.com/locate/tet

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

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ARTICLE INFO

Article history:
Received 27 July 2007
Received in revised form 5 November 2007
Accepted 13 November 2007
Available online 16 November 2007

Keywords:
o-phthalaldehyde
Condensation reaction
Regioselectivity
Mechanism; understanding

ABSTRACT

Our approach for the synthesis of isoalloxazines, a privileged bioactive heterocyclic core structure involves a condensation reaction of *o*-phthalaldehydes with a suitable nitrogen-containing nucleophile. This favouring reaction is revisited here in the context of the use of *o*-phthalaldehydes that contain additional substituents in the aromatic ring leading to a detailed analysis of the regioselectivity of the reaction. Eleven mono-substituted *o*-phthalaldehydes were synthesized and reacted with alanine. The regioselectivity observed across the eleven substrates led to the design of a disubstituted substrate that reacted with very high control. A gram-scale reaction followed by esterification gave one major regioisomer in high yield. In addition, the regioselectivity observed on reaction of two novel mono-substituted substrates led to an increased mechanistic understanding.

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1. Introduction

The isoalloxazines make up an important class of bioactive molecules that includes the known drugs Patrnaxone (1),¹ Indoprofen (2),² and Chlorothalidone (3).³ (Fig. 1a).

Common methods of obtaining isoalloxazines that are unsubstituted in the aromatic ring, for example compound 4 (Fig. 1b), include selective reduction of 5,⁴ reductive amination-cyclization of 6⁵ or 7⁶ with a primary amine (RNH₂) and, of interest here, the condensation reaction of *o*-phthalaldehyde (8) with a primary amine (RNH₂).^{7,8}

To date, the majority of studies performed on this condensation reaction have focused on evaluating the scope of the amine nucleophile that can be tolerated in the reaction,^{9,10,11} and/or proposing potential reaction mechanisms.^{12,13} In contrast, examples of the use of this condensation reaction with mono-substituted *o*-phthalaldehydes are rare (SI part 1). One report describes a regioselectivity of 1:1 for the products 1E:1Z resulting from the condensation of 9 with 10 (Scheme 1a).¹ However, the observed regioselectivity was measured only after filtration or purification by column chromatography. Isolated yields for the formation of a single isomer, 1E is most cases, resulting from the condensation of 13 with various amines have also been reported (Scheme 1b).⁴

Other studies have provided only isolated yield(s) after purification (for one or for each isomer), incomplete regioisomeric ratio (rr) data within a series or have claimed to form a single regioisomer (no yield provided) without discussing the other possible isomer (SI part 1).^{7,9}

The work reported here revisits this issue by presenting a detailed study of the regiochemical outcome of the condensation of alarins (16) with 3-mono-substituted *o*-phthalaldehydes 17 (to give 1E and 1Z, Scheme 1c) and with 4-mono-substituted *o*-phthalaldehydes 20 (to give 2E and 2Z, Scheme 1d). Based on the initial results, the design of a highly regioselective substrate was achieved consistent with an improved understanding of the reaction. Further mechanistic insights were provided by the use of novel mono-substituted substrates.

2. Results and discussions

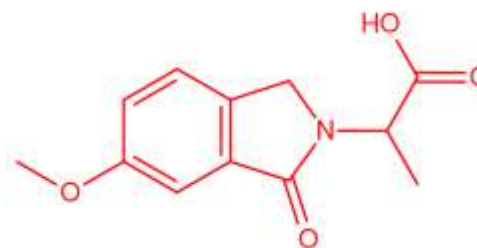
2.1. Synthesis of mono-substituted *o*-phthalaldehydes

Five 3-substituted *o*-phthalaldehydes 17a–e were synthesized using 2–5 step routes involving either a Swern oxidation of the corresponding diol 23 or an acetal deprotection of the corresponding monoacetal 24 or diacetal 25 (Scheme 2 and SI) part S.1 for more details). It should be noted that the synthesis of pure samples of 17a–e was particularly challenging (in line with literature reports¹⁴) with significant decomposition occurring during purification attempts and on storage. In several cases freshly

这是一篇常见的化学文献，包含：

1. 16页PDF全文
2. 2个Supporting Information的Word文档，一个是44页，一个37页

已知文献中报道了这个化合物，如何在上述的97页文档中找到有关这个化合物的描述？



Query Builder下的检索方式

Reaxys® Quick search Query builder Results Synthesis planner History

Search in: Reactions > Targets > **Substances >** Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

Find search fields and forms
Q title X

Reaxys ^

Journal Title

Document Title

Feedback

添加结构与文献名称，并检索物质

COc1ccc2c(c1)c(=O)n(C(C)C)C2=O

As drawn

AND

Document Title

is Title Assessment of the regioselectivity in the condensation reaction

检索到的结果

The screenshot shows the Reaxys search results page for the compound 2-(6-methoxy-1-oxoisindolin-2-yl)propanoic acid. The interface includes a navigation bar with 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. A left sidebar titled 'Filters and Analysis' contains 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 Accession'. The main content area displays the search results for '1 Substances: 1 Documents, 7 Reactions, 0 Targets'. The compound name is '2-(6-methoxy-1-oxoisindolin-2-yl)propanoic acid' with the molecular formula $C_{12}H_{13}NO_4$, molecular weight 235.24, and CAS number 32021463. A chemical structure is shown with a red highlight on the propanoic acid group. The 'Hit Data - 7' section is expanded, showing the following data points:

- 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
- IR Spectroscopy - 1 hits out of 1
- Mass Spectrometry - 1 hits out of 1

Other data categories visible include 'Preparations - 7', 'Reactions - 7', and 'Documents - 1'. A text box on the right side of the image states: '这个物质在这篇文献中的所有数据都在Hit Data中' (All data for this substance in this literature is in Hit Data).

关键性的标识性数据

^ Hit Data - 7

- ✓ 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
- ✓ IR Spectroscopy - 1 hits out of 1
- ✓ Mass Spectrometry - 1 hits out of 1

21a表示的是这个化合物在文献中的标识符。可以用21a对上述97页文档进行搜索，用于化合物定位

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

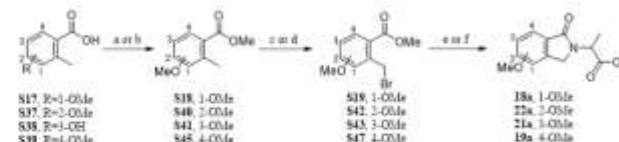
全文和Supporting Information中的搜索结果

2.2. Regioselectivity of the condensation reaction of mono-substituted *o*-phthalaldehydes

The mono-substituted *o*-phthalaldehydes **17a-e** and **20a-f** were refluxed for 4 h with alanine (**16**, 1.2 equivalents) in anhydrous acetonitrile before the reaction was concentrated *in vacuo*. The crude reaction mixtures (except when specified, [Table 1](#)) were then analysed using a quantitative ^1H NMR experiment. A baseline correction was applied using MestReNova-9 software and integrations were calculated relative to one proton on deconvoluted peaks (see [Fig. 2](#) for an example of the analysis applied to the formation of **18a/19a** and [SI1 part III.1](#) for the rest of the NMR analysis; also see the experimental section below for a detailed explanation of the analytical protocol used).

In two of the condensation reactions the structure of the major regioisomer was identified by comparison with the ^1H NMR spectrum of a pure sample of one of the regioisomers (for **18a/19a**, **21a/22a**, for the synthesis of authentic isomers see [SI1 part III.2](#)). In the rest of the cases, advanced NMR techniques (HSQC, HMBC, COSY) applied to the crude reaction mixture were used to assign the structure of the major regioisomer. Considering the analysis of the regioisomeric mixture of **18b/19b** as an example ([Fig. 3](#)), the proximity of a carbonyl was observed to shift the signal corresponding to the aromatic H7 proton in **18b** and the methyl H1' protons in **19b** downfield ([Fig. 3a](#) and [b](#)). Identification of H7 in **18b** was further validated by its correlation with C1 in the HMBC analysis of the regioisomeric mixture ([Fig. 3a](#)). In contrast, H4 in **19b** showed a correlation with C3 in this HMBC analysis ([Fig. 3c](#)). Using the correlations observed in the COSY spectrum ([Fig. 3d](#)), the signals corresponding to H5 and H6 for **18b** and **19b** were finally assigned. The value of the integrals in the 1D quantitative ^1H NMR

III.2. Synthesis of pure isoindolinones **18a**, **19a**, **21a** and **22a**.



Scheme S 10: Synthesis of **18a**, **19a**, **21a** and **22a**. Reagents and conditions: (a) MeOH, H_2SO_4 , reflux, 7-24 h, quant. for **S18**, 84% for **S40**; (b) MeI, K_2CO_3 , DMF, 70 °C 17-18 h, 92% for **S41**, 99% for **S45**; (c) NBS, AIBN, CHCl_3 , reflux, 2.5-21.0 h, 97% for **S19**, crude **S42** and **S43** were directly used in the next step; (d) NBS, AIBN, CCl_4 , reflux, 2 h, crude **S47** was directly used in the next step; (e) alanine (**16**), MeOH, K_2CO_3 , reflux 19-21 h, 61% for **18a**, 55% (2 steps) for **19a**; (f) alanine (**16**), MeOH, NEt_3 , reflux 2-23 h, 4% (2 steps) for **21a**, 4% (2 steps) for **22a**.

Esterification of **S17**, **S37**, **S38** and **S39** was achieved in excellent yield using iodomethane or methanol with sulfuric acid (Scheme S 10).⁸ Radical monobromination⁹ of **S18**, **S40**, **S41** formed **S19**, **S42**, **S43** which were directly reacted⁹ with alanine (**16**) to obtain **18a**, **22a** and **21a** respectively. To investigate the poor yield over two steps (2% for **18a**, 4% for **21a** and 4% for **22a**), radical monobromination of **S18** was repeated and the succinimide side product from *N*-bromosuccinimide was removed by a basic wash using NaOH (1 M) leading to pure **S19** in 97% yield. Reaction of **S19** with **16** and NEt_3 afforded **18a** in only 8% yield. However, concentration of the aqueous phase showed **S44** as the major product (identified by NMR spectroscopy (Figure S 5) and supported by mass spectrometric analysis (HRMS (ES⁻) m/z calculated for $\text{C}_{16}\text{H}_{26}\text{NO}_3$ [M]⁻: 280.1907; found: 280.1910) along with the remaining NEt_3 and alanine (**16**). Formation of **S44** was prevented by reacting **S19** with K_2CO_3 instead of NEt_3 to provide **18a** in good yield. This optimisation could be applied for the synthesis of **21a** and **22a** but was not performed since sufficient material was available.

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**If you have questions feel
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