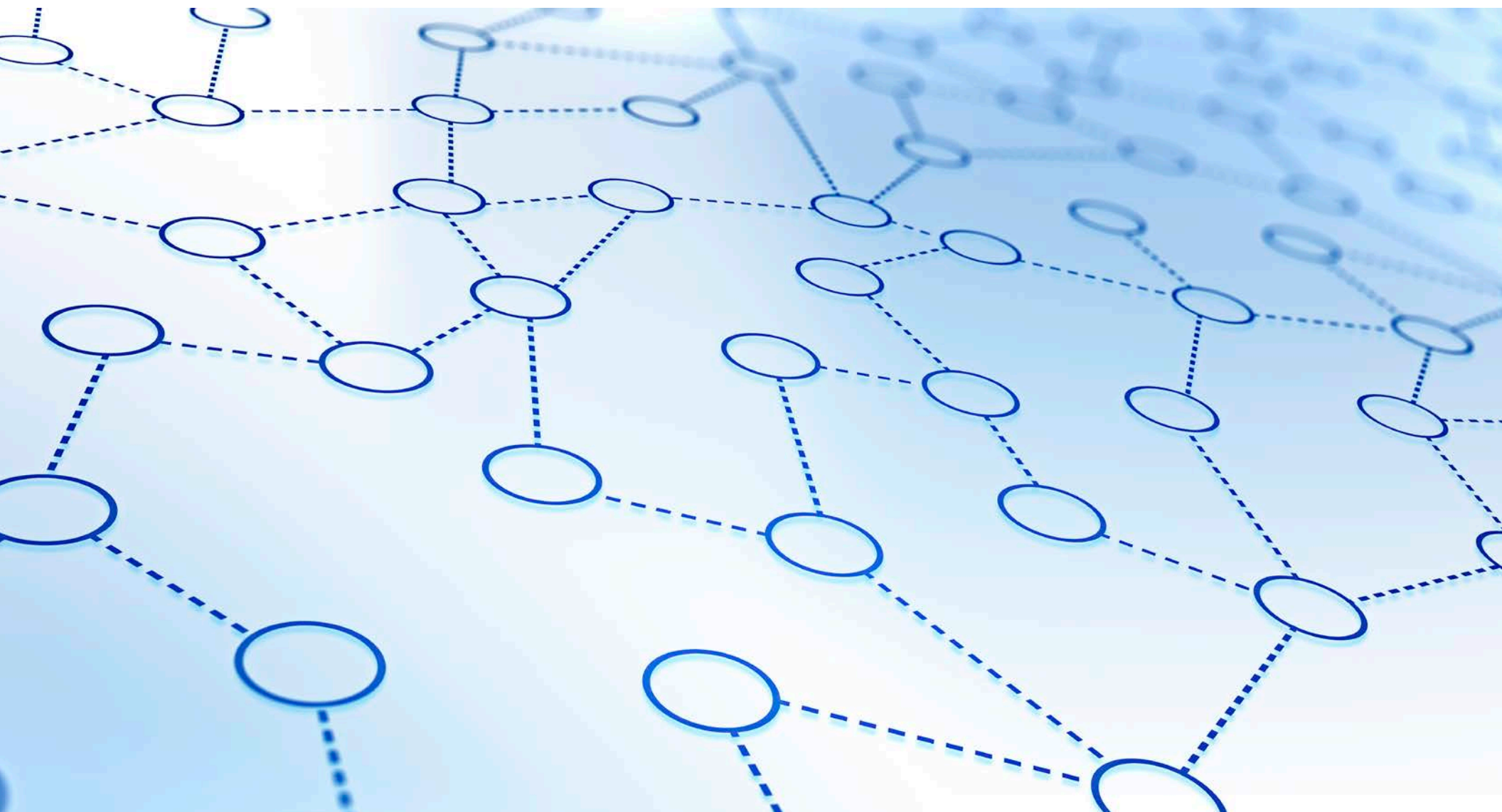


Reaxys<sup>®</sup>

QUICK START GUIDE



## WELCOME TO YOUR QUICK START GUIDE FOR REAXYS.

Reaxys is a Java-free web solution that runs on modern browsers. The various available browsers present a complex landscape. The Reaxys team has tested the system on the following browser versions.

- Firefox (version 49 or higher)
- Chrome (version 53 or higher)
- Edge (version 14 or higher)
- Safari (version 9 or higher)
- Internet Explorer (version 11)

We recommend using one of these browsers to achieve best performance. While Reaxys may work on other browsers, some features and functionalities may not work properly.

Please contact us if you have question regarding browser support.

**NOTE to Reaxys users in China:** We noticed a significant performance increase if Google Chrome is used. If you encounter any performance issues, then try switching to Google Chrome.

**NOTE to all users:** We recommend not using addins and plugins or at least reducing their number to the absolutely necessary minimum. All such components influence the performance and memory usage of a browser.

QUICK SEARCH

Drag your structure file or click here to browse and import it.

Navigate easily between **Quick search**, **Query builder**, **Results**, **Synthesis planner** and **History**.

Click the bell icon to access alerts created from the results of your queries.

Click the question mark to access Reaxys Help, with guides, training material and the FAQ.

The **Quick Search** text option accepts natural language keywords.

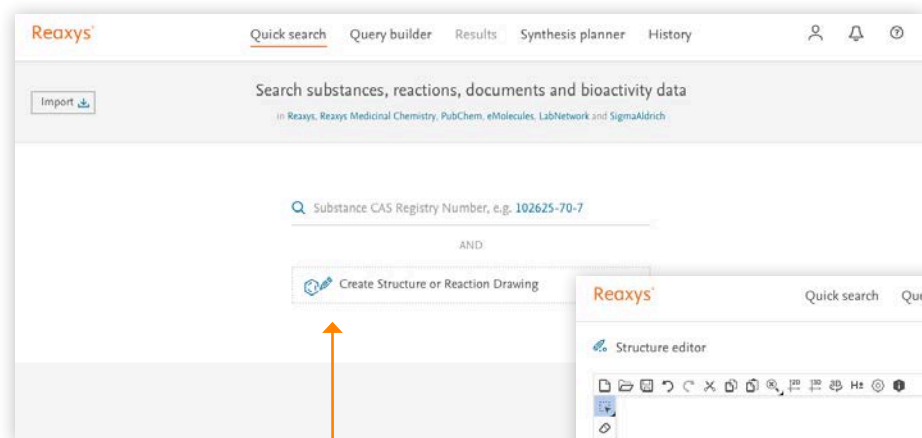
Truncations and wildcards are accepted.

**Structure Search** enables the creation of structure and reaction drawings.

Use these as the main query or combine them with keywords for added search power.

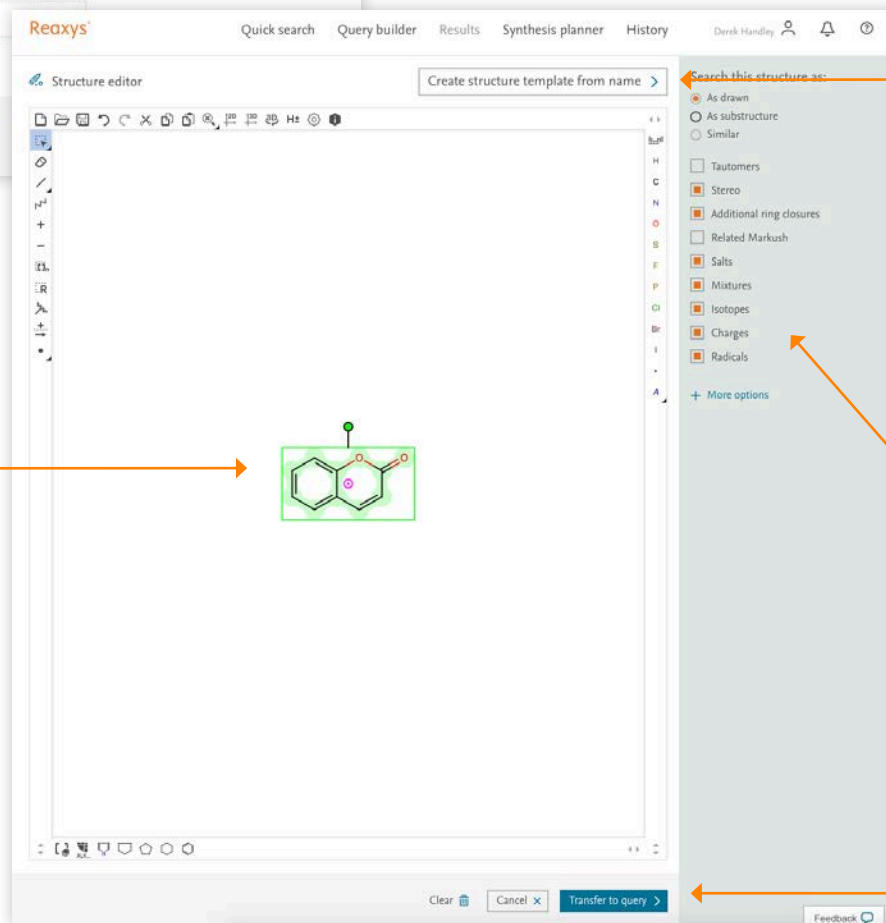
Create a user profile to enable customized results displays (hits per page) as well as alerts and saved searches.

## QUICK SEARCH USING STRUCTURE OR REACTION DRAWINGS



1. Click the **Create Structure or Reaction Drawing** box.

2a. Use ChemAxon's Marvin JS to create a structure or reaction drawing.



2b. Use **Create structure template from name** to generate a drawing from the name of the substance.

3. Define whether the query should be **As drawn**, **As substructure** or as a **Similar** structure. Add limits (e.g., tautomers, additional ring closures), if required.

4. Click **Transfer to query** to add the drawing to your query.

### QUICK TIPS:

- Atom Mapping: draw a reaction arrow between the mapped atoms
- Substitution Counts: Click in the white space and type the period key (.), then select .s+ from the Atom Query Properties menu, and click to change count
- Click [here](#) for more tips

## QUICK SEARCH RESULTS PREVIEW

When the query is ready, click **Find**.

Reaxys analyzes the Quick search query input and provides options based on query interpretation (Substances, Reactions and/or Documents).

Click **Preview Results** to view the top three results for that result set.

Click **View Results** to view all results for that result set.

## QUERY BUILDER FIELDS, FORMS AND HISTORY PANEL

Click here to open  
Query builder.

To find search **Fields** or **Forms**, enter keywords here. For example, "boil" would help to find the *boiling point* fields.

Click **Forms** to access predefined or customized search forms covering certain subjects.

Click **History** to display Recent and Saved searches that can be used in **Query builder** in combination with each other or with other search fields.

The initial view shows the search field categories.

The screenshot displays the Reaxys Query Builder interface. At the top, there is a navigation bar with tabs for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. Below this is a toolbar with icons for 'Import', 'Save', 'Reset forms', and 'Delete all', along with search filters for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'. The main area is a large grid with a textured background and the text 'Drag & Drop to build a new query'. On the right side, there is a panel titled 'Find search fields and forms' with a search input field and three tabs: 'Fields', 'Forms', and 'History'. The 'Fields' tab is active, showing a list of search categories such as 'Basic Indexes', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', 'Bibliography', 'PubChem', 'eMolecules', 'LabNetwork', 'SigmaAldrich', and 'Structure'. Each category has a dropdown arrow. An arrow points from the 'Forms' tab to the search input field, and another arrow points from the 'History' tab to the search input field.

Drag & Drop to build a new query

## QUERY BUILDER

Save enables the user to save the query for re-use later.

Chosen fields and forms appear in the main working area for Query builder.

Click Show or Hide fields to show all the parameters that can be chosen in that query field or form.

When fields and forms are found, click or drag-and-drop to add them to the main working area.

AND

OR

● AND

NOT

NEAR

NEXT

PROXIMITY

Define the search criteria

Click Search when the query is ready.

### CLICK TO ADD BOOLEAN OPERATORS:

- OR: contains data from at least one of the fields
- AND: contains data from both fields
- NOT: contains the first field's data and excludes the second's
- PROXIMITY: ensures the content of both fields relate to each other (typically used with parameter fields, e.g., melting point and solvent)

**Note:** If a field or form consists of multiple parameters, they are automatically combined using the PROXIMITY operator.

DOCUMENT RESULTS PAGE

Use **Filters and Analysis** options to narrow your results.

Default sorting is by descending relevance, but other options are available:

- Publication Year.
- Document Type.
- Cited By.

Sort search results ✕

Relevance ↑ ↓

Publication Year

Document Type

Cited By

Use **Index Terms (List)** and/or **Index Terms (ReaxysTree)** to filter documents by topic.

Click an author's name to explore details about their publications and get additional analysis options in Scopus®.

50

From history

**Filters and Analysis**

Index Terms (List) ▾

Index Terms (ReaxysTree) ▾

Publication Year ▾

Document Type ▾

Authors ▾

Patent Assignee ▾

Journal Title ▾

Substance Classes ▾

Reaction Classes ▾

**50 Documents** with 114 Substances, 147 Reactions, 45 Targets

0 Limit To Exclude Export

Relevance ▾ Heatmap

**Compositions and methods for prevention and treatment of chronic diseases and disorders including the complications of diabetes mellitus**

<sup>1</sup> Kosbab, John V. - US2001/31744, 2001, A1

Patent Family Members: CA2280093 A1; WO1998/33494 A1; AU6141498 A; EP1021177 A1; JP2001/511153 A; ...

[Abstract](#) ▾ [Front Page](#) ▾ [Info](#) ▾ [Substances](#) 12 ▾ [Reactions](#) 11 ▾ [Full Text](#) ↗

[Hit Reactions](#) 1 ▾

**DNA encoding human K casein and process for obtaining the protein**

<sup>2</sup> Symbicom Aktiebolag - US6232094, 2001, B1

Patent Family Members: DK8892 D0; CA2128110 A1; WO1993/15196 A1; AU3346493 A; EP625197 A1; ...

[Abstract](#) ▾ [Front Page](#) ▾ [Info](#) ▾ [Substances](#) 14 ▾ [Reactions](#) 14 ▾ [Full Text](#) ↗

[Hit Reactions](#) 1 ▾

**No title**

<sup>3</sup> [Lythgoe, B. et al.](#) - Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), 1978, p. 590 - 595

[Substances](#) 32 ▾ [Reactions](#) 36 ▾ [Full Text](#) ↗

[Hit Reactions](#) 5 ▾

Click these links to view the **Abstract**, the **Index Terms** for this record, the **Substances** and **Reactions** in the record, the **Front Page** information (for patents) or the **Full Text** of the document.

[Cited 43 times](#)

To export results:

- Click **Export** in the toolbar (if the export button is not visible, click Options)
- Define **Format**, **Range**, **Export data** and **Additional options**
- Click **Export** – the progress will be displayed in the lower right of the screen
- When the export is complete, click **Download**

Click this citation number to view citation information in Scopus.

**Note:** Use the checkboxes beside the results to select individual results and only export those.



## USING FILTERS

147 Reactions out of 50 Documents containing 114 Substances, 45 Targets

Reaction ID: 338987

4 Conditions Find Similar >

Yield Conditions References

With benzene Irradiation UV-Licht; unter Luftausschluss; Reinigung ueber das O-<3.5-Dinitro-benzoyl>-Derivat, das O-<3.5-Dinitro-4-methyl-benzoyl>-Derivat oder das Allophanoyl-Derivat;

Windaus; Deppe; Wunderlich - Justus Liebig's Annalen der Chemie, 1938, vol. 533, p. 118,126  
Full Text > Details >

Windaus; Schenck; v. Werder - Hoppe-Seyler's Zeitschrift fuer Physiologische Chemie, 1936, vol. 241, p. 100,103  
Full Text > Details >

Schenck - Naturwissenschaften, 1937, vol. 25, p. 159  
Full Text > Cited 8 times > Details >

Winthrop Chem. Co. - US20  
Full Text > Details >

Inhoffen - Naturwissenschaften  
Full Text > Details >

van der Vliet - Recueil des Tr

1. Click text or to expand the filter.

2. Click **More** to display additional filter options.

3a. Applying this filter will reduce the original 147 reactions to 19.

Catalyst Classes 19

|                  |     |
|------------------|-----|
| Catalyst Classes | 147 |
| active center    | 106 |
| Al               | 69  |
| Cr               | 38  |
| B                | 32  |
| Si               | 19  |
| Pd               | 19  |
| Zn               | 14  |
| Fe               | 9   |
| Os               | 6   |
| Ti               | 2   |
| Mn               | 1   |

Selected search items:  
Pd

Clear selected

Limit To > Exclude >

Click [here](#) to learn more about Filters

3b. Click **Limit To** to see just these 19 results or **Exclude** to see all results except these 19.

## SYNTHESIS PLANNER: MANUAL PLANNING

Reaction ID: 338987

Options

Synthesize

4 Condition

Yield

Synthesize

- Manually
- Autoplan

1. Click **Synthesize** under a substance and then click **Manually**.

3. Click **Add # to plan**.

Add preparation - 49

Preparation

85.4%

+ others

+ Load more Cancel x Add 2 to plan >

2. In the **Add preparation** window, select reactions to add to your plan.

Synthesis Planner Edit

Synthesis plan 1

Import Save Export

+ Create new

Feedback

6. Click **Export** to export reactions or documents.

7. To save the query (as a .json file), click **Save**.

4. From the **Synthesis planner**, click the Synthesis plan to view.

5. Click the Synthesis step options (⋮) to access:

- Show conditions
- Hide preparations
- Add preparations
- Remove preparations

Show conditions

Hide preparation

+ Add preparations

Remove preparation

Conditions

Abstract >

With water; sodium hydroxide In methanol at 28 - 70°C; Temperature; Experimental Procedure v

FERMENTA BIOTECH LIMITED; DATLA, Anupama; TAMORE, Jagdish; TRIVIKRAM, Sreenath - WO2015170341, 2015, A1 Location in patent: Page/Page column 14 Full Text > Details > Abstract >

Preparation - 1b

| Yield | Conditions   | Reference  |
|-------|--|--|
|       | Stage #1: C <sub>12</sub> H <sub>22</sub> O <sub>5</sub> With pyridine; methanesulfonyl chloride at 0 - 20°C; for 1.25h; | Xu, Libin; Porter, Ned A. - Journal of the American Chemical Society, 2014, vol. 136, # 14, p. 5443 - 5450 |
|       | Stage #2: With tetrabutyl ammonium fluoride In tetrahydrofuran at 20°C; for 2h;  | Full Text > Cited 11 times > Details > Abstract >  |

SYNTHESIS PLANNER: AUTOPLAN

Reaction ID: 338987

Options

Synthesize

4 Conditions

Yield

Find Similar

Synthesize

- Manually
- Autoplan

1. Click **Synthesize** under a substance and then click **Autoplan**.

Synthesis Planner

Plan 1

1 Plan 1

2 Plan 2

Autoplan 2 2

1 Plan 1

2 Plan 2

Autoplan 3 2

1 Plan 1

2 Plan 2

Autoplan 4 2

+ Create new



2. Define parameters for automatically generating synthetic pathways.

Create plans by autoplan

Number of plans to create: 10

Max. alternative branches: 5

Max. number of steps: 5

Stop searching if starting material is commercially available:  Yes  No

Default yield for reactions without a given yield: [Slider]

Always show screen before creating autoplan

Create Plans



3. Click **Create Plans**

Show conditions

Hide preparation

+ Add preparations

Remove preparation

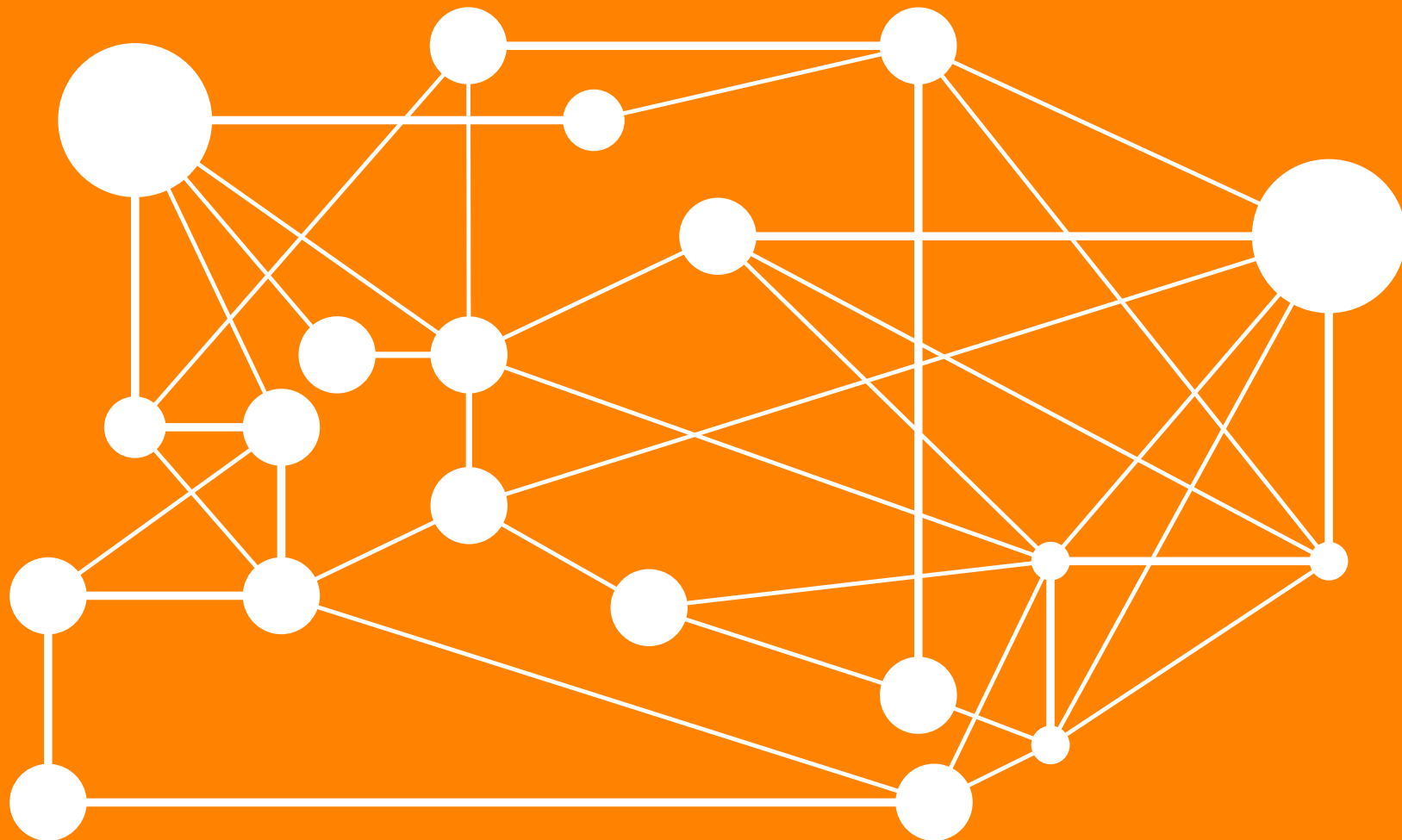
4. Click the Synthesis step options (⋮) to access:

- Show conditions
- Hide preparations
- Add preparations
- Remove preparations

Conditions

Preparation - 1a

| Yield | Conditions  | Reference  |
|-------|---|--|
| 85.4% | With sodium hydroxide in ethanol at 80°C for 0.5h   | Jiu, Mengqi; Zhao, Rui; Xu, Bing; Yin, Wenqiang; Chu, Fuhao; Gu, Hongshun; Gu, Tianan. J. Wang. Beijing: Lin. Huan. MedChemComm, 2017, vol. 8, 4, p. 343-351<br>Full Text > Details > Abstract > |
|       | With sodium tetraborate in methanol   | U; Babunan, Faz; Tan, Tian. Bull. of the Chemical Society of Ethiopia, 2011, vol. 25, # 2, p. 247-254<br>Full Text > Cited 2 times > Details > Abstract >  |
|       | With water: sodium hydroxide in methanol at 28-29°C; Temperature: Experimental Procedure: > | FERMENTA BIOTECH LIMITED; DATLA, Anupama; TAMORE, Jagdish; THEVIRAM, Sreerath - WQU005176141_2015_A1<br>Location in patent: Page/Page column: 14<br>Full Text > Details > Abstract >             |



# REAXYS

Visit <https://www.reaxys.com> to log in.

Visit the **Reaxys Support Center** for more helpful information about using Reaxys