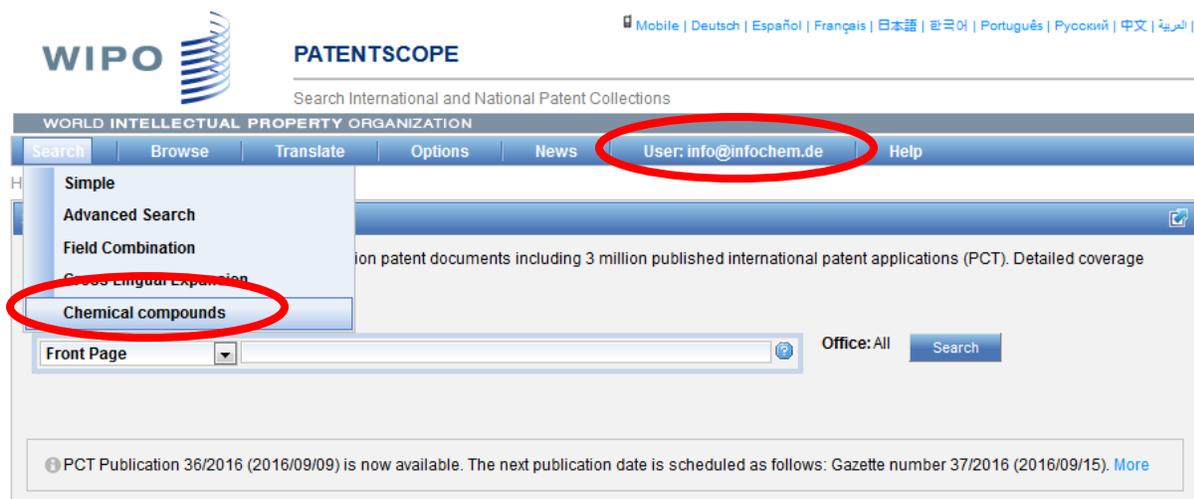


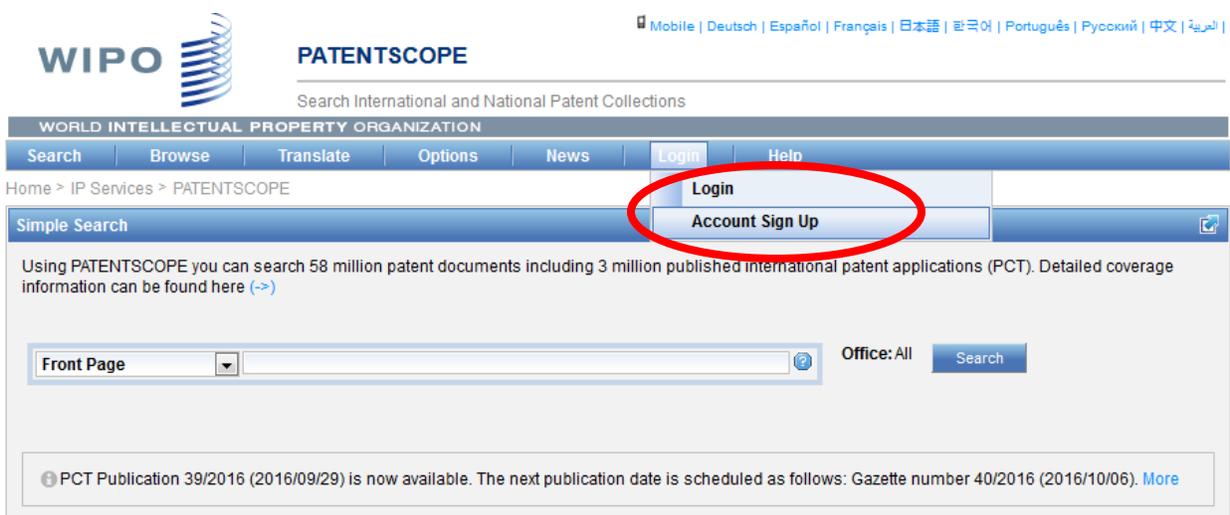
Chemical structure search

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



The screenshot shows the WIPO PATENTSCOPE interface. At the top, the WIPO logo and 'PATENTSCOPE' are displayed, along with a language menu. Below this is a navigation bar with 'Search', 'Browse', 'Translate', 'Options', 'News', 'User: info@infochem.de', and 'Help'. The 'User: info@infochem.de' text is circled in red. A dropdown menu is open under 'Search', with 'Chemical compounds' highlighted in red. The main content area shows a search box with 'Front Page' selected and a 'Search' button. A notification at the bottom states: 'PCT Publication 36/2016 (2016/09/09) is now available. The next publication date is scheduled as follows: Gazette number 37/2016 (2016/09/15). More

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



The screenshot shows the WIPO PATENTSCOPE interface. At the top, the WIPO logo and 'PATENTSCOPE' are displayed, along with a language menu. Below this is a navigation bar with 'Search', 'Browse', 'Translate', 'Options', 'News', 'Login', and 'Help'. The 'Login' and 'Account Sign Up' options are circled in red. The main content area shows a search box with 'Front Page' selected and a 'Search' button. A notification at the bottom states: 'PCT Publication 39/2016 (2016/09/29) is now available. The next publication date is scheduled as follows: Gazette number 40/2016 (2016/10/06). More

3 options to perform a search

Chemical compounds search

[Help]

Structure editor Convert structure Upload structure

Compound name [v] Type an accepted name, commercial name, CAS name, IUPAC name

Search Show in editor Reset

Search for scaffold: Office: All Specify ⇨

Tooltip Help

1. 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;
2. Convert a structure allows users to select the input type of the search such as the name the chemical compound: commercial name, CAS name, trivial name are handled in an equal manner, the international NonProprietary Name, InCHI, InChIkey or SMILES;
3. 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 InChIKey. The scaffold is Basic skeleton of a molecule to which further groups and moieties are attached

Structure editor tab

The screenshot displays the 'Chemical compounds search' application window. The 'Structure editor' tab is active, showing a toolbar with various drawing tools such as a square, undo, redo, eraser, lasso, rotate, add, delete, and ring selection tools. Below the toolbar is a large empty canvas for drawing chemical structures. At the bottom of the window, there are search options: 'Search for scaffold:' with a checkbox, 'Office:' with 'All' selected and a 'Specify' link, and 'Tooltip Help' with a checkbox. 'Search' and 'Reset' buttons are located in the bottom right corner of the editor area.

The structure editor allows you to draw chemical formulas like you would do on paper.

Convert structure tab

The screenshot shows the 'Chemical compounds search' interface with the 'Convert structure' tab selected. At the top, there are three tabs: 'Structure editor', 'Convert structure', and 'Upload structure'. Below the tabs is a search input field with a dropdown menu. The dropdown menu is open, showing options: 'Compound name', 'INN', 'InChI', and 'SMILES'. The input field contains the placeholder text 'Type an accepted name, commercial name, CAS name, IUPAC name'. To the right of the input field are three buttons: 'Search', 'Show in editor', and 'Reset'. Below the input field, there is a 'Search for scaffold' checkbox and an 'Office' dropdown menu set to 'All' with a 'Specify' link. At the bottom left, there is a 'Tooltip Help' checkbox.

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.

Upload structure tab

The screenshot shows the 'Chemical compounds search' interface with the 'Upload structure' tab selected. At the top, there are three tabs: 'Structure editor', 'Convert structure', and 'Upload structure'. Below the tabs is a large text box with the instruction: 'Select a structure file (MOL) or image file (PNG, GIF, TIFF, JPEG) and upload it.' Below this text box is a file selection area with a 'Browse...' button and the text 'No file selected.' To the right of the file selection area are two buttons: 'Show in editor' and 'Reset'. Below the file selection area, there is a 'Search for scaffold' checkbox and an 'Office' dropdown menu set to 'All' with a 'Specify' link. At the bottom left, there is a 'Tooltip Help' checkbox.

Select a file from your computer.

FAQs

- 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.**
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