

## Integrating Peaks with NMRFAM-Sparky Macro Methods 2017

1. Navigate to the spectrum you would like to integrate peaks for. Be sure the peak labels are displayed and the contour level has been set to an appropriate cutoff so the resonances are clearly observed.

2. Type **it** and a peak integration window will appear (shown at left). Change the check boxes and values in the window so it matches those shown:

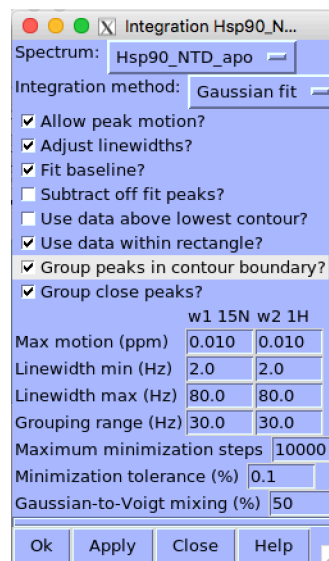
*Note:* Be sure to select the proper spectrum each time since you can apply different settings to individual spectra.

3. Click **Apply**.

4. Navigate to the Pointer Mode window and switch to *integrate* (hold the function key and type F10).

5. Click and draw a box around the peaks you would like to integrate. Once you release the mouse, Sparky will begin calculating the volume. This may take a few minutes to complete but you can tell when the integration is done when a circle appears around the peak (as shown in the screenshot for L207N-H).

6. In order to record the peak volumes, display the peak list by typing **lt** and click **Options**. A separate window will appear with a variety of variables to include in the peak list. Check the box next to Volume and click **Apply**. The peak list should now be populated with an additional column containing the calculated volume for a given peak:



Assignment	w1	w2	Volume
L185N-H	111.214	7.280	2.91e+06 ga
E186N-H	117.766	7.483	2.23e+06 ga
E187N-H	127.665	9.104	1.66e+06 ga
K188N-H	126.955	8.911	2.86e+06 ga
R189N-H	120.117	6.932	2.01e+06 ga
L190N-H	118.805	8.161	1.96e+06 ga
K191N-H	116.798	8.511	1.19e+06 ga
E192N-H	119.818	7.694	2.53e+06 ga
V193N-H	120.950	8.660	8.01e+06 ga
L194N-H	119.935	8.397	2.75e+06 ga
K195N-H	119.452	7.919	2.45e+06 ga
R196N-H	115.889	7.528	1.54e+06 ga
H197N-H	115.480	7.742	1.28e+06 ga
S198N-H	115.970	8.457	8.03e+05 ga
E199N-H	121.511	8.859	2.17e+06 ga
F200N-H	114.809	8.854	1.49e+06 ga
V201N-H	122.685	7.234	1.88e+06 ga
K202N-H	129.718	8.951	1.51e+06 ga
V203N-H	116.717	6.728	2.10e+06 ga
L205N-H	121.436	7.995	0.89e+06 ga
O206N-H	128.925	9.578	1.07e+06 ga
L207N-H	129.238	7.733	1.93e+06 ga

7. Click **Save** to write the peak list. As is the case for moving peaks, any time you re-integrate a peak, be sure to click **Update** and re-save the list.