



Search Examples

Table of Contents

TABLE OF CONTENTS	1
SEARCHING USING IDENTITY OR SIMILARITY SEARCH TYPES	2
FINDING A CHEMICAL STRUCTURE BY NAME:.....	2
IMPORT A MOL FILE OR SMILE STRING	4
SEARCHING USING A SUBSTRUCTURE SEARCH	5
DRAWING A SIMPLE CHEMICAL STRUCTURE	5
OR, UPLOAD THE SAME SIMPLE CHEMICAL STRUCTURE AS A MOL FILE OR SMILE STRING.	8
LIST ATOM FEATURE.....	8
SEARCH FILTERS	9
<i>FILTER BY MOLECULAR WEIGHT:</i>	9
<i>FILTER BY MOLECULAR FORMULA:</i>	9
<i>FOUND IN CLAIMS/ALL:</i>	9
<i>COUNTRY FILTER:</i>	9
<i>NUMBER OF STRUCTURES TO RETURN:</i>	10
CONTACT US	10

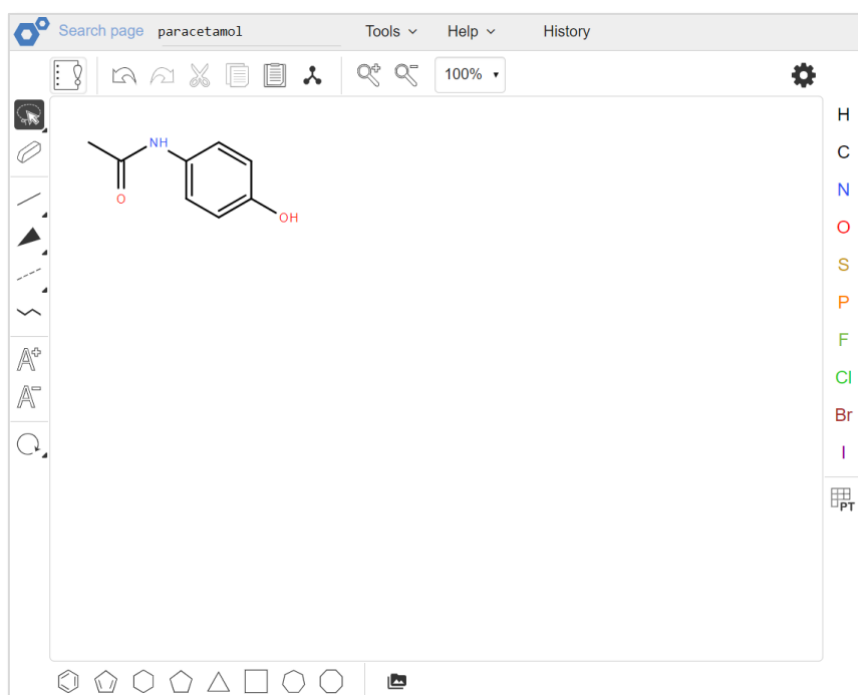
Searching using Identity or Similarity search types

For an *Identity Search*, use one of the examples below and use the default selections of *Broad*, *All text*, *All countries* and *50 structures to return*.

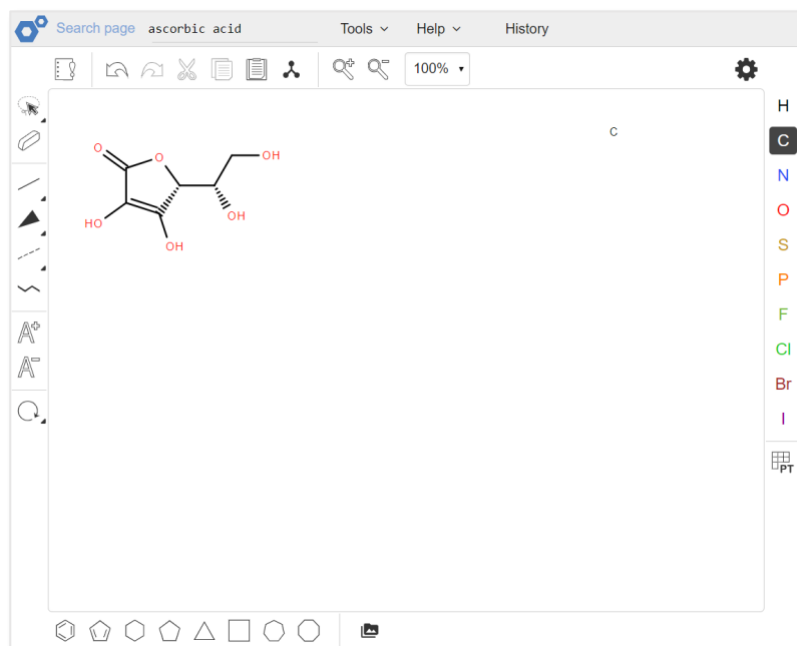
For a *Similarity Search*, use one of the examples below and select a Tanimoto threshold of 95-98% and *All Text*, *All countries*, and *50 structures to return*.

Finding a chemical structure by name:

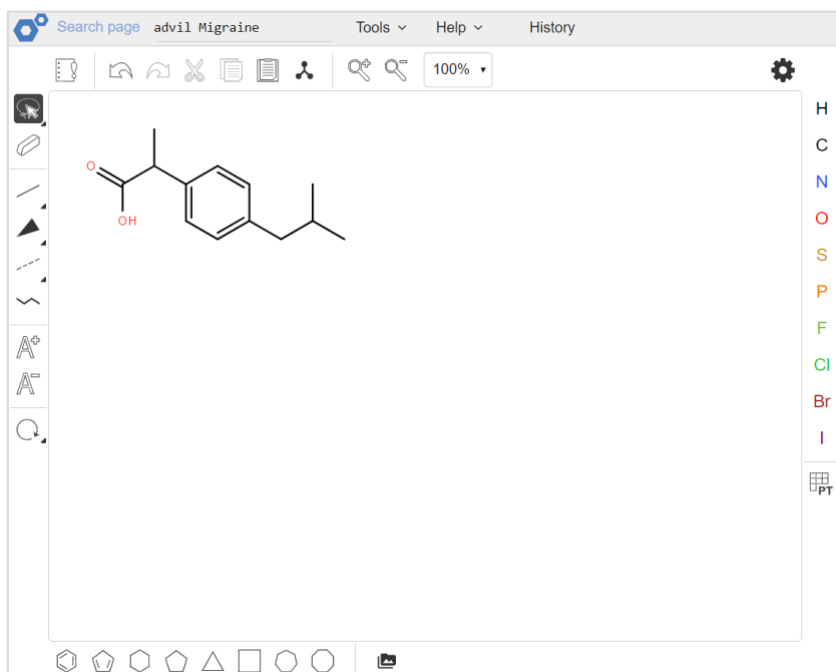
Examples of active ingredients: Simvastatin, Codeine, Aspirin, Paracetamol (see screenshot below).



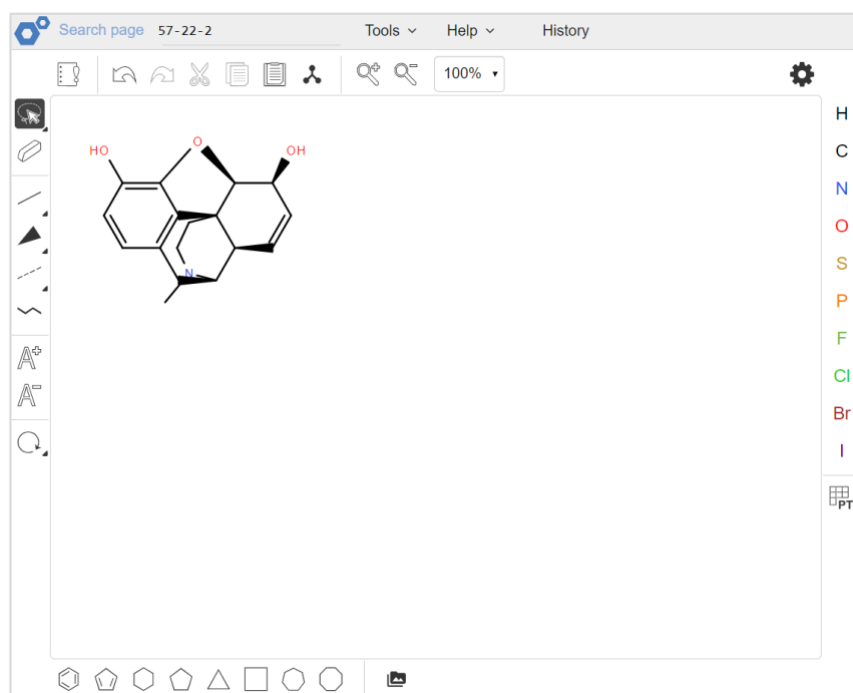
Examples of a generic chemical name: Acetylsalicylic acid (Aspirin), [Ascorbic acid](#) (Vitamin C)



Examples of a tradename: Prozac (antidepressant), Amoxil (antibiotic), [Advil](#) (pain killer)



Example of a CAS Registry Number: 67-66-3 (Chloroform), 10024-97-2 (Nitrous Oxide – Laughing Gas), 132-22-9 (Chlorpheniramine – antihistamine), [57-27-2](#) (Morphine – pain killer)



Import a MOL file or SMILE string

Go to the *Tools* menu and *Upload a MOL file* – examples are attached below:



Or, go to *Tools* and *Upload a SMILE string*:

Codeine: CN1CCC23C4C1CC5=C2C(=C(C=C5)OC)OC3C(C=C4)O

Paracetamol: CC(=O)NC1=CC=C(C=C1)O

Aspirin: CC(=O)OC1=CC=CC=C1C(=O)O

Searching using a Substructure Search

For a *Substructure Search*, draw the chemical compound below (if you are feeling brave) or upload the MOL file (attached) and leave all other options as default settings. I would not select any of the further options to return molecules based on [Resonance](#) form (where the charge on the chemical does not allow it to be expressed as a single formula) or [Tautomer](#) (different forms or isomers of the same chemical compound) but I have linked both of these to Wikipedia for more information. I would also use following options when conducting a substructure search:

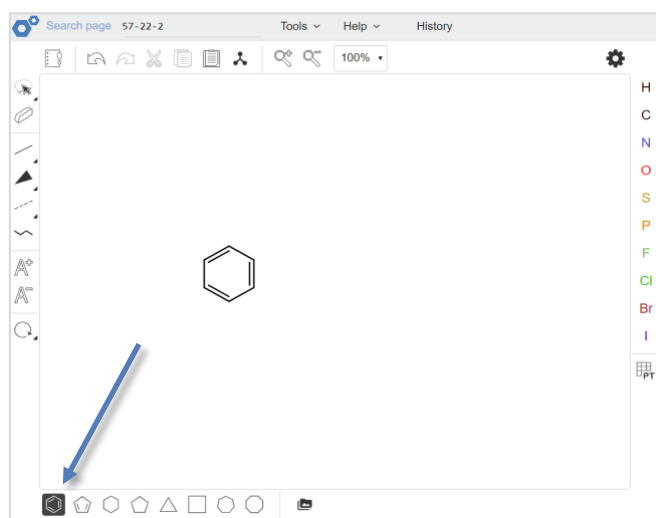
Claims only

Pick a single country of interest – e.g. USA

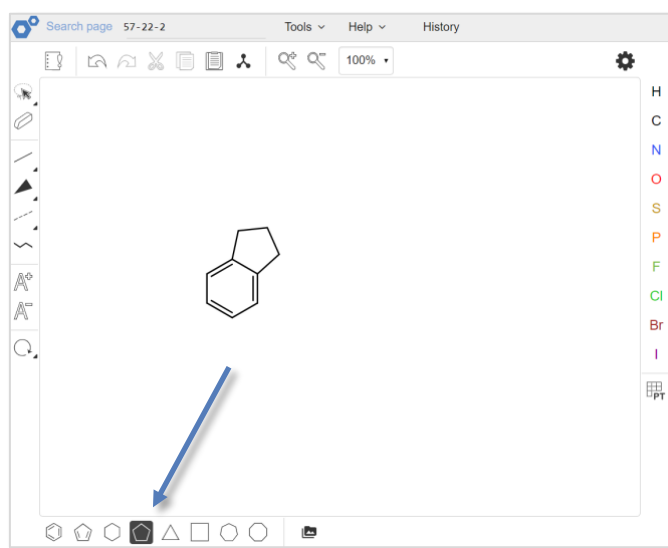
Return 50 structures

Drawing a simple chemical structure

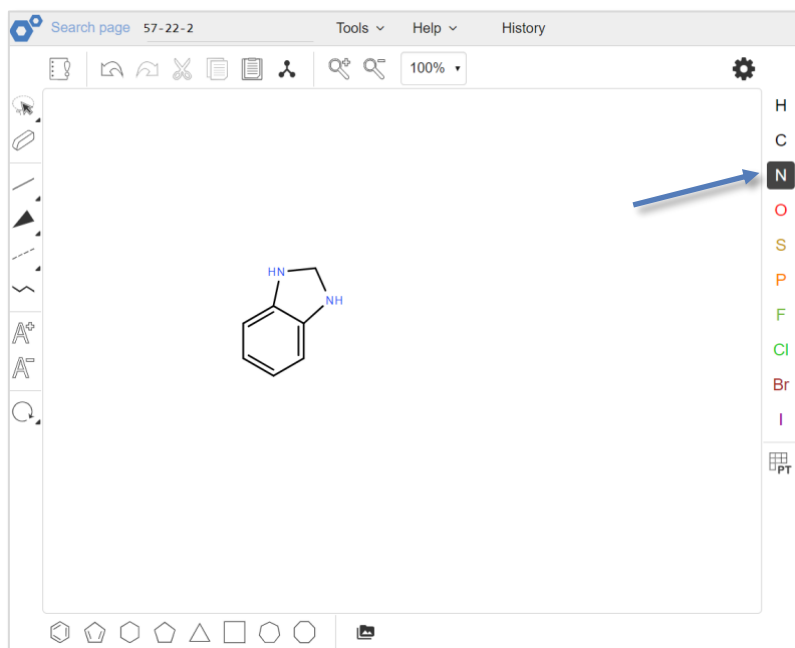
- 1) Click on the Benzene ring (indicated by the blue arrow) and add it to your editor window



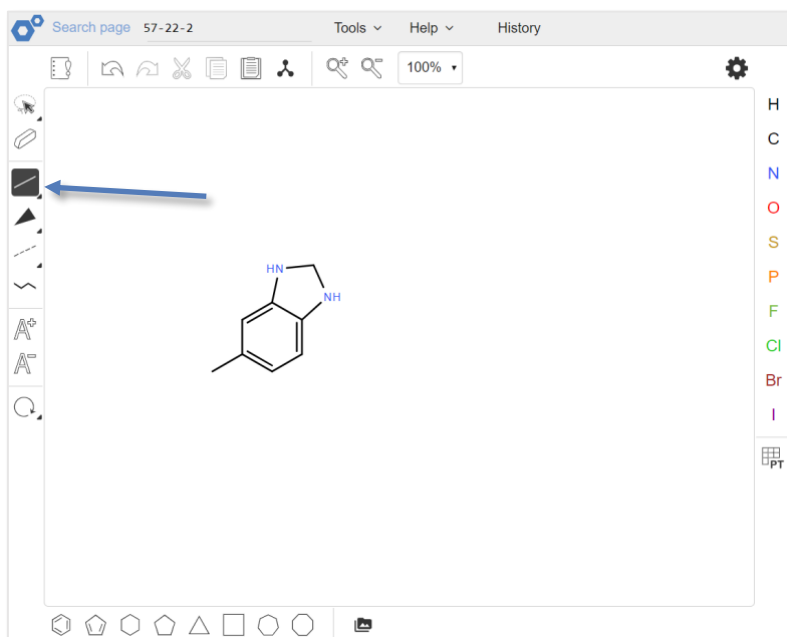
- 2) Click on the Cyclopentane ring (indicated by the blue arrow) and add it to the Benzene ring



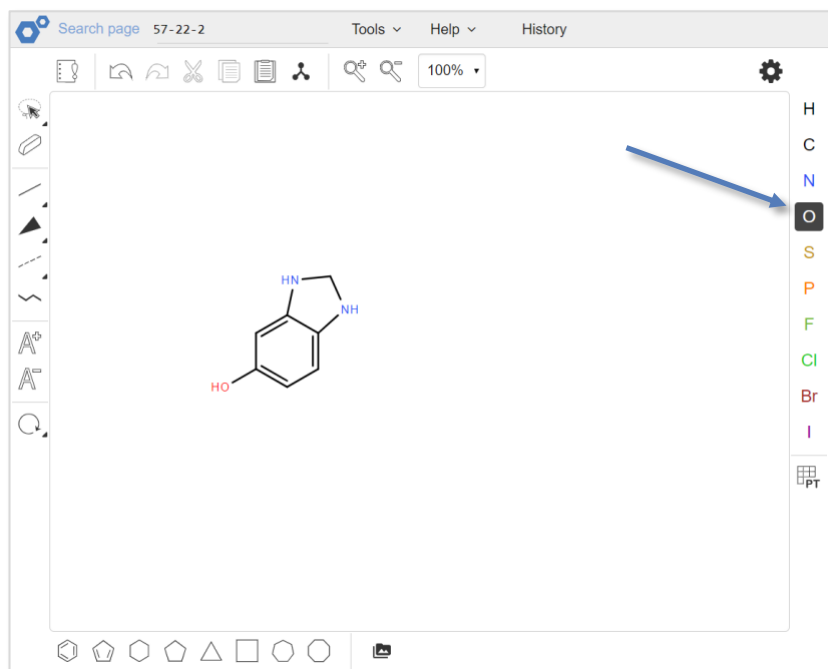
- 3) Click on the Nitrogen (indicated by the blue arrow) and add two of them to the Cyclopentane ring



4) Click on a single bond (indicated by the blue arrow) and add it to the Benzene ring



5) Finally, add an Oxygen atom (O) to the single bond



Or, upload the same simple chemical structure as a MOL file or SMILE string.

Go to *Tools* and *Upload MOL file* – same structure as a MOL file is attached:

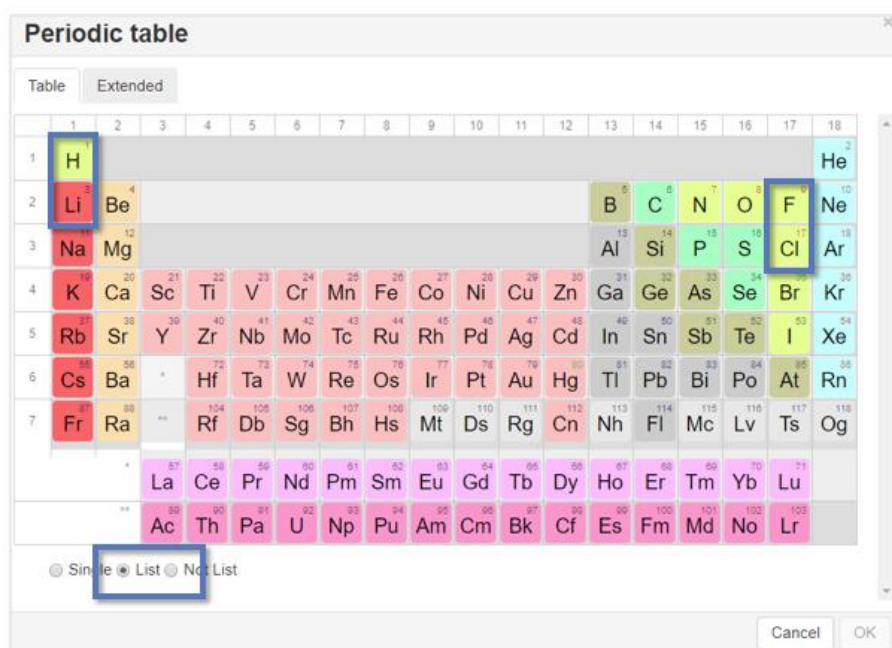


Or go to *Tools* and *Upload a SMILE string*, e.g. C1(=CC=C2C(=C1)NCN2)O

List atom feature

The list/not list atom features are available when conducting a sub-structure search.

This feature allows users to define multiple atoms that either can or must not appear at a given position within a chemical structure. To use the list/not list function, open the periodic table option from the sketch tool, and select either the List or the Not List options (by default, "single" atom will be selected when the periodic table is first opened).



This function allows users to define broad ranges of entities within a single query without having to run multiple structure queries.

Search filters

Search filters can be applied to Chemical Explorer searches by entering criteria into the *Return structures* section found below the search type selection to the right of the sketcher frame.

Return structures:

Filter by molecular weight: -

Filter by molecular formula: contains ▾

Found in claims All

Country: All ▾

Number of structures to return: 50 ▾

Filter by Molecular weight: entering an upper and lower limit to these boxes will apply a weight range filter to your results, only returning structures that fall in between your set limits.

Filter by Molecular formula: the returned structured must either contain or be identical to the input formula (depending on which option is selected via the dropdown). If no formula is inserted, no filter is applied.

Found in claims/All: this option set controls whether your returned structures should be found in the claims section of patent documents only, or if the system should return all hits found across the full text.

Country filter: this drop-down allows you to restrict your returned results to only documents from a specific jurisdiction/country.

Number of structures to return: this drop-down allows you to set how many structures that match your query structure should be loaded per page when reviewing your results, by default this is set to 50.

Contact us

If you have any questions about anything mentioned in this guide, please contact support@minesoft.com, or call us on +44 (0)20 8404 0651.