



ISI CHEMISTRYSM

Powered by ISI Web of KnowledgeSM



Benefits

*ISI Chemistry*SM provides Web access to reports of new compounds published in leading journals and reports of new reactions published in journals and international patents. As part of *ISI Web of Knowledge*SM a seamless integration with *ISI Web of Science*[®] (for mutual subscribers) opens up all the rich possibilities inherent in cited reference searching, as well as links to electronic full-text journal articles through ISI Links.

Updated weekly, *ISI Chemistry* provides researchers with timely information from the world's most prestigious chemistry journals and international patents, selective indexes which include the most significant reactions and novel compounds and eliminate redundancy, and easy-to-use drawing software for substructure or reaction searching.

Features

Information is stored in two databases: *Reaction Center*SM and *Compound Center*SM. They may be searched simultaneously by:

- **structure or reaction** using a fully integrated structure drawing program
- **bibliographic** fields such as title, abstract, and author
- **data fields** such as biological activity and product yield

Reaction Center—a comprehensive database of single-and multi-step new synthetic methods, includes reaction conditions, product yields, and accurate atom-atom mappings. This database is supplemented by data from the Institut National de la Propriete Industrielle (INPI). INPI data include reactions from 1840 through 1989, and adds approximately 139,000 classical reactions to the database. It includes:

- complete bibliographic data with abstracts
- graphical displays of each chemical reaction
- detailed reaction conditions
- new synthetic method data
- capability to export reactions as RDfiles

Compound Center—provides easy access to new organic compound data, and covers over one million compounds, including synthetic intermediates and labeled compounds. In it, users can find:

- biological activity alerts
- complete bibliographic information and searchable author abstracts
- structures of new compounds
- graphical abstracts of each indexed article
- capability to export structures as SDfiles

Search Field Rules

- Searches are not case sensitive
- Enter words and phrases *without* quotation marks
- Truncate terms to find plurals and variant spellings, using * for any group of characters including no characters, or ? for a single character
In Topic searches, the asterisk must be preceded by at least three characters
- Use Boolean operators AND, OR, SAME, and NOT to combine terms
- Terms entered in multiple fields are combined by AND logic
- Click the Help button for more information about entering terms



Searching Options

ISI Chemistry supports two types of searches: **structure search** and **text search**. In a structure search, the database(s) are searched for reactions or for structures that contain those you have drawn using the Structure Drawing Program. In a text search, *ISI Chemistry* retrieves database records containing words and phrases, bibliographic information, or compound/reaction data that you specify.

Enter search criteria on the **Search** form, which is divided into three sections:

- **Reaction/Structure Query**
- **Bibliographic Query**
- **Reaction/Compound Data Query**

If you enter search criteria in more than one section, *ISI Chemistry* will use **AND** logic to search the database(s) for information that satisfies the search.

If, for example, you enter a structure in the Structure Query section and specify a biological activity in the Reaction/Compound section, the program will find compounds that contain the structure **and** that have the specified biological activity.

If you subscribe to both Reaction Center and Compound Center, you can limit your search to one database by checking the appropriate box. If you do not check a box, *ISI Chemistry* will search both databases.

Reaction/Structure Query

A structure search allows you to search the database for structures or reactions that you create using the Structure Drawing program. *ISI Chemistry* will search the database(s) for exact matches or for structures or reactions that contain your drawing as a substructure.

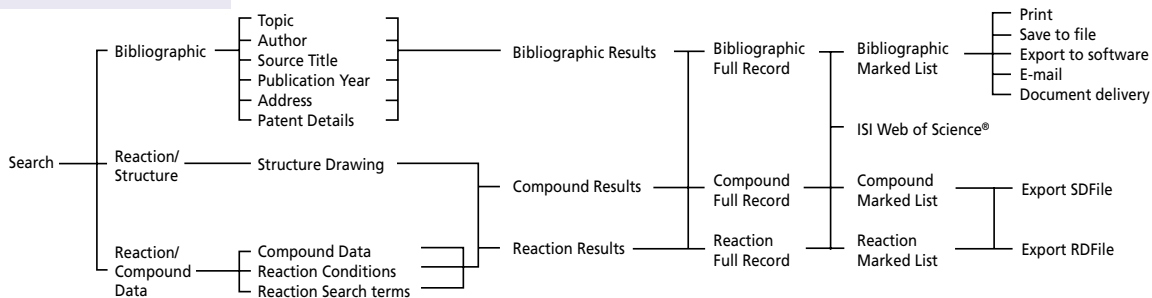
If you subscribe only to Compound Center, you cannot search by reactions.

In the **Structure Drawing** window, draw structures and reactions. Use the tool palette on the left-hand side of the **Structure Drawing** window to draw a single structure or a reaction. It is similar to using a drawing or paint program. Transfer the drawing to the **Query** form to perform structure searches.

Use the **Back** arrow on the **Structure Drawing** toolbar or **Back** on the **Search** menu (NOT your Web browser's **Back** button) to return to the **Search** form.

Consult the **Sample Reaction Structure Query** in **Help** for an introduction to drawing structures/reactions and performing a structure/reaction query.

Functionality Flow



Select a search mode:

- **Substructure** (to find compounds or reactions that contain what's in the **Query** box), or
- **Exact Match** (to find compounds or reactions that match what's in the **Query** box).

Click the **Search** button to search.

You can save structure queries for future searches, and search on them.

Bibliographic Query

A bibliographic query searches the domain for records containing bibliographic information that you specify. The bibliographic information identifies the source article or source patent.

Topic:

Enter a word or phrase that might appear in the article title, abstract, or keyword list. Use the Title Only check box to restrict the search to article titles. **Search Field Operators:** AND, OR, NOT, SAME.

Examples for the Topic field:

Enter Starfish*; Lewis acid; epoxid* SAME olefin*

Author:

Enter an author's last name first, followed by a space and up to five initials. Unless you know all initials in an author's first name, enter an asterisk after the initial(s). You may also enter last names without initials. **Search Field Operators:** AND, OR, NOT

Examples for the Author field:

Singh S; VanHummel G*; Singh S* AND Nicholas K*

Source Title:

The Source Title field is phrase indexed. To select titles directly from the source title list, click the [list](#) link for a list of journal titles. Enter titles directly. **Search field operator:** OR

Examples for the Source Title field:

"JOURNAL OF HETEROCYCLIC CHEMISTRY"; "SYNTHESIS-STUTTGART"

Publication Year:

Enter a four-digit year. Use <, > or OR combined with AND logic to specify a range. **Search field Operator:** OR.

Examples for the Publication Year field:

1995; >1998; >1989 AND <2000

Address:

Enter term(s) to be found in an author's address. Click the [Abbreviations](#) link for a list of address abbreviations.

Examples for the Address field:

Pfizer; Caltech; Univ Texas SAME Austin

Patent Country Code:

Select a patent country code from the drop-down list.

Examples for the Patent Country Code field:

GB; JP; US

Patent Number:

Enter patent number, preceded by abbreviation for the issuing agency.

Examples for the Patent Number field:

EP881214; US5834588; WO9851716



Patent Kind:

Patent kind depicts the type of patent issued (unexamined, granted, reissue, translated, etc.) and is denoted by a letter, a series of letters, or a letter followed by a number. The meaning of each code is determined by each patent office.

Examples for the Patent Kind field:

A1; A2; B1

Patent Date:

Enter date as mm-dd-yy or yyyy.

Examples for the Patent Date field:

05/02/97; 1996

Reaction/Compound Data Query

A reaction/compound data query finds reactions or compounds that have certain data associated with them such as a reaction type (Diels-Alder, Rearrangement) or biological activity (hormonal, insecticidal).

To create a reaction/compound query, in the **Reaction/Compound Data Query** section of the Search form, enter **Compound Data**, **Reaction Conditions**, and/or **Reaction Search Terms**. If you subscribe to Compound Center only, the Reaction Conditions and Reaction Terms fields are not available. Follow the basic rules for entering terms. You can combine a **Reaction/Compound Data Query** with a structure query or a bibliographic query. Click **Search**.

Compound Name: Enter name of natural product or compound name without a prefix.

Examples for the Compound Name field:

salinomycin; mycotrien*; carbacyclin (for(+/-)-carbacyclin)

Compound Biological Activity: Click the [biol act](#) link for a list of biological activities.

Examples for the Compound Biological Activity field:

“Antiviral activity”; Insect pheromone activity”

Molecular Weight: Enter single value, or value preceded by > or <.

Examples for the Molecular Weight field:

340; > 500

Reaction Role

Check a box to indicate a reaction role: **Reactant**, **Product**, **Catalyst**, and/or **Solvent**. If no box is checked, the compound can have any role.

Marked Records

The **Marked Records List**, **Marked Compound List**, and **Marked Reaction List** pages display lists of the records, compounds and/or reactions you marked during the current session.

You can mark records on the relevant **Search Results Summary** page by clicking the **check box** beside the journal item, compound, or reaction, then clicking the **Submit Marks** button. Or click the **Mark** button on the **Full Record** page. You can see the available options on the **Marked Records** page to:

Print records:

Select the bibliographic information you want to print in each record by selecting the check box beside each field name you want. Note that the author/inventor, title, and source information fields always print. Click **FORMAT TO PRINT**, and use your Web browser's **Print** command to print.

Save records:

Save journal article records to a text file suitable for import into a bibliographic management program.

Export journal article records:

Export records directly into *EndNote*[®], *ProCite*[®] or *Reference Manager*[®]

Export compounds and reactions:

For compounds on the **Marked Compound Records** list, you can **Export SDfile**. For reactions on the **Marked Reaction Records** list, you can **Export RDfile**.

E-mail records:

E-mail records with a note to any e-mail address you enter.

Order Full-text:

Click **FORMAT FOR DOCUMENT DELIVERY** for information about ordering Full-text copy of the articles on your **Marked List**.

Note:

To clear all **Marked Records**, click **CLEAR MARKED LIST** at the top of the **Marked Records** page.



Reaction Conditions

Atmosphere:

Select a value from the drop-down box:

Any, Air, O₂, N₂, H₂, He, Ar, CO, or CO₂

Time (hrs):

Enter single value, or value preceded by > or <.

Examples for the Time field:

24; <10; >2

Product Yield:

The product yield is expressed as a percentage. Enter as single value, or value preceded by > or <.

Examples for the Time field:

100; >60

Pressure (Atm):

Enter single value, or value preceded by > or <.

Examples for the Pressure field:

>1; >5 AND <20

Temperature:

(in degrees Celsius): Enter single value, or value preceded by > or <.

Examples for the Temperature field:

25; >-40; <0

Other:

Click the [Terms list](#) link for list of terms.

Examples of Terms:

irradiation; ultrasound

Refluxed flag:

Check the box to retrieve reactions that have been flagged as refluxed.

Reaction Search Terms

Reaction Keyphrases:

Click the [Keyphrase list](#) link for list of terms. Note that words on the list may be combined with other words.

Examples of Reaction Search Terms:

DIELS ALDER; RING CLOSURE; SOLID PHASE SYNTHESIS

Comments:

Comments can include advantages, limitations, warnings and other qualitative data. Enter single term or terms.

Examples of Comments:

commercial* AND cheap; simple OR efficient; explosive



Link to *Web of Science*

After you run a search, records are retrieved. In the full record, click on the **Go to Web of Science** button to see the cited references and citing articles for the results of your search (*Web of Science* subscribers).

Getting Help

Click **Help** for detailed online help, which is available at all times.

If you have questions about *ISI Chemistry*, please contact the Technical Help Desk nearest you. Use the contact information listed on the right. The Help Desk answers questions about *ISI Chemistry*, as well as questions about appropriate search and retrieval techniques. Questions about network connections and/or the use of your Web browser should be directed to your network administrator.

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