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# Introduction

SpecSurf is a unique platform independent spectroscopic information system. It combines the most frequently used spectroscopic techniques in an easy-to-use client-server architecture. SpecSurf is designed for groups of people working together sharing databases, being connected by a network.

SpecSurf is a new Java based applet which runs inside a web browser and offers all necessary tools for structure drawing and import of experimental spectra. Using your Netscape or Microsoft Internet Explorer browser and SpecSurf you can access the world's largest spectra collection. SpecInfo and its more than 660,000 spectra is available on the Internet. Use the browser for data display, spectrum similarity searches, substructure searches or NMR shift prediction. The easy-to-use client offers spectra similarity searches for all methods, substructure searches, name, MW and formula searches as well as precise NMR shift prediction for various nuclei. Search results can be compared with experimental spectra and printed by using a report generator.

SpecSurf delivers maximum efficiency for structure elucidation and structure identification. The platform independent SpecInfo client SpecSurf includes the powerful Structure Editor tool. Create a structure and within seconds you can predict NMR spectra for candidate structures based on well-established rules. The predicted spectra of the new compounds will be compared with database signal assignments. An easy-to-use Hitlist displays link hits to the SpecSurf Result Zone. Any query, a spectrum search, a property search or a structure search results in such a list of hits. Select hits by a left mouse-button click.

The software allows MOL-file format suitable for the import of structures as well as spectrum/data import from JCAMP-DX format.

## Search

### Structure Searching

- Searching across different databases connectivity can be achieved using Intranet, Internet or a remote modem/ISDN access from anywhere in the world.

- Searching for chemical structures

- Quick chemical substructure searching

### Spectral Searching

- Searching across different databases

- Searching for the most important NMR nuclei

- Searching for MS, UV, IR, Raman

### General Searching

- Searching across different databases

- Wildcard search on all entries of the Search Pattern, including chemical names, formulas, molecular weight, or Original Numbers (ID).

## The Workspace

The screenshot shows the SpecSurf Workspace interface. At the top is a menu bar with options: File, Edit, Search, Predict, Show, Float, Clear, Settings, Help. Below the menu bar is a toolbar with various icons. The main workspace is divided into several sections:

- Query area (top left):** Contains an 'Estimated spectrum' plot with the y-axis labeled 'Arbitrary Unit' (0 to 100) and the x-axis labeled 'ppm' (140 to 120). A chemical structure of 3-chloro-aniline is shown to the right.
- Result area (middle left):** Contains a spectrum plot with the y-axis labeled 'Arbitrary Unit' (0 to 75) and the x-axis labeled 'ppm' (140 to 120). A chemical structure of 3-chloro-aniline is shown to the right.
- Hitlist (bottom):** A table with the following data:
 

Rank	Quality	Folder ID	Property
1/1	1000	1.FO0000000039	3-Chloro-aniline
- Table on the right:** A table with columns 'Type' and 'St'. The data is:
 

Type	St
13C	st
15N	st
ir	

### SpecSurf Workspace

The Workspace is what you see on your screen - the Title Bar, Menu Bar, Query as well as Result area, Hitlist and Status Log area. The workplace also includes elements such as menu commands, dialog boxes, and windows.

The Menu Bar contains a list of menus. A menu contains a list of related commands or functions. Thus, the Search menu contains the standard functions for general search, whereas the commands of the Settings menu help you to setup your favorite preferences and to customize the software.

The Query as well as the Result area is divided into three main parts. Spectra are displayed on the left side whereas structures are located in the middle. The table on the right contains additional information about how many and what kind of objects are inside a folder.

<b>Type</b>	Type of spectrum: IR, 13C, ...
<b>St</b>	Structure

Search results are displayed in the Hitlist. By default the first entry of a hitlist will automatically displayed in the Result area. When moving the pointer over a result and pressing a mouse button a connection to the SpecInfo server will be established again and the content of this folder will be displayed.

### The Folder principle

#### Data storage

Within a SpecInfo database information are stored in so-called "Folders". A folder consists of objects such as spectra, structures and property information. Any folder may contain a number of different spectra and structures even of the same type. A folder may contain the NMR spectra of the same compound acquired using different solvents or observation frequencies. All data is stored unmodified, the resolution, the number of data points or any other property of a spectrum is not changed.

The advantage of this concept is to store all relevant information of a compound, a set of compounds, a measurement or even a series of measurements in one folder.

All primary objects in a folder are on the same hierarchical level. There are no objects on a higher level - but there are some interdependencies possible. For example, spectra can be assigned to a certain structure within the folder, or vice versa different structures could be connected to one spectrum (if e.g. you have measured a  $^{13}\text{C}$ -NMR spectrum of a mixture of compounds). Another type of dependency between a structure and a NMR spectrum (whatever type) is obtained if peaks of the spectrum are assigned to the corresponding atoms in the structure.

The stored information objects generally consist of several parts:  
The structure and spectra information, which is given as connection tables and full or peak spectra, respectively is complemented by textual information (notes) describing e.g. the source, measure date, literature references, the kind of the experiment etc of the chemical compound and/or spectra.

## Dialogs

The user communicates with the software via dialogs. You can control the functionality of commands by entering or modifying the parameters or values in the respective dialog. The message dialogs display additional information, warnings, or messages concerning the respective task.

## Zoom

### Zoom in/out a structure

Controls how large or small the current structure appears on the screen.  
Pressing the Shift key and moving the mouse up or down moves a structure to the front or to the rear.

### Zoom in/out a spectrum

Controls how large or small the current spectrum appears on the screen.  
To zoom in/out a part of a spectrum, move the pointer in the window containing the respective spectrum. Press the left mouse button and drag a frame to the desired size. Releasing the mouse button fixes the size of the frame and allows moving it to the desired zoom area. Another left mouse-click zooms framed area to full window size. Double-click the right mouse button to switch back to your previous view.

## Security

SpecSurf uses JavaScript, which supports importing datasets. When JavaScript is active, the upload process is more convenient, the browse window is resized to a small window and shifted to the foreground. Since JavaScript is not necessarily required, you can disable it.

### Java Sandbox

As an unsigned Java applet, SpecSurf does not have any access to the file system of your computer.

When importing files from your hard disk, SpecSurf opens a window of your web browser, which enables you to select a file or invoke a path and transfer this file to the web server hosting your SpecSurf installation. This web server sends the file back to SpecSurf on your computer. So SpecSurf can only get any knowledge about the data you intentionally select for this purpose.

Another Java applet restriction for your security should be mentioned: SpecSurf cannot contact any host different from the host it has been downloaded from.

### SSL

When you start SpecSurf using https (SSL, this is an optional product), all data transfer between your computer and SpecSurf's web server is encrypted.

### Cookies

A future release of SpecSurf will use cookies to save your settings. If you do not accept these cookies or your firewall filters cookies, your next SpecSurf session will start with default settings. Other functionality is not affected.

## Tutorial

# Create a spectrum

If there is no spectrum in the Query spectrum area you can easily create hetero NMR or mass spectra of your own. From the Edit menu select Peaklist. The Peaklist editor dialog opens

X	Y	Multi
20.300	1.000	q
25.400	2.000	t
143.500	1.000	s

In case the Query area contains a peak spectrum the table contains data. If you want to enter new values click the New button to clear its contents. Select the method of your choice and enter X- and Y-values in the edit boxes below the table. Click Add Row to transfer the values into the table.

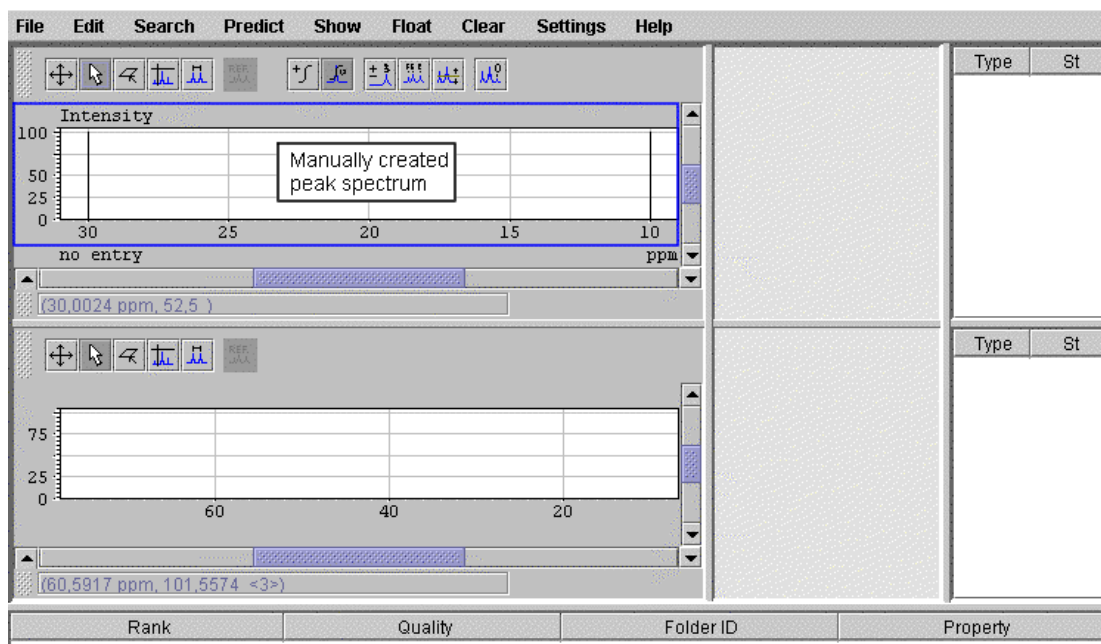
For a later change of any cell value double click the cell, enter a new value and finish the change by pressing "Return". Click OK to leave the dialog. Your "new" spectrum will be displayed in the spectrum query area. You can use this spectrum for a search in all databases.

## Using the Search Spectrum command:

Import a spectrum from your local source or create a special one from publication data with the Edit/Peaklist command.

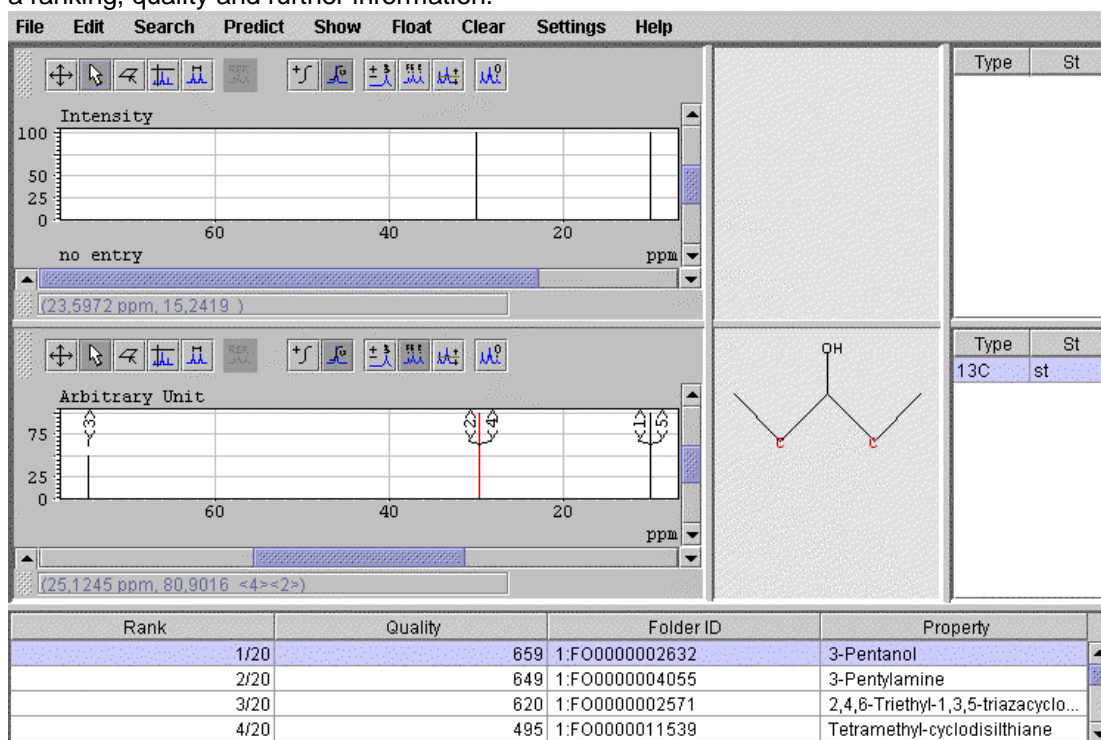
Create a spectrum manually.

In this example the search was performed with a manually created  $^{13}\text{C}$  NMR spectrum with two signals at 10 and 30 ppm.



## Start structure search

Open the Spectrum command of the Search menu. A connection to the SpecInfo Server is established. This will take a moment. You receive a folder hitlist shown in the Hitlist area with a ranking, quality and further information.



Ranking and Quality affect the search remarkable. You can change the Quality value in the Settings/Databases/Set selection/Searches dialog.

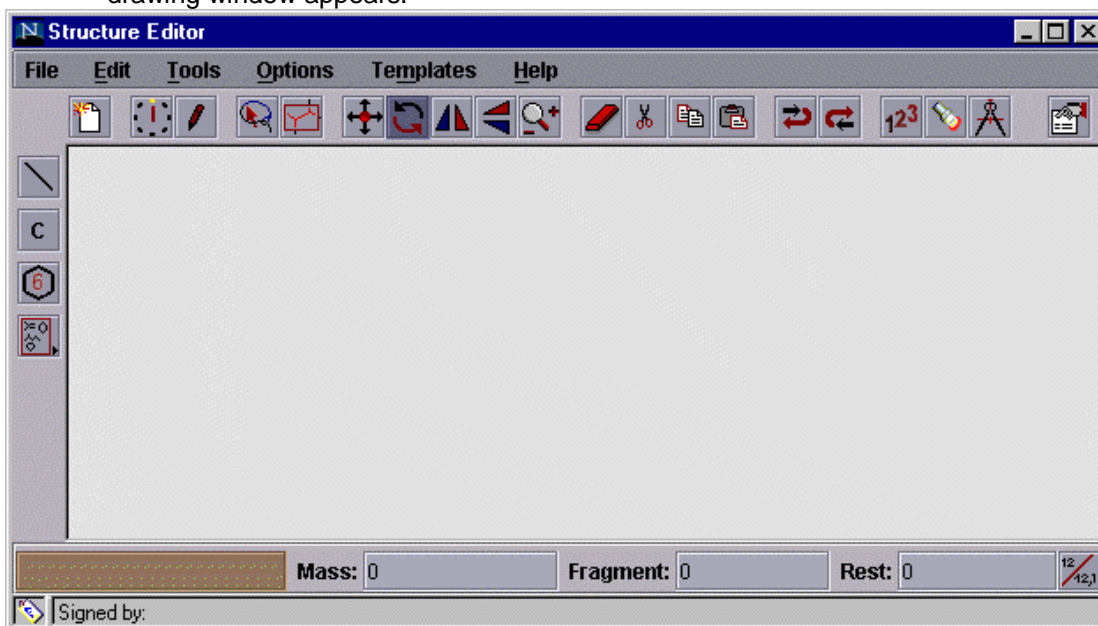
The higher a quality value in the folder hitlist the better the match to the spectrum. The first dataset of this list is automatically displayed in the Result Zone.

If nothing meets the search the message "No hits found" will be displayed in the status line.

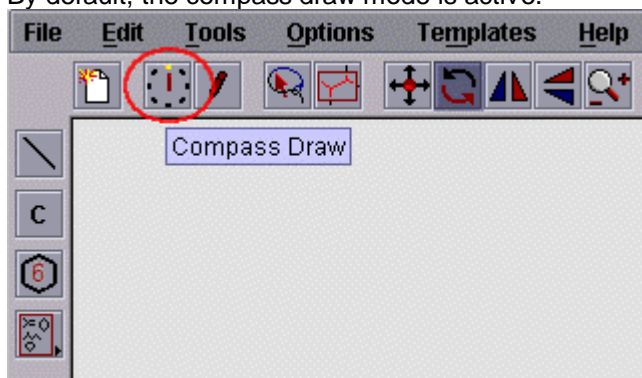
## Draw a new structure

The Structure Editor extensively supports the generation and processing of single chemical structures. It provides a wide range of features, which help you to draw accurate, chemically significant structures quickly and intuitively. Its functionality is optimized for the fast creation of even most complex chemical structures.

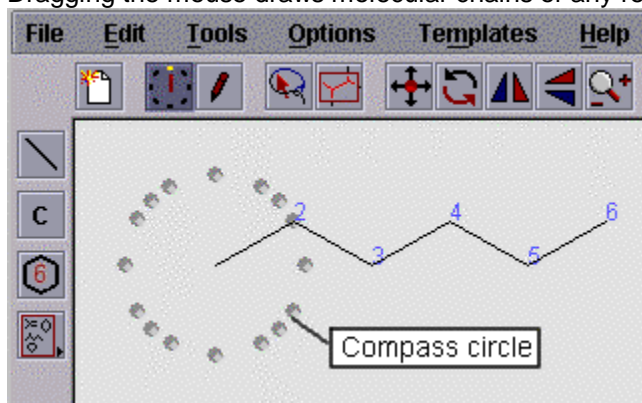
1. From the Structure menu select New structure. After a few seconds an empty drawing window appears.



2. By default, the compass draw mode is active.

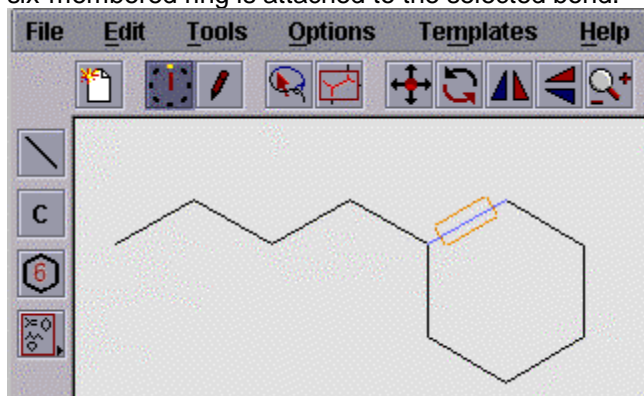


3. Move the pointer into the window. Clicking the left mouse button in an empty area creates a circle of points around a carbon atom. It is also possible to click on an already displayed atom; in this case, this particular atom will form the center of the circle. The points constituting the circle represent the most common angles of chemical structures.
4. Dragging the mouse draws molecular chains of any required length.

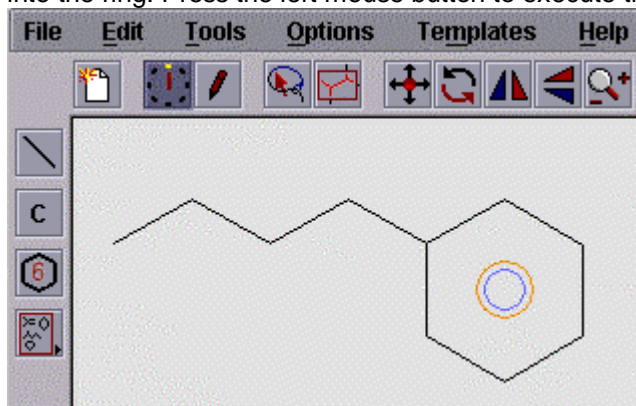


5. Adding a ring is quite easy. Simply move the pointer over the terminated bond, but

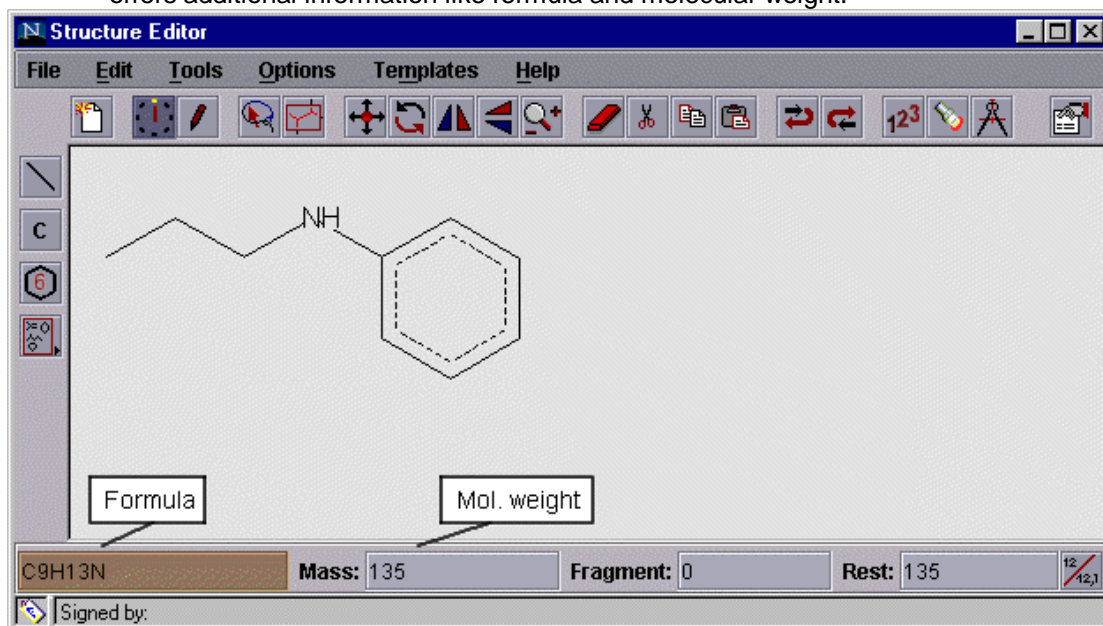
don't press the mouse button. The color of the bond changes to blue and a rectangular hit box appears. Now press the „6“ key on the keyboard. Automatically a six-membered ring is attached to the selected bond.



6. You can convert this aliphatic ring into an aromatic one by simply moving the pointer into the ring. Press the left mouse button to execute the command.



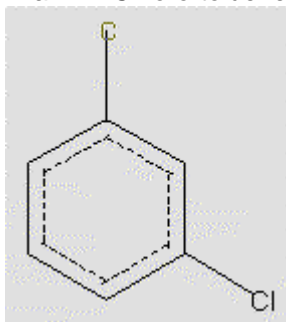
7. Inserting heteroatoms is simple too. Select the carbon atom which you would like to replace by pressing the left mouse button and then enter e.g. „N“ to substitute the carbon by the nitrogen sign. As you can see from the screenshot the structure editor offers additional information like formula and molecular weight.



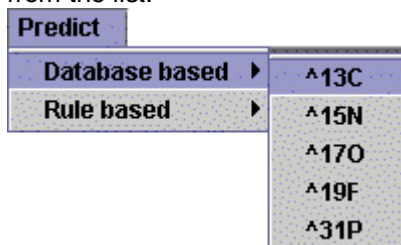
8. After finishing your drawing select Transfer from the File menu to transfer the structure into SpecSurf

# Using the Database based prediction command

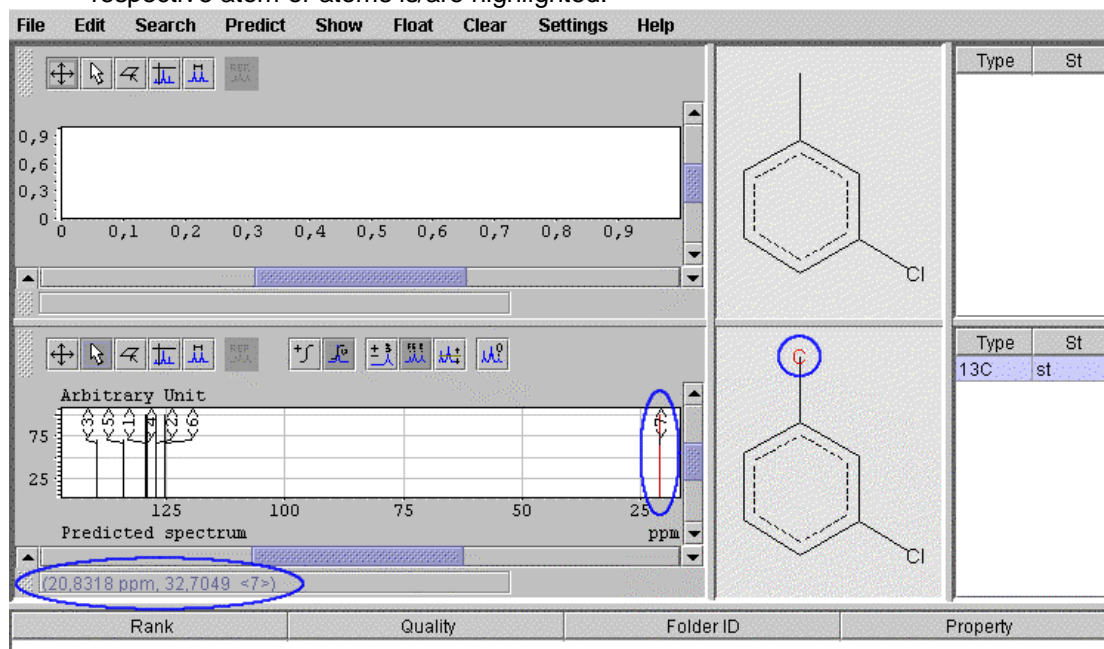
1. Drawn 2-Chloro-toluene using the internal Structure Editor.



2. Click Settings/Databases/Predictions to select one or more databases.
3. On the Predict menu, click Database based and select one of the given elements from the list.



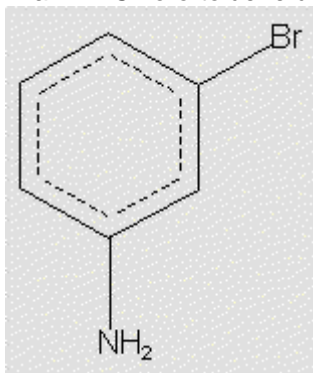
4. A connection to the SpecInfo Server is established. The structure, displayed in the Query Structure Zone, is sent to the server.
5. As a result you will receive a predicted spectrum in the Spectrum Result zone.
6. Activate the Select mode inside the Result area. When pointing with the mouse on an atom, the respective peak is highlighted. When pointing with the cursor on a peak, the respective atom or atoms is/are highlighted.



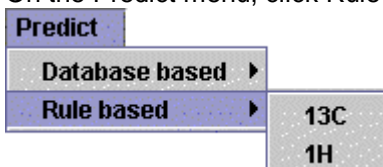
# Using the Rule based prediction

# command

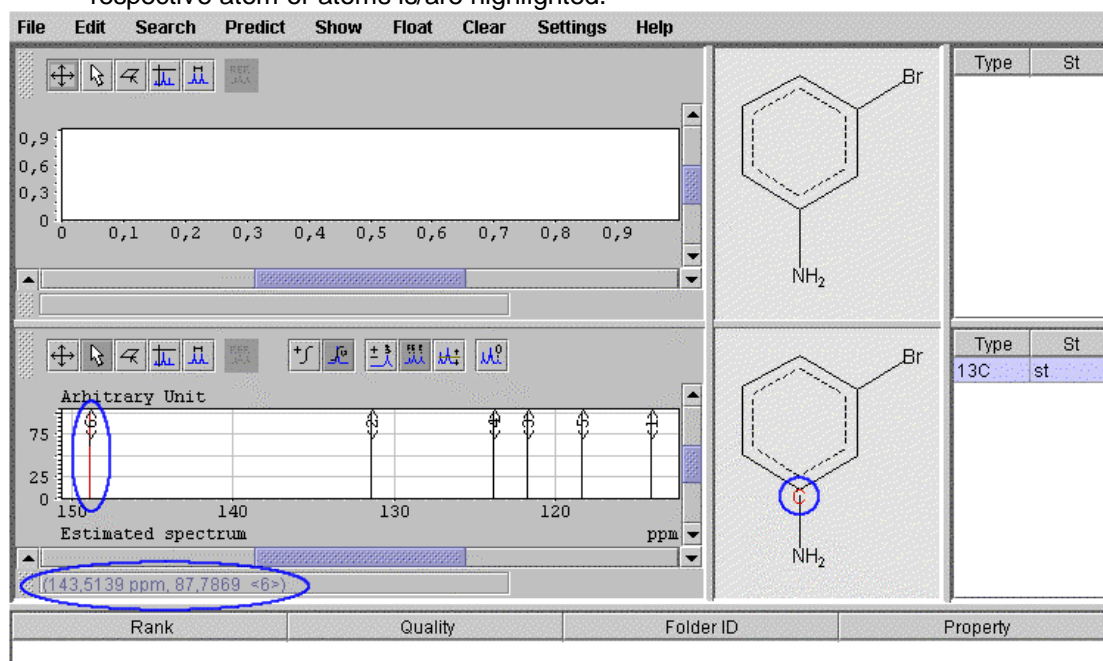
1. Draw 2-Chloro-toluene using the internal Structure Editor.



2. Click Settings/Databases/Predictions to select one or more databases.
3. On the Predict menu, click Rule based and select <sup>13</sup>C or <sup>1</sup>H from the list.



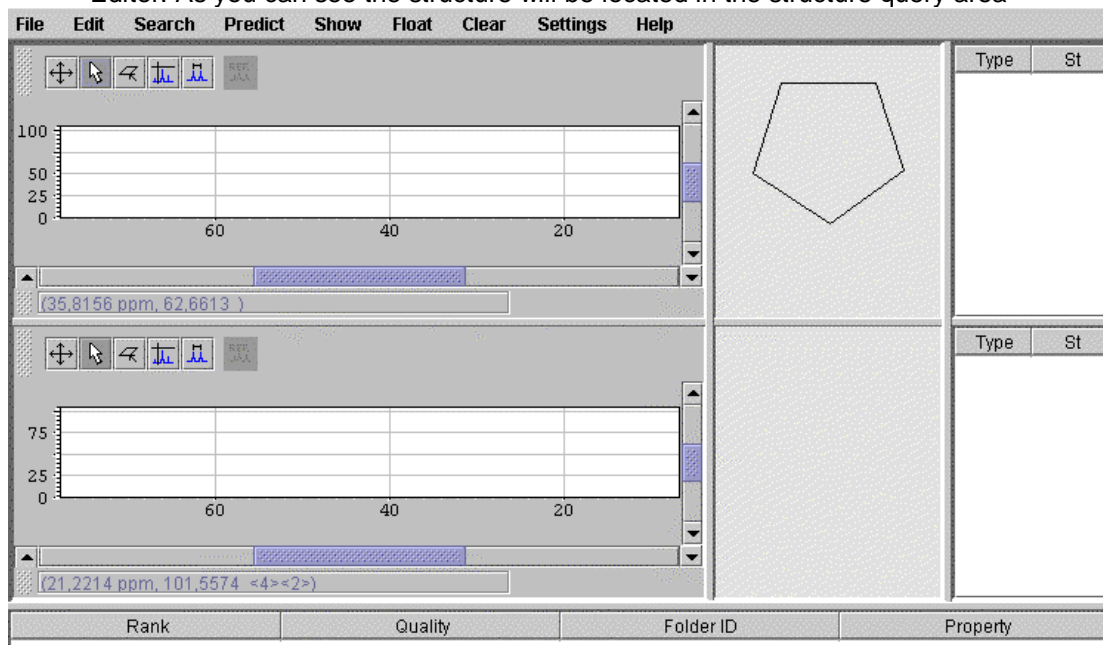
4. A connection to the SpecInfo Server is established. The structure, displayed in the Query Structure Zone, is sent to the server.
5. As a result you will receive a predicted spectrum in the Spectrum Result zone.
6. Activate the Select mode inside the Result area. When pointing with the mouse on an atom, the respective peak is highlighted. When pointing with the cursor on a peak, the respective atom or atoms is/are highlighted.



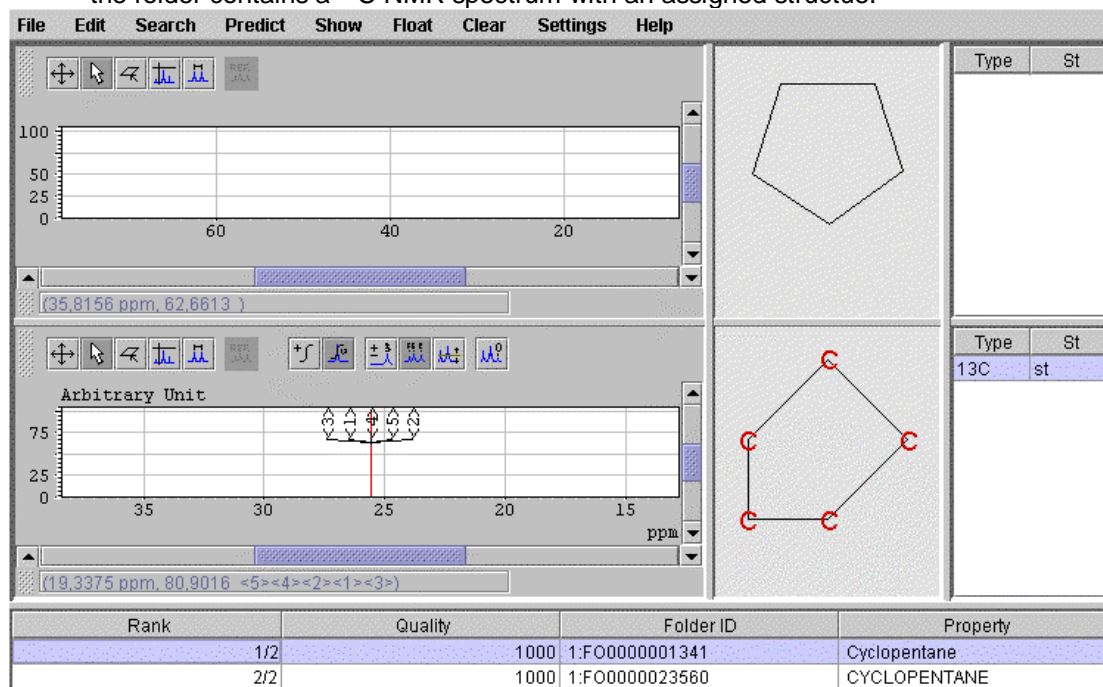
## Using the Search Structure command

1. Import a previously drawn structure or create a new one using the internal Structure

Editor. As you can see the structure will be located in the structure query area



2. From the Settings menu select Databases/Searches and select one or more databases.
3. Click Search/Structure to start the query. A connection to the SpecInfo server is established and the structure, located in the Query Structure Zone, is sent to the server.
4. After a few seconds you receive a hitlist and the first dataset of this list will be displayed automatically in the result area. The table on the right hand of the result area gives you information about all objects in the transferred folder. In our example the folder contains a  $^{13}\text{C}$  NMR spectrum with an assigned structure.



If nothing meets a search the message "No hits found" will be displayed in the status line.

## Substructure search

### Important remarks:

The positions where substitution is allowed in the search fragments are identified by

a) "?" (question mark)

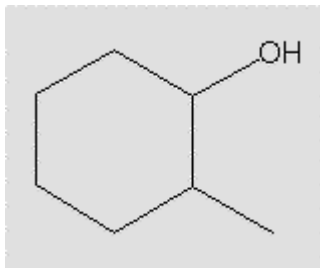
A "?" will be interpreted as „any atom except hydrogen“.

b) "A" (any atom)

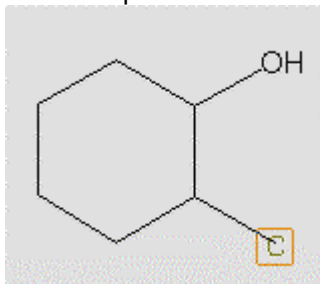
An "A" will be interpreted as „any atom including hydrogen“.

a) Question mark search

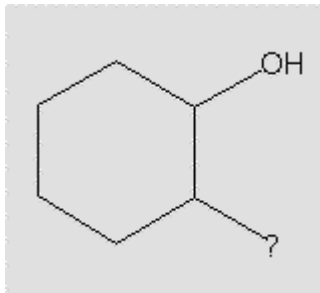
1. Import a previously drawn structure or create a new one using the internal Structure Editor.
2. To modify any structure to define substitution positions with an explicit question mark select **Edit/Structure**. After the editor was opened draw the following structure



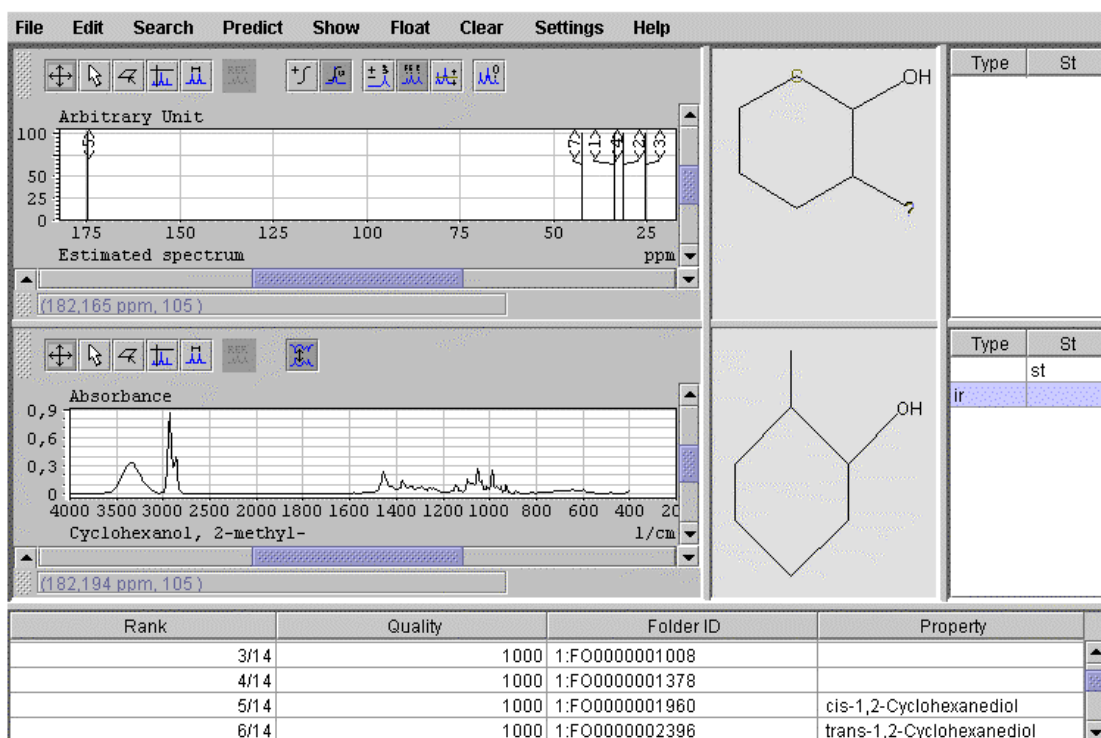
3. Move the pointer over the carbon atom as indicated in the screen shot



4. Replace the carbon symbol by typing the "?". You are free to replace more than one carbon atom with the "?" and start a substructure search.

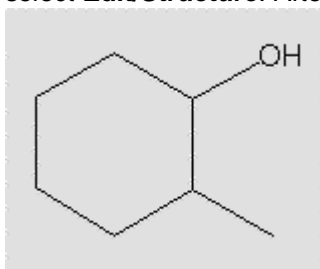


5. From the **File** menu select **Transfer** to transfer the structure to the SpecSurf query area.
6. From the **Settings** menu select **Databases/Searches** and select one or more databases.
7. Click **Search/Structure** to start the query. A connection to the SpecInfo server is established and the structure, located in the query structure area, is sent to the server.
8. After a few seconds you receive a hitlist (14 hits) and the first dataset of this list will be displayed automatically in the result area. The table on the right hand of the result area gives you information about all objects in the transferred folder. In our example the folder Cyclohexanol, 2-methyl- contains two objects, an IR spectrum and a structure.

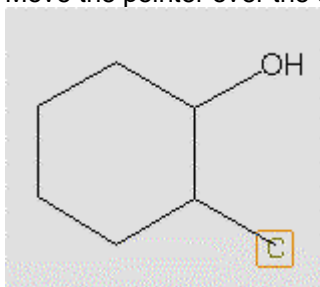


b) Any Atom search

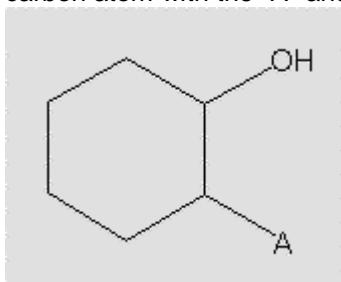
1. Import a previously drawn structure or create a new one using the internal Structure Editor.
2. To modify any structure to define substitution positions with an explicit question mark select **Edit/Structure**. After the editor was opened draw the following structure



3. Move the pointer over the carbon atom as indicated in the screen shot



4. Replace the carbon symbol by typing the "A". You are free to replace more than one carbon atom with the "A" and start a substructure search.



- From the **File** menu select **Transfer** to transfer the structure to the SpecSurf query area.
- From the **Settings** menu select **Databases/Searches** and select one or more databases.
- Click **Search/Structure** to start the query. A connection to the SpecInfo server is established and the structure, located in the query structure area, is sent to the server.
- After a few seconds you receive a hitlist (16 hits) and the first dataset of this list will be displayed automatically in the result area. The table on the right hand of the result area gives you information about all objects in the transferred folder. In our example the folder Cyclohexanol contains four objects, two  $^{13}\text{C}$  NMR spectra, one  $^{17}\text{O}$  NMR spectrum and a structure.

The screenshot displays the SpecInfo software interface. It features two NMR spectra plots on the left, each with a y-axis labeled 'Arbitrary Unit' and an x-axis labeled 'ppm'. The top plot is an 'Estimated spectrum' with a peak at 182.194 ppm. The bottom plot has a peak at 72.056 ppm. To the right of the plots are two chemical structures: the top one is 2-methylcyclohexanol (labeled 'A') and the bottom one is cyclohexanol. On the far right, there is a table with columns 'Type' and 'St'. Below the plots and structures is a hitlist table with columns 'Rank', 'Quality', 'Folder ID', and 'Property'.

Rank	Quality	Folder ID	Property
1/16	1000	1:FO0000000387	Cyclohexanol, 2-methyl-
2/16	1000	1:FO0000000391	1,2-Cyclohexanediol
3/16	1000	1:FO0000000198	Cyclohexanol
4/16	1000	1:FO0000001008	

If nothing meets a search the message "No hits found" will be displayed in the status line.

## Note Field search

### An overview

Another quick way to find information in SpecInfo is through a Notes search. The Notes search is a very easy to handle but powerful tool for data retrieval. This function allows you to search every folder in a database for a particular string. It is different from the object search because note fields may contain keywords or other data. The Notes search finds only folders containing the string you are looking for. It uses the predefined fields in the databases dealing with the most frequently used properties of spectra and structures such as:

- compound name
- formula
- molecular weight.

### Compound Name

Search Text	Comment	Result (example)
-------------	---------	------------------

(example)		
Benzene, Cyclohexane	Searches for full names.	Benzene, Cyclohexane
Benz*	Searches for partial names. Wildcard for an unlimited number of characters is * „asterisk“.	Benzoic acid, Benzo-15-crown-5

### MW

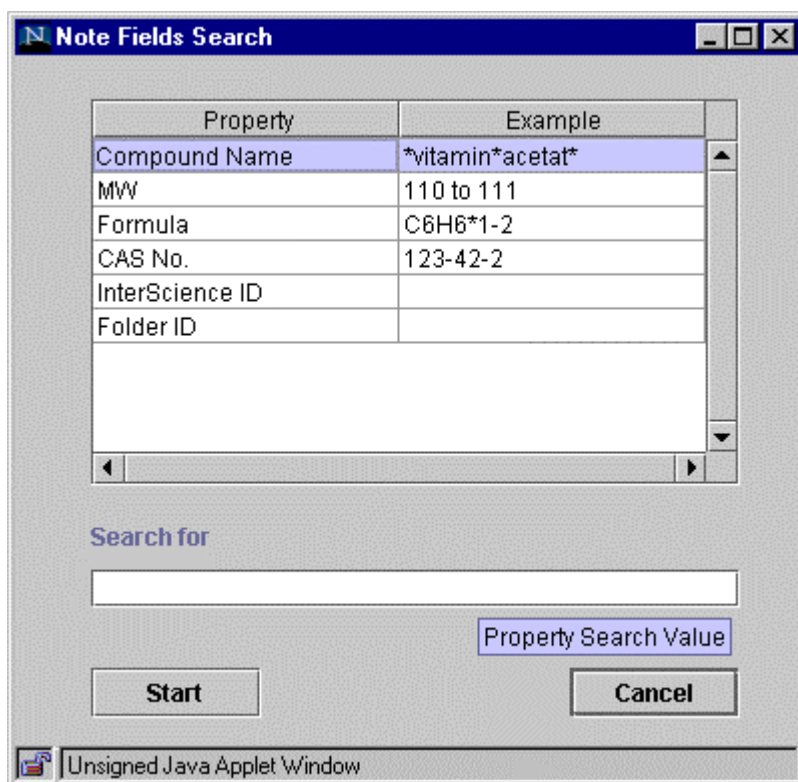
Search Text (example)	Comment	Result (example)
78 to 78.1	Searches the molecular weight by a user-defined range.	78.0468 (for Benzene and other C <sub>6</sub> H <sub>6</sub> compounds)

### Formula

Search Text (example)	Comment	Result (example)
C <sub>6</sub> H <sub>6</sub>	Searches for all compounds with exact six carbons and six protons.	C <sub>6</sub> H <sub>6</sub>
C-5H <sub>6</sub>	Searches for all compounds with # C <= 5 but exact six protons but an unlimited number of other hetero atoms..	C <sub>2</sub> H <sub>6</sub> O, C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>
C <sub>3</sub> -5H <sub>6</sub>	Searches for all compounds with 3 <= # C <= 5 but exact six protons.	C <sub>3</sub> H <sub>6</sub> , C <sub>4</sub> H <sub>6</sub> , C <sub>5</sub> H <sub>6</sub>
C <sub>3</sub> H <sub>5</sub> Cl	Searches for all compounds with exact three carbons, five protons, one chlorine atom but an unlimited number of other hetero atoms.	C <sub>3</sub> H <sub>5</sub> ClNO <sub>2</sub>
C <sub>3</sub> H <sub>5</sub> Cl*1	Searches for all compounds with exact three carbons and five protons, one chlorine atom and any other atom that occur one time in a molecule.	C <sub>3</sub> H <sub>5</sub> ClO, C <sub>3</sub> H <sub>5</sub> ClO

### a) Normal search without wildcard

1. Select the Note Fields ... command of the Search menu. This opens a Note Field Search dialog with a list of keywords for a search across different databases.



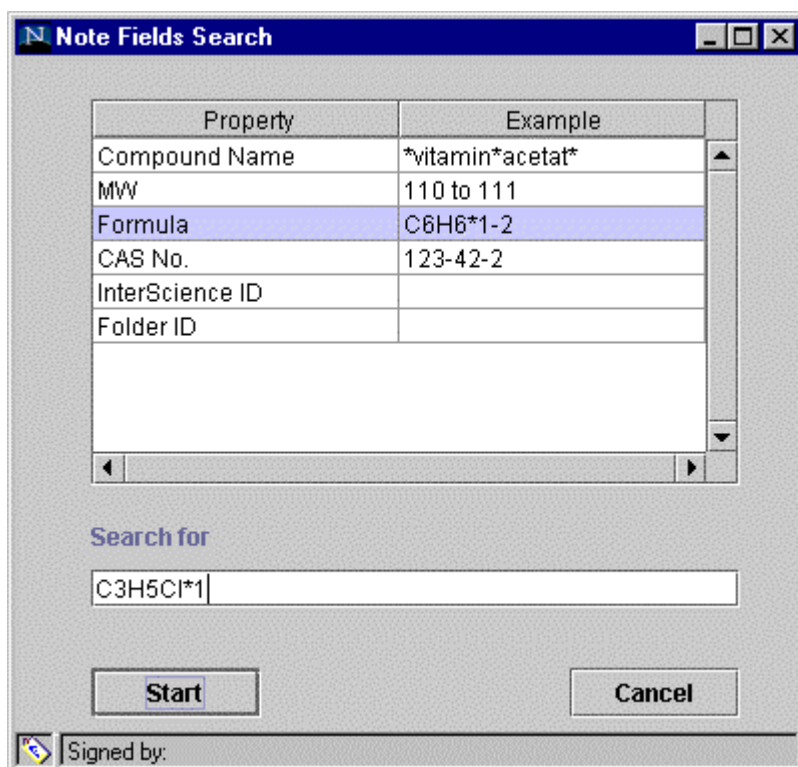
- From the Property column select Compound name and enter the search string "Benzylchloride" in the Search for edit field.
- Press the Start button. A connection to the SpecInfo server is established.
- After a while you receive a hitlist containing a folder which matches your query.

Rank	Quality	Folder ID	Property
1/1	1000	1:F00000002883	Benzylchloride

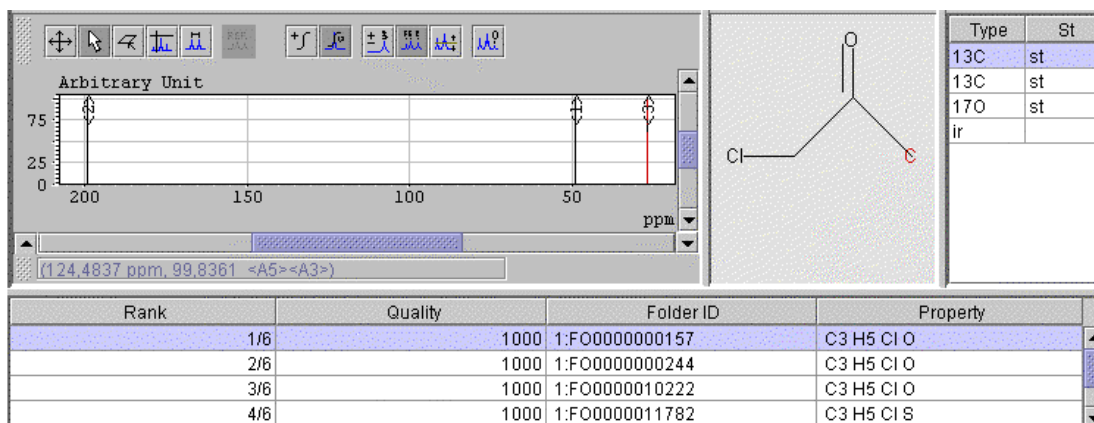
- The folder contains two  $^{13}\text{C}$  NMR spectra and one IR spectrum. The first object is automatically displayed in the Result area.

## b) Advanced search using wildcards

- Select the Note Fields ... command of the Search menu. This opens a Note Field Search dialog with a list of keywords for a search across different databases.
- From the Property column select Compound name and enter the search string "C3H5Cl\*1" in the Search for edit field.



3. Press the Start button. A connection to the SpecInfo server is established.
4. After a while you receive a hitlist containing six folders matching your query. There are five folders with a formula  $C_3H_5ClO$  and one with  $C_3H_5ClS$ .



The folder contains a structure, two  $^{13}C$  NMR and one  $^{17}O$  NMR peak tables as well as one IR spectrum.

As you can see the fourth folder has a different formula but matches your query too.

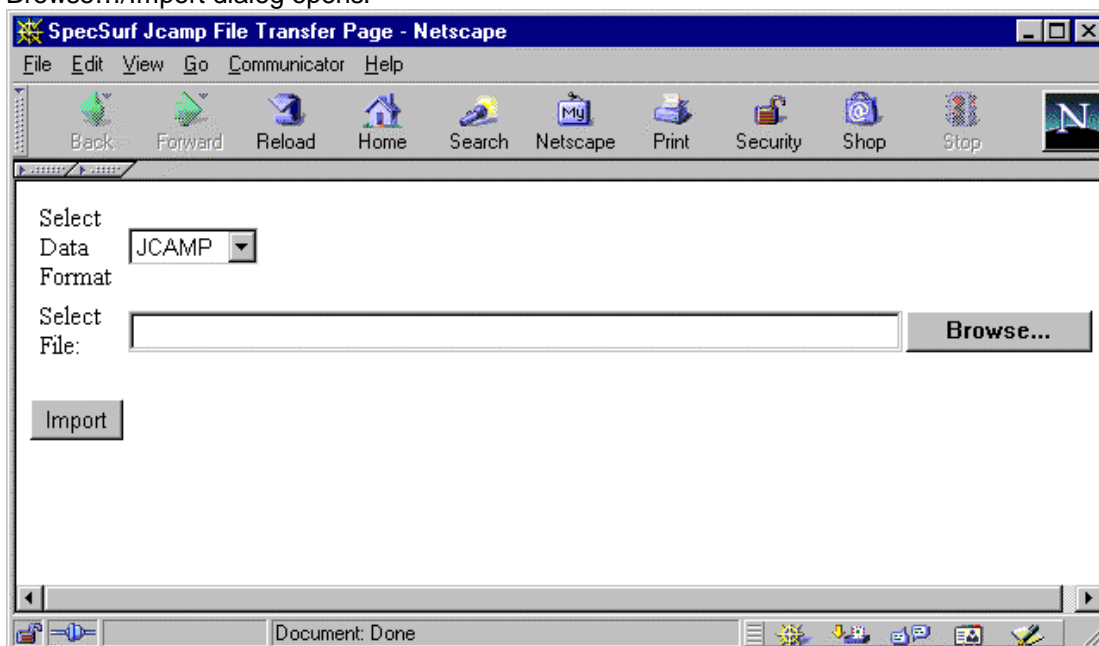
To retrieve the entry simply click with the mouse pointer to the row and click the left mouse button. The request is sent to the SpecInfo server. After a few seconds you receive the new folder.

## File menu

## Import

This command is available as the first one from the File menu. It imports datasets from your

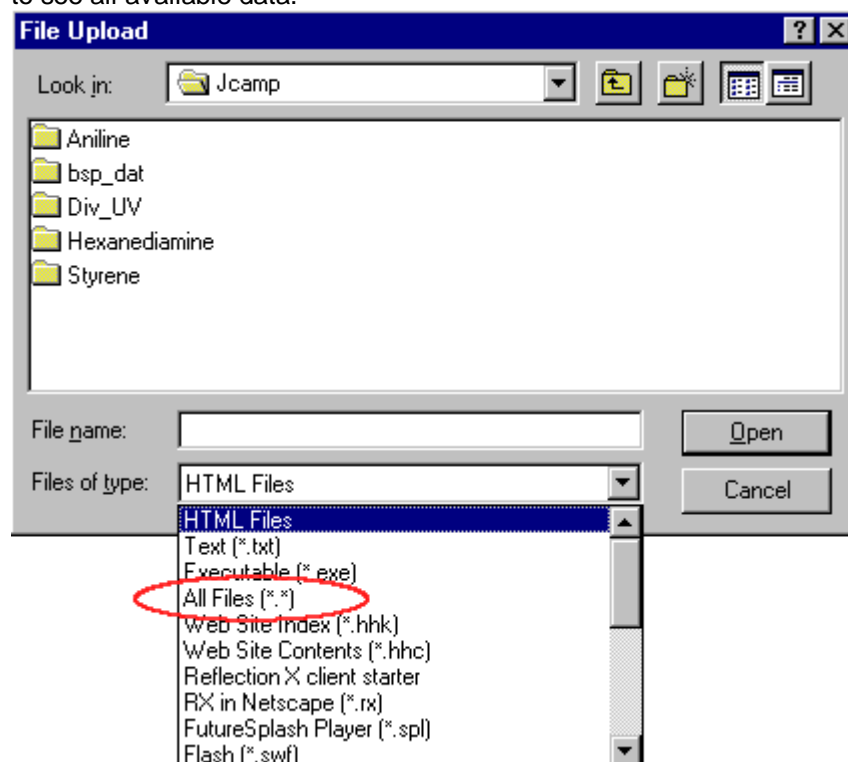
local file system into SpecSurf. The standard data format for spectra and structures is JCAMP-DX and additional MDL Molefile for chemical structures. On the **File** menu click **Import** to open a submenu with additional commands. After selecting an import command, a Browse.../Import dialog opens.



#### SpecSurf File Transfer Window

Select a Mol file, JCAMP data, or any Peaktable for an upload into SpecSurf. Enter a data file name in the text box or click the **Browse...** button to open a File Upload Box.

Note that the default extension of \*.html will of course mean that you will not be shown any JCAMP-DX files with the extension \*.dx. Select from the drop-down menu the option **All Files** to see all available data.



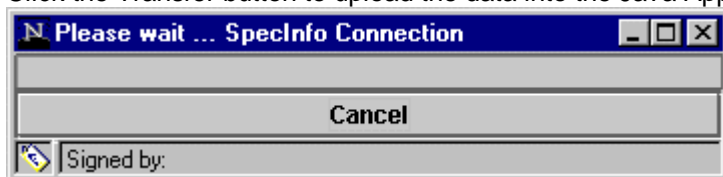
In File Name, enter the name of the dataset you want to open. Click OK or double-click on a file name to select this file without clicking OK.

If the dataset you want to import is not listed, do the following:

In Look in, select a new drive.

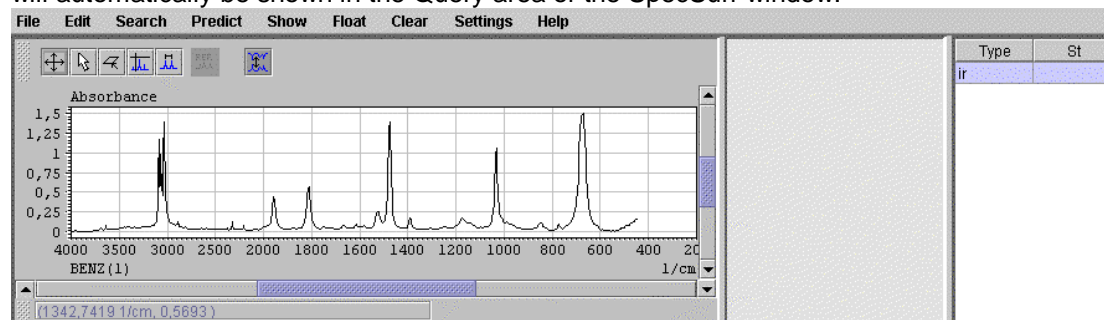
In Folders, select a new folder.  
Select a file and click OK.

Click the Transfer button to upload the data into the Java Applet.



SpecInfo Connection Window

If you chose JCAMP data, the information from the first row of the query window peak table will automatically be shown in the Query area of the SpecSurf window.



In case of a Mol file, only a structure is displayed.

SpecSurf supports the following import formats:

Structures	MDL-Mol JCAMP-CS		
Spectra	JCAMP Versions 4.24 and 5.0	IR UV MS NMR	Bruker, Varian, Jeol

## Export

Lets you export a drawn structure located in the structure query area. MOL-File extension is \*.mol, JCAMP-CS is \*.cs.

File name	Enter the name and the extension of the file you want to export. You can also change the directory by entering a new valid path here.
File list	Alternatively, you can select a filename from this list. If the file which you want to save is not listed, do the following: In Drives, select a new drive. In Folders, select a new folder. Select a file and click OK.

## Print

Note: if you want to print the report during a Specs surf session it is necessary to have a version of the Adobe Reader installed on your system. Otherwise Specs surf will create a PDF document for a later use.

From the File menu select Print/Report. A second browser window opens with the Specs surf Report Page.

Report Title

Include the following graphic display areas and corresponding notes from SpecSurf

**Data Notes**

Query Structure

Query Spectrum

Result Structure

Result Spectrum

Hitlist

Please do not bookmark this page.

The Report Title entry will be the heading of your report. Query structure and spectrum are displayed on the first page, the search result on the second one and the Hitlist on the third.

## Edit menu

# Structure

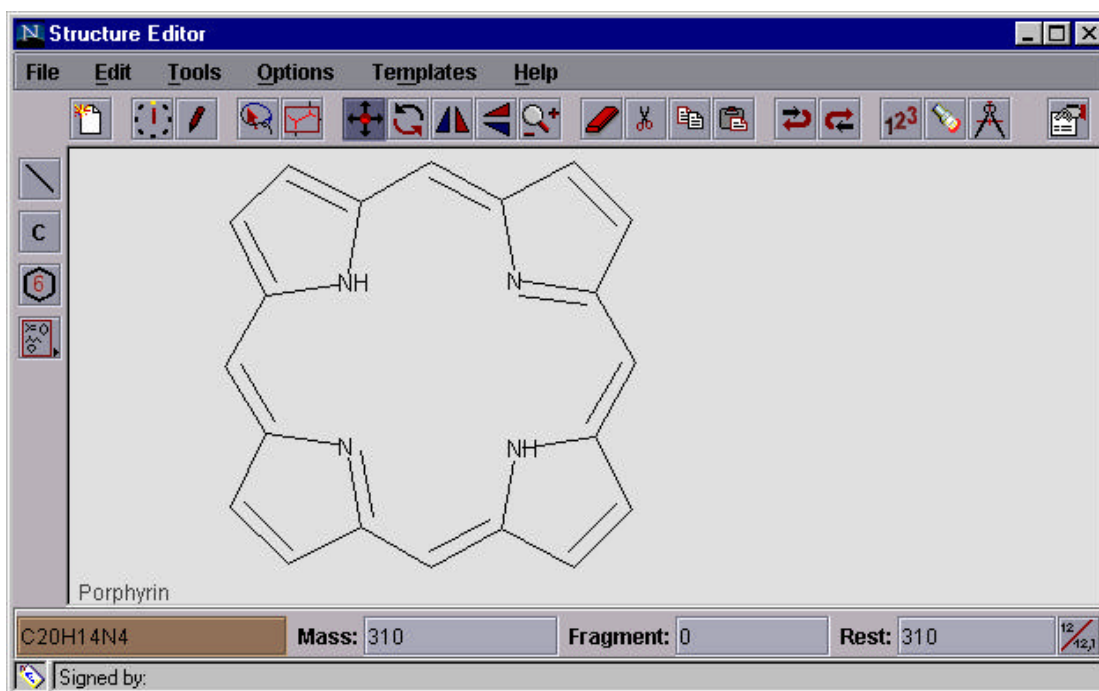
The SpecSurf Structure Editor is a powerful tool to create chemical structures. You can draw chemical structures with just a few mouse clicks. Written in Java, the Structure Editor is platform independent.

It's chemical intelligence helps you to draw accurate, chemically significant structures quickly and intuitively; letters are identified as atoms with valence limits, lines as bonds that attach at correct lengths and angles. The editor also checks for maximal allowed valences of elements. Free valences are automatically saturated with Hydrogen; atom charges are considered.

Based on the generated structure and the automatically complemented hydrogen atoms the empirical formula, the molar or, switchable, the nominal mass are calculated and displayed for whole molecules, selections, and the corresponding loss. For the nominal mass individual isotopes are considered.

These are especially interesting features for scientists involved with mass spectroscopy. On demand, The Structure Editor highlights possible errors and improbable structural features.

On the Edit menu, click Structure to start the SpecSurf Structure Editor.



Structure Editor screen

The central part of the screen contains the so-called workspace where an existing structure will be displayed or new one can be drawn.

The horizontal toolbar enables access to most of the commands of the File, Edit, Tools, and Template menu. The vertical toolbox contains most of the drawing tool-buttons. Just click an icon to perform the respective command.

Using the icons and pop-up menus you can quickly and easily create molecule structures. Simple mouse-clicks set or move atoms and define bonds. All elements can be entered in your active structure just by a mouse-click on the respective atom of the displayed periodic system. Additionally the editor offers a menu from which the mostly used elements can be chosen directly.

For experienced users, using the keyboard eases the generation and manipulation of structures; every element of the periodic system as well as any bond and the most common rings can be activated via the respective keyboard combination.

All structures can be presented with various accompanying information, e.g. the empirical formula, the atom numbering, charge, carbons, carbon protons are displayed if desired. Furthermore, you can activate a context dialog, which indicates and allows you to edit the name, charge, isotope, and weight of the respective atom.

The editor provides different drawing modes, such as Compass Draw, Freehand Draw and Single Draw. By using the Compass Draw mode for example, you can create molecular chains of any required length just by dragging the mouse. While dragging the mouse, the editor displays the number of added atoms.

You can move and rotate complete molecules or selections while bonds are preserved and adjusted automatically. Various selection modes, e.g. the Lasso Tool, enable you to select irregularly shaped fragments freehand. The selected fragment can be extended easily.

The editor offers a wide selection of pre-defined ring types. You can select from three-membered up to nine-membered saturated hydrocarbon rings and Benzene. As well, a rich set of pre-defined structure templates from various areas of organic chemistry is available. The user can enter these templates and combine them with/at any chosen bond or atom of the active structure.

## Edit Peaklist

SpecSurf contains a built-in peaklist editor, which allows you to create peak spectra of your own. If there is any spectrum in the query area, the peaks of this spectrum are listed.

Selecting Edit/Peaklist opens a dialog box with an empty table or the peaklist of the spectrum located in the query spectrum area. Dependent on the kind of spectrum the dialog should look similar to this:

Method:

Title:

X Unit:  Y Unit:

X	Y	Multi
20.300	1.000	q
25.400	2.000	t
143.500	1.000	s

X:  Y:  Multi:

Buttons: Add Row, Delete, New, OK, Cancel

Signed by:

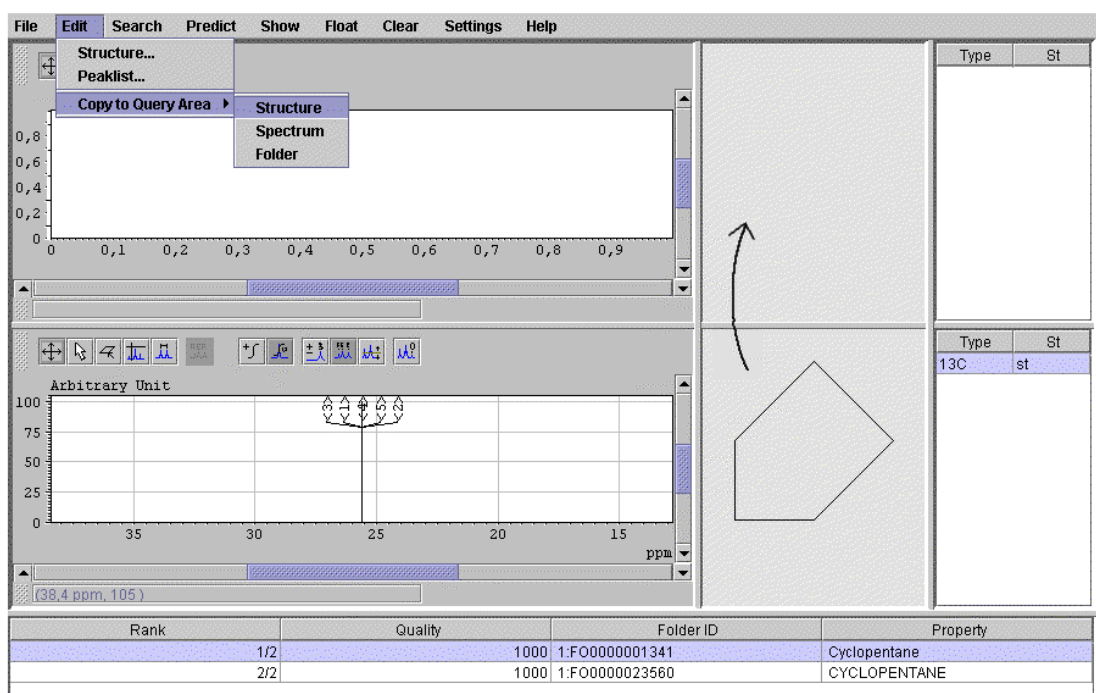
Peaklist for a <sup>13</sup>C-NMR spectrum

Method	Available methods like NMR, UV, IR, ... Note: there is a difference between Full spectrum and Peaklist. A Full spectrum isn't editable.
Title	JCAMP label "Title". This title is displayed in the information line under the spectrum.
X Unit	E.g. ppm, nm (corresponds to the method).
Y Unit	Intensity Units corresponding to the method.

With the Peaklist editor it is very easy to create peak spectra manually.

## Copy to Query area

Copies a structure, spectrum, or folder from the Result area to the respective Query area.



# Search menu

## Search Structure

SpecSurf delivers maximum efficiency for structure elucidation and structure identification. The platform independent SpecInfo client SpecSurf includes the powerful Structure Editor tool. The Edit/Structure command enables you to define a structure or substructure that is searched against a structure database. An easy-to-use hitlist displays link hits to the SpecSurf Result Zone. Select hits by a left mouse-button click. How to use the Search Structure command

## Search substructure

Substructure searches are used to retrieve structures containing the drawn part of the molecule.

Substructure searching means you only want to search for a part of a molecule and you want to see all chemical structures containing this fragment in your hitlist. The positions where substitution is allowed in the search fragments are identified by the following wildcards:

- "?" (question mark)  
A "?" will be interpreted as „any atom except hydrogen“.
- "A" (any atom)  
An "A" will be interpreted as „any atom including hydrogen“.

The number of substructures, including identical ones, is taken into account during the search. Please note that using small substructures which are common in the database may lead to long substructure search times.

Search substructure

## Search Spectrum

Search Spectrum is a spectral search across different databases. The spectrum displayed in

the Query Spectrum Zone is sent to the server.  
Using the Search Spectrum command

## Search Note Fields

A quick way to find information in SpecInfo is through a Note Fields Search. The Note Fields Search is a very easy to handle but powerful tool for data retrieval. This function allows you to search every folder in a database for a particular string. It is different from the object search because note fields may contain keywords or other data. The Note Fields Search finds only folders containing the string you are looking for. It uses the predefined fields in the databases dealing with the most frequently used properties of spectra and structures such as:

- compound name
- formula
- molecular weight.

Using the Search Note Fields command

## Predict menu

# Prediction

An important feature of SpecSurf is the prediction of a spectrum - Database based or Rule based. SpecSurf allows you to predict spectra for novel or known compounds and use the predictions to assign peaks.

The following two sections will give you a quick insight on prediction and estimation.

Estimation and prediction differ in algorithms. Estimation gives you the chemical shifts as results of increment calculations, whereas prediction is calculated on HOSE codes, i.e. the chemical shift information in the database.

The quality of the spectrum prediction and automatic assignment is dependent on the contents of a database.

## Database based prediction

Predicts the X-NMR-spectrum of a structure on the basis of data stored in the database. This function for each X-atom of the structure searches the database for atoms in a similar chemical environment, until the predicted spectrum is complete. Because the prediction result depends strongly on the amount of data stored in a database you have to select a database from the Select database dialog.

How to use the database based prediction command

## Rule based prediction

Estimates the <sup>1</sup>H- or <sup>13</sup>C-NMR-spectrum of a structure on the basis of empirical increment-systems. Founded on the data of many known <sup>1</sup>H- and <sup>13</sup>C-NMR-spectra empirical rules for the absorption of proton or carbon depending on their chemical environment can be stated. The increment-method supposes that the influence of substituents is additive, which of course is inexact. Nevertheless, with the exception of structures that show special sterical or electronical reciprocal action the received values for  $\delta$  are quite useful.

The estimation process will be started by clicking on the <sup>1</sup>H or <sup>13</sup>C command.

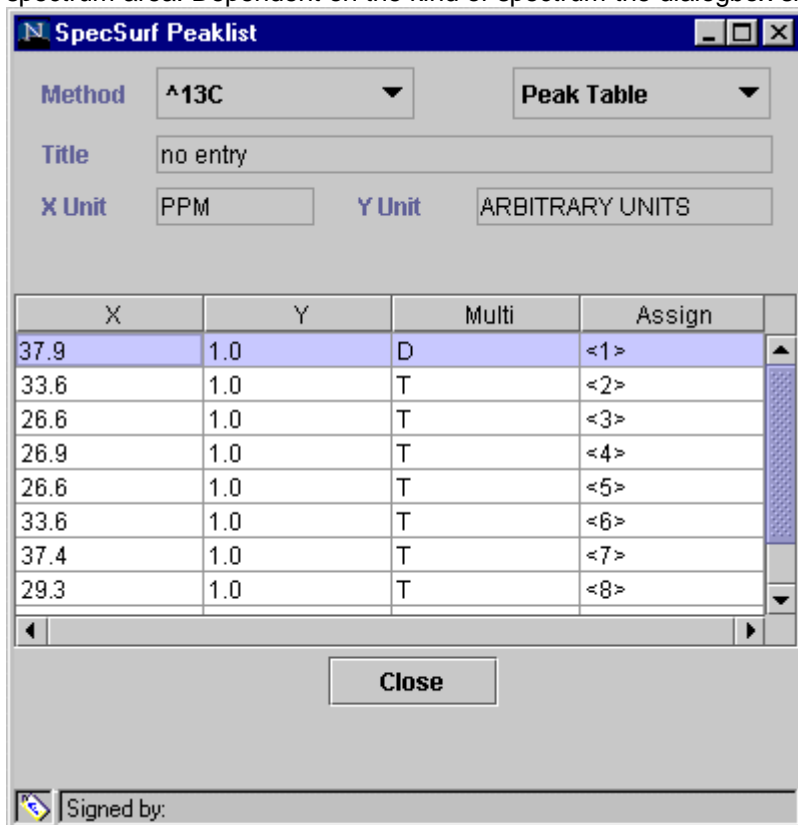
How to use the rule based prediction command

When pointing with the mouse on an atom, the respective peak is highlighted. When pointing with the cursor on a peak, the respective atom or atoms is/are highlighted.

# Show menu

## Peaklist

Opens a dialog box with the peaklist of the spectrum currently displayed in the Result spectrum area. Dependent on the kind of spectrum the dialogbox should look similar to this:



Peaklist for a <sup>13</sup>C-NMR spectrum

Method	Lists the corresponding method like NMR, UV, IR...
Title	Name of the compound, if available.
X Unit	Corresponding to the method like ppm, nm, ...
Y Unit	Intensity units, corresponding to the method.

All fields are read-only.

Note fields contain notices related to the kind of object. That may be for example information about an experiment or a solvent used during a NMR measurement. These attributes are stored within the JCAMP-DX or JCAMP-CS data file.

## Structure notes

Opens a dialog box with the note fields of the structure currently displayed in the Result structure area.

Note-Fields	Value
Title	Cyclohexanol
Owner	COPYRIGHT (C) 1995 by Chemical Concepts
Origin	Chemical Concepts, Tel. +49(0)6201-606433, P.O. Box 10...
Input Date	Jan 03 1980 05:02AM
Original No.	1:ST00::STCC-65563-409S
Special No.	EPA:69805 CCF:00200200
SpecInfo ID	1:ST0000000642
Sp-Litera	OW#000195168

**Close**

Signed by:

## Spectrum

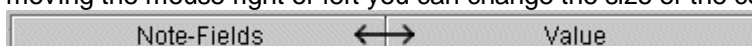
Opens a dialog box with the note fields of the spectrum currently displayed in the Result spectrum area.

Note-Fields	Value
Title	Cyclohexanol
NMR SPECTRUM	
Owner	COPYRIGHT (C) 1995 by Chemical Concepts
Input Date	Jan 03 1980 05:02AM
Literature	G.C. Lewy, R.A. Komoroski, Org. Magn. Resonance 7, 172 (1975).
Original No.	1:CN00::CNCC-29239-197L
Quality	100
Solvent	Neat liquid
SpecInfo ID	1:CN0000002021
Standard	TMS
Update Date	Feb 12 1995 09:17AM
Nucleus	<sup>13</sup> C
Instrument	Bruker WH-270
State	soluted
Temperature (K)	308

**Close**

Signed by:

Note, that all dialogs are resizable. Move the mouse pointer to the vertical divider. When the pointer changes to a small double arrow press the left mouse button and hold it down. By moving the mouse right or left you can change the size of the columns.



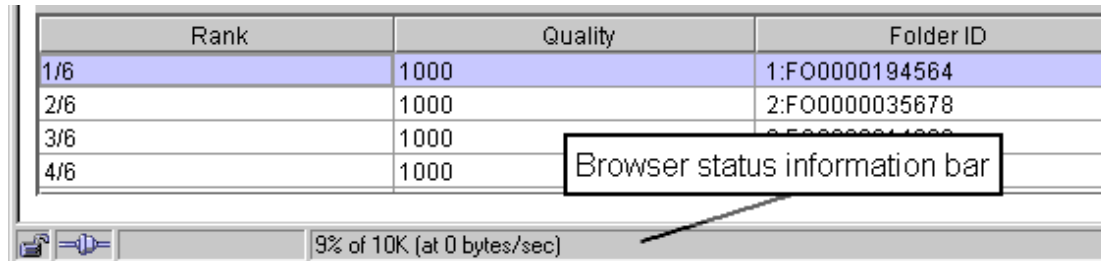
## Float menu

# Float menu

Shows structures, spectra, index, hitlist or the whole application in separate windows.

## Float all

The **Float all** option will detach the Java window from your browser. This allows you to change the scale of the SpecSurf window to any other than the default size. But note, after floating all you will lose the browser status information bar which gives you information about data transfer status. This bar is useful to see if a datatransfer was completed successfully or not.



Rank	Quality	Folder ID
1/6	1000	1:FO0000194564
2/6	1000	2:FO0000035678
3/6	1000	3:FO0000011999
4/6	1000	

Browser status information bar

9% of 10K (at 0 bytes/sec)

## Clear menu

# Clear menu

Clears structures or spectra in the Query or Result area. The clear All command clears everything inside the SpecSurf working area, including the hitlist.

## Settings menu

# Settings menu

The Settings menu commands are primary designed to organize the usage of databases. Additional functionality is given to adapt the online display to the user requirements. The following commands are available

Databases

Options

Spectrum display

Structure display

Optimize the settings for an optimal handling during a SpecSurf session. But note that settings are not stored when you leave SpecSurf.

# Databases

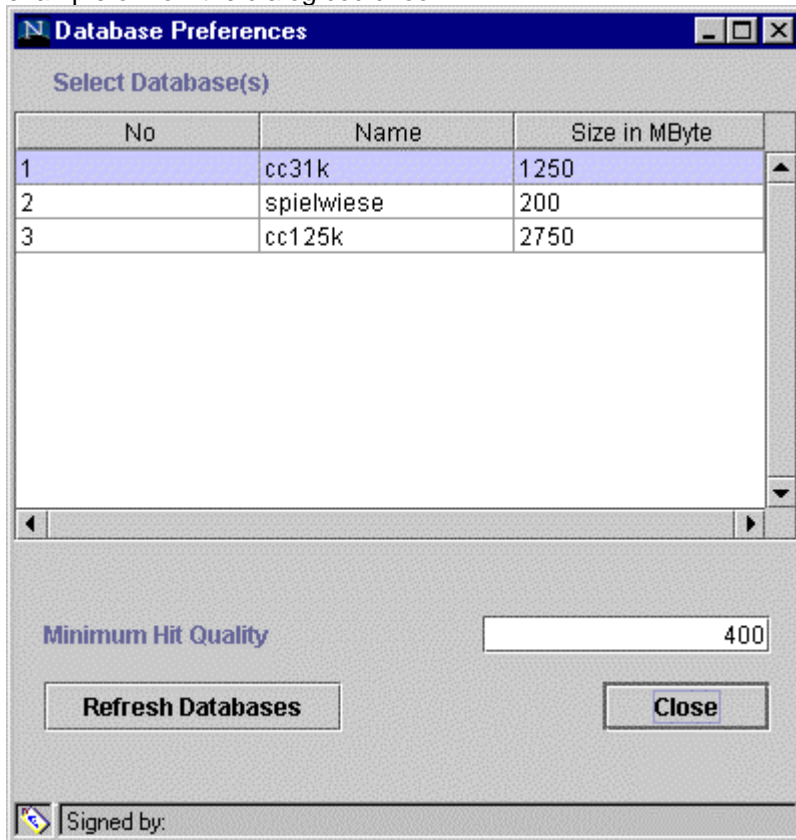
Set Settings/Databases: Searches

Shows all selectable databases for spectrum or structure search. Each database has an ID and an unequivocal name (External Name). Within this dialog you can define values for Maximum Number of Hits and Minimum Hit Quality. Change these values with care - a huge number of hits increases the connection time as well as a small quality value leads to a lot of unspecified hits.

### Set Settings/Databases: Predictions

Shows selectable databases for spectrum prediction. The more databases are selected the better is a prediction. No further options are available.

SpecSurf offers the possibility to select several databases at once. The figure shows an example of how the dialog could look.



To select more than one database use the standard keyboard/mouse combinations: Shift + left mouse button for sequential selection or Ctrl + left mouse button for a non-sequential selection.

## Options

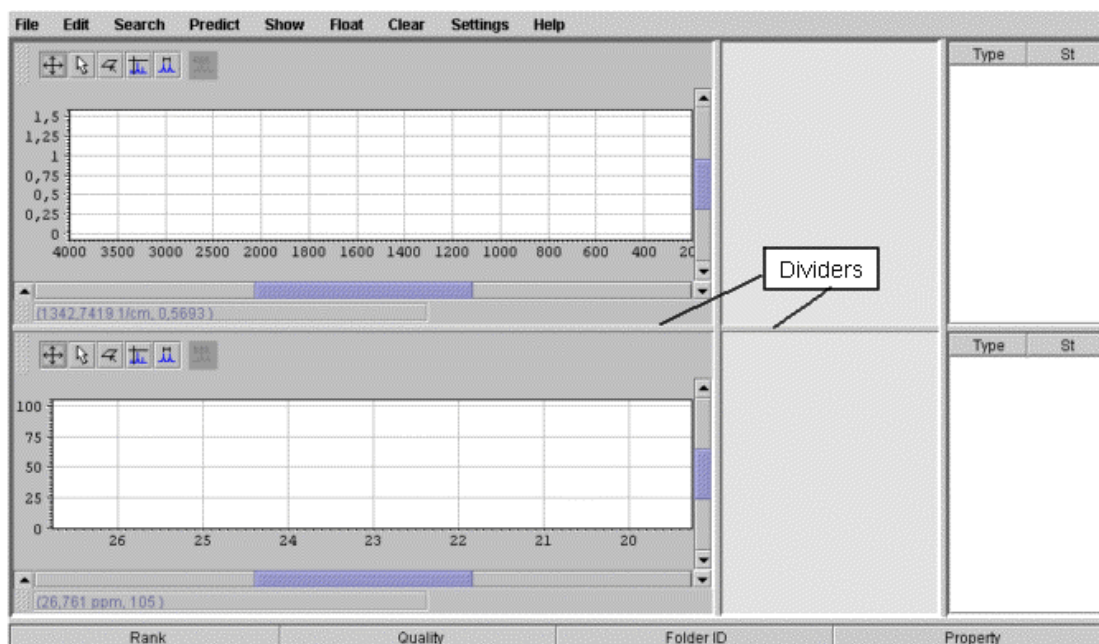
This command is available as the second one from the Settings menu.

### Get First Entry

If the select box is checked the first entry of a hitlist is automatically displayed.

### Synchronize Dividers

Synchronizes the movement of the dividers.



## Spectrum display

Shows a checklist with display attributes.

Show Grid	Hides or displays gridlines in the spectra.
Hide Status Line	Hides or displays the Status Line.
Synchro Zoom X	Shows a spectrum in the query as well as in the Result zone with identical x-axis zoom factors.
Synchro Zoom Y	Shows a spectrum in the query as well as in the Result zone with identical y-axis zoom factors.

A check mark (✓) on the left side of the command means the command is active. Click the command again to remove the check mark and to deactivate the command.

## Structure display

Shows a checklist with display attributes.

Hide Carbons	Hides the carbon element symbol.
Hide Numbers	Hides the atom numberings.
Hide Charge	Hides charge of a molecule.
Hide Carbon Auto-Protons	Hides the protons bonded to the carbon atoms except the explicitly added protons. Protons bonded to heteroatoms are always displayed.
Hide All Auto-Protons	Hides all protons except the explicitly drawn.

A check mark (✓) on the left side of the command means the command is active. Click the command again to remove the check mark and to deactivate the command.

## Help menu

## GUI overview

The Quick Start is designed to illustrate the workspace and to introduce the nomenclature of the most important working areas.

See the screenshot for further information.

The screenshot shows the software interface with three main sections:

- Query area (top):** Contains an 'Estimated spectrum' plot with 'Arbitrary Unit' on the y-axis (0 to 100) and 'ppm' on the x-axis (140 to 120). It also shows a chemical structure of 3-chloro-aniline (Nc1cccc(Cl)c1) and a table with columns 'Type' and 'St'.
- Result area (middle):** Contains a spectrum plot with 'Arbitrary Unit' on the y-axis (0 to 75) and 'ppm' on the x-axis (140 to 120). It shows the same chemical structure of 3-chloro-aniline and a table with columns 'Type' and 'St' containing entries for '13C', '15N', and 'ir'.
- Hitlist (bottom):** A table with columns 'Rank', 'Quality', 'Folder ID', and 'Property'. It contains one entry: Rank 1/1, Quality 1000, Folder ID 1:FO0000000039, Property 3-Chloro-aniline.

### GUI Overview

The Query as well as the Result area is divided into three main parts. Spectra are displayed on the left side whereas structures are located in the middle. The table on the right contains additional information about how many and what kind of objects are inside a folder.

### The Query area

Imported spectra or structures as well as manually created objects are located in the Query area. Objects of that area are searched against the selected database(s).

### The Result area

Contains the result folder.

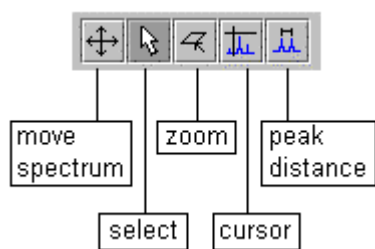
### The Hitlist

Any successful query, a spectrum search, a property search or a structure search result in a list of hits – called Hitlist. Listed are by default the sequential numbers, the quality (Ranking) factors and a descriptor like Title. Of these, the Rank is, perhaps, most interesting, since it tells you how well your query matches the found database entries. The value of the factor ranges from 1 to 1000 (best ranking). By default the first entry of a hitlist will automatically displayed in the Result area. When moving the pointer over a result and pressing the left mouse button a connection to the SpecInfo server will be established and the content of this folder will be displayed.

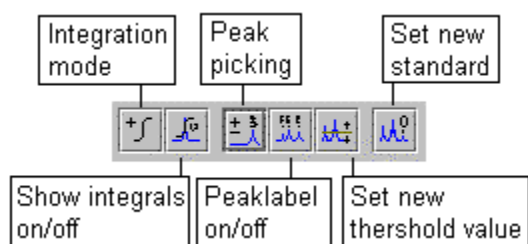
### The Icon bar

The view of the Icon bar depends on the type of spectrum.

Standard icons (are always available):



NMR-icons (only NMR spectra):



IR-icon

