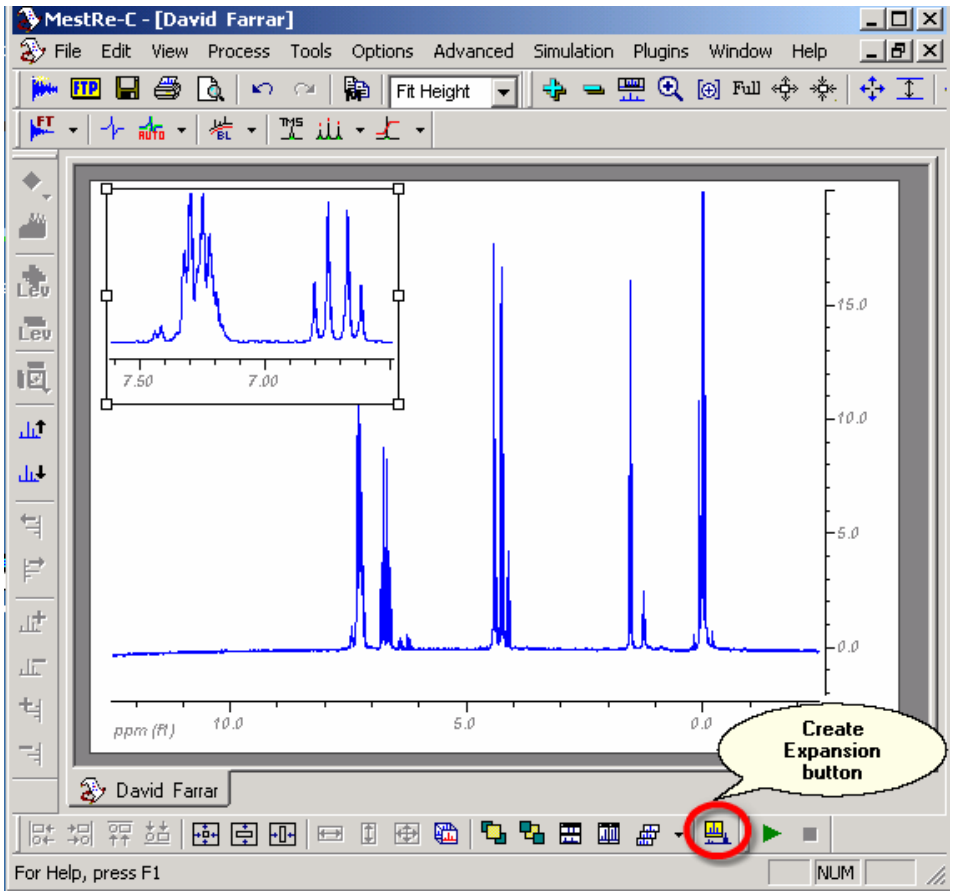
What's new in MestRe-c 3.4.0

Create expansions with a single mouse click!

In the previous versions of MestRe-C, the procedure needed to plot multiple regions of the same spectrum on one plot was somewhat cumbersome. Now you can do it with a single mouse click! Once the desired spectral region is displayed, click on the expansion toolbar button (see below). That's it!

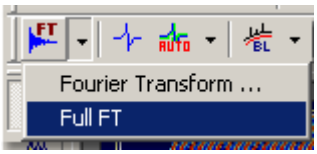


Automatic creation of stacked plots of 1D spectra

Even though the program already included a stacked plot routine for arrayed experiments, sometimes it is necessary to create stacked plot of individual 1D spectra. This option is now included in this new version.

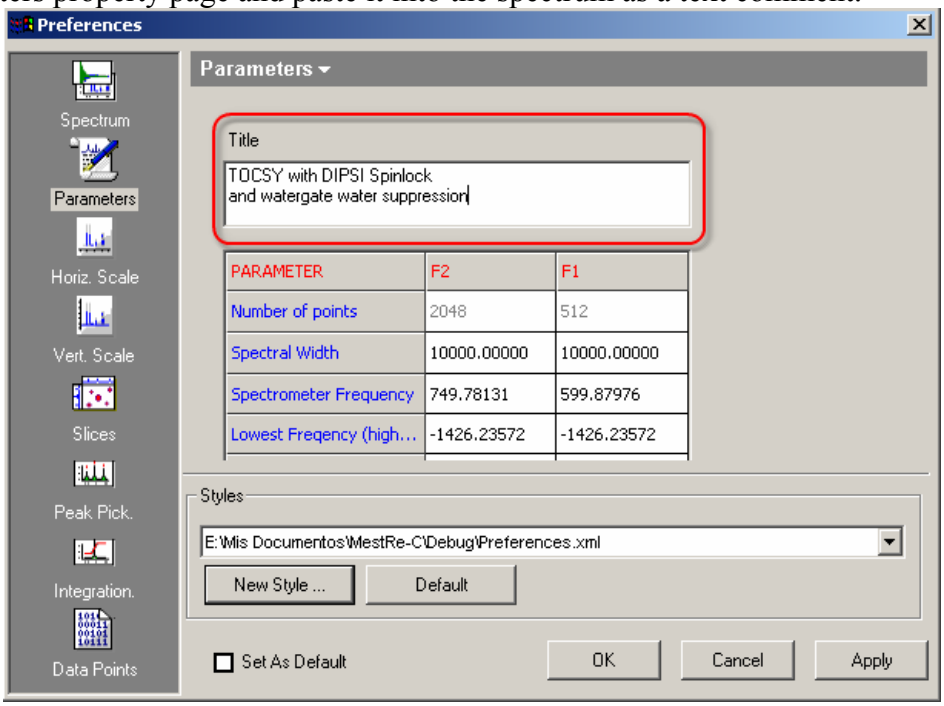
Full FT

This command is intended to automatically transform a 2D spectrum from the time domain to the fully transformed frequency domain. The program uses the default values read from the parameters file.



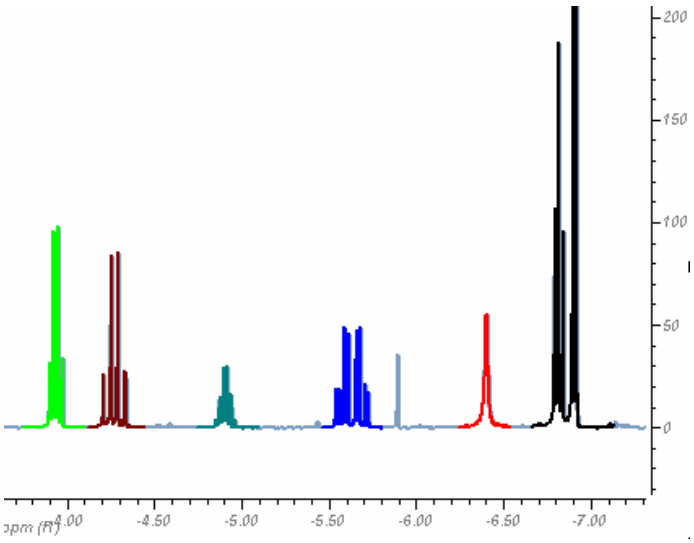
Comment/Title

We have received a great deal of requests to make the program to be able to read the 'title' (Bruker) or the 'text' (Varian) files. Well, this feature is now incorporated into this new version. Moreover, you can edit the spectrum title from the spectrum parameters property page and paste it into the spectrum as a text comment.



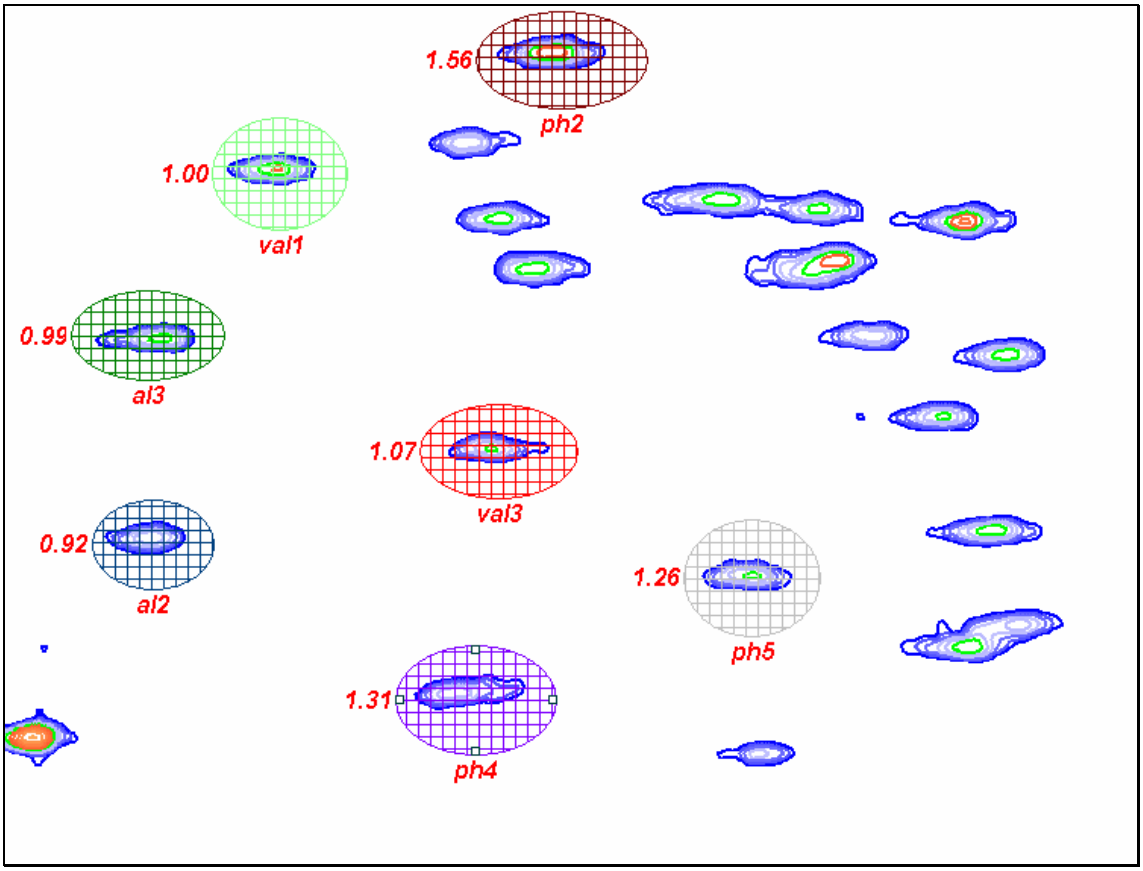
Marking peaks with different colors

I believe a picture worth a thousand words …



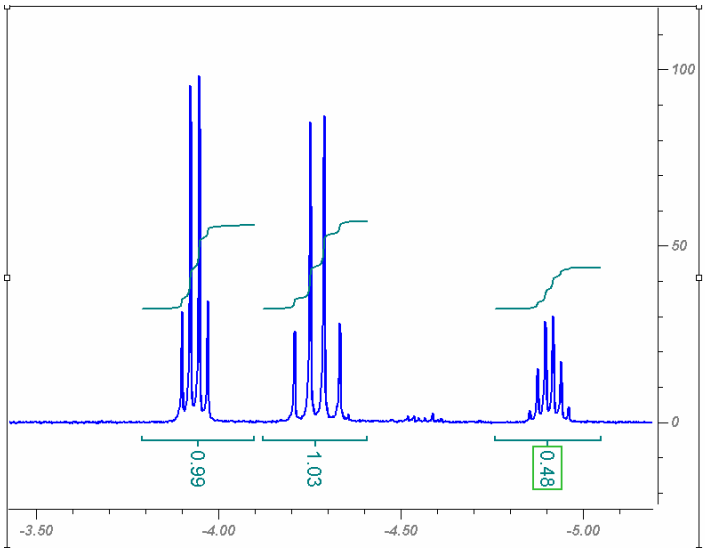
To create such a spectrum, you need to integrate each region you want to draw using a different color. Then go to “List integrals”, select the color you wish for each interval and check the “Fill” button.

In the case of 2D spectra, if you follow the same procedure you can achieve effects like this:



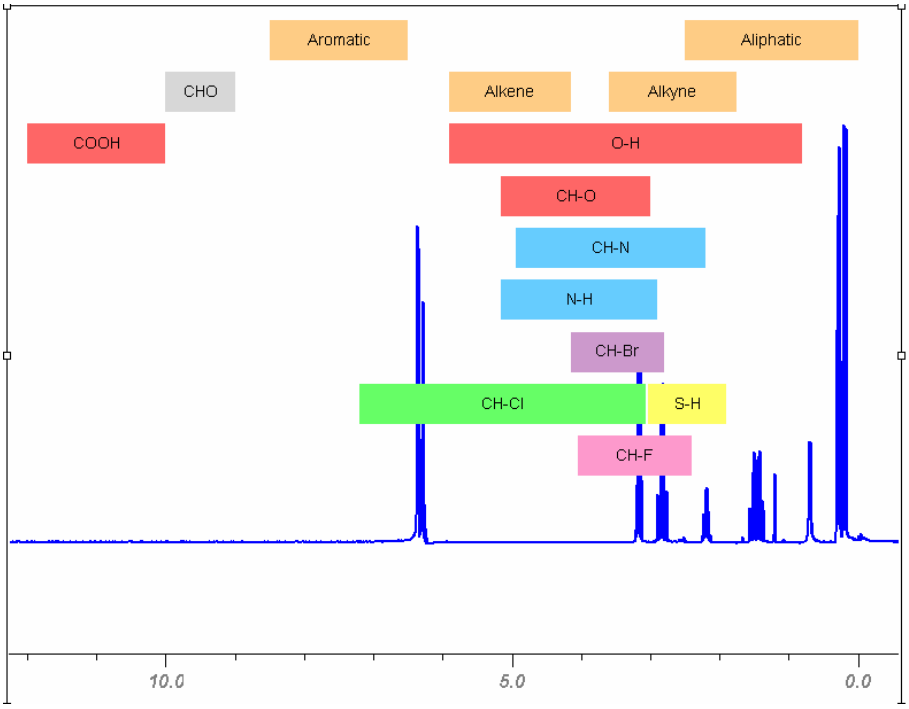
Integration labels are now displayed vertically

In order to avoid labels overlap, now the numerical values are displayed vertically.

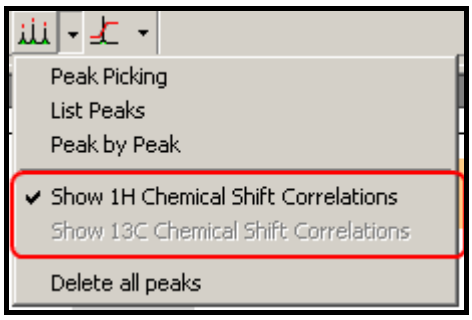


Simple chemical shift correlation (experimental)

Very simple chemical shift correlation (1H and 13C) can be displayed along with the spectrum.



This option is available from the Peak-Picking menu bar:



Other new features:

- ✓ Export metafile to disk.
- ✓ The Bruker converter is now more 'intelligent'. It has been rewritten in order to improve the automatic detection of phase-sensitive protocols of indirect dimensions. This means that you will not need to know anything about TPPI, Ruber-States, Echo-antiecho, etc … to be able to process a phase sensitive experiment.
- ✓ Text labels: now the program 'remembers' the settings used for the text comments.