

Research Databases for Chemistry and Materials Science

Chemistry databases provide information about substance properties, reactions, and references to published research in biochemistry, chemistry,

materials, physics, pharmacology, medicine and more. In this task, you will search the **SciFinder** and **Reaxys** database.



SciFinder has excellent coverage of the 20th century chemistry literature. You can use it to search the literature by topic, substance or reaction structure.

Go to **SOLO** at <https://solo.bodleian.ox.ac.uk/>

Search for **SciFinder**, click on **Online access** and follow the link to **CAS Registration page** (sign in using your SSO credentials).

Fill in an online registration form, create user name and password.

Go back to SciFinder and sign in.

SciFinder: Research Topic

- A research topic search can help you find literature and substance information related to a particular subject.
- If it is not already selected, choose the **References: Research Topic** search option from the left of the SciFinder search home screen.
- Enter a topic to search, you can use natural language, such as *“Lead contamination in water supply”*
- SciFinder will try to identify documents containing your search terms, choose which set you would like to view from the options SciFinder gives you and then click **Get References**.
- SciFinder will show you a list of matching references. You can further refine these by using the **Analyze, Refine and Categorize** options on the left of the screen.
- Try using the **Refine** options to view only records from Conferences.
- If you open one of the records in your results list by clicking its title, you will see that the records contain information such as links to CAS records for chemical substances. These contain extensive information on physical and experimental properties.

SciFinder: Substances (substance properties)

- Click on **Explore** at the top left of the screen and choose **Substances: Chemical Structure**
- Click the **Structure Editor**. A box into which you can draw a chemical structure will open. We are going to draw the structure of ethanol.
- Make sure that carbon ‘C’ and single bond is selected in the row of icons underneath the drawing screen. Draw two connected carbon atoms on the screen (note that symbols for carbon and hydrogen are not shown as you draw). Click on the oxygen ‘O’ button and add an Oxygen to one end of the molecule you have drawn.
- On the right of the drawing screen check the **Exact** search option and click **OK**.
- The structure you’ve drawn will now be displayed in search box. Click on **Search**.
- After a few seconds, you will be shown chemical substances related to your search structure. Again you can use the analyse and refine options on the left to further narrow down your search results.

For more information and to arrange consultations:

Contact your subject librarian alessandra.vetrugno@bodleian.ox.ac.uk

Reaxys

This database covers research information in organic, inorganic and organometallic chemistry dating as far back as 1771. Discover chemical structures, properties and synthesis reactions; find relevant chemistry literature, or check availability for purchasing. You can open Reaxys by searching SOLO for Reaxys and clicking on the Online Access link.

Searching Reaxys: Substances, Reactions and Documents

Reaxys: Quick Search

You can use the quick search to look up a natural language enquiry such as '*boiling point of acetone*'. An initial selection of results will be shown, to display a results set click on the **View Results** button for the results set you are interested in viewing.

Reaxys: Structure search

- Reset the search and then click on the **Draw** button which is just underneath the main search box. We are going to draw the structure of hydrogen cyanide.
- From the right hand element selection bar, click the carbon **C** symbol and add this to the drawing panel. Add a nitrogen close to the carbon in the same way.
- On the left hand bond selection bar, click on the symbol for a single covalent bond. From the menu that pops out, choose the triple bond symbol. Drag this triple bond symbol between the nitrogen and carbon to connect the two.
- Click **Transfer to Query** at the bottom right of the drawing window. Now you can click the Find button.
- From the results, click the **View Results** button in the Substances section. You should now find results to access publications, reactions and substance information related to hydrogen cyanide.

Reaxys: Reactions Synthesis Planner

- Reset your search again. This time do a quick search for *Aspirin*.
- Next to the Substances set of results, click the **View Results** button.
- The top hit in your results should now show the chemical structure of aspirin. Beneath the structure diagram, find the icon that looks like this –



- This icon allows you to access the synthesis planner. Click the icon and from the options that appear, select **Autoplan**.
- You will be asked to choose some basic options for the planner. Leave the default settings as they are and click the **Create Plans** button. Reaxys uses information sourced from the chemistry literature to produce a list of alternative plans to synthesise your target molecule (aspirin in this case).
- Reaxys will show you a synthesis plan for aspirin. More detailed information and links to the literature is shown at the bottom of the screen.
- Options at the top of the screen allow you to save and export the displayed synthesis plan.

Subject Guides – LibGuides link to subject specific sources available at University of Oxford.

<https://libguides.bodleian.ox.ac.uk/chemistry>

<https://libguides.bodleian.ox.ac.uk/materials>

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