

2022.9 新增功能

- ✓ 文献知识图谱 (P1-7)
- ✓ 下载详细的检索历史(P8-12)
- ✓ 根据反应产率来排序反应结果(P13-16)
- ✓ 根据反应步数来排序反应结果(P17-21)

CAS SciFinderⁿ 使用技巧|文献知识图谱

在 CAS SciFinderⁿ 文献检索结果集页面，新增文献结果的知识图谱（Knowledge Graph），可以直观地展示多篇文献中的数据（作者、机构、概念词和物质）关联。

1. 在 CAS SciFinderⁿ 文献结果集页面，点击页面上方 Knowledge Graph，即可打开文献结果集的知识图谱。知识图谱最多可以作用于 150 篇文献。如果结果集的文献超过 150 篇，则会根据当前的排序方式，展示结果集中前 150 篇文献的知识图谱。

References search for "'organic semiconductor" and dop*"

Substances Reactions Citing Knowledge Graph

Filter Behavior: Filter by Exclude

Document Type: Journal (15), Patent (29), Preprint (1)

Substance Role: Uses (45), Properties (19)

Filtering: Substance Role: Uses

45 Results | Sort: Relevance | View: Partial Abstract

1

Organic Zener Diodes: Tunneling across the Gap in Organic Semiconductor Materials
By: Kleemann, Hans; Gutierrez, Rafael; Lindner, Frank; Avdoshenko, Stanislav; Manrique, Pedro D.; Lussem, Bjorn; Cuniberti, Gianuario; Leo, Karl
Nano Letters (2010), 10(12), 4929-4934 | Language: English, Database: CAlplus and MEDLINE

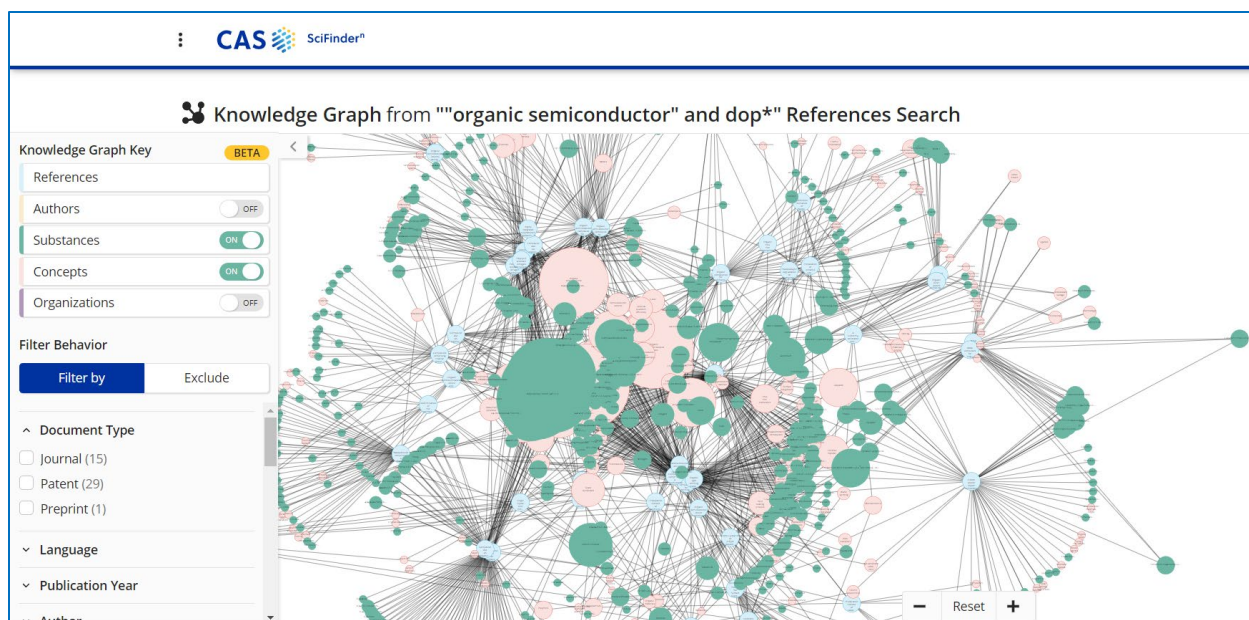
Organic Zener diodes with a precisely adjustable reverse breakdown from -3 to -15 V without any influence on the forward current-voltage curve are realized. This is accomplished by controlling the width of the charge depletion zone in a pin-diode with an accuracy of 1 nm independently of the doping concentration and the thickness of the intrinsic layer. The

2. 在展开的知识图谱 (Knowledge Graph) 页面中, 右侧是完整的知识图谱, 左侧是对知识图谱的分析项。图谱中含有节点和连接线。节点代表文献、文献中的概念词、文献中的物质、作者和发表文献的机构名。连接线代表多个节点之间的关联。节点越大, 连接线越多, 代表某个概念词/物质/作者/机构关联的文献越多。

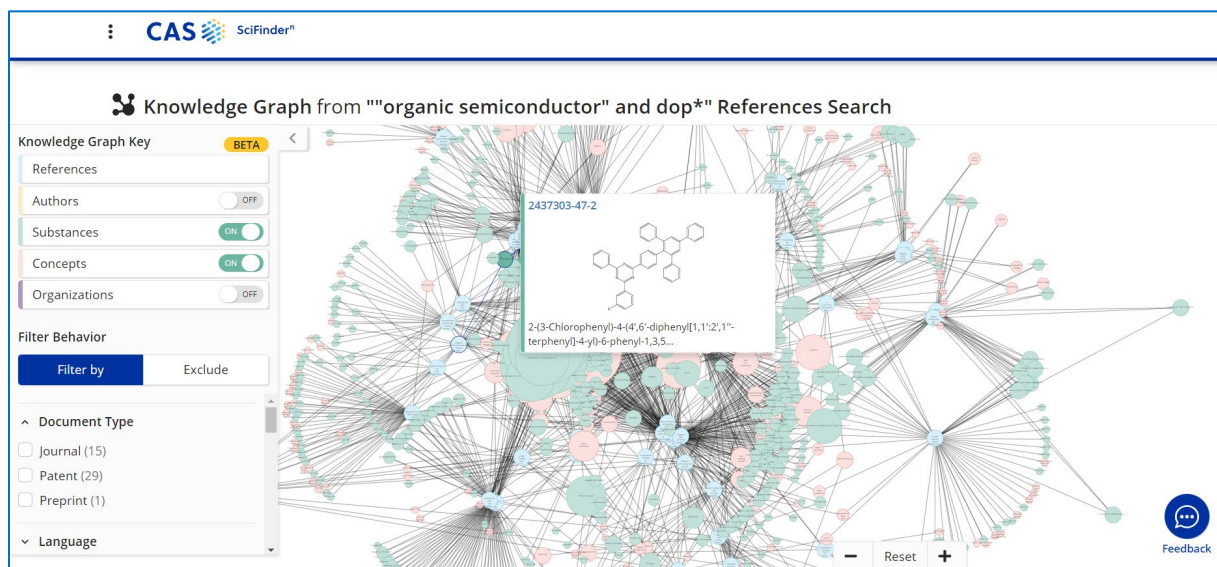
(1) 通过鼠标点击右侧空白处, 可以自由地移动图谱的位置; 也可以点击页面下方的 Reset (+和-) 对图谱进行放大或缩小。

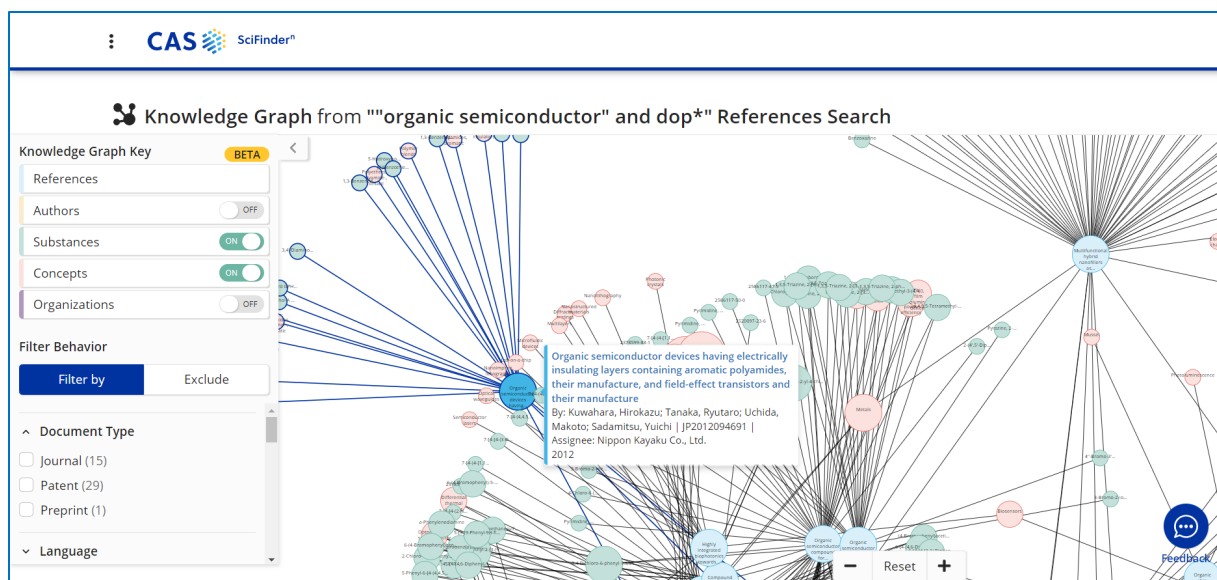
(2) 左侧 Knowledge Graph Key 下方显示了 References (默认始终出现中右侧的图谱中)、Authors、Substances、Concepts 和 Organizations, 点击 ON/OFF 选择性地展示或关闭相关项目。这五项内容分别使用了不同的颜色标签, 鼠标悬在某一项的字体上, 右侧的图谱则会标亮显示这一项。例如, 鼠标悬在左侧 Substances 上面, 右侧的图谱中代表文献中物质 (Substances) 的绿色节点会标亮显示。

The screenshot shows the CAS SciFinder Knowledge Graph interface. The main heading is "Knowledge Graph from \"\"organic semiconductor\"\" and dop*\"\" References Search". On the left side, there is a "Knowledge Graph Key" section with a "BETA" label and a list of categories: References, Authors, Substances, Concepts, and Organizations, each with an "ON" toggle switch. Below this is the "Filter Behavior" section with "Filter by" and "Exclude" buttons, and two expandable sections: "Document Type" (Journal (15), Patent (29), Preprint (1)) and "Language" (English (40), Chinese (2)). The main area displays a complex network graph with nodes of various sizes and colors (purple, green, orange, blue) connected by lines. A "Reset" button with "-" and "+" symbols is located at the bottom right of the graph area.



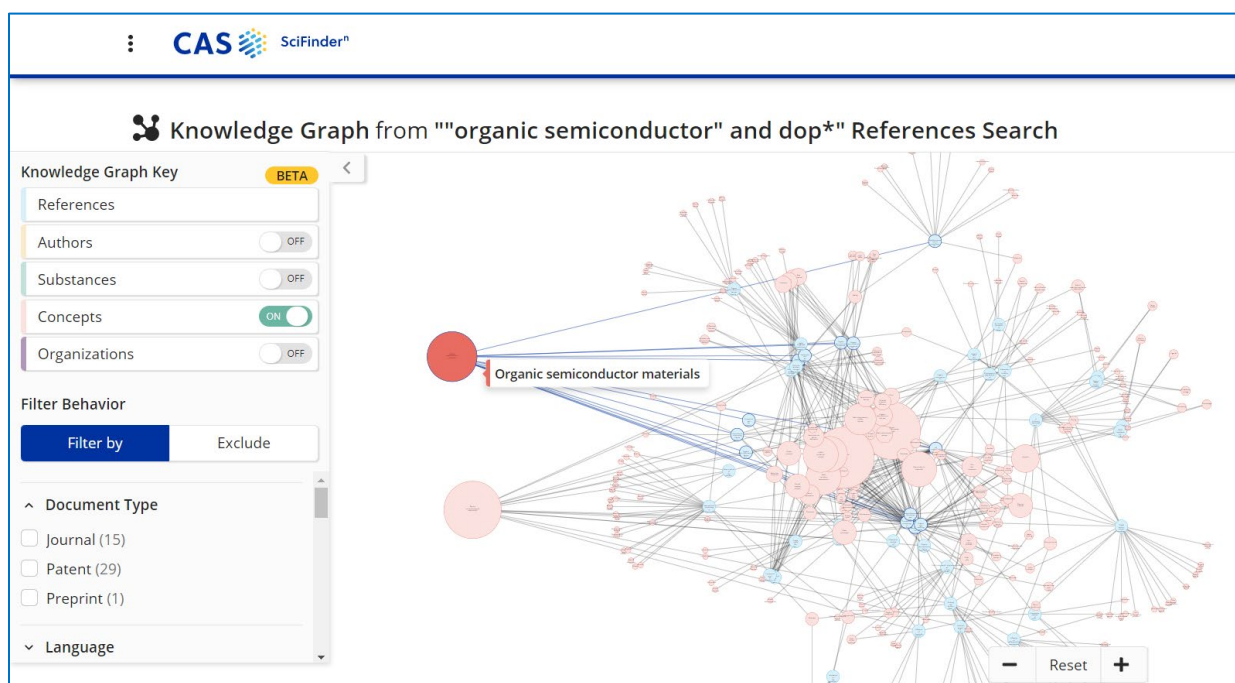
3. 在知识图谱（Knowledge Graph）页面右侧，点击任何一个节点即可展示其代表的具体内容。例如点击绿色的节点，则在弹出窗口中展示其代表的具体物质信息（CAS 登记号、结构和名称），点击 CAS 登记号可以链接至物质详情；点击蓝色的节点，则在弹出窗口中展示其代表的具体文献信息（标题、作者、刊物名/专利号和年份等），点击文献标题可以链接至文献详情。

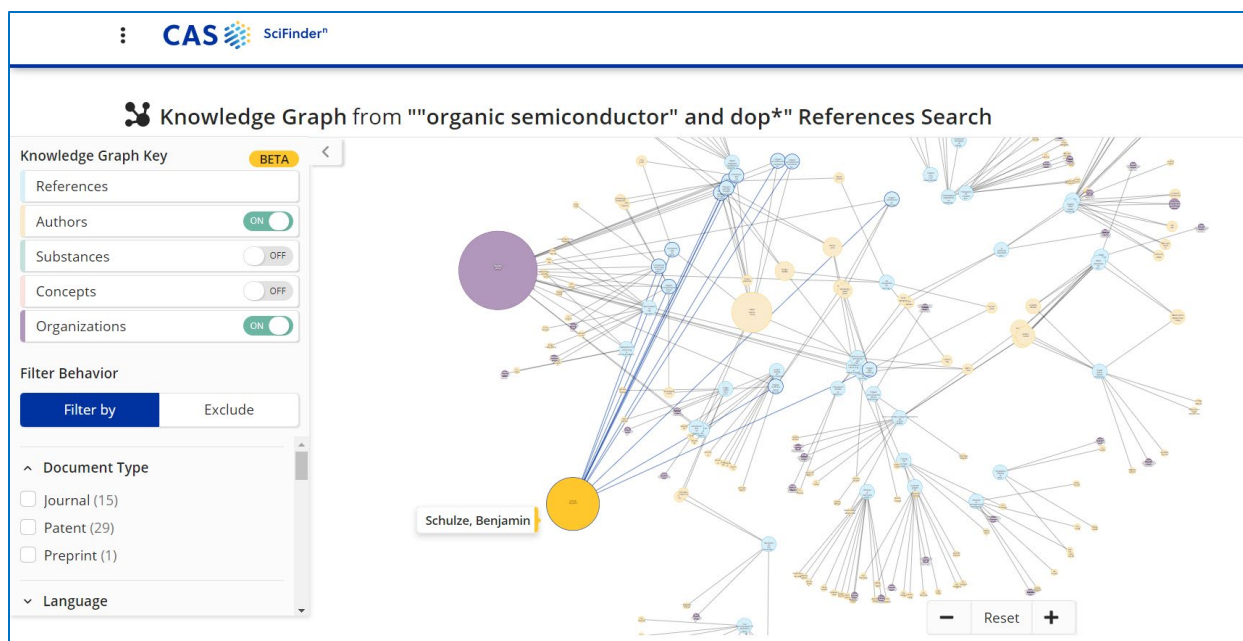




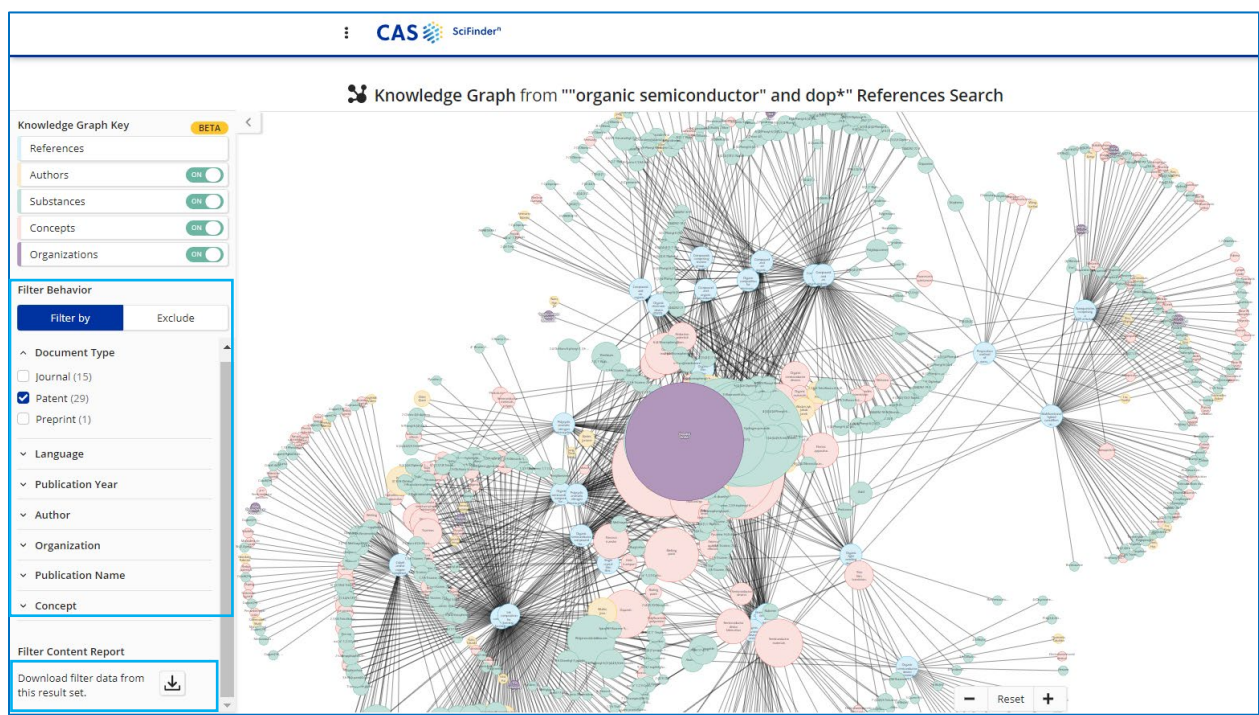
4. 在知识图谱 (Knowledge Graph) 页面右侧, 点击拖拽任何一个节点即可展示其关联的文献内容。节点越大, 连线越多, 代表此节点 (概念词/物质/机构/作者) 关联的文献越多。

例如, 拖拽某个红色的节点, 即可查看某个概念词(concept)关联的文献; 绿色的节点, 可查看某个物质(substance)关联的文献; 紫色的节点, 可查看某个结构(organization)发表的文献; 黄色的节点, 可查看某位作者(author)发表的文献。





5. 在知识图谱（Knowledge Graph）页面左下侧，可以通过 Filter Behavior: Filter by（精炼）或 Exclude（排除）下面的聚类项，比如文献类型、语言、发表年份、作者名、机构名、刊物名和概念词。聚类项中的内容可以被下载为 excel 格式的文件。



Download Reference Filter Content ✕

File Type

Excel (.xlsx)

Select Quantity

All Filter Values

Applied Filter Values

File Name

Reference_Filters_20220929_1031

Filters

Document Type

Language

Publication Year

Author

Organization

Publication Name

Concept

Download

Cancel

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Concept	Count
Semiconductor films	16
Electric current-potential relationship	15
Organic electroluminescent devices	15
Organic semiconductor materials	13
Glass transition temperature	9
HOMO (molecular orbital)	9
LUMO (molecular orbital)	9
Semiconductor materials	9
Electroluminescent display devices	8
Melting point	8
Dopants	7
Light sources	7
Dipole moment	6
Electron transfer	6
Glass substrates	6
Optical imaging devices	6
Electric apparatus	5
Organic semiconductor devices	5
Semiconductor device fabrication	5
Thin film transistors	5
Aromatic nitrogen heterocycles	4
Bias potential	4
...	4

Document Type | Publication Year | Organization | Publication Name | **Concept** | +

CAS SciFinderⁿ 使用技巧 | 下载详细的检索历史

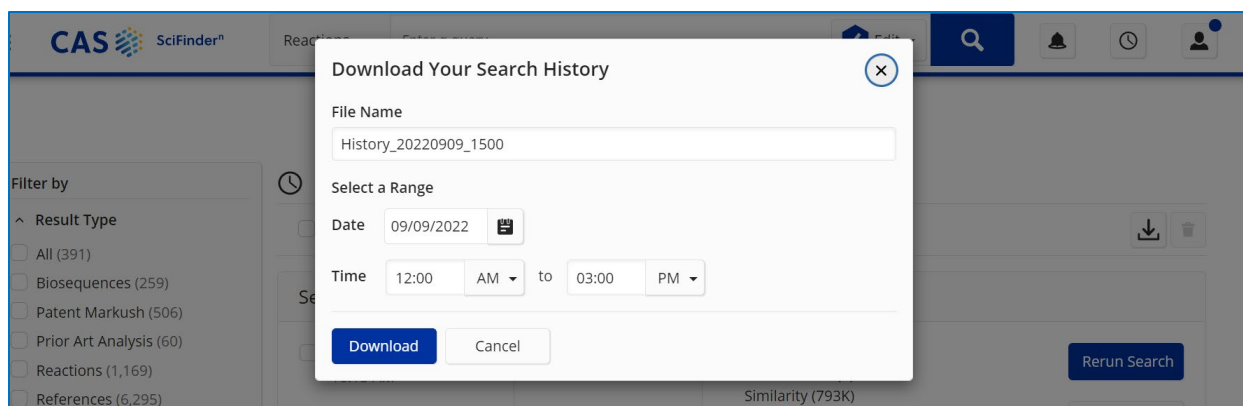
在 CAS SciFinderⁿ 检索历史页面，可选择下载特定时间范围内的详细检索历史。

1. 在 CAS SciFinderⁿ 检索历史界面，点击右上角下载标志，即可打开下载选项，选择检索日期和时间范围。

The screenshot displays the CAS SciFinderⁿ Search History interface. At the top, there is a navigation bar with the CAS SciFinderⁿ logo, a search bar with the text "Enter a query...", and several utility icons including "Edit", a magnifying glass, a notification bell, a clock icon (highlighted with a red box), and a user profile icon. Below the navigation bar, the main content area is titled "Search History" and shows a total of 13,564 searches. A "Download History" button (highlighted with a red box) is located in the top right corner of the search history section. The search results are organized by date, with the current view for "September 9, 2022". Three search results are listed:

- Reactions** (10:15 AM): Includes a chemical structure image and options for "As Drawn (2)", "Substructure (4)", and "Similarity (793K)". Buttons for "Rerun Search" and "Edit Search" are present.
- References** (10:03 AM): Title: "Development of macrocyclic peptides containing epoxyketone with oral availability as proteasome inhibitors, (1 Result)". Buttons for "Rerun Search" and "Edit Search" are present.
- References** (10:02 AM): Title: "Molecular Glues for Targeted Protein Degradation: From Serendipity to Rational Discovery (1 Result)". Buttons for "Rerun Search" and "Edit Search" are present.

On the left side of the interface, there is a "Filter by" section with two expandable categories: "Result Type" and "Date". The "Date" section includes a date range selector and a calendar for "September, 2022".



2. 下载文件为.rtf 格式。下面是详细的检索历史样本。检索历史记录精确到分钟。

注：下载文件中显示的时间为美国时间。如果在中国进行检索操作，则下载文件中的检索时间和实际检索操作的时间有 12 小时时差，比如下面导出文件中第一项显示 9 月 8 日 9: 53PM 的检索历史，实际上是在中国时间 9 月 9 日 9: 53AM 操作的。

**September 8,
2022**

09:53 PM	Reference Search: Molecular Glues for Targeted Protein Degradation: From Serendipity to Rational Discovery Sort by: Relevance (1 Result)
09:54 PM	Reference Search: PROTACs: An Emerging Therapeutic Modality in Precision Medicine Sort by: Relevance (1 Result)
09:55 PM	Reference Search: Molecular Glues for Targeted Protein Degradation: From Serendipity to Rational Discovery Sort by: Relevance (1 Result)
10:02 PM	Reference Search: Molecular Glues for Targeted Protein Degradation: From Serendipity to Rational Discovery Sort by: Relevance (1 Result)
10:03 PM	Reference Search: Development of macrocyclic peptides containing epoxyketone with oral availability as proteasome inhibitors, Sort by: Relevance (1 Result)
10:14 PM	Get Reactions from References Group By: Document Sort by: Relevance

11:14 PM	Get Reactions from Reactions Group By: Scheme Sort by: Relevance (3 Results)
11:25 PM	Reaction Search: synthesis of 2242433-98-1 Group By: Document Sort by: Relevance (9 Results)
11:30 PM	Upload Structure to CAS Draw
11:31 PM	Upload Structure to CAS Draw
11:37 PM	Download RD File for Reaction Search: synthesis of 2242433-98-1 (1 Result)
11:40 PM	Download RD File for Reaction Search: synthesis of 2242433-98-1 (1 Result)
11:53 PM	Reference Detail: Development of macrocyclic peptides containing epoxyketone with oral availability as proteasome inhibitors

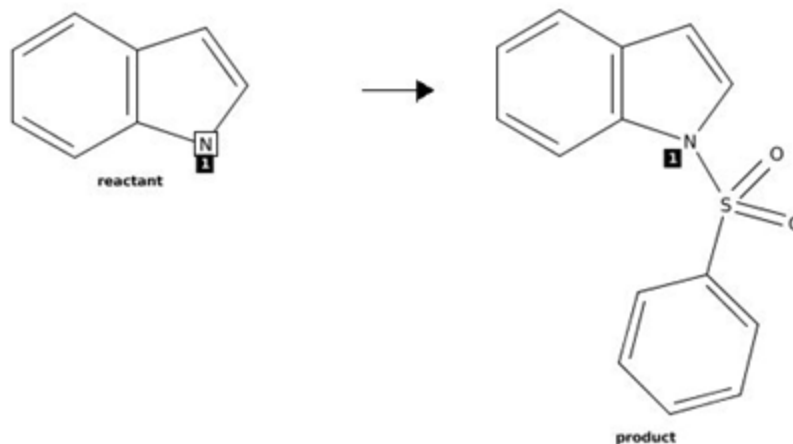
02:42 AM

Reaction Substructure Structure Search

Group By: Document

Sort by: Yield

(7,760 Results)



02:43 AM

Get Reactions from Reactions

Group By: Scheme

Sort by: Yield

(12 Results)

02:46 AM

Get Reactions from Reactions

Group By: Scheme

Sort by: Yield

(9 Results)

02:46 AM

Get Reactions from Reactions

Group By: Scheme

Sort by: Yield

(2 Results)

02:59 AM

Reference Search: **DOI: 10.1021/jacs.1c12071**

Sort by: Relevance

CAS SciFinderⁿ 使用技巧|根据反应产率来排序反应结果

在 CAS SciFinderⁿ 反应检索结果集页面，新增根据反应产率对结果进行排序的功能，且默认以降序排列。

1. 在 CAS SciFinderⁿ 反应结果集页面，点击右上角 Sort 旁的箭头，再点击 Yield，即可根据反应产率排序结果。当反应结果以 Scheme 分组（Group: by scheme）时，每个 Scheme 中的反应也默认以反应产率从高到底排序。

Reactions search for drawn structure

References

Structure Match

- As Drawn (99)
- Substructure (7,760)
- Similarity (152)

Filter Behavior

Filter by Exclude

Yield

- 90-100% (1,007)
- 80-89% (975)
- 70-79% (720)
- 50-69% (880)
- 30-49% (445)

View All

7,760 Results

Group: By Scheme Sort: Yield View: Expanded

Scheme 1 (94 Reactions)

Yield: 100%

Suppliers (106) Suppliers (76) Suppliers (78)

31-081-CAS-13977940 Steps: 1 Yield: 100% Preparation of as 2-oxindoles CGRP receptor antagonists

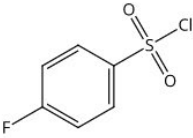
1.1 Reagents: Sodium hydride
Solvents: Tetrahydrofuran; cooled; 15 min, cooled
1.2 cooled; overnight, rt

By: Gottschling, Dirk; et al
World Intellectual Property Organization, WO2009065920 A2
2009-05-28

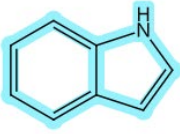
PatentPak Full Text

31-081-CAS-11195608 Steps: 1 Yield: 100% Preparation of as piperidinobenzamides CGRP receptor antagonists

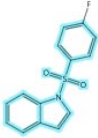
Scheme 4 (4 Reactions) Steps: 1 Yield: 81-100% ...



Suppliers (90)



Suppliers (106)



Suppliers (3)

<input type="checkbox"/>	31-081-CAS-13526390	Steps: 1 Yield: 100%	<p>Quinols as Novel Therapeutic Agents. 2. 4-(1-Arylsulfonylindol-2-yl)-4-hydroxycyclohexa-2,5-dien-1-ones and Related Agents as Potent and Selective Antitumor Agents</p> <p>1.1 Reagents: Sodium hydroxide, Tetrabutylammonium hydrogen sulfate Solvents: Toluene, Water; 0 °C; 16 h, rt</p> <p>By: Berry, Jane M.; et al Journal of Medicinal Chemistry (2005), 48(2), 639-644</p> <p>Experimental Protocols Full Text ▾</p>
<input type="checkbox"/>	31-081-CAS-15975625	Steps: 1 Yield: 89%	<p>Heterocyclic compounds as inhibitors of bromodomain CB P and EP300 and their preparation</p> <p>1.1 Reagents: Sodium hydride Solvents: Tetrahydrofuran; 0 °C; 30 min, 0 °C 1.2 2 h, 20 °C</p> <p>By: Romero, F. Anthony; et al World Intellectual Property Organization, WO2016055028 A1 2016-04-14</p> <p style="text-align: right;">PatentPak ▾ Full Text ▾</p>
<input type="checkbox"/>	31-081-CAS-7263657	Steps: 1 Yield: 81%	Preparation of 4-[1-(sulfonyl)-1H-indol-2-yl]-4-(hydroxy)-

2. 当 CAS SciFinder[®] 反应结果以 Document 分组 (Group: by document) 时, 每篇 Document 中的反应优先显示产率最高的那条反应。

Reactions search for drawn structure

References ▾

Structure Match

As Drawn (99)

Substructure (7,760)

Similarity (152)

Filter Behavior

Filter by Exclude

Yield

90-100% (1,007)

80-89% (975)

70-79% (720)

50-69% (880)

30-49% (445)

[View All](#)

7,760 Results

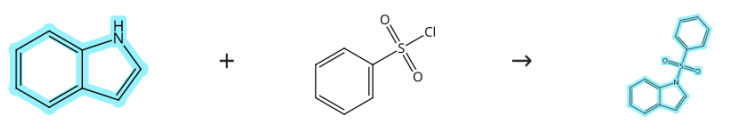
Group: By Document ▾ Sort: Yield ▾ View: Expanded ▾

1

Preparation of as 2-oxoindoles CGRP receptor antagonists

By: Gottschling, Dirk; Dahmann, Georg; Doods, Henri; Heimann, Annkatrin; Mueller, Stephan Georg; et al
World Intellectual Property Organization, WO2009065920 A2 2009-05-28 | Language: German, Database: CAplus

PatentPak ▾ Full Text ▾



[Suppliers \(106\)](#) [Suppliers \(76\)](#) [Suppliers \(78\)](#)

31-081-CAS-13977940

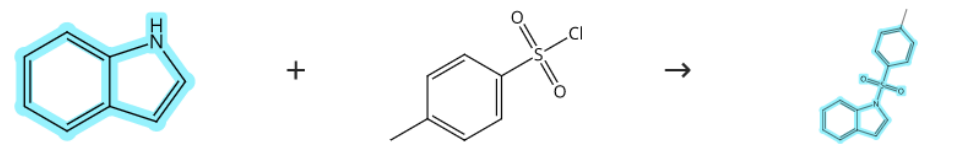
Steps: 1 Yield: 100%

7

Discovery and characterization of an acridine radical photoreductant

By: MacKenzie, Ian A.; Wang, Leifeng; Onuska, Nicholas P. R.; Williams, Olivia F.; Begam, Khadiza; et al
Nature (London, United Kingdom) (2020), 580(7801), 76-80 | Language: English, Database: CAplus and MEDLINE

Full Text ▾ [View 2 Related Reactions](#)



[Suppliers \(106\)](#) [Suppliers \(76\)](#) [Suppliers \(39\)](#)

31-081-CAS-22393643

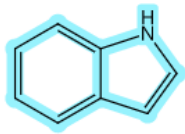
Steps: 1 Yield: 100%

1.1 Reagents: [Pyridine](#); 0 °C; 2 - 3 h, rt

[Experimental Protocols](#)

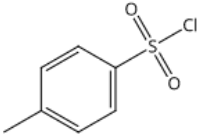
2 Results Group: By Scheme ▾ Sort: Yield ▾ View: Expanded ▾

Scheme 1 (1 Reaction) Steps: 1 Yield: 100% ⋮



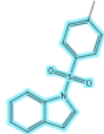
Suppliers (106)

+



Suppliers (76)

→



Suppliers (39)

31-081-CAS-22393643 Steps: 1 Yield: 100% [Discovery and characterization of an acridine radical photoreductant](#)

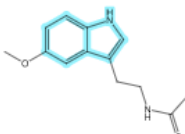
1.1 Reagents: [Pyridine](#); 0 °C; 2 - 3 h, rt

By: MacKenzie, Ian A.; et al
Nature (London, United Kingdom) (2020), 580(7801), 76-80

[Experimental Protocols](#) [Full Text ▾](#)

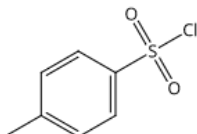
[Collapse Scheme ▾](#)

Scheme 2 (1 Reaction) Steps: 1 Yield: 85% ⋮



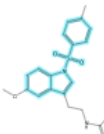
Suppliers (134)

+



Suppliers (76)

→



Supplier (1)

31-081-CAS-22393668 Steps: 1 Yield: 85% [Discovery and characterization of an acridine radical photoreductant](#)

1.1 Reagents: [Potassium hydroxide](#), [Tetrabutylammonium hexafluorophosphate](#)
Solvents: [Dichloromethane](#); 0 °C; 5 min, rt

By: MacKenzie, Ian A.; et al
Nature (London, United Kingdom) (2020), 580(7801), 76-80

CAS SciFinder[®] 使用技巧|根据反应步数来排序反应结果

在 CAS SciFinder[®] 反应检索结果集页面，新增根据反应步数对结果进行排序的功能，且可以选择按照降序或升序来排列。

1. 在 CAS SciFinder[®] 反应结果集页面，点击右上角 Sort 旁的箭头，再点击 Number of Steps: Ascending，即可根据反应步数的升序排列。当反应结果以 Scheme 分组（Group: by scheme）时，每个 Scheme 中的反应也默认以反应步数从少到多排序。

The screenshot displays the CAS SciFinder[®] interface for a reaction search. The search criteria are set to "Reactions" and "Enter a query...". The results are grouped by scheme, and the sorting is set to "Number of Steps: Ascending". The first result is expanded to show the reaction scheme and associated information.

Search Results Summary:

- Group: By Scheme
- Sort: Number of Steps: Ascending
- View: Expanded
- Yield: 74%
- Supplier: (1)
- Suppliers: (11)

Reaction Details:

- 31-367-CAS-19350143
- Steps: 1
- Yield: 74%
- Development of macrocyclic peptides containing epoxyketone with oral availability as proteasome inhibitors
- By: Li, Daqiang; et al
- Journal of Medicinal Chemistry (2018), 61(20), 9177-9204
- Full Text

1.1 Reagents: 1-Hydroxybenzotriazole, Diisopropylethylamine, 1-[Bis(dimethylamino)methylene]-1H-benzotriazolium hexafluorophosphate(1-) 3-oxl...

Solvents: Tetrahydrofuran; 0 °C; 3 h, rt

Experimental Protocols

Suppliers (11) Suppliers (6) Suppliers (19)

View Reaction Detail Steps: 3 **Fibonacci's Route to Regioregular Oligo(3-hexylthiophene)s**

1.1 Catalysts: [Tetrakis\(triphenylphosphine\)palladium](#)
Solvents: [Toluene](#); 24 - 72 h, 90 °C

2.1 Reagents: [Lithium diisopropylamide](#)
Solvents: [Tetrahydrofuran](#), [Hexane](#); -78 °C; 2 h, -78 °C

2.2 -78 °C; -78 °C → rt

3.1 Catalysts: [Tetrakis\(triphenylphosphine\)palladium](#)
Solvents: [Toluene](#); 24 - 72 h, 90 °C

Experimental Protocols

By: Koch, Felix P. V.; et al
Journal of the American Chemical Society (2013), 135(37), 13695-13698

Full Text ▾

View Reaction Detail Steps: 5 **Fibonacci's Route to Regioregular Oligo(3-hexylthiophene)s**

1.1 Catalysts: [Tetrakis\(triphenylphosphine\)palladium](#)
Solvents: [Toluene](#); 24 - 72 h, 90 °C

2.1 Reagents: [Lithium diisopropylamide](#)
Solvents: [Tetrahydrofuran](#), [Hexane](#); -78 °C; 2 h, -78 °C

2.2 -78 °C; -78 °C → rt

3.1 Catalysts: [Tetrakis\(triphenylphosphine\)palladium](#)
Solvents: [Toluene](#); 24 - 72 h, 90 °C

4.1 Reagents: [N-Bromosuccinimide](#)
Solvents: [Dimethylformamide](#); 5 h, -20 °C; overnight, -20 °C → rt

View All ▾

Experimental Protocols

By: Koch, Felix P. V.; et al
Journal of the American Chemical Society (2013), 135(37), 13695-13698

Full Text ▾

2. 当 CAS SciFinderⁿ 反应结果以 Document 分组 (Group: by document) 时, 每篇 Document 中的反应优先显示步数最少的那条反应。如果某篇文献中含有多条反应, 展开后的多条反应也是按照步数从少到多排列。

Reactions from Substances

References 🔗 📄 📧 🔔 Save and Alert

Filter Behavior: **Filter by** Exclude

Substance Role: Product (10K) Reactant (299) Reagent (227) Catalyst (99) Solvent (6)

Yield: Number of Steps: Experimental Protocols: Synthetic Methods (2,538) Experimental Procedure (2,384)

Reaction Type: Stereochemistry: Reagent: Catalyst:

Filtering: Substance Role: **Product** ✕ Clear All Filters

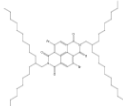
10,211 Results Group: By Document Sort: Number of Steps: Ascending View: Expanded

1

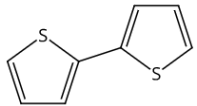
Rational Use of Aromatic Solvents for Direct Arylation Polycondensation: C-H Reactivity versus Solvent Quality

By: Matsidik, Rukiya; Komber, Hartmut; Sommer, Michael
ACS Macro Letters (2015), 4(12), 1346-1350 | Language: English, Database: CPlus and MEDLINE

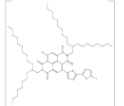
Full Text ▾



🛒 Suppliers (42)



🛒 Suppliers (93)



🛒 Suppliers (6)

31-614-CAS-29750154 Steps: 1 Yield: 100%

1.1 Reagents: [Pivalic acid](#), [Potassium carbonate](#)
Catalysts: [Tris\(dibenzylideneacetone\)dipalladium](#)

□ 2



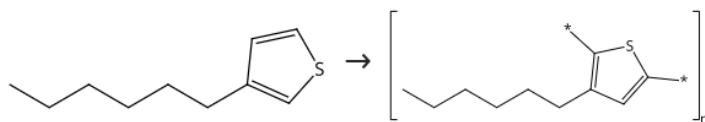
An in depth study of solvent effects on yield and average molecular weight in poly(3-hexylthiophene)

By: Gadiant, Jennifer; Groch, Rebecca; Lind, Cora

Polymer (2017), 115, 21-27 | Language: English, Database: CAplus

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[View 2 Related Reactions](#)



Suppliers (84)

Suppliers (19)

31-614-CAS-27863986

Steps: 1 Yield: 100%

1.1 Reagents: [Iron chloride \(FeCl₃\)](#)

Solvents: [Dichloromethane](#), [Nitrobenzene](#); 24 h, rt

[Experimental Protocols](#)

2 Results
 Group: By Scheme ▾ Sort: Number of Steps: Ascending ▾ View: Expanded ▾

Scheme 1 (1 Reaction)
Steps: 1 Yield: 100% ⋮

Suppliers (84)

Suppliers (19)

31-614-CAS-27863986
 Steps: 1 Yield: 100%
An in depth study of solvent effects on yield and average molecular weight in poly(3-hexylthiophene)

1.1 Reagents: [Iron chloride \(FeCl₃\)](#)
 Solvents: [Dichloromethane](#), [Nitrobenzene](#); 24 h, rt

By: Gadiant, Jennifer; et al
Polymer (2017), 115, 21-27

Experimental Protocols
Full Text ▾

Collapse Scheme ^

Scheme 2 (1 Reaction)
Steps: 2 ⋮

Suppliers (32)

Suppliers (85)

Suppliers (19)

View Reaction Detail
 Steps: 2
An in depth study of solvent effects on yield and average molecular weight in poly(3-hexylthiophene)

1.1 Catalysts: [Dichloro\[1,1'-\(1,3-propanediyl\)bis\[1,1'-diphenylphosphine-kP\]\]nickel](#)
 Solvents: [Diethyl ether](#); overnight, rt