A Guide to Using Reaxys
For NUS users
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ACCESSING REAXYS

1. Click or enter the following URL to access the NUS Libraries portal: lib.nus.edu.sg.

2. Select the “Databases” tab.

3. Click “Reaxys”.

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A Guide to Using Reaxys
4. Users will be prompted to log in before accessing the E-Resources such as Reaxys. To proceed, perform EITHER of the following steps:

**A: If you are accessing Reaxys in campus**
- Click “Campus Login”

**B: If you are accessing Reaxys outside campus (e.g. home)**
- Select your Network Domain
- Enter your User ID (NUSNET ID). Examples are:
  - E0192923 (for students matriculating after AY 2015/2016)
  - g0700625, u0700423 (for students before AY 2010/2011)
  - ecettt (for staff)
- Enter your NUSNET password (same as the password for NUS email & IVLE)
- Click “Login”

Click [here](#) for Frequently Asked Questions (FAQs) on access to E-Resources.
5. Upon successful login, users will be advised to view the Appropriate Use Policy. Once the policy is read, click “I accept”.

NUS Libraries E-Resources Appropriate Use Policy

You are reminded that the Copyright Act applies to the whole National University of Singapore Library collection. The usage of materials/information retrieved from the Digital Library Collection by users from the NUS must abide by the conditions set out in the Copyright Act.

These materials can be used for academic research, learning and teaching purposes only for yourself. Under no circumstances should the data be disseminated to another person or used for commercial purposes.

Violation of the Copyright Act is an offence in Singapore and the use of NUS facilities for illegal copying is a violation of NUS rules and regulations. The University takes a serious view of copyright infringement. Anyone found violating the Copyright Act may face disciplinary action.

Please note that this service will not be available between 5:00 AM to 5:30 AM (Singapore Time) daily for maintenance.

If you have any problems accessing this service, please refer to the Frequently Asked Questions or contact Helpdesk.

I have read the Appropriate Use Policy for E-Resources and agree to abide by it.

I Accept

6. The homepage of Reaxys will be displayed.
PERFORMING A SEARCH

There are two ways through which users can conduct a search in Reaxys: by using Ask Reaxys or the specific search form (e.g. Reactions, Substances). While the design of the former resembles the search boxes in commonly-used search engines, it intelligently interprets the query and directs user conveniently to the right information needed. For more accurate results, a search done via the specific search form may be a better option.

USING ASK REAXYS

1. Enter a query in the search box and click “Go”.

2. Ask Reaxys automatically recognizes the term “phenyl styryl ketone” as a substance query and directs users to the Substances tab (see step 1 of REFINING YOUR SEARCH). On the other hand, for terms that fit into more than 1 category (e.g. citations and reactions), a box appears and prompts users to select the most suitable option. For instance, the term “Barton McCombie” is interpreted in 3 ways:

   - Citation search based on the author name “Barton McCombie”
   - Reaction search based on the reaction “Barton-McCombie deoxygenation”
   - Citation search in the title, abstract and keyword based on the term “Barton McCombie”
Useful Tips

For a start, you may wish to view the query examples by clicking “See examples” below the search box. Through these examples, you can learn how to construct search statements in a manner that can be interpreted correctly by Ask Reaxys.

Using Specific Search forms

1. Select the search form that best describes the nature of your search.

2. If you require fields from multiple search forms (e.g. finding spectra of substances), click “Add/Remove Fields” at the bottom of the search form to add the fields from another search form. In example below, fields related to IR spectroscopy are added in the “Substances” search form.
Users can view the list the fields that can be included in the popup box. Search for the property, select the relevant field(s) and click “Add >>”. When completed, click “Save”.

The added fields will be displayed.
3. In the selected field, choose the appropriate relational operators (e.g. is, contains, =, <) and enter the search term. Users can also select from a list of related terms suggested automatically by Reaxys.

Alternatively, users can click “lookup” to view a list of index items for each respective field.

A box containing the list of items appears. Enter the term and select the most appropriate index item. The number (in brackets) next to the index item shows how many of such items can be found in the database. Click “Transfer”.

Performing a Search
4. Users do not need to complete all the fields. Once sufficient search information is provided, click “Search Substances” at the bottom of the search form.

**STRUCTURE SEARCH**

In addition to chemical name search, a structure search is also possible in both Substances and Reactions search forms. There are two ways to perform a structure search on a single substance in the **Substances** search form. **Create Structure Template from Name** allows users to build a structure by entering a chemical identifier (e.g. name):
Alternatively, users can click the box to **sketch** the molecule from scratch or edit the created molecule. Use the tools at the sides of the pop-up box to complete the sketch. When done, click “Transfer Query”.

Once a structure is constructed, view and select the options on the right to broaden or narrow your search.
The same methods can be applied to the structure search in the **Reactions** search form. You can sketch a substance or equation:

**MOLECULAR FORMULA SEARCH**

The field “Molecular Formula” can be added to any search form. Once the field is added, users can use type or use the formula builder to construct the formula. In the formula builder, users can specify the range of charges and atom counts in the formula.
Performing a Search

For instance, based on the search statement “Hg[1-2]Cl[1-2]”, mercury compounds such as HgCl, HgCl₂ and Hg₂Cl₂ can be retrieved.

<table>
<thead>
<tr>
<th>Cl₂Hg</th>
<th>Cl–Hg–Hg–Cl</th>
<th>Cl₂Hg₂</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="#" alt="Synthesize" /></td>
<td><img src="#" alt="Synthesize" /></td>
<td><img src="#" alt="Synthesize" /></td>
</tr>
<tr>
<td><img src="#" alt="Find similar" /></td>
<td><img src="#" alt="Find similar" /></td>
<td><img src="#" alt="Find similar" /></td>
</tr>
<tr>
<td>Identification: Physical Data (1865) Spectra (235) Reactivity (76) Use/Application (36) Quantum Chemical Data (33)</td>
<td>Identification: Physical Data (2773) Spectra (12) Use/Application (28) Quantum Chemical Data (12)</td>
<td>Identification: Physical Data (86) Spectra (5) Use/Application (4) Quantum Chemical Data (1)</td>
</tr>
</tbody>
</table>

**Finding Metal Alloys**

The field “Alloy” can be added to any search form. Once the field is added, the component formula and its corresponding percentage can be specified.
LITERATURE SEARCH

A literature search is recommended for complex molecules such as polymers. In the Literature search form, enter the search term in “Citation Basic Index” field so that a search can be done in the title, author, abstract and keywords of the indexed articles. Where possible, use Boolean operators (AND, OR, NEAR, NEXT, NOT), truncation (*) and/or Lookup to enhance your search.

Based on the above search statement, Reaxys retrieves articles that contain both words “surface” and “tension” in close proximity as well as any word containing “polyvinyl”.

**Polyvinylamine-g-galactose is a route to bioactivated silica surfaces**

Polyvinylamine (PVAm) was derivatized with lactobionic acid to give PVAm-GAL with pendant galactose groups along the PVAm chain. The galactose substituents: types of specific interactions: (1) condensation with phenolic and acidic moieties on polymers and on surfaces and, (2) the specific binding of RCA120, a galactose binding and assembly was monitored with Quartz Crystal Microbalance (QCM-D) measurements. Multilayer assemblies based on boronic ester formation were destabilized by introducing sorbitol. We propose that the physical adsorption of PVAm-GAL onto silica or other negatively charged support surfaces is a simple route to galactose useful for affinity separations, cell targeting and cell culturing.

Keywords:
- Author: Boronate complexes; Galactose; Layer-by-layer; Lectin; Polyvinylamine; QCM-D
- Compound: Boronate; Complexes; Galactose; Layer-by-layers; Lectins; Polyvinylamines; QCM-D
- Compound Description: Boronate; Complexes
- Compound Mainhead: Silica
- EMTREE drug term: boronate; boronic acid; galactose; lactobionic acid; lectin; polyvinylamine-g-galactose; silicate; sorbitol; unclassified drug
- EMTREE medical term: adsorption; article; concentration (parameters); derivatization; esterification; ionization; molecular weight; p; pH; polymerization; porosity; binding; proton nuclear magnetic resonance; quartz crystal microbalance; steady state; substitution reaction; surface properties; surface tension
- Medicine Description: Galactose; Magnetic Resonance Spectroscopy; Polyvinyl; Silicon Oxide; Surface Properties
- Reaxys Terms: Polyvinylamine; galactose-specific lectin; lactobionic acid; sorbitol - physical adsorption
A Close Look at the Search Results

There are three tabs in the search results page: Reactions, Substances and Citations. Users will be directed to the Substances tab automatically whenever the search term is recognized as a substance (e.g. phenyl styryl ketone). This principle applies to both Reactions and Citations tab.

In the Substances tab, the compounds are sorted according to the number of references (N° of ref.) by default. The order of the substances can be adjusted by clicking the drop-down menu beside “Sort by”.

It is interesting to note that a search on “phenyl styryl ketone” returns a total of 52 substance results. Reaxys also extracts the cis-trans isomers, isotopes and compounds with the same substructure as phenyl styryl ketone.

The number of results per page can be adjusted at the bottom of the page.
The property data of the substances can be found under the column “Available Data”. For example, to obtain the NMR spectrum of phenyl styryl ketone, click “Spectra”.

<table>
<thead>
<tr>
<th>Structure</th>
<th>Structure/Compound Data</th>
<th>Nº of preparations</th>
<th>Nº of ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Chemical Structure" /></td>
<td>Chemical Name: phenyl styryl ketone  Reaxys Registry Number: 50985  CAS Registry Number: 94-41-7  Type of Substance: bicyclic  Molecular Formula: C_{12}H_{10}O  Linear Structure Formula: C=CH(C)(CH=CH)_CH_CH_CH_O</td>
<td>209 prep out of 4066 reactions.</td>
<td>2559</td>
</tr>
</tbody>
</table>

Expand the “Spectra” list in which the NMR spectroscopic data can be found.

- Identification
- Physical Data
- Spectra
  - NMR Spectroscopy (51)
    - IR Spectroscopy (13)
    - Mass Spectrometry (13)
    - UV/VIS Spectroscopy (20)
    - ESR Spectroscopy (1)
    - Raman Spectroscopy (1)
    - Fluorescence Spectroscopy (1)
    - Other Spectroscopic Methods (1)

Details of the NMR spectroscopy carried out in each research experiment are summarized in a table form for easy viewing. To view a spectrum, see the full text of the article (refer to Accessing Full Text in this manual).
Information about reactions involving the compound can be found under the column “\textbf{N\textdegree\ of preparations}”. Select the figures to obtain the corresponding list of reactions in the Reactions tab.

<table>
<thead>
<tr>
<th>Structure</th>
<th>Structure/Compound Data</th>
<th>\textbf{N\textdegree\ of preparations}</th>
<th>Available Data</th>
<th>\textbf{N\textdegree\ of reactions}</th>
</tr>
</thead>
<tbody>
<tr>
<td>\includegraphics[width=1cm]{structure1}</td>
<td>\begin{itemize} \item Chemical Name: \textit{phenyl styryl ketone} \item Reaxys Registry CAS Registry N: \item Type of Subst. \item Molecular Form \item Linear Structure formula: \item Molecular Weight: \item InChI Key: \end{itemize}</td>
<td>209 prep \ out of 4066 reactions.</td>
<td>Identification \ Physical Data (198) \ Bioactivity (123) \ Ecological Data (2) \ Use/Application (49) \ Quantum Chemical Data (3)</td>
<td>2550</td>
</tr>
</tbody>
</table>

Out of 4066 reactions, 209 involve the synthesis of phenyl styryl ketone

In the Reactions tab, the articles are grouped according to the reactions. Details such as the condition of the experiment and the corresponding percentage yield are recorded in the table. Refer to Accessing Full Text in this manual for obtaining the full texts of these articles.
Useful Tips

You can magnify chemical structures without enlarging the fonts in the table at the same time. Click “Zoom In”.

To find information on another substance in the reaction equation, click under the substance and select “Copy Structure to Query”.

Performing a Search
The structure of the substance will be transferred to the homepage and a search can be carried out.
REFINING YOUR SEARCH

The search results can be refined by two ways: the filter panel and the analysis view. The available filter criteria are similar in both but the latter shows a graphical distribution of the data under a particular criteria.

USING FILTER PANEL

Located at the side of the search results page, the filter panel is divided into three parts:

- **Substance-focused**
  - Substructure
  - Molecular Weight
  - Number of Fragments
  - Physical Data
  - Spectroscopic Data
  - Bioactivity
  - Ecological Data
  - Natural Product
  - Availability
  - Availability in other DBs

- **Reaction-focused**
  - Yield
  - Record Type
  - Reagent/Catalyst
  - Solvent
  - Reaction Type
  - No. of Steps
  - Product Availability
  - Reactant Availability
  - Availability in other DBs

- **Citation-focused**
  - Document Type
  - Authors
  - Patent Assignee
  - Journal Title
  - Publication Year
1. For instance, to filter the search results by reaction type, expand the “Reaction Type” pane and click “More”. A box appears with more reaction types. The number beside each reaction type refers to the number of reactions associated with it. Select the desired reaction type(s) by ticking the box beside them. Click “Limit to” to show only these reaction types or “Exclude” to eliminate them from the list.

In this case, when the reaction types are limited to those associated with Friedel-Crafts reaction, only records containing these selected reaction types will be displayed. An example is shown here.
2. Repeat step 1 to apply another filter (if required) to the existing filtered results. For instance, limit the experimental yield to 95-100%. As a result, only reactions that contain records of the selected reaction type \text{AND} yield will be displayed. Observe the drop in the number of reactions after the filters are applied.

3. Every action taken in a search is traced and indicated on top of the search results. To undo one or more actions, click the box which displays the original list of results before the change was applied.
Sometimes it would be more effective to filter by substructure. In this example, from a list of reactions involving butadiene, we are interested in limiting reactions to those that produce 1,5-cyclooctadiene. This can be done without filtering by reaction type.

Expand the Substructure pane in the filter panel. In the popup box, the structure of 1,5-cyclooctadiene can be created by sketching or creating the structure template from name (refer to pages 11-12). Make sure the role “Product” is selected. Click “Limit to”.

The results are effectively retrieved. Note that certain reactions do not contain any record that specifies the reaction type.
**USING ANALYSIS VIEW**

1. Open the analysis view by clicking the icon above the search results.

2. The expanded Analysis View contains 2 histograms. Select the filter criteria from the drop-down list for Histogram A.
3. Mouse over each category to view the full category name and click it to view the sub-categories. Click 🔄 to view the next page. Click the bar graph(s) to select one or more (sub)categories. These graphs will be highlighted in red.

![Histogram A and B](image)

4. The yellow regions in Histogram B represent the distribution of the filtered results from Histogram A when the second filter criteria is selected. Repeat steps 2-3 for Histogram B.

![Histogram B](image)
5. A total of 124 reactions satisfy both criteria. Click “Limit to” to show only these reaction types or “Exclude” to eliminate them from the list.
ACCESSING FULL TEXT

1. Click available in every article record.

2. A new tab or window appears with the publisher’s record that allows the full-text access to the selected article.
An error message (similar to the screenshot below) may appear instead of a publisher’s record. In this case, the online title may not be subscribed by NUS Libraries.

You can check if the title is available in the Library catalogue by clicking “By ISSN” and “By Title”. If the title is not available in the catalogue, you may request for Document Delivery Service (if eligible). More details can be found here.
EXPORTING CITATIONS

1. Click “Show Details” in the article record of interest.

2. Users will be directed to the Citations tab containing the article record of interest. Click “Export” below the tabs.
3. In the popup box, select the format “Literature Management Systems”. Users can decide if the export contains abstract. Once done, click “Export Data”.

4. When the export is complete, click “Download”.

![Reaxys Export Citation Results](image)
5. If a reference management software (i.e. EndNote) is installed in the computer, it will be launched and the newly-imported title can be found in “Imported References”.

6. With these imported references, users can use EndNote’s Cite While You Write (CWYW) feature to insert citations in Microsoft Word. For more information on EndNote, refer to the EndNote LibGuide.

References


COMBINING DATASETS

The History tab records every action taken by the user during the current session. The datasets generated in this series of actions can be combined via Merge, Overlap or Exclusion. Merge allows the selected datasets to unite and form a new, bigger dataset. On the other hand, overlap identifies and extracts the common information in these datasets and hence a new, smaller dataset forms. Exclusion subtracts information in one dataset from the other. These functions help to broaden or narrow the search results.

1. In this example, we are interested in merging the preps of both cis- and trans-isomers (cis-chalcone and 1,3-diphenyl-propen-3-one) of phenyl styryl ketone. A search on the term “phenyl styryl ketone” returns both information on cis-chalcone and 1,3-diphenyl-propen-3-one.
2. Retrieve information on the preps of both substances by selecting the highlighted figures.

- Select the first figure (which displays the prep of trans-isomer in the Reactions tab)
- Go back to the Substances tab (which re-displays the list shown below)
- Select the second figure (which displays the prep of cis-isomer in the Reactions tab)

3. Select History Tab at the top of the page.
4. The actions carried out in step 2 have been recorded in the search history. Tick the boxes beside the datasets to be merged. Click “Combine hitsets”.

5. Select “Overlap”.

![Diagram showing Combine hitsets feature with options to select datasets and merge them.](image)
6. As a result, reactions in the combined dataset involve the synthesis of both cis-trans isomers. In certain experiments, the yield ratio is stated in the full text.
SAVING YOUR SEARCH HISTORY

This is a useful tool to users who wish to save their search results for future reference.

CREATING A REAXYS ACCOUNT

1. Click the Register Tab at the top right hand corner of the homepage.

2. Fill in the required details. Tick the box below the mandatory fields and click “Register”.

![Register Tab in Reaxys](image1)

![Register Form in Reaxys](image2)
3. Upon successful registration, a notification box appears. Click “ok”. Users can now proceed to save the search history as they are automatically logged in.

**SAVING SEARCH HISTORY**

1. **Skip this step if you are automatically logged in.** Log in to Reaxys by clicking the Login Tab at the top right hand corner of the homepage.

   Upon successful login, your login name will appear on instead of “Anonymous user”.

2. Conduct a search via Ask Reaxys or a specific search form. Refine your results (if applicable).

3. Select the History Tab.
4. Click “Store” beside the search that you wish to save.

5. Name the search and enter a comment. Click “Save”.

6. Your search is now permanently saved. To view the search in a new Reaxys session, log in and view the History tab. Click “View” to see the results.