Not So Short Introduction To TopSpin

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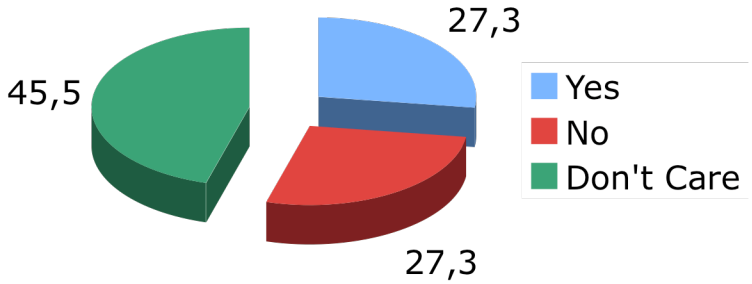
TopSpin:

The Next Generation of NMR Data Processing Software

1) new software package for acquisition, processing and analyzing NMR data, streamlined for your convenience
2) **TopSpin** was designed for Windows® and Linux® users with a highly intuitive interface
3) Java™ Technology - this superior programming language, which evolved in the past half decade, ensures the platform independence of **TopSpin** on the one hand, while providing for increased programming productivity on the other
4) may run under Windows 2k/XP, or Red Hat Enterprise Linux WS 3
5) according to survey done by KK people do not like TopSpin more than XWinNMR but neither the other way around!

Do you like TopSpin more than XWinNMR? 22 respondents!!!



A) Starting TopSpin

i) type **`xhost +`**, or type **`xhost +bloch`**
ii) i) doesn‘t work, type **`/usr/X11R6/bin/xhost +`**
iii) **`hostname`**
iv) **`ssh bloch`**
v) on bloch type **`setenv DISPLAY $hostname:0.0`**
vi) **`echo $DISPLAY`**
vii) **`topspin`**

```
dione.nmr.mpibpc.mpg.de:kaku > xhost +
access control disabled, clients can connect from any host
dione.nmr.mpibpc.mpg.de:kaku > xhost +bloch
bloch being added to access control list
dione.nmr.mpibpc.mpg.de:kaku > hostname
dione.nmr.mpibpc.mpg.de
dione.nmr.mpibpc.mpg.de:kaku > ssh bloch
Password:
Last login: Mon Jan 23 15:13:41 2006 from dione.nmr.mpibpc.mpg.de
Have a lot of fun...
Directory: /home/kaku
Have a lot of fun...
Directory: /home/kaku
Mon Jan 23 15:44:57 CET 2006
bloch:kaku > seten
setenforce  setenv
bloch:kaku > setenv DISPLAY dione.nmr.mpibpc.mpg.de:0.0
bloch:kaku > echo $DISPLAY
dione.nmr.mpibpc.mpg.de:0.0
bloch:kaku > topspin
CPR : Path to prog : "/opt/topspin/prog"
CPR : Path to exp  : "/opt/topspin/exp"
CPR : Path to conf : "/opt/topspin/conf"
```

B) TopSpin is on strike and doesn‘t work!

Unfortunately too many things can be wrong, hence go ahead and resolve them on your own

1) can‘t connect to X11 window server using ‚$hostname‘ as the DISPLAY variable

⇒ probably you‘ve set your display wrong, check it as shown at point **vi)** on previous slide

2) a session with your id is already running.

⇒ type **`ps -aux | grep kaku`** - lists processes for kaku, if TopSpin appears kill it with prefix -9: **`kill -9 11276 11281`** (11276 and 11281 are two jobs with TopSpin)

⇒ than type what suggested by TopSpin, namely /opt/topspin/prog/bin/shmrm

⇒ type topspin again, if problems with running session are still occuring, repeat ALL what‘s written in point 2) and additionally, type:
`rm -r /opt/topsin/prog/curdir/kaku` kaku just in case you‘re logged in as me ...

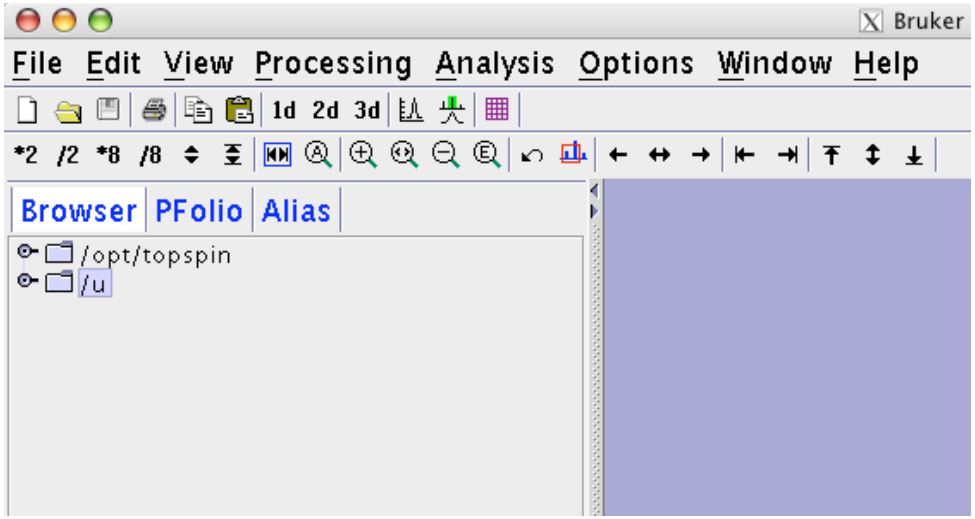
In case anything else happens, don‘t blame me but (you can) look for me, chfa or whoever more experienced with TopSpin than you! Generally, after this steps, TopSpin works, but as Forrest Gump is saying ...

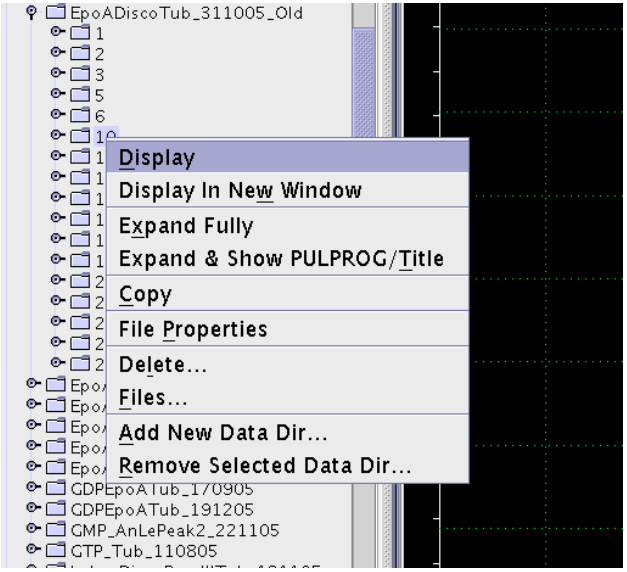
C) Opening spectra

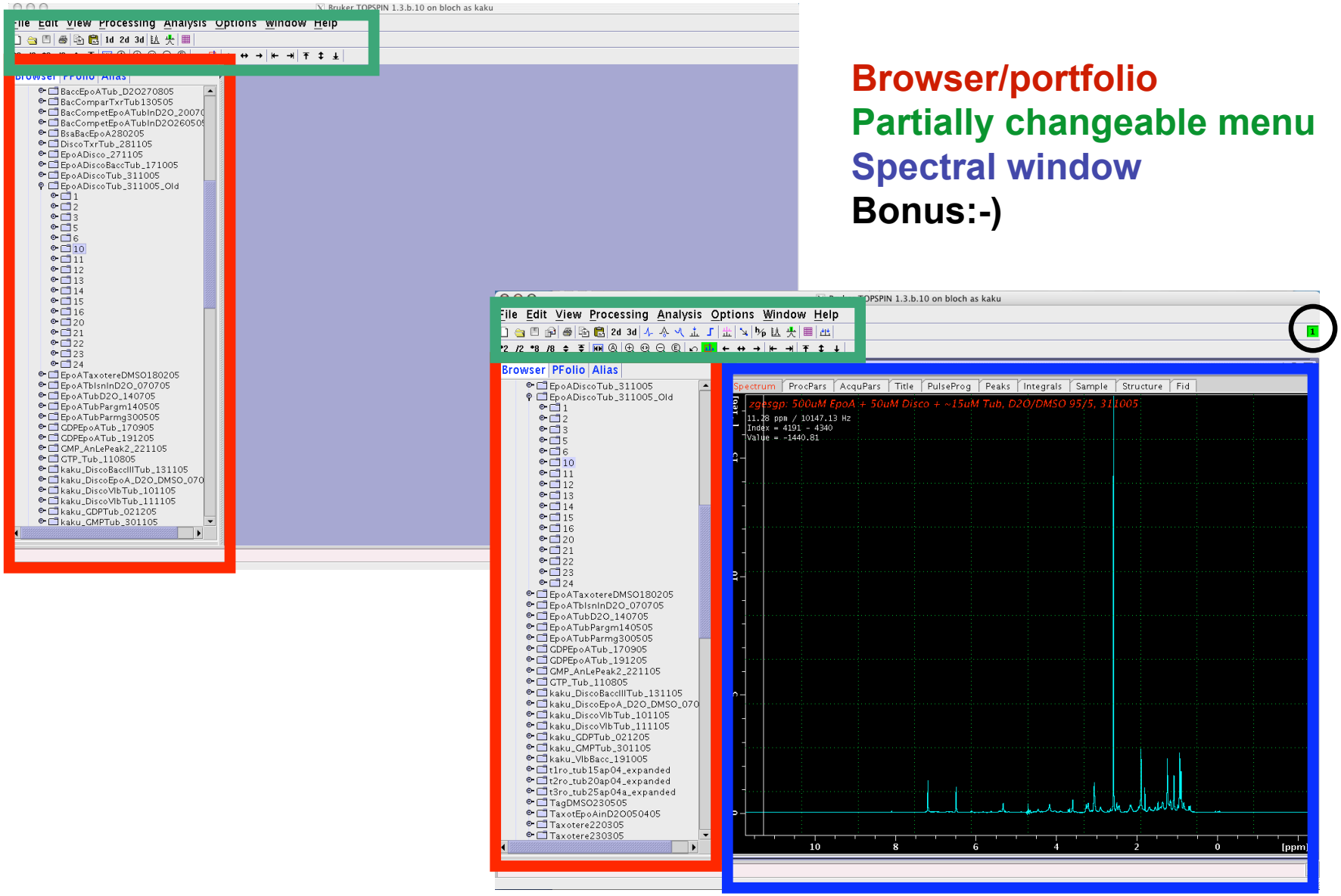
Easy and rather straightforward:

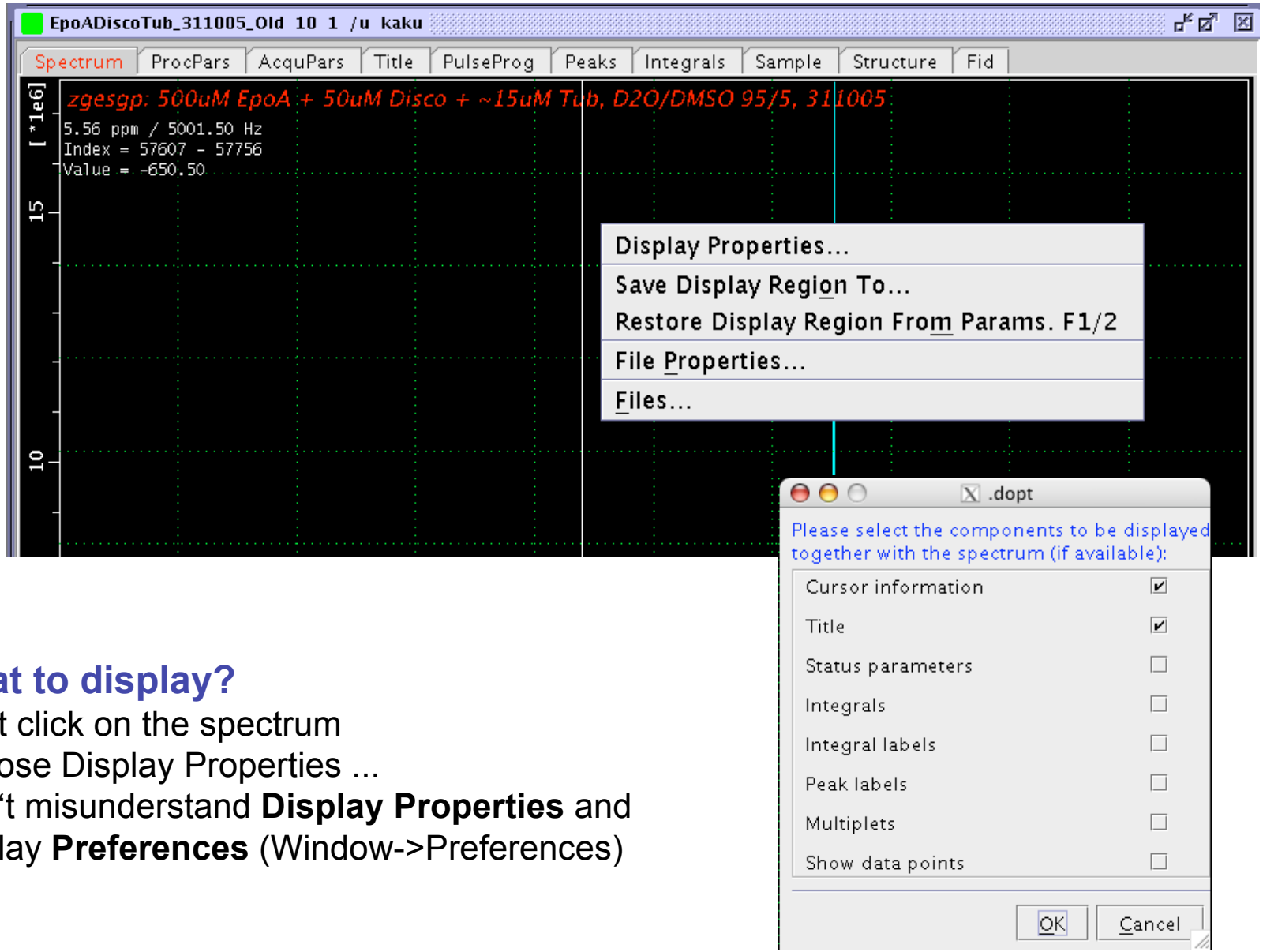
a) type ‚**re**‘ as you‘re used from XWinNMR
b) double click on epxno in the tree structure of your directory list
c) drag the expno and drop it on the display next to the tree structure
d) right click on the chose expno and selecting ***Display*** option

⇒ ***Spectrum will appear*** (see next slide)
⇒ a-d) work the same for 1-3D






Browser/portfolio
Partially changeable menu
Spectral window
Bonus:-)
File Edit View Processing Analysis Options Window Help
Browser PFolio Alias
Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Fid
zgesgp: 500uM EpoA + 50uM Disco + ~15uM Tub, D2O/DMSO 95/5, 311005
11.28 ppm / 10147.13 Hz
Index = 4191 - 4340
Value = -1440.81
10
8
6
4
2
0
[ppm]

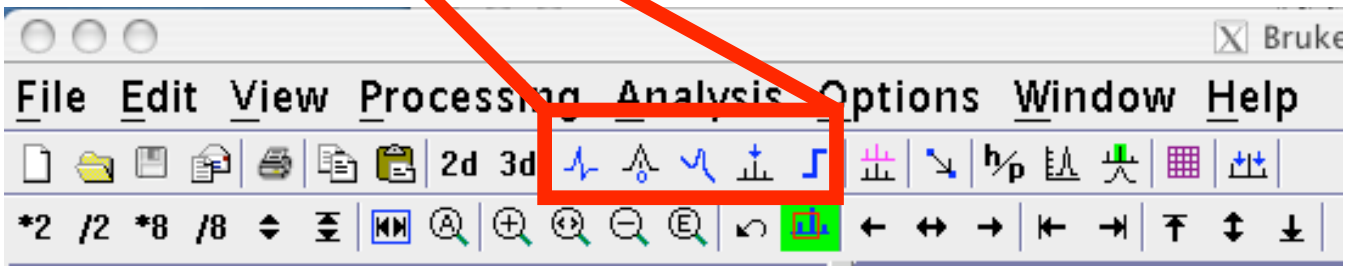


What to display?

-right click on the spectrum
-choose Display Properties ...
-don‘t misunderstand **Display Properties** and Display **Preferences** (Window->Preferences)

D) Processing spectra

.works the same way as in XWinNMR, but some exceptions are there
.commands like **`fp, qsin, efp, xfb, xfb n, abs[ 12]`** are working
.some of the commands are changed - **`apk`** => **`apkf`**, not sure if **`abs`** doesn‘t do something more than in XWinNMR
.phasing, calibrating, integrating and peak-picking - so similar and still so different

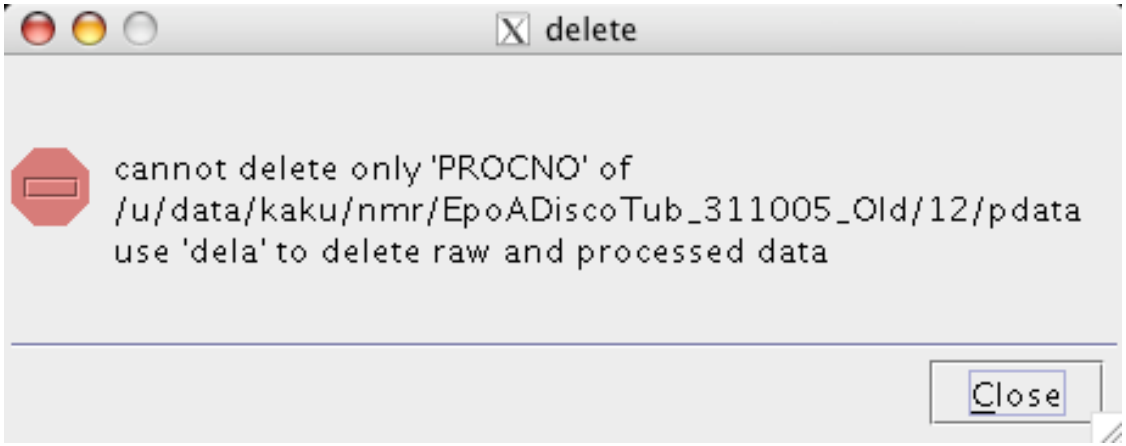


Troubleshooting

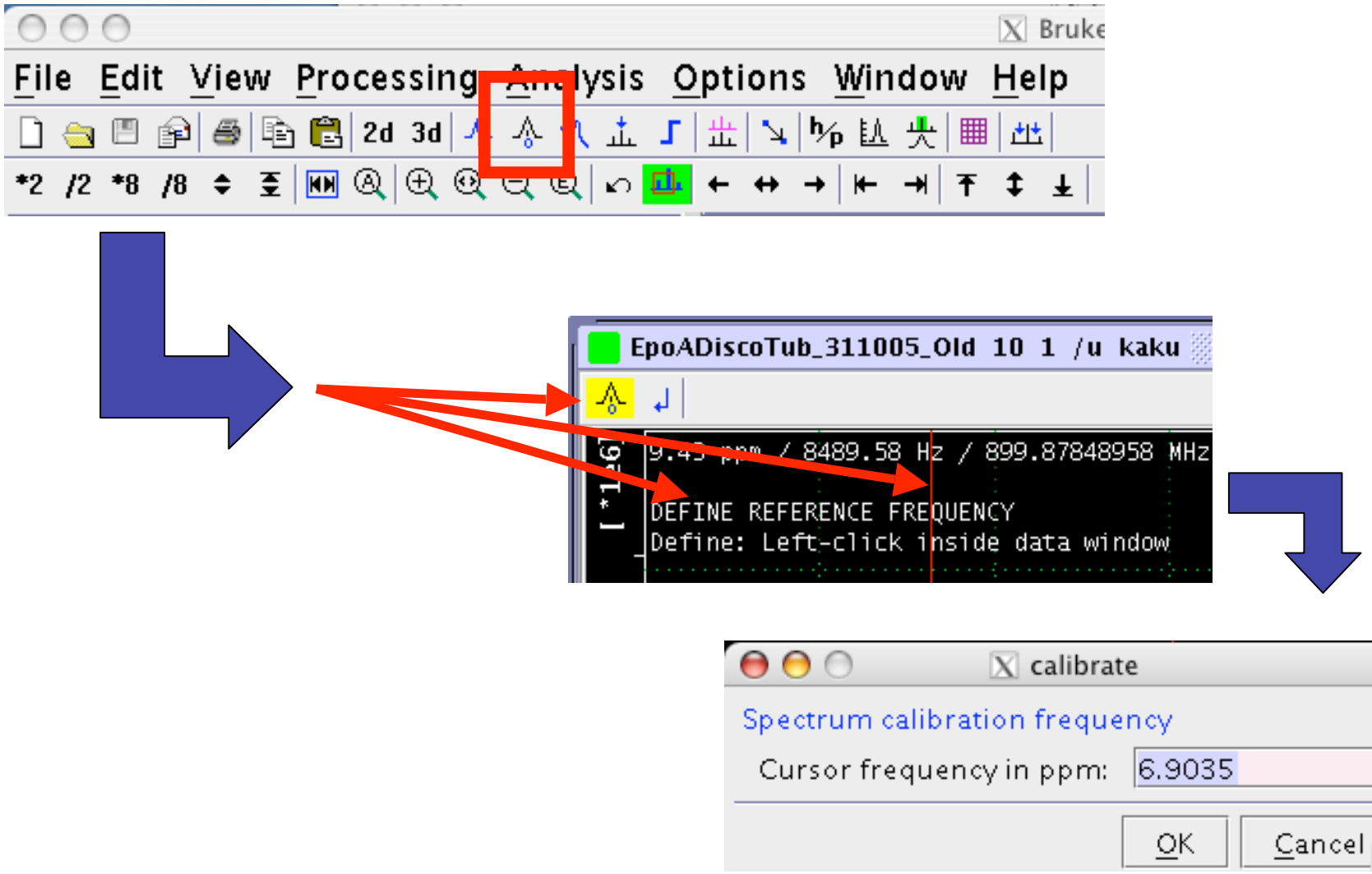
??? processing doesn‘t work
⇒check your ser-file size: if your data is 4k*512 points, the size of the ser-file should be 4k*512*4=8388608

??? processed data are not displayed properly
⇒type **`delp`** to remove any processed parts of your spectrum (2rr, 2ri, 2ir, 2ii) and process the spectrum once again
⇒If the data are still processed badly and you expect to see something else, go to pdata directory **[**/*disc*/**data**/*user*/**]nmr**/*dataset*/*expno*/**pdata**/**1**/ and remove the 2/3* processed files by hand by typing **`rm 2rr 2ri 2ir 2ii`** and than **`rm *dsp* -`** by this you‘re not going to loose your acquisition data, just the processed part, but be **CAREFUL**

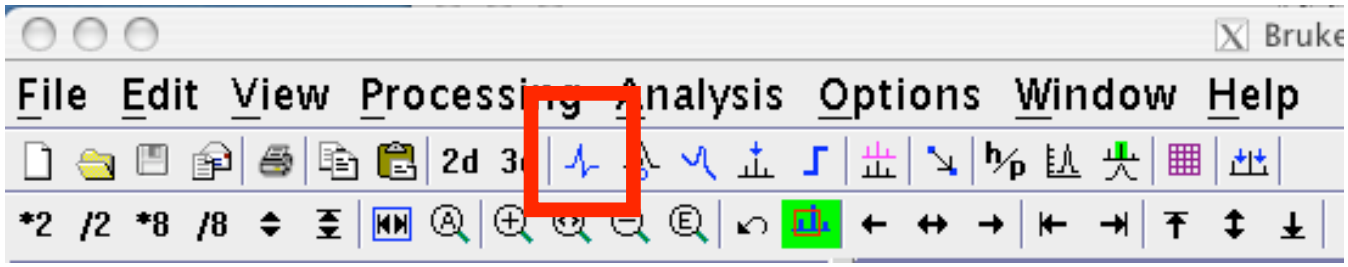
Extremely Dangerous Hint from TopSpin !!!

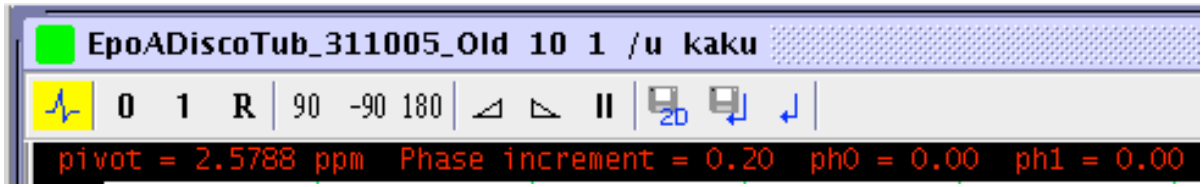


Calibrating spetrum/a

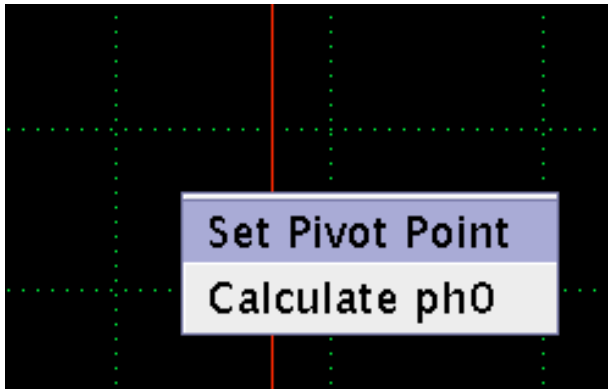


Phasing spetrum/a

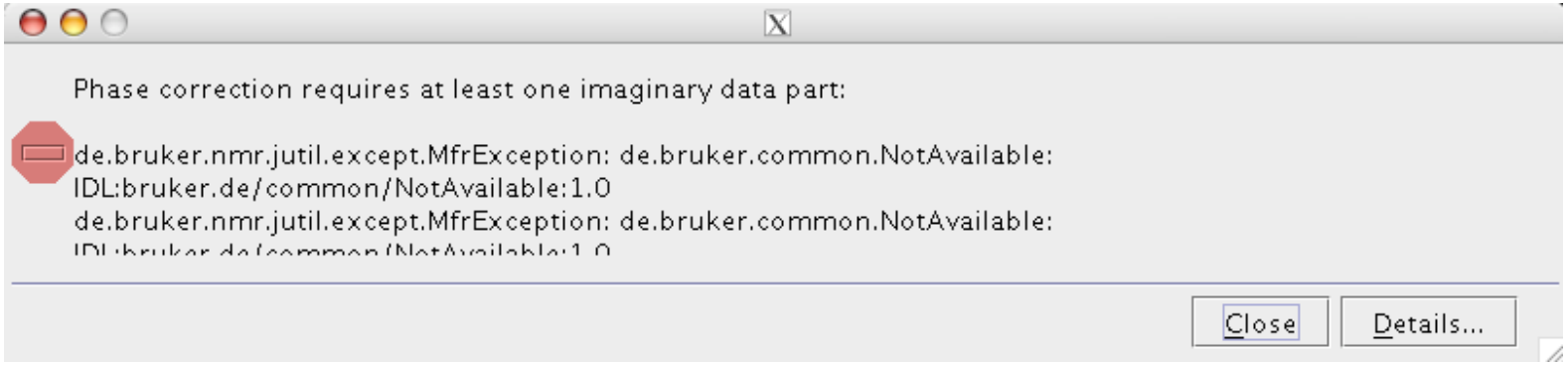


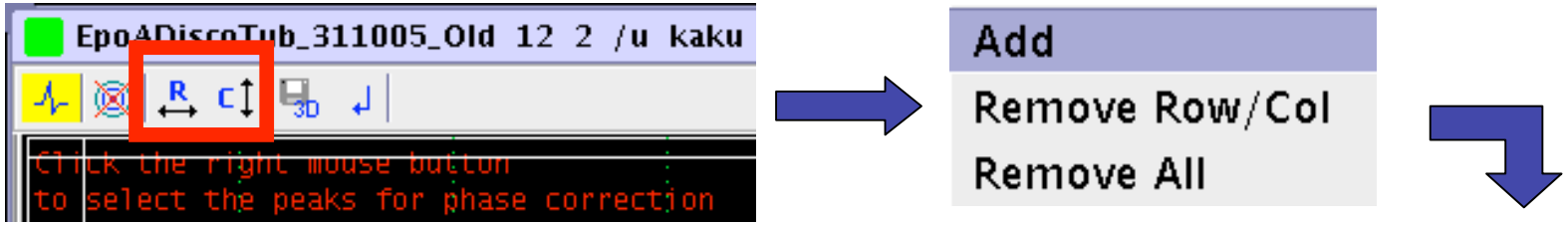


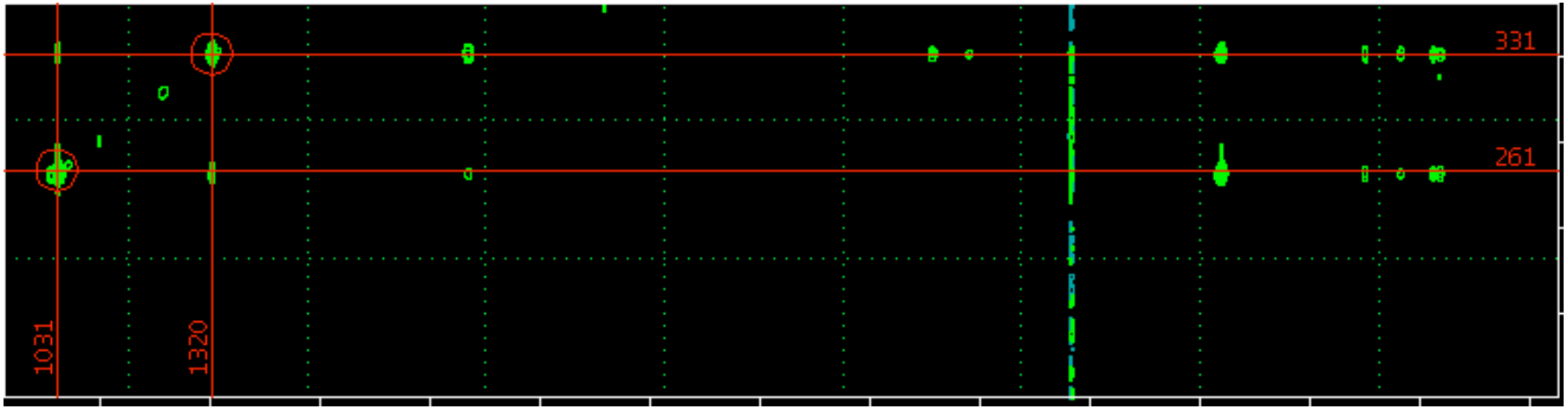
1) set the pivot => right mouse-button
2) **click** left mouse-button on 0/1, **hold** the button and drag mouse up/down until the phase is fine, **then release** the button
3) if the mouse is insensitive, set the sensitivity
4) you can reset [**R**], save, save as 2D, or return

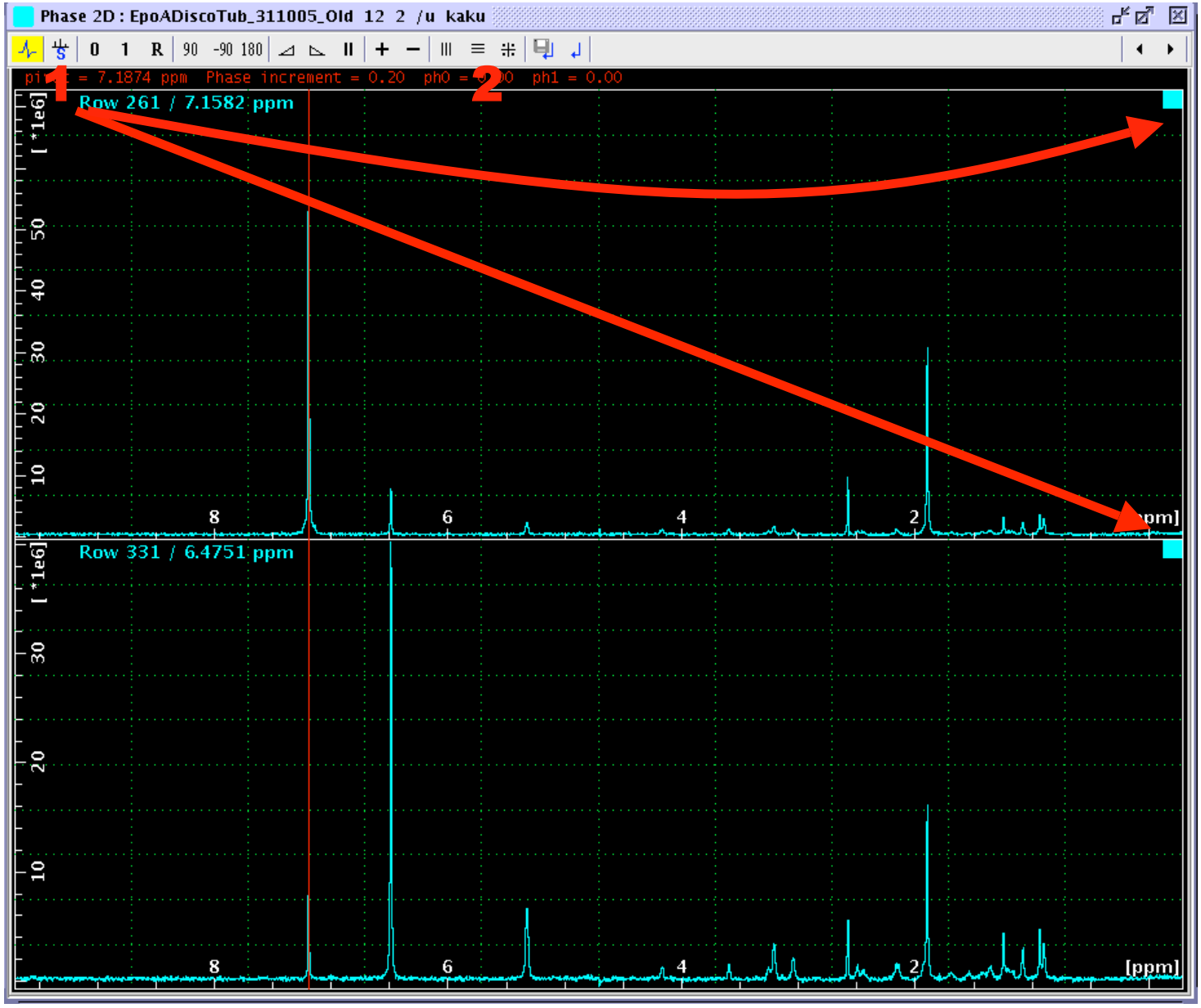


Phasing 2D


Phase correction requires at least one imaginary data part:
de.bruker.nmr.jutil.except.MfrException: de.bruker.common.NotAvailable:
IDL:bruker.de/common/NotAvailable:1.0
de.bruker.nmr.jutil.except.MfrException: de.bruker.common.NotAvailable:
Close
Details...

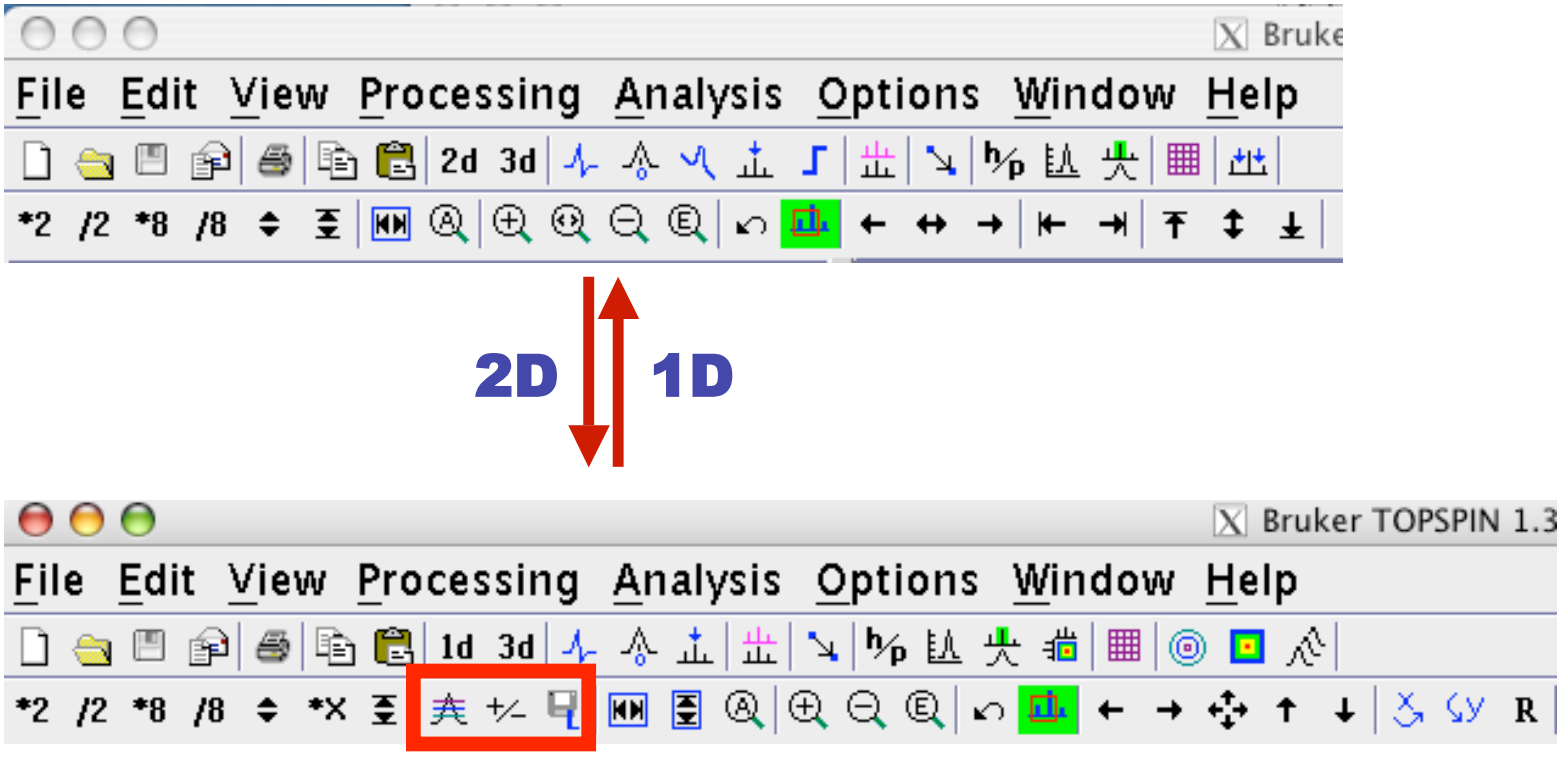

EpoADiscoTub_311005_Old 12 2 /u kaku
R
C
3D
Click the right mouse button
to select the peaks for phase correction
Add
Remove Row/Col
Remove All


331
261
1031
1320


Phase 2D : EpoADiscoTub_311005_Old 12 2 /u kaku
0 1 R 90 -90 180
Row 261 / 7.1582 ppm
Row 331 / 6.4751 ppm
[*1e6]
8
6
4
2
[ppm]
1
2

„Playing around“

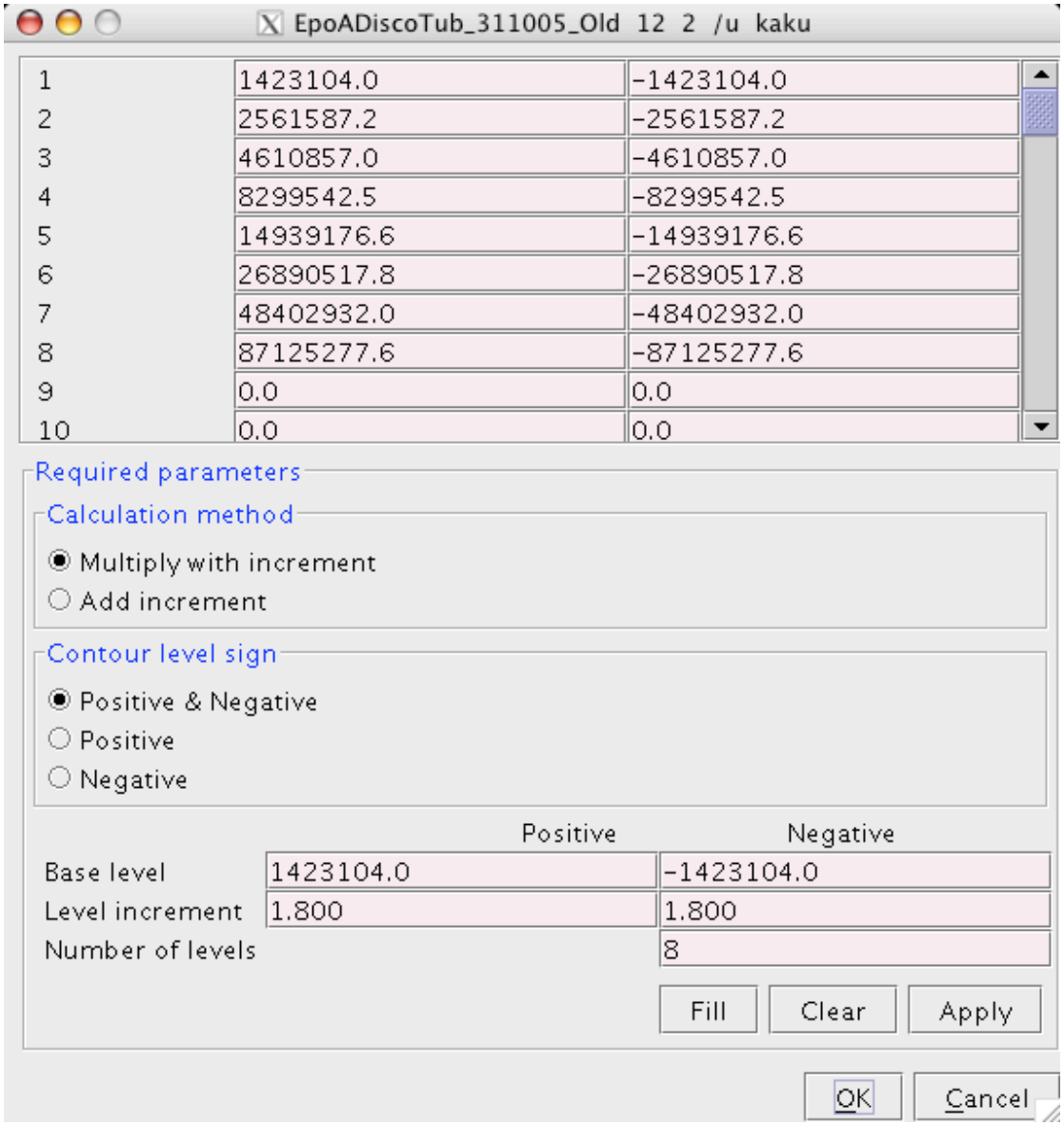
a) Editing contour levels



„Playing around“

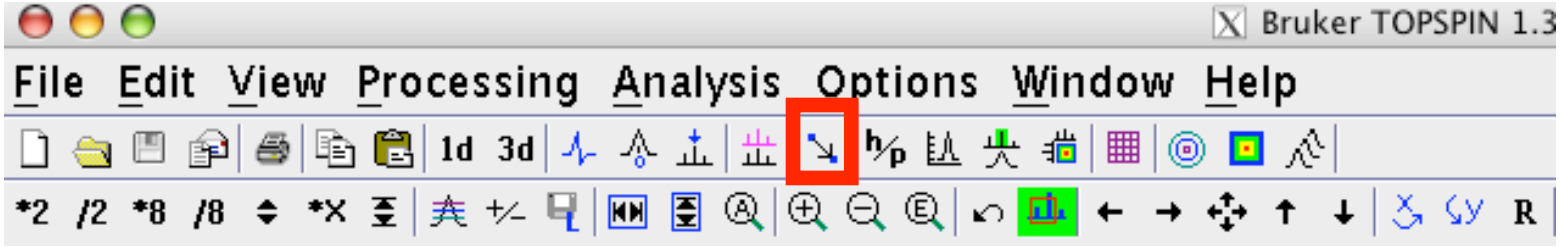
a) Editing contour levels

.choose cont. level sign to be manipulated/displayed
.set base level
.set increment
.number of levels for each sign
.fill
.apply

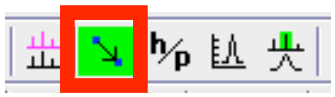


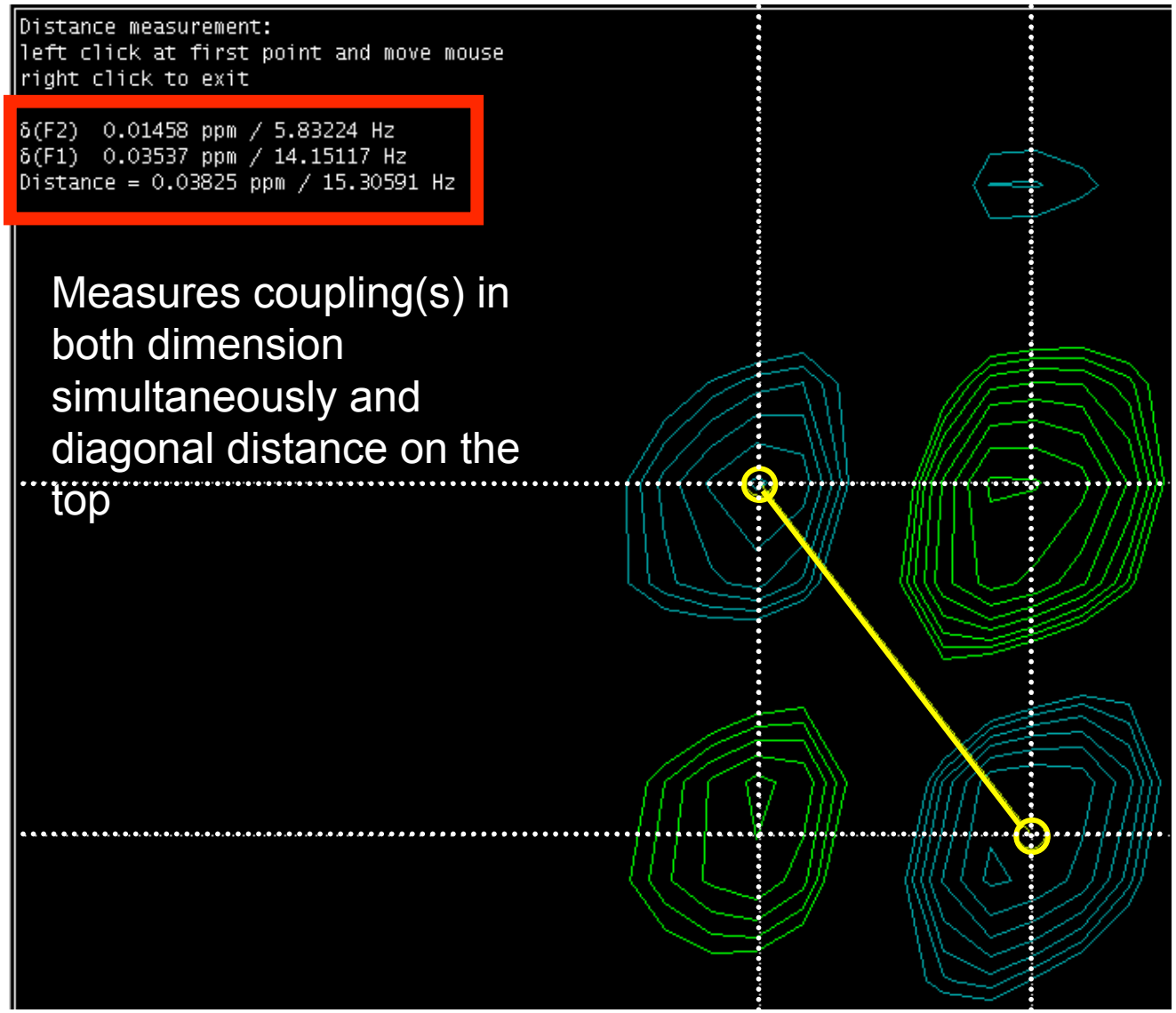
„Playing around“

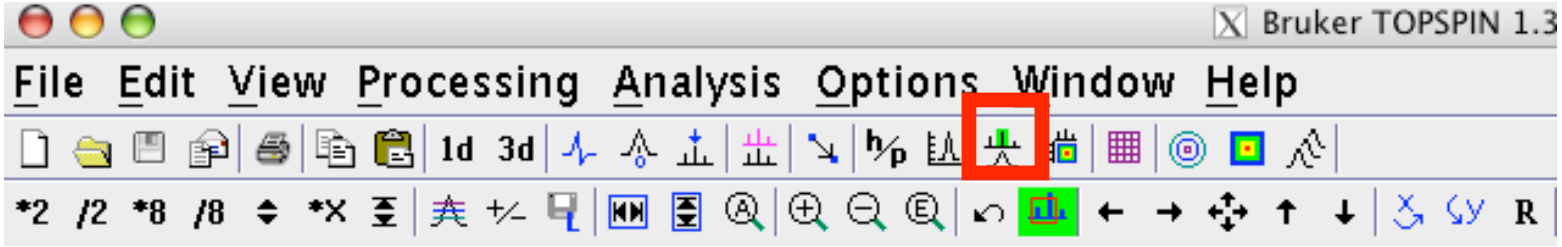
b) Measuring couplings (distances)



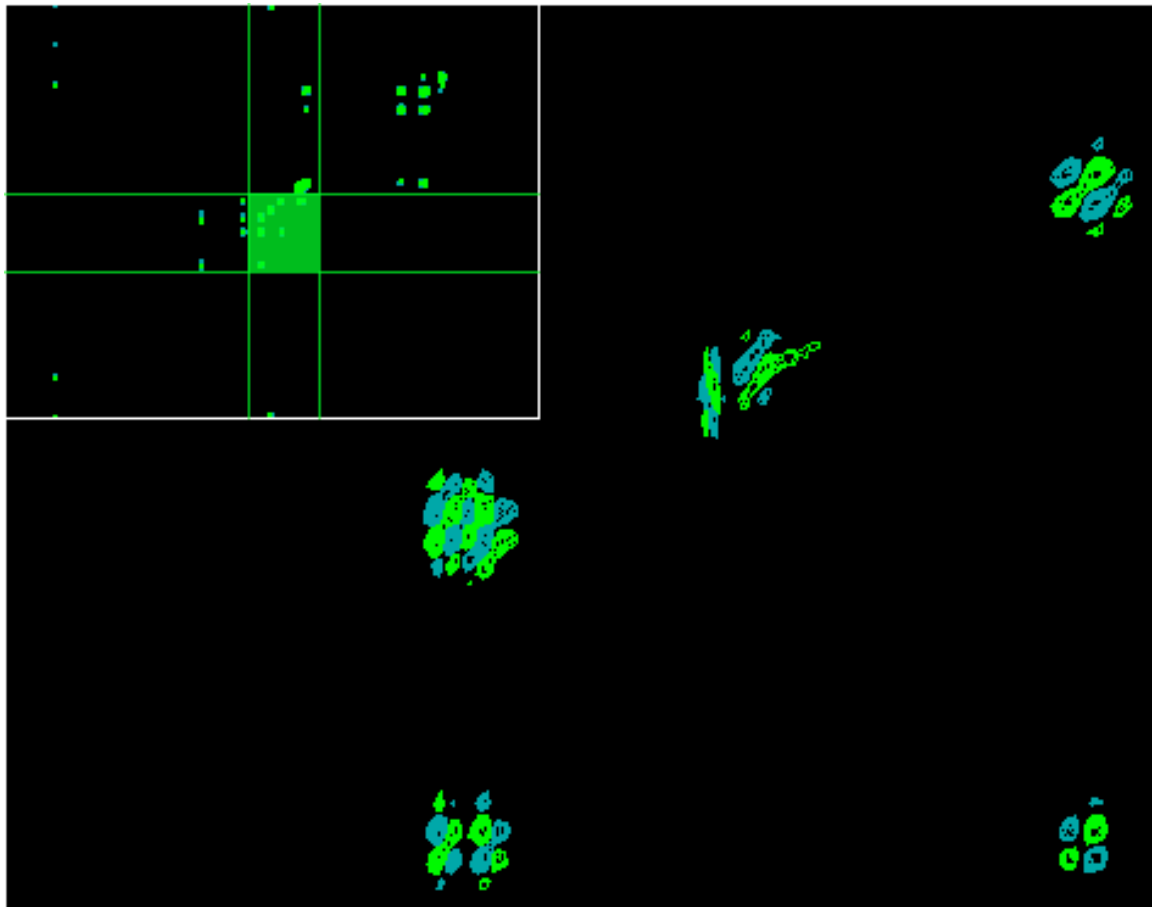
-click the icon
-green background of the icon means the measure-distance option is active
-move the cursor into the spectrum and follow the hints given by TopSpin
-to deactivate the measure-distance either move the cursor away from the spectrum (e.g., to the tree structure of your directories) or right click

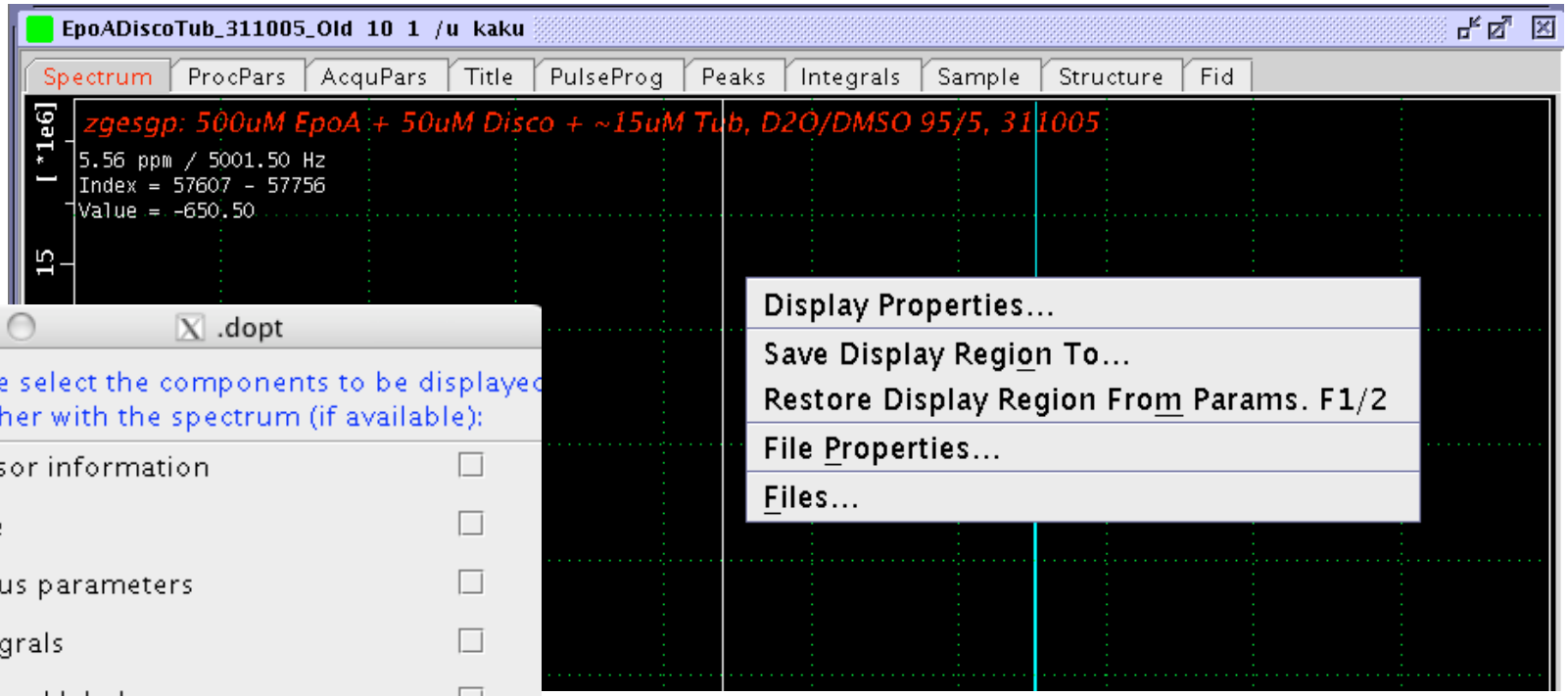


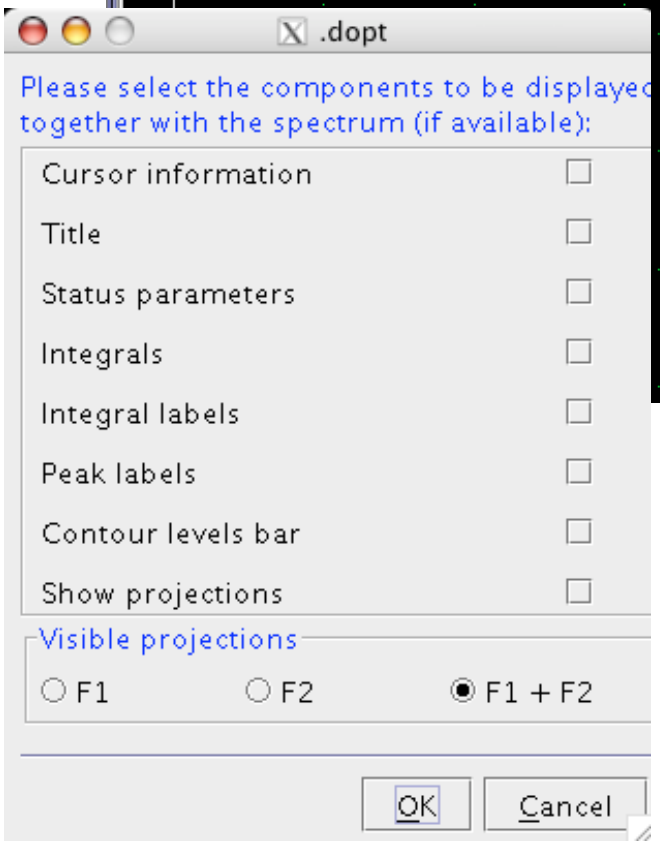

Distance measurement:
left click at first point and move mouse
right click to exit
δ(F2) 0.01458 ppm / 5.83224 Hz
δ(F1) 0.03537 ppm / 14.15117 Hz
Distance = 0.03825 ppm / 15.30591 Hz
Measures coupling(s) in both dimension simultaneously and diagonal distance on the top



Overview window







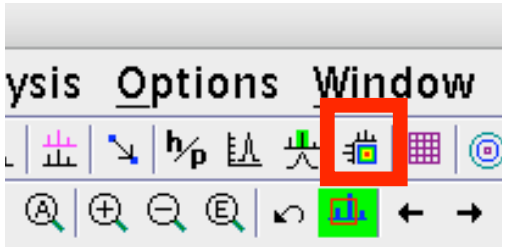
1D Projections

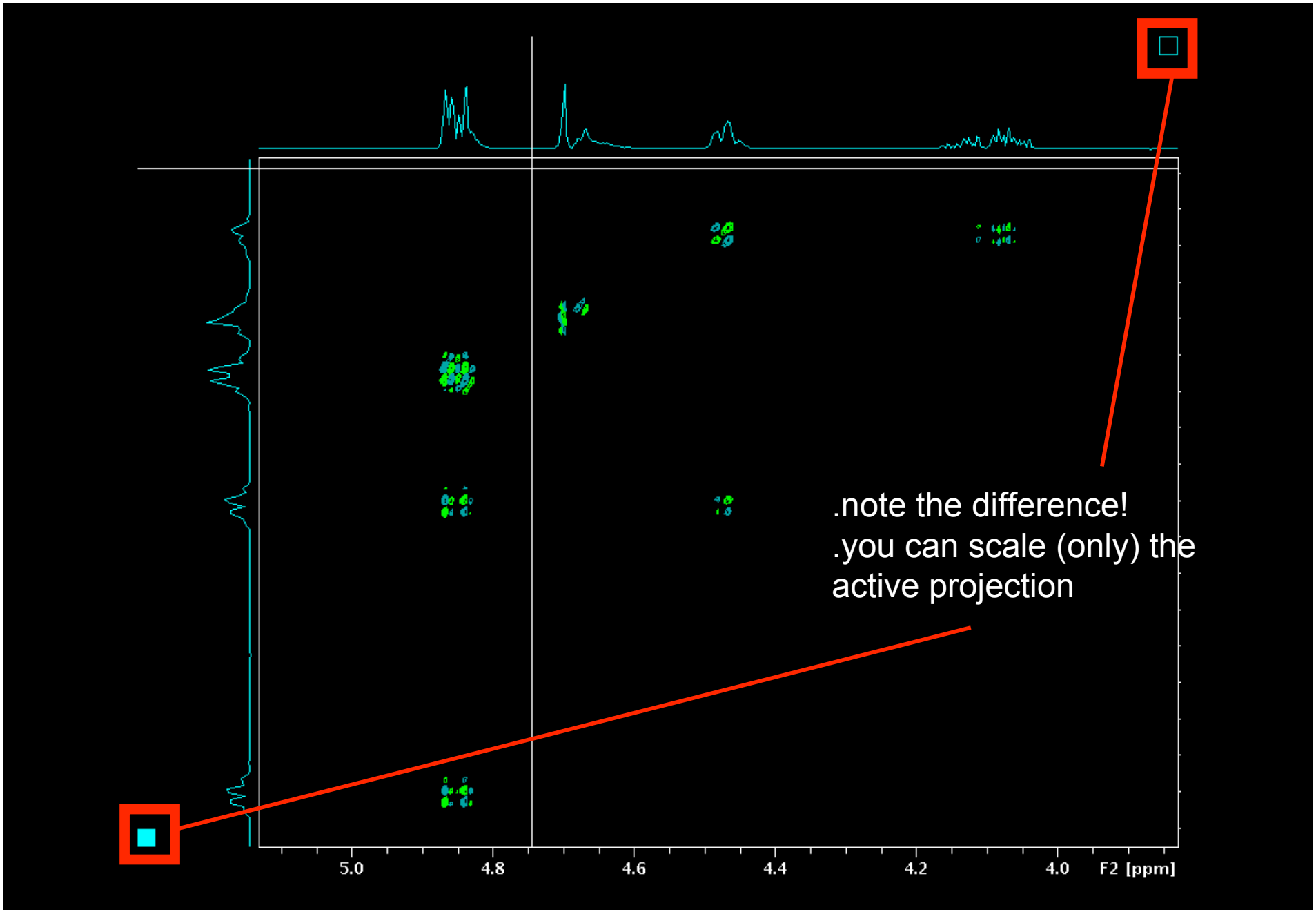
=>3 ways to obtain them:

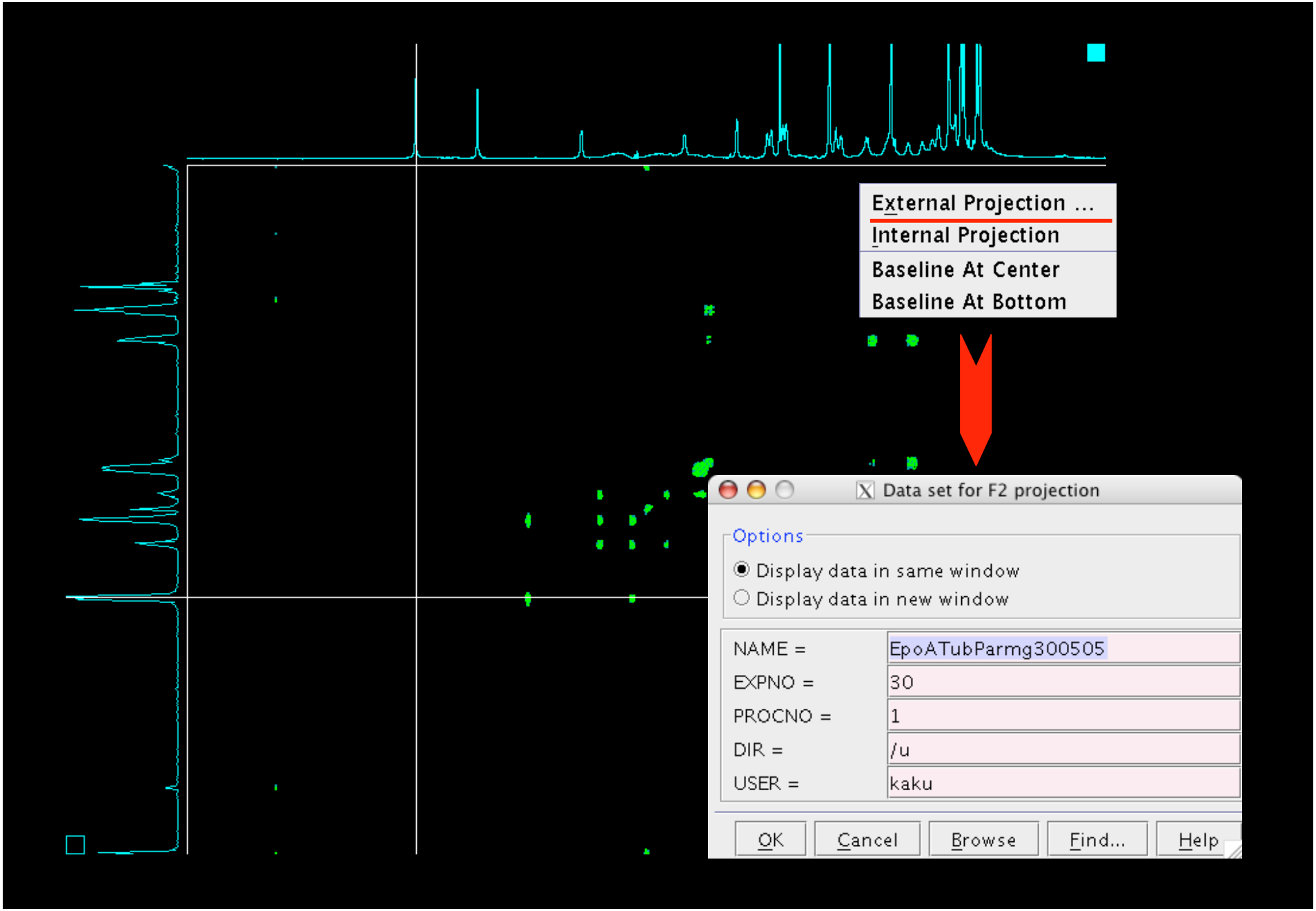
i) type **`.dopt`**

ii) right click

iii) click the icon

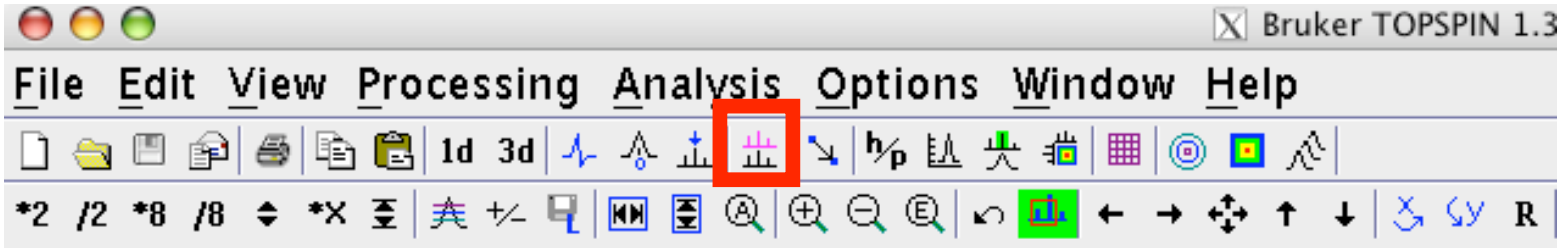



.note the difference!
.you can scale (only) the active projection
5.0
4.8
4.6
4.4
4.2
4.0
F2 [ppm]

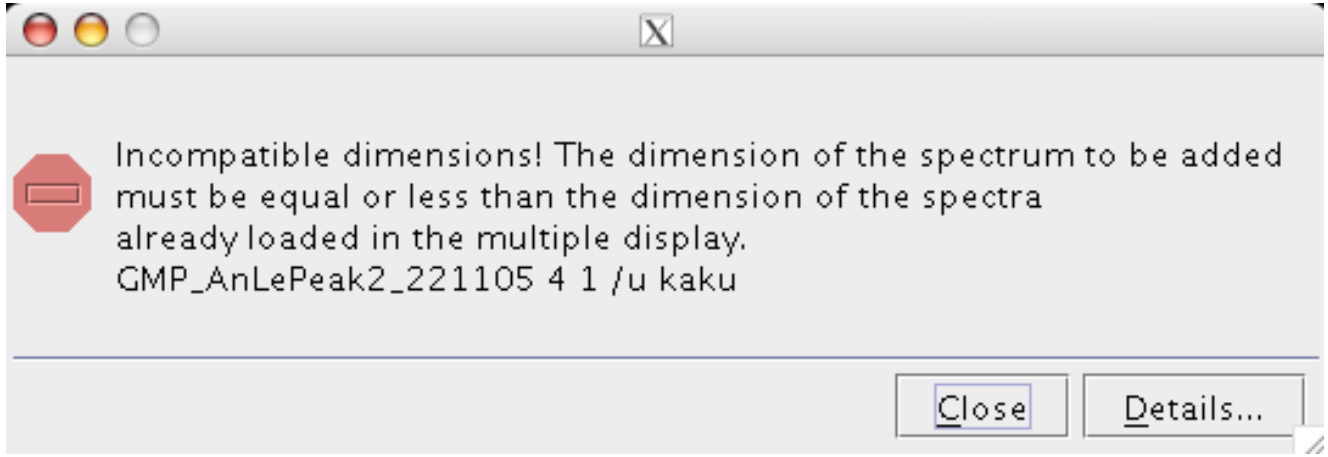

External Projection ...
Internal Projection
Baseline At Center
Baseline At Bottom
Data set for F2 projection
Options
Display data in same window
Display data in new window
NAME = EpoATubParmg300505
EXPNO = 30
PROCNO = 1
DIR = /u
USER = kaku
OK
Cancel
Browse
Find...
Help

„Playing around“

Overlaying spectra (and scanning rows/columns)



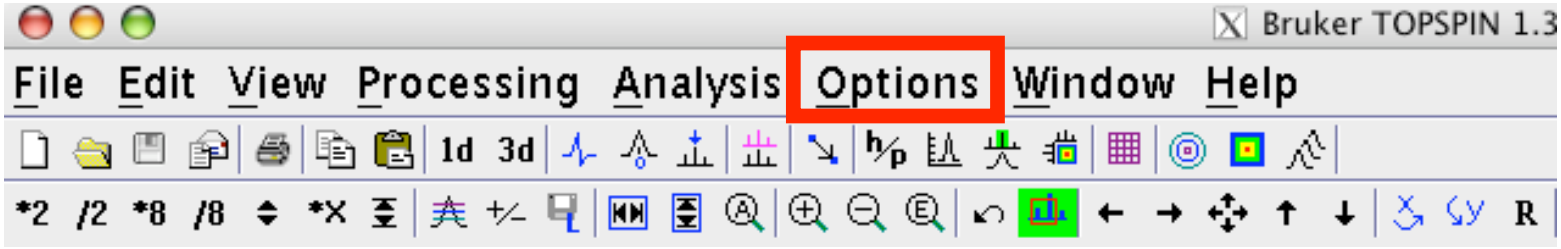
You only can overlay 1Ds‘; 1D on the top of 2/3D; 2Ds‘; 2D on the top of 3D but not the other way around!!! Otherwise:

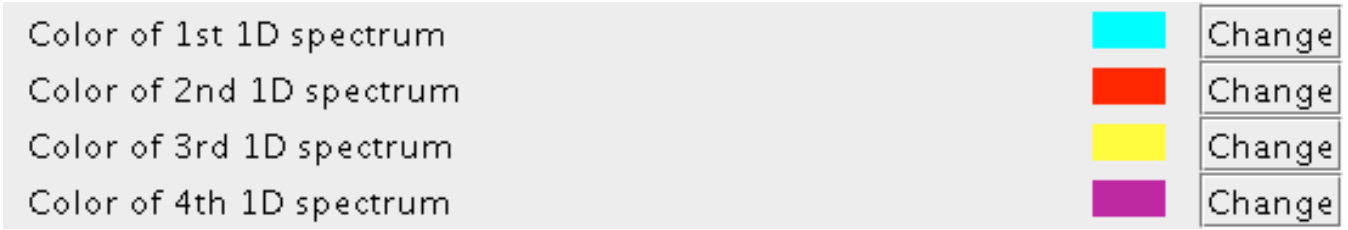


„Playing around“

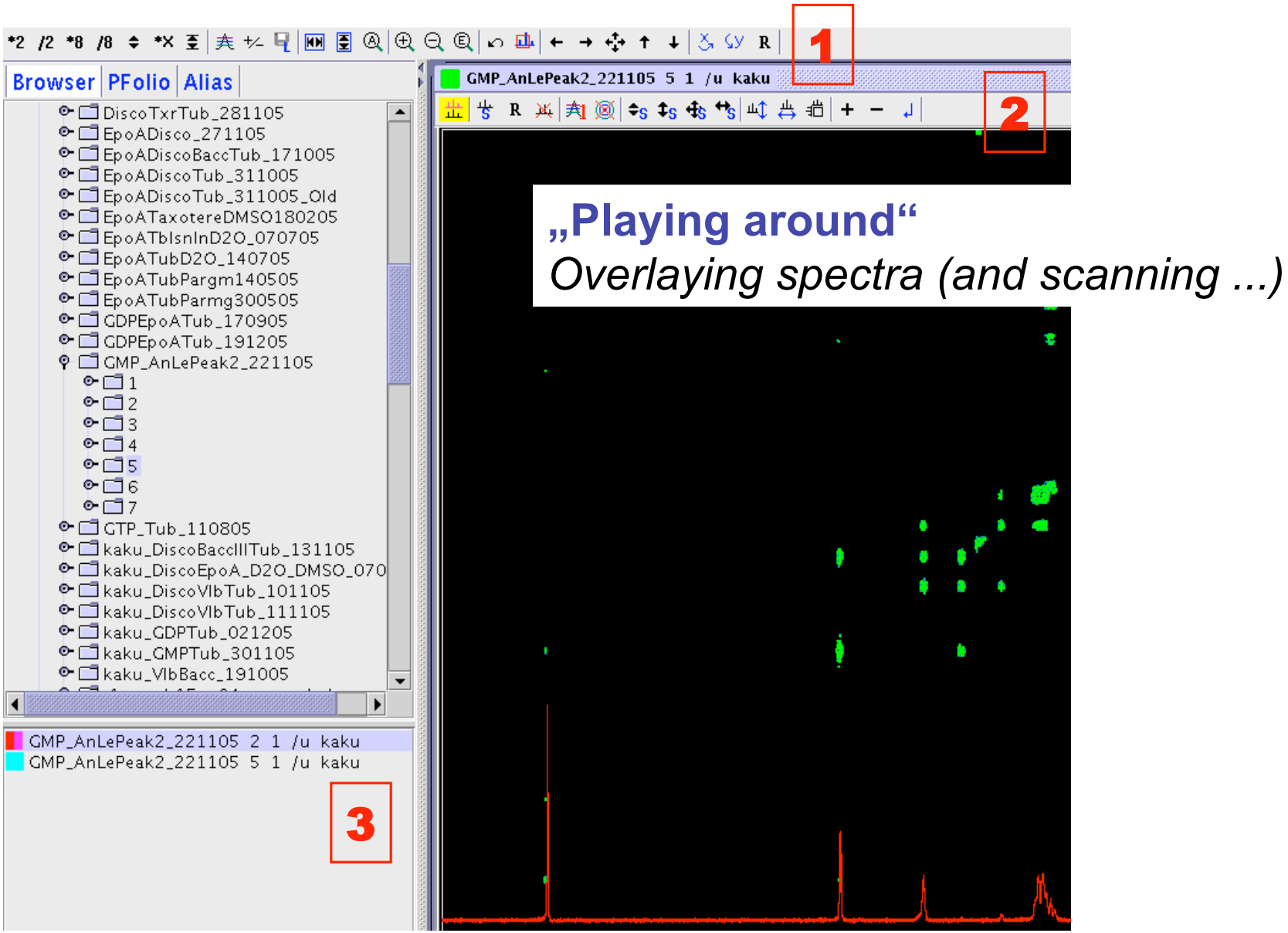
Overlaying spectra (and scanning rows/columns)

Choose the colours for your spectra (and don‘t criticize mine:-):
Options-> Preferences ...





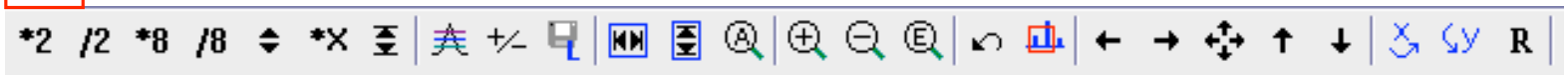
Overlaying spectra is simple as opening a single spectrum: display the first spectrum, click the overlay icon (Bruker calls it multiple display) and display second, third ... spectrum in exactly the same way as you did with the first one


1
2
3
Browser
PFolio
Alias
DiscoTxrTub_281105
EpoADisco_271105
EpoADiscoBaccTub_171005
EpoADiscoTub_311005
EpoADiscoTub_311005_Old
EpoATaxotereDMSO180205
EpoATblsnInD2O_070705
EpoATubD2O_140705
EpoATubPargm140505
EpoATubParmg300505
GDPEpoATub_170905
GDPEpoATub_191205
GMP_AnLePeak2_221105
1
2
3
4
5
6
7
GTP_Tub_110805
kaku_DiscoBaccIIITub_131105
kaku_DiscoEpoA_D2O_DMSO_070
kaku_DiscoVIbTub_101105
kaku_DiscoVIbTub_111105
kaku_GDPTub_021205
kaku_GMPTub_301105
kaku_VIbBacc_191005
GMP_AnLePeak2_221105 2 1 /u kaku
GMP_AnLePeak2_221105 5 1 /u kaku
GMP_AnLePeak2_221105 5 1 /u kaku
„Playing around“
Overlaying spectra (and scanning ...)

„Playing around“

Overlaying spectra

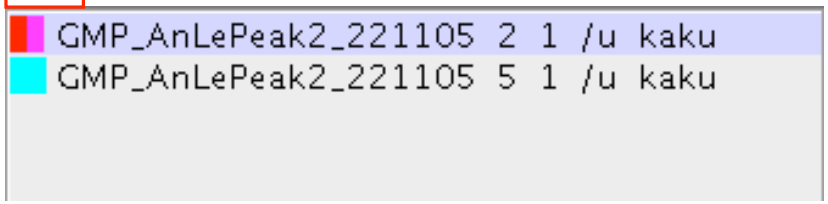
1



Don‘t mess up these two menu-bars

2

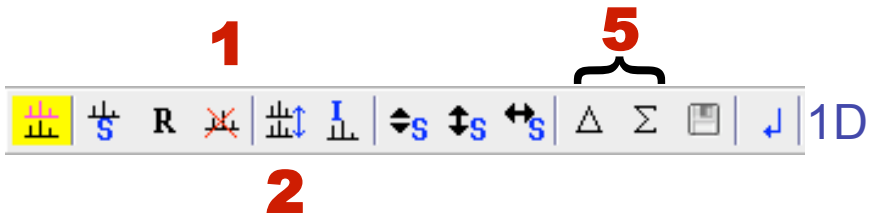
3

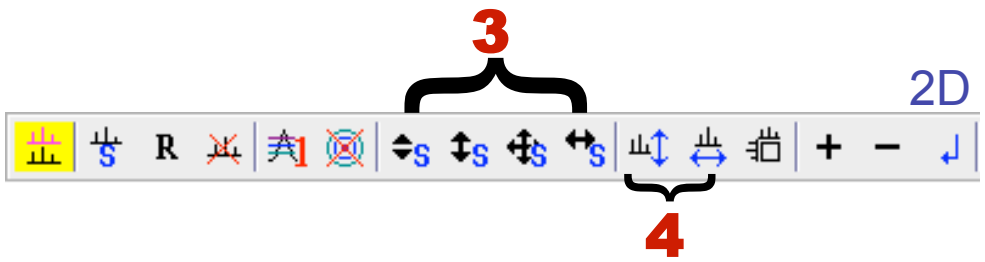


MB-**1** scales **ALL** spectra
MB-**2** scales (and allows other manipulation) **ONLY** spectra **SELECTED** in **3**

„Playing around“

Overlaying spectra (1D) and scanning rows/columns (2D)



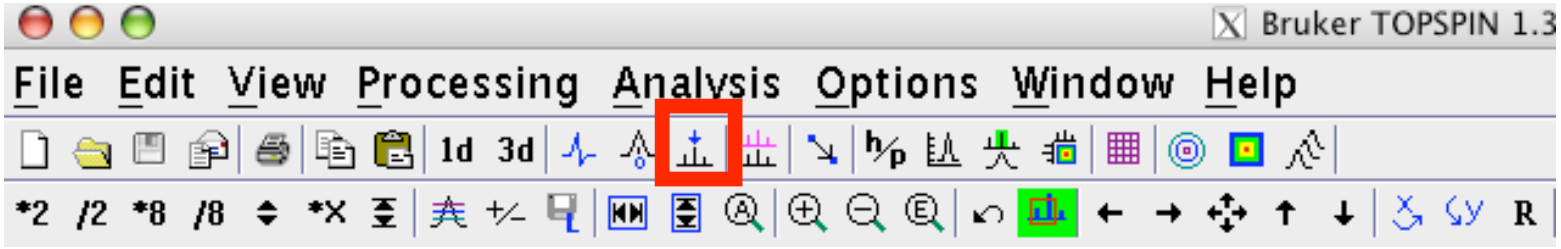


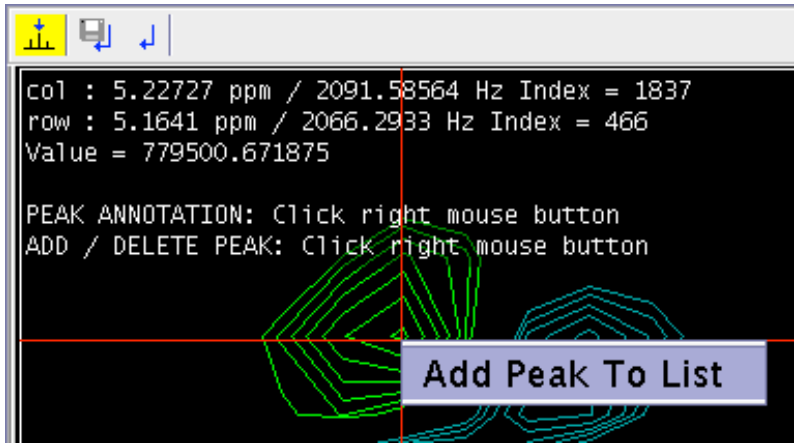
.note the difference between 1D and 2D overlay MB! => same icons but different functions

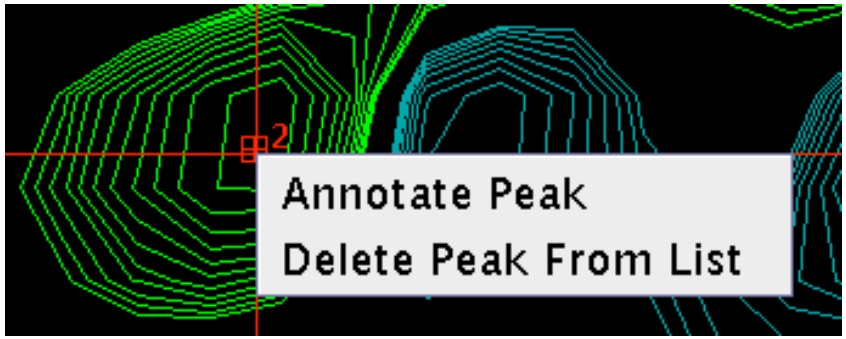
.you can never remove first spectrum (the one from which you called overlay option)

1) removes spectrum
2) **a)** in 1D overlays two spectra on the top of each other or creates displays them in two separate windows; **b)** in 2D scans row/columns
3) scales/shifts selected spectrum
4) see point **2b),** scanned r/cs‘ are scaled by left/middle mouse-button up/down respectively
5) summs/subtracts 1Ds‘

Peak picking & integrating 2D - Manually



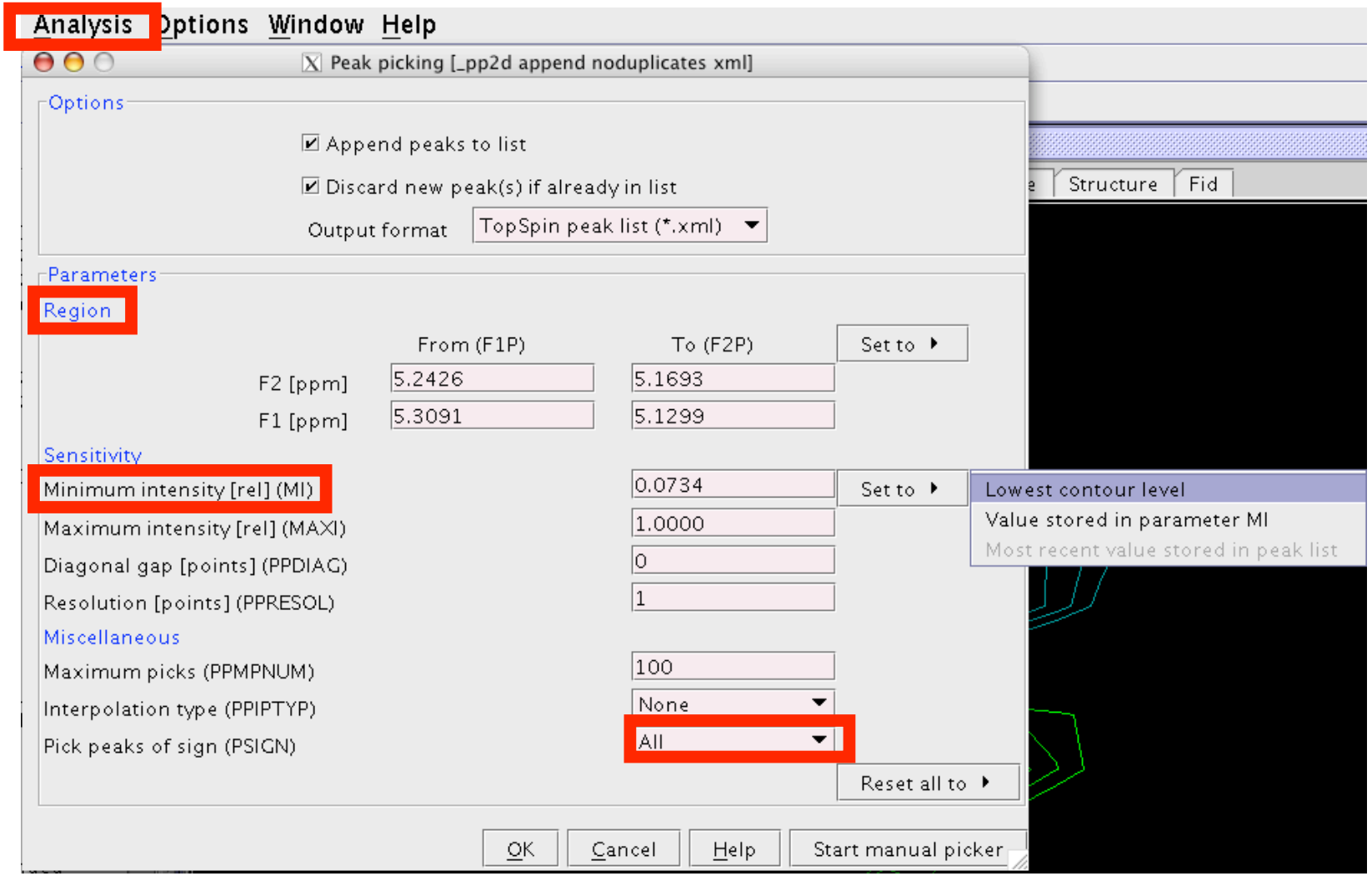




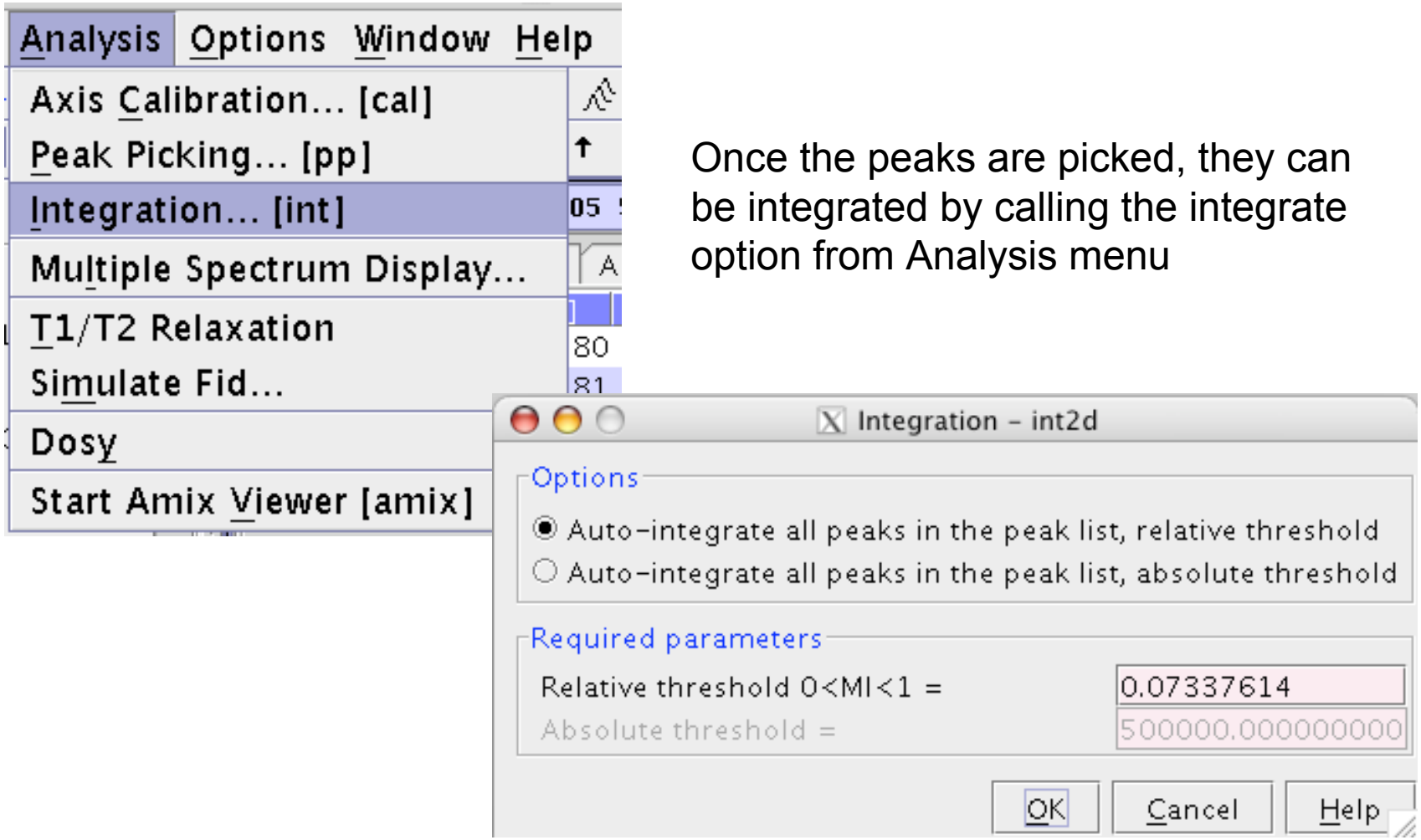
Spectrum | ProcPars | AcquPars | Title | PulseProg | Peaks | Integrals | Sample | Structure | Fid

Peak	v(F2) [ppm]	v(F1) [ppm]	Intensity	Annotation
1	5.2280	5.1942	-2235944.83	Pokus1
2	5.2281	5.2291	1592654.66	
3	5.2273	5.1635	779500.67	

Peak picking & integrating 2D - Automatically



Peak picking & integrating 2D



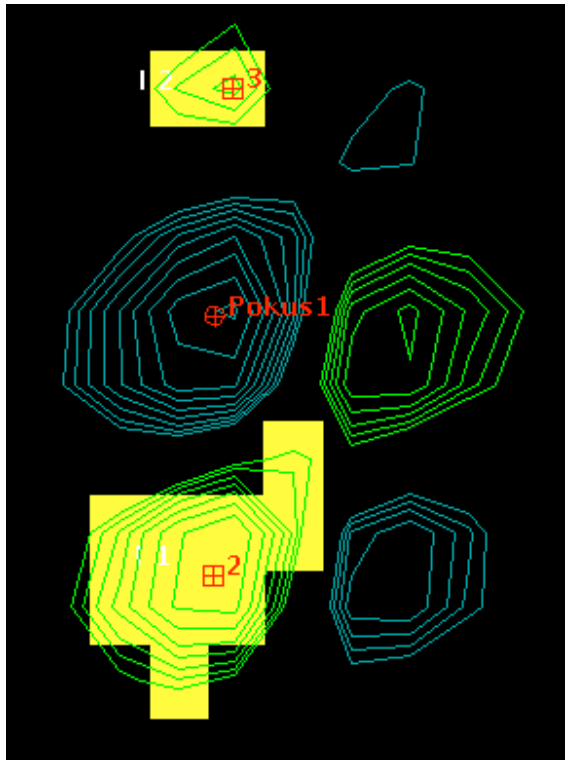
Once the peaks are picked, they can be integrated by calling the integrate option from Analysis menu

Peak picking & integrating 2D

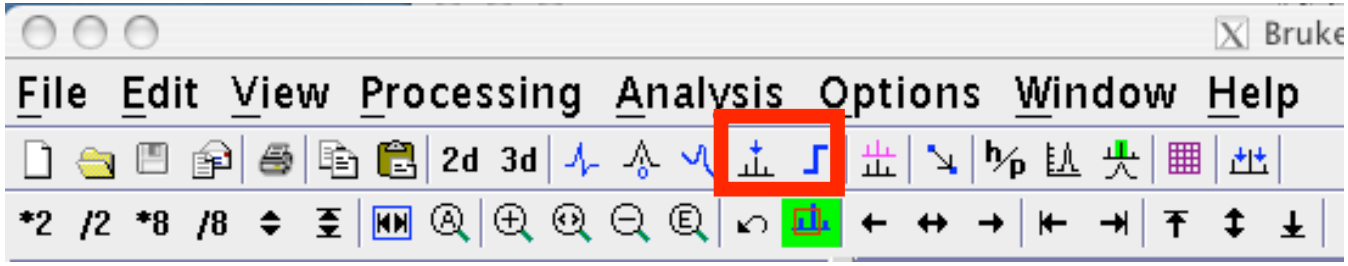
Spectrum | ProcPars | AcquPars | Title | PulseProg | Peaks | Integrals | Sample | Structure | Fid

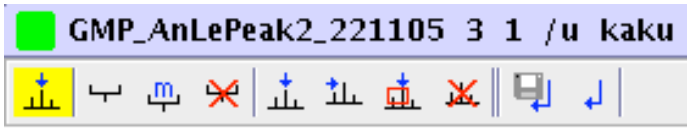
Object	Integral [abs]	Integral [rel]	Peaks	ν(F2) [ppm]	ν(F1) [ppm]	Intensity
Integral 1	9885378.17	1.0000	1			
Integral 2	1392927.27	0.1409	1			
Peak 3				5.2273	5.1635	779500.67

The integrated peaks have yellow background. The info about integrals can be seen in the Integrals-folder of your spectrum. The integrals items are expandable and the table can be sorted by any field present in the header of the table



Peak picking & integrating 1D

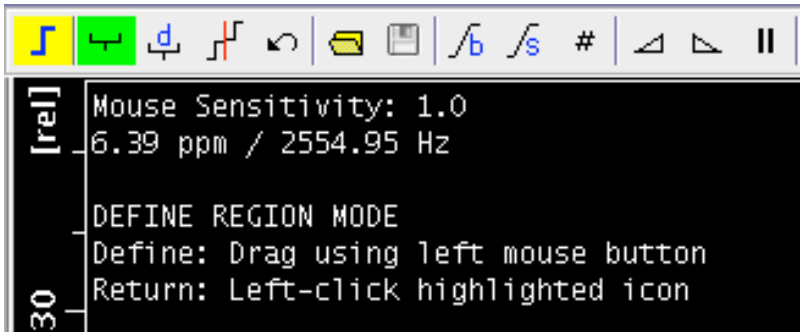


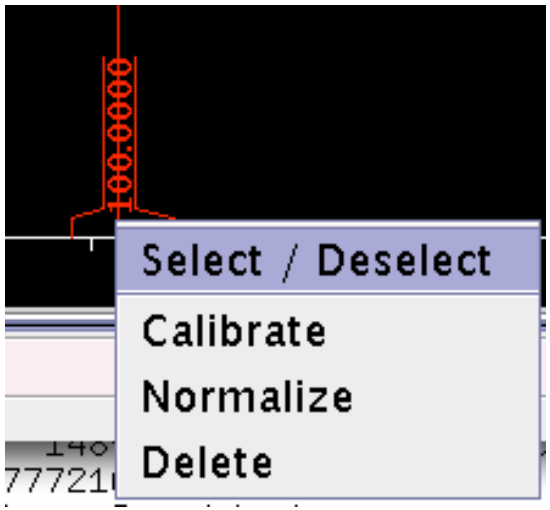


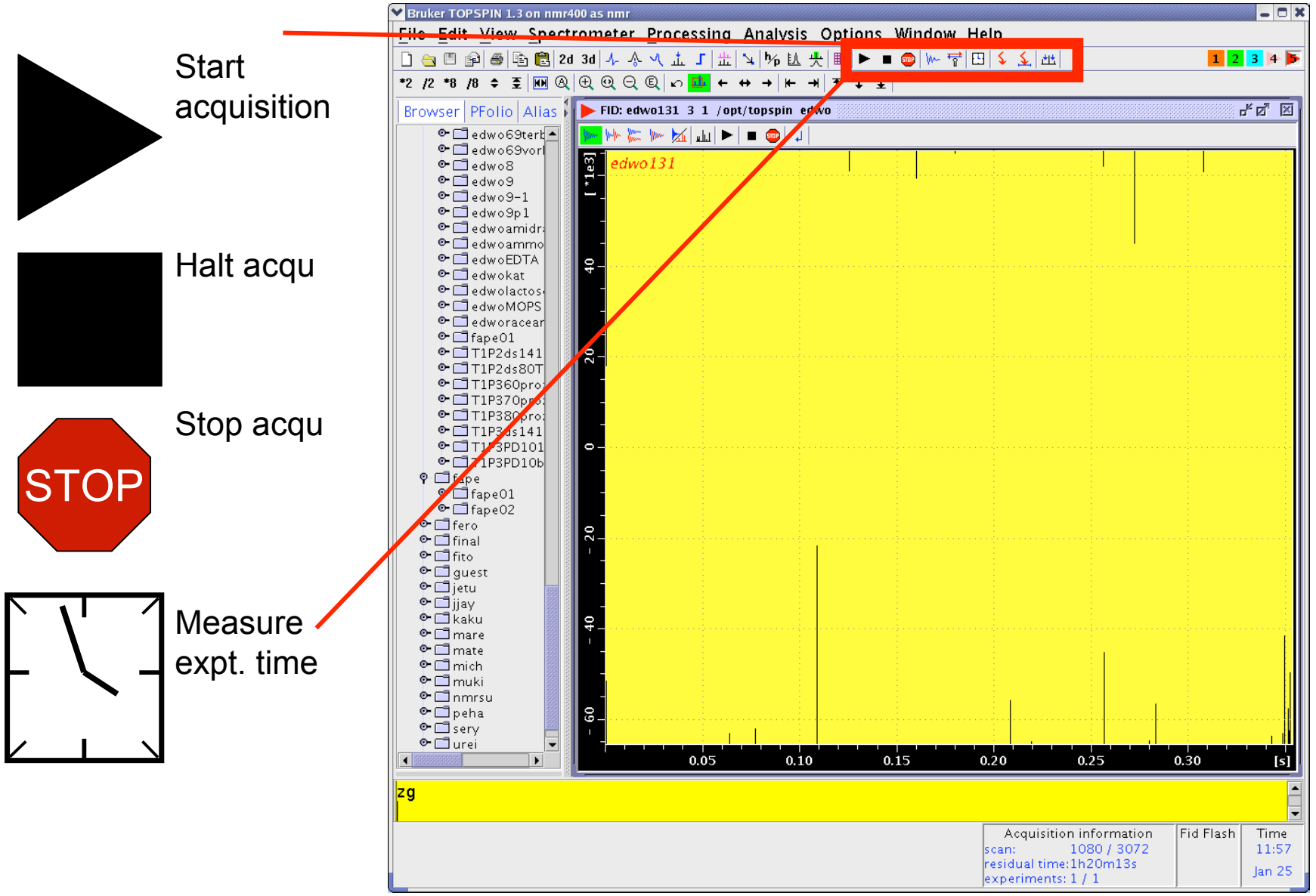
I personally fail to make it work automatically, volunteers are welcome, manually it works well, but that‘s not the way we want it to be

Peak picking & integrating 1D

Contrary to peak-picking, the integration is straightforward and works fastly. The relative values are displayed, to see the absolute values, one has to check the Integrals folder of your dataset






Start acquisition
Halt acqu
STOP
Stop acqu
Measure expt. time
Bruker TOPSPIN 1.3 on nmr400 as nmr
File Edit View Spectrometer Processing Analysis Options Window Help
Browser PFolio Alias
edwo69terb
edwo69vorl
edwo8
edwo9
edwo9-1
edwo9p1
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edwoEDTA
edwokat
edwolactos
edwoMOPS
edworacear
fape01
T1P2ds141
T1P2ds80T
T1P360pro
T1P370pro
T1P380pro
T1P3ds141
T1P3PD101
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fape
fape01
fape02
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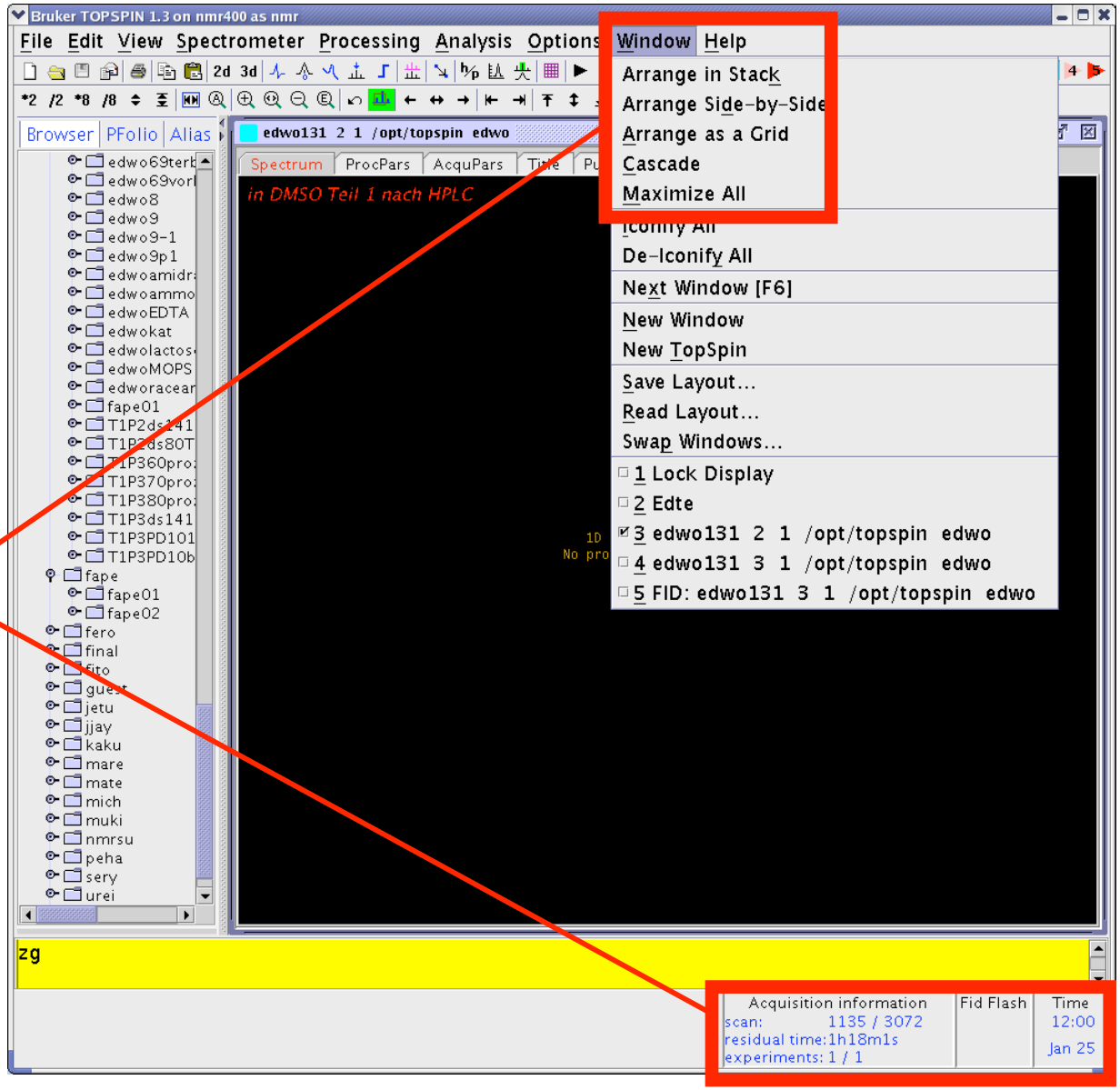
FID: edwo131 3 1 /opt/topspin edwo
edwo131
[*1e3]
40
20
0
- 20
- 40
- 60
0.05
0.10
0.15
0.20
0.25
0.30
[s]
zg
Acquisition information
scan: 1080 / 3072
residual time:1h20m13s
experiments: 1 / 1
Fid Flash
Time
11:57
Jan 25

Not all things work as we are used from XWinNMR, e.g. temperature window is not an independent window anymore, **`acbdisp`** doesn‘t work (yet?), but we get something instead:

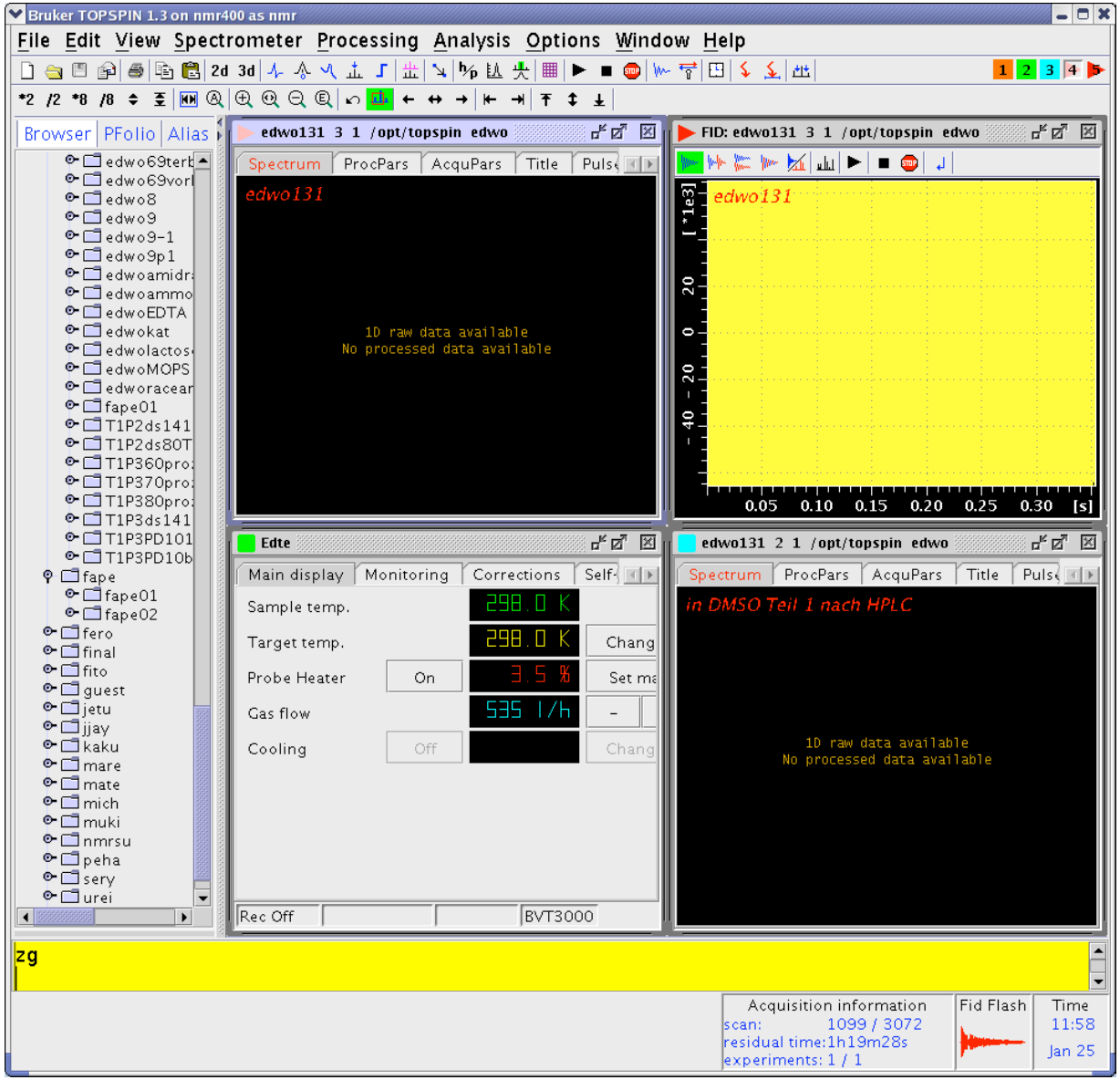
1) status window
2) possibility of arranging windows
3) icons from last slide
4) many other nice things

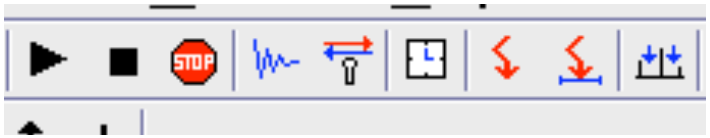


Most of the common commands are still working:

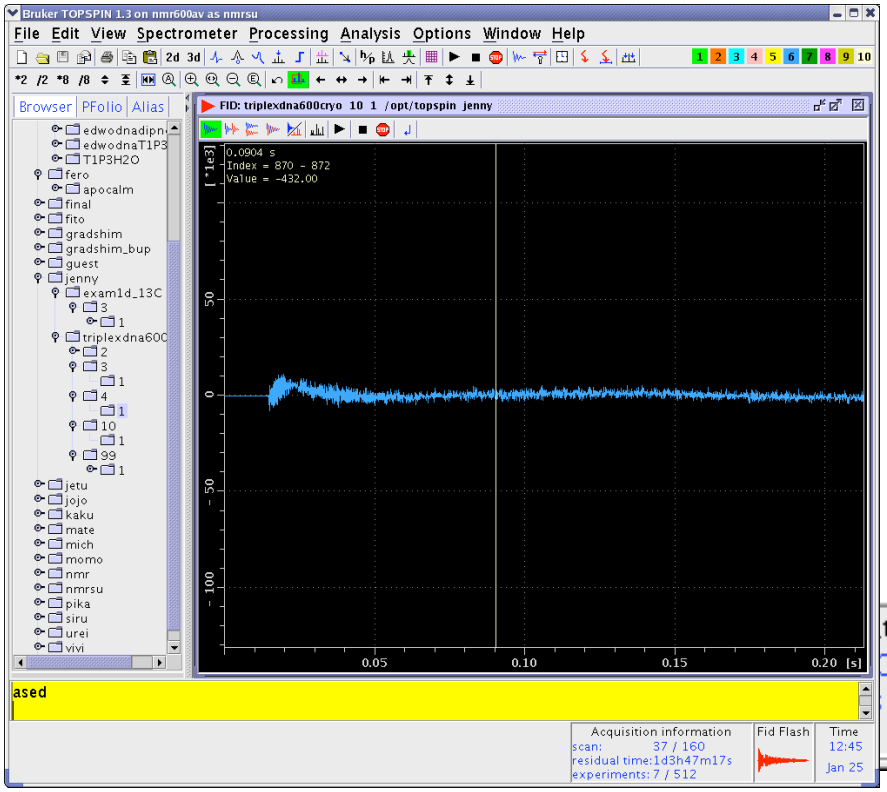
.zg, qsin, fp, efp
.ased, edp, eda, edasp
.wobb, gs
.list_pp, expt, multiexpt, multizg
.stdisp
.etc.

Example of grid arrangement






1
2
3
4
5
6
7
8
9
10


Bruker TOPSPIN 1.3 on nmr600av as nmrsu
File Edit View Spectrometer Processing Analysis Options Window Help
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FID: triplexdna600cryo 10 1 /opt/topspin jenny
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Value = -432.00
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0.15
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Acquisition information
scan: 37 / 160
residual time:1d3h47m17s
experiments: 7 / 512
Fid Flash
Time
12:45
Jan 25


tion
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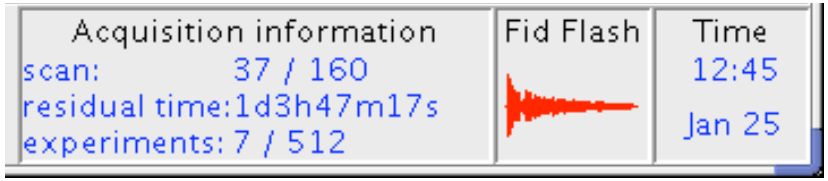
Fid Flash
Time
12:00
Jan 25


Acquisition information
scan: 37 / 160
residual time:1d3h47m17s
experiments: 7 / 512
Fid Flash
Time
12:45
Jan 25


Thank you for your attention !
END