

Searching by Chemical Structure

The Structure Search allows you to search by structure or substructure and to optionally add a drug action term or compound name and date range. It offers a quick and convenient way of searching the *Thomson Reuters Pharma* Chemical registry.

- Avoid missing a related structure patent due to incorrect use of keywords or not knowing structure names given by your competitors
- Allows cross-referencing of compounds appearing in multiple Therapy Areas
- Eliminates uncertainty regarding search terms
- Can comprehensively investigate your company's promising early-stage molecule, of which little might be known other than structure information.

1. System requirements and plug-ins for chemical structure search

To perform a structure query in *Thomson Reuters Pharma* you will require the following software:

MDL Chime plug-in (Version 2.6 Service Pack 6 recommended)

Drawing structures software (MDL ISIS/Draw version 2.5 or higher recommended)

The MDL Chemscape Chime plug-in is downloadable free of charge from the MDL website:
<http://www.mdli.com/downloads/downloadable/index.jsp>

You can choose either one of the following structure drawing packages:

- ISIS/Draw (Recommended)
- ChemDraw (Pro or Ultra version)
- Any drawing package capable of copying a structure to the clipboard as a molfile and/or which is capable of saving structures in molfile format.

To perform a structure search, simply draw a structure, or import an existing structure from a file you have saved previously. Please note that structures must be in molfile format.

2. Structure query search options

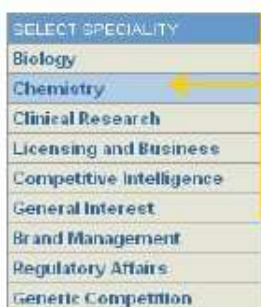
You can search *Thomson Reuters Pharma* by chemical structure from the following areas. The resulting report types will correspond to the area where the search was performed, eg, Drug Reports from the Form Search – Drug search page

Search Area	Report Type in Results
"Quick structure search" portlet on Chemistry homepage	Chemistry Report
Form Search – Drugs	Drug Report

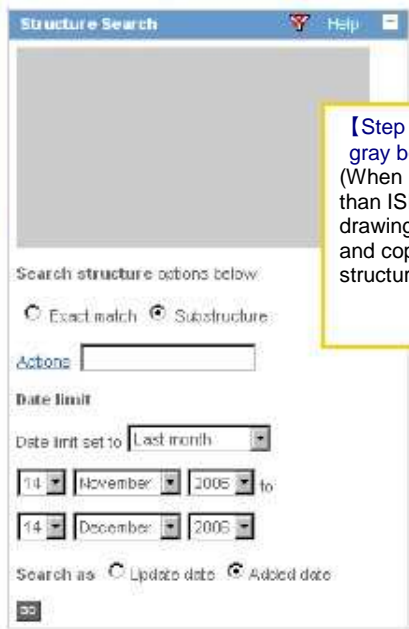
Form Search - Intellectual Property	Intellectual Property Report
Form Search – Literature and News	Literature and News Report
Guided Search - Biology -ADMET	Drug Report, Drugdex Monograph, Literature and News Report

Search Example

How to search for compounds in *Thomson Reuters Pharma*, e.g. Anthracene as a sub-structure.

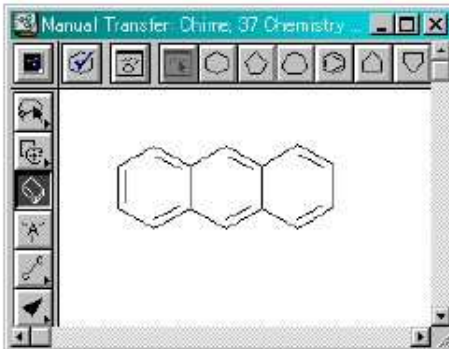


[Step 1] Select "Chemistry" in the "Select Speciality" menu bar to display the Structure Search portlet.

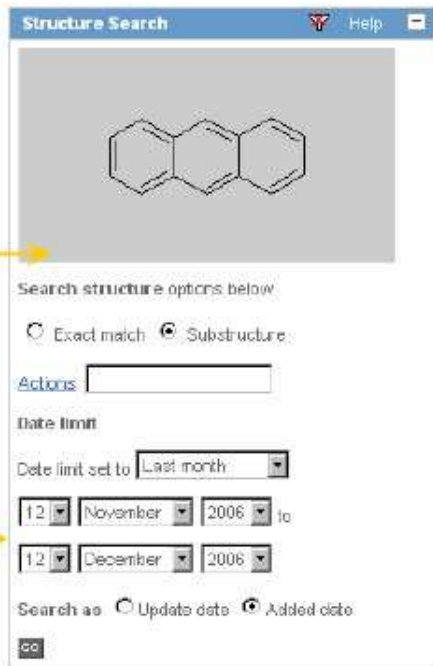


[Step 2] Double click in the gray box to open ISIS/Draw. (When using software other than ISIS/Draw, open the drawing program independently and copy & paste the drawn structure into the gray box.)

[Step 3] Click the transfer mode icon on the top left corner.



The structure is transferred into the gray box automatically.



[Step 4] Set the Date Limit as "Last Month" and select "Added Date". Click "Go".

3. Results Summary display

Type/number of Reports

Export option

The screenshot displays a search results page with several interactive elements:

- Number of Reports:** A box showing "Chemistry CH 4" and a "Go to Form Search" link.
- Display by:** A dropdown menu set to "Summary".
- Sort by:** A dropdown menu set to "Date", with radio buttons for "Ascending OR" and "Descending order".
- Rank by:** A dropdown menu set to "Select".
- Display options:** Radio buttons for "Bar Chart", "Pie Chart", and "Matrix Chart".
- Process results:** A menu with options: "Print", "Export", "Star Tree", and "Save".
- Results Table:** A table with columns for checkboxes, chemical names, update dates, and report types (all "CH").

Check	Chemical Name	Updated on	Report Type
<input checked="" type="checkbox"/>	9,16-bis-(3,5-dimethoxy-phenyl)-anthracene	7 December 2006	CH
<input checked="" type="checkbox"/>	C25H21O2 Cited in: LISNews 1	24 November 2006	CH
<input checked="" type="checkbox"/>	11-anthracen-9-ylmethyl-1,4,7-trithia-11-aza-cyclotetradecane Cited in: LISNews 1	22 November 2006	CH
<input checked="" type="checkbox"/>	5,12-diethyl-6,11-diphenyl-1,2,3,4-tetrahydro-naphthalene Cited in: LISNews 1	22 November 2006	CH

Type of report

Type of Report

Results can be sorted according to your requirements, e.g. "Summary with abstract", "Rank by".