

# Chemical Database Service (CDS)

## SpecSurf self-paced tutorial

This manual is intended for the novice user and covers getting started and the basic functionality of SpecSurf. The most up to date version can always be found on the CDS website at <http://cds.dl.ac.uk>.

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. It was designed to aid in structure elucidation, but has many more generally useful facilities.

SpecSurf is available to the UK academic community through the Chemical Database Service (see <http://cds.dl.ac.uk>).

The main features of the package are:

- (Sub)-structure searching – the ability to search the database for all spectra corresponding to a specified (sub)-structure.
- Spectrum prediction – the ability to predict a NMR spectra from a structure.
- Spectrum searching – finds the spectra from the database which most closely match the query spectrum.

The associated database now contains over 400,000 high quality spectra covering 8 spectroscopic techniques. The number of spectra for each technique is shown below.

Technique	<sup>13</sup> C NMR	<sup>15</sup> N NMR	<sup>17</sup> O NMR	<sup>31</sup> P NMR	<sup>19</sup> F NMR	<sup>1</sup> H NMR	IR	Mass spectra
Spectra	102,369	992	856	16,561	25,442	117,379	20,898	138,727

### Accessing SpecSurf

The SpecSurf interface is a Java applet and will run in most modern, Java enabled browsers. For access go to <http://cds.dl.ac.uk/specsurf> or follow the SpecSurf links from the CDS home page. You will be prompted for your CDS id and password and then see the following purple background screen.



## Welcome to SpecInfo on the Internet

A number of online demos illustrating the use of SpecSurf are available [here](#).

Please have a look at the [IllustratedGuide](#).

Screen Size

The applet has a size of about 500 kbyte and needs several minutes for the first download. Please allow some computation time after the download. You can follow this by watching your CPU usage meter on your task manager or system monitoring tool, generally CPU usage is 100% during this period.

Here there are important links to electronic help information about SpecSurf. The Illustrated Guide is an online guide to using SpecSurf, whilst the online demos contain a number of Flash-based movies demonstrating use of the program.

Press the Start SpecSurf button to begin. There will be a short delay whilst the applet downloads, and then you should see the main SpecSurf applet. Below is a screenshot, highlighting the main areas of the interface (query area, result area and hitlist area).

The screenshot displays the SpecSurf interface with three main areas highlighted by colored boxes:

- Query area (red box):** Shows an empty spectrum plot with an x-axis labeled 'ppm' (140, 130, 120) and a y-axis labeled 'Arbitrary Unit' (0, 25, 50, 100). The plot is titled 'Estimated spectrum'. To the right is a chemical structure of 3-chloro-aniline (Nc1cccc(Cl)c1) and a table with columns 'Type' and 'St'.
- Result area (blue box):** Shows a spectrum plot with an x-axis labeled 'ppm' (140, 130, 120) and a y-axis labeled 'Arbitrary Unit' (0, 25, 75). The plot is titled 'Estimated spectrum'. To the right is the same chemical structure of 3-chloro-aniline, but with a red 'C' label on the benzene ring. The table below it has columns 'Type' and 'St' and contains the following data:

Type	St
13C	st
15N	st
ir	
- Hitlist area (green box):** A table with columns 'Rank', 'Quality', 'Folder ID', and 'Property'. It contains one entry:

Rank	Quality	Folder ID	Property
1/1	1000	1:FO00000000039	3-Chloro-aniline

Selecting Help Index from the Help menu opens a new browser window and presents you with the online help system for SpecSurf.

Contents		Index	Search
[-]		Specsurf	
		Introduction	
		Spectrum handling and icons	
		Dialogs	
		Zoom	
		Security	
[-]		Tutorial	
		Create a spectrum	
		search spectrum	
		<b>Draw a new structure</b>	
		Using the Database based pr	
		Using the Rule based predict	
		Using the Search Structure c	
		Substructure search	
		Using the Search Note Fields	
[+]		File menu	
[+]		Edit menu	
[+]		Search menu	
[+]		Predict menu	
[+]		Show menu	
[+]		Float menu	
[+]		Clear menu	
[+]		Settings menu	
[+]		Help menu	

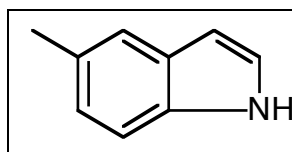
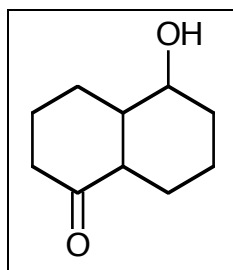
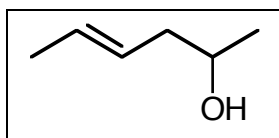
Click on the + icon next to SpecSurf and then Tutorial, to open up the tutorial index as shown above. Go through sections 3 (Draw a new structure), 4 and 5, then you will be equipped to work through the training examples 1 to 3 below. Next read sections 1,2 and 6, then try examples 4-6 below.

If you have trouble with any of the examples, see the next page for hints about how to approach each problem. Once you are comfortable with the examples try the structure solving problems on the last page.

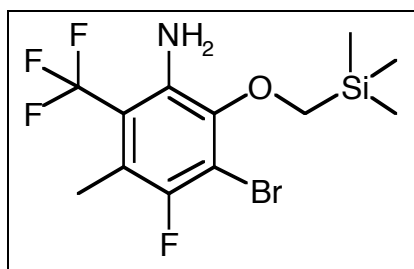
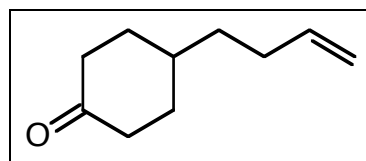
If you have any difficulties, please contact the Chemical Database Service, [cdsbb@dl.ac.uk](mailto:cdsbb@dl.ac.uk) or 01925 603162.

## SpecSurf Training Examples

1. Draw the following structures using the structure generator



2. What is the  $^{13}\text{C}$  NMR shift of the terminal  $\text{CH}_2$  group of this molecule?



3. Run a database based  $^{13}\text{C}$  NMR prediction on this compound. What can you say about the quality of the prediction and why is this the case?

4. The following  $^{13}\text{C}$  NMR spectrum was recorded for a simple alkane sample.

Shift (ppm)	Multiplicity	Relative intensity
11.5	quartet	0.51
22.0	quartet	1.0
30.0	doublet	0.46
31.5	triplet	0.48

Find the structure of the sample.

5. A chemist has synthesised one of the geometric isomers of 2-buten-1-ol. What spectral differences will help the chemist decide which isomer is present ?

6. What spectra are available for acetaldehyde ?

## Hints for training examples

2. You can choose between predication and estimation of the spectrum.
3. Notice the number of missing values in the prediction data. Compare with an estimation of the spectrum.
4. Try a <sup>13</sup>C-NMR spectra search using the data provided.
5. Run a CNMR prediction for the two isomers and look for different shifts, or run a structure search and examine the spectra available for the two isomers.
6. A structure search is most reliable. Don't forget to check each hit, which may have more than one spectrum.

## SpecSurf structure solving problems

Find the most likely structure given the following spectral data

1) Significant MS peaks at 29 43 57 72.

C-13 NMR signals, quartets at 8 and 29 ppm, triplet at 36.5 ppm and singlet at 207.6 ppm.

2) Significant MS peaks at 29 77 105 148.

C-13 NMR signals

Position(ppm)	Intensity	Multiplicity	Position(ppm)	Intensity	Multiplicity
19	2	Q	132	1	D
35	1	D	136	1	S
128	2	D	204	1	S
129	2	D			

3) Significant MS peaks at 121 134 194.

C-13 NMR signals

Position(ppm)	Intensity	Multiplicity	Position(ppm)	Intensity	Multiplicity
28	1	T	129	2	D
35	1	T	133	1	S
50	1	Q	159	1	S
53	1	Q	174	1	S
114	2	D			