

My experience using Sparky to integrate peak volumes in 2-D NMR spectra (by Dave H.):

Open the integrate settings panel by typing "it"

I have been getting reproducible and believable results using the following settings:

|                                 |   |              |
|---------------------------------|---|--------------|
| Integration method              | = | Gaussian fit |
| allow peak motion               | = | yes          |
| adjust linewidths               | = | yes          |
| fit baseline                    | = | yes          |
| subtract off fit peaks          | = | no           |
| use data above lowest contour   | = | no           |
| use data within rectangle       | = | yes          |
| group peaks in contour boundary | = | yes          |
| group close peaks               | = | yes          |
| maximum motion (ppm)            | = | 0.01, 0.01   |
| linewidth minimum (Hz)          | = | 2.0, 2.0     |
| linewidth maximum (Hz)          | = | 80.0, 80.0   |
| grouping range (Hz)             | = | 30.0, 30.0   |
| maximum minimization steps      | = | 10000        |
| minimization tolerance          | = | 0.1 %        |

Procedure:

Pick peaks to be integrated by selecting "Find/add peak" in the pointer mode box.

Next, set the pointer mode box to "integrate".

Next, use the mouse to define a box around the peaks to be integrated. The regions within the box that are not defined as peaks will be used to determine the baseline. A correction will be made for a non-zero baseline.

To view progress of the integration, under the "peak menu" select "peak list" (the shortcut for this is "lt").

The output from the peak volume integration can be sent to a text file as follows:

In the "peak list" box (that appears when "lt" is typed), select "options", then select "frequency", "volume", "linewidth", and sort by frequency. Save the peak list, which will include the volumes, as a text file.