Searching Reaxys

1. What subjects and publication types are included in the database?
   There are three databases in Reaxys and they index facts about compounds that are found in the primary literature. Facts can be chemical, physical pharmacological, toxicological, etc. The publication types indexed are journal articles and patents.

2. What are the coverage dates?
   - Beilstein is 1771 to the present.
     176 journals are indexed
     Organic compounds
     11,196,514 substances
     22,732,872 reactions
   - Gmelin is 1772 to the present.
     62 journals are indexed
     Organometallic and Inorganic compounds
     2,687,265 substances
     2,044,673 reactions
   - Patent Chemistry Database is 1976 to the present.
     World, European, and US patents
     Organic chemistry & Life Science patents

3. What Boolean or Proximity operators are used by the database?
   - AND
   - OR
   - NOT
     The following three are all versions of the AND operator:
     - NEAR
       Find the terms adjacent to one another in any order
     - NEXT
       Find the first term immediately preceding the second term
     - PROXIMITY
       Use it when searching for facts that contain subfields or parameter field.
       (bp.bp=120 proximity bp.p=750-760)

4. If truncation is allowed then what symbols are used?
   - Asterisk (*) – represents any group of characters, including no character.
   - Question mark (?) – represents any single (1) character.
   - Double Question mark (??) – represents any two (2) characters.
   Right and Left truncation is permitted.

5. If wildcards are allowed then what symbols are used?
   Same as in question 4.

6. How do you search for a phrase?
   Use the NEXT operator.

6. Is it possible to group words from the same concept?
   Not Applicable.

7. Any unique features?
   Can search for a range of numbers
   (Example: den.den=150-160)
Accessing the database:
1. Go to the Chemistry Library web page (chemistry.library.nd.edu).
2. Click the Reaxys link.

Looking at the screen – it has three section tabs
1. Reactions – this is for building structures, substructures, and reactions. We will look at this in two weeks.
2. Substances and Properties
3. Text, Authors and more – this is for finding articles if you have a known citation or are looking for what an author has published. We won’t use this.

The focus for today will be the Substances and Properties tab.

This section has two contextual tabs at the bottom of the screen
1. Properties (Form-based)
2. Properties (Advanced)

**BOOLEAN OPERATORS**

AND, OR, NOT – these are standard

PROXIMITY – the two connected search terms will be retrieved if they are present in the same occurrence of a fact. This is very important when you search for facts that contain related fields. So when searching for a boiling point measured at a particular pressure, this operator should be used.

NEAR – both search terms are adjacent to each other but in any order

NEXT – the first search term will appear before the second search term

**Example:** You have an unknown in your org lab. The unknown has a melting point between 10-12 in a petroleum ether solvent, a density between 1.0-1.5, a molecular weight between 146-151 and you have a proton nmr for your unknown. What are the possibilities?

\[ (\text{DEN.DEN}=1.0-1.5 \ \text{AND \ IDE.MW = 146-151} \ \text{AND \ MP.MP =10-12} \ \text{AND \ MP.SOL = 'petroleum ether'} \ \text{AND \ NMR.NUC = '1h'}) = 1 \text{ compound} \]

1. Select the Query tab. Select the Substances & Properties tab. Click on the Generate structure from name button. Type 50-00-0 into search box. Click the Submit button. Click the Submit button for structure 1of 2 in the Found Chemical Structures window

Notice the Search Strategy section now has the structure associated with the name or CAS registry number you searched for.

Be sure the As drawn radio button is selected.
Click the **Search** button (lower right). Search Progress window opens to inform you of the progress of the search.

Then a results page appears. The results are shown with the compounds that have the most number of references first. You can change the sort by criteria.

1a. How many compounds do you get with this search?  
(You just did a structure search. You should get between 1900 - 2000 substances)

On the left side of the window there is a way to filter your results.

1b. How many compounds have a molecular weight between 24 and 36?  
(You should get between 50 - 75 compounds)

Click on the **Query** tab. Click on the **Clear Query** button. Then click on the **Properties (Form-based)** tab. Then click on the phrase **Substance Data**. Then click on the phrase **Identification Data**. **CAS Registry Number** is 50-00-0. Then click the **Search** button.

1c. How many compounds do you get with this search?  
(You searched for records with a certain CAS Registry Number. You should get fewer than 10.)

This view gives you a preview for each result.  
* In the **Compound Structure** section there are up to three icons and two links.

- ![Availability](image) Availability – check for commercial availability of the compound.
- ![Display](image) Display further options and data
- ![Enlarge](image) Enlarge the structure and rotate in 3D

  Synthesize – to create a synthesis plan for the compound

  Show Details – to display more information about the compound

* In the **Structure/Compound Data** section

  1d. What is the InChI Key?  

* In the **N° of preparations** section:

  1e. For the first result, How many reactions involve this compound?  
  (You should get between 75,000 – 77,000 reactions)

  1f. Of those, how many are for the preparation of this compound?  
  (You should get between 3,300 – 3,400 reactions)
* In the Available Data section shows what facts are associated with compound within broad categories.

1g. How many categories are listed? ________________

Click the Show Details link in the Structure Section for result #1 (Reaxys Registry Number = 1209228).

1h. Compare the categories with those in the Available Data Section. Are they the same? Yes No Kind of

Click on the Physical Data link.

1i. Click on the Boiling Point link.

What is the boiling point value for the first item? ________________________

In the reference column there are lists of citations that contain the data displayed. The citations include author’s last name, journal name, et al., and if there is full text available (of course, the library must have a subscription to it in order for you to be able to access the full text.)

1j. What is the journal title that reported this boiling point value? ________________

(If there is more than one citation then pick one of them.)

1k. Write the author’s name that reported this boiling point value? ________________

(If there is more than one citation then pick one of them.)

1l. Write the dissociation exponent for this compound? (Pick just one) ________________

(Scan all the entries in the Physical Data section to find it or <ctrl><F> to search the page.)

On the right side of the window are four triangles vertically stacked.

Click on the top one to go back to your Summary Information.

Click on the Physical Data link to collapse the listing. Then click on the Spectra link.

1m. How many times has Carbon NMR data been found in the literature for this compound? ________________

(You should get fewer than 10)
Click on the **Natural Product** link.

1n. In the Isolation from Natural Product section, how many articles are there? _______

**ALWAYS DO THE FOLLOWING BEFORE BEGINNING A NEW SEARCH**

Click the **Clear Query** button

**ALWAYS DO THE PRECEDING BEFORE BEGINNING A NEW SEARCH**

1. **Known compound to unknown property**
   (follow the instructions on page 10)

2. Find the following facts for dibenzopyrrole (Reaxys RN 3956).
   - What is the ionization potential? ________
     (pick one)
   - What is the solubility? 100 g of solvent dissolves ________ g of substance at ________ °C
     (there will be 83 entries - look at the 55th through 75th)
   - What is the mortality of mosquito larvae after 24 hours of exposure? ________ %
     (In the Bioactivity/Ecotox section look at the Pharmacological Data – entry 39 of 41)

3. Spinatoside is isolated from what natural product?
II. Known property to unknown compound
   (follow the instructions on page 10)

4. Find compounds which have a sublimation between 120C and 140C at pressures lower than $10^{-4}$ Torr

You should get between 35-40.  __________
   Did you get an error?  Check Common Mistakes – Number
   Did you get 41?  Check Common Mistakes - Operator
   Did you get 98?  Check Common Mistakes – Relation
   Did you get 102?  Check Common Mistakes – Operator & Relation
   Did you get more than 150?  Check your translation of $10^{-4}$.

5. How many substances have a molecular weight from 135 to 137, a boiling point from 105 to 110, and a dissociation exponent?

You should get between 55 – 65.  __________

6. How many substances have a dissociation exponent from 7.5 to 8.0 in methanol and a melting point from 150 to 160?

You should get between 10 – 15.  __________
   Did you get 31?
      Look at the dissociation exponent for substances 2 & 3.
      All are wrong because they don’t meet the criteria in the question.
      What was your mistake?
III. Group name to specific compounds within that group
(follow the instructions on page 10)

7. Find pyridines which have a density greater than 1.5 g/ml

You should get more than 25.

Did you get zero? Check Common Mistakes – Substance Name

8. How many succinics have been isolated from natural product spinach? (Newer records use the English word while the older records use the German word, spinat.)

You should get between 4 – 14.

Did you get more than 15? Check Common Mistakes - Parentheses

IV. General info about a reaction to specifics about a reaction
(follow the instructions on page 10)

9. How many reactions are there for the preparation of coumarin from salicylaldehyde?

You should get between 15 – 20 reactions.
For the last 9 questions you will need to identify which search strategy to employ to help you answer the question.

10. How many reactions give you synthesis information for aspirin?

11. How many compounds have a melting point of 75 in ethanol or methanol and a boiling point greater than 300?

12. How many compounds have been isolated from the natural product, digitalis purpurea?

13. How many compounds have a boiling point of 152 at a pressure of 700 torr?

14. How many compounds have a melting point of 119-121 degrees and a boiling point less than 300 degrees?

15. How many reactions describe the synthesis of a compound using acyclovir as a starting material?

16. How many compounds have a dissociation exponent value of 2.6 measured in ethanol or methanol?

17. What is the acidity of acetic acid in water and picric acid in water only. (There will be more than one number so pick one.)

18. You have an unknown compound that has a melting point of 70 °C and a boiling point of 200 °C at a pressure of 760 torr. What is the CAS registry number for the compound?
Which choice best describes your problem?

The Roman numeral represents the search strategy you should use.

What do you know?

I Name of one compound or substance
II Property or properties
III Group of compounds or substances – alcohols, lipids, etc.
IV Reaction info – key compound or reaction partner (reactant, reagent, catalyst, etc.) or product

What are you looking for?

I Property or properties
II Name of one compound or substance
III Name of compounds or substances within a group
IV Info about a reaction

Common Mistakes

Operator mistake: Using AND when PROXIMITY should be used

Relation mistake: Using = when < should be used

Number mistake: Typing .0001 when 0.0001 should be used (always begin a number with a number not a decimal)

Substance name mistake: Using the plural (pyridines) when the singular (pyridine) should be used

Parentheses mistake: Using the OR operator without using parentheses
Example: ham OR pork and dinner vs (ham OR pork) and dinner
Search strategies:

I  Known compound to unknown property

1  Query – Substances and Properties – Properties (Form-based) – Substance Data – Identification Data – Chemical Name/Synonyms
2  Find the full record for the compound
3  Look at the hyperlinked list under the Available Data column-header or look at the hyperlinks below the structure
4  Click the hyperlinks to get to the answer

II  Known property to unknown compound

1  Query – Substances and Properties – Properties (Advanced) – Find search box below “Check Syntax” – type the <property name> to find the correct search code – click Search for Field button
2a  If you have one value, then click field name, select the correct relation (=, <, >, etc.), click grey box with dots, select desired value, then click the Transfer button.
2b  If you have a range of values then type the correct field code, type the appropriate relation, type the range
3  Do you have another property? Add the appropriate Boolean operator and go back to step 2 until all properties are identified
4  Double check to make sure you have used the correct operator and relation

III  Group name to specific compounds within that group

1  Query – Substances and Properties – Properties (Advanced) – Find search box below “Check Syntax” – type Chemical Name Segment to find the correct search code – click Search for Field button
2  Click field name, select content operator, click grey box with dots, select content, then click the transfer button
3  Do you have another property? Add the appropriate Boolean operator and go back to step 2 until all properties are identified
4  Double check to make sure you have used the correct operator and relation

IV  General info about a reaction to specifics about a reaction

1  Query – Reactions – Conditions (Advanced) – Reaction Data – Reaction – Select either Reactant or Product – click grey box with dots, find compound name then click the Transfer button.
2  Repeat until all compounds have been given a role
3  Double check to make sure you have used the correct operator and relation