Signal to Noise Calculation in 2D Spectrum

Written by Markus Voehler, January 17, 2013

2D sino requires a 2D signal region and a 2D noise region stored in an "int2drng" formatted file according to the following example:

```
0 0
a 512 90 112 125.456032 124.324229  ⎤
  1024 314 336 8.865432 8.739681    ⎦ Signal of interest
a 512 100 419 124.933661 108.740169 ⎤
  1024 65 260 10.322998 9.179809    ⎦ Noise region
```

Format description of int2drng file:

Mode	SI_F1	row1	row2	row1(ppm)	row2(ppm)
	SI_F2	col1	col2	col1(ppm)	col2(ppm)

Integration:

You may setup the file by hand, by a program, or most comfortably in the 2D integration mode:

1) Open a 2D spectrum in TopSpin

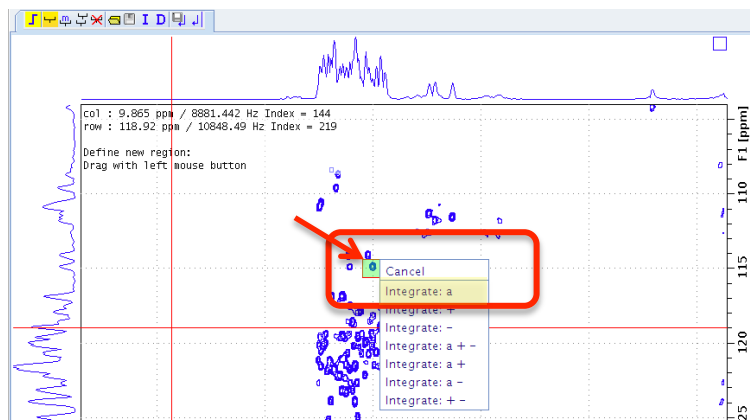2) Enter interactive integration mode using a menu entry or tool button or by entering the command ".int".
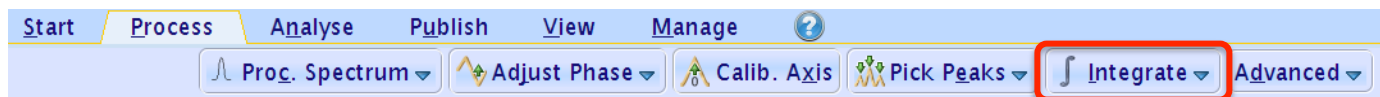
3) Click on the tool button "delete all regions" to start from scratch. Confirm to delete all integral regions.

4) Click on the tool button "define new integration region"

5) **First Integrate the signal of interest**: Drag a region around a signal while keeping the left mouse button depressed. When the button is released, a popup menu is opened. Click on an "integrate" entry, e.g. the first one (which one doesn't matter).

6) **Then define the noise area**: Move the mouse to a signal-free region and drag again the mouse to mark the region. Again click on an "integrate" entry when releasing the left mouse button.

7) Click on the diskette icon and select "Export integration regions".
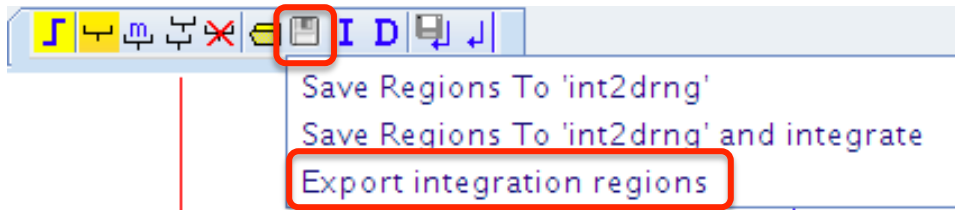
8) The "wmisc" window is opened. Click on "Write new...". Enter a filename. The file is stored in the .../list/intrng2d directory, which can be inspected using the "rmisc" command.
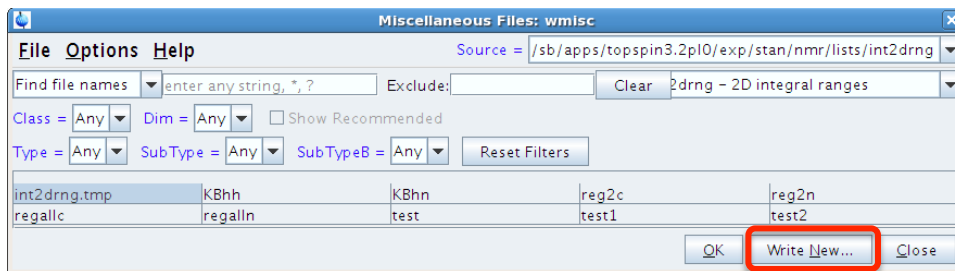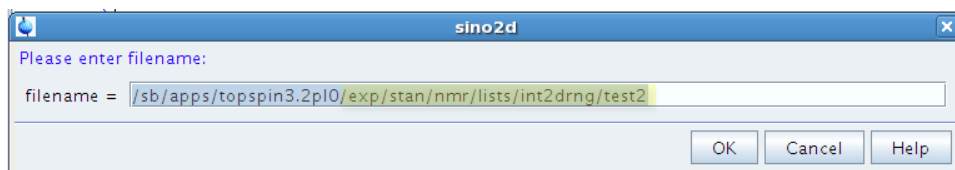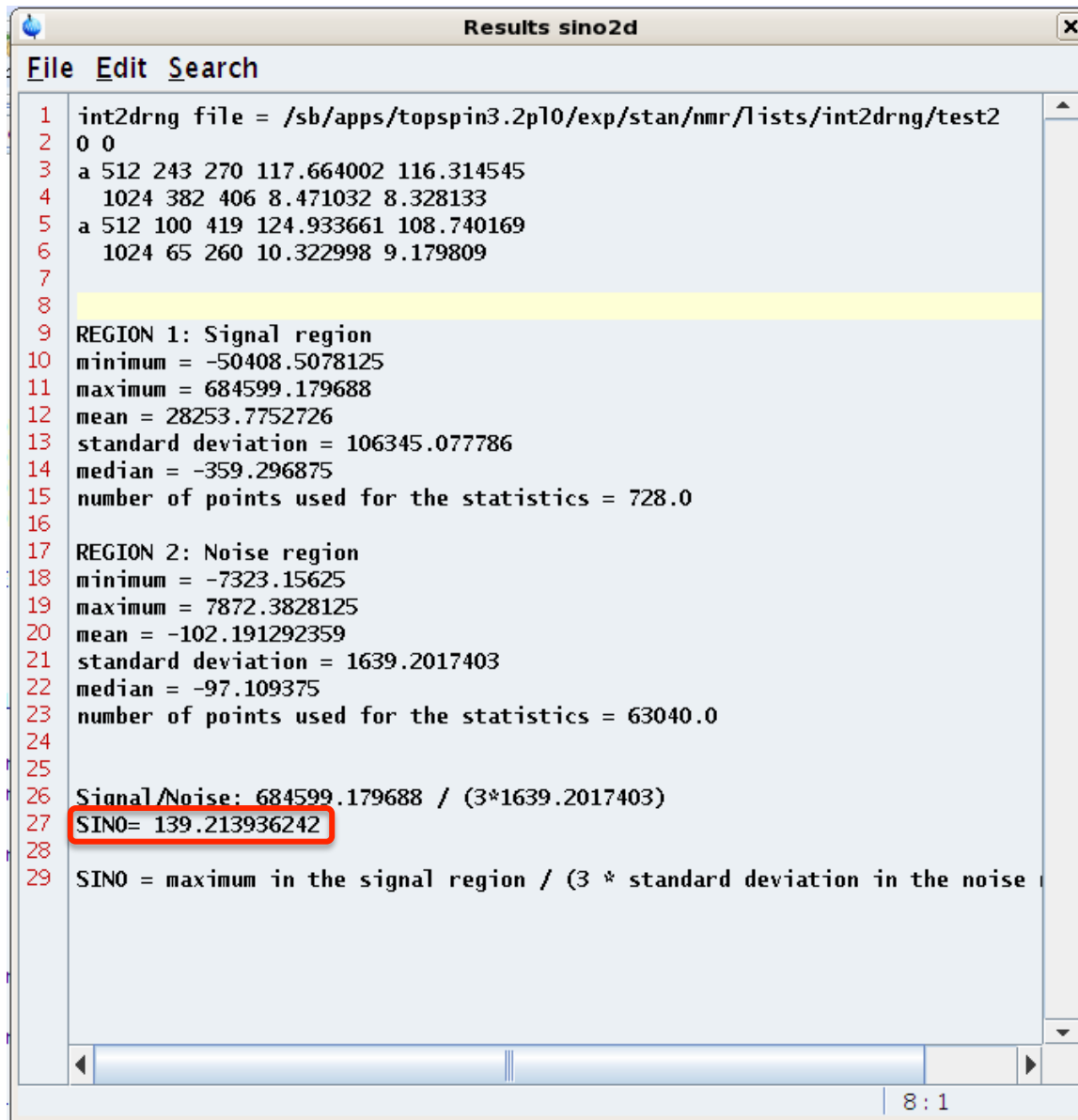

9) Exit the integration mode
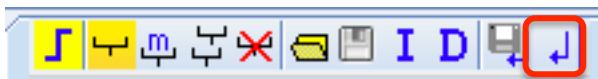
Perform 2D-SINO Calculation:

10) Start the python program sino2d.py, either by typing "sino2d.py" into the command line, or by typing "xpy 2dsino".

11) 2dsino requests the region file. Enter the filename you used in 8) (e.g. by completing the proposed path) and hit OK.

12) The result is displayed in a text window, which allows you to store the result in a file.

```
Results sino2d                                    ✕

File  Edit  Search

 1  int2drng file = /sb/apps/topspin3.2pl0/exp/stan/nmr/lists/int2drng/test2
 2  0 0
 3  a 512 243 270 117.664002 116.314545
 4    1024 382 406 8.471032 8.328133
 5  a 512 100 419 124.933661 108.740169
 6    1024 65 260 10.322998 9.179809
 7
 8
 9  REGION 1: Signal region
10  minimum = -50408.5078125
11  maximum = 684599.179688
12  mean = 28253.7752726
13  standard deviation = 106345.077786
14  median = -359.296875
15  number of points used for the statistics = 728.0
16
17  REGION 2: Noise region
18  minimum = -7323.15625
19  maximum = 7872.3828125
20  mean = -102.191292359
21  standard deviation = 1639.2017403
22  median = -97.109375
23  number of points used for the statistics = 63040.0
24
25
26  Signal/Noise: 684599.179688 / (3*1639.2017403)
27  SINO= 139.213936242
28
29  SINO = maximum in the signal region / (3 * standard deviation in the noise

                                                          8:1
```