



Reaxys®

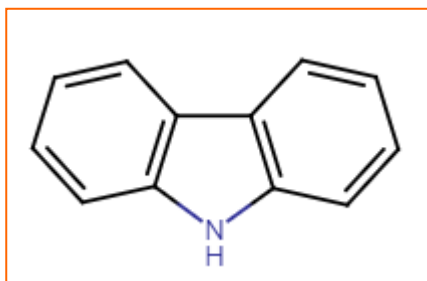
# Workflow example

Searching for the properties and preparation methods for new carbazole-based organic light-emitting device materials

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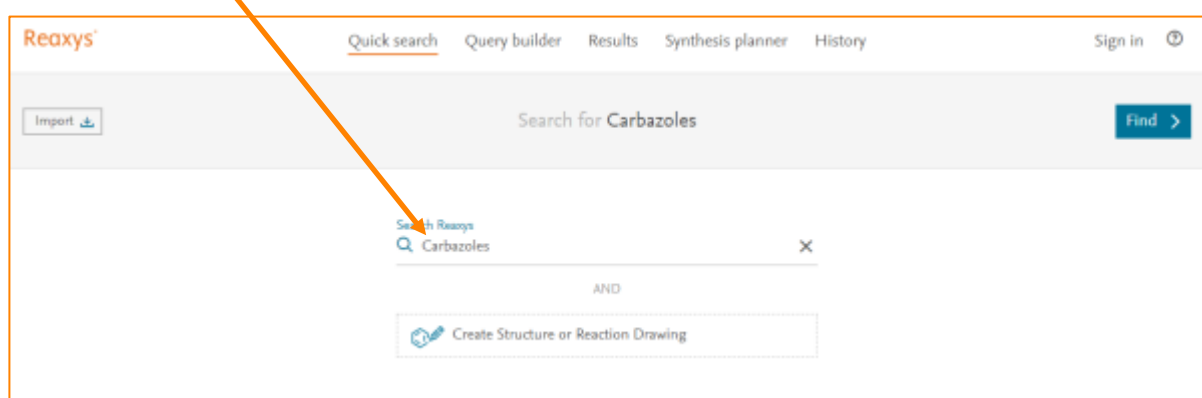
## Workflow concept

Using Reaxys, the scientist wishes to find the properties and preparation methods for new carbazole-based organic light-emitting device (OLED) materials.

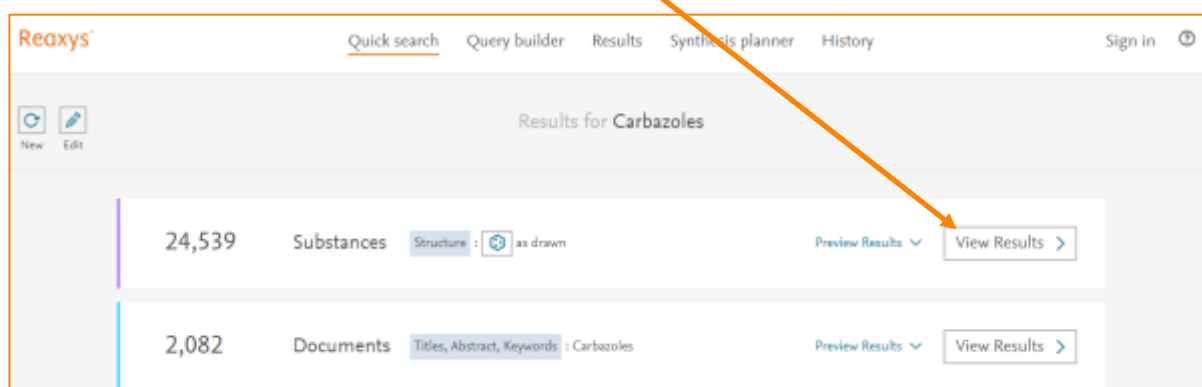


### 1. Perform a Quick Search for carbazole

Type “Carbazole” in the **Quick Search** field in Reaxys.



Review the search preview, which shows that the term will retrieve 24,539 substance and 2,082 documents. Click on **View Results for Substances**.



## 2. Apply Filters

The **Substances Results** page shows the structural diversity of the carbazoles. This can be further investigated using the **Filters and Analysis** function.

Click on **Substance Class**.

The screenshot shows the Reaxys interface. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The 'Results' section displays '24,539 Substances out of 13,681 Documents, containing 65,395 Reactions, 1,008 Targets'. The 'Filters and Analysis' sidebar on the left has 'Substance Classes' selected. The main content area shows a list of substances, including 9H-carbazole and carvedilol, with their chemical structures and associated data.

Substance	Chemical Formula	Identification	Bioactivity (All)	Spectra	Preparations	Reactions	Targets	Documents
9H-carbazole	C <sub>12</sub> H <sub>9</sub> N	167.21 3950 86-74-8		500	478	7,929	9	4,901
carvedilol	C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>	406.481 1514452 72956-09-3		50	32	88	107	1,486

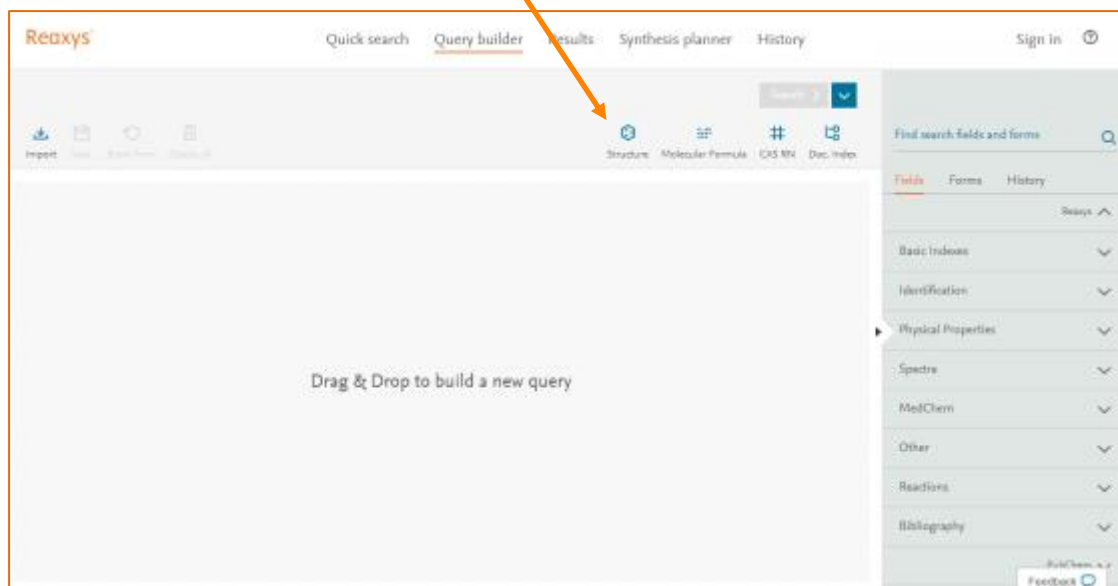
Select **Richter Classification** to see details on *n*-membered heterocyclic carbazoles.

The screenshot shows the 'Filters and Analysis' sidebar on the left and the 'Substance Classes' panel on the right. The 'Substance Classes' panel displays a tree view of classification categories, with 'Richter Classification' selected. The 'Richter Classification' category is expanded, showing a list of sub-categories and their corresponding counts.

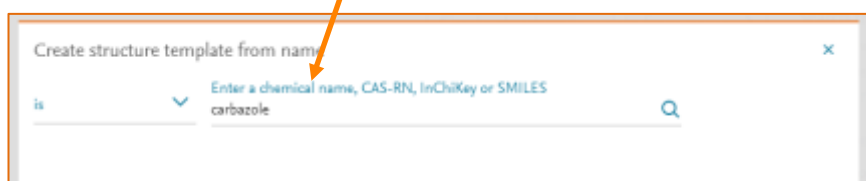
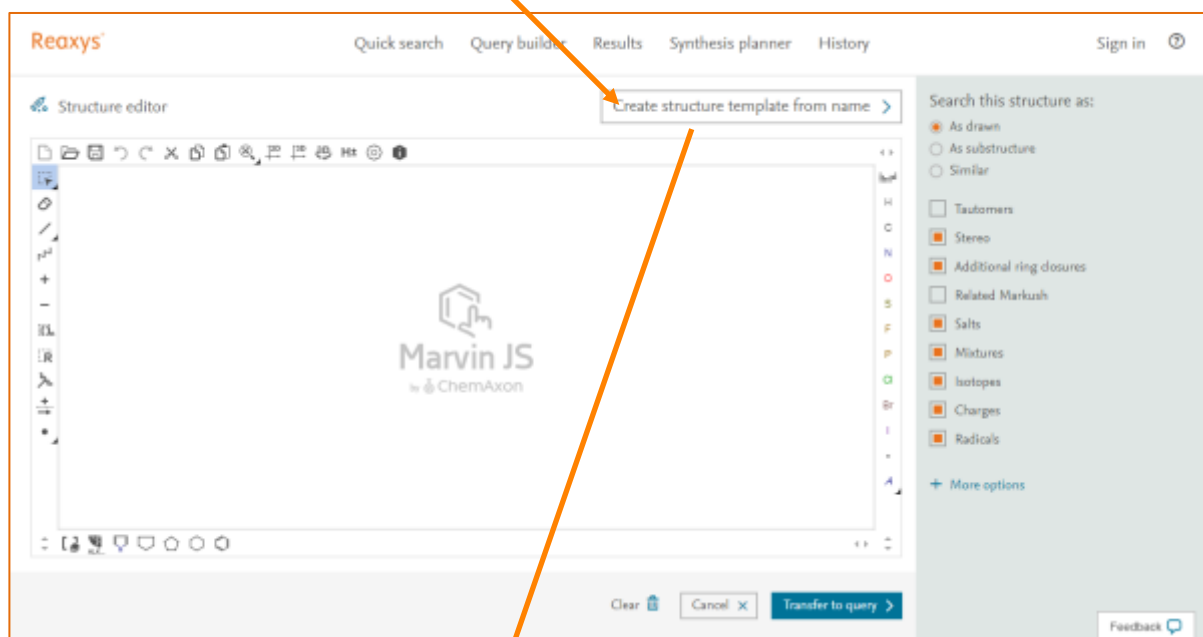
Substance Class	Count
Substance Classes	24,539
Functional Group Classification	24,207
Richter Classification	24,206
Ring Classification	24,206
Heterocyclic Compounds	24,191
5-Membered Heterocycles Containing a Single Heteroatom in the Ring	24,183
6-Membered Heterocycles Containing a Single N Atom	1,972
6-Membered Heterocycles Containing Two Heteroatoms	1,389
5-Membered Heterocycles Containing Two Heteroatoms from Groups 15 and, or 16	1,202
5-Membered Heterocycles Containing More than Two Heteroatoms	716
6-Membered Heterocycles with Two or More Fused Rings	662
3- and 4-Membered Heterocycles	248
6-Membered Heterocycles Containing O, S, Se, Te, Si, Ge, Sn, Pb or I	240

### 3. Use Query Builder to investigate which carbazoles are used in OLEDs

Click on **Query Builder** and then on the structure icon to open the structure editor.



Click **Create structure template from name** and type "Carbazole".



Select **Search this structure as:** and then **As substructure**.

Reaxys

Quick search Query builder Results Synthesis planner History Sign in

Structure editor

Create structure template from name

Search this structure as:

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

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

Charges

Radicals

+ More options

Clear Cancel Transfer to query

Feedback

Type "Use" in the **Find field and form field** and click on it to add it to the main form.

Reaxys

Quick search Query builder Results Synthesis planner History Sign in

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

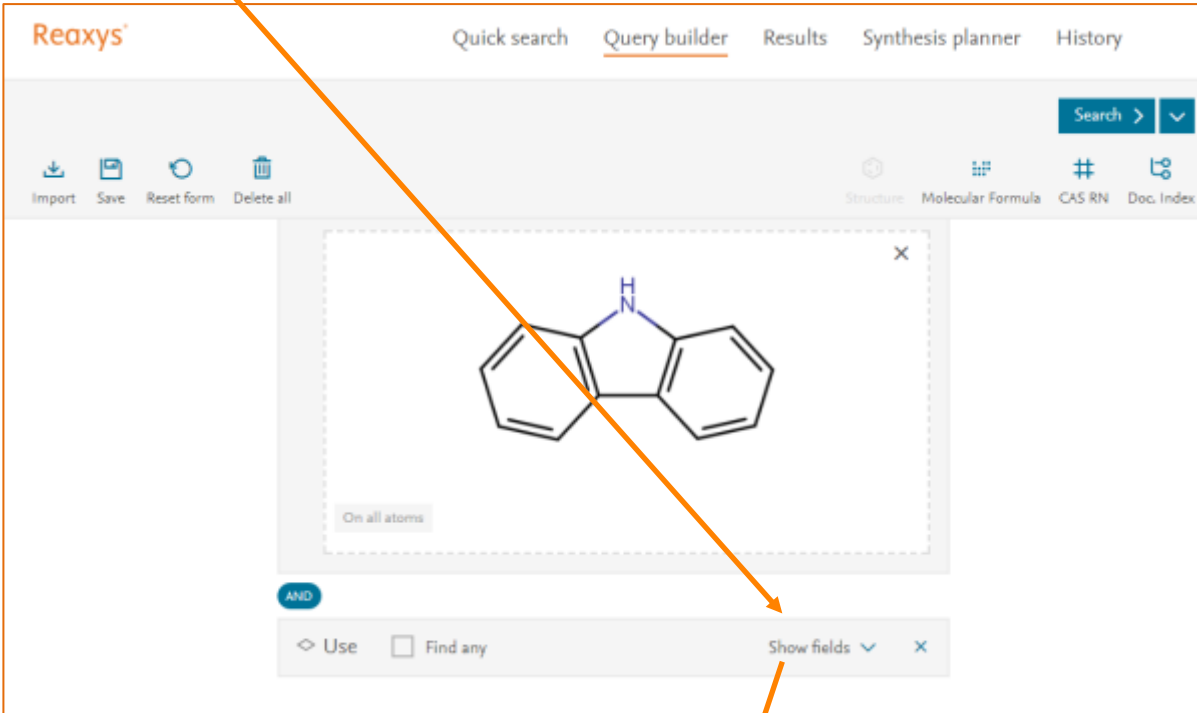
Find search fields and forms

Use

Use

Feedback

Click **Show fields** and type OLED\*.



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

Search > ▾

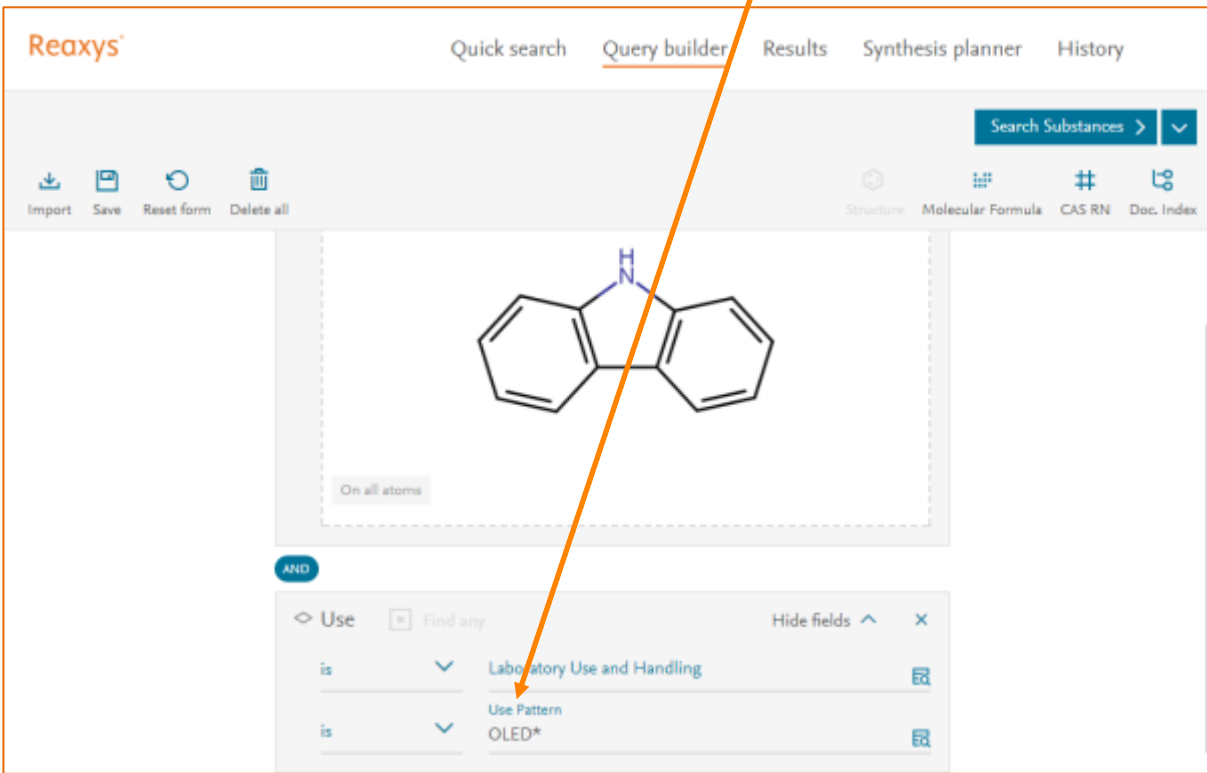
Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

On all atoms

AND

◇ Use  Find any Show fields ▾ ×



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

Search Substances > ▾

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

On all atoms

AND

◇ Use  Find any Hide fields ^ ×

is ▾ Laboratory Use and Handling

is ▾ Use Pattern

OLED\*

#### 4. Review results

Review all the carbazoles with applications as OLEDs.

The screenshot shows the Reaxys search results page. On the left is a 'Filters and Analysis' sidebar. The main area displays '36 Substances' with a list of results. Two results are visible: 'N-phenylcarbazole' and '4,4'-bis(N-carbazolyl)N,N'-diphenylamine'. Each result includes a chemical structure icon, a list of data categories (e.g., Hit Data, Identification, Physical Data), and a 'References' link.

The **Hit Data** include links to the relevant literature.

This close-up shows the 'Hit Data - 1' section for N-phenylcarbazole. It features a table with two columns: 'Use Pattern' and 'References'. The 'Use Pattern' column contains the text 'hole transport layer (HTL) material for organic light emitting diode (OLED)'. The 'References' column contains the citation 'Samsung SDI Co., Ltd. - EP1925618, 2008, A1'. An orange arrow points from the text 'The Hit Data include links to the relevant literature.' to the 'References' column.

Where relevant, information about the location within the references is included.

This close-up shows the 'Hit Data - 4' section for 4,4'-bis(N-carbazolyl)N,N'-diphenylamine. It features a table with three columns: 'Use Pattern', 'Location', and 'Reference'. The 'Use Pattern' column contains the text 'Material for hole-transporting layer in (OLED)'. The 'Location' column contains 'Page/Page column 11, 15, 16, 35'. The 'Reference' column contains the citation 'Cheng, Chen-Hong - US2009/110705, 2009, A1'. An orange arrow points from the text 'Where relevant, information about the location within the references is included.' to the 'Location' column.

## 5. Search for substance properties

The previous search gives the user the CAS numbers of the relevant carbazoles.

N-phenylcarbazole  
C<sub>12</sub>H<sub>10</sub>N<sub>2</sub> 243.308 189982 1150-62-5

Hit Data - 1  
Identification  
Druglikeness

Bioactivity (All)  
Physical Data - 77  
Spectra - 218

Other Data - 8  
Preparations - 74  
Reactions - 283  
Documents - 338

Hit Data - 1  
Use - 1 hits out of 6

Use Pattern	Reference
hole transport layer (HTL) material for organic light emitting diode (OLED)	Samsung SDI Co., Ltd. - EP1925018, 2008, A1 Full Text Details Abstract

Use this CAS number with the relevant property to quickly retrieve precise property data. For example, in **Quick Search**, type “Melting point of 1150-62-5” or “MP of 1150-62-5”.

Reaxys Quick search Query builder Results Synthesis planner History Sign in

Import Search for MP of 1150-62-5 Find

Search Reaxys  
MP of 1150-62-5

AND

Create Structure or Reaction Drawing

Click on **View Results** for **Substances** in the search preview.

Reaxys Quick search Query builder Results Synthesis planner History Sign in

Results for MP of 1150-62-5

1	Substances	CAS : 1150-62-5 AND Property : MP	Preview Results View Results
0	Documents	Title, Abstract, Keywords : MP, 1150-62-5	Preview Results View Results
174,640	Documents	Title, Abstract, Keywords : MP	Preview Results View Results
8	Documents	Title, Abstract, Keywords : 1150-62-5	Preview Results View Results



The selected property data (melting points) and the related literature is shown on the results page.

1 Substances out of 338 Documents, containing 283 Reactions, 0 Targets

**N-phenylcarbazole**  
C12=CC=C(C=C1)C3=CC=CC=C3  
 C<sub>12</sub>H<sub>11</sub>N 243.308 169962 1150-42-9

Hit Data - 26  
 Identification  
 Druglikeness

Bioactivity (All)  
 Physical Data - 77  
 Spectra - 2

Other Data - 8  
 Preparations - 74  
 Reactions - 283  
 Documents - 338

**Hit Data - 26**  
 Melting Point - 26 hits out of 26

Melting Point, °C	Location	Reference
94		Sanyal, Sonali B.; Mahajan, Prasad G.; Bodale, Anita J.; Kulkarni, Govind B.; Patel, Shivraj B. - Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, vol. 183, p. 232 - 238 Full Text > Details > Abstract >
90	supporting information	Hollén, Catherine M.; Söhl, Sharar M. A.; Greaney, Michael P. - Angewandte Chemie - International Edition, 2016, vol. 55, # 7, p. 2493 - 2493; Angew. Chem., 2016, vol. 128, # 7, p. 2496 - 2499,4 Full Text > Details > Abstract >
88 - 89	supporting information	Wu, Jun; Xia, Yanjun; Chen, Xiangqi; Deng, Qianjun - Advanced Synthesis and Catalysis, 2016, vol. 338, # 25, p. 5206 - 5211 Full Text > Cited 1 times > Details > Abstract >
88 - 90	supporting information	Kerner, Lukas; Gmucová, Katarína; Kozáček, Josef; Peřínák, Viktor; Putala, Martin - Tetrahedron, 2016, vol. 72, # 44, p. 7881 - 7892 Full Text > Details > Abstract >
82 - 83		Chen, Pei; Liu, Ning; Li, Enhui; Dai, Bin - RSC Advances, 2015, vol. 5, # 64, p. 51512 - 51525 Full Text > Cited 2 times > Details > Abstract >
94 - 96		Lee, Jung; Hahn - Asian Journal of Chemistry, 2003, vol. 25, # 1, p. 381 - 504

In the same manner, any property can be retrieved. All other physical data for a given substance can be reviewed by clicking **Physical Data**.

## 6. Find preparation methods

Click on **Preparations** to review the methods to make this substance.

1 Substances out of 338 Documents, containing 283 Reactions, 0 Targets

**N-phenylcarbazole**  
C12=CC=C(C=C1)C3=CC=CC=C3  
 C<sub>12</sub>H<sub>11</sub>N 243.308 169962 1150-42-9

Hit Data - 26  
 Identification  
 Druglikeness

Bioactivity (All)  
 Physical Data - 77  
 Spectra - 218

Other Data - 8  
**Preparations - 74**  
 Reactions - 283  
 Documents - 338

**Hit Data - 26**  
 Melting Point - 26 hits out of 26

Melting Point, °C	Location	Reference
94		Sanyal, Sonali B.; Mahajan, Prasad G.; Bodale, Anita J.; Kulkarni, Govind B.; Patel, Shivraj B. - Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, vol. 183, p. 232 - 238 Full Text > Details > Abstract >
90	supporting information	Hollén, Catherine M.; Söhl, Sharar M. A.; Greaney, Michael P. - Angewandte Chemie - International Edition, 2016, vol. 55, # 7, p. 2493 - 2493; Angew. Chem., 2016, vol. 128, # 7, p. 2496 - 2499,4 Full Text > Details > Abstract >
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88 - 90	supporting information	Kerner, Lukas; Gmucová, Katarína; Kozáček, Josef; Peřínák, Viktor; Putala, Martin - Tetrahedron, 2016, vol. 72, # 44, p. 7881 - 7892 Full Text > Details > Abstract >
82 - 83		Chen, Pei; Liu, Ning; Li, Enhui; Dai, Bin - RSC Advances, 2015, vol. 5, # 64, p. 51512 - 51525 Full Text > Cited 2 times > Details > Abstract >
94 - 96		Lee, Jung; Hahn - Asian Journal of Chemistry, 2003, vol. 25, # 1, p. 381 - 504

The Reactions Results page displays the reactions and conditions

Filters can be used to filter by yield, reagent, solvent and solvent class. If a certain yield range is selected (it will turn orange), certain reagents and solvents will turn green.

These reagents and solvents are most likely to give the desired yield.

Selecting solvent classes allows you to limit the results to solvents with, for example, low or high boiling points or a green nature.

For more information on using the **Synthesis Planner** to plan substance synthesis, see pages 22 and 23 of the user guide available in [Reaxys Support Center](#).