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 – (1771 - )
     Organic
     105,000,000+ substances
     42,000,000+ reactions
   * Gmelin – (1772 - )
     Organometallic & Inorganic
     53,000,000+ citations
     Organic Chem & Biology patents
     500,000,000+ experimental properties
     105,000,000+ substances
     42,000,000+ reactions
     53,000,000+ citations
     500,000,000+ experimental properties

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.

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.

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

8. Any unique features?
   Can search for a range of numbers
   (Example: 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 six links near the top.
1. Quick search
2. Query builder
3. Results
4. Synthesis planner – in two weeks
5. History
6. Sign-in

The focus for today will be **Query builder, Results, & History**. Click on **Query builder**.

This section has two sections
1. Drag & Drop section
2. Fields & Forms section (on the right)

**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

**The Practice Starts Here**

There are 2 ways to find data on a compound – 1. by structure & 2. by registry number

1. **By Structure**: Make sure **Quick Search** is underlined. Click the **Create Structure / Reaction Drawing** link. Click the **Create structure template from name** link. Type **50-00-0** into search box and make sure **is** is there. Click the **magnifying glass** icon.

   The matching structures are displayed below you search.

   Click the **Load template** button for the top structure.

   Make sure the **As drawn** radio button to the right of the structure is selected. Click the **Transfer to query** button (lower right). Click the **Find** button. Identify the **Substances: as drawn** result then click **View Results**.

   The results page appears. The default sort for the results are by the number of documents associated with each structure – the higher number is at the top of the list. You can change the **Sort by** criteria.
1a. How many substances do you get with this search? ________
(You just did a structure search. You should get between 2,400 – 2,500 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 Query builder link.

2. By Registry Number: Click the CAS RN link at the top of the page. Type 50-00-0 into the CAS Registry Number search. Click the Substances 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.)

Registry Number Searches give fewer results than a Structure Search because a structure search is looking for similar structure rather than a specific compound.

The Overview for each compound has 2 sections: Structure and Summary. For example:

* In the Structure section (on the left) has up to two icons and two drop-down menus.
  - Commercial availability – where can I buy this compound?
  - Zoom: Enlarge the structure and rotate in 3D
  - Create synthesis plan – to create a synthesis plan for the compound
  - Options – for copying the structure or to do a similarity search

* The Summary (on the right) section tells you the areas that have data and how much is in each area.

To answer the following questions, pick the first result.
On the far-right side of the summary section for this compound:

1d. For the first result, How many reactions involve this compound? ____________
   (You should get between 106,000 – 111,000 reactions)

1e. How many reactions are for the preparation of this compound? ____________
   (You should get between 3,500 – 4,000 reactions)

* In the Identification section

1f. What are the first 6 characters of the InChI Key? ___________________________

Click on the Physical Data link.

1g. 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.)

1h. What is the journal title for the oldest article reporting this boiling point value?

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

Click the +Load More button

1j. Write the dissociation exponent for this compound? (Pick just one) ______________

Click on the caret symbol to the left of the Physical Data link to collapse this section

Click on the Spectra link

1k. How many times has Carbon NMR data been found in the literature for this
   compound? ______________
   (You should get more than 1 and less than 6)

Click on the Other Data link

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

Click the Query builder link at the top of the page
ALWAYS DO THE FOLLOWING BEFORE BEGINNING A NEW SEARCH

Click the Delete All link

ALWAYS DO THE PRECEDING BEFORE BEGINNING A NEW SEARCH

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

2. Find the following facts for carbazole
   (if there is more than one result, then pick the first structure).

   What is the most common density reported in the literature? ________________

   What is the contamination concentration in the ground water in Escambia County Florida?
   __________ mg/l
   (In the Other Data section look at the Concentration in the Environment)

3. How many heteroatom nmr spectras do you find for 2,4-Dinitrofluorobenzene?

   15N _____  17O _____  19F _____

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

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

You should get between 45-50. __________
Did you get a Warning window? Check Common Mistakes – Number
Did you get 95-145? Check Common Mistakes – Relation
Did you get more than 150? Check your translation of $10^{-4}$.

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

(If sure to pick the property in Reaxys and not some other database)

You should get between 55 – 65. __________

7. 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 36?
Look at the dissociation exponent for substance 1. All are wrong because they don’t meet the criteria in the question. Check Common Mistakes – Operators.
III. Group name to specific compounds within that group

(follow the instructions on page 10)

8. Find pyridines which have a density greater than 1.5 g/ml and molecular weight from 156 to 168.

You should get more than 10.

Did you get zero? Check Common Mistakes – Substance Name

9. 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 more than 4 and fewer than 14.

How do you put multiple terms into the same search field? Two ways:

1. Click on this icon and select the terms you need. 2. Type the terms and separate them by OR.

IV. General info about a reaction to specifics about a reaction

(follow the instructions on page 10)

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

You should get between 30 – 40 reactions.
For the last 9 questions you will need to identify which search strategy to employ to help you answer the question.

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

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

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

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

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

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

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

18. 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.)

19. 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
Search strategies:

I  Known compound to unknown property

1  Query Builder – Fields – Identification – Chemical Name – type the `<chemical name>`
2  Search Substances
3  Find the full record for the compound
4  Click the hyperlink to the appropriate category to get to the answer

II  Known property to unknown compound

1  Query Builder – Fields – Find search fields and forms – type the `<property name>` to get the right form.
2  Type your information into the correct field of the form Select the correct relation (=, <, >, etc.), click Lookup link, select desired value, then click the Transfer button.
3  Select the correct relation (=, <, >, etc.).
4  Do you have another property? Redo steps 1-3 and then add the appropriate Boolean operator between the two forms
5  Double check to make sure you have used the correct operator and relation
6  Search Substances

III  Group name to specific compounds within that group

1  Query Builder – Fields – Find search fields and forms – type Chemical Name Segment – select the form in the Reaxys database.
2  Type the group name (singular is preferred to plural)
3  Do you have a property? Add the appropriate Boolean operator AND go back to strategy II until all properties are identified
4  Double check to make sure you have used the correct operator and relation
5  Search Substances

IV  General info about a reaction to specifics about a reaction

1  Query Builder – Fields – Find search fields and forms – type either Reactant or Product – select either Reactant or Product – type compound name
2  Repeat step 1 until all compounds have been given a role
3  Double check to make sure you have used the correct operator and relation
4  Search Substances