



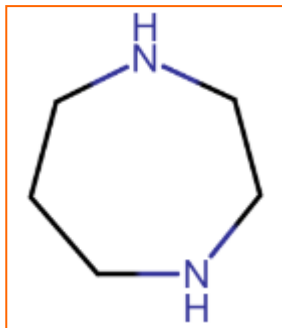
Reaxys®

Workflow example

Preparation of homopiperazine derivatives
with up to 3 rings and no ring fused to the parent

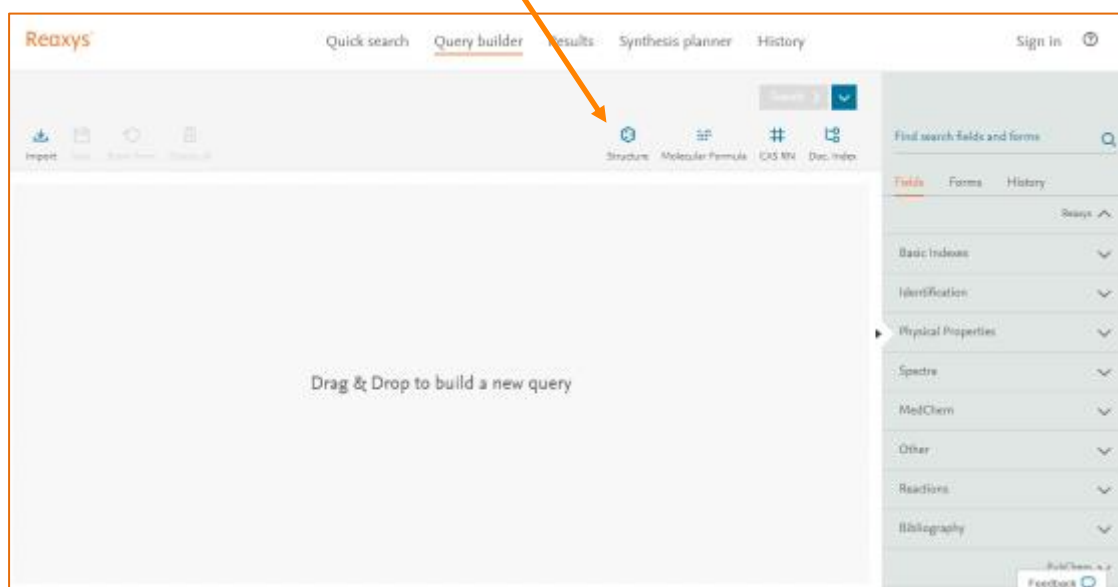
Workflow concept

Using Reaxys, the scientist wishes to prepare homopiperazine derivatives with up to 3 rings, including at least one 6-membered heterocyclic ring, and with no ring fused to the parent. They would also like to know if microwave-assisted synthesis would save time.



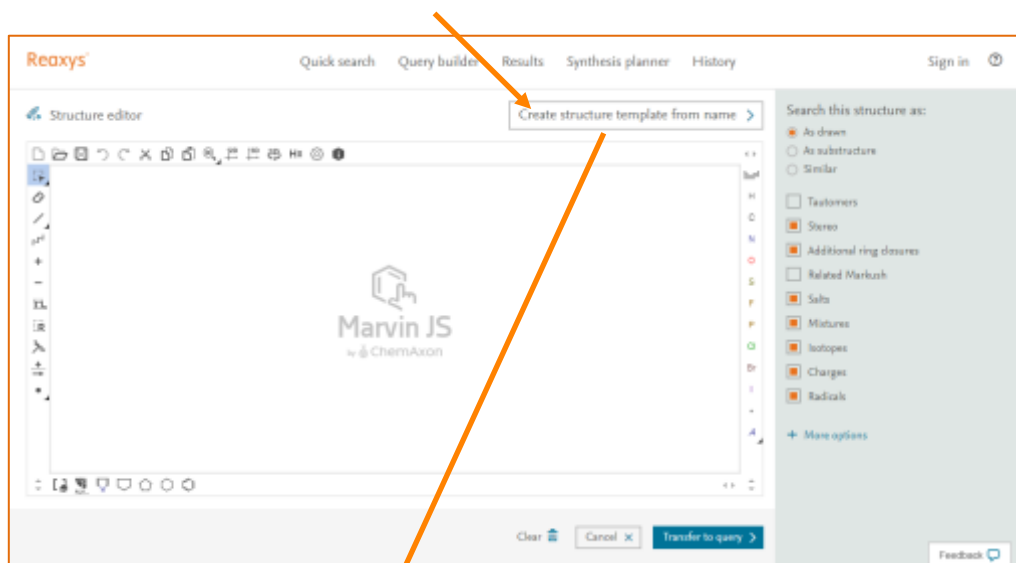
1. Use Query Builder to create the desired structure

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



The screenshot shows the Reaxys interface with the 'Query builder' tab selected. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The 'Structure' icon is highlighted with an orange arrow. The main workspace contains the text 'Drag & Drop to build a new query'. The right sidebar features a search bar and a list of search fields and forms, including 'Basic Indexes', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'.

Click **Create structure template from name** and type “homopiperazine”.



Reaxys

Quick search Query builder Results Synthesis planner History Sign in

Structure editor

Create structure template from name

Marvin JS
by ChemAxon

Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals
- + More options

Clear Cancel X Transfer to query Feedback

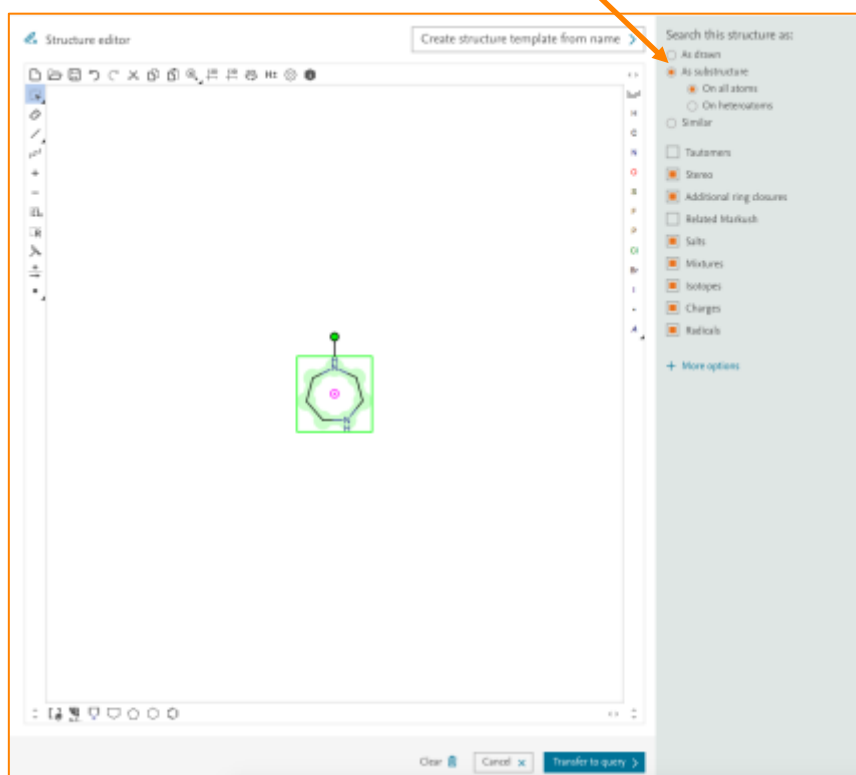


Create structure template from name

is Enter a chemical name, CAS-RN, InChIKey or SMILES

homopiperazine

Under **Search this structure as:**, select **As substructure**.



Structure editor

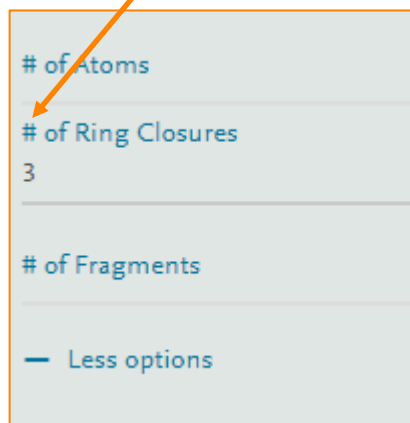
Create structure template from name

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 X Transfer to query

Click + **More options** and add 3 in **# of Ring Closures**. Click **Transfer** to query.



Reaxys retrieves over 7,400 homopiperazine analogs.

A screenshot of the Reaxys search results interface. The top header shows '7,468 Substances out of 2,488 Documents, containing 11,759 Reactions, 1,220 Targets'. On the left is a 'Filters and Analysis' sidebar with various filter categories. The main results area shows a list of substances. The first entry is '1-(5-isquinolinesulfonyl)homopiperazine' with its chemical structure and associated data. The second entry is 'diazep' with its chemical structure and associated data. The third entry is 'bumazosin'. At the top right of the results area, there is a dropdown menu showing 'Reaxys - 7,468'. At the bottom right, there is a 'Feedback' button.

2. Apply filters to limit to substances with the desired substructure

Click the **Substance Classes** filter and select **+ More**.

The image shows two panels from the Reaxys interface. On the left is the 'Filters and Analysis' sidebar, which includes categories like 'By Structure', 'Measurement pK', 'Highest Clinical Phases', 'Targets', 'Parameters', 'Substance Classes', and 'Molecular Weight'. The 'Substance Classes' filter is expanded, showing options for 'Functional Group Classification', 'Richter Classification', and 'Ring Classification', each with a count of 7,443. A '+ More' button is visible below these options. On the right is the 'Substance Classes' filter panel, which displays a tree view of classification categories under 'Richter Classification'. The 'Heterocyclic Compounds' category is expanded, showing sub-categories like '7-Membered Heterocycles Containing One or More Heteroatoms' (7,444), '6-Membered Heterocycles Containing a Single N Atom' (1,956), and '6-Membered Heterocycles Containing Two Heteroatoms' (782). Below the tree is a 'Selected search items' section with three active filters: '6-Membered Heterocycles Containing a Single N Atom', '6-Membered Heterocycles Containing Two Heteroatoms', and '6-Membered Heterocycles Containing Three or More N Atoms'. A 'Limit to' button is highlighted in blue.

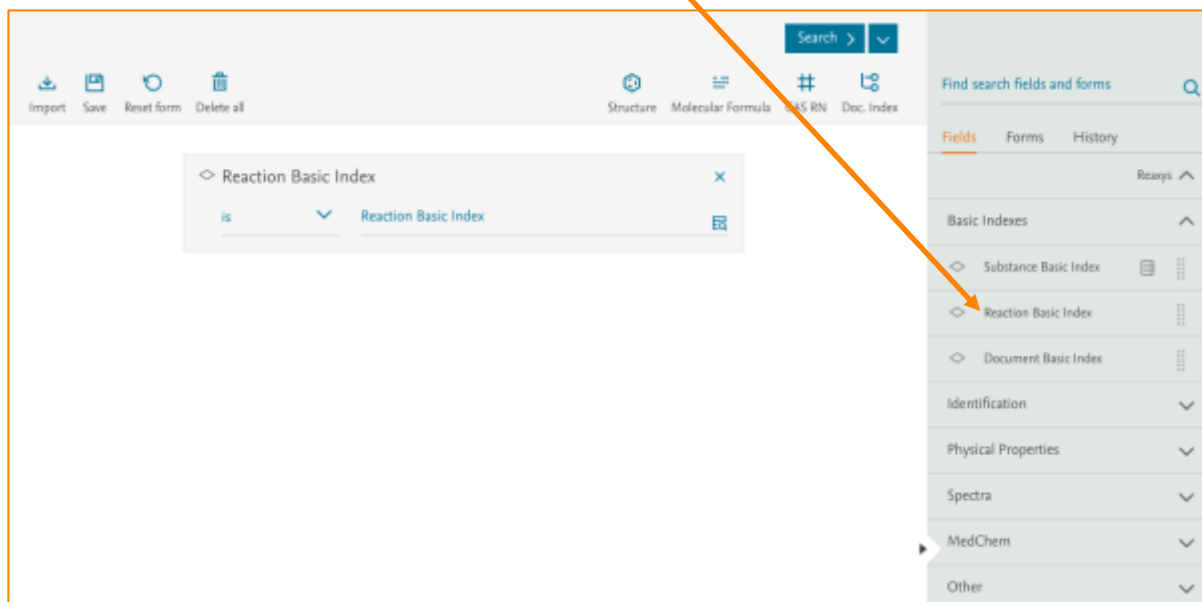
Select the **Richter Classification**, select all the substance classes with 6-membered heterocyclic rings, and click **Limit to**.

Reaxys retrieves over 2,700 substances meeting these criteria.

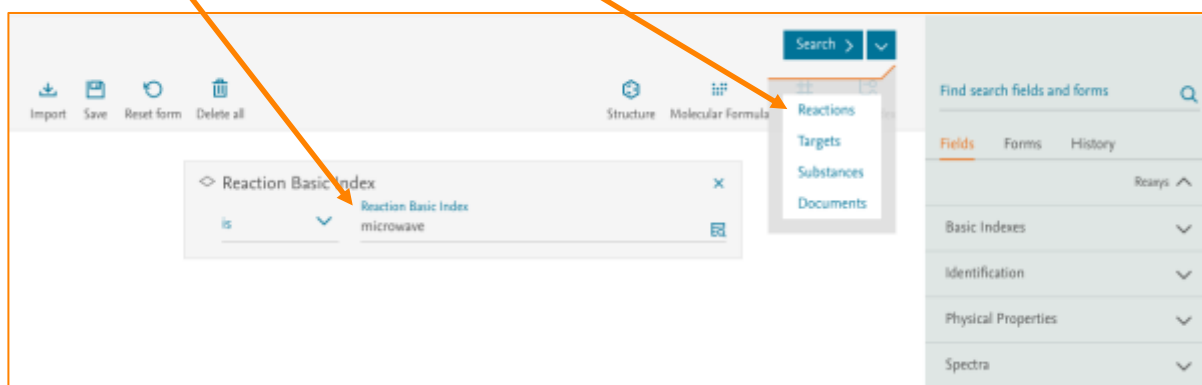
The image shows the Reaxys search results page. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The 'Results' section shows '2,724 Substances' out of '1,278 Documents, containing 3,450 Reactions, 866 Targets'. The 'Filters and Analysis' sidebar is visible on the left, with the 'Substance Classes' filter expanded to show 'Functional Group Classification' (2,724), 'Richter Classification' (2,724), and 'Ring Classification' (2,724). The main search results area displays two substance cards. The first card is for '1-(5-isoquinolinesulfonyl)homopiperazine' (C₁₄H₁₂N₂O₅S), with 291,374 documents, 548,273 reactions, and 103,746 targets. The second card is for 'benacezin' (C₁₄H₁₂N₂O₂), with 373,455 documents, 71,203 reactions, and 80,758 targets. The 'Limit to' button is highlighted in blue.

3. Use Query Builder to search for the desired reaction types

Open **Query Builder** and select **Reaction Basic Index** from the **Fields** options.



Type "microwave" and search for **Reactions**.



Reaxys retrieves over 900,000 reactions.

4. Use Query Builder to construct a merged search query

Click **History** in **Query Builder** and drag the relevant searches to the main field to build a merged query.

The image shows two screenshots of the Reaxys Query Builder interface. The top screenshot shows the 'History' tab selected in the right-hand sidebar, with a list of previous searches including '928,102 Reactions reactions: (RDLB:REA is "microwave")' and '2,724 Substances'. An orange arrow points from the 'History' tab to the main query field. The bottom screenshot shows the main query field containing the merged query: '928,102 Reactions reactions: (RDLB:REA is "microwave") AND 2,724 Substances'. An orange arrow points from the 'AND' button to the main query field.

Reaxys retrieves around 200 reactions that have microwave reactions and the desired derivative, with links to the source literature and the possibility to explore reaction details.

The image shows a screenshot of the Reaxys Results page. The left sidebar contains filters and analysis options. The main area displays 211 reactions, with one reaction selected and its details shown. The reaction details include the reaction scheme, reagents, conditions, and a list of references.

Further information on using Reaxys can be found in the user guide in the [Reaxys Support Center](#).