



ELSEVIER

Elsevier Reaxys中化学信息的获取

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Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
 - Reaxys对文献的提炼
 - Reaxys中物质与物性数据获取反向检索
 - Reaxys中结构面板与反应数据获取
 - Reaxys中的实用小案例
- Q&A

什么是Reaxys

Reaxys是Elsevier旗下Life Science产品线中基于数据深度提炼与挖掘的**化学及相关学科**的科研信息平台

6,000万文献

(Elsevier, ACS, Nature-Springer, Blackwell, Taylor and Francis, etc)

105家专利机构专利

WPO, USPO, EPO [≈ mid 70's >]

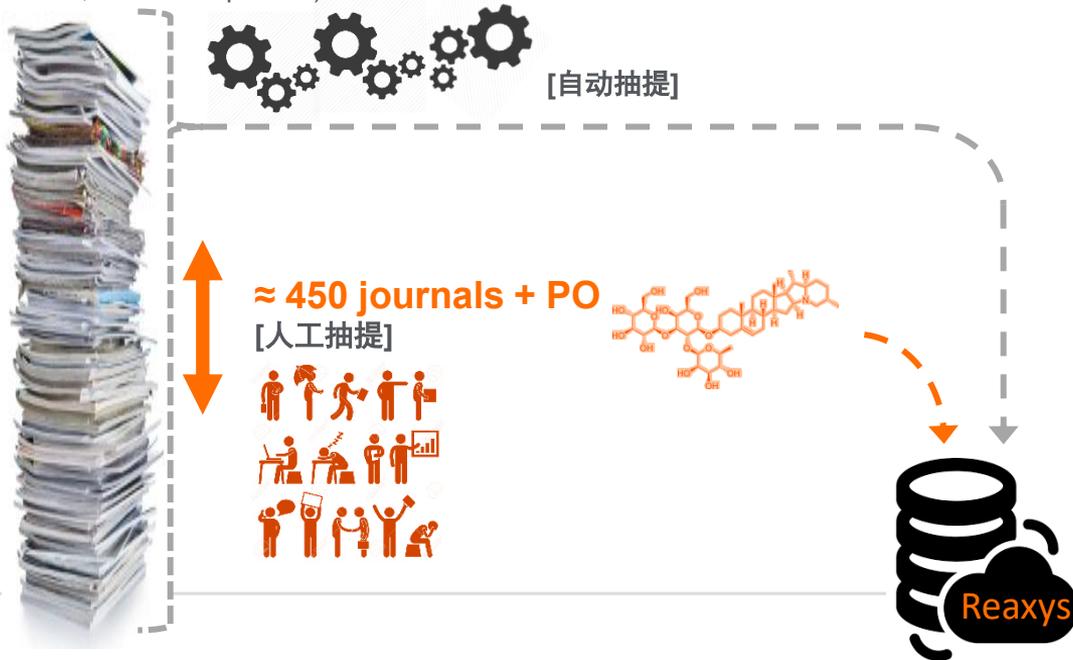
PO: JP, KR, CN, TW [2015 >]

2021年底前完成105家专利机构专利回溯与抽提

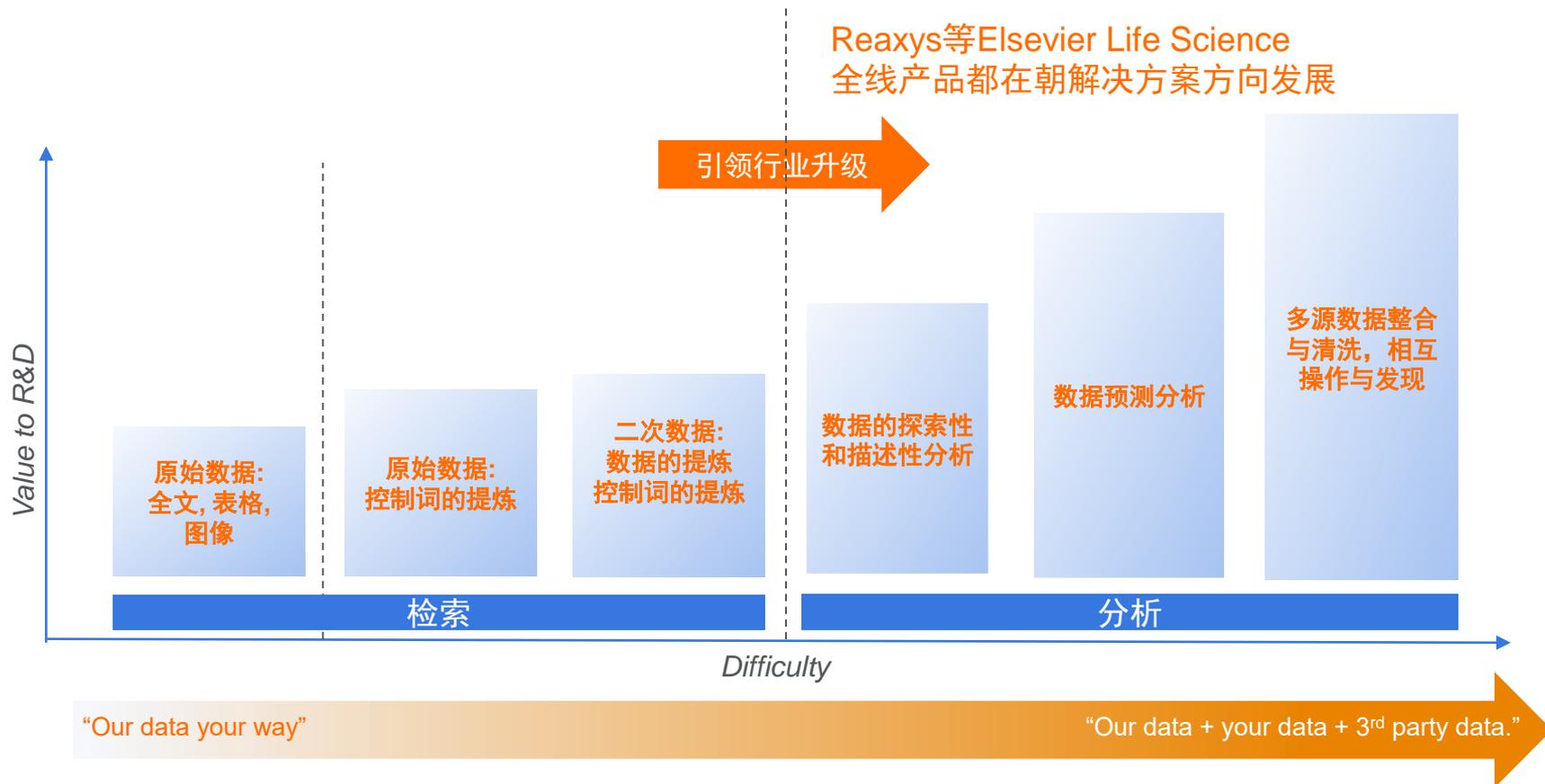
38万书的章节

Beilstein, Gmelin,....

16,300 期刊
(journals, books and patents)

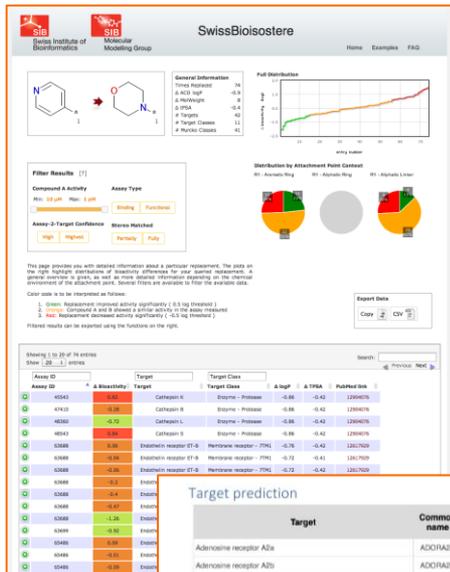


Reaxys已经在不断利用AI/ML技术， 引领数据库到解决方案的行业升级



越来越多的AI/ML技术融入到数据库中

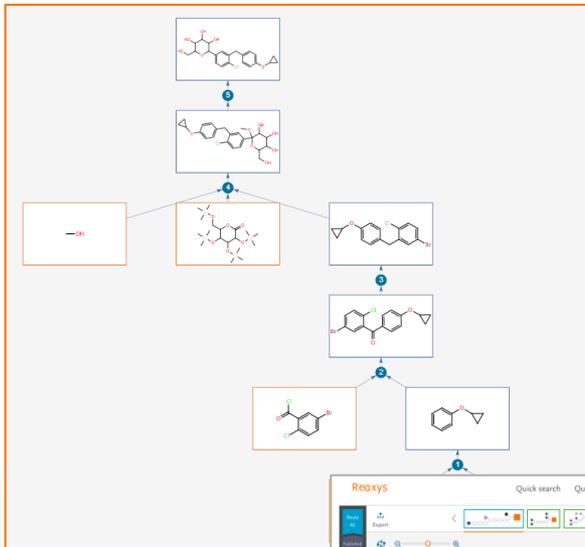
MMP分析



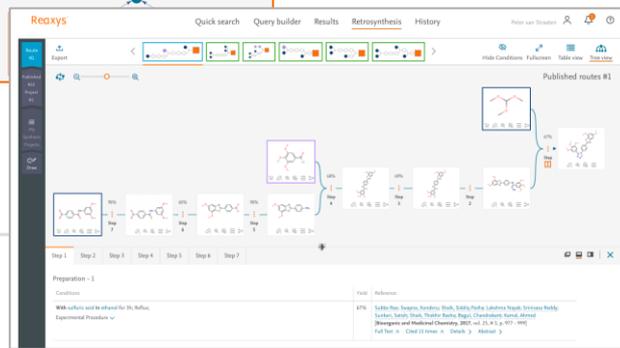
靶点预测



AI合成预测



2021年将于现有Synthesis Plan整合到一个平台



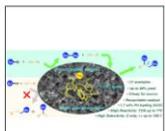
Agenda

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一篇常见的化学相关文献的构成

Chem | Article

Porous Ligand Creates New Reaction Route: Bifunctional Single-Atom Palladium Catalyst for Selective Distannylation of Terminal Alkynes



Abstract: We report a porous ligand that allows for the bifunctional single-atom palladium catalyzed distannylation of terminal alkynes. The porous ligand is a porous metal-organic framework (MOF) with a large surface area and high porosity. It is used as a support for a single-atom palladium catalyst. The porous ligand creates a new reaction route for the distannylation of terminal alkynes, which is more selective than the traditional method. The porous ligand also allows for the recycling of the catalyst. The porous ligand is a porous metal-organic framework (MOF) with a large surface area and high porosity. It is used as a support for a single-atom palladium catalyst. The porous ligand creates a new reaction route for the distannylation of terminal alkynes, which is more selective than the traditional method. The porous ligand also allows for the recycling of the catalyst.

Chem | Article

Experimental Section

Starting Materials, Reagents, Solvents, and Purification: All reagents and solvents were used as received unless otherwise specified. Purification was performed by column chromatography on silica gel (40-60 μm) using the indicated eluent. The yield and purity of the products were determined by ¹H NMR and ¹³C NMR.

General Procedure for the Synthesis of **3:** A solution of **1** (0.5 mmol) and **2** (1.0 mmol) in THF (10 mL) was stirred at room temperature for 16 h. The reaction mixture was then purified by column chromatography on silica gel using a gradient of ethyl acetate in hexanes to give **3** as a colorless oil. Yield: 42%.

Characterization Data: ¹H NMR (400 MHz, CDCl₃) δ = 7.52 (1H, d, J = 7.8 Hz), 7.15 (1H, d, J = 8.2 Hz), 7.08-7.03 (1H, m), 7.01-6.95 (1H, m), 6.93 (1H, d, J = 3.1 Hz), 6.46 (1H, s, J = 168.4 Hz, 65.5 Hz), 6.40 (1H, d, J = 3.1 Hz), 4.78 (2H, d, J = 1.3 Hz), 1.40-1.25 (12H, m), 1.22-1.14 (12H, m), 0.88-0.72 (30H, m). ¹³C NMR (400 MHz, CDCl₃) δ = 160.6, 144.4, 136.4, 128.8, 128.0, 121.2, 120.7, 119.2, 110.1, 101.0, 60.1, 29.2, 29.1, 27.4, 27.3, 13.7, 13.6, 10.8, 10.2. HRMS (m/z) (ESI): calcd for C₃₅H₆₃KNSn₂[M+K]⁺ 774.2630, found 774.2654.

Chem | Article

Experimental Section

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

Reaction Scheme: $R-C\equiv C-H + H-SnBu_3 \xrightarrow{Pd@POL-PPh_3, THF, r.t., 16 h} R-C(SnBu_3)=C(SnBu_3) + R-C(SnBu_3)=C(SnBu_3) + \text{other isomers}$

O-containing terminal alkynes:

- 3a** 72% (50:1)
- 3b** 66% (100:1)
- 3c** 65% (100:1)
- 3d** 84% (50:1)
- 3e** 68% (71:1)[†]
- 3f** 63% (5:1)[†]
- 3g** 71% (7:1)
- 3h** 72% (10:1)
- 3i** 60% (10:1)

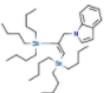
N-containing terminal alkynes:

- 3j** 89% (100:1)
- 3k** 58% (25:1)
- 3l** 61% (50:1)
- 3m** 81% (50:1)
- 3n** 81% (100:1)
- 3o** 41% (14:1)[†]

Support Information中的化合物理化性质描述

(Z)-1-(2,3-bis(tributylstanny)allyl)-1H-indole 3j: colorless oil. Petroleum ether as eluent for column chromatography (**3j**, R_f = 0.75; **2j**, R_f = 0.4, 42% of alkyne was isolated and recovered); ¹H NMR (400 MHz, CDCl₃) δ = 7.52 (1H, d, J = 7.8 Hz), 7.15 (1H, d, J = 8.2 Hz), 7.08-7.03 (1H, m), 7.01-6.95 (1H, m), 6.93 (1H, d, J = 3.1 Hz), 6.46 (1H, s, J = 168.4 Hz, 65.5 Hz), 6.40 (1H, d, J = 3.1 Hz), 4.78 (2H, d, J = 1.3 Hz), 1.40-1.25 (12H, m), 1.22-1.14 (12H, m), 0.88-0.72 (30H, m). ¹³C NMR (400 MHz, CDCl₃) δ = 160.6, 144.4, 136.4, 128.8, 128.0, 121.2, 120.7, 119.2, 110.1, 101.0, 60.1, 29.2, 29.1, 27.4, 27.3, 13.7, 13.6, 10.8, 10.2. HRMS (m/z) (ESI): calcd for C₃₅H₆₃KNSn₂[M+K]⁺ 774.2630, found 774.2654.

Reaxys对文献中的化合物的结构化数据提炼



1

(Z)-1-(2,3-bis(tributylstanny)allyl)-1H-indole
 C₃₅H₆₃N₅Sn₂ 735.312 36450188

Hit Data - 6
 Identification
 Druglikeness
 Physical Data - 2
 Spectra - 3

Preparations - 1 >
 Reactions - 1 >
 Documents - 1 >

Hit Data - 6

- ✓ Substance Label - 1 hits out of 1
- ✓ Chromatographic Data - 1 hits out of 1
- ✓ Crystal Property Description - 1 hits out of 1
- ✓ NMR Spectroscopy - 2 hits out of 2
- ✓ Mass Spectrometry - 1 hits out of 1

文献中出现的化合物性质，全部直接抽提，或者给出文献中出现的位置，方便科研人员直接获取，或节省查找阅读全文的时间。

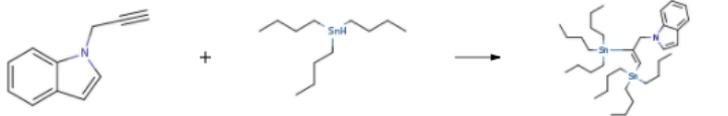
Label	Reference
3j	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie[Chem, 2020 , vol. 6, # 9, p. 2300 - 2313] Full Text Details Abstract >

Colour & Other Properties	Location	Reference
colourless	supporting information	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie[Chem, 2020 , vol. 6, # 9, p. 2300 - 2313] Full Text Details Abstract >

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Solvents (NMR Spectroscopy)	Frequency (NMR Spectroscopy), MHz	Location	Reference
Chemical shifts, Spectrum	¹ H	chloroform-d ₁	400	supporting information	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie[Chem, 2020 , vol. 6, # 9, p. 2300 - 2313] Full Text Details Abstract >
Chemical shifts, Spectrum	¹³ C	chloroform-d ₁		supporting information	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie[Chem, 2020 , vol. 6, # 9, p. 2300 - 2313] Full Text Details Abstract >

Reaxys对原文反应的提炼 (3J)

1



1 Conditions [Find Similar](#) > Reaction ID: 54835331 [View](#)

Conditions	Yield	Reference
<p>With porous vinyl functionalized tri(2-methoxyphenyl)phosphine derived polymer supported palladium in tetrahydrofuran at 25°C; Schlenk technique; Sealed tube; stereoselective reaction;</p> <p>Experimental Procedure ^</p>	89%	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie [Chem, 2020, vol. 6, # 9, p. 2300 - 2313] Full Text ↗ Details > Abstract >

General Procedure for Distannylation of Terminal Alkynes

General procedure: A flame-dried Schlenk tube was flushed under an atmosphere of nitrogen and charged with 15.5 mg of Pd₁@POL-5 (0.0025 mmol, 0.005 equiv-). The vial was sealed with a rubber septum and 2 mL of distilled THF was added followed by addition of the alkyne (0.5 mmol). Tributyltin hydride (0.5 mmol, 1 equiv) was added dropwise to the reaction vial. The reaction mixture was left to stir for 24–36 h at room temperature. When the reaction was completed (monitored by TLC), the solution was filtered and washed with EtOAc. The filtered solution was evaporated under vacuum. The crude product was purified directly by silica gel column chromatography eluting with petroleum ether, ethyl acetate, and 1% triethylamine to afford the corresponding product.

Reaxys从文献中提炼出来的内容

文献 Database

>63 million records

源自16000本刊以及
105专利机构的专利
(2021年底前完成
专利回溯)

化合物 Database

>150 million

源自文献专利中的
报道, 供应商品库
(2021将继续扩大
供应商名录)

化学反应Database

>54.8 million

单步多步反应, 同
时提炼文献与专利
中的实验过程

性质 Database

> 500 million

化合物实验数据,
并提炼实验数据检
测条件

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 - Reaxys中结构面板与反应数据获取
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- Q&A

Reaxys的登录界面

- IP范围内，浏览器输入www.Reaxys.com，可以直接进行检索，推荐Chrome，Firefox浏览器，
- 收藏夹收藏的链接建议只收藏www.Reaxys.com

Reaxys

Quick search Query builder Results Synthesis planner History Register > Sign in

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

Search Reaxys
Substance Effect, e.g. anticoagulant
AND
Draw

Content Overview | Latest update: 07. August 2020 >

118M 49M 59M 37M
Substances Reactions Documents Bioactivities

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Tips:

1. 账号注册（可选），注册帐号后，可以使用提醒，结果集保存，结果导出功能（2020.8以后）
2. Quick Search，快速检索，结构反应检索，或者输入自然语言，Reaxys智能分析语义进行检索。
3. Query Builder，组合检索，利用Reaxys中的各种字段进行组合，实现不同检索需求。

视频介绍:

1. Reaxys主界面：
<https://www.bilibili.com/video/BV1T5411L7Ec>
2. Quick Search：
<https://www.bilibili.com/video/BV1az4y1C7ZL>
3. Query Builder：
<https://www.bilibili.com/video/BV1UK4y1774Q>
4. Reaxys账号注册与应用
<https://www.bilibili.com/video/BV1NA41147if>

Case 1: 快速获取化合物的理化性质

Reaxys® [Quick search](#) [Query builder](#) [Results](#) [Synthesis planner](#) [History](#) [Register >](#) [Sign in](#)

Search for **solubility of gefitinib** [Import](#)

Search Reaxys

[Find >](#)

Substance Properties, e.g. [ferroelectric materials](#)

AND

Draw

Tips:
快速获取某个化合物
溶解性数据。

[Content Overview](#) | Latest update: 30. March 2020 >

118M	49M	59M	37M
Substances	Reactions	Documents	Bioactivities

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RELX Group™

Reaxys中的结果

Quick search Query builder Results Synthesis planner History

Results for solubility of gefitinib

1	Substances	Structure as drawn AND Property: solubility	Preview Results > View Results >
178	Documents	Titles, Abstracts, Keywords: "solubility", "gefatinib"	Preview Results > View Results >
341,792	Documents	Titles, Abstracts, Keywords: "solubility"	Preview Results > View Results >
23,178	Documents	Titles, Abstracts, Keywords: "gefatinib"	Preview Results > View Results >

1 Substances out of 9,928 Documents, containing 148 Reactions, 1,149 Targets

0 selected Limit To Exclude Export Preparations

Sort by No of References > Grid Heatmap

Reaxys - 1

gefatinib
C22H24N4ClFO3 446,909 8949523 184475-35-2

Hit Data - 4 Bioactivity (All) Other Data - 4,132 Preparations - 83 >

Identification Physical Data - 115 Reactions - 148 >

Druglikeness Spectra - 80 Targets - 1,149 >

Documents - 9,928 >

Hit Data - 4

Solubility (MCS) - 4 hits out of 4

抽提的数据包括具体的数值，或者相关的文字性描述

^ Solubility (MCS) - 4 hits out of 4

Show/Hide columns >

Solubility, g l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Location	Comment (Solubility (MCS))	Reference
					freely soluble in DMSO THP and PEG-400, sparingly soluble in 2-butanol and slightly soluble in 1-butanol, IPA, ethanol, methanol, EG and PG	Alanazi, Abdullah; Alshehri, Sultan; Altamimi, Mohammad; Shakeel, Faiyaz [Journal of Molecular Liquids, 2020, vol. 299, art. no. 112211] Full Text > Details > Abstract >
					soluble in water and 1-octanol	Wu, Kuen-Da; Chen, Grace Shiahuy; Liu, Jia-Rong; Hsieh, Chen-En; Chern, Ji-Wang [ACS Medicinal Chemistry Letters, 2019, vol. 10, # 1, p. 22 - 26] Full Text > Cited 1 times > Details > Abstract >
0.009832	in pure solvent	25	water	supporting information		Wang, Xin-Xin; Tian, Fei-Yang; Liu, Ming; Chen, Kai; Zhang, Yun-Qian; Zhu, Qian-Jiang; Tao, Zhu [Tetrahedron, 2019, vol. 75, # 37, art. no. 130488] Full Text > Details > Abstract >
0.0021	in pure solvent	20	water			Zhao, Feng; Lin, Zhaohu; Wang, Feng; Zhao, Weili; Dong, Xiaochun [Bioorganic and Medicinal Chemistry Letters, 2013, vol. 23, # 19, p. 5385 - 5388] Full Text > Cited 22 times > Details > Abstract >

Reaxys中化合物更多的理化性质

1 Substances out of 9,928 Documents, containing 148 Reactions, 1,149 Targets

0 selected Limit To Exclude Export Preparations

Sort by No of References ↓ Grid Heatmap

gefitinib
C22H24N4ClFO3 446.909 8949523 184475-35-2

Hit Data - 4 Bioactivity (All) Other Data - 4,132 Preparations - 83 >
Identification Physical Data - 115 Reactions - 148 >
Druglikeness Spectra - 80 Targets - 1,149 >
Documents - 9,928 >

Hit Data - 4
Solubility (MCS) - 4 hits out of 4

直接获取化合物的理化性质或者谱图数据

^ Spectra - 80

- ✓ NMR Spectroscopy - 46
- ✓ IR Spectroscopy - 9
- ✓ Mass Spectrometry - 17
- ✓ UV/VIS Spectroscopy - 6
- ✓ Raman Spectroscopy - 1
- ✓ Fluorescence Spectroscopy - 1

^ Physical Data - 115

- ✓ Melting Point - 27
- ✓ Density - 1
- ✓ Association (MCS) - 12
- ✓ Chromatographic Data - 5
- ✓ Conformation - 1
- ✓ Crystal Phase - 9
- ✓ Crystal Property Description - 25
- ✓ Crystal System - 2
- ✓ Dissociation Exponent - 3
- ✓ Further Information - 1

Reaxys中与化合物分析有关文献的获取

1 Substances out of 9,928 Documents, containing 148 Reactions, 1,149 Targets

0 selected Limit To Exclude Export Preparations

Sort by No of References ↓ Grid Heatmap

gefitinib
C22H24N4ClFO3 446,909 894,9523 184475-35-2

Hit Data - 4 Bioactivity (All) Other Data - 4,132 Preparations - 83
Identification Physical Data - 115 Reactions - 148
Druglikeness Spectra - 80 Targets - 1,149
Documents - 9,928

Hit Data - 4
Solubility (MCS) - 4 hits out of 4

可以一次性获取与该化合物有关的文献

Reaxys® Quick search Query builder Results Synthesis planner History Alerts

9,928 Documents with 61,309 Substances, 72,101 Reactions, 2,279 Targets

0 selected Limit To Exclude Export

Filters: Limit to Exclude

- Index Terms (List)
- Index Terms (ReaxysTree)
- Publication Year
- Document Type
- Authors
- Patent Assignee
- Patent Office
- Journal Title
- Substance Classes
- Reaction Classes
- Manually processed content only

1 Current progress and future perspectives of polypharmacology: From the view of non-small cell lung cancer
Karuppasamy, Ramanathan; Veerappapillai, Shanthi; Maiti, Sayoni; Shin, Woong-Hee; Khara, Daisuke [Seminars in Cancer Biology, 2021, vol. 68, p. 84 - 91]
Abstract Index Terms Substances (48) Full Text
Hit Substances (1)

2 Repurposing of plant alkaloids for cancer therapy: Pharmacology and toxicology
Effarth, Thomas; Oesch, Franz [Seminars in Cancer Biology, 2021, vol. 68, p. 143 - 163]
Abstract Index Terms Substances (43) Full Text
Hit Substances (1)

3 Repurposing old drugs as new inhibitors of the ubiquitin-proteasome pathway for cancer treatment
Yang, Huanjie; Chen, Xin; Li, Kai; Chealto, Hassan; Yang, Qianqian; Wu, Guojun; Liu, Jinbao; Dou, Q. Ping [Seminars in Cancer Biology, 2021, vol. 68, p. 105 - 122]
Abstract Index Terms Substances (64) Full Text
Hit Substances (1)

4 Kinases as potential targets for treatment of pulmonary hypertension and right ventricular dysfunction
Weiss, Astrid; Boehm, Mario; Egemnazarov, Bakytbek; Grimminger, Friedrich; Savai Pullamsetti, Soni; Kwapiszewska, Grazyna; Schermuly, Ralph T. [British Journal of Pharmacology, 2021, vol. 178, #1, p. 31 - 53]
Abstract Index Terms Substances (28) Full Text
Hit Substances (1) Cited 1 times

Reaxys中的文献分析工具

9.93 K

1

Preview

Filters

Limit to > Exclude >

- Index Terms (List) v
- Index Terms (ReaxysTree) v
- Publication Year v
- Document Type v
- Authors v
- Patent Assignee v
- Patent Office v
- Journal Title v
- Substance Classes v
- Reaction Classes v

Manually processed content only

Index Terms (ReaxysTree) ^

- physico chemical properties 4,729
- chemical transformations 4,540
- physico chemical analysis... 1,658
- quantum chemical calculati... 196

[View more](#)

Reaxys中与分析有关的文献分类

Index Terms (ReaxysTree) x

- Index Terms (ReaxysTree) 9,928
 - physico chemical properties 4,729
 - chemical transformations 4,540
 - physico chemical analysis methods 1,658
 - separation method 781
 - spectroscopical analysis 760
 - fluorescence spectroscopy 267
 - luminescence spectroscopy 245
 - mass spectrometry 116
 - NMR spectroscopy 55
 - IR spectroscopy 35
 - Raman spectroscopy 28
 - photoelectron emission spectroscopy 12

Clear selected x

Limit to > Exclude >

Case 2: 理化性质的高级应用

- 获取KCl在乙醇中的溶解度

Reaxys

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

Register > Sign in

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Drag & Drop to build a new query

Search fields

Fields Forms History

Reaxys ^

Topics and Keywords v

Identification v

Physical Properties v

Spectra v

MedChem v

Other v

Reactions v

Bibliography v

PubChem v

eMolecules v

LabNetwork v

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

检索策略的构建

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 "Register" and "Sign in" buttons. Below the navigation, a "Search in:" section contains buttons for "Reactions", "Targets", "Substances", and "Documents". A toolbar includes "Import", "Save", "Reset form", and "Delete all" icons. The main search area shows a query structure: "Molecular Formula" is linked to "Molecular Formula" via an "is" operator. Below this, a blue "AND" button is followed by a "Solubility" section. This section includes a "Find any" checkbox and a "Hide fields" link. The "Solubility" section is expanded to show several criteria: "Solubility, g-l-1", "Saturation", "Temperature (Solubility (MCS)), °C", "Solvent (Solubility (MCS))", and "Ratio of Solvents". On the right side, a "Search fields" dropdown menu is open, showing "solubility" as the selected field. Below it, a list of available fields includes "Solubility" and "Solubility Product". An orange arrow points from the "Solubility" field in the dropdown to the "Solubility" section in the main query builder. Another orange arrow points from the "Solubility" section in the main query builder to a text box containing a tip.

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

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all Structure Molecular Formula CAS RN TI, AB & KW

◇ Molecular Formula is Molecular Formula

AND ◇ Solubility Find any Hide fields ^

- = Solubility, g-l-1
- is Saturation
- = Temperature (Solubility (MCS)), °C
- is Solvent (Solubility (MCS))
- is Ratio of Solvents

Search fields Q solubility

- Solubility
- Solubility Product

Reaxys ^

Tips:
手动添加MF 与 Solubility的字段

条件的输入

Reaxys[®] Quick search [Query builder](#) Results Synthesis planner History

Search in: [Reactions](#) [Targets](#) [Substances](#) [Solvents](#)

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

◇ Molecular Formula is KCl

AND

◇ Solubility

- Find any Hide fields ^
- = Solubility, g l-1
- is Saturation
- = Temperature (Solubility (MCS)), °C
- is ethanol
- is Ratio of Solvents

Step3: 进行物质检索

Step1: 输入分子式KCl

Step2: 在溶剂一块选择乙醇

Solvent (Solubility (MCS)) 1 eth

<input type="checkbox"/>	ethane-1,2-diamine	23
<input type="checkbox"/>	ethane-1,2-diol	100
<input type="checkbox"/>	ethanesulfonic acid	1
<input checked="" type="checkbox"/>	ethanol	5,024
<input type="checkbox"/>	ethanol (99.4percent)	1
<input type="checkbox"/>	ethanol (99.8percent)	1
<input type="checkbox"/>	ethanol (99.9percent)	2
<input type="checkbox"/>	ethanol (99percent)	3
<input type="checkbox"/>	ethanolamine	3
<input type="checkbox"/>	ethyl acetate	1,062
<input type="checkbox"/>	ethyl benzoate	7
<input type="checkbox"/>	ethyl carbamate	6
<input type="checkbox"/>	ethyl nitrate	2

38 of 67 Go to page >

Clear selected × Transfer >

最后的结果

1 Substances out of 7,363 Documents, containing 4,322 Reactions, 68 Targets

0 selected Limit To Exclude Export Preparations Reaxys - 1

Sort by No of References Grid Heatmap

potassium chloride
CIK 74.5513 3534978

Hit Data - 20 Bioactivity (All) Other Data - 791 Preparations - 415
Identification Physical Data - 2,976 Reactions - 4,322
Druglikeness Spectra - 184 Targets - 68 Documents - 7,363

Hit Data - 20
Solubility (MCS) - 20 hits out of 429

Solubility (MCS) - 20 hits out of 429

Show/Hide columns

Solubility, g ⁻¹	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Comment (Solubility (MCS))	Reference
	20	ethanol	Solubility: 0.012 mol/kg solvent	El-Dossoki [Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
	25	ethanol	Solubility: 0.025 mol/kg solvent	El-Dossoki [Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
	30	ethanol	Solubility: 0.037 mol/kg solvent	El-Dossoki [Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
	35	ethanol	Solubility: 0.043 mol/kg solvent	El-Dossoki [Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical and Analytical, 2005, vol. 44, # 8, p. 1594 - 1596] Full Text Cited 6 times Details Abstract
0.320571		ethanol		Abakshin, V. A., Eliseeva, O. V., Krasnoperova, A. P., Lebedeva, L. T., Krestov, G. A. [Doklady Physical Chemistry, 1991, vol. 317, p. 303 - 306][Dokl. Phys. Chem. (Transl. of Dokl. Akad. Nauk.), 1991, vol. 317, p. 1140 - 1143] Full Text Details
	20	ethanol	Solubility: 1.270E0 mol/1000mol solvent	Kirm; Dunlap [Journal of the American Chemical Society, 1931, vol. 53, p. 393] Full Text Details
	45	ethanol	Solubility: 1.277E0 mol/1000mol solvent	Kirm; Dunlap [Journal of the American Chemical Society, 1931, vol. 53, p. 393] Full Text Details

Reaxys直接给出具体的数据和数据的文献出处，其实也可以设定更多的条件，如温度.....

Case 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

Reaxys

Quick search Query builder Results Synthesis planner History

Register > Sign in ?

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Search fields
Q catalyst

Reaxys ^

◇ Catalyst Investigation

◇ Reagent/Catalyst

◇ Molecular Formula is Molecular Formula

AND

◇ 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 name

Tips :
手动添加MF 与
Catalyst
Investigation的字段.

条件的输入

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

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

◇ Molecular Formula contains Fe

AND

◇ Catalyst Investigation

- is Investigated characteristic(s)
- is stereoselective catalysis
- is Classification of catalysis
- is Type of reaction
- is Co-catalyst/co-substrate name

Step3: 进行物质检索

Step1: 输入分子式Fe, 并将逻辑关系改成“Contains”, 即只要分子式中包含Fe, 就检索出来

Step2: Specification of Catalysis部分选择
立体选择性催化

Specification of catalysis 1

Search

<input type="checkbox"/> chemoselective catalysis	2,481
<input type="checkbox"/> immobilised catalyst	452
<input type="checkbox"/> phase-transfer catalysis	419
<input type="checkbox"/> regioselective catalysis	2,516
<input checked="" type="checkbox"/> stereoselective catalysis	9,365

最后的结果

Reaxys® Quick search Query builder **Results** Synthesis planner History Register > Sign in ⓘ

311 Filters
Limit to > Exclude >

311 Substances out of 33,712 Documents, containing 28,346 Reactions, 70 Targets
0 selected Limit To Exclude Export Preparations Search Sort by No of References ↓ Grid Heatmap

ferrocene
((C₅H₅)₂Fe) 186.036 11756767 102-54-5

Hit Data - 2 Bioactivity (All) Other Data - 241 Preparations - 896 >
Identification Physical Data - 3,483 Reactions - 3,636 >
Druglikeness Spectra - 514 Targets - 1 >
Documents - 13,609 >

Hit Data - 2
Catalyst Investigation - 2 hits out of 25 Show/Hide columns

Investigated characteristic(s)	Specification of catalysis	Type of reaction (Catalyst Investigation)	Location	Co-catalyst/co-substrate name	Reference
Catalytic activity, Diastereomeric excess	Stereoselective catalysis	Olefination		bathophenanthroline	Gao, Pin; Wu, Hao; Yang, Jun-Cheng; Guo, Li-Na[Organic Letters , 2019, vol. 21, # 17, p. 7104 - 7108] Full Text > Details > Abstract >
Catalytic activity, Diastereomeric excess	Stereoselective catalysis	Annulation	supporting information		Hou, Zhong-Wei; Yan, Hong; Song, Jin-Shuai; Xu, Hai-Chao[Chinese Journal of Chemistry , 2018, vol. 36, # 10, p. 909 - 915] Full Text > Cited 26 times > Details > Abstract >

Case 4: 钙钛矿类化合物的获取

- 检索含特定组分的“钙钛矿”类化合物如必须含Fe0.8, O3, 但是一定不含 La

The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, Query builder (selected), Results, Synthesis planner, History, and Alerts. The user's name, Sam Yu, is visible in the top right corner. Below the navigation, there is a search bar with the text "Search in:" and four buttons: Reactions, Targets, Substances, and Documents. Below the search bar, there are icons for Import, Save, Reset form, and Delete all. To the right of these icons are icons for Structure, Molecular Formula, CAS RN, and TI, AB & KW. The main area of the interface displays a query builder with three rows of search criteria:

- Linear Structure Formula contains Fe0.8
- AND Linear Structure Formula contains O3
- NOT Linear Structure Formula contains La

On the right side, there is a "Search fields" panel with a search input field containing "Linear|". Below this panel, there are sections for "Reaxys", "PubChem", and "Commercial Substances", each with a search input field and a list of search fields.

全部选择Contains, 并且根据逻辑关系定义Fe0.8 and O3 not La

Reaxys中的检索结果

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

263 Substances out of 217 Documents, containing 211 Reactions, 0 Targets

0 selected Limit To Exclude Export Preparations

Sort by No of References ↓ Grid Heatmap

Reaxys ID: 16164828
Bi(Fe0.8Mn0.2)O3 312.644 16164828

Identification
Druglikeness
Physical Data - 23
Spectra - 2

Preparations - 3 >
Reactions - 3 >
Documents - 9 >

Reaxys ID: 18094170
Co0.2Fe0.8O3Sr 192.094 18094170

Identification Physical Data - 18 Other Data - 1
Druglikeness Spectra - 4

Preparations - 6 >
Reactions - 6 >

Physical Data - 23
Crystal Phase - 6
Crystal System - 2
Electrical Data - 2
Magnetic Data - 5
Space Group - 6

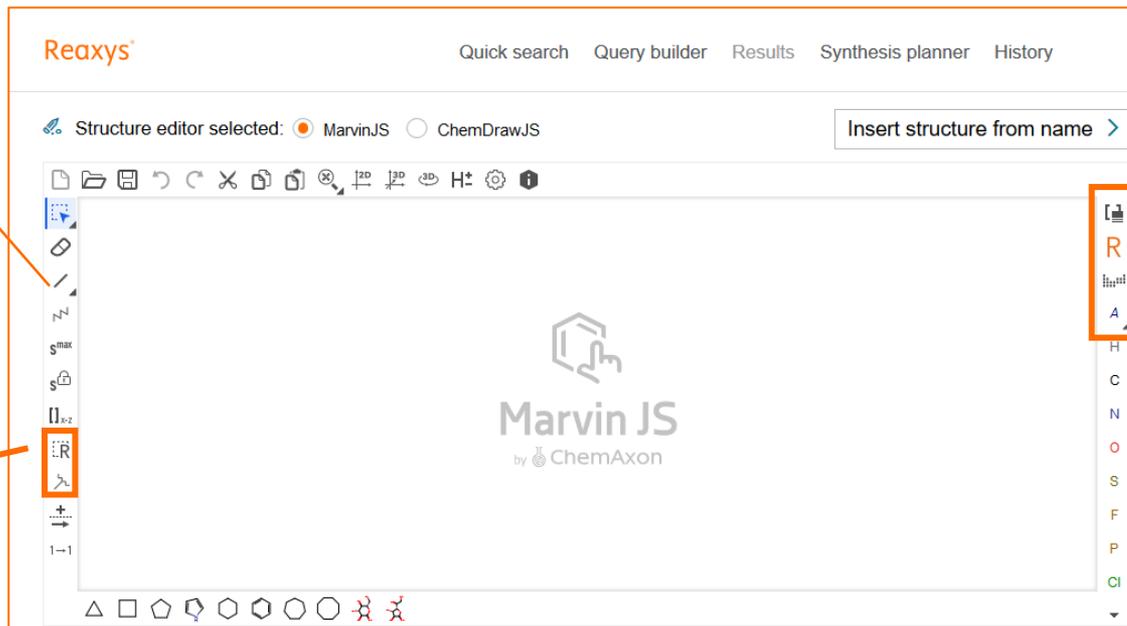
与该物质有关的XRD
有关的报道

Description (Crystal Phase)	Reference
Powder X-ray Diffraction	Kumar, Manoj; Yadav[Applied Physics Letters, 2007, vol. 91, # 24, art. no. 242901] Full Text ↗ Cited 118 times ↗ Details > Abstract >
	Jayakumar; Achary; Girija; Tyagi; Sudakar; Lawes; Naik; Nisar; Peng; Ahuja[Applied Physics Letters, 2010, vol. 96, # 3, art. no. 032903] Full Text ↗ Cited 63 times ↗ Details > Abstract >
Electron Diffraction	Jayakumar; Achary; Girija; Tyagi; Sudakar; Lawes; Naik; Nisar; Peng; Ahuja[Applied Physics Letters, 2010, vol. 96, # 3, art. no. 032903] Full Text ↗ Cited 63 times ↗ Details > Abstract >
Crystal growth forms	Lee; Yang; Jeong; Birge[Physica B: Condensed Matter, 2006, vol. 383, # 1, p. 31 - 32] Full Text ↗ Cited 6 times ↗ Details > Abstract >
	Takahashi, Kouhei; Tonouchi, Masayoshi[Journal of Magnetism and Magnetic Materials, 2007, vol. 310, # 2 SUPPL. PART 2, p. 1174 - 1176] Full Text ↗ Cited 37 times ↗ Details > Abstract >
	Xu; Ihlefeld; Lee; Ezekoye; Vlahos; Ramesh; Gopalan; Pan; Schliom; Musfeldt[Applied Physics Letters, 2010, vol. 96, # 19, art. no. 192901] Full Text ↗ Cited 49 times ↗ Details > Abstract >
crystal defects	Ianculescu, Adalina; Gheorghiu, Felicia Prihor; Postolache, Petrone; Oprea, Ovidiu; Mitoseriu, Liliana[Journal of Alloys and Compounds, 2010, vol. 504, # 2, p. 420 - 426] Full Text ↗ Cited 81 times ↗ Details > Abstract >

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
 - Reaxys对文献的提炼
 - Reaxys中物质与物性数据获取反向检索
 - Reaxys中结构面板与反应数据获取
 - Reaxys中的实用小案例
- Q&A

Reaxys中的结构面板



R基团定
义工具

缩写官能团，通
用官能团，原子
列表/列表非
原子属性列表

一些常见的功能使用视频

常用功能	视频链接
最基本功能	https://www.bilibili.com/video/BV13i4y177wV
不定位键	https://www.bilibili.com/video/BV1LK411P7nW
通用/缩写官能团	https://www.bilibili.com/video/BV1PV41117J6
原子列表与列表非	https://www.bilibili.com/video/BV1Ay4y1z7a5
R基团定义	https://www.bilibili.com/video/BV1654y1r7be
原子锁定与环锁定	https://www.bilibili.com/video/BV175411V77h
G Group与通用原子	https://www.bilibili.com/video/BV1fy4y1B7LU
原子属性列表	https://www.bilibili.com/video/BV1uD4y1R7K2
盐, 自由基, 同位素	https://www.bilibili.com/video/BV1Rr4y1c7AL

一些简单案例视频

常用功能	视频链接
合成计划的制作	https://www.bilibili.com/video/BV1Ni4y1L7Lt
机理性文献查询	https://www.bilibili.com/video/BV1pK4y1E7Qx
反应定义基本操作	https://www.bilibili.com/video/BV19r4y1w7Z5
反应条件的定义	https://www.bilibili.com/video/BV1Af4y1q7xk

Case 5: Reaxys中最简单的反应定义与筛选

- 检索以下核心结构反应并进行反应筛选操作
- 视频操作过程
 - <https://www.bilibili.com/video/BV1BT4y1F7vT>

The screenshot displays the Reaxys web interface. At the top, there are navigation links: "Quick search", "Query builder", "Results", "Synthesis planner", and "History". On the right side, there are buttons for "Register >" and "Sign in".

The main workspace shows a chemical reaction: benzaldehyde (a benzene ring with a formyl group, O=Cc1ccccc1) reacting to form benzyl alcohol (a benzene ring with a hydroxymethyl group, OCCc1ccccc1). The reaction is indicated by a right-pointing arrow.

Below the reaction, the text "原子匹配与原子锁定" (Atom matching and atom locking) is written. Two orange arrows point from this text to the left-hand side of the reaction diagram, specifically to the carbonyl carbon and the oxygen atom of the benzaldehyde molecule.

On the right side of the interface, there is a search filter panel titled "Search this structure as:". It contains several options with radio buttons and checkboxes:

- As drawn
- As substructure
- On all atoms
- On heteroatoms
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

At the bottom of the interface, there are buttons for "Clear", "Cancel", and "Transfer to query".

Reaxys中的结果

Reaxys® Quick search Query builder **Results** Synthesis planner History Register > Sign in ⓘ

10.11 K Filters

Limit to > Exclude >

By Structure > Yield > Reagent/Catalyst > Solvent > Catalyst Classes > Solvent Classes > Product Availability > Reactant Availability > Reaction Classes > Document Type > Publication Year >

10,112 Reactions out of 7,263 Documents containing 13,573 Substances, 2,788 Targets

0 Limit To Exclude Export Syn-Plan Show Conditions

Reaxys Ranking ↓ >

1  **Show/Hide Conditions, 选择显示/隐藏条件**

2  **55 Conditions** Find Similar > Reaction ID: 2407606

3  **38 Conditions** Find Similar > Reaction ID: 305004

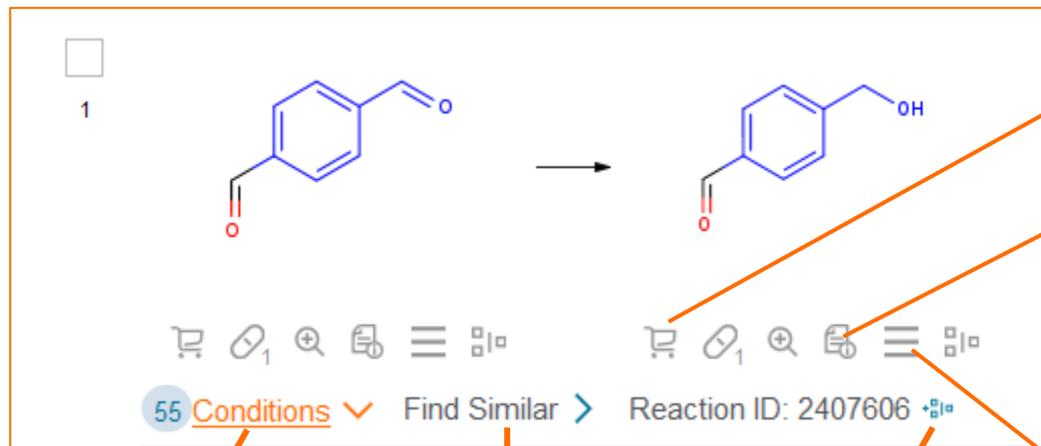
Single step reactions only

Experimental procedure only

1  **55 Conditions** Find Similar > Reaction ID: 2407606

Conditions	Yield	Reference
With formic acid, [(η ⁵ -C ₅ H ₅)Ru(κ ¹ -P-Ph ₂ Py)](PPh ₃)Cl; sodium hydroxide In water; acetonitrile at 80°C; for 8h;	92%	Kumar, Prashant; Singh, Ashish Kumar; Sharma, Sanjeev; Pandey, Daya Shankar [Journal of Organometallic Chemistry, 2009, vol. 694, # 22, p. 3643 - 3652] Full Text > Cited 21 times > Details > Abstract >
With bis(η ⁵ -cyclopentadienyl)hafnium dihydride In isopropyl alcohol at 80°C; for 8h;	91%	Nakano, Tatsuya; Umano, Shigetoshi; Kino, Yoshio; Ishii, Yasutaka; Ogawa, Masaya [Journal of Organic Chemistry, 1988, vol. 53, # 16, p. 3752 - 3757] Full Text > Details > Abstract >
With sodium tetrahydroborate In ethanol at 0°C; for 1h; Experimental Procedure >	91%	AKITA INNOVATIONS LLC; BARDON, Kevin M.; MINNS, Richard, A.; SELFRIDGE, Scott, D.; TAKIFF, Larry; ADAMS, Timothy WO2018/217266, 2018, A1 Location in patent: Page/Page column 52; 53 Full Text > Details > Abstract >

Reaxys的一条反应的界面



查看商业来源

查看物质详情

4-(hydroxymethyl)benzaldehyde ×
HCO₂C₆H₄CH₂OH 136.15 878348 52010-97-6

Identification	Physical Data - 28	Preparations - 35
Druglikeness	Spectra - 84	Reactions - 745
Bioactivity (All)		Targets - 1
		Documents - 251

[View Details >](#)

查看条件

寻找相似反应

合成计划按钮

更多与物质相关操作

Find Similar Reactions... ×

Click on one of the hyperlinks below for getting similar reactions according to the selected scope: the reactions were determined by regarding similar transition states based on your reaction query

Query Reaction	Tight ⌵	Near ⌵	Medium ⌵	Wide ⌵	Widest ⌵
	1,612	6,822	6,827	6,878	40,060

Options ×

- [Find Similar](#)
- [View related Markush](#)
- [View details](#)

- [Copy structure to query](#)
- [Copy reaction to query](#)
- [Use as filter](#)
- [Open in database](#)

Reaxys的筛选操作

Filters

Limit to > Exclude >

- By Structure ▾
- Yield ▾
- Reagent/Catalyst ▾
- Solvent ▾
- Catalyst Classes ▾
- Solvent Classes ▾
- Product Availability ▾
- Reactant Availability ▾
- Reaction Classes ▾
- Document Type ▾
- Publication Year ▾
- Single step reactions only
- Experimental procedure only

Yield

<input type="checkbox"/> >95 - 100	924
<input type="checkbox"/> >90 - 95	835
<input type="checkbox"/> >85 - 90	614
<input type="checkbox"/> >80 - 85	456
<input type="checkbox"/> >75 - 80	375
<input type="checkbox"/> >70 - 75	287
<input type="checkbox"/> >65 - 70	223

Filter by value ▾ [View more](#)

Reagent/Catalyst

<input type="checkbox"/> sodium tetrahydroborate	7,079
<input type="checkbox"/> methanol	1,387
<input type="checkbox"/> potassium carbonate	1,236
<input type="checkbox"/> water	690
<input type="checkbox"/> lithium aluminium tetrahydride	639
<input type="checkbox"/> hydrogen	620
<input type="checkbox"/> hydrogenchloride	599

Filter by value ▾ [View more](#)

Solvent

<input type="checkbox"/> methanol	4,014
<input type="checkbox"/> tetrahydrofuran	3,375
<input type="checkbox"/> ethanol	2,025
<input type="checkbox"/> water	1,395
<input type="checkbox"/> dichloromethane	1,268
<input type="checkbox"/> n,n-dimethyl-formamide	1,105
<input type="checkbox"/> toluene	515

Filter by value ▾ [View more](#)

Document Type

<input type="checkbox"/> article	7,543
<input type="checkbox"/> patent	3,181
<input type="checkbox"/> review	68
<input type="checkbox"/> conference paper	44
<input type="checkbox"/> letter	11
<input type="checkbox"/> short survey	4
<input type="checkbox"/> note	4

[View more](#)

Publication Year

<input type="checkbox"/> 2020	393
<input type="checkbox"/> 2019	788
<input type="checkbox"/> 2018	834
<input type="checkbox"/> 2017	780
<input type="checkbox"/> 2016	921
<input type="checkbox"/> 2015	829
<input type="checkbox"/> 2014	755

Filter by value ▾ [View more](#)

Tips:

常见的一些反应筛选工具，
如：收率，催化剂/试剂，溶剂，
文献类型，出版年限等

Reaxys中的一些特殊筛选工具—溶剂分类

The image displays two panels from the Reaxys interface. The left panel shows a list of solvent classes with checkboxes and counts. The right panel shows a detailed view of the 'Solvent Classes' filter, including a tree view of the categories and their counts, along with control buttons like 'Clear selected', 'Limit to', and 'Exclude'.

Solvent Class	Count
Low boiling (<100°C)	8,385
Green	6,424
Protic	6,352
Aprotic apolar	4,172
Yellow	4,056
Aprotic dipolar	3,179
Red	3,119
High boiling (>150°C)	1,354
Middle boiling(100°C - 150°C)	912
Inorganic	88

[View more](#)

Solvent Classes (Total: 10,112)

- Solvent Classes (10,112)
- Low boiling (<100°C) (8,385)
- Green (6,424)
- Protic (6,352)
- Aprotic apolar (4,172)
- Yellow (4,056)
- Aprotic dipolar (3,179)
- Red (3,119)
- High boiling (>150°C) (1,354)
- Middle boiling(100°C - 150°C) (912)
- Inorganic (88)

Clear selected X Limit to > Exclude >

Reaxys中的一些特殊筛选工具—催化剂分类

Catalyst Classes ^

- active center 8,926
- heterogeneous 297
- organism / enzymes 52

[View more](#)

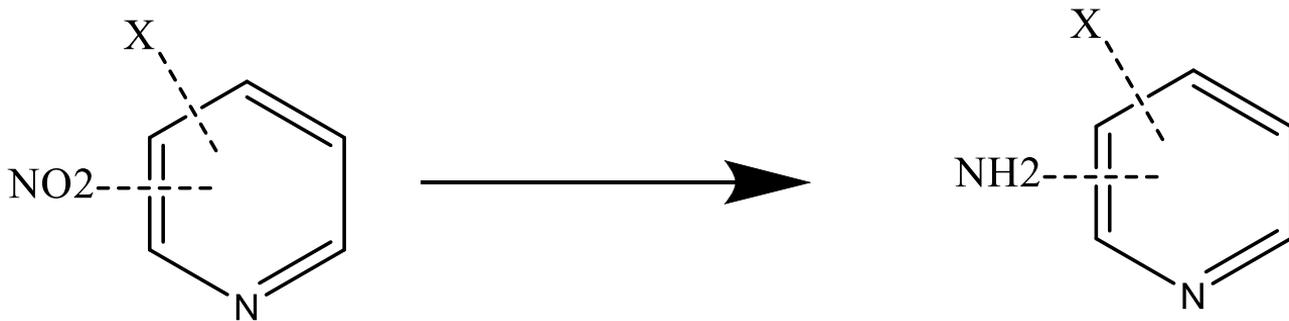
Catalyst Classes ×

- ▼ Catalyst Classes 10,112
 - ▼ active center 8,926
 - > B 7,587
 - > Al 956
 - > Pd 803
 - ▼ Cu 288
 - copper(I) iodide 160
 - copper 40
 - copper(II) oxide 35
 - copper(I) chloride 13
 - copper diacetate 11
 - copper oxide-chromium oxide 10

Clear selected × Limit to > Exclude >

Case 6: 结构中有特殊需求的反应定义

- 检索以下反应
 - 吡啶环上存在一个硝基，一个卤素，且这两个官能团处于邻位
 - 反应过后硝基还原成氨基
 - 定义难点：如果确保NO₂和卤素处于邻位



视频操作过程:

<https://www.bilibili.com/video/BV1si4y177as>

Reaxys中的结构定义

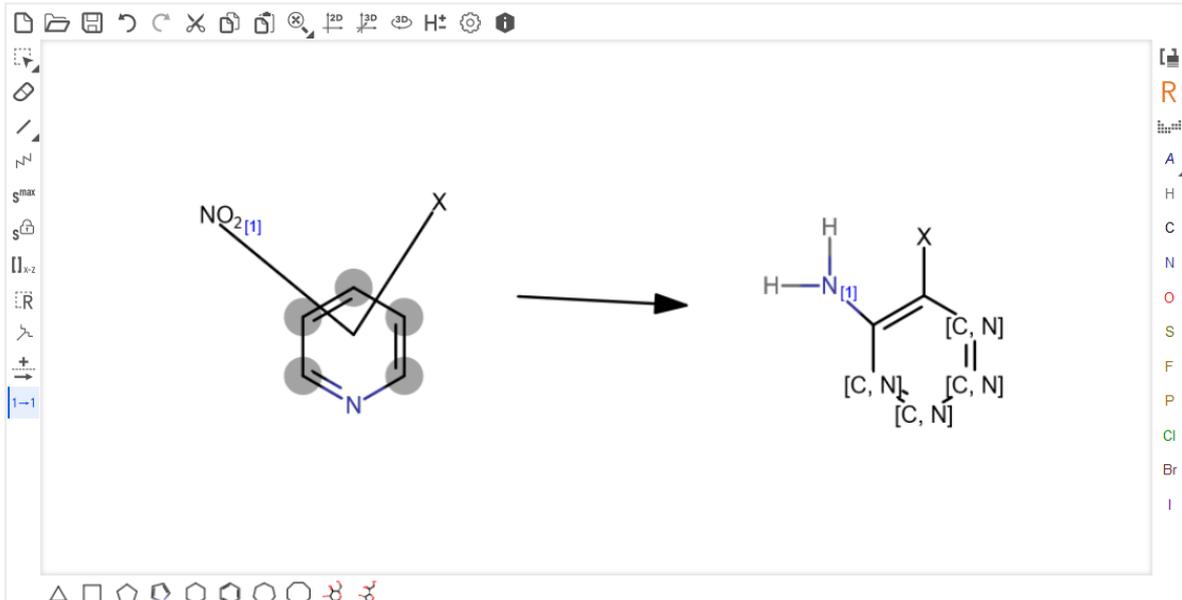
Reaxys

Quick search Query builder Results Synthesis planner History

Register > Sign in ⓘ

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >



Search this structure as:

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

- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Clear  Cancel × Transfer to query >

最后的结果

Reaxys[®] Quick search Query builder **Results** Synthesis planner

624 Filters 624 Reactions out of 434 Documents containing 791 Substances, 37 Targets

Limit to > Exclude > 0 selected Limit To Exclude Export Syn-Plan Show Conditions

By Structure > Yield > Reagent/Catalyst > Solvent > Catalyst Classes > Solvent Classes > Product Availability > Reactant Availability > Reaction Classes > Document Type > Publication Year >

Single step reactions only
 Experimental procedure only

1



6 Conditions Find Similar > Reaction ID: 149845

2



7 Conditions Find Similar > Reaction ID: 22895930

3



1



6 Conditions Find Similar > Reaction ID: 149845

Conditions	Yield	Reference
With hydrogen in methanol at 20°C, for 2h; Experimental Procedure >	96%	LIFESCI PHARMACEUTICALS, INC.; MCDONALD, Andrew, QIAN, Shawn WO2017/1936, 2017, A2 Location in patent: Paragraph 00159 Full Text > Details > Abstract >
With hydrogen, nickel in ethanol at 20°C, under 760.051 Torr, for 4h; Experimental Procedure >	95%	UNIVERSITY OF GEORGIA RESEARCH FOUNDATION, INC. WO2007/47793, 2007, A2 Location in patent: Page/Page column 87 Full Text > Details > Abstract >
With iron, acetic acid Erwärmen des Reaktionsgemisches mit HgCl ₂ und Zink.		Talík, Plazek. [Roczniki Chemii. 1956, vol. 30, p. 1130,1145.][Chem.Abstr., <1957> 12089] Full Text > Details >

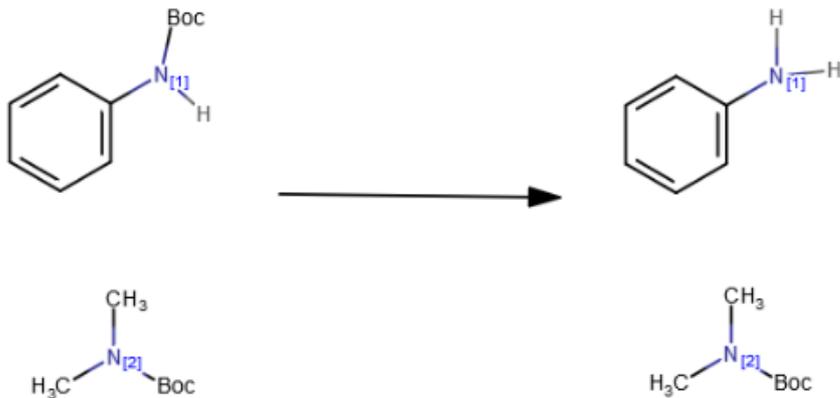
Experimental Procedure

4-Amino-2-chloro-3-nitropyridine (6.0 g, 34.57 mmol) in 150 mL of ethanol was hydrogenated over Raney nickel catalyst (6.0 g wet) for 4h at room temperature under 1.0 atm of H₂ atmosphere. After addition of 4.0 g of celite to the solution, the mixture was stirred vigorously and filtered over celite pad. The filtrate was concentrated and purified with silica gel column chromatography (CH₂Cl₂:MeOH = 20:1 v/v) to give 2-Chloro-3,4-diaminopyridine (4.72 g, 32.84 mmol) in 95% yield. ¹H-NMR (DMSO, 500 MHz) δ 7.31 (d, J = 5.0, 1H), 6.45 (d, J = 5.0, 1H), 5.79 (s, 2H), 4.68 (s, 2H); ¹³C-NMR (DMSO, 125 MHz) δ 143.41, 138.03, 135.61, 126.66, 108.73, 1.

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

Case 7: 选择性氧化还原脱保护反应的定义

- 结构中两个带Boc的片段，两个片段以任意的形式相接在一个分子中
- 反应过后把其中一个片段的Boc脱掉，但是另外一个Boc不变



视频操作过程:

<https://www.bilibili.com/video/BV1Vv411r7Bc>

Reaxys中的结构定义

Reaxys

Quick search Query builder Results Synthesis planner History Register > Sign in

Structure editor selected: MarvinJS ChemDrawJS

Insert structure 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

Ignore Atom Mappings

Keep fragments

Separate Together

Clear Cancel Transfer to query >

Reaxys可以直接设定这些片段在一个结构中

Reaxys中结果

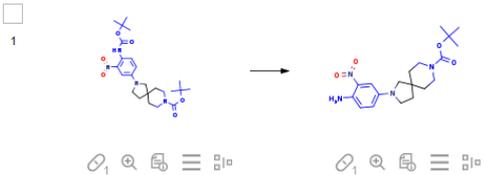
Reaxys[®] Quick search Query builder **Results** Synthesis planner History

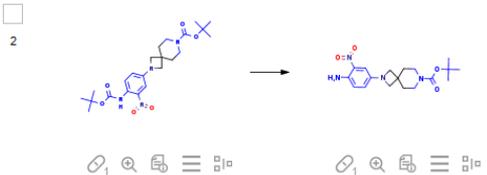
12 Reactions out of 8 Documents containing 22 Substances, 5 Targets

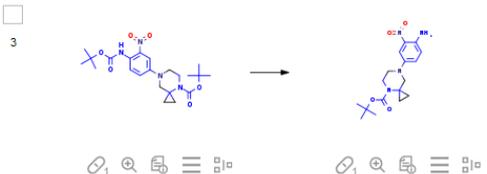
Limit to > Exclude >

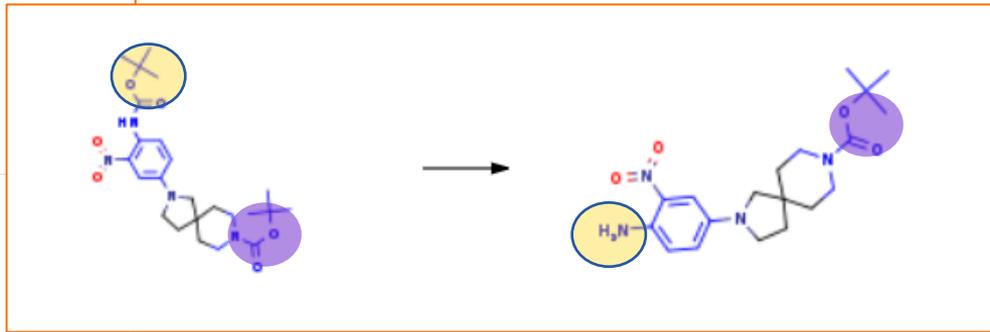
By Structure > Yield > Reagent/Catalyst > Solvent > Catalyst Classes > Solvent Classes > Product Availability > Reactant Availability > Reaction Classes > Document Type > Publication Year >

Single step reactions only
 Experimental procedure only

1 
1 Conditions Find Similar > Reaction ID: 51038227

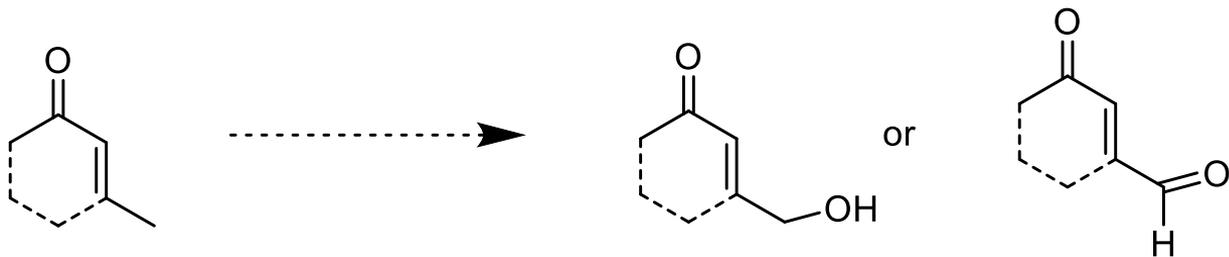
2 
1 Conditions Find Similar > Reaction ID: 51038186

3 



Case 8: 涉及环系变化的反应定义

- 获取以下反应



Requirement:

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

<https://www.bilibili.com/video/BV1gv411r7oc>

Reaxys中的定义

The screenshot displays the Reaxys software interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Synthesis planner, History, and Alerts. The user's name, Sam Yu, is visible in the top right corner. The main workspace is the Structure editor, which is currently set to MarvinJS. It shows a chemical structure of a bicyclic compound with a methyl group (CH₃) and a nitrogen atom (N1) at position 1-10. An arrow points to the same structure with the methyl group replaced by a generic R₁ group. To the right, the R₁ definition is shown as a CH₂OH group. The search options panel on the right is titled "Search this structure as:" and includes several options: As drawn, As substructure (selected), On all atoms, On heteroatoms, and Similar. There are also checkboxes for Tautomers, Stereo, Additional ring closures, and Related Markush. A list of elements (R, A, H, C, N, O, S, F, P, Cl, Br, I) is visible on the left side of the search panel. At the bottom of the interface, there are buttons for Clear, Cancel, and Transfer to query.

定义方法:

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

最后的结果

Reaxys®

Quick search Query builder Results Synthesis planner History

63 Reactions out of 41 Documents containing 92 Substances, 72 Targets

0 selected Limit To Exclude Export Syn-Plan Show Conditions

83 Preview

Filters

- Limit to > Exclude >
- By Structure ▾
- Yield ▾
- Reagent/Catalyst ▾
- Solvent ▾
- Catalyst Classes ▾
- Solvent Classes ▾
- Product Availability ▾
- Reactant Availability ▾
- Reaction Classes ▾
- Document Type ▾
- Publication Year ▾
- Single step reactions only
- Experimental procedure only

1



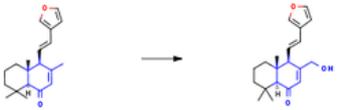
1 Conditions ▾ Find Similar > Reaction ID: 39179987

2



1 Conditions ▾ Find Similar > Reaction ID: 53952384

3



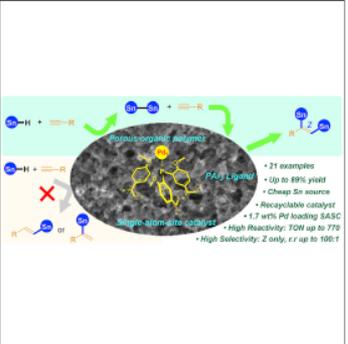
Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
 - Reaxys对文献的提炼
 - Reaxys中物质与物性数据获取反向检索
 - Reaxys中结构面板与反应数据获取
 - Reaxys中的实用小案例
- Q&A

Case 9: 化合物的文献定位

Chem 

Article
Porous Ligand Creates New Reaction Route:
Bifunctional Single-Atom Palladium Catalyst
for Selective Distannylation of Terminal
Alkynes



Wen-Yong Huang, Guo-Qing Wang, Wen-Hao Li, ..., Hai-Tao Tang, Ying-Ming Pan, Yun-Jie Ding
htang@pku.edu.cn (H.-T.T.),
panym@mailbox.pku.edu.cn (Y.-M.P.),
dyj@pku.edu.cn (Y.-J.D.)

HIGHLIGHTS
Design a single-atom-site catalyst based on organic synthesis mechanism

Utilizing pores, ligands, and SAS for synergistic controlling reaction paths

A highly selective distannylation of terminal alkynes was achieved

We proposed a unique research concept of "mechanism-oriented catalyst design": The structural elements of single-atom catalyst are designed according to the requirements of organic synthesis mechanism. This concept is totally different from the previous "electrocatalytic" single-atom-site research concept. This work suggests that single-atom-site catalysts not only afford an efficient platform for transforming homogeneous reactions into heterogeneous reactions, but also possess many interesting potentials in developing new synthetic reactions and solving homogeneous reaction problems.

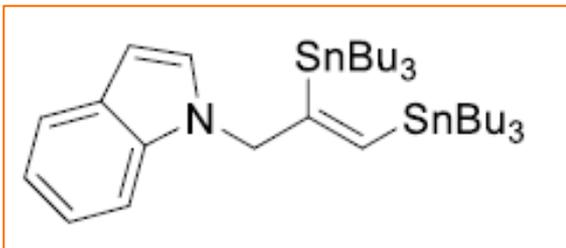
Huang et al., Chem 6, 200–213
September 10, 2020 © 2020 Elsevier Inc.
<https://doi.org/10.1016/j.chem.2020.08.020>



这是一篇常见的化学文献，包含：

1. 15页PDF全文
2. 52页Support Information文档

已知文献中报道了这个化合物，如何在上述的67页文档中找到有关这个化合物的描述？



视频操作过程：

<https://www.bilibili.com/video/BV1gA411x7KE>

Reaxys中的检索

- Query Builder联合化合物结构与文献DOI号

The screenshot displays the Reaxys Query Builder interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', 'History', and 'Alerts' are on the right. Below this is a search bar with 'Search in:' and four buttons: 'Reactions >', 'Targets >', 'Substances >', and 'Documents >'. A secondary toolbar contains icons for 'Import', 'Save', 'Reset form', 'Delete all', 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The main workspace is a large dashed box labeled 'Structure' containing a chemical structure of a tin(IV) complex. The structure features a central tin atom coordinated to two ethyl groups and two butyl groups, with a double bond to a carbon atom that is also bonded to a nitrogen atom in a five-membered ring system. Below the structure, the text 'As drawn' is visible. At the bottom of the interface, there is a search query field with a dropdown menu set to 'AND', a search icon, and the query text 'DOI is 10.1016/fj.chempr.2020.06.020'.

Reaxys中的结果

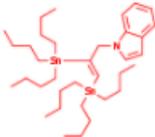
1 Substances out of 1 Documents, containing 1 Reactions, 0 Targets

0 selected Limit To Exclude Export Preparations

Reaxys - 1

Sort by No of References ↓ Grid Heatmap

1



(Z)-1-(2,3-bis(tributylstannyl)allyl)-1H-indole
C₃₅H₆₃N₅Sn₂ 735.312 36450188

Hit Data - 6 Druglikeness Spectra - 3 Preparations - 1 >
Identification Physical Data - 2 Reactions - 1 >
Documents - 1 >

Hit Data - 6

- Substance Label - 1 hits out of 1
- Chromatographic Data - 1 hits out of 1
- Crystal Property Description - 1 hits out of 1
- NMR Spectroscopy - 2 hits out of 2
- Mass Spectrometry - 1 hits out of 1

Hit Data - 6

Substance Label - 1 hits out of 1

Label	Reference
3j	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, - 2313]

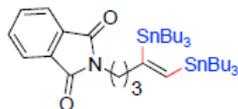
Full Text ↗ Details > Abstract >

全文检索3J定位化合物

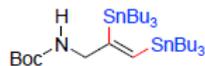
N-containing terminal alkynes



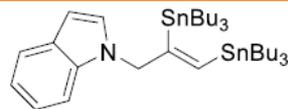
3j 89% (100:1)



3k 58% (25:1)



3n 81% (100:1)



(Z)-1-(2,3-bis(tributylstannyl)allyl)-1H-indole **3j**: colorless oil. Petroleum ether as eluent for column chromatography (**3j**, $R_f = 0.75$; **2j**, $R_f = 0.4$, 42% of alkyne was isolated and recovered); ^1H NMR (400 MHz, CDCl_3) $\delta = 7.52$ (1H, d, $J = 7.8$ Hz), 7.15 (1H, d, $J = 8.2$ Hz), 7.08-7.03 (1H, m), 7.01-6.95 (1H, m), 6.93 (1H, d, $J = 3.1$ Hz), 6.46 (1H, s, $J = 168.4$ Hz, 65.5 Hz), 6.40 (1H, d, $J = 3.1$ Hz), 4.78 (2H, d, $J = 1.3$ Hz), 1.40-1.25 (12H, m), 1.22-1.14 (12H, m), 0.88-0.72 (30H, m). ^{13}C NMR (400 MHz, CDCl_3) $\delta = 160.6, 144.4, 136.1, 135.9, 135.8, 135.7, 135.6, 135.5, 135.4, 135.3, 135.2, 135.1, 135.0, 134.9, 134.8, 134.7, 134.6, 134.5, 134.4, 134.3, 134.2, 134.1, 134.0, 133.9, 133.8, 133.7, 133.6, 133.5, 133.4, 133.3, 133.2, 133.1, 133.0, 132.9, 132.8, 132.7, 132.6, 132.5, 132.4, 132.3, 132.2, 132.1, 132.0, 131.9, 131.8, 131.7, 131.6, 131.5, 131.4, 131.3, 131.2, 131.1, 131.0, 130.9, 130.8, 130.7, 130.6, 130.5, 130.4, 130.3, 130.2, 130.1, 130.0, 129.9, 129.8, 129.7, 129.6, 129.5, 129.4, 129.3, 129.2, 129.1, 129.0, 128.9, 128.8, 128.7, 128.6, 128.5, 128.4, 128.3, 128.2, 128.1, 128.0, 127.9, 127.8, 127.7, 127.6, 127.5, 127.4, 127.3, 127.2, 127.1, 127.0, 126.9, 126.8, 126.7, 126.6, 126.5, 126.4, 126.3, 126.2, 126.1, 126.0, 125.9, 125.8, 125.7, 125.6, 125.5, 125.4, 125.3, 125.2, 125.1, 125.0, 124.9, 124.8, 124.7, 124.6, 124.5, 124.4, 124.3, 124.2, 124.1, 124.0, 123.9, 123.8, 123.7, 123.6, 123.5, 123.4, 123.3, 123.2, 123.1, 123.0, 122.9, 122.8, 122.7, 122.6, 122.5, 122.4, 122.3, 122.2, 122.1, 122.0, 121.9, 121.8, 121.7, 121.6, 121.5, 121.4, 121.3, 121.2, 121.1, 121.0, 120.9, 120.8, 120.7, 120.6, 120.5, 120.4, 120.3, 120.2, 120.1, 120.0, 119.9, 119.8, 119.7, 119.6, 119.5, 119.4, 119.3, 119.2, 119.1, 119.0, 118.9, 118.8, 118.7, 118.6, 118.5, 118.4, 118.3, 118.2, 118.1, 118.0, 117.9, 117.8, 117.7, 117.6, 117.5, 117.4, 117.3, 117.2, 117.1, 117.0, 116.9, 116.8, 116.7, 116.6, 116.5, 116.4, 116.3, 116.2, 116.1, 116.0, 115.9, 115.8, 115.7, 115.6, 115.5, 115.4, 115.3, 115.2, 115.1, 115.0, 114.9, 114.8, 114.7, 114.6, 114.5, 114.4, 114.3, 114.2, 114.1, 114.0, 113.9, 113.8, 113.7, 113.6, 113.5, 113.4, 113.3, 113.2, 113.1, 113.0, 112.9, 112.8, 112.7, 112.6, 112.5, 112.4, 112.3, 112.2, 112.1, 112.0, 111.9, 111.8, 111.7, 111.6, 111.5, 111.4, 111.3, 111.2, 111.1, 111.0, 110.9, 110.8, 110.7, 110.6, 110.5, 110.4, 110.3, 110.2, 110.1, 110.0, 109.9, 109.8, 109.7, 109.6, 109.5, 109.4, 109.3, 109.2, 109.1, 109.0, 108.9, 108.8, 108.7, 108.6, 108.5, 108.4, 108.3, 108.2, 108.1, 108.0, 107.9, 107.8, 107.7, 107.6, 107.5, 107.4, 107.3, 107.2, 107.1, 107.0, 106.9, 106.8, 106.7, 106.6, 106.5, 106.4, 106.3, 106.2, 106.1, 106.0, 105.9, 105.8, 105.7, 105.6, 105.5, 105.4, 105.3, 105.2, 105.1, 105.0, 104.9, 104.8, 104.7, 104.6, 104.5, 104.4, 104.3, 104.2, 104.1, 104.0, 103.9, 103.8, 103.7, 103.6, 103.5, 103.4, 103.3, 103.2, 103.1, 103.0, 102.9, 102.8, 102.7, 102.6, 102.5, 102.4, 102.3, 102.2, 102.1, 102.0, 101.9, 101.8, 101.7, 101.6, 101.5, 101.4, 101.3, 101.2, 101.1, 101.0, 100.9, 100.8, 100.7, 100.6, 100.5, 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83.8, 83.7, 83.6, 83.5, 83.4, 83.3, 83.2, 83.1, 83.0, 82.9, 82.8, 82.7, 82.6, 82.5, 82.4, 82.3, 82.2, 82.1, 82.0, 81.9, 81.8, 81.7, 81.6, 81.5, 81.4, 81.3, 81.2, 81.1, 81.0, 80.9, 80.8, 80.7, 80.6, 80.5, 80.4, 80.3, 80.2, 80.1, 80.0, 79.9, 79.8, 79.7, 79.6, 79.5, 79.4, 79.3, 79.2, 79.1, 79.0, 78.9, 78.8, 78.7, 78.6, 78.5, 78.4, 78.3, 78.2, 78.1, 78.0, 77.9, 77.8, 77.7, 77.6, 77.5, 77.4, 77.3, 77.2, 77.1, 77.0, 76.9, 76.8, 76.7, 76.6, 76.5, 76.4, 76.3, 76.2, 76.1, 76.0, 75.9, 75.8, 75.7, 75.6, 75.5, 75.4, 75.3, 75.2, 75.1, 75.0, 74.9, 74.8, 74.7, 74.6, 74.5, 74.4, 74.3, 74.2, 74.1, 74.0, 73.9, 73.8, 73.7, 73.6, 73.5, 73.4, 73.3, 73.2, 73.1, 73.0, 72.9, 72.8, 72.7, 72.6, 72.5, 72.4, 72.3, 72.2, 72.1, 72.0, 71.9, 71.8, 71.7, 71.6, 71.5, 71.4, 71.3, 71.2, 71.1, 71.0, 70.9, 70.8, 70.7, 70.6, 70.5, 70.4, 70.3, 70.2, 70.1, 70.0, 69.9, 69.8, 69.7, 69.6, 69.5, 69.4, 69.3, 69.2, 69.1, 69.0, 68.9, 68.8, 68.7, 68.6, 68.5, 68.4, 68.3, 68.2, 68.1, 68.0, 67.9, 67.8, 67.7, 67.6, 67.5, 67.4, 67.3, 67.2, 67.1, 67.0, 66.9, 66.8, 66.7, 66.6, 66.5, 66.4, 66.3, 66.2, 66.1, 66.0, 65.9, 65.8, 65.7, 65.6, 65.5, 65.4, 65.3, 65.2, 65.1, 65.0, 64.9, 64.8, 64.7, 64.6, 64.5, 64.4, 64.3, 64.2, 64.1, 64.0, 63.9, 63.8, 63.7, 63.6, 63.5, 63.4, 63.3, 63.2, 63.1, 63.0, 62.9, 62.8, 62.7, 62.6, 62.5, 62.4, 62.3, 62.2, 62.1, 62.0, 61.9, 61.8, 61.7, 61.6, 61.5, 61.4, 61.3, 61.2, 61.1, 61.0, 60.9, 60.8, 60.7, 60.6, 60.5, 60.4, 60.3, 60.2, 60.1, 60.0, 59.9, 59.8, 59.7, 59.6, 59.5, 59.4, 59.3, 59.2, 59.1, 59.0, 58.9, 58.8, 58.7, 58.6, 58.5, 58.4, 58.3, 58.2, 58.1, 58.0, 57.9, 57.8, 57.7, 57.6, 57.5, 57.4, 57.3, 57.2, 57.1, 57.0, 56.9, 56.8, 56.7, 56.6, 56.5, 56.4, 56.3, 56.2, 56.1, 56.0, 55.9, 55.8, 55.7, 55.6, 55.5, 55.4, 55.3, 55.2, 55.1, 55.0, 54.9, 54.8, 54.7, 54.6, 54.5, 54.4, 54.3, 54.2, 54.1, 54.0, 53.9, 53.8, 53.7, 53.6, 53.5, 53.4, 53.3, 53.2, 53.1, 53.0, 52.9, 52.8, 52.7, 52.6, 52.5, 52.4, 52.3, 52.2, 52.1, 52.0, 51.9, 51.8, 51.7, 51.6, 51.5, 51.4, 51.3, 51.2, 51.1, 51.0, 50.9, 50.8, 50.7, 50.6, 50.5, 50.4, 50.3, 50.2, 50.1, 50.0, 49.9, 49.8, 49.7, 49.6, 49.5, 49.4, 49.3, 49.2, 49.1, 49.0, 48.9, 48.8, 48.7, 48.6, 48.5, 48.4, 48.3, 48.2, 48.1, 48.0, 47.9, 47.8, 47.7, 47.6, 47.5, 47.4, 47.3, 47.2, 47.1, 47.0, 46.9, 46.8, 46.7, 46.6, 46.5, 46.4, 46.3, 46.2, 46.1, 46.0, 45.9, 45.8, 45.7, 45.6, 45.5, 45.4, 45.3, 45.2, 45.1, 45.0, 44.9, 44.8, 44.7, 44.6, 44.5, 44.4, 44.3, 44.2, 44.1, 44.0, 43.9, 43.8, 43.7, 43.6, 43.5, 43.4, 43.3, 43.2, 43.1, 43.0, 42.9, 42.8, 42.7, 42.6, 42.5, 42.4, 42.3, 42.2, 42.1, 42.0, 41.9, 41.8, 41.7, 41.6, 41.5, 41.4, 41.3, 41.2, 41.1, 41.0, 40.9, 40.8, 40.7, 40.6, 40.5, 40.4, 40.3, 40.2, 40.1, 40.0, 39.9, 39.8, 39.7, 39.6, 39.5, 39.4, 39.3, 39.2, 39.1, 39.0, 38.9, 38.8, 38.7, 38.6, 38.5, 38.4, 38.3, 38.2, 38.1, 38.0, 37.9, 37.8, 37.7, 37.6, 37.5, 37.4, 37.3, 37.2, 37.1, 37.0, 36.9, 36.8, 36.7, 36.6, 36.5, 36.4, 36.3, 36.2, 36.1, 36.0, 35.9, 35.8, 35.7, 35.6, 35.5, 35.4, 35.3, 35.2, 35.1, 35.0, 34.9, 34.8, 34.7, 34.6, 34.5, 34.4, 34.3, 34.2, 34.1, 34.0, 33.9, 33.8, 33.7, 33.6, 33.5, 33.4, 33.3, 33.2, 33.1, 33.0, 32.9, 32.8, 32.7, 32.6, 32.5, 32.4, 32.3, 32.2, 32.1, 32.0, 31.9, 31.8, 31.7, 31.6, 31.5, 31.4, 31.3, 31.2, 31.1, 31.0, 30.9, 30.8, 30.7, 30.6, 30.5, 30.4, 30.3, 30.2, 30.1, 30.0, 29.9, 29.8, 29.7, 29.6, 29.5, 29.4, 29.3, 29.2, 29.1, 29.0, 28.9, 28.8, 28.7, 28.6, 28.5, 28.4, 28.3, 28.2, 28.1, 28.0, 27.9, 27.8, 27.7, 27.6, 27.5, 27.4, 27.3, 27.2, 27.1, 27.0, 26.9, 26.8, 26.7, 26.6, 26.5, 26.4, 26.3, 26.2, 26.1, 26.0, 25.9, 25.8, 25.7, 25.6, 25.5, 25.4, 25.3, 25.2, 25.1, 25.0, 24.9, 24.8, 24.7, 24.6, 24.5, 24.4, 24.3, 24.2, 24.1, 24.0, 23.9, 23.8, 23.7, 23.6, 23.5, 23.4, 23.3, 23.2, 23.1, 23.0, 22.9, 22.8, 22.7, 22.6, 22.5, 22.4, 22.3, 22.2, 22.1, 22.0, 21.9, 21.8, 21.7, 21.6, 21.5, 21.4, 21.3, 21.2, 21.1, 21.0, 20.9, 20.8, 20.7, 20.6, 20.5, 20.4, 20.3, 20.2, 20.1, 20.0, 19.9, 19.8, 19.7, 19.6, 19.5, 19.4, 19.3, 19.2, 19.1, 19.0, 18.9, 18.8, 18.7, 18.6, 18.5, 18.4, 18.3, 18.2, 18.1, 18.0, 17.9, 17.8, 17.7, 17.6, 17.5, 17.4, 17.3, 17.2, 17.1, 17.0, 16.9, 16.8, 16.7, 16.6, 16.5, 16.4, 16.3, 16.2, 16.1, 16.0, 15.9, 15.8, 15.7, 15.6, 15.5, 15.4, 15.3, 15.2, 15.1, 15.0, 14.9, 14.8, 14.7, 14.6, 14.5, 14.4, 14.3, 14.2, 14.1, 14.0, 13.9, 13.8, 13.7, 13.6, 13.5, 13.4, 13.3, 13.2, 13.1, 13.0, 12.9, 12.8, 12.7, 12.6, 12.5, 12.4, 12.3, 12.2, 12.1, 12.0, 11.9, 11.8, 11.7, 11.6, 11.5, 11.4, 11.3, 11.2, 11.1, 11.0, 10.9, 10.8, 10.7, 10.6, 10.5, 10.4, 10.3, 10.2, 10.1, 10.0, 9.9, 9.8, 9.7, 9.6, 9.5, 9.4, 9.3, 9.2, 9.1, 9.0, 8.9, 8.8, 8.7, 8.6, 8.5, 8.4, 8.3, 8.2, 8.1, 8.0, 7.9, 7.8, 7.7, 7.6, 7.5, 7.4, 7.3, 7.2, 7.1, 7.0, 6.9, 6.8, 6.7, 6.6, 6.5, 6.4, 6.3, 6.2, 6.1, 6.0, 5.9, 5.8, 5.7, 5.6, 5.5, 5.4, 5.3, 5.2, 5.1, 5.0, 4.9, 4.8, 4.7, 4.6, 4.5, 4.4, 4.3, 4.2, 4.1, 4.0, 3.9, 3.8, 3.7, 3.6, 3.5, 3.4, 3.3, 3.2, 3.1, 3.0, 2.9, 2.8, 2.7, 2.6, 2.5, 2.4, 2.3, 2.2, 2.1, 2.0, 1.9, 1.8, 1.7, 1.6, 1.5, 1.4, 1.3, 1.2, 1.1, 1.0, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2, 0.1, 0.0, -0.1, -0.2, -0.3, -0.4, -0.5, -0.6, -0.7, -0.8, -0.9, -1.0, -1.1, -1.2, -1.3, -1.4, -1.5, -1.6, -1.7, -1.8, -1.9, -2.0, -2.1, -2.2, -2.3, -2.4, -2.5, -2.6, -2.7, -2.8, -2.9, -3.0, -3.1, -3.2, -3.3, -3.4, -3.5, -3.6, -3.7, -3.8, -3.9, -4.0, -4.1, -4.2, -4.3, -4.4, -4.5, -4.6, -4.7, -4.8, -4.9, -5.0, -5.1, -5.2, -5.3, -5.4, -5.5, -5.6, -5.7, -5.8, -5.9, -6.0, -6.1, -6.2, -6.3, -6.4, -6.5, -6.6, -6.7, -6.8, -6.9, -7.0, -7.1, -7.2, -7.3, -7.4, -7.5, -7.6, -7.7, -7.8, -7.9, -8.0, -8.1, -8.2, -8.3, -8.4, -8.5, -8.6, -8.7, -8.8, -8.9, -9.0, -9.1, -9.2, -9.3, -9.4, -9.5, -9.6, -9.7, -9.8, -9.9, -10.0, -10.1, -10.2, -10.3, -10.4, -10.5, -10.6, -10.7, -10.8, -10.9, -11.0, -11.1, -11.2, -11.3, -11.4, -11.5, -11.6, -11.7, -11.8, -11.9, -12.0, -12.1, -12.2, -12.3, -12.4, -12.5, -12.6, -12.7, -12.8, -12.9, -13.0, -13.1, -13.2, -13.3, -13.4, -13.5, -13.6, -13.7, -13.8, -13.9, -14.0, -14.1, -14.2, -14.3, -14.4, -14.5, -14.6, -14.7, -14.8, -14.9, -15.0, -15.1, -15.2, -15.3, -15.4, -15.5, -15.6, -15.7, -15.8, -15.9, -16.0, -16.1, -16.2, -16.3, -16.4, 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Case 10: 机理性文献的检索

- Query Builder中结构与Subject Study联合检索
- 视频操作: <https://www.bilibili.com/video/BV1pK4y1E7Qx>

The screenshot displays the Reaxys Query Builder interface. At the top, there are navigation tabs for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', 'History', and 'Alerts'. The user 'Sam Yu' is logged in. Below the navigation, there are search filters for 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar includes 'Import', 'Save', 'Reset form', and 'Delete all' buttons, along with search criteria options: 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The main workspace is divided into two sections: 'Structure' and 'Subject Studied'. The 'Structure' section contains a chemical reaction scheme: $R_1-CH=CH_2 + Sn-H \rightarrow R_1-CH=CH-Sn$. An orange arrow points from this reaction to a larger, detailed view on the right. The 'Subject Studied' section has a search criteria of 'is mechanism'. On the right side, a sidebar lists search fields: 'Fields', 'Form', 'Topics and Keyw', 'Identification', 'Physical Propert', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'. The detailed view on the right shows the chemical reaction $R_1-CH=CH_2 + Sn-H \rightarrow R_1-CH=CH-Sn$ with a large black arrow indicating the reaction direction.

最后的结果

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

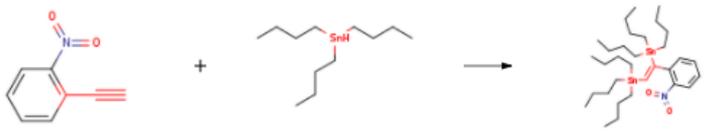
1 Filters
Limit to > Exclude >

By Structure >
Yield >
Reagent/Catalyst >
Solvent >
Catalyst Classes >
Solvent Classes >
Product Availability >
Reactant Availability >
Reaction Classes >
Document Type >
Publication Year >

1 Reactions out of 1 Documents, containing 3 Substances, 0 Targets

0 Limit To Exclude Export Syn-Plan Hide Conditions

1



1 Hits/Conditions Find Similar > Reaction ID: 54835337

Conditions	Yield	Reference
With porous vinyl functionalized tri(2-methoxyphenyl)phosphine derived polymer supported palladium in tetrahydrofuran at 25°C; Mechanism; Schlenk technique; Sealed tube; stereoselective reaction; Experimental Procedure >	82%	Huang, Wen-Yong; Wang, Guo-Qing; Li, Wen-Hao; Li, Ting-Ting; Ji, Guang-Jun; Ren, Shi-Cheng; Jiang, Miao; (...) Pan, Ying-Ming; Ding, Yun-Jie [Chem, 2020, vol. 6, # 9, p. 2300 - 2313] Full Text > Details > Abstract >

1 hit out of 1

Case 11: 文献关键词检索时词语之间距离的设置

- 希望在主题，摘要，关键词中进行检索低温润滑剂的文献
- Low temperature与lubricant两单词之间距离小于7

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

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all Structure Molecular Formula CAS RN TI, AB & KW

◇ Titles, Abstracts & K... is ▾ lubrican* [🔍] [X]

NEAR 7

◇ Titles, Abstracts & K... is ▾ |\"Low temperature\" [🔍] [X]

Search fields [🔍]

Fields Forms History

Reaxys ^

Topics and Keywords ^

◇ Substance Properties & Comments [📄] [⋮]

◇ Reaction Data & Conditions [⋮]

◇ **Titles, Abstracts & Keywords** [⋮]

◇ All Keywords [⋮]

OR
AND
NOT
NEAR
• NEXT
PROXIMITY

Tips:

1. 逻辑关系的选择, And, Or, Not
2. Near没有前后次序, Next有前后次序

Reaxys中的结果

Reaxys® Quick search Query builder **Results** Synthesis planner History Register > Sign in ⓘ

358 Filters

Limit to > Exclude >

Index Terms (List) v

Index Terms (ReaxysTree) v

Publication Year v

Document Type v

Authors v

Patent Assignee v

Journal Title v

Substance Classes v

Reaction Classes v

358 Documents with 242 Substances, 76 Reactions, 0 Targets

0 Limit To Exclude Export

Publication Year v Heatmap

1 Automating ASTM D2983 low-temperature viscosity measurements
Henderson, Kenneth O.; Mastropiero, Joseph T.; Patterson, Reid A. [Journal of Testing and Evaluation, 2020, vol. 48, no. 4, p. 4225 - 4237]
Abstract v Index Terms v Full Text ↗
Abstract hit: {...The low-temperature viscosity of lubricants and hydraulic fluids is a key performance...

2 Facile fabrication of biomimetic slippery lubricant-infused transparent and multifunctional omniphobic surfaces
Yu, Mengnan; Liu, Mingming; Hou, Yuanyuan; Fu, Shaohai; Zhang, Liping; Li, Min; Wang, Dong [Journal of Materials Science, 2020, vol. 55, # 10, p. 4225 - 4237]
Abstract v Index Terms v Substances 1 v Full Text ↗
Index Terms hit: {...Hierarchical structures, High/low temperature, Mechanical resistance...}

3 Chemical modification of castor oil fatty acids (Ricinus communis) for biolubricant applications: An alternative for Brazil's green market
Rios, Ítalo C.; Cordeiro, João P.; Arruda, Tathilene B.M.G.; Rodrigues, F. Eduardo A.; Uchoa, Antonia F.J.; Luna, F. Murilo T.; Cavalcante, Célio L.; Ricardo, Nágila M.P.S. [Industrial Crops and Products, 2020, vol. 145, art. no. 112000]

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- Document Type
- Cited By** ↑ ↓

Reaxys中的专利的筛选

Filters

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- Index Terms (List) ▾
- Index Terms (ReaxysTree) ▾
- Publication Year ▾
- Document Type 1 ▲
 - article 220
 - conference paper 83
 - patent 36
 - note 6
 - review 4
 - abstract report 3
 - conference review 2

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36 Documents with 110 Substances, 74 Reactions, 0 Targets

0 [Limit To](#) [Exclude](#) [Export](#) [Publication Year](#) ▾ [Heatmap](#)

- PROCESS AND APPARATUS FOR WATER PURIFICATION**
 - Buchsbaum, Norbert Nathan - EP2663529, 2020, B1
Patent Family Members: CA2807640 A1; WO2012/21402 A2; WO2012/21402 A3; AU2011289648 A1; SG187759 A1; ...
[Abstract](#) ▾ [Claims](#) ▾ [Front Page Info](#) ▾ [Full Text](#) ↗
Claims hit: {...oil or lubricant, and a low temperature synthetic base fluids.7. The process of...} ▾
- Sublingual tablet pharmaceutical composition for treating acute spastic pain and preparation method thereof (by machine translation)
 - Yaoyuan Bio-technology (Qidong) Co., Ltd.; Wang Yuan; Wu Jianpeng; Zhu Lei; He Xungui; Tang Wensheng - CN111419809, 2020, A
Patent Family Members: CN111419809 A
[Abstract](#) ▾ [Claims](#) ▾ [Front Page Info](#) ▾ [Full Text](#) ↗
Claims hit: {...and the lubricant is directly pressed. Step 2: Using low temperature vacuum drying,...} ▾
- LUBRICANT FOR MEDICAL DEVICE TO BE SUBJECTED TO GAS LOW-TEMPERATURE STERILIZATION, MEDICAL DEVICE TO BE SUBJECTED TO GAS LOW-TEMPERATURE STERILIZATION, AND METHOD OF MANUFACTURING MEDICAL DEVICE TO BE SUBJECTED TO GAS LOW-TEMPERATURE STERILIZATION
 -

Agenda

- Reaxys内容与发展规划
- Reaxys中的检索
 - Reaxys对文献的提炼
 - Reaxys中物质与物性数据获取反向检索
 - Reaxys中结构面板与反应数据获取
 - Reaxys中的实用小案例
- Q&A

Reaxys小结

- Reaxys从大量文献中摘取和物质性质相关的所有数据，帮助科研人员获得标准化，规范化，格式化的物性数据列表及参考文献
- Reaxys中的Query Builder检索帮助科研人员通过简便的方式，获得精准，跨学科精确答案
- Reaxys中的结构面板，能实现科研人员绝大部分的结构绘制要求，帮助科研人员用最直接的方式获得相应的物质和反应
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请就今天的培训
进行问卷调查





Thank you

