

Chemical Search

Available from the Search menu, for logged-in users, the chemical structure search allows users to search for chemical information in PATENTSCOPE

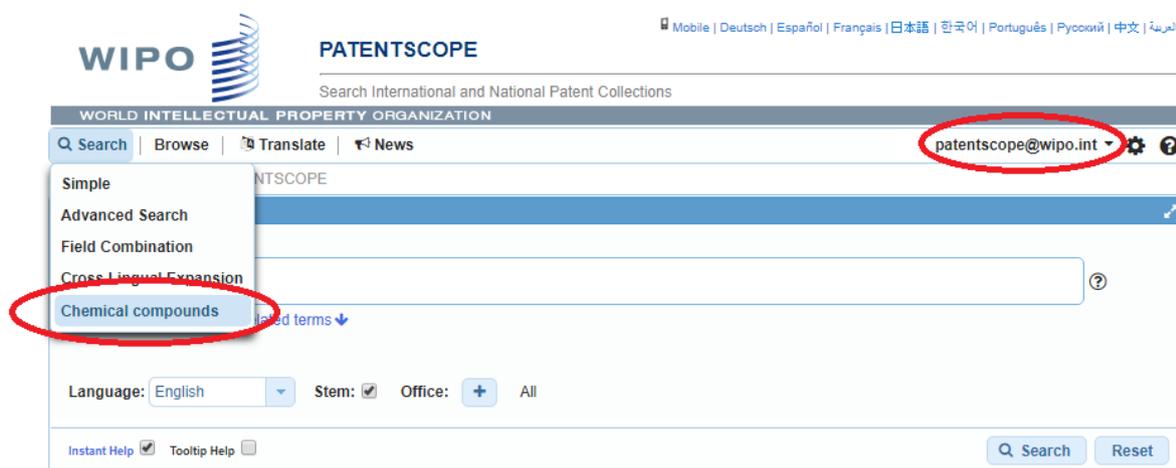


Fig. 1: The chemical menu is available for logged-in users

If you do not have a PATENTSCOPE account to login-in, you can create one free of charge in the Login menu.

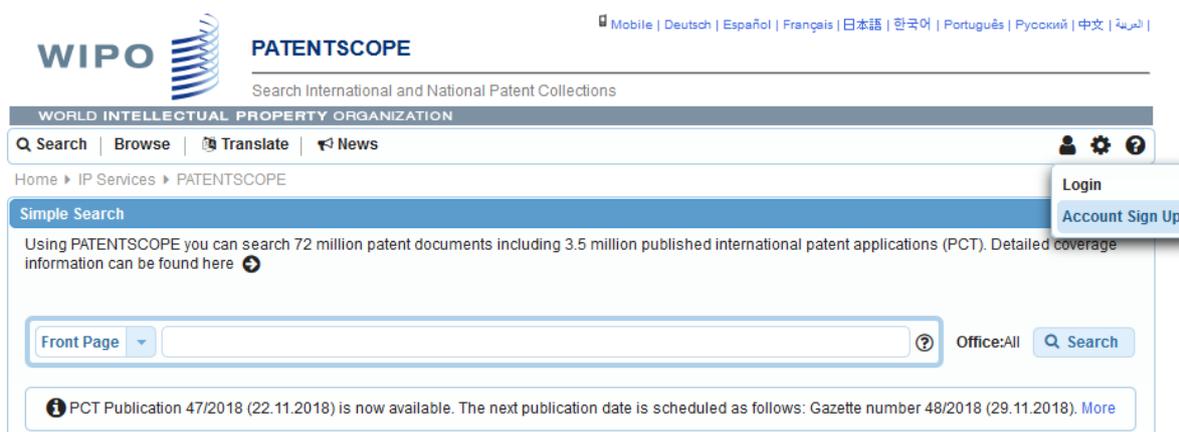


Fig. 2: Creating a new account is possible from the drop down menu

There are four options to perform a search

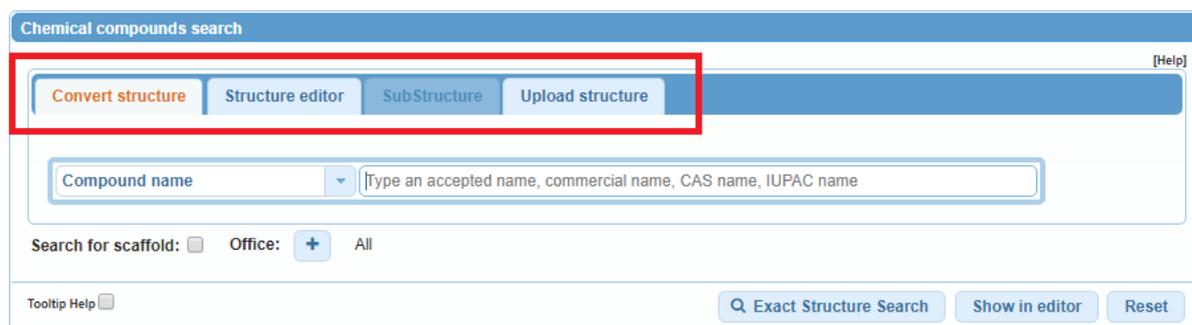


Fig. 3: There are four types of search

1. Convert structure tab

Convert a structure allows users to select the input type of the search such as the name of the chemical compound.



Fig. 4: Convert a structure tab allows the user to search by different types of names

Different options to enter your search are available: name of the chemical compound such as trivial name, commercial name, IUPAC name or CAS name, the International NonProprietary Name INN, InChI, InChIkeys or SMILES.

You can submit your query directly or check the structure using the show in editor. This button will process the input data to convert the compound name, INN, InChI or SMILES into the corresponding structure.

2. Structure editor tab

Structure editor allows users to draw or edit a structure. Chemical structures, reactions and fragments can be drawn in a very intuitive way using the symbols familiar from chemical sketches on paper.

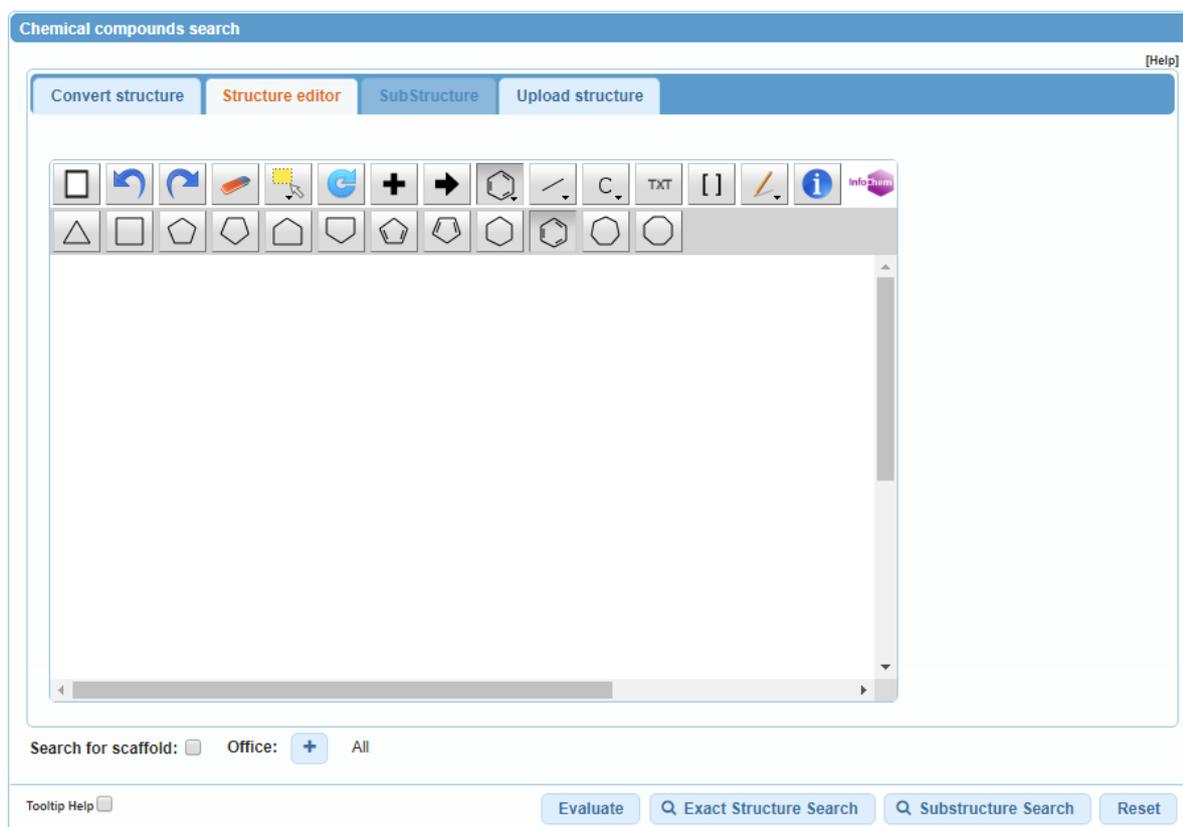


Fig. 5: The structure editor allows you to draw chemical formulas, as you would do on paper.

3. Upload structure tab

Upload a structure allows users to upload a chemical description file in a supported format for example MOL, SMILES as well as a bitmap representation of the chemical compound such as png, gif, tiff, jpeg format The Search for scaffold button will enlarge your search as the compound will be searched more generally, taking into consideration only the 1st part of the InchKey. The scaffold is Basic skeleton of a molecule to which further groups and moieties are attached Structure editor tab



Fig. 6: The upload structure tab enables the user to upload a file

4. Substructure search

Additionally to the “Exact Structure Search”, the functionality to search substructures within chemical compounds is now also available. The “Substructure Search” can be submitted from the “Structure editor” (Fig. 1).

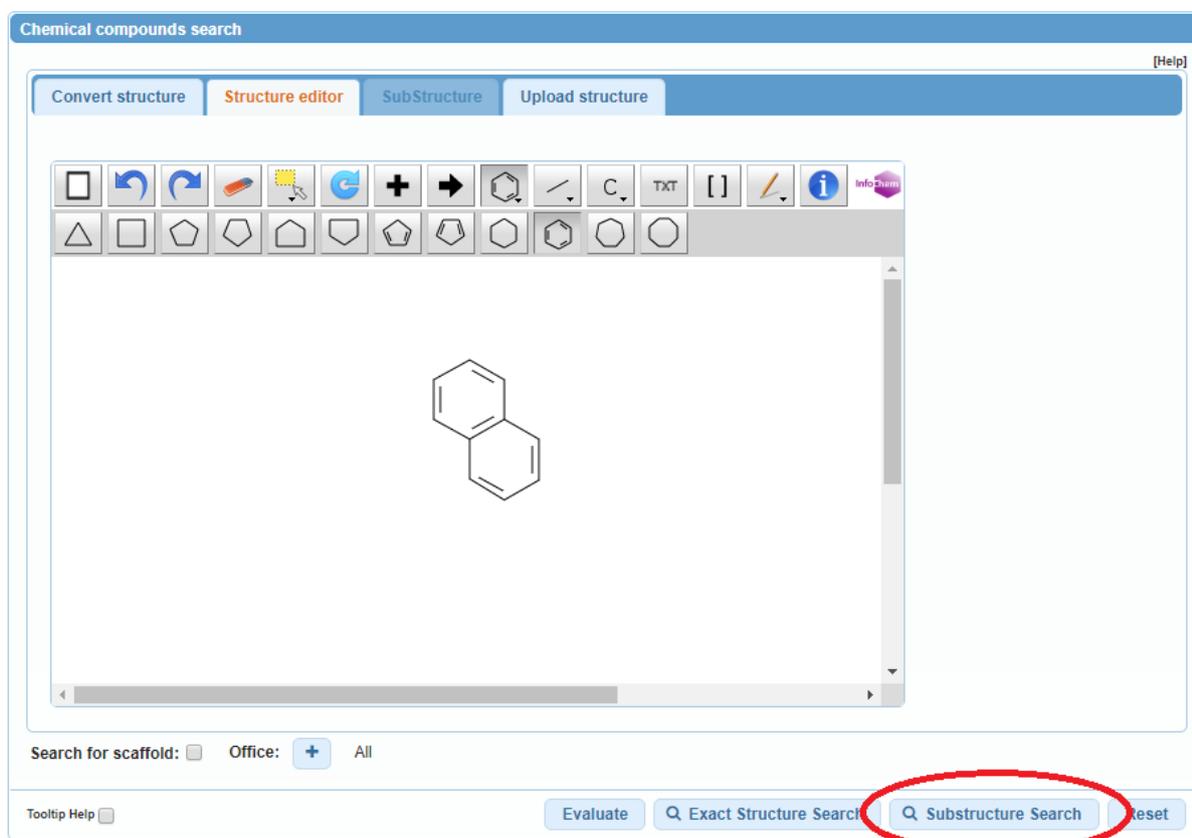


Fig. 7: New action „Substructure Search” in Structure editor panel

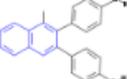
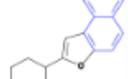
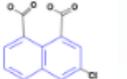
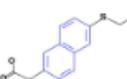
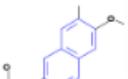
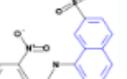
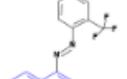
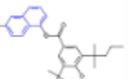
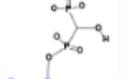
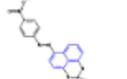
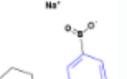
After a substructure search has been launched, a list of structures containing the query molecule will be returned (ordered as a grid). The matching substructure is shown highlighted (blue color) by each molecule hit.

Chemical compounds search [Help]

Convert structure Structure editor **SubStructure** Upload structure

Substructure search results (47787+ 15%)

(1 of 1992) 1 2 3 4 5 6 7 8 9 10 24 ▾

<input type="checkbox"/> 	<input type="checkbox"/> 	<input checked="" type="checkbox"/> 	<input checked="" type="checkbox"/> 	<input checked="" type="checkbox"/> 	<input type="checkbox"/> 
<input type="checkbox"/> 	<input type="checkbox"/> 	<input type="checkbox"/> 	<input type="checkbox"/> 	<input type="checkbox"/> 	<input type="checkbox"/> 
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(1 of 1992) 1 2 3 4 5 6 7 8 9 10 24 ▾

Search for scaffold: Office: All

Tooltip Help Search Select all Clear all Reset

Fig. 8: Substructure Search result

You can select one or several structures before submitting the search of the patents clicking on the checkboxes or you can select (or deselect) all the chemical compounds *on the page* clicking the buttons "Select all" (or "Clear all").

A maximum of 1024 chemical compounds can be selected for the search of the patents. If selection contains more than 1024 chemical compounds, a message will be displayed as shown in Fig. 9:.

The screenshot shows the 'Chemical compounds search' interface. At the top, there are navigation tabs: 'Convert structure', 'Structure editor', 'SubStructure' (highlighted), and 'Upload structure'. Below the tabs, a yellow message box states: 'You can select max. 1024 compounds or refined your search'. The main section is titled 'Substructure search results (47676+ 15%)' and shows '(1 of 1987)' results. There are navigation buttons for page 1, and a dropdown menu set to '24'. Below this, there is a grid of 12 search results, each in a blue-bordered box. Each box contains a chemical structure and a checked selection box. The results are labeled with alphanumeric codes such as 'AAPAGLBSROJFGM-UHFFFAOYSA-N'.

Fig. 9: Selection of all "Substructure Search" results and message after the "search" action for patents was sent with more than 1024 selected chemical compounds.

If the "substructure search" takes longer than 4 sec., a link with the label "Show more" will appear on the last page indicating that the substructure search is not completed (s. Fig. 8:). This information may also be inferred by the percentage of the result list at the top of the substructure list.

The screenshot shows the 'Chemical compounds search' interface. At the top, there are navigation tabs: 'Convert structure', 'Structure editor', 'SubStructure' (highlighted), and 'Upload structure'. Below the tabs, a yellow message box states: 'You can select max. 1024 compounds or refined your search'. The main section is titled 'Substructure search results (47787+ 15%)' and shows '(1992 of 1992)' results. There are navigation buttons for years 1983 through 1992, and a dropdown menu set to '24'. Below this, there is a grid of 3 search results, each in a blue-bordered box. Each box contains a chemical structure and a selection box. A 'Show more...' link is highlighted with a red circle. At the bottom, there are buttons for 'Search', 'Select all', 'Clear all', and 'Reset'.

Fig. 10: "Show more action"

5. FAQ

1. Typically, how many structures are revealed in an patent for an INN drug?

It is difficult to compute. The system has no limit in terms of maximum number of chemical structures recognized by a document.

2. Can we search by "CAS name" "CAS number"?

CAS name. CAS numbers can't be converted into InChIKey's, therefore they can't be associated with a chemical search but only with a simple text search.

3. Is it possible to upload structures from ChemDraw if we get inchi from the chemdraw or chemsketch. is it possible to search by simply pasting it in chemical search?

Yes, the CDX format not supported for file loading

4. Can generic formulae for polymers containing parameters such as n an m for the repeating units be searched?

No, only exact structures that can be represented by an Inchi

5. Will alerting on structures be available?

Yes using RSS feed

6. How far back in time will PCT/US be chemically indexed?

PCT 1978 and US 1979

7. Is it limited to small molecules or can I search for (small) proteins too?

Only exact structures that can be represented by an Inchi

8. Structure search for compound where only chemical name is given in patent..is that patent also get picked in the search?

Yes

9. How does this affect drafting and filing applications - is there a size requirement for proper data capture?

The clearer the embedded images are the better. min 300dpi

10. Are the data annotated with InChI or InChIkeys or do you use the Inchi and Inchi keys to generate IUPAC names and search with the names.

They are annotated with InChIkeys

11. OK so the trivial name is also indexed as an InChI string or InChiKey?

Yes

12. Can we search the compounds by using code names like GS1101?

Yes 13. Do we have option for Markush search? No