

Displaying ellipses in Sparky



The screenshot shows a window titled "testm.save" containing a text-based configuration file for Sparky. The file includes various parameters for processing NMR spectra, such as integration methods, motion ranges, and peak picking thresholds. A red arrow points from the text "insert code for ellipses here in Sparky .save file" to the line "<end ornament>".

```
integrate.methods 1 0 1
integrate.allow_motion 1
integrate.adjust_linewidths 1
integrate.motion_range 0.040 0.010
integrate.min_linewidth 0.0133 0.0033
integrate.max_linewidth 1.3252 0.3333
integrate.fit_baseline 0
integrate.subtract_peaks 0
integrate.contoured_data 1
integrate.rectangle_data 0
integrate.maxiterations 10000
integrate.tolerance 0.001000
peak.pick 0.000000 0.000000 0.000000 0
peak.pick-minimum linewidth 0.000000 0.000000
peak.pick-minimum-dropoff 0.00
noise.sigma 744251.000000
ornament.label.size 2.500000
ornament.line.size 0.400000
ornament.peak.size 1.200000
ornament.grid.size 0.400000
ornament.peakgroup.size 0.800000
ornament.selectsize 0.500000
ornament.pointersize 0.500000
ornament.lineendsize 0.500000
<attached data>
<end attached data>
<view>
name TASLlanneal_090430_303K_D20_700_6_hsqc13C
precision 0
precision_by_units 0 0 0
viewmode 0
show 1 label line peak grid peakgroup
axisstype 2
flags crosshair crosshair2
contour.pos 20 4e+06 1.400000 0.000000 red-blue
contour.neg 20 -4e+06 1.400000 0.000000 purple
<params>
orientation 1 0
location 315 446
size 500 500
offset 92.324284 479.000003
scale 1.000000 0.748696
zoom 2.344901
flags 0
<end params>
<params>
orientation 1 0
location 315 446
size 500 500
offset 92.324284 479.000003
scale 1.000000 0.748696
zoom 2.344901
flags 0
<end params>
<params>
orientation 1 0
location 315 446
size 500 500
offset 92.324284 479.000003
scale 1.000000 0.748696
zoom 2.344901
flags 0
<end params>
<end view>
<ornament>
<end ornament>
<end spectrum>
```

insert code
for ellipses
here in Sparky .save file

For each ellipse a separate text file is available, e.g.
C8H8_GG.txt will display the GGX ellipse in the ^{13}C -HSQC.
For the 2D TOCSY ellipses above the diagonal (H5H6_XX.txt) and
below the diagonal (H6H5_XX.txt) are given