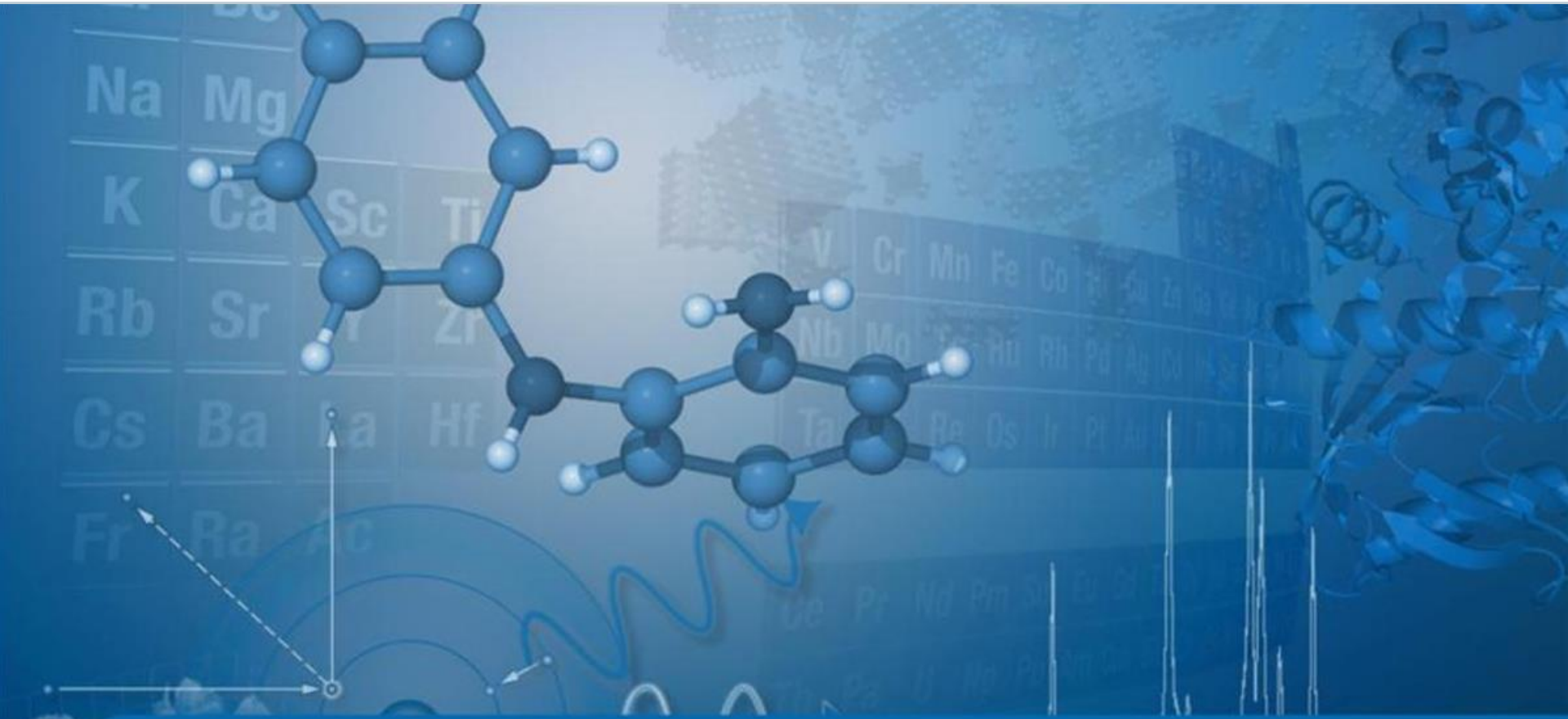
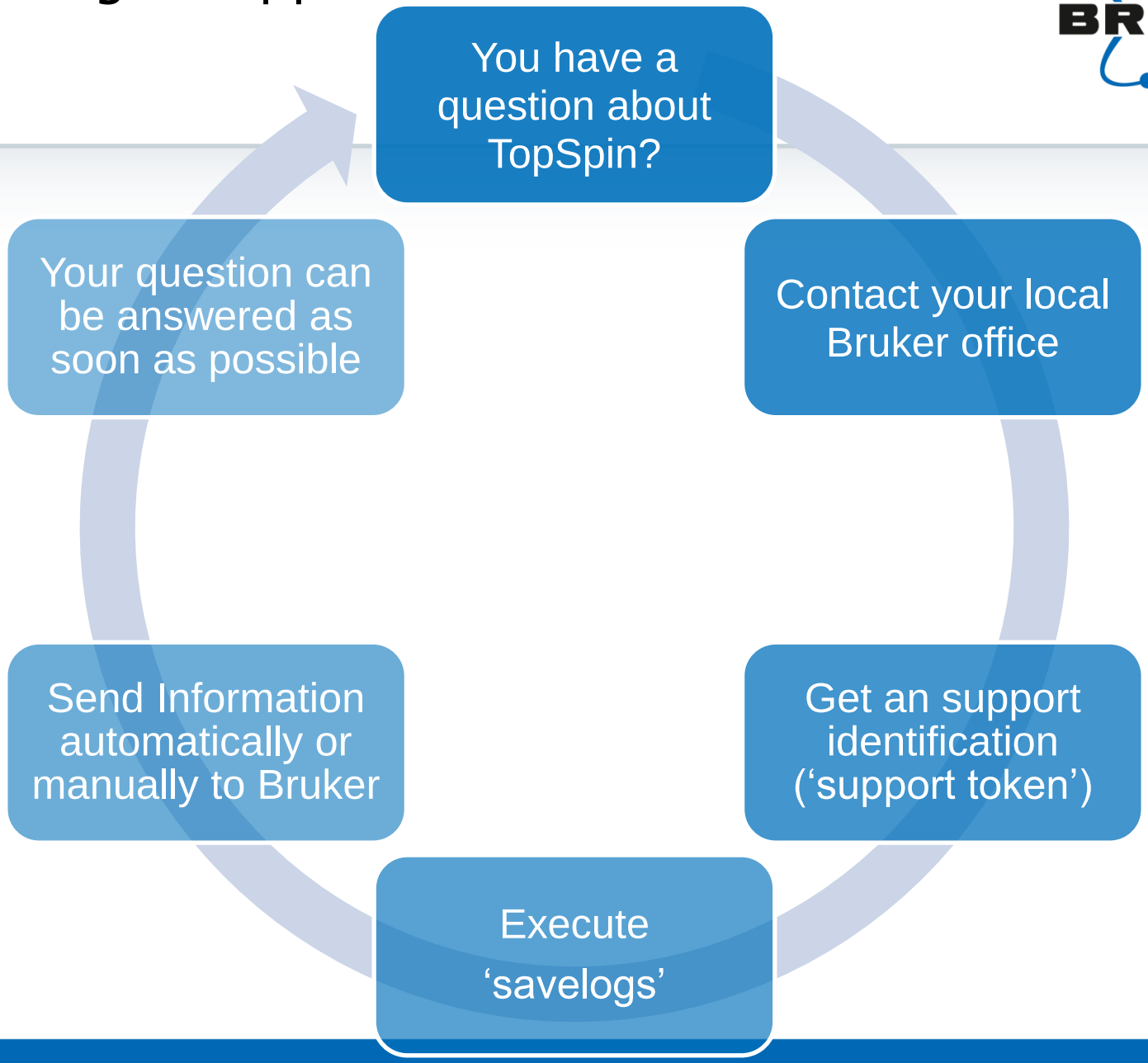
Tips & Tricks

Dr. Benjamin Görling

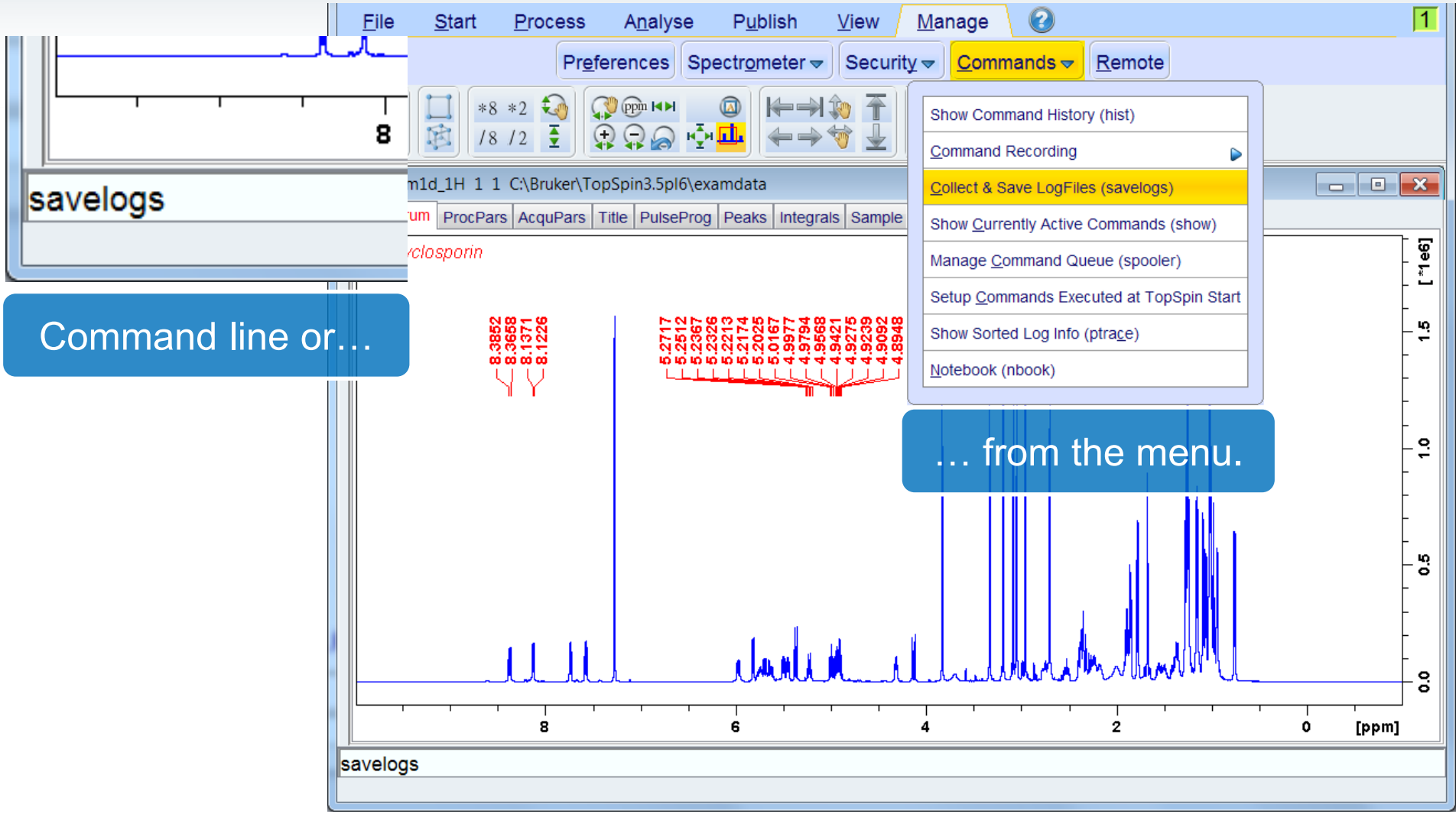


- **General Troubleshooting**

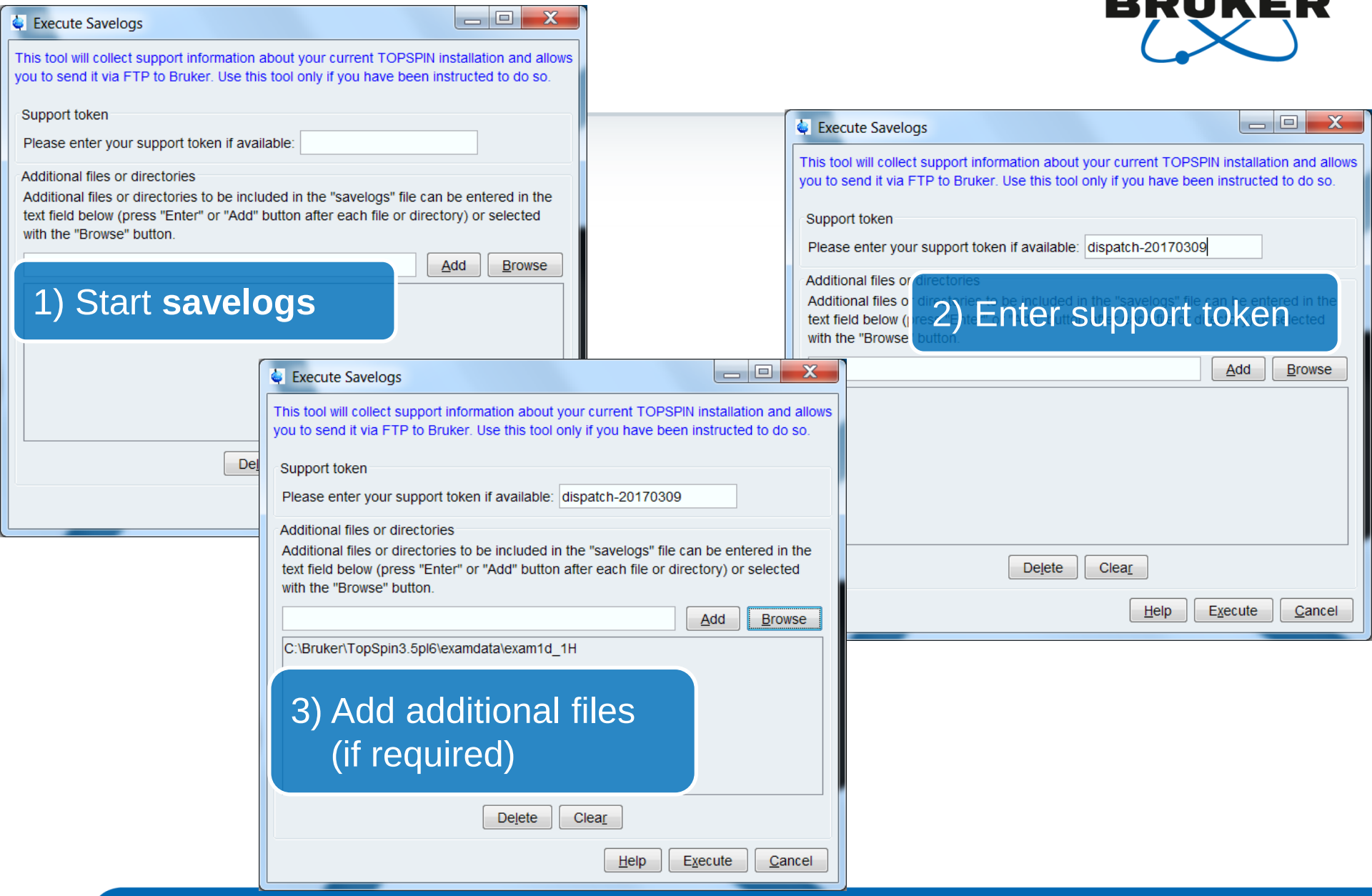
How to get support



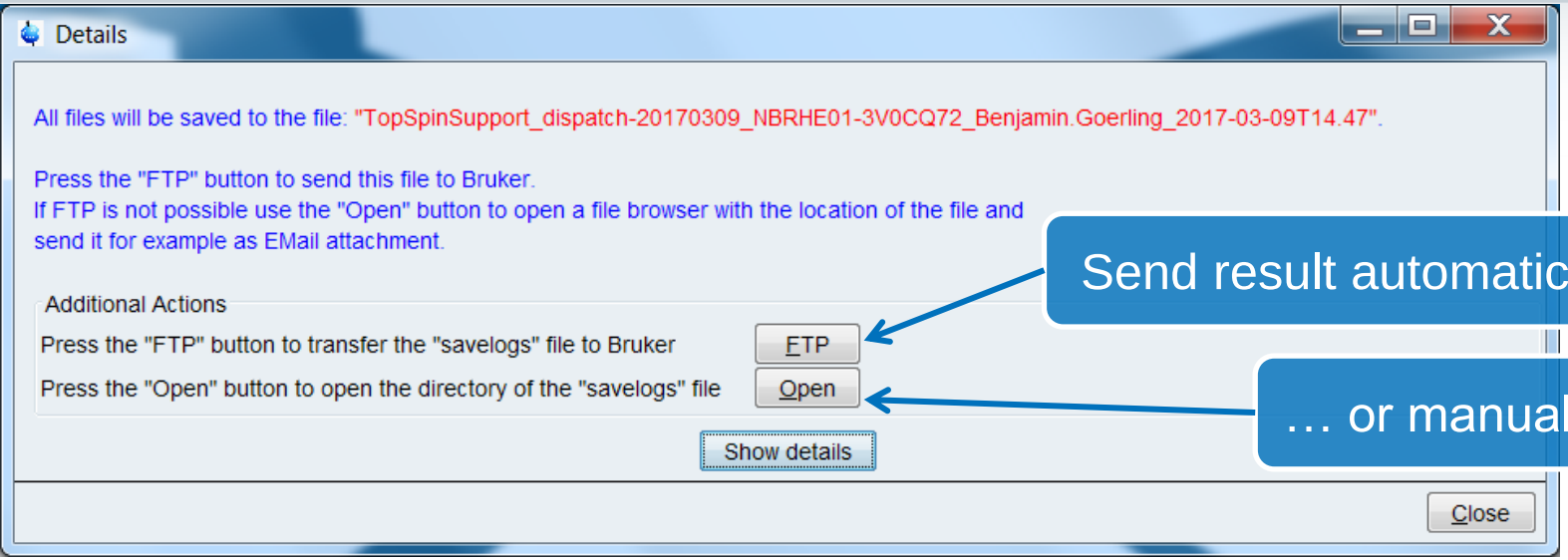
Hot to start **savelogs**

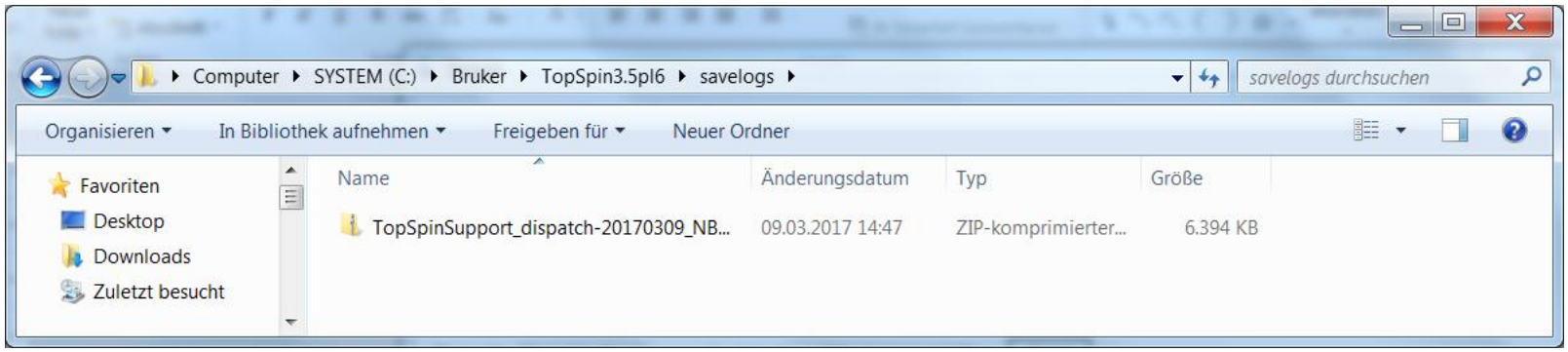


How to use **savelogs**



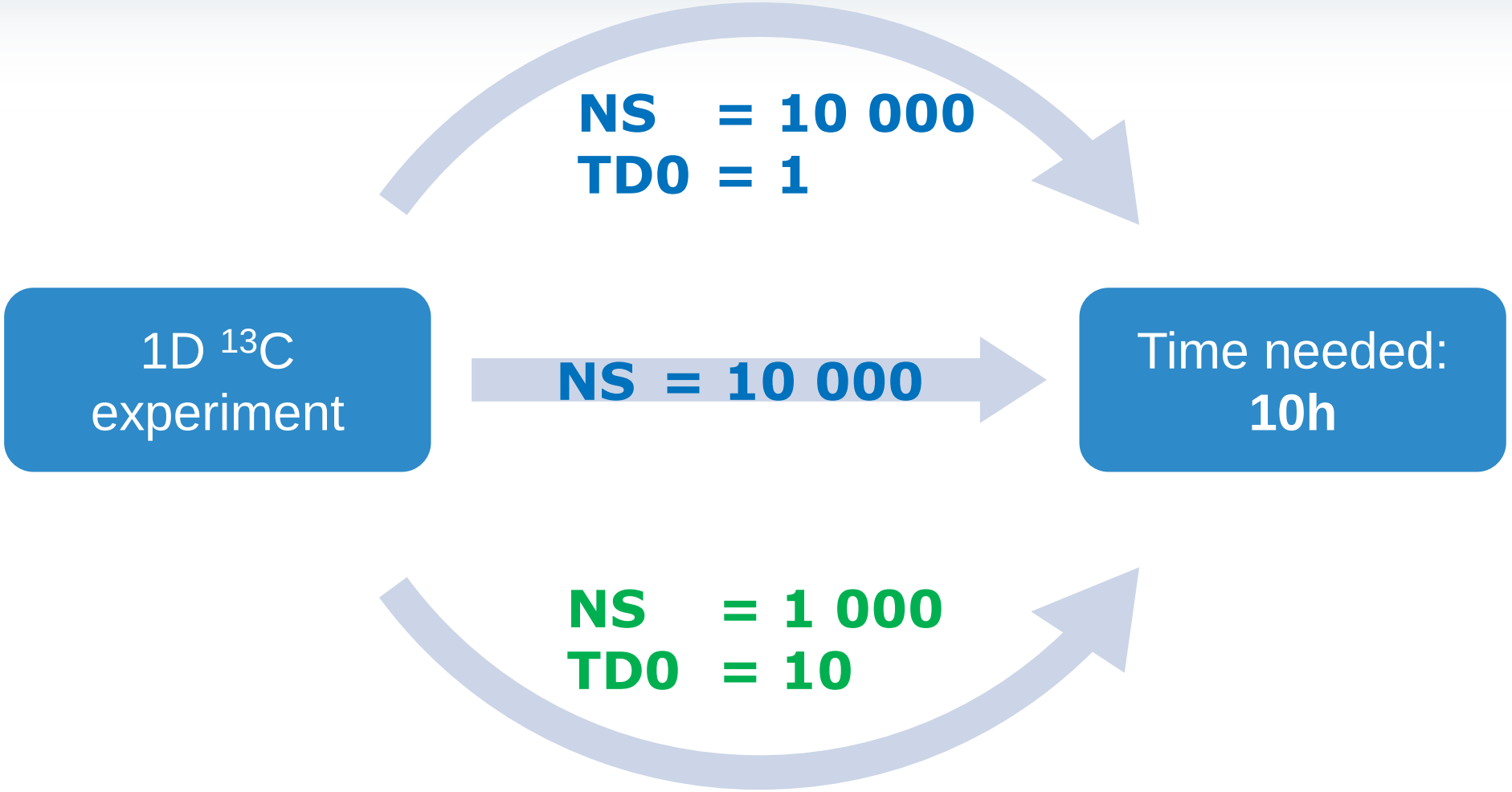
How to use **savelogs**





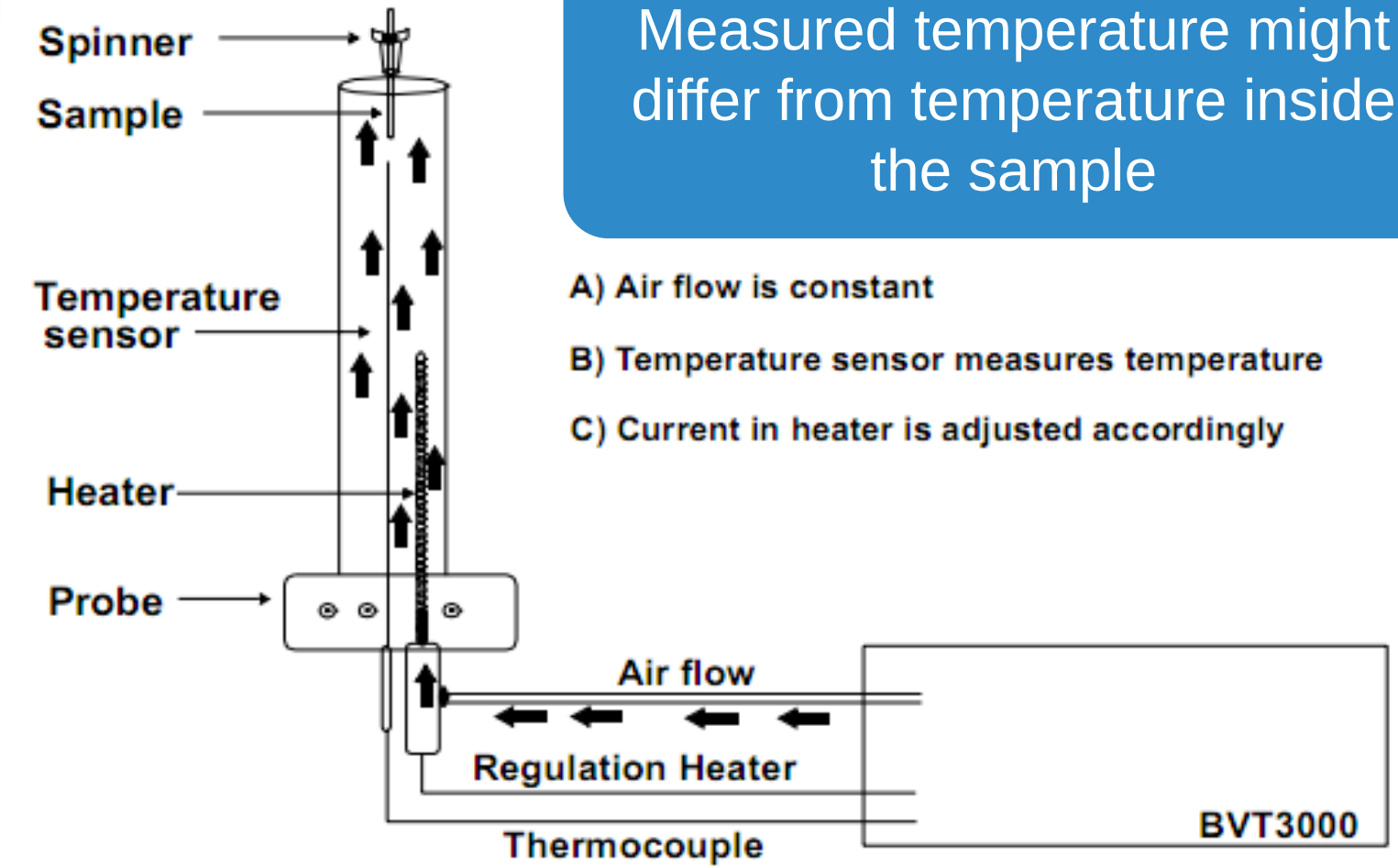
- **TD0**

TD0


NS = 10 000
TD0 = 1
1D ^{13}C experiment
NS = 10 000
Time needed:
10h
NS = 1 000
TD0 = 10

- **Temperature Calibration**

Basic Principle of Temperature Control



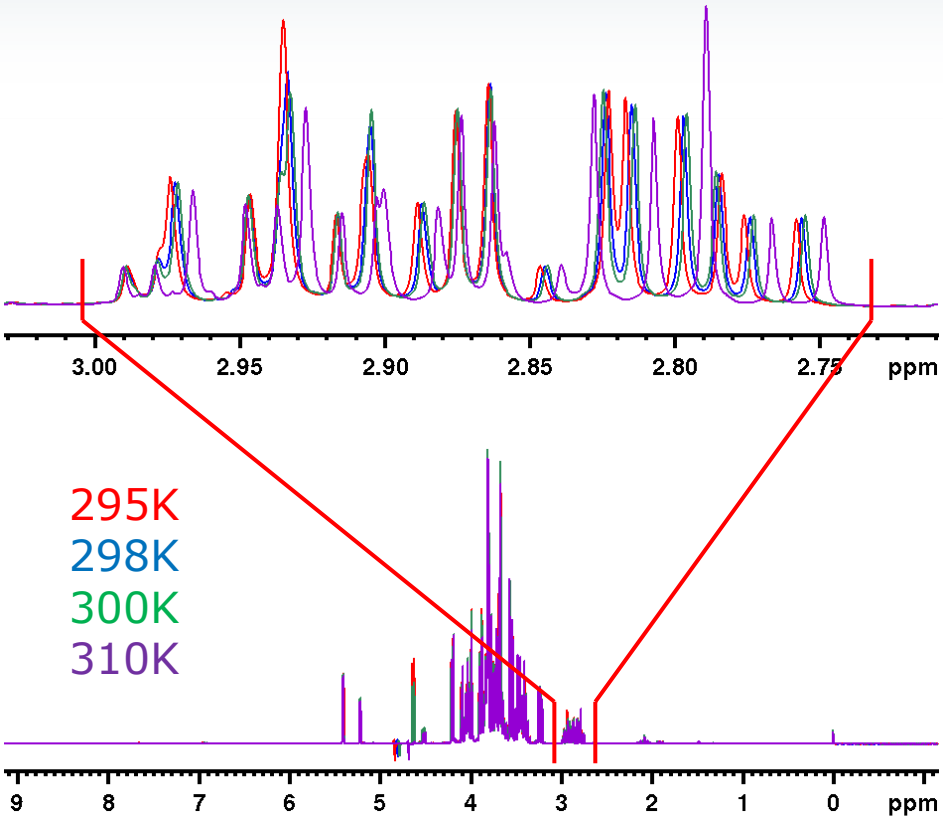
Measured temperature might differ from temperature inside the sample

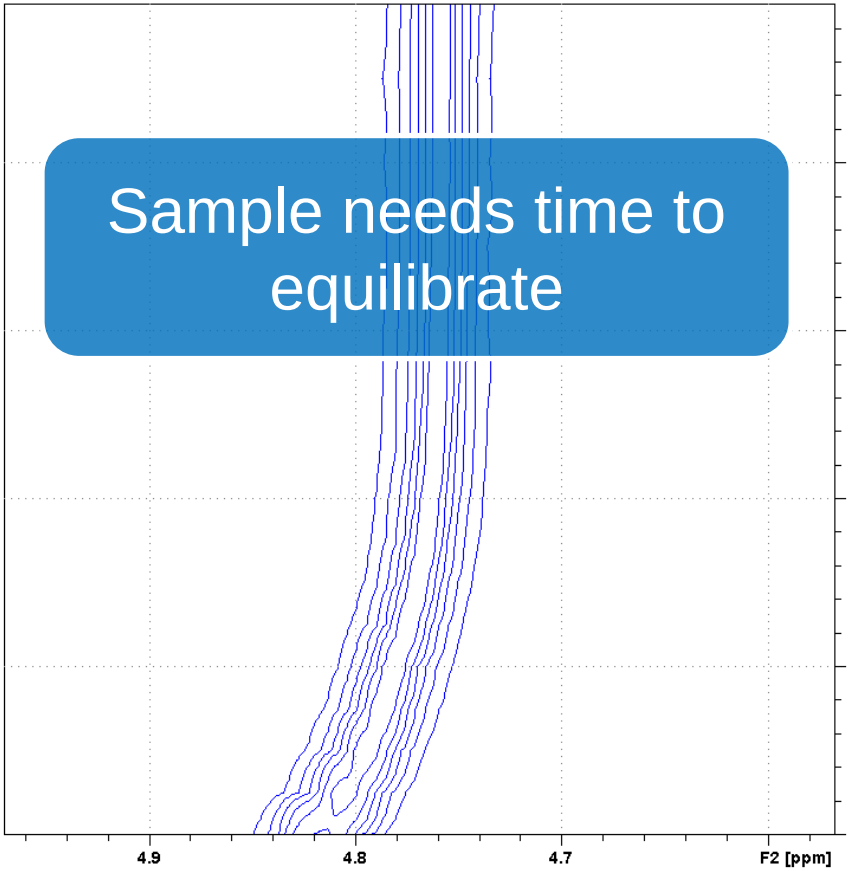
A) Air flow is constant

B) Temperature sensor measures temperature

C) Current in heater is adjusted accordingly

Effects of different/unstable temperature

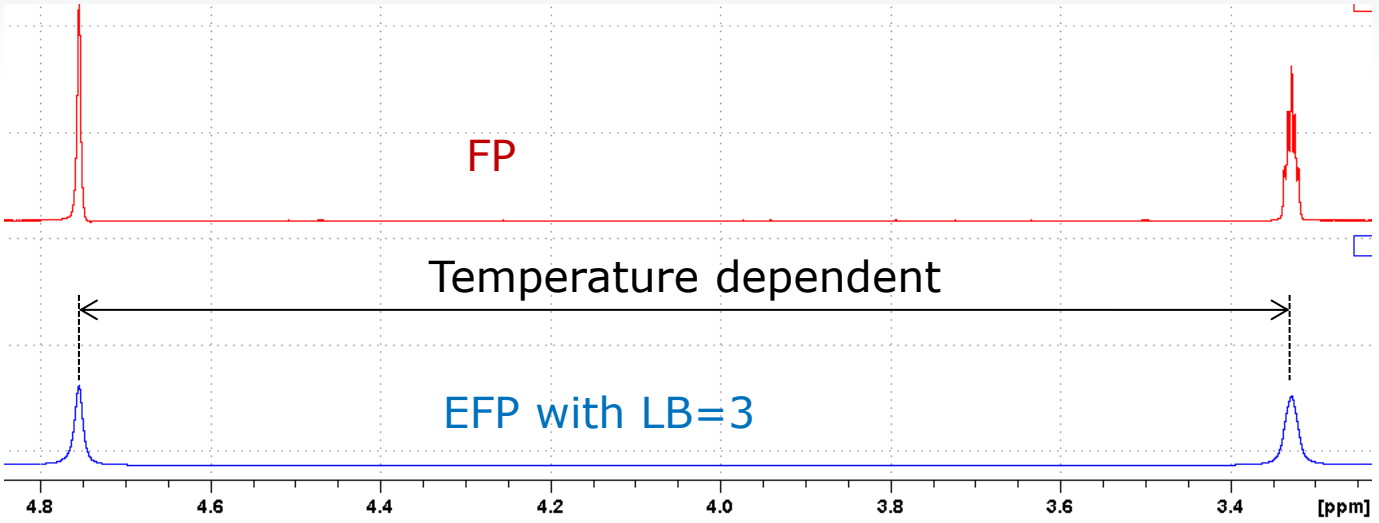




Sample needs time to equilibrate

Temperature must be identical to compare spectra

How to calibrate?

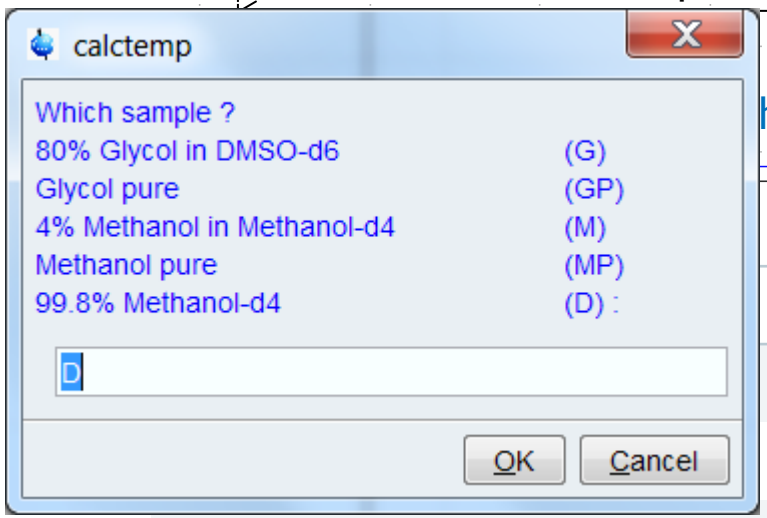


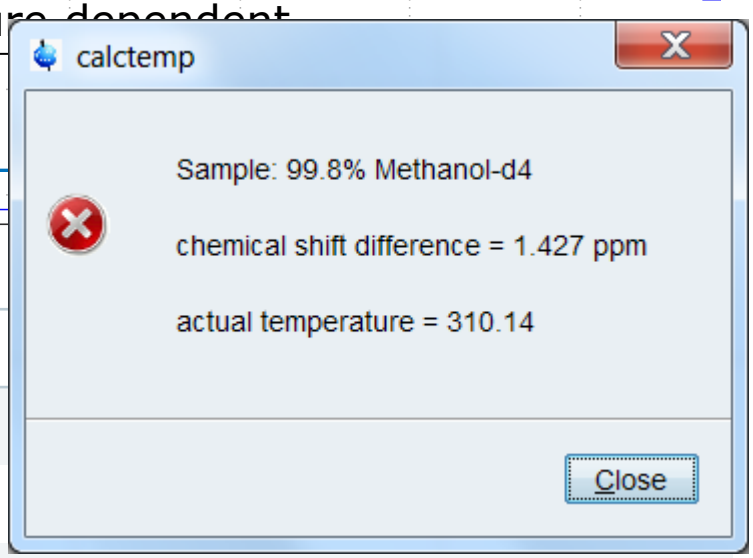
Sample	Range
80% Glycol in DMSO-d6	300 – 380K
Glycol, pure	300 – 380K
4% Methanol in Methanol-d4	181.2 – 300K
Methanol, pure	180.1 – 299.9K
99.8% Methanol-d4	282 – 330K

How to calibrate?

AU program:
CALCTEMP

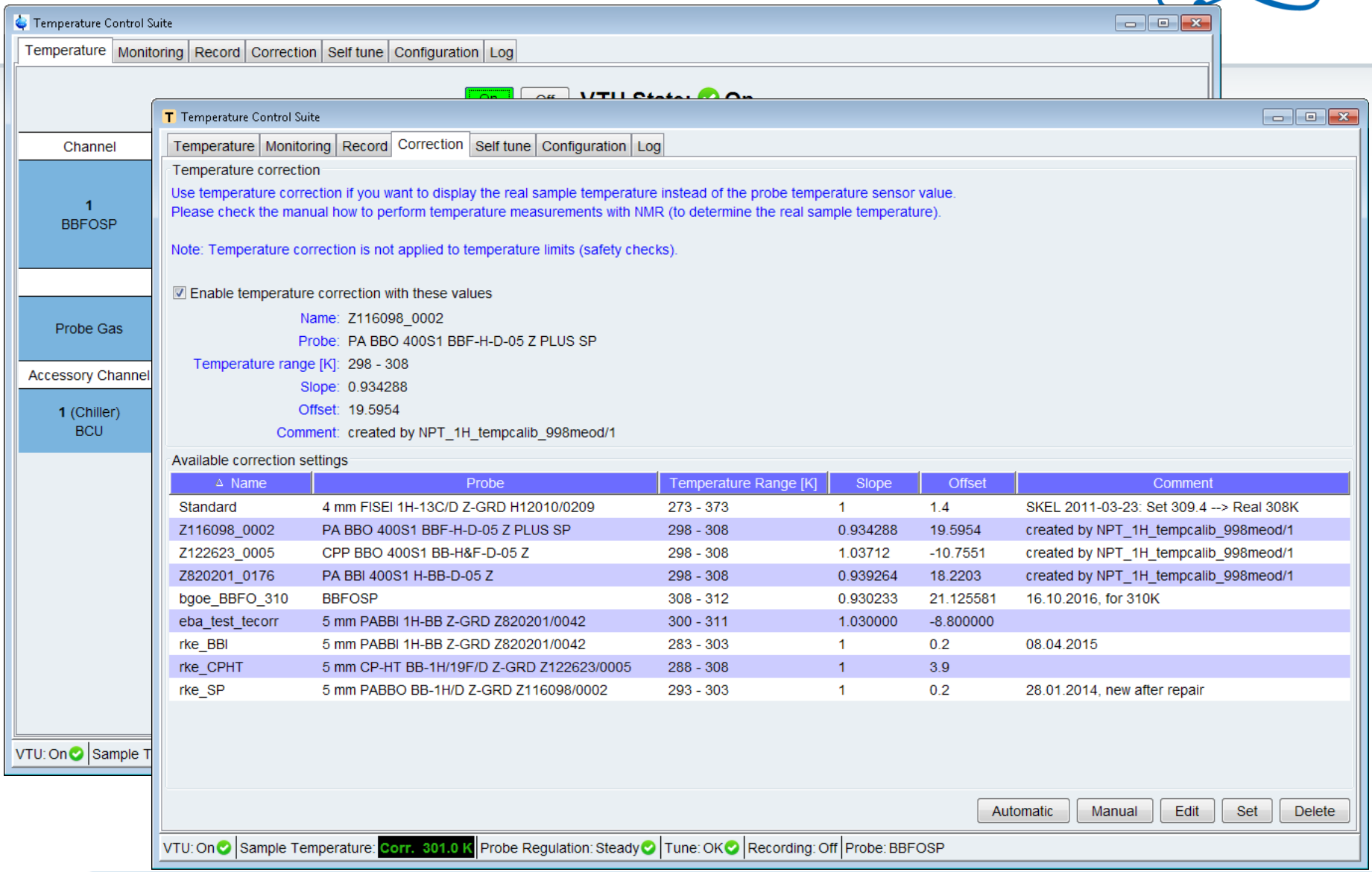
Temperature dependent





4% Methanol in Methanol-d4	181.2 – 300K
Methanol, pure	180.1 – 299.9K
99.8% Methanol-d4	282 – 330K

Set correction in Temperature Control [edte]



- **User Directories**

Summary

- each user starts with a list of default directories (e.g. lists/pp and lists/pp/user)
- each user can remove one or more default directories from its list
- each user can specify one or more additional source directories
- each user can define the order of the directories which defines the search order within TopSpin

How to use different source directories

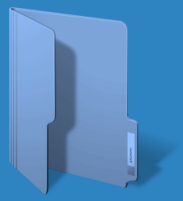
<shared folder>

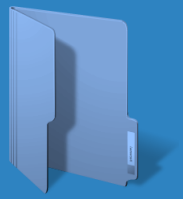
<Home>/myPP

../pp/user

../pp

How to use different source directories





Bruker files in:

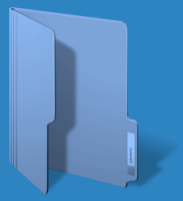
.../exp/stan/nmr/lists/pp

These files are write protected!

You can be sure that these files always contain the original Bruker library file!

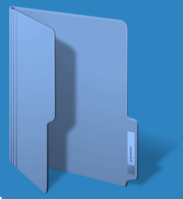
How to use different source directories

<shared folder>



<Home>/myPP

../pp/user



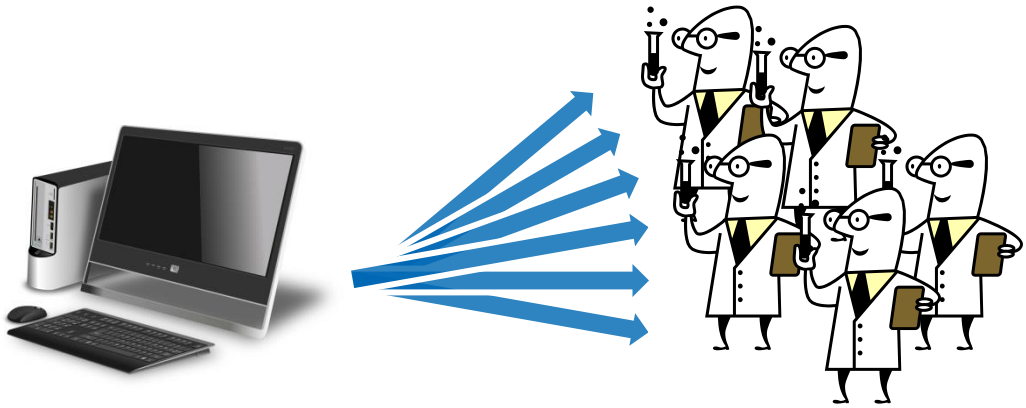
../pp

User files in:

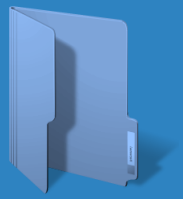
…/exp/stan/nmr/lists/pp/user

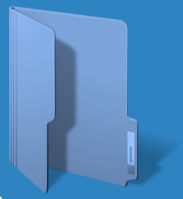
By default all user-specific files will be stored here; read- and writable

You have an easy setup to distribute user-specific files to all colleagues



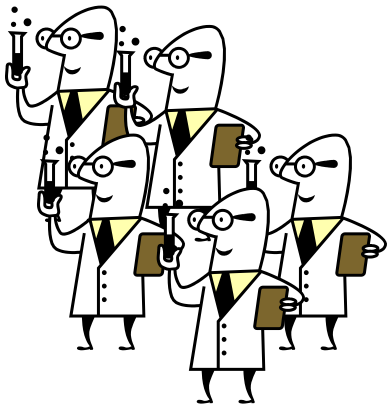
How to use different source directories



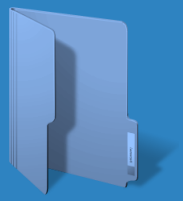


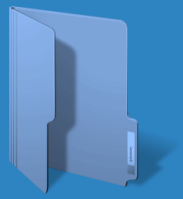
Each user can define his **own source directories**

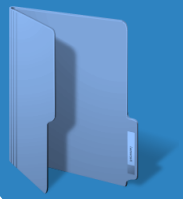
If you store them e.g. in your home directory, then they are automatically read and write protected for anybody else



How to use different source directories

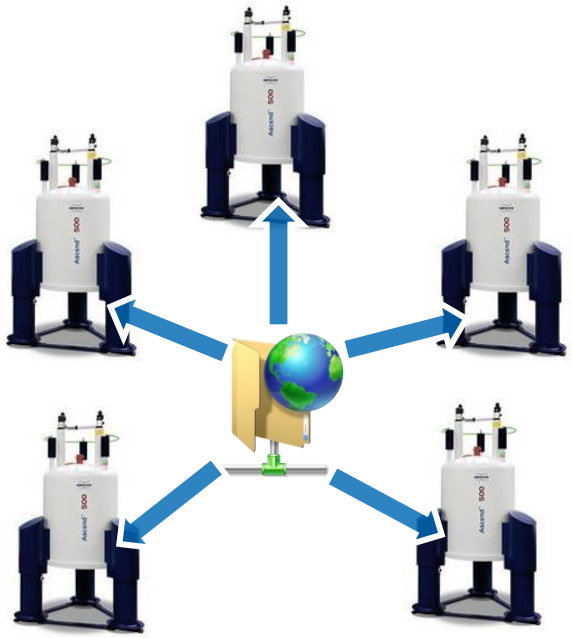




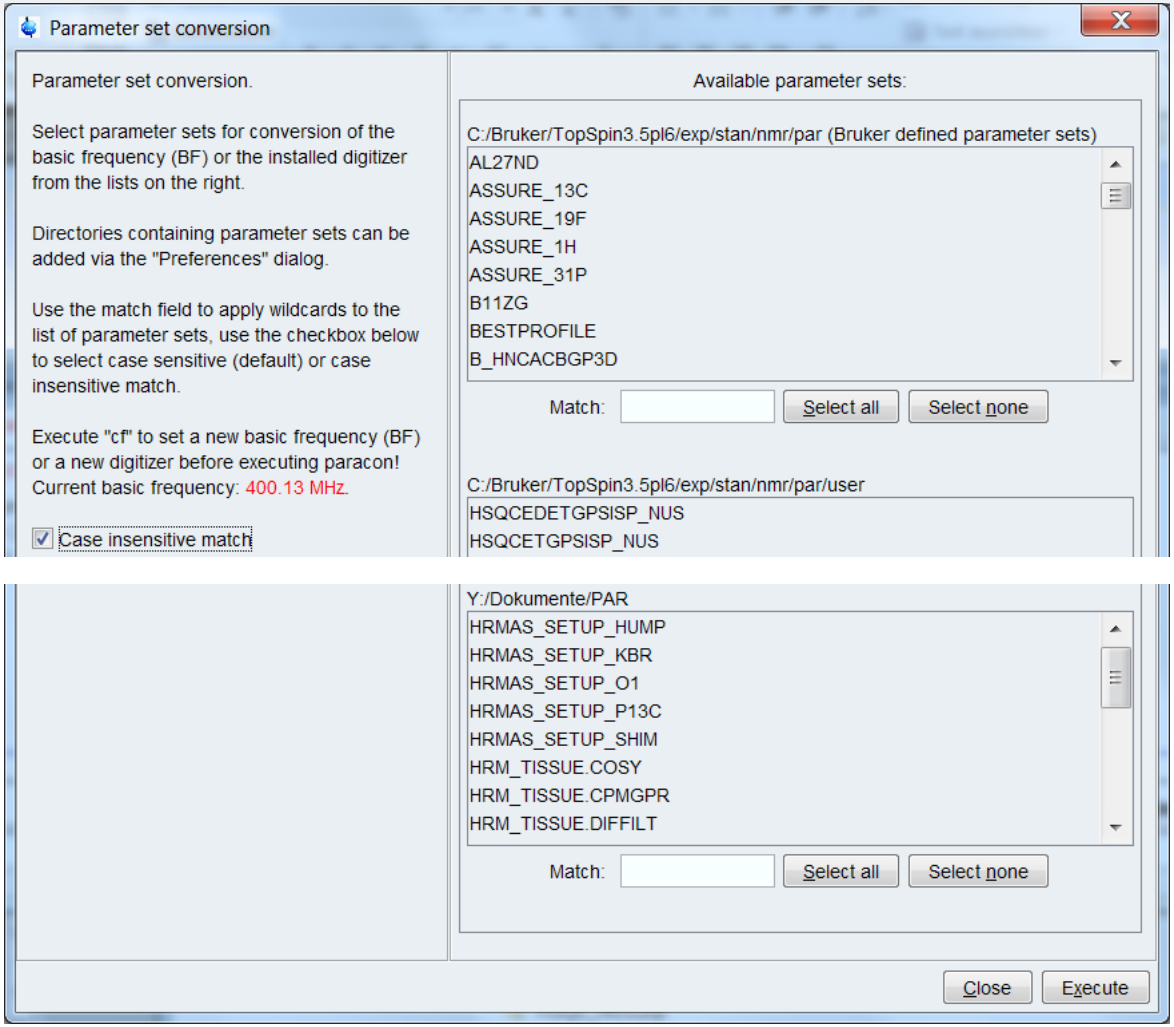


These files can be easily distributed!

It is easy to use e.g. your pulse programs on different spectrometers, just define a network drive as a source directory.



Convert parameter sets [**paracon**]



Parameters of one spectrometer cannot be used at another spectrometer.

Need to be converted to spectrometer frequency and routing:

paracon

Supports user defined directories

- **Serial processing**

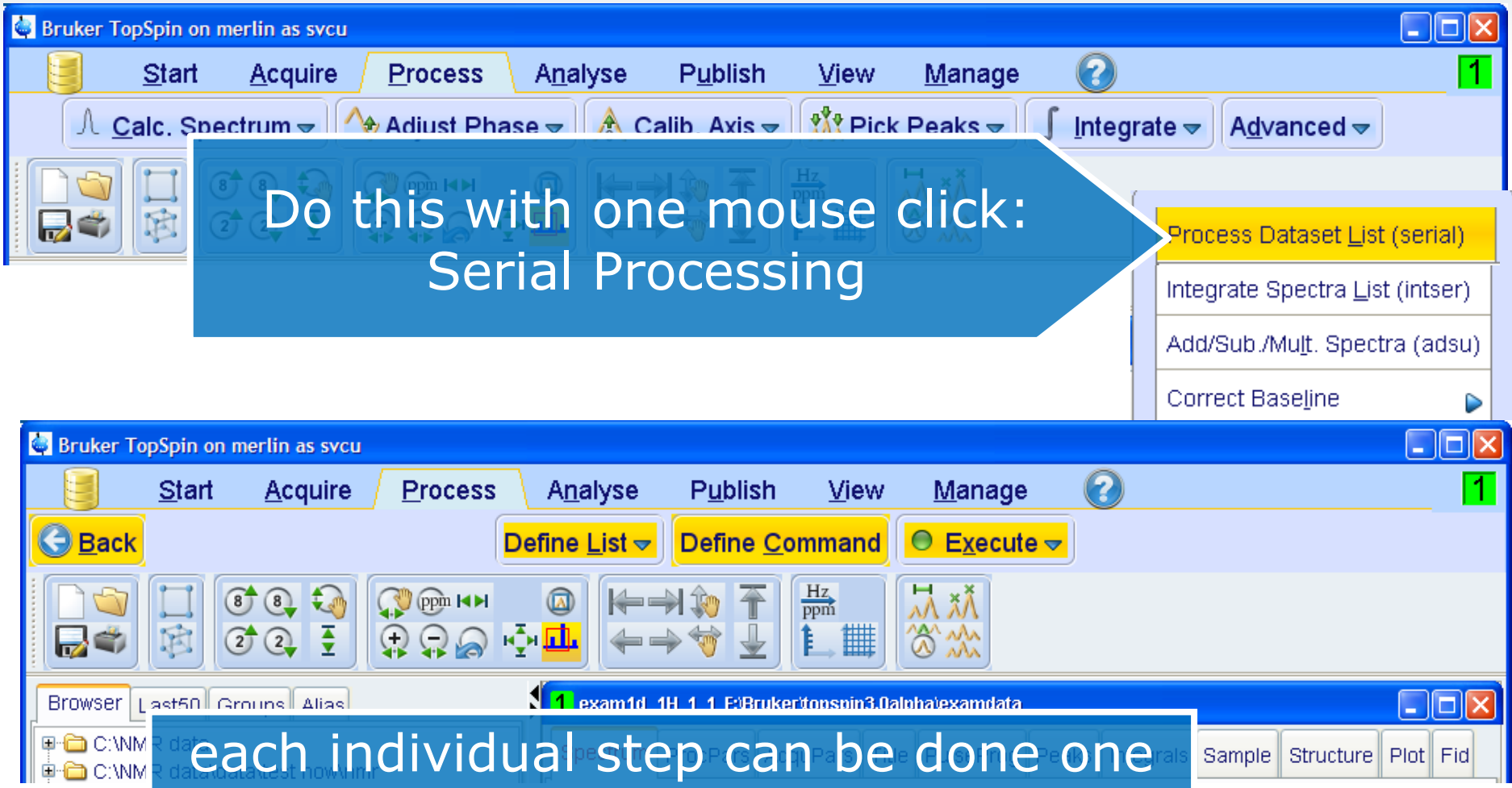
Repetitive Tasks …

You would like to run a sequence of processing steps?

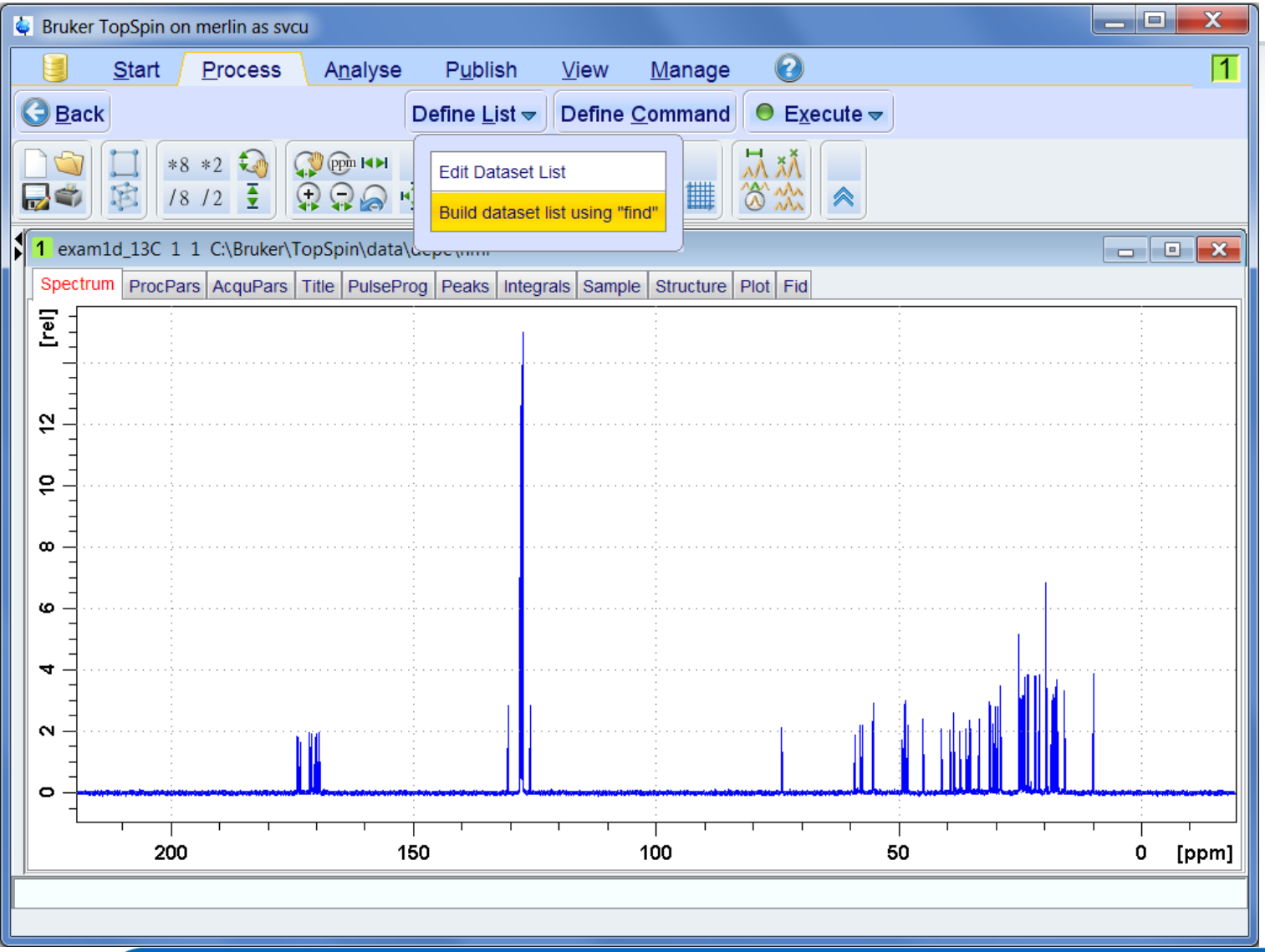
and these should be executed on several datasets?

SERIAL PROCESSING

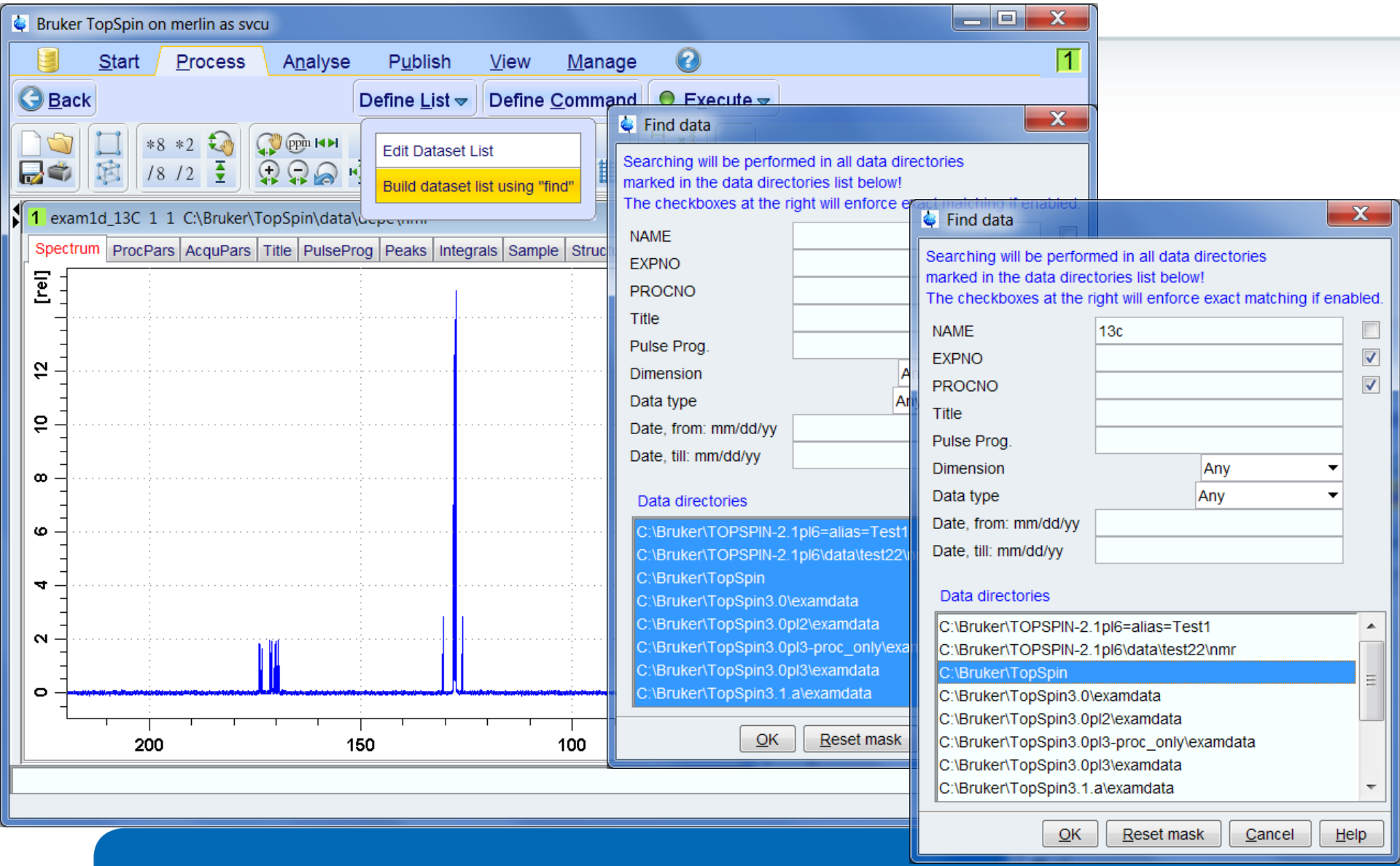
Serial Processing



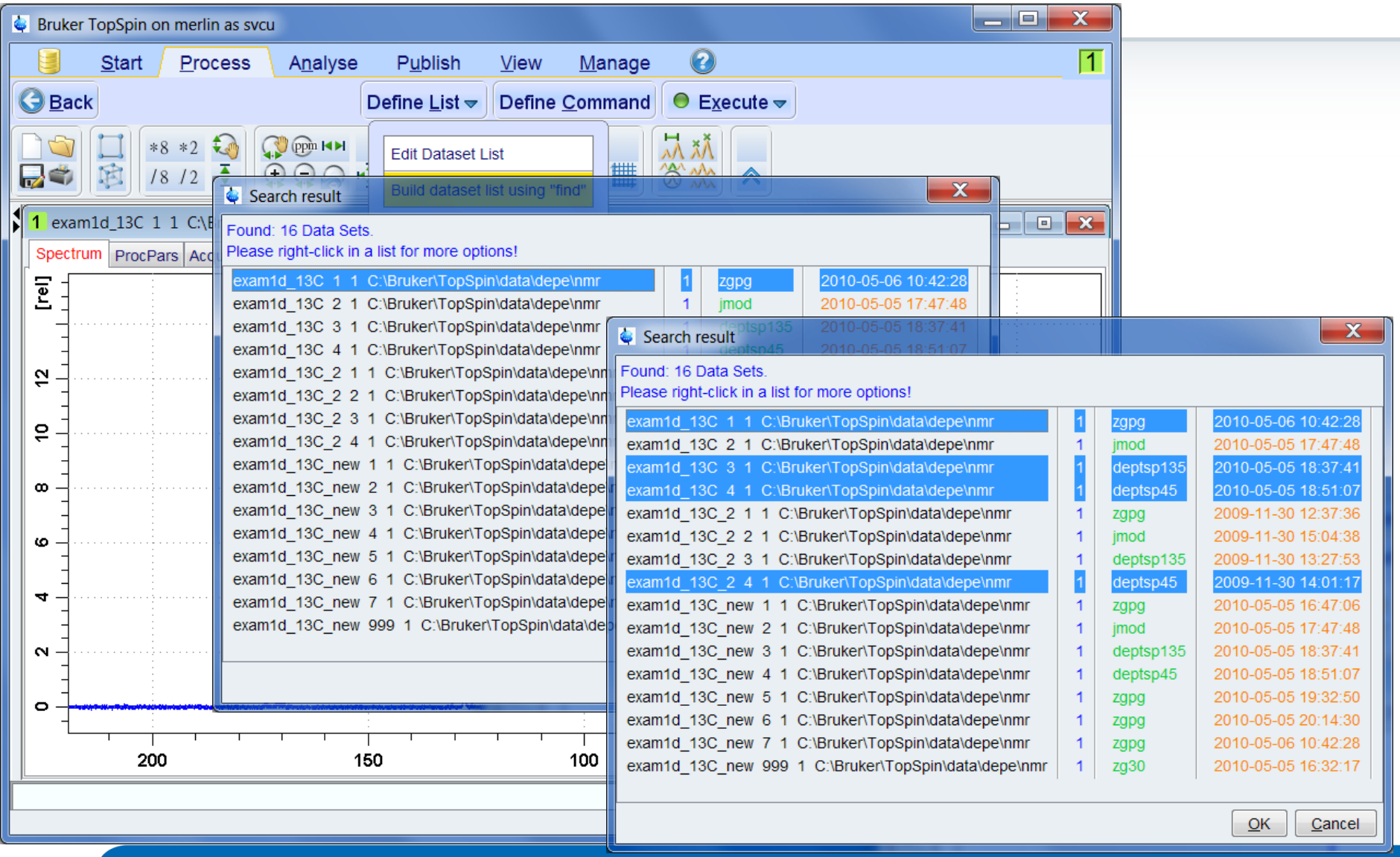
Serial Processing – find datasets



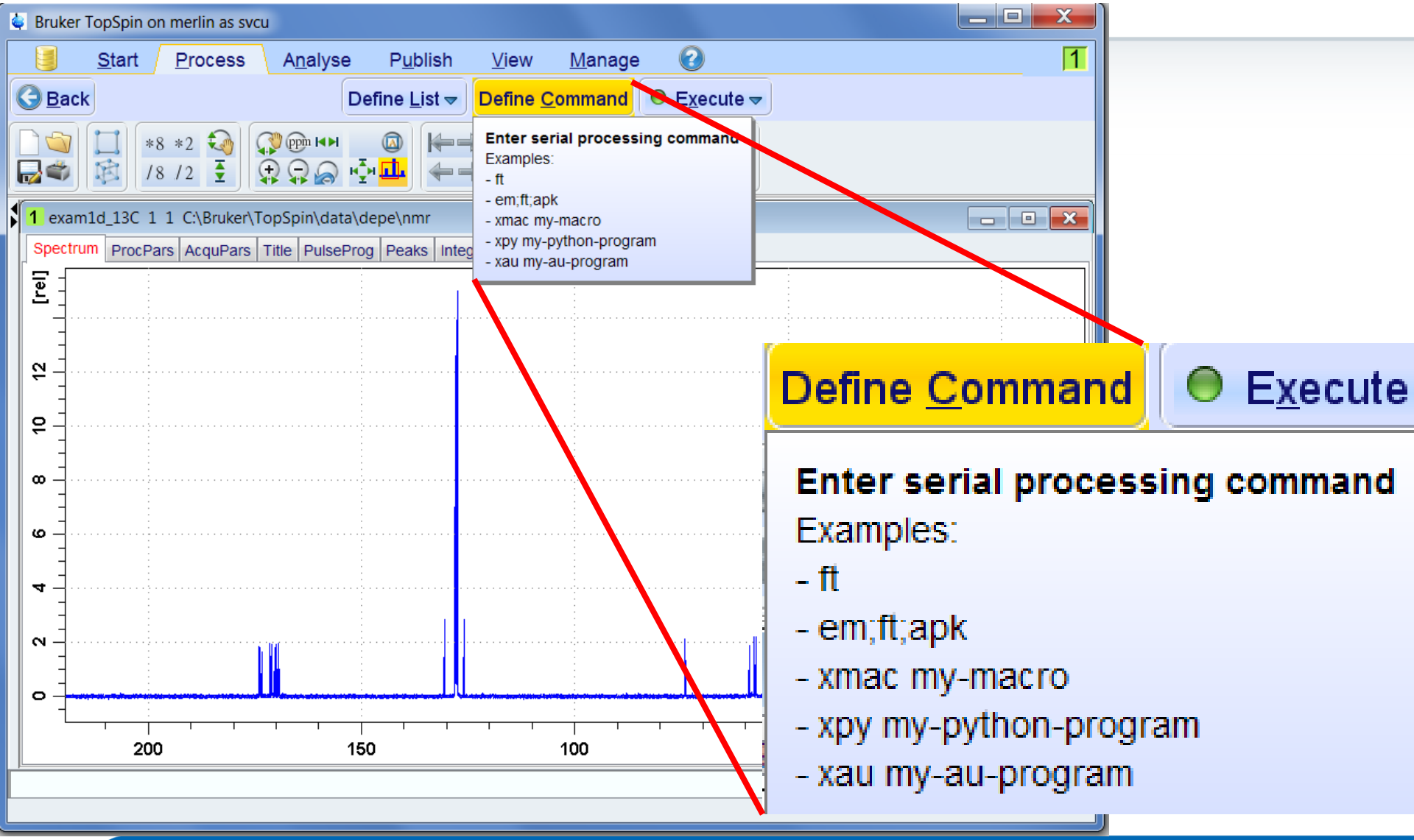
Serial Processing – find datasets



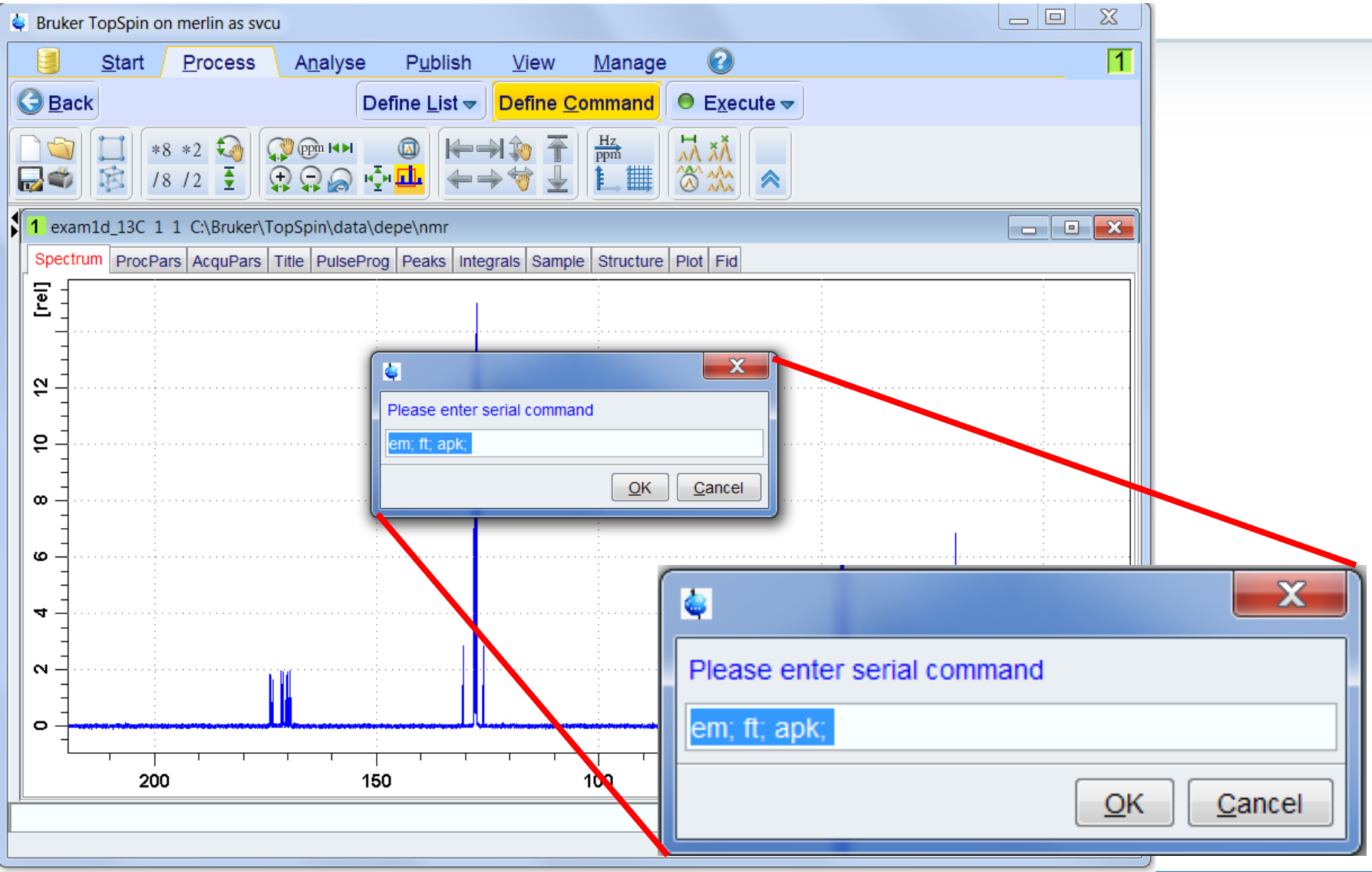
Serial Processing – find datasets



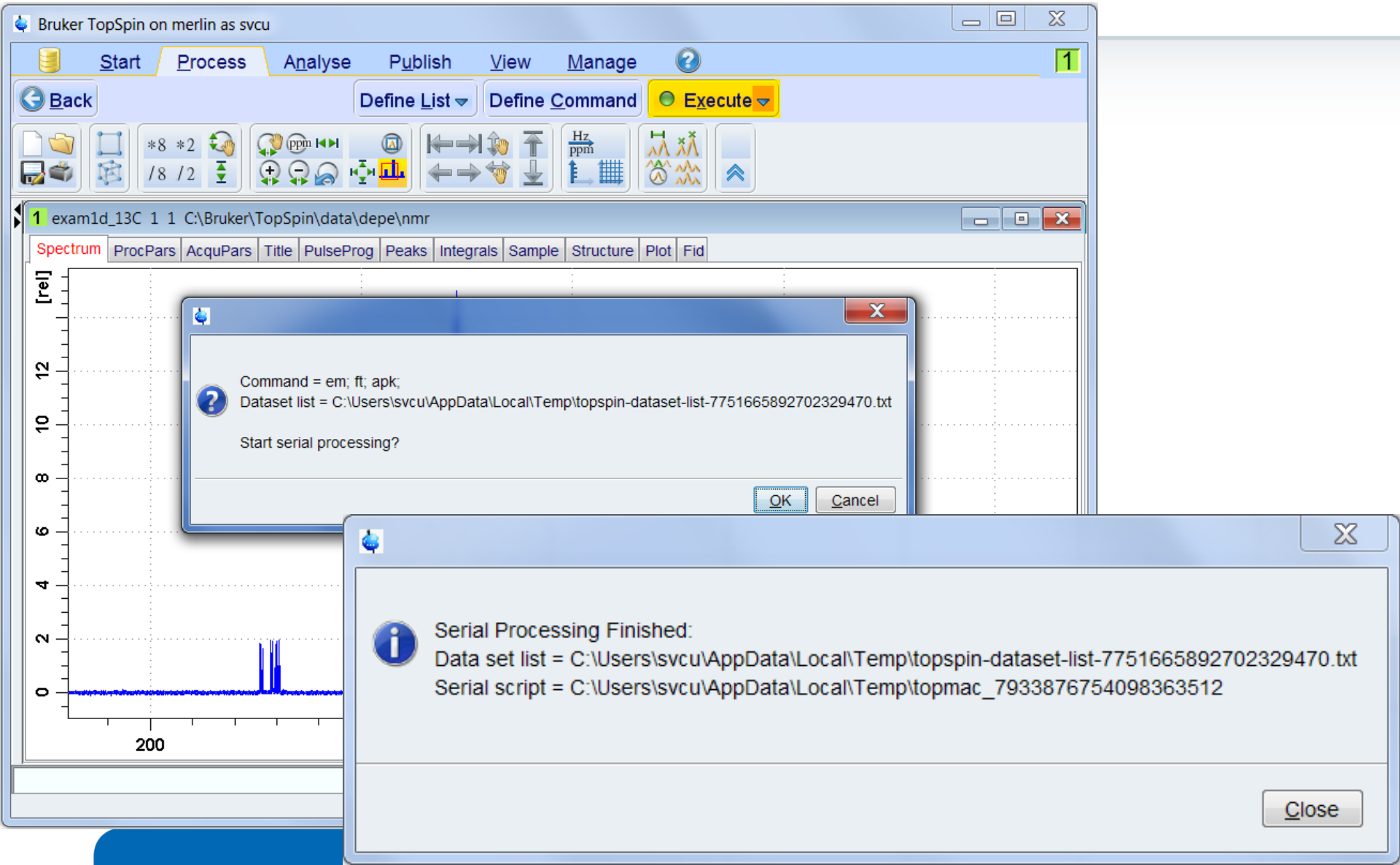
Serial Processing – commands



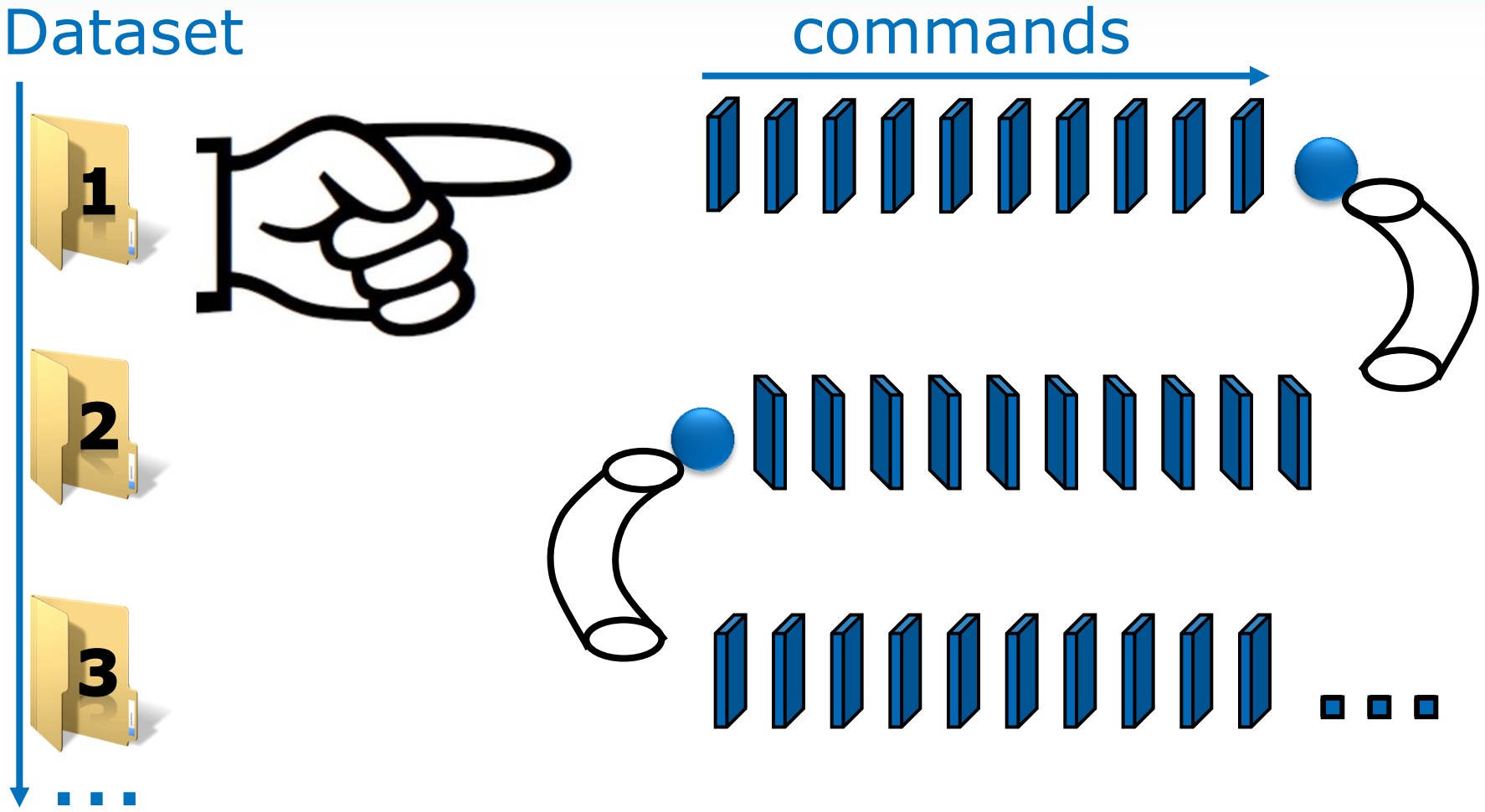
Serial Processing – commands example



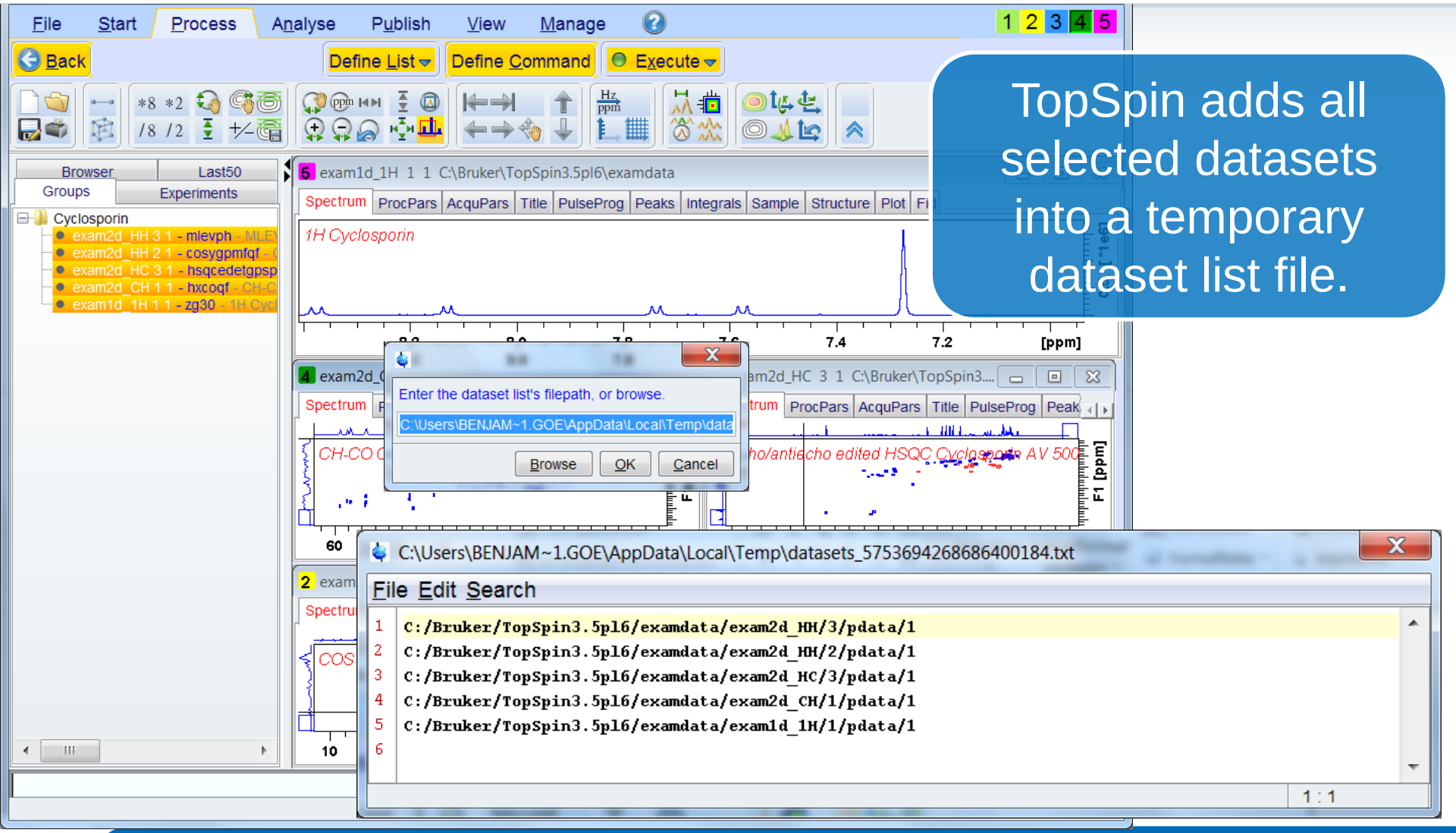
Serial Processing – execute



Serial Processing



Group members meet serial processing



TopSpin adds all selected datasets into a temporary dataset list file.

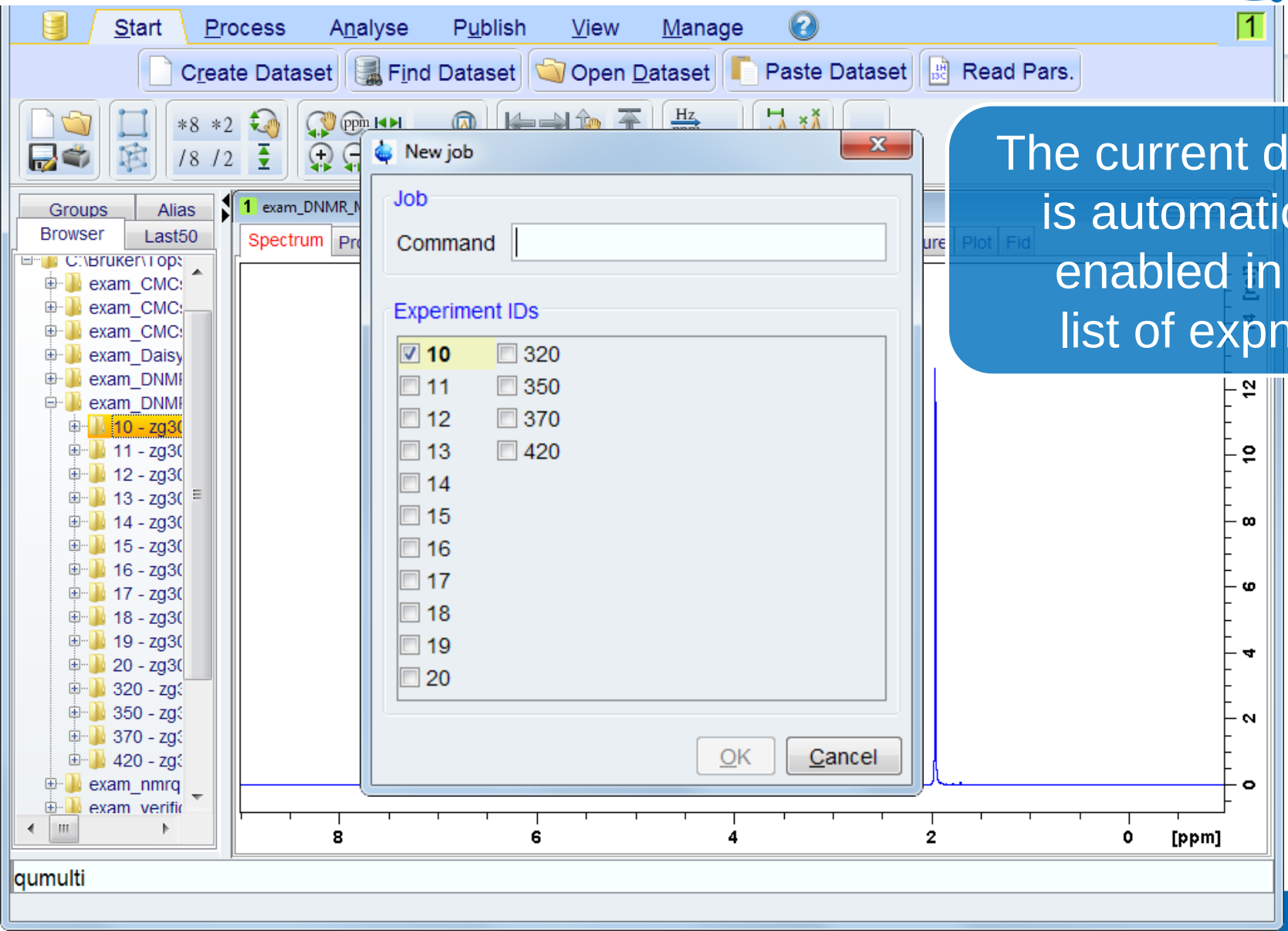
- **qumulti**

Command spooler

- Any command in TopSpin can be sent to the spooler (**qu <command>**)
- Tasks in the spooler are executed sequentially
- It is possible to define the experiment number on which a command should be queued:

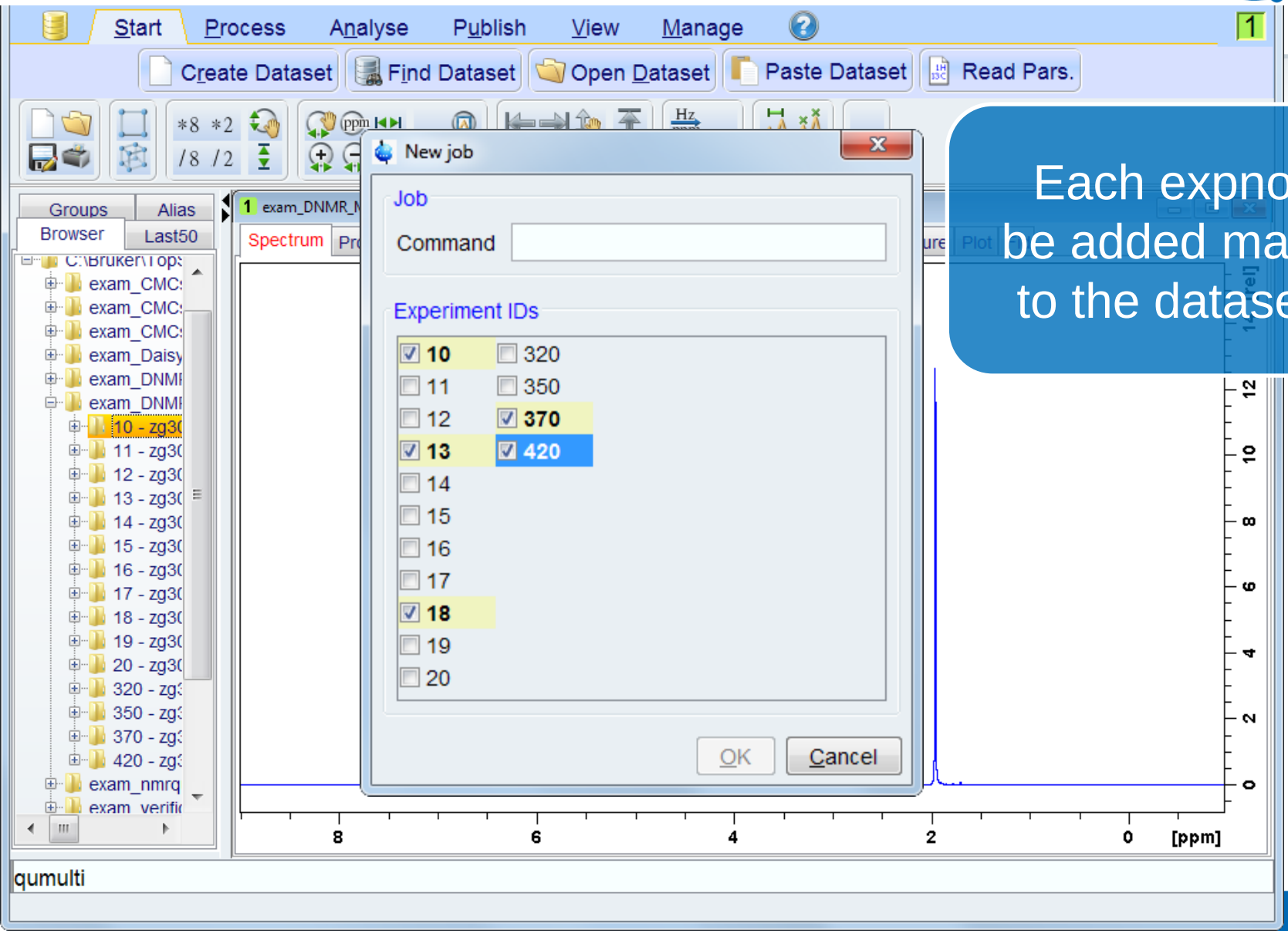
QUMULTI

qumulti



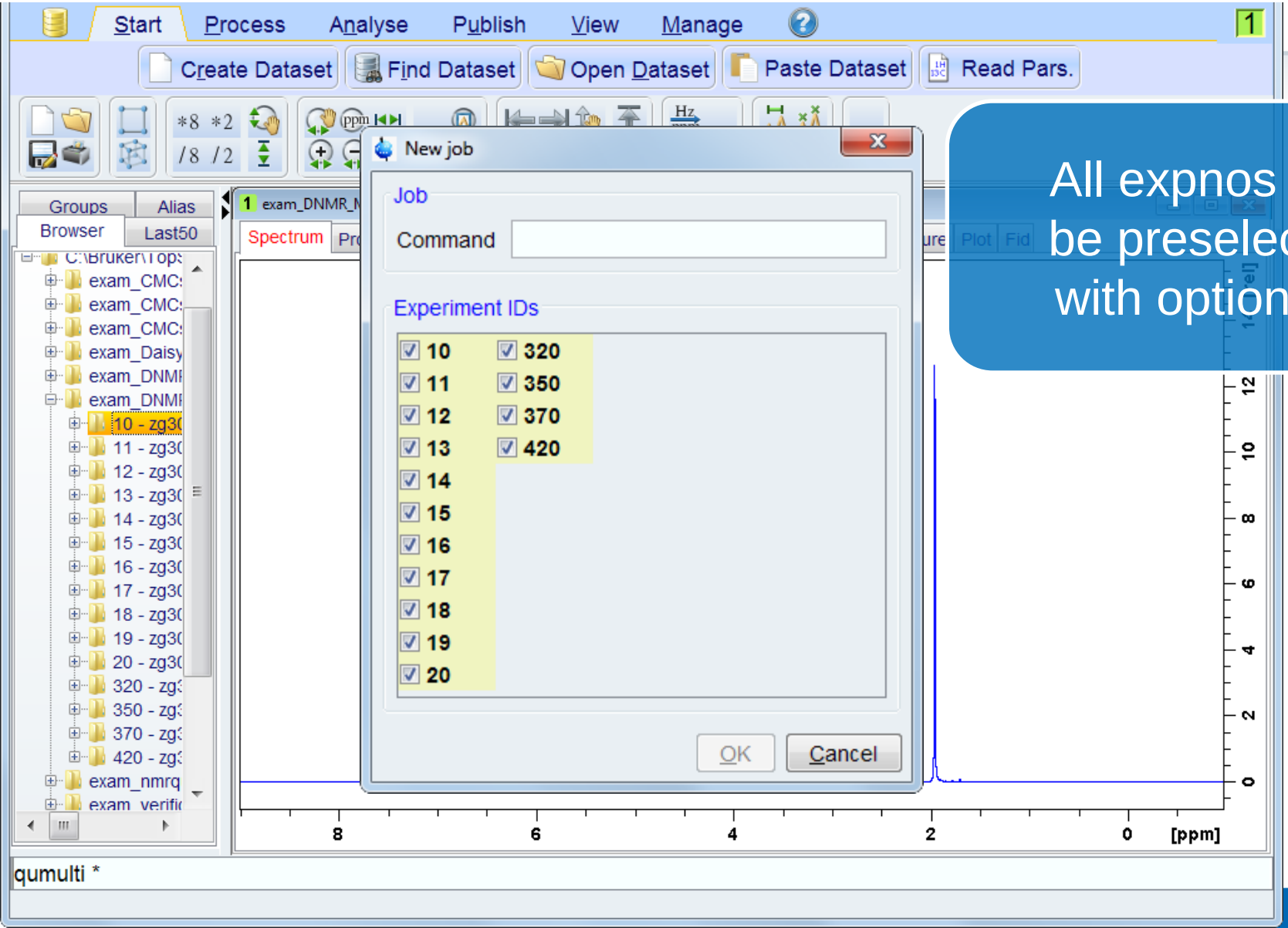
The current dataset is automatically enabled in the list of expnos.

qumulti



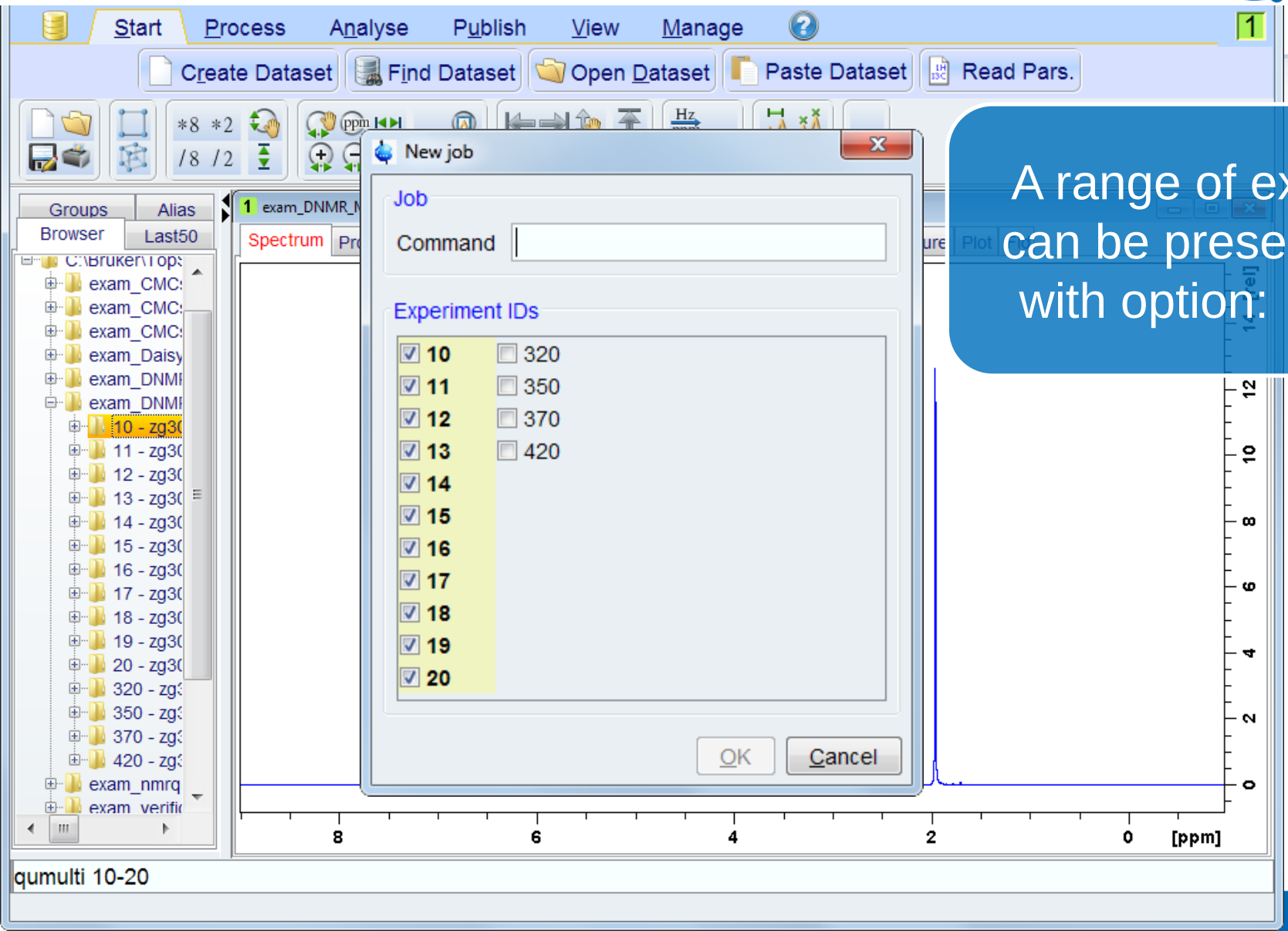
Each expno can be added manually to the dataset list.

qumulti *



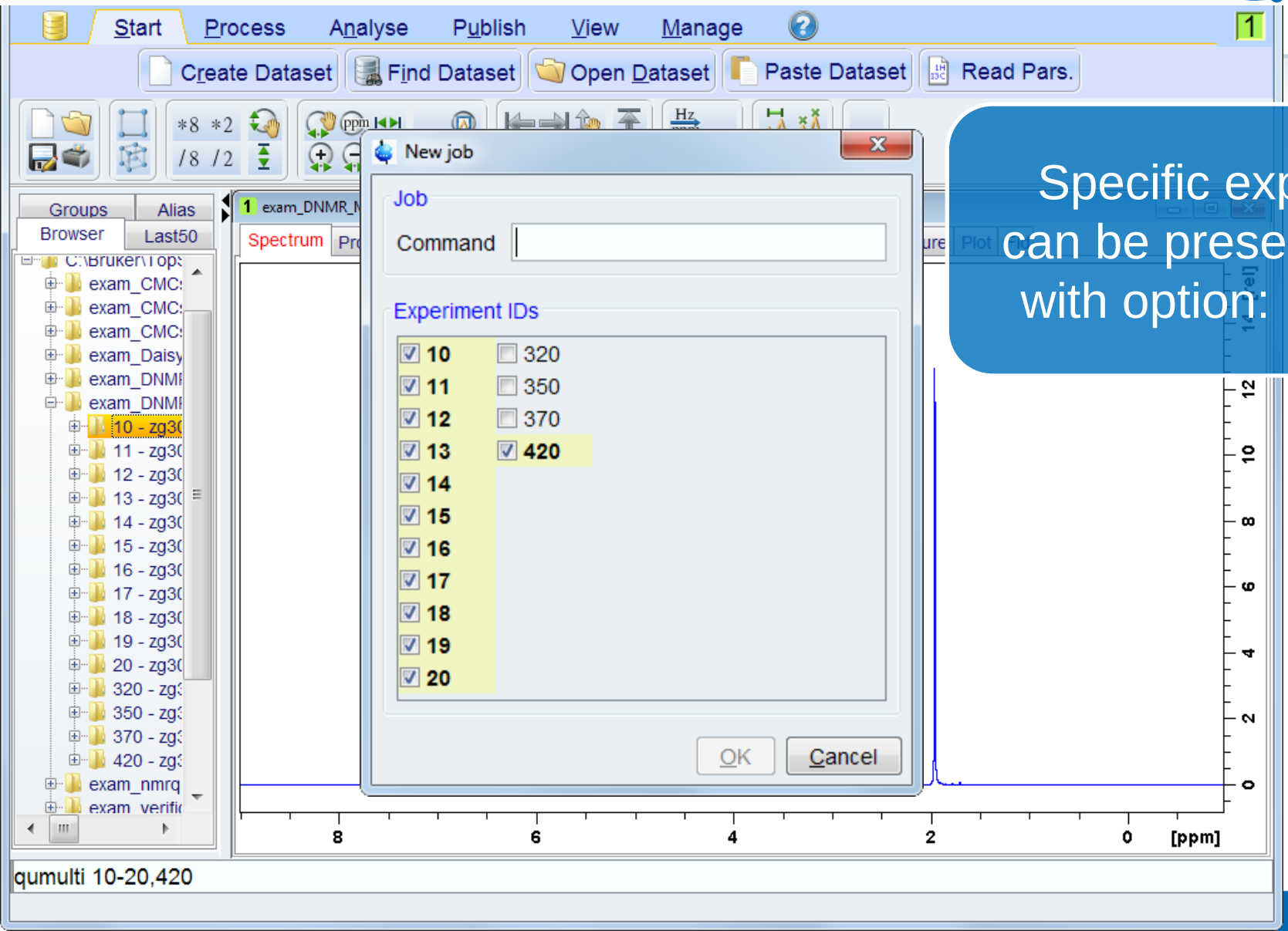
All expnos can be preselected with option: *

qumulti n-m



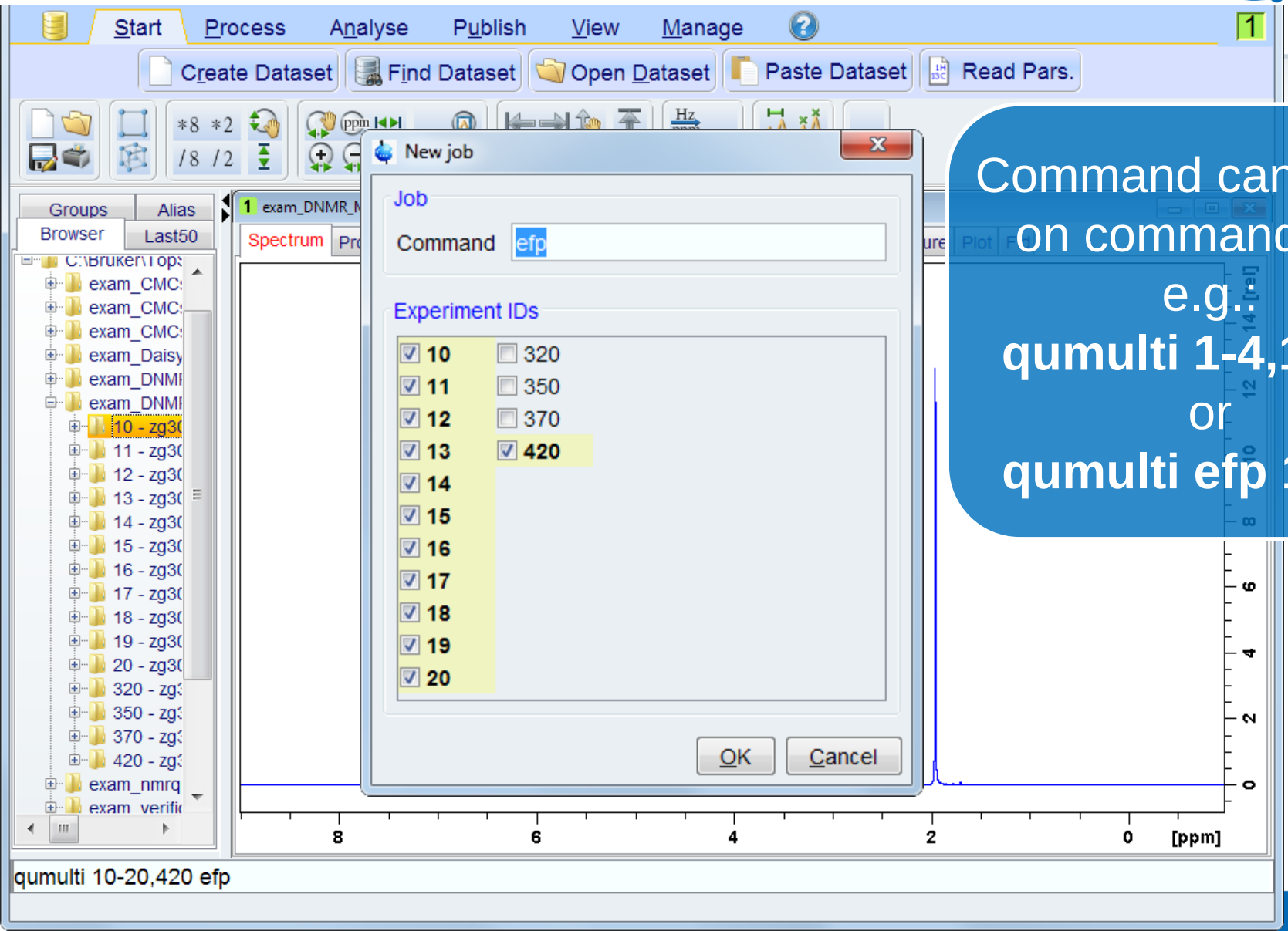
A range of expnos can be preselected with option: **n-m**

qumulti n,m



Specific expnos can be preselected with option: **n,m**

qumulti



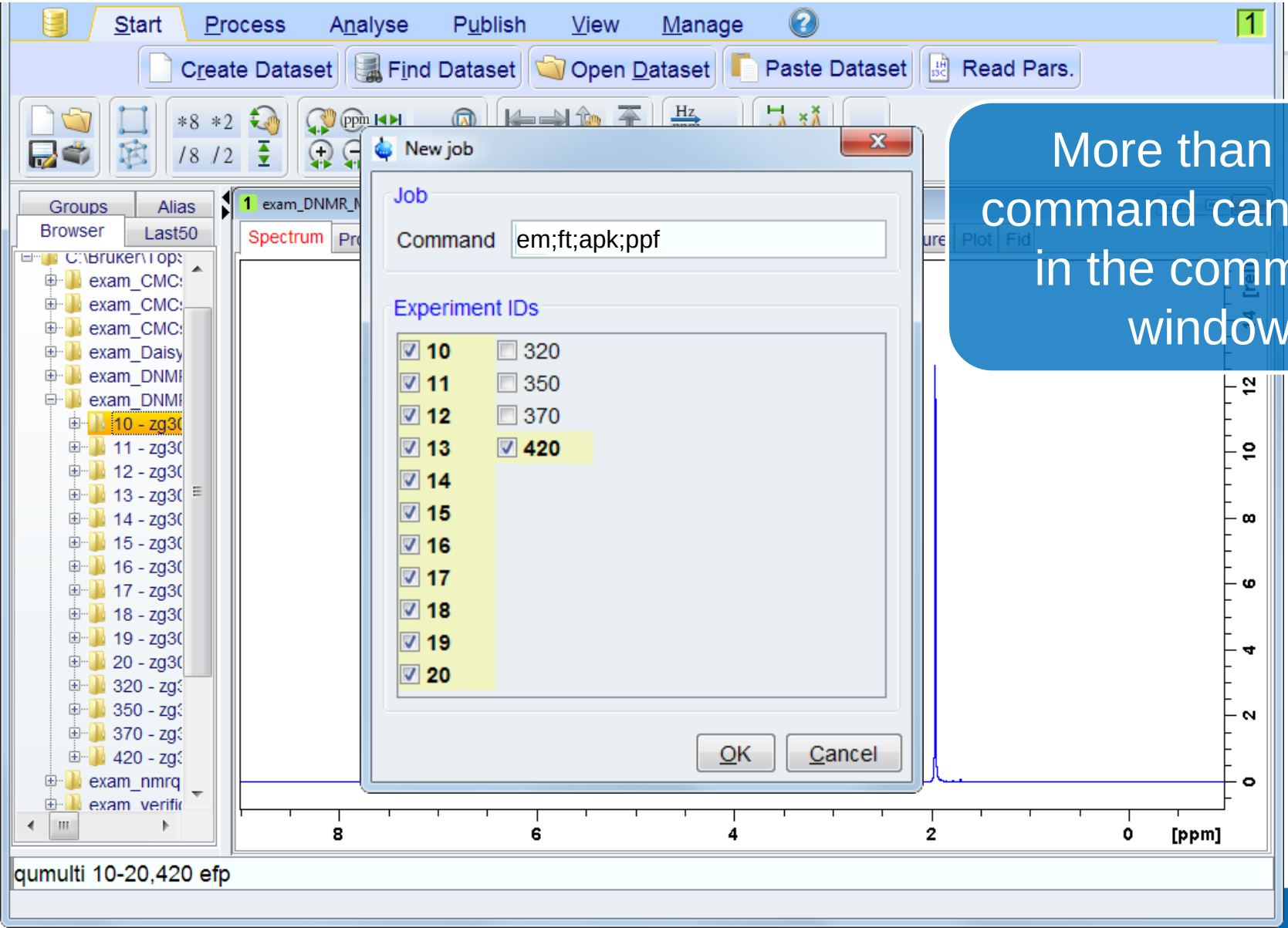
Command can be set on command line, e.g.:

qumulti 1-4,11 efp

or

qumulti efp 1-4,11

qumulti



More than one command can be set in the command window

qumulti vs. Serial Processing

qumulti

For NMR data stored under one dataset name
=
Using of Expnos

fast ✓

Serial Processing

For NMR data stored under several dataset names
=
Using of Names

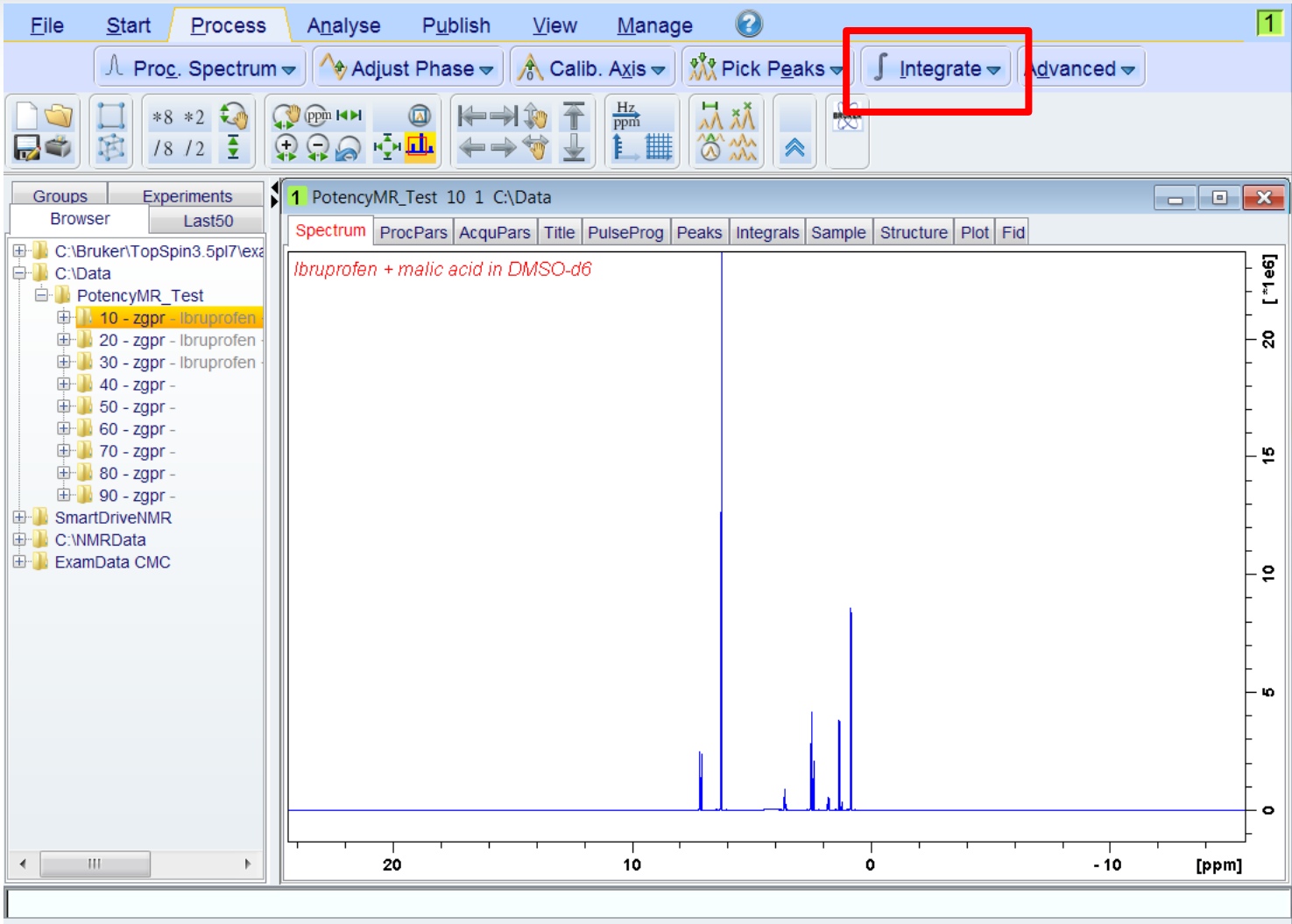
powerful ✓

- **Serial Integration**

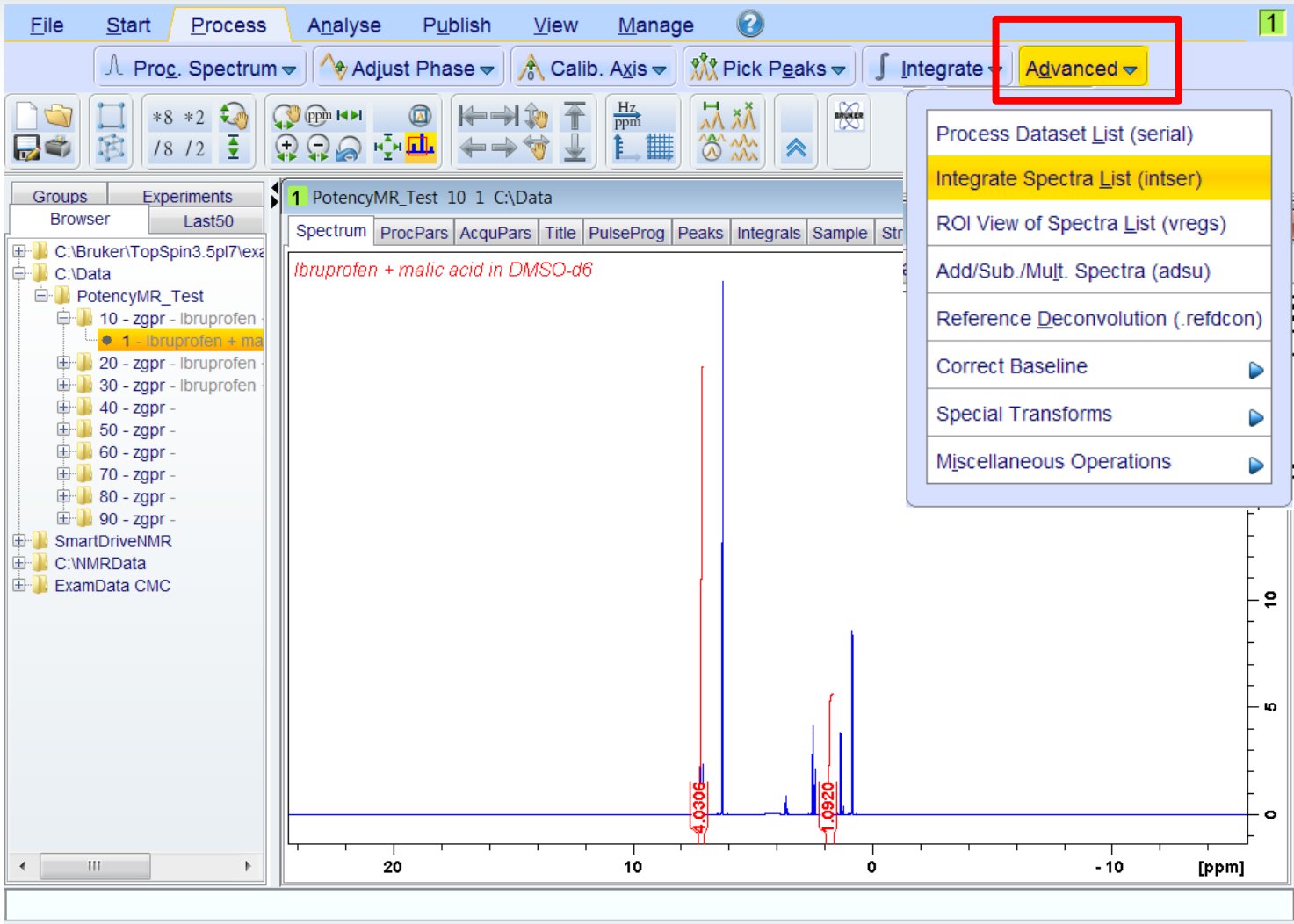
intser – automatic integration of a series of spectra

- User defined list of datasets
- Use integrals of first dataset in list
- Allows easy normalization of any integral
- For 1D and 2D

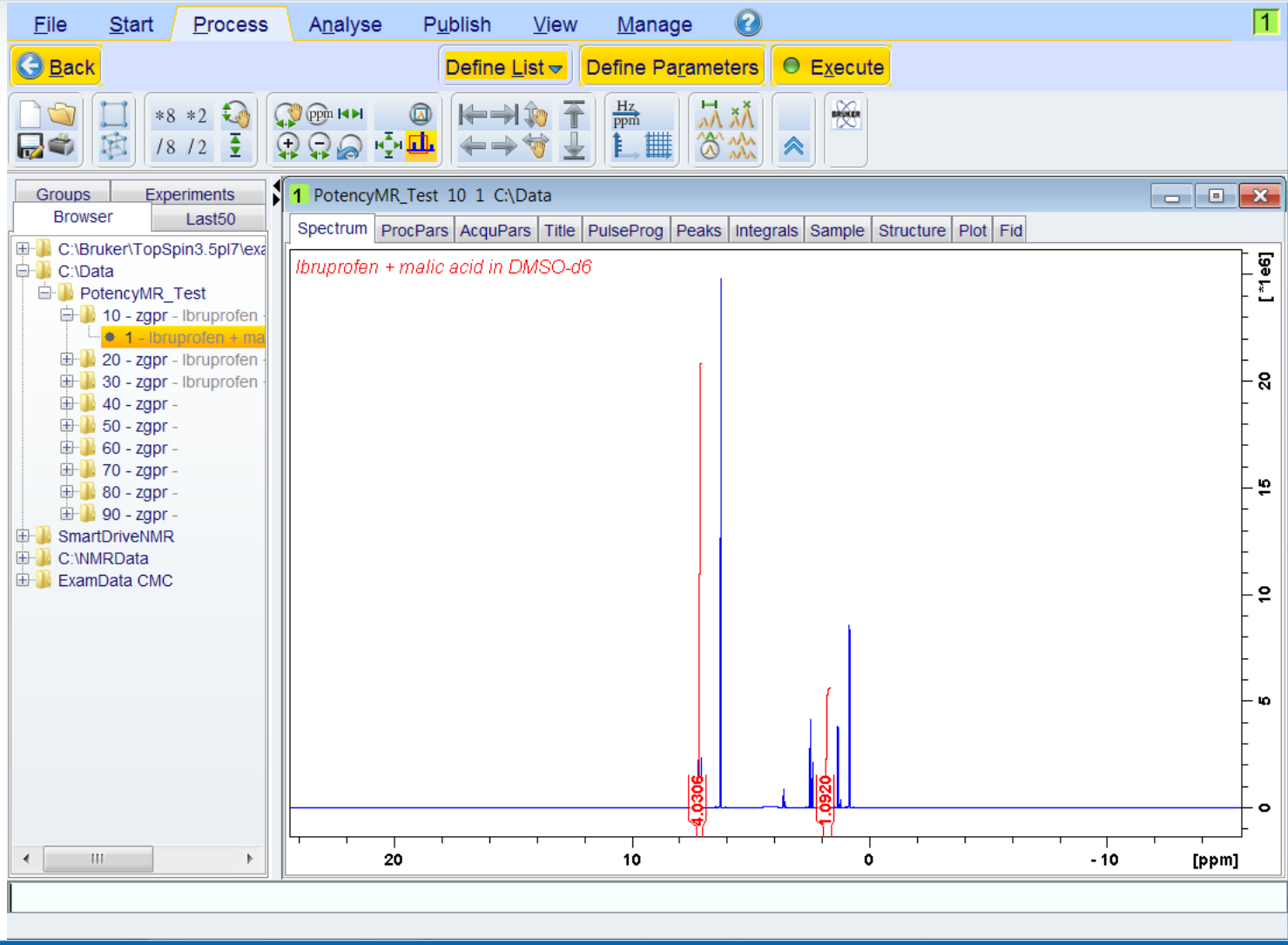
Define integrals in first dataset



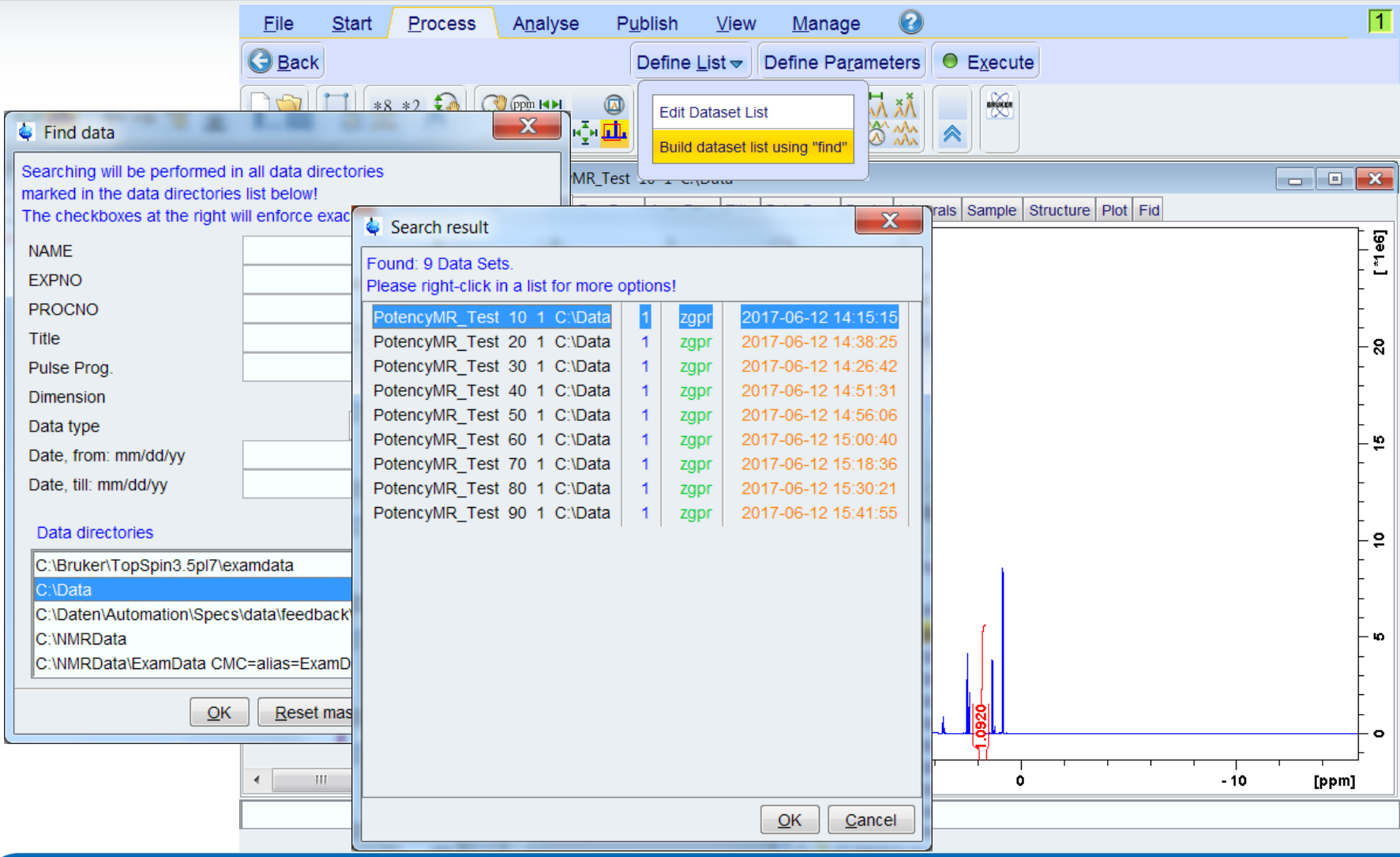
Advanced processing – **intser**



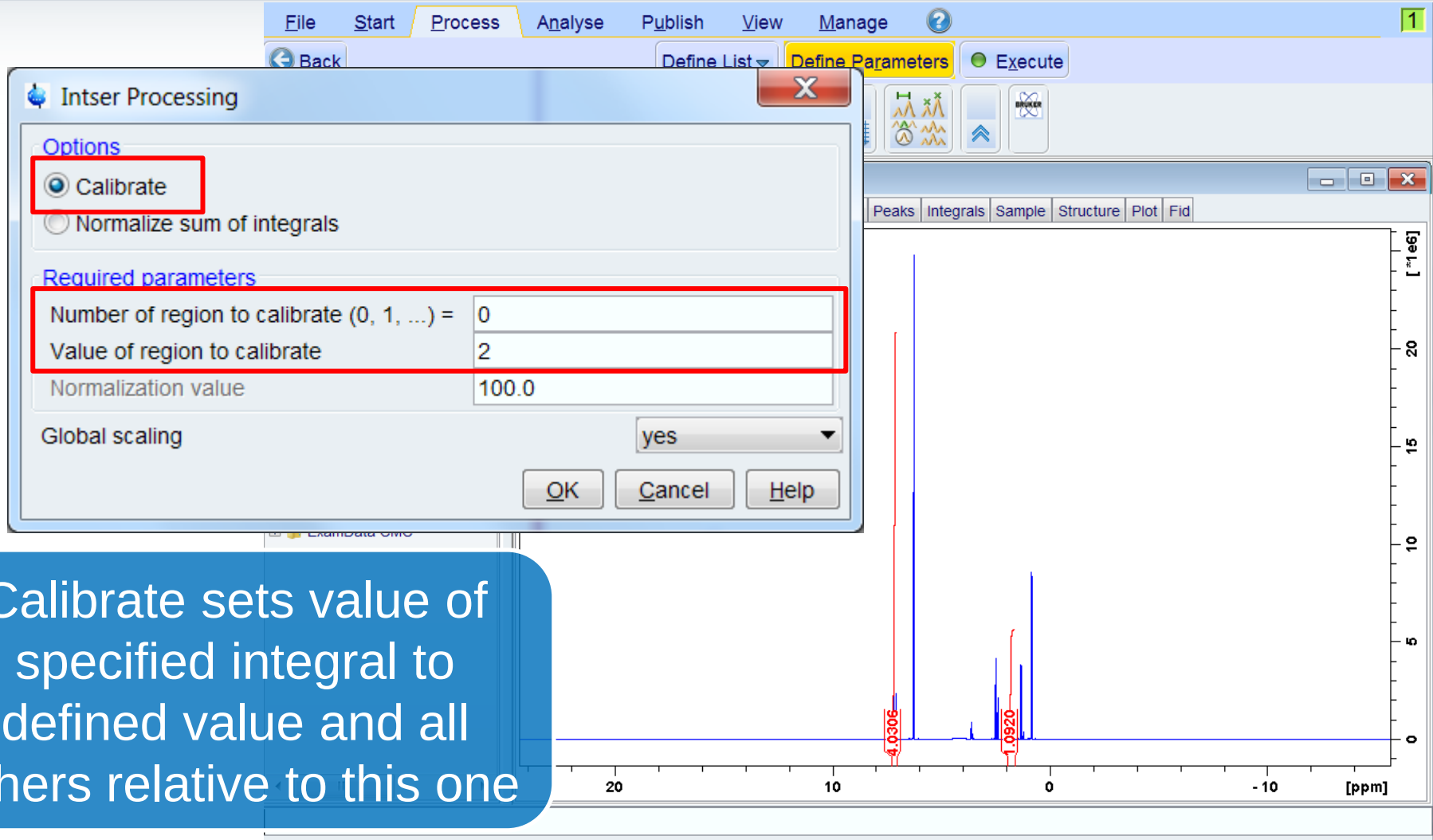
intser – flowbar



intser – define list

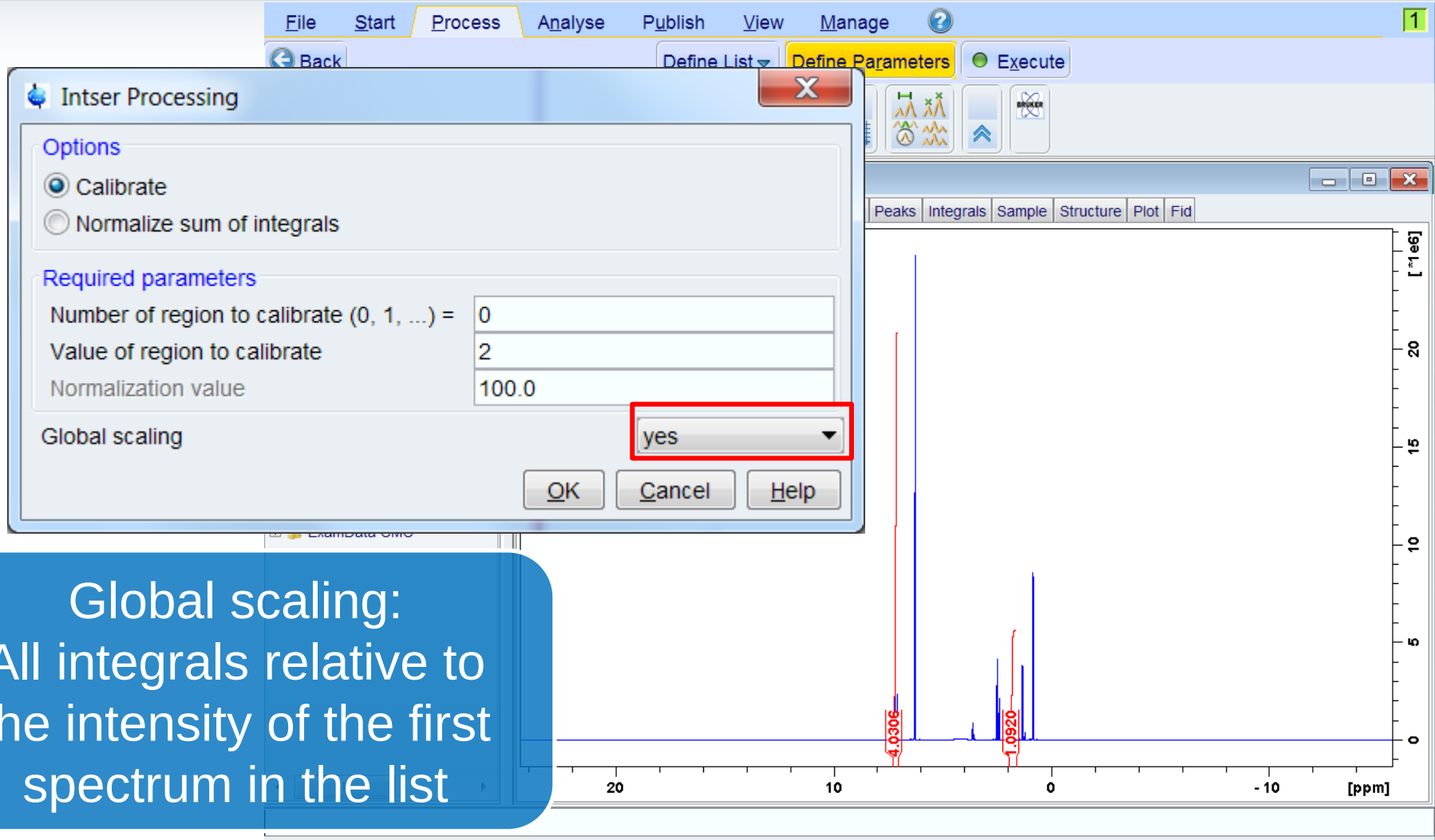


intser – parameters



Calibrate sets value of specified integral to defined value and all others relative to this one

intser – parameters



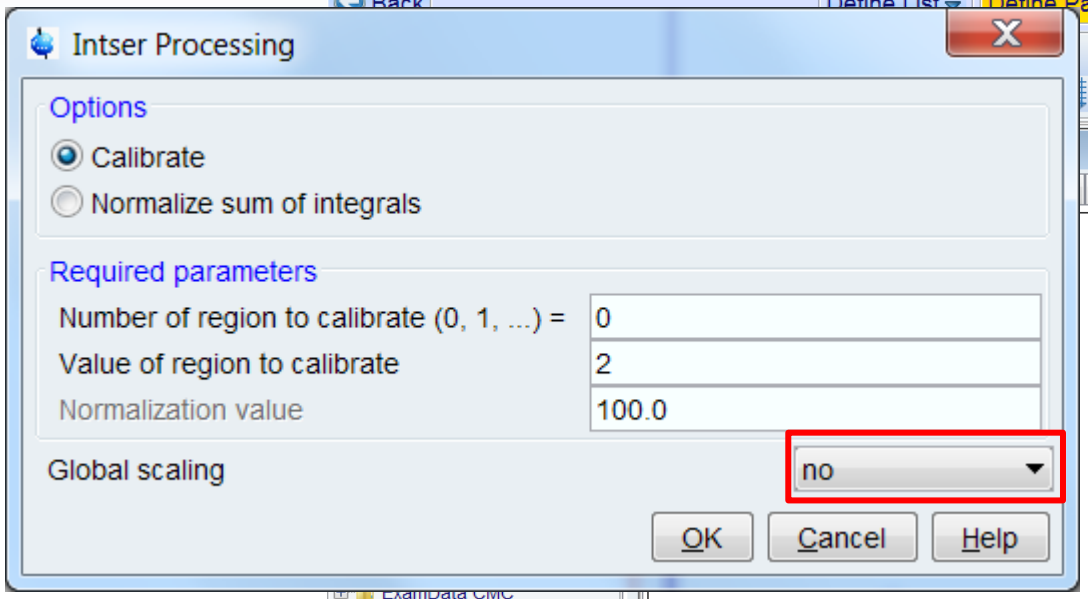
Global scaling:
All integrals relative to the intensity of the first spectrum in the list

intser – results with global scaling

```
# Result of 'intser'
# Date/time = Tue Jun 13 10:39:52 CEST 2017
# Data set list (full path) = C:\Users\BENJAM~1.GOE\AppData\Local\Tem
# Region to calibrate = 0
# Value of region to calibrate = 2.0
# Global scaling = yes

# --- Integral info ---
# A 1.0 #regions in PPM
# # low field   high fie
#   7.308494264941776  7
#   1.9668447801240367

# Spectrum#; Integral 0;
0;2.0;0.541879110289391;
1;4.1420599921166925;1.0
2;2.0174270965987207;0.5
3;3.0562284571461933;0.8
4;4.136608194179254;1.07
5;2.0072924645941086;0.5
6;3.054762441695267;0.84
7;4.218547545095421;1.12
8;2.0057743467025406;0.5
```

```
# Result of 'intser'
# Date/time = Tue Jun 13 10:39:52 CEST 2017
# Data set list (full path) = C:\Users\BENJAM~1.GOE\AppData\Local\Tem
# Region to calibrate = 0
# Value of region to calibrate = 2.0
# Global scaling = yes

# --- Integral info ---
# A 1.0 #regions in PPM
# # low field   high field  bias        slope
#   7.308494264941776  7.018304051480852  0.0  0.0  # for region 1
#   1.9668447801240367  1.6014200668769478  0.0  0.0  # for region 2

# Spectrum#; Integral 0; Integral 1;
0;2.0;0.541879110289391;
1;4.1420599921166925;1.0845876325140709;
2;2.0174270965987207;0.5748499797054847;
3;3.0562284571461933;0.8323333205988354;
4;4.136608194179254;1.0794343635429302;
5;2.0072924645941086;0.5646915621179266;
6;3.054762441695267;0.8419335886413671;
7;4.218547545095421;1.129945036314264;
8;2.0057743467025406;0.5722091049434685;
```

intser – parameters

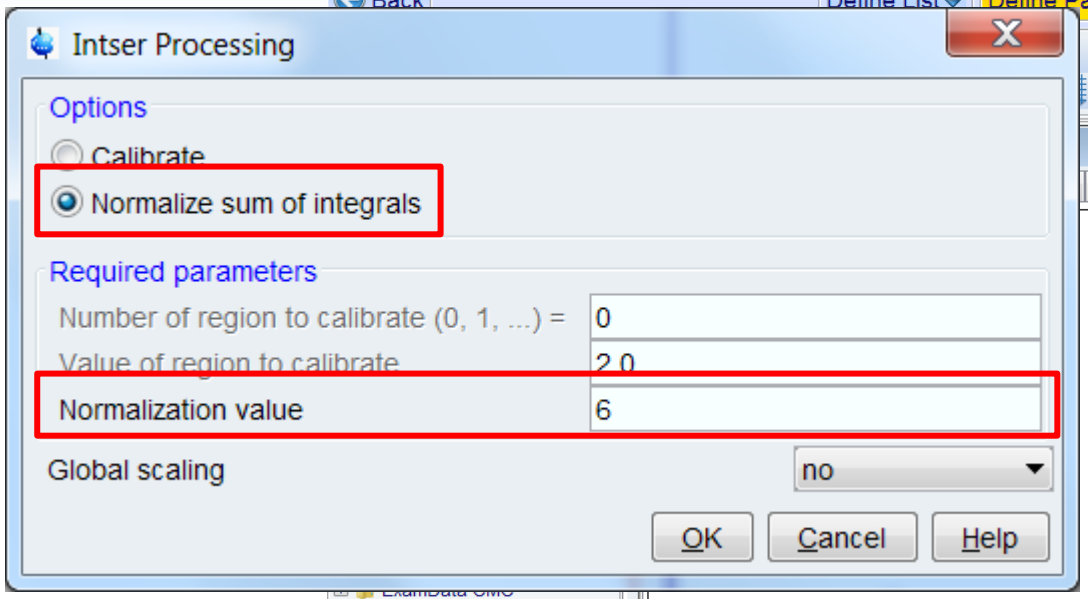


Global scaling:
All integrals relative to the intensity of the first spectrum in the list

intser – results without global scaling

```
# Result of 'intser'
# Date/time = Tue Jun 13 10:45:42 CEST 2017
# Data set list (full path) = C:\Users\BENJAM~1.GOE\AppData\Local\Tem
# Region to calibrate = 0
# Value of region to calibrate = 2.0
# Global scaling = no

# --- Integral info ---
# A 1.0 #regions in PPM
# # low field   high field  bias        slope
#   7.308494264941776  7.018304051480852  0.0  0.0  # for region 1
#   1.9668447801240367  1.6014200668769478  0.0  0.0  # for region 2

# Spectrum#; Integral 0; Integral 1;
0;2.0;0.541879110289391;
1;2.0;0.5236947965883133;
2;2.0;0.5698842656318559;
3;2.0;0.544680040952201;
4;2.0;0.5218934512878619;
5;2.0;0.5626400458112735;
6;2.0;0.5512268824243687;
7;2.0;0.5357033548800292;
8;2.0;0.5705617941361856;
```

intser – parameters



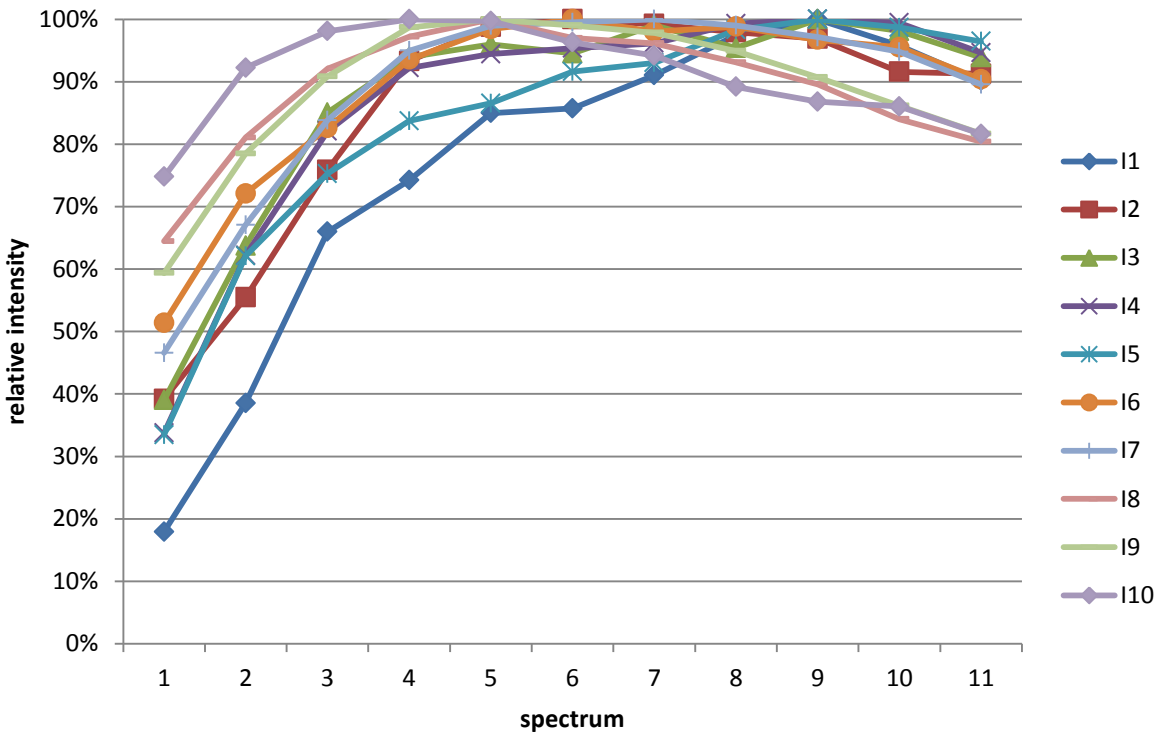
Normalize sets sum of all integral of one spectrum to defined value

intser – results without global scaling

```
# Result of 'intser'
# Date/time = Tue Jun 13 10:56:30 CEST 2017
# Data set list (full path) = C:\Users\BENJAM~1.GOE\AppData\Local\Tem
# Normalization value = 6.0
# Global scaling = no

# --- Integral info ---
# A 1.0 #regions in PPM
# # low field   high field  bias        slope
#   7.308494264941776  7.018304051480852  0.0  0.0  # for region 1
#   1.9668447801240367  1.6014200668769478  0.0  0.0  # for region 2

# Spectrum#; Integral 0; Integral 1;
0;4.720916880517504;1.279083119482496;
1;4.754933130671087;1.2450668693289133;
2;4.669470979872927;1.330529020127073;
3;4.715720564817920;1.2842794351820803;
4;4.758329497969840;1.2416705020301595;
5;4.682670911825649 5;1.3173290881743505;
6;4.703619298882854;1.2963807011171453;
7;4.732414766461415;1.2675852335385849;
8;4.668240237357334;1.3317597626426665;
```

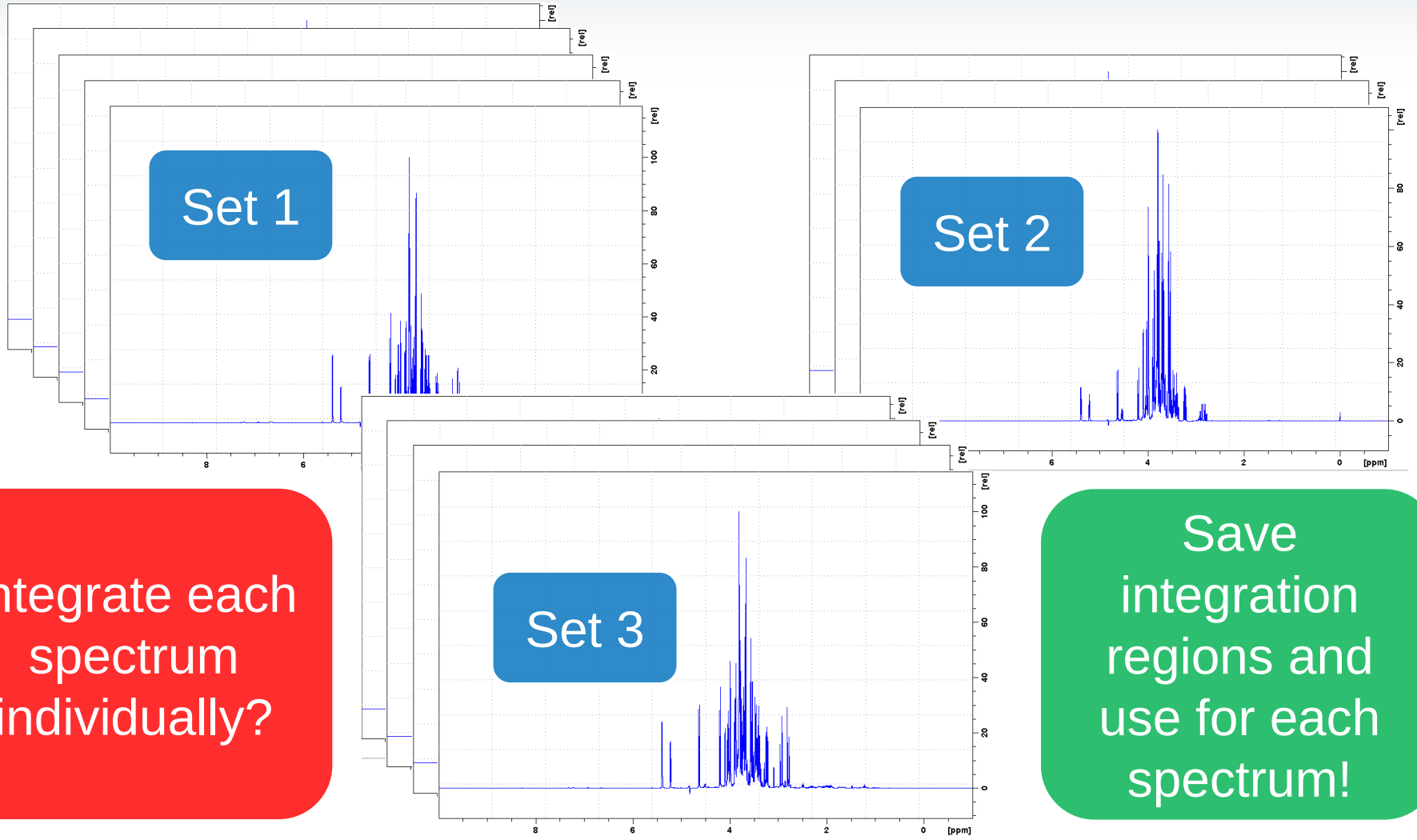
intser – results

Result file can be easily imported into excel
→ Simple graphical presentation



- **Write/read lists for integration**

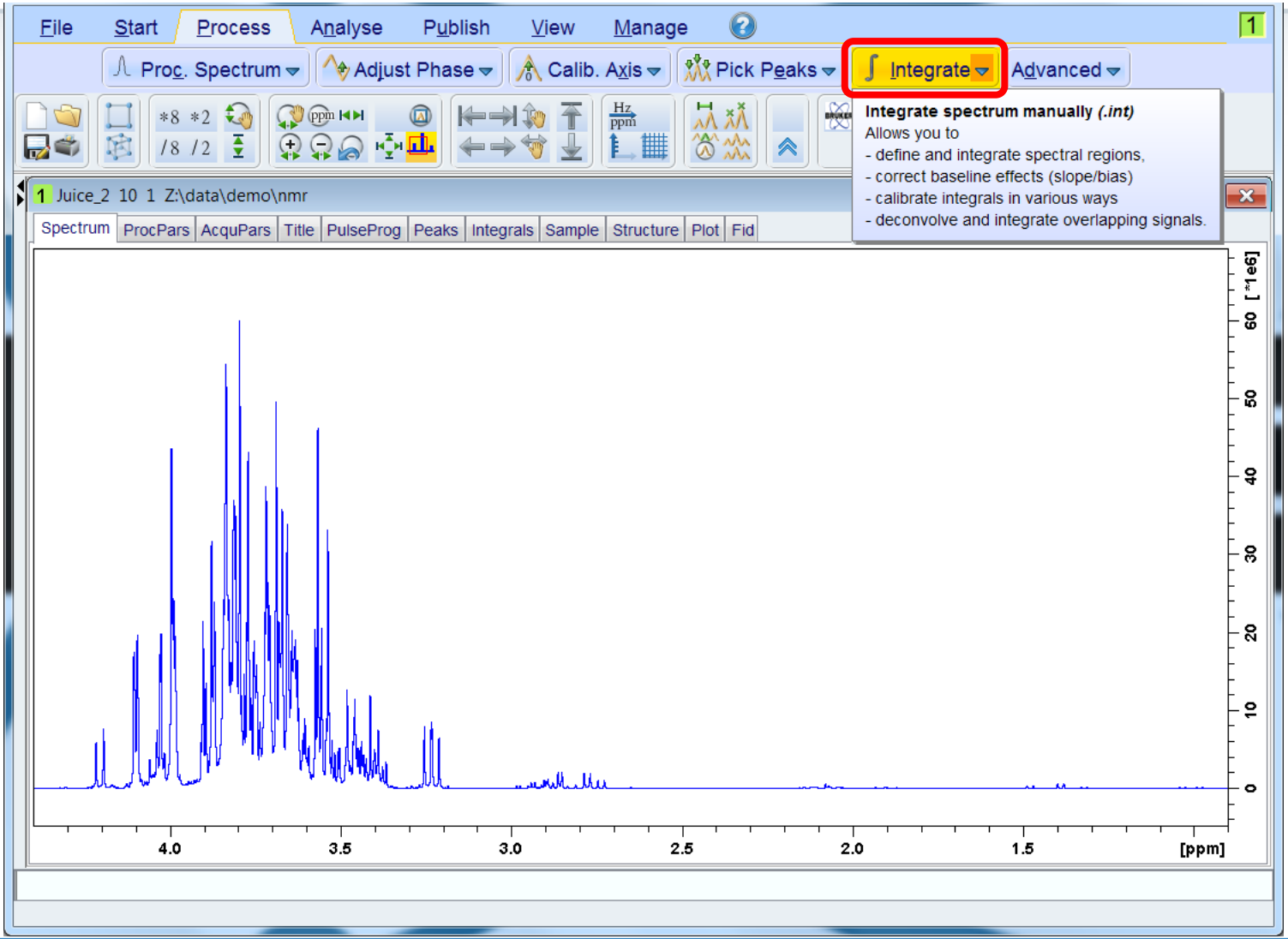
Integrate small set of spectra



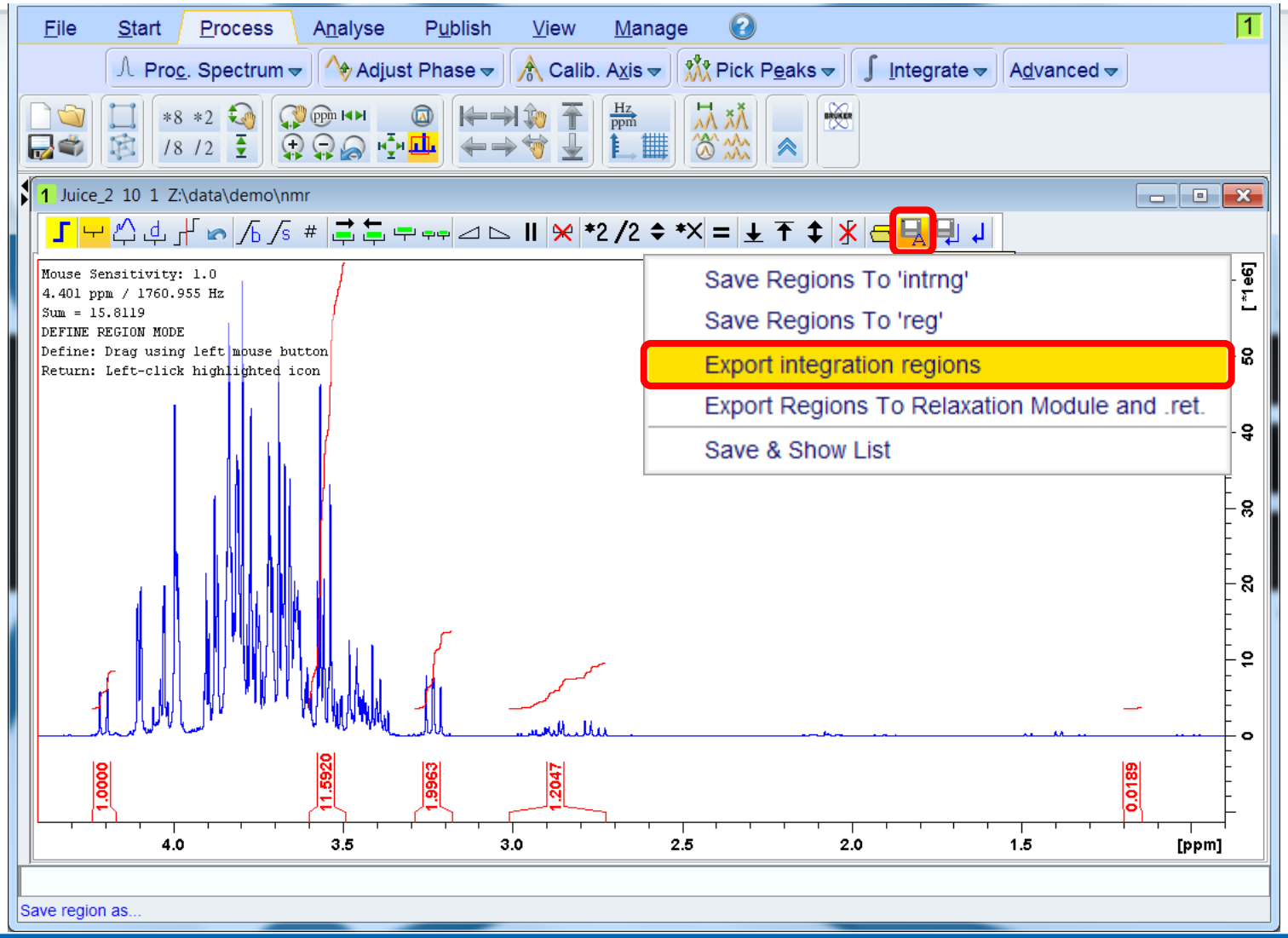
Integrate each spectrum individually?

Save integration regions and use for each spectrum!

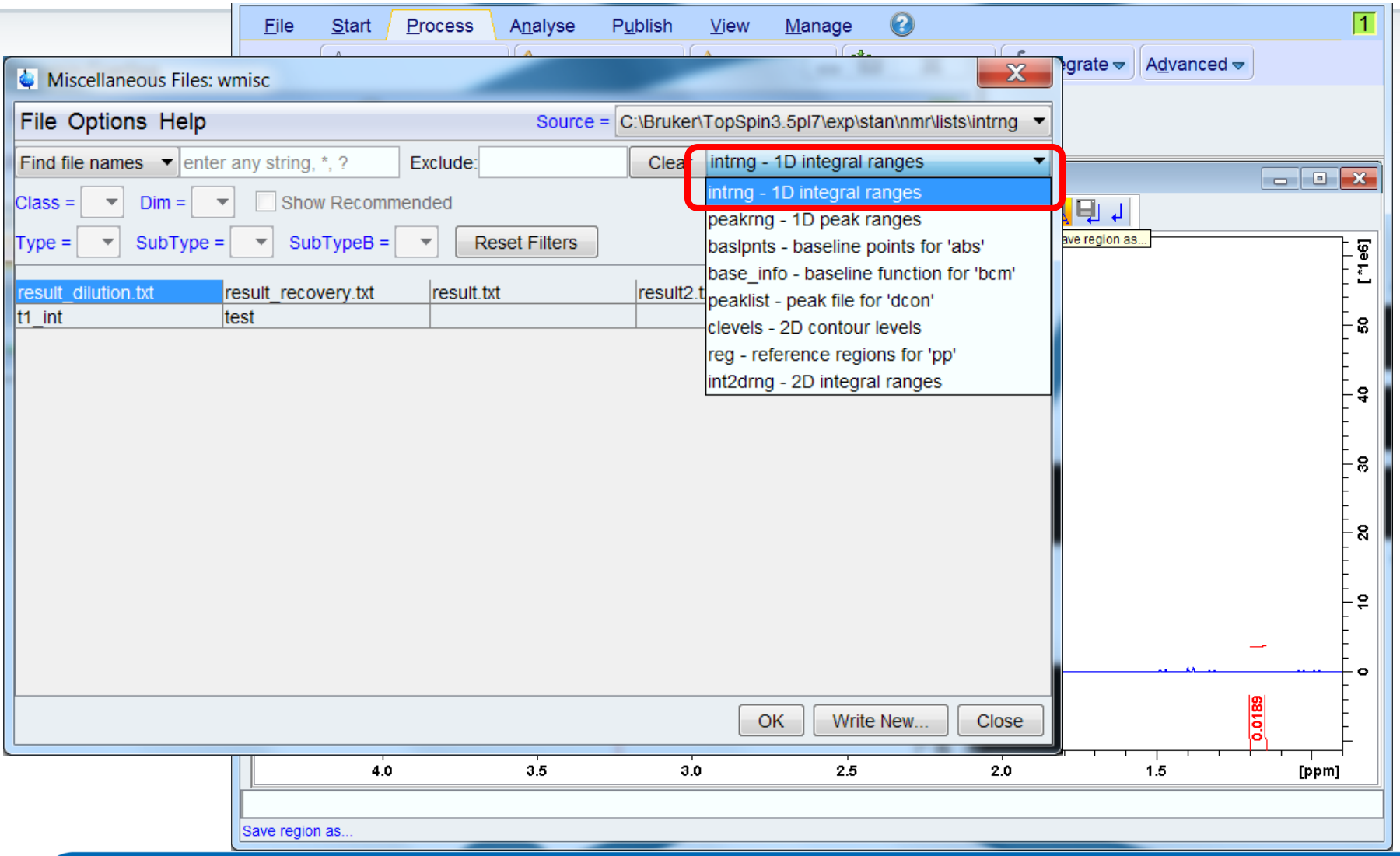
Load first spectrum and integrate it



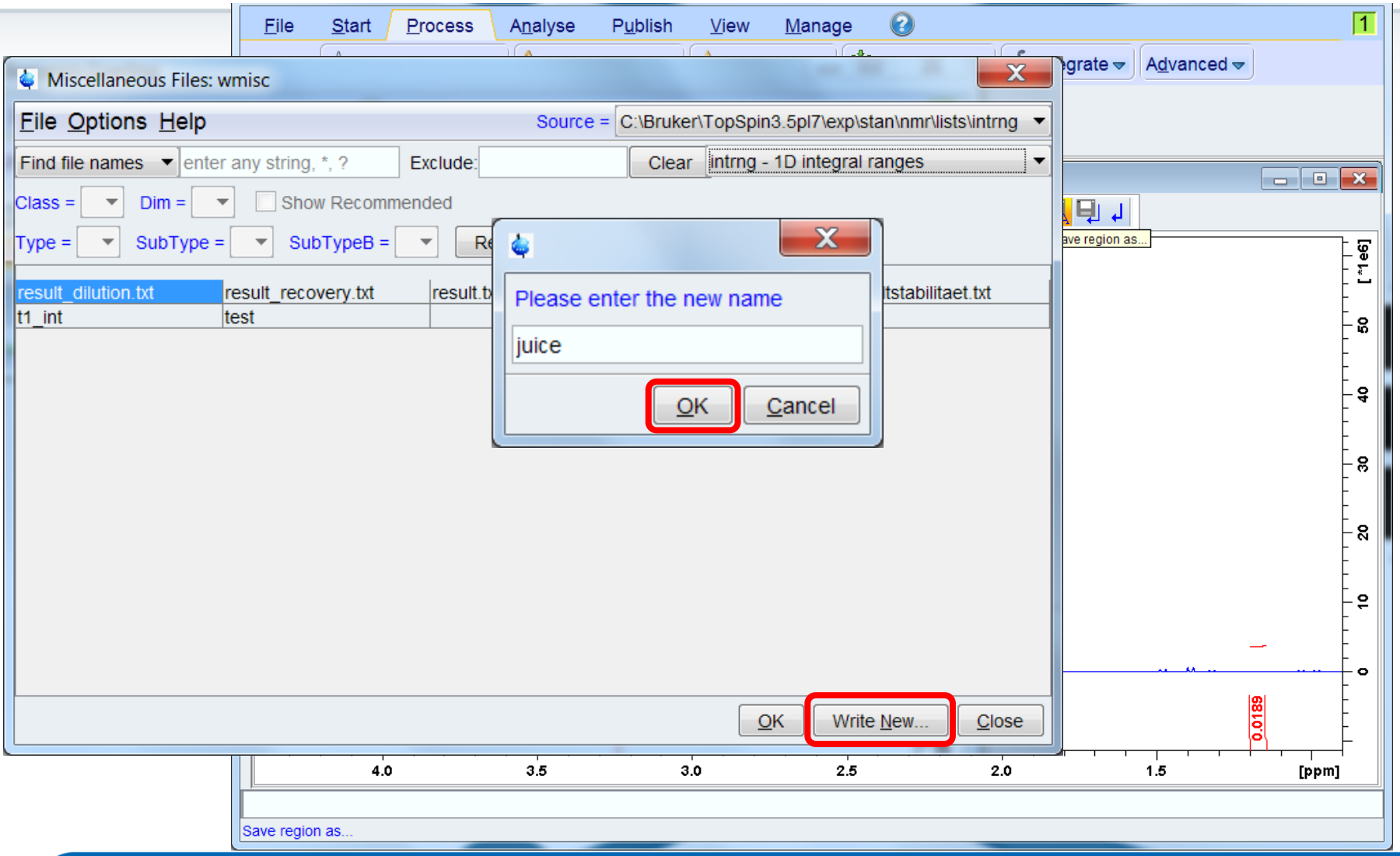
Export integral regions



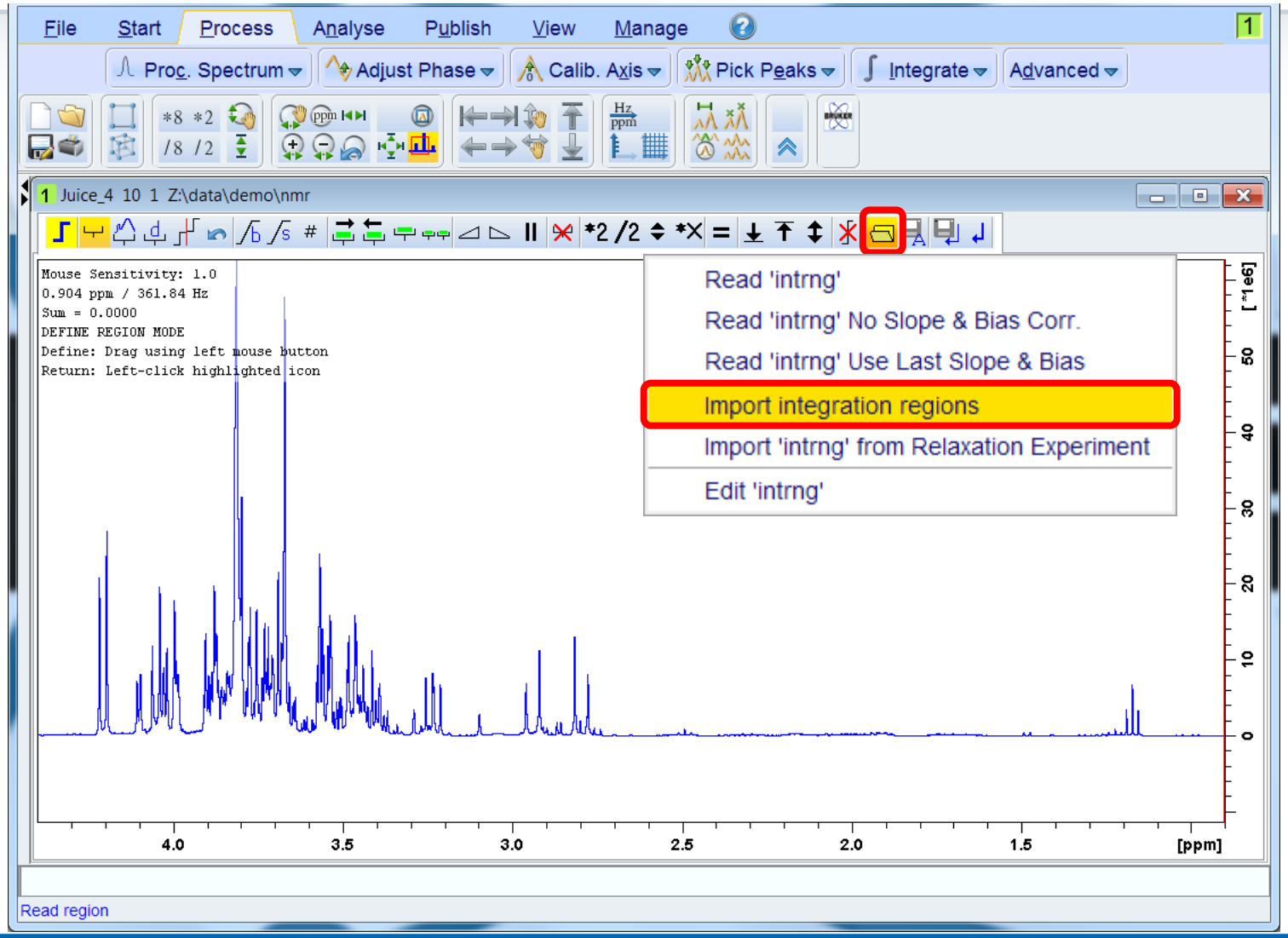
Save as intrgn



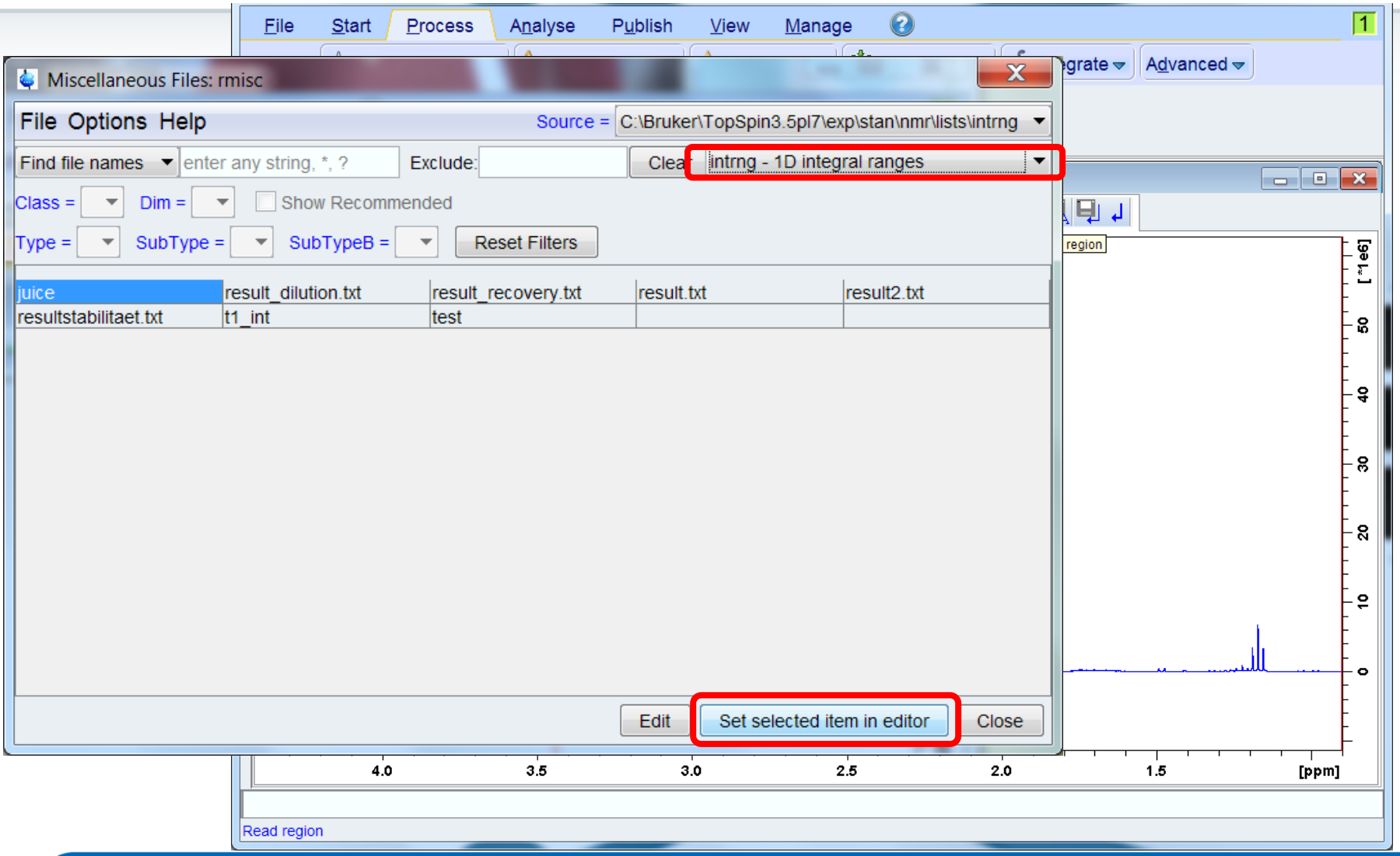
Save as intrgn



Load next spectrum and import region list

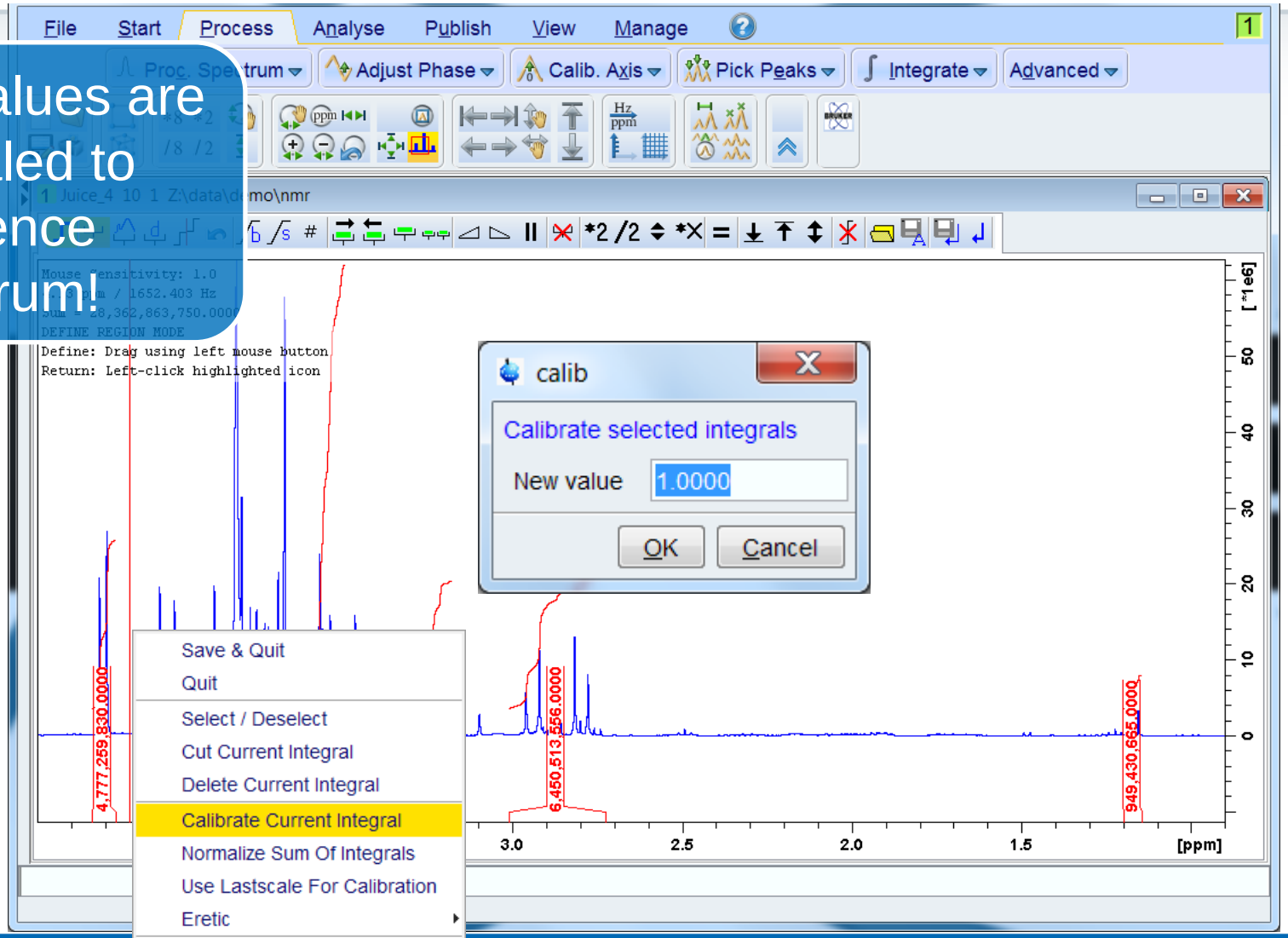


Load next spectrum and import region list

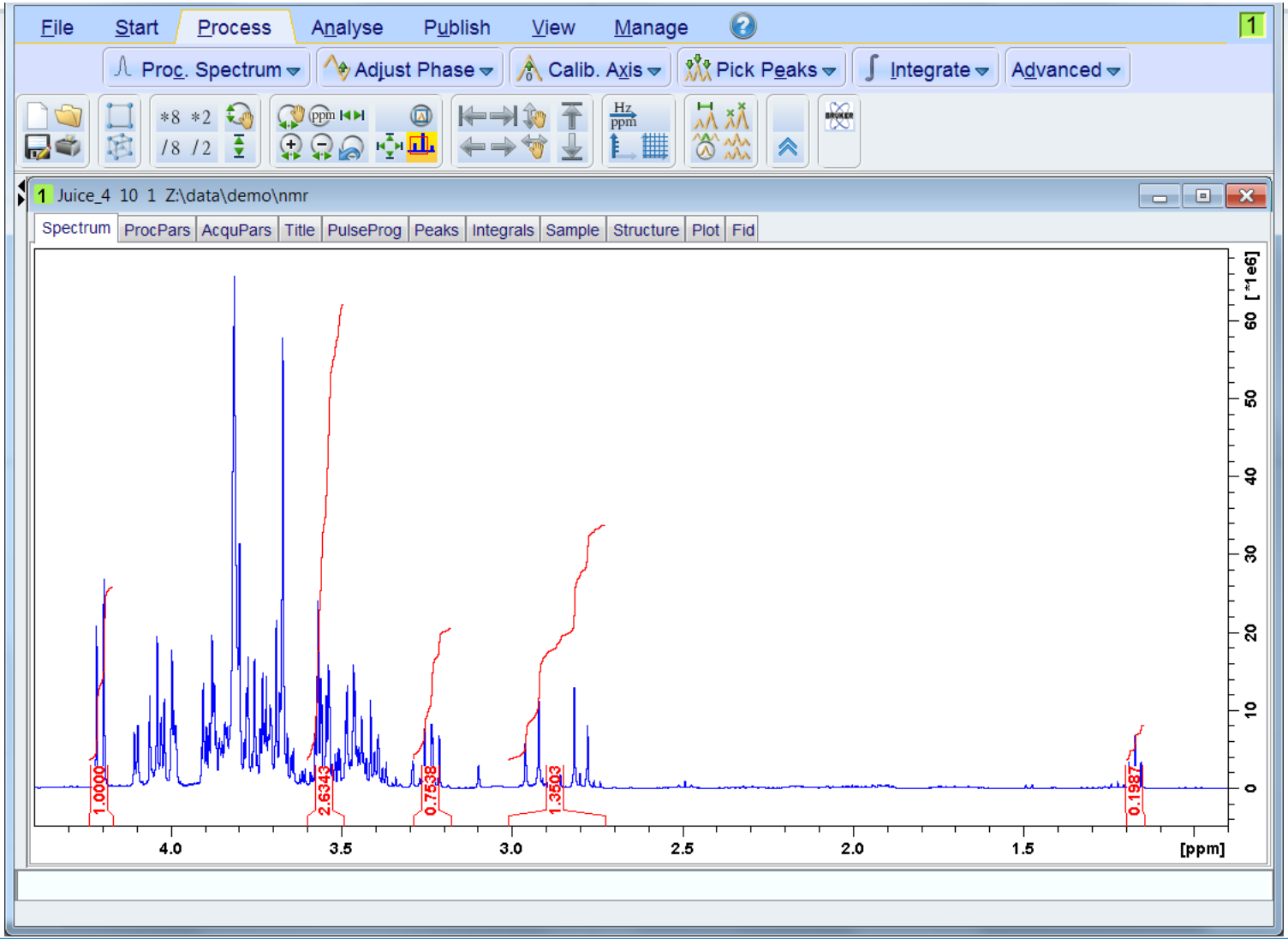


Integrals need to be calibrated

Integral values are not scaled to reference spectrum!

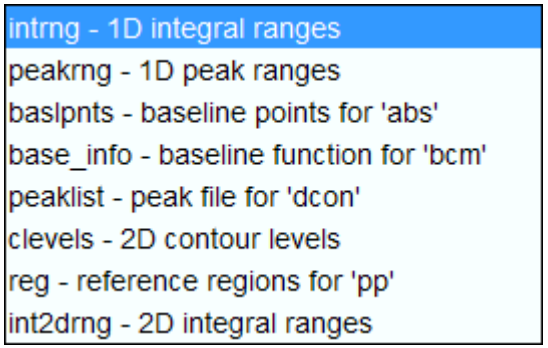


Load next spectrum and import region list



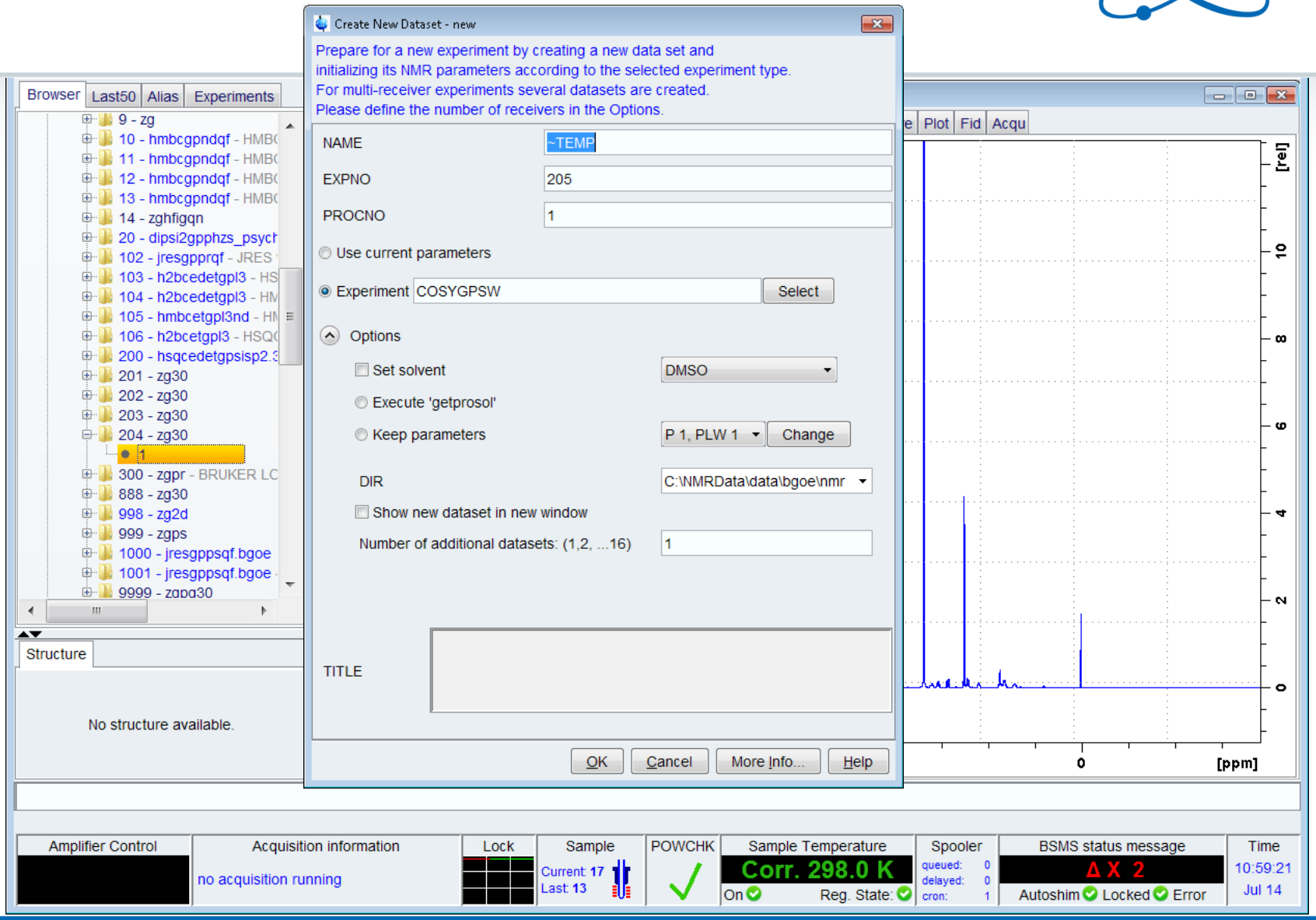
wmisc/rmisc

- Can be called from command line as well
- Commands are: **wmisc** and **rmisc**
- To call specific file, the type of list and the name need to be specified (**wmisc/rmisc <type> <name>**)
- Example: **rmisc intrng juice**

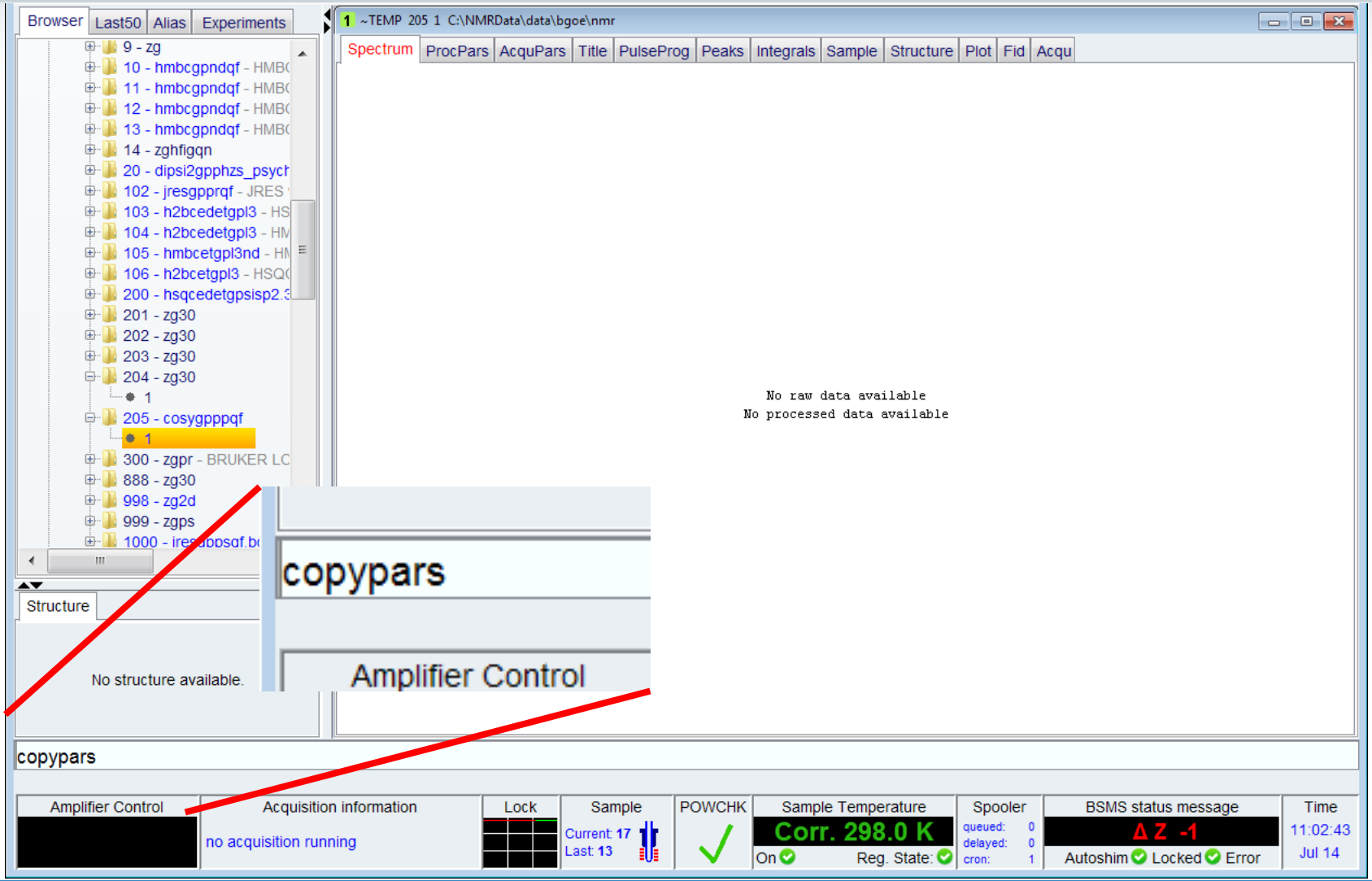


- **Useful commands**

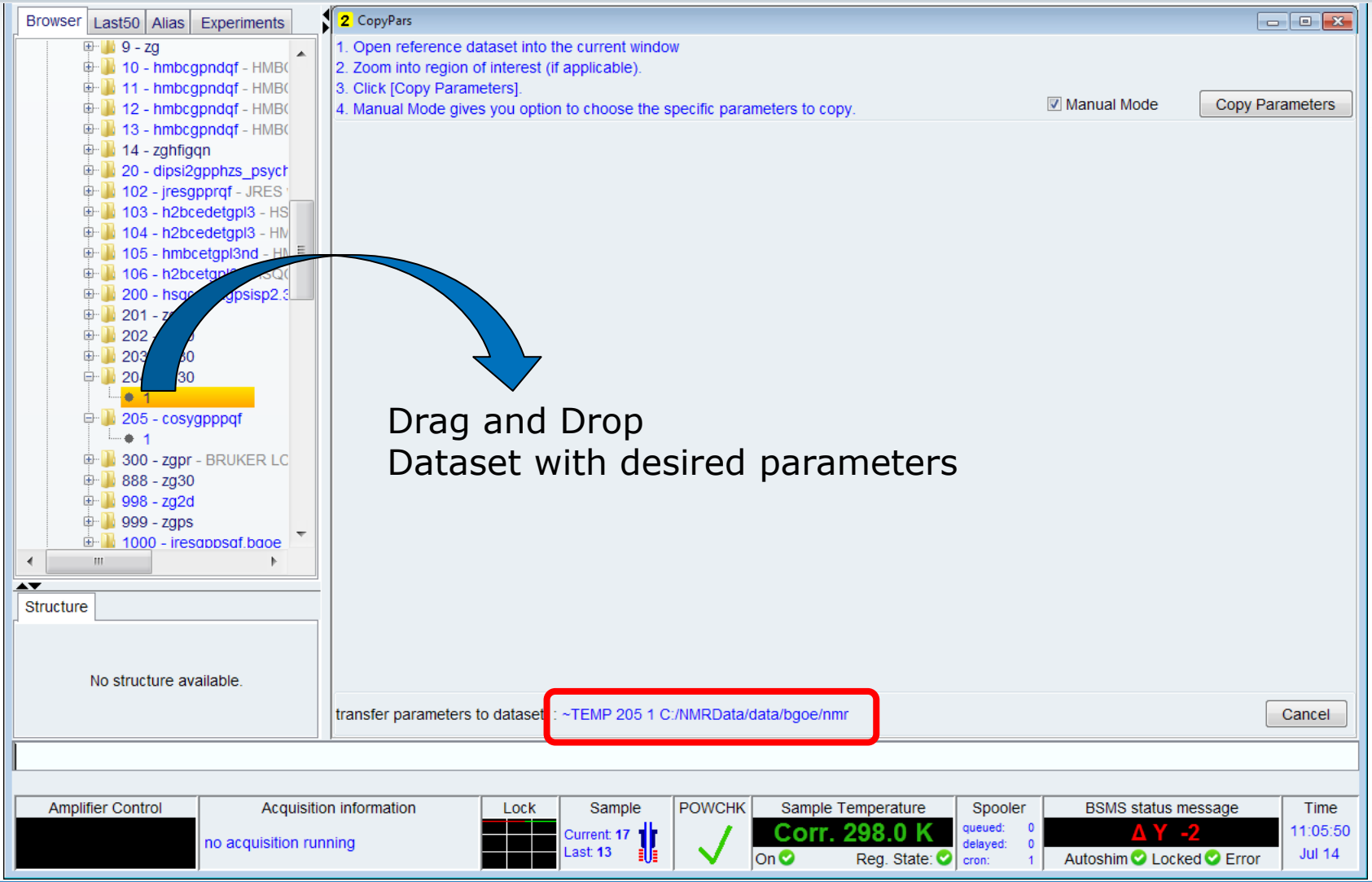
Copy parameters between datasets



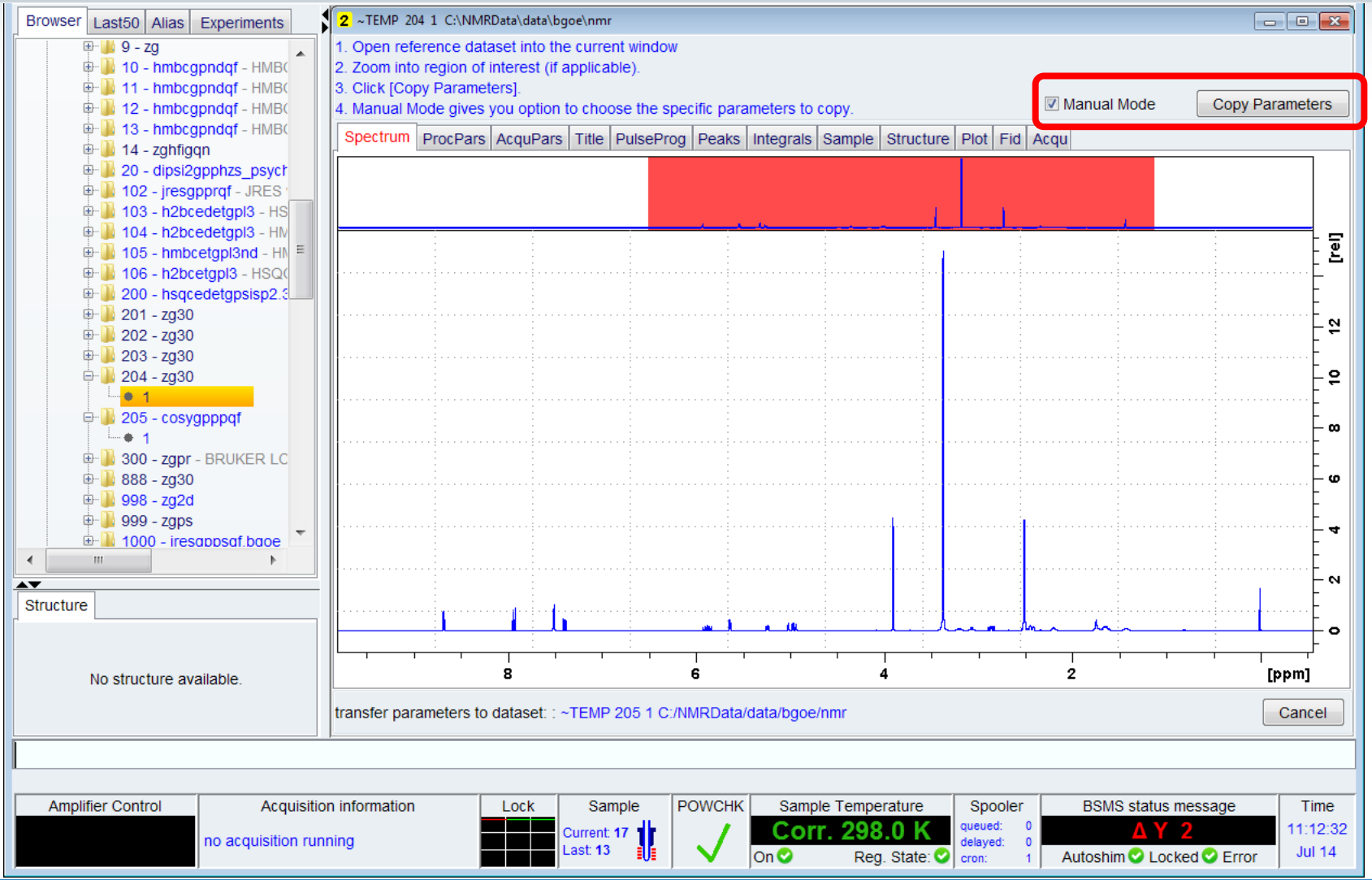
Copy parameters between datasets



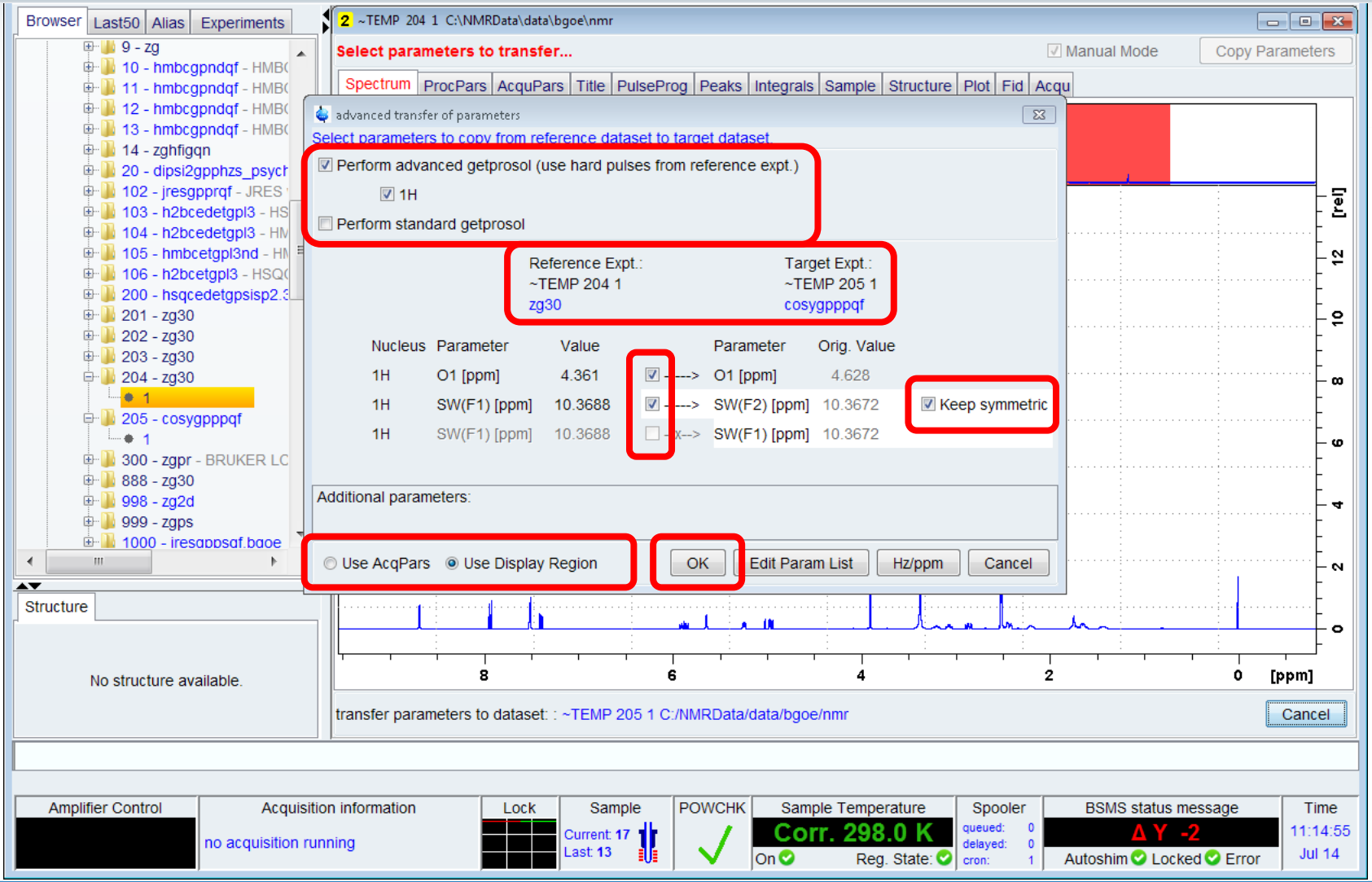
Copy parameters between datasets



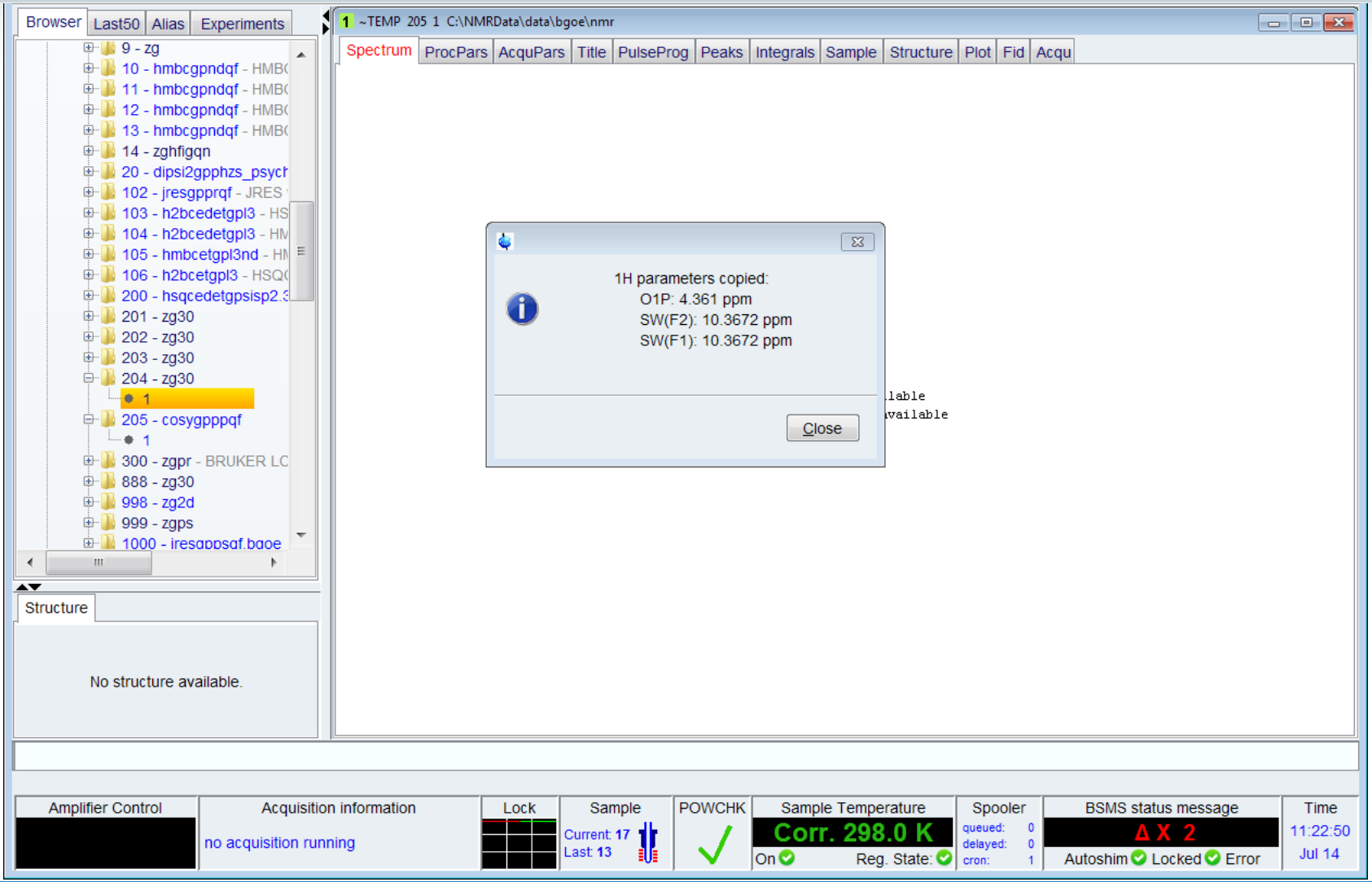
Copy parameters between datasets



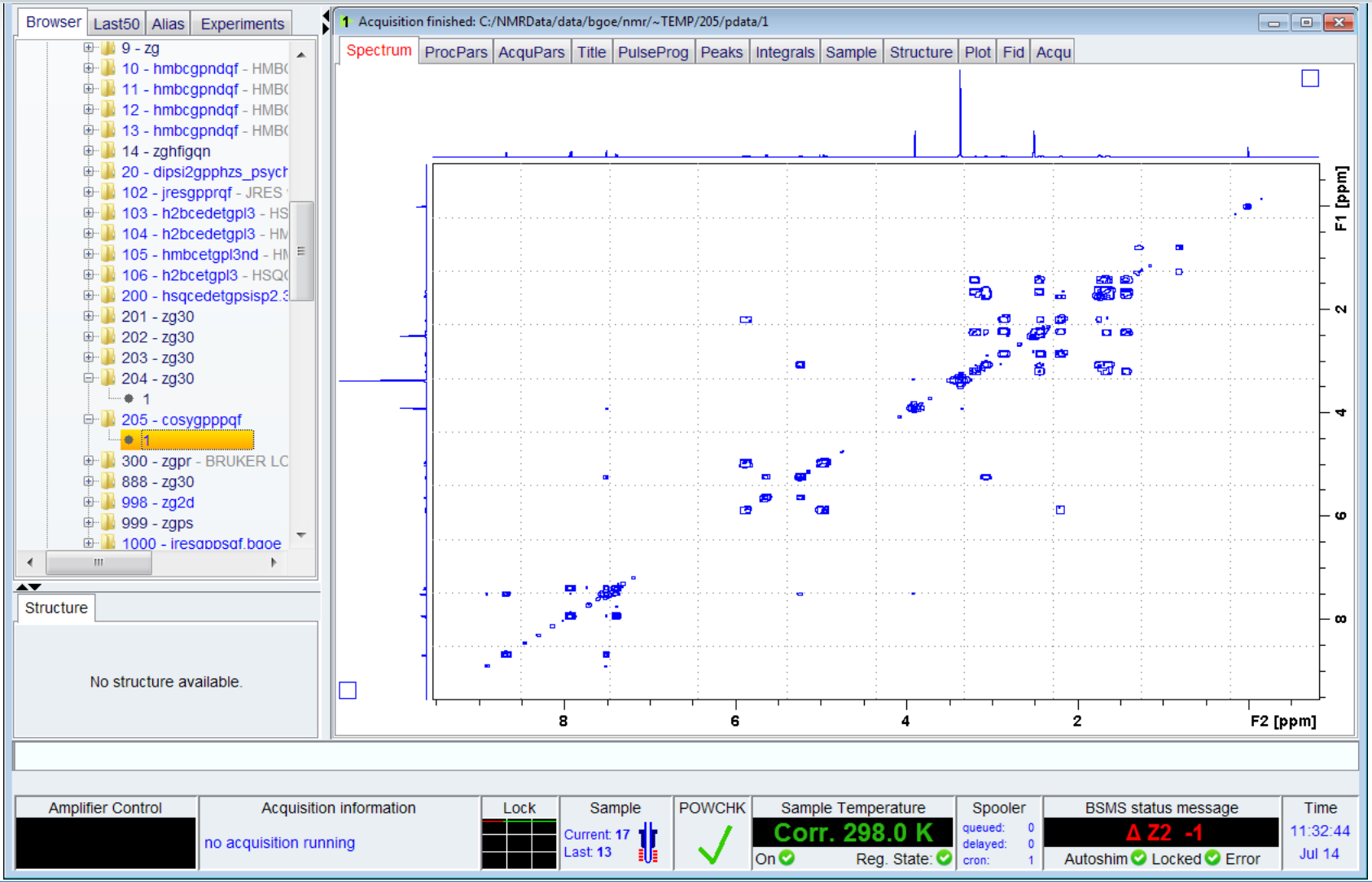
Copy parameters between datasets



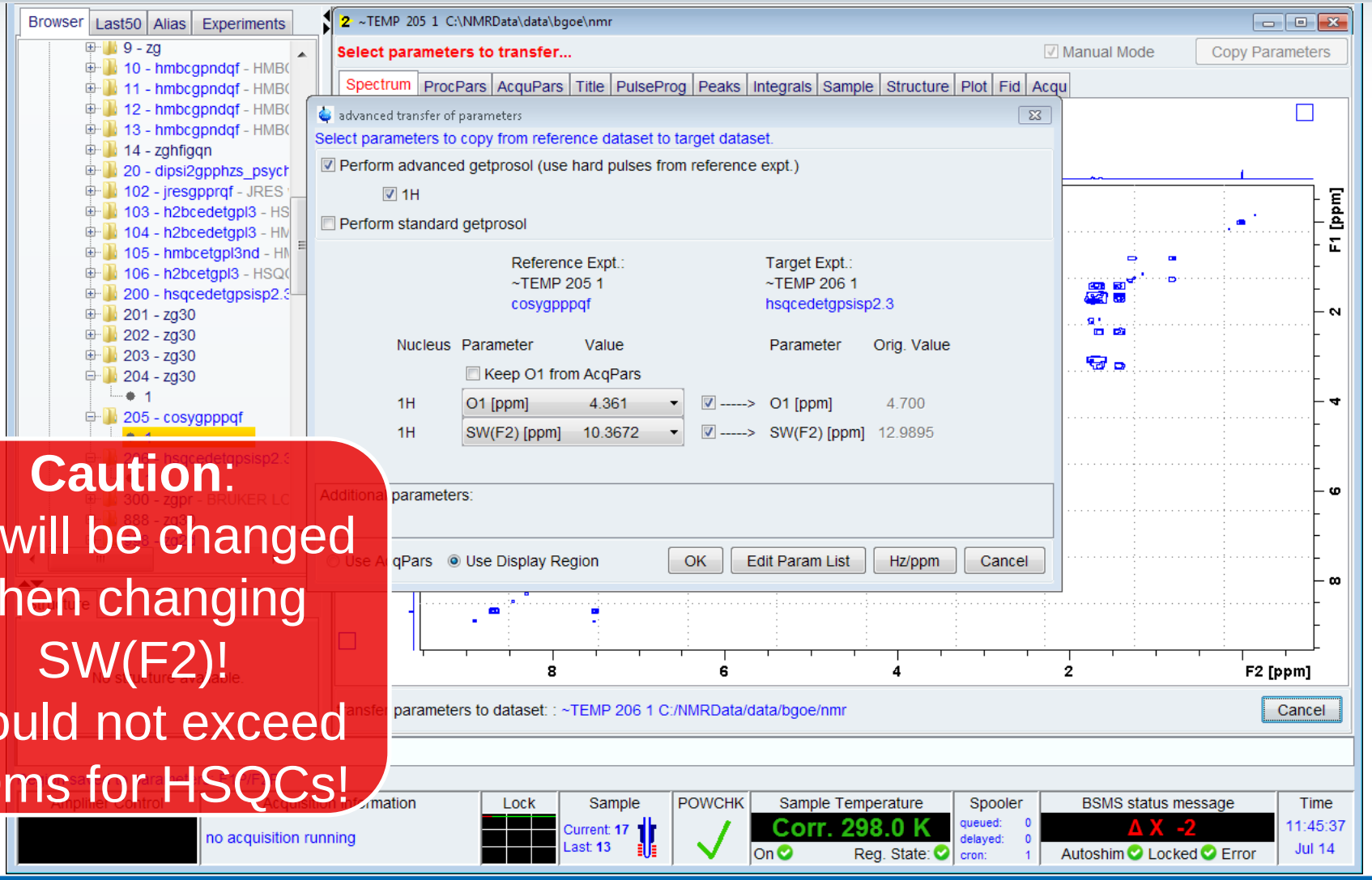
Copy parameters between datasets



Copy parameters between datasets

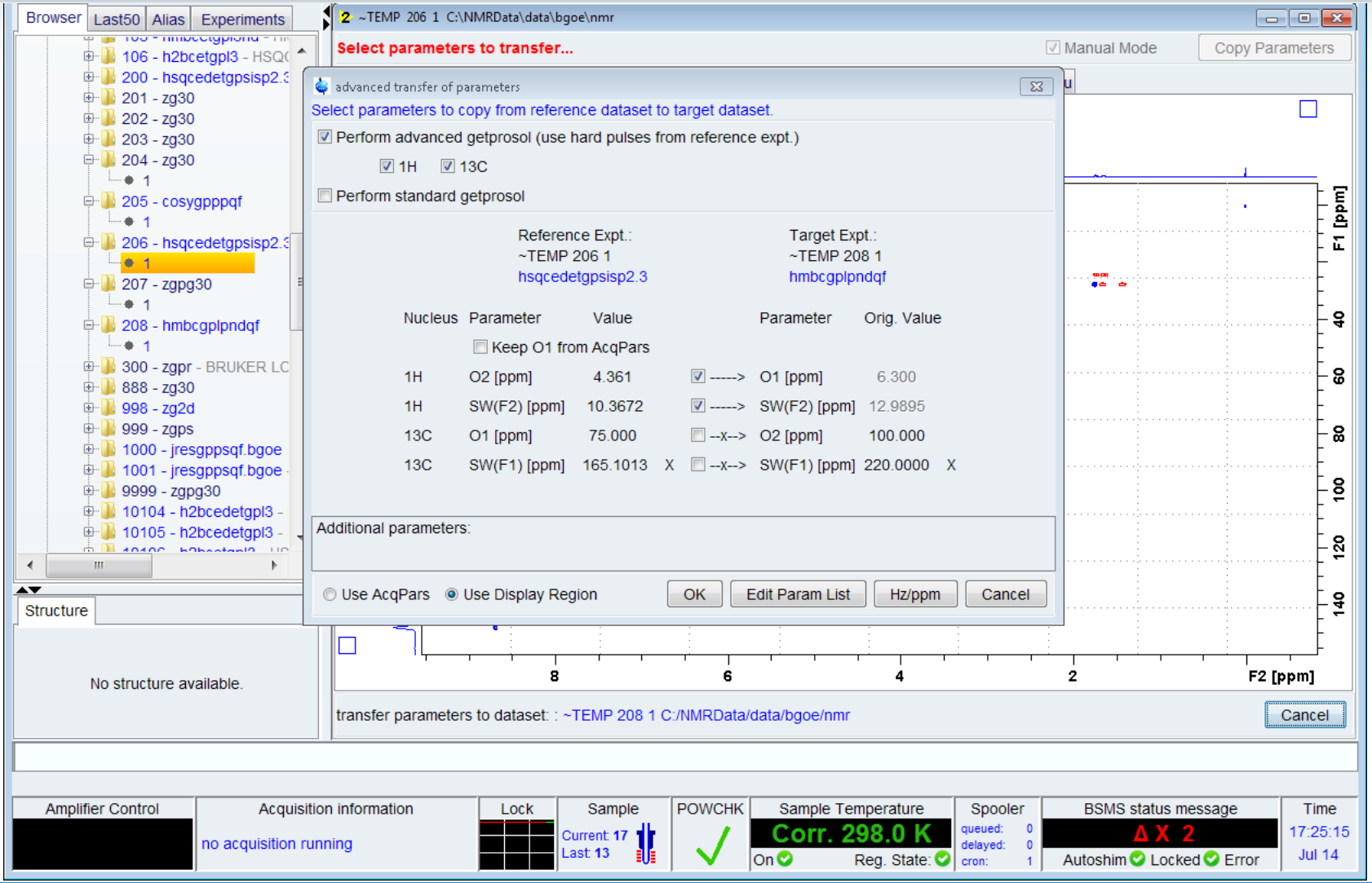


COSY → HSQC



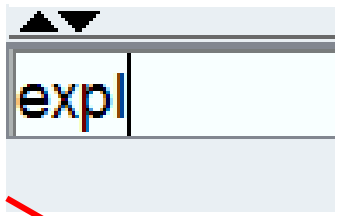
Caution:
AQ will be changed when changing SW(F2)!
Should not exceed 200ms for HSQCs!

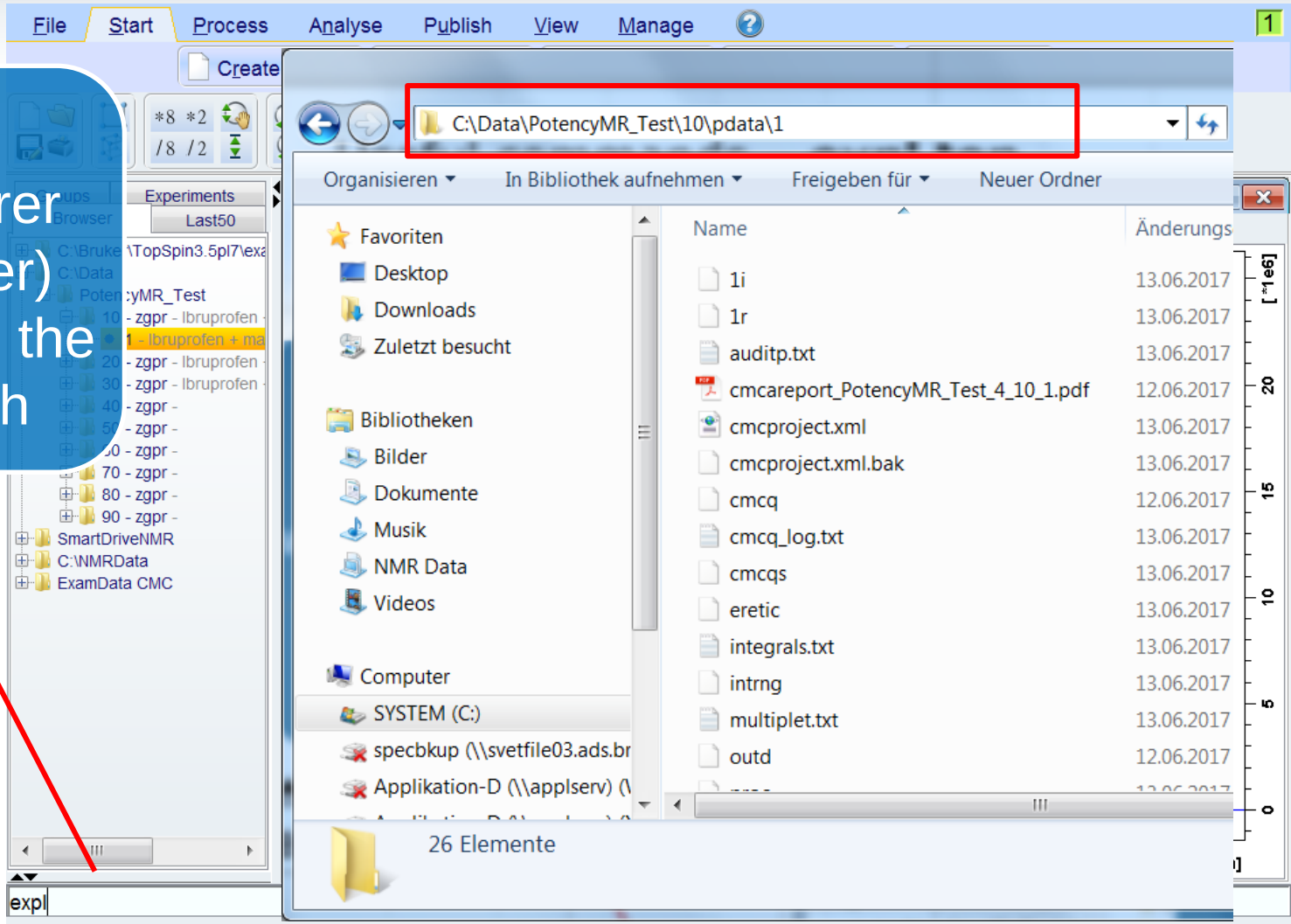
HSQC → HMBC


Browser
Last50
Alias
Experiments
106 - h2bcetgpl3 - HSQC
200 - hsqcedetgpsisp2.3
201 - zg30
202 - zg30
203 - zg30
204 - zg30
205 - cosygpppqf
206 - hsqcedetgpsisp2.3
207 - zgpg30
208 - hmbcgplpndqf
300 - zgpr - BRUKER LC
888 - zg30
998 - zg2d
999 - zgps
1000 - jresgppsqf.bgoe
1001 - jresgppsqf.bgoe
9999 - zgpg30
10104 - h2bcedetgpl3
10105 - h2bcedetgpl3
Structure
No structure available.
~TEMP 206 1 C:\NMRData\data\bgoe\nmr
Select parameters to transfer...
Manual Mode
Copy Parameters
advanced transfer of parameters
Select parameters to copy from reference dataset to target dataset.
Perform advanced getprosol (use hard pulses from reference expt.)
1H
13C
Perform standard getprosol
Reference Expt.:
~TEMP 206 1
hsqcedetgpsisp2.3
Target Expt.:
~TEMP 208 1
hmbcgplpndqf
Nucleus Parameter Value Parameter Orig. Value
Keep O1 from AcqPars
1H O2 [ppm] 4.361 -----> O1 [ppm] 6.300
1H SW(F2) [ppm] 10.3672 -----> SW(F2) [ppm] 12.9895
13C O1 [ppm] 75.000 --x--> O2 [ppm] 100.000
13C SW(F1) [ppm] 165.1013 X --x--> SW(F1) [ppm] 220.0000 X
Additional parameters:
Use AcqPars
Use Display Region
OK
Edit Param List
Hz/ppm
Cancel
F1 [ppm]
F2 [ppm]
transfer parameters to dataset: : ~TEMP 208 1 C:/NMRData/data/bgoe/nmr
Cancel
Amplifier Control
Acquisition information
no acquisition running
Lock
Sample
Current: 17
Last: 13
POWCHK
Sample Temperature
Corr. 298.0 K
On
Reg. State:
Spooler
queued: 0
delayed: 0
cron: 1
BSMS status message
Δ X 2
Autoshim
Locked
Error
Time
17:25:15
Jul 14

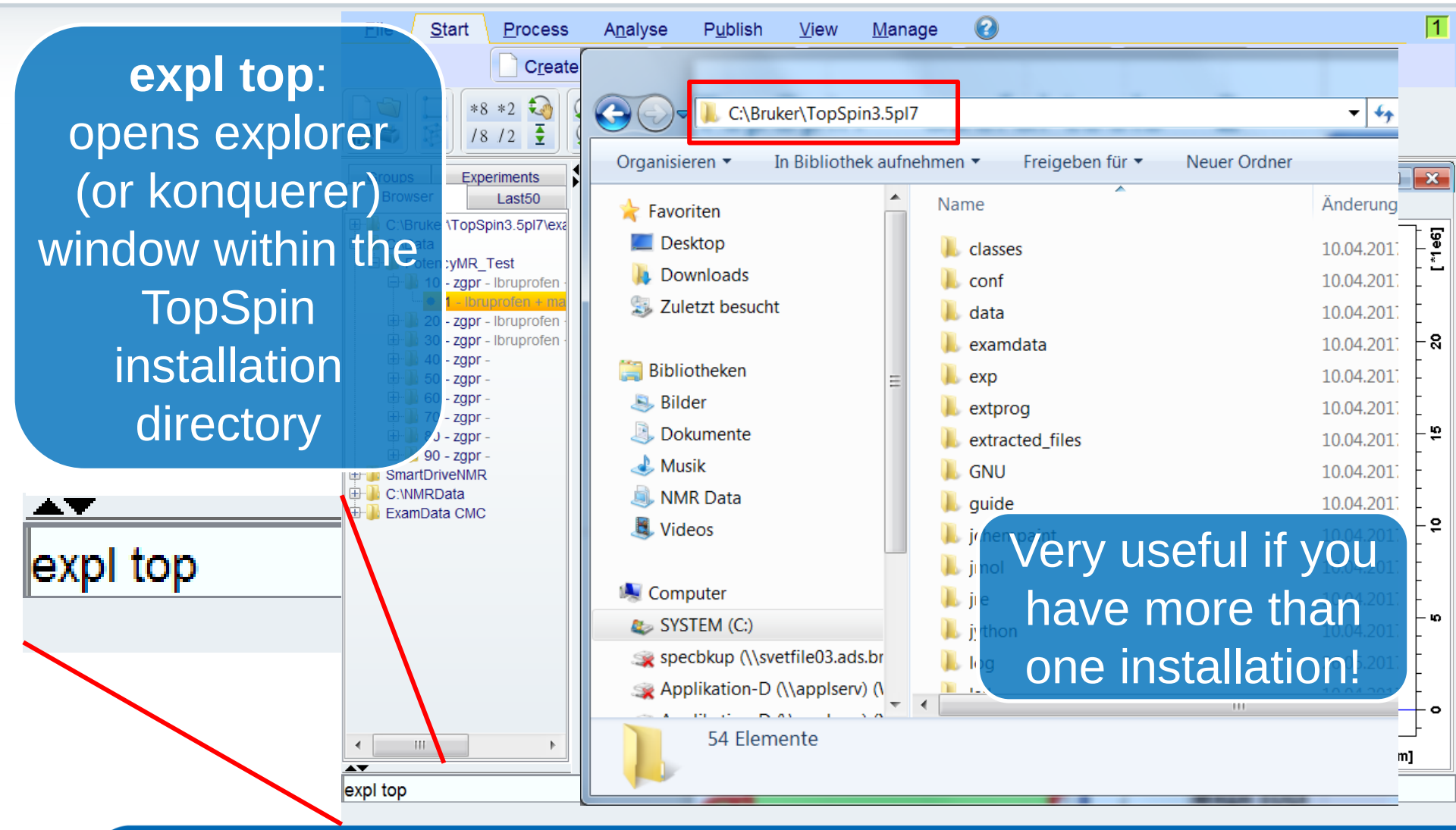
Useful commands – **expl**

expl:
opens explorer (or konquerer) window within the dataset path



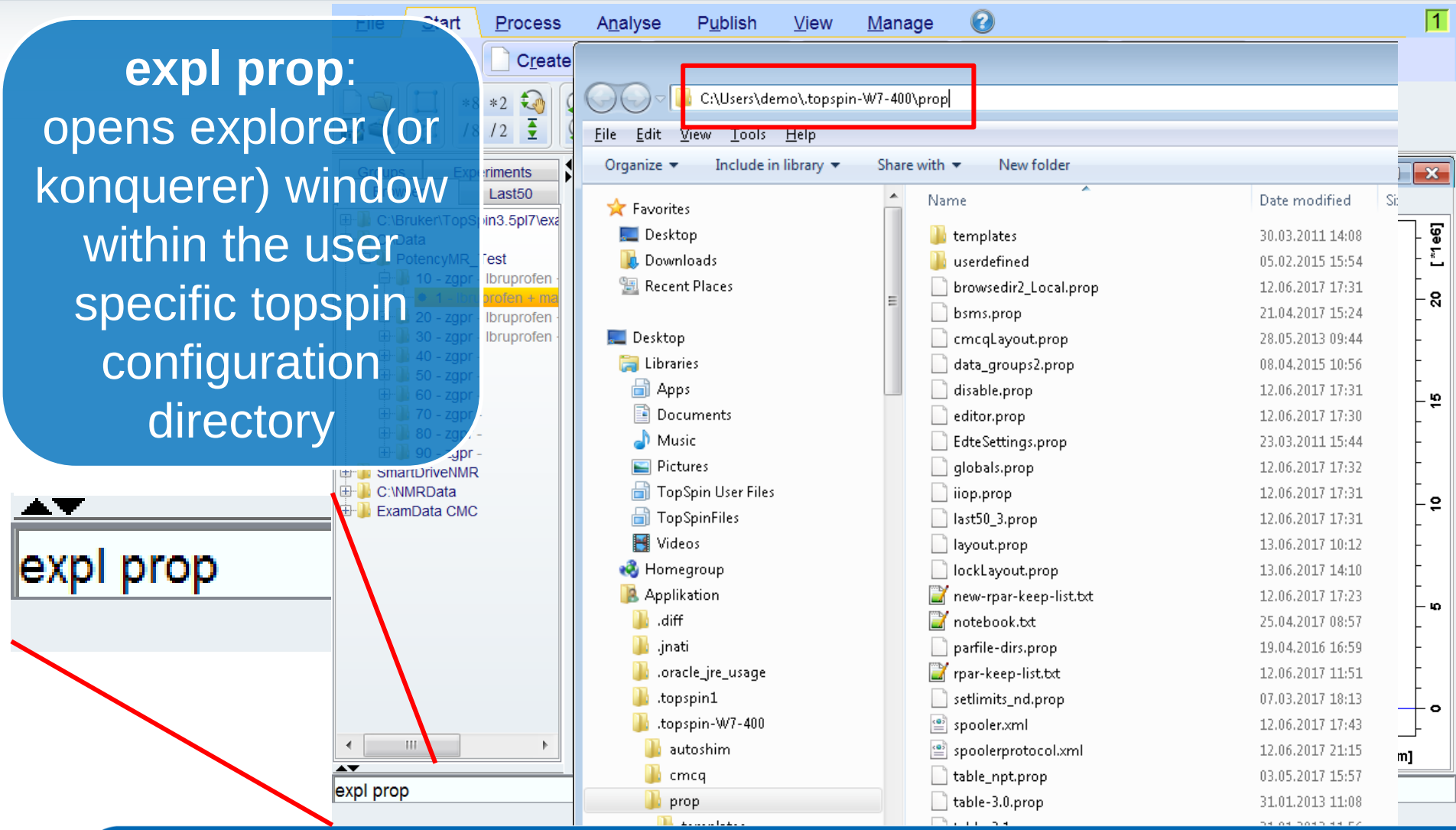


Useful commands – **expl top**



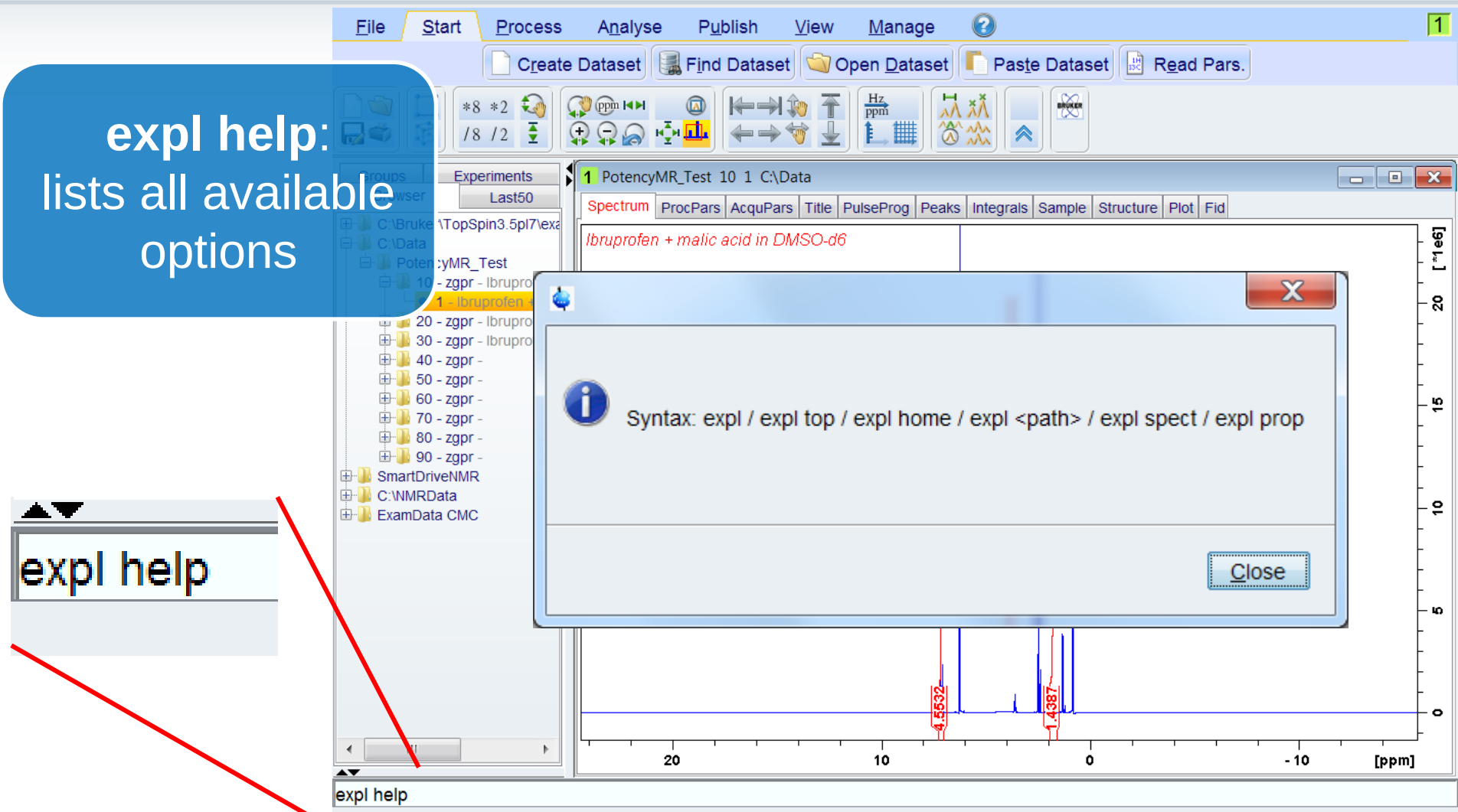
Useful commands – **expl prop**

expl prop:
opens explorer (or konquerer) window within the user specific topspin configuration directory



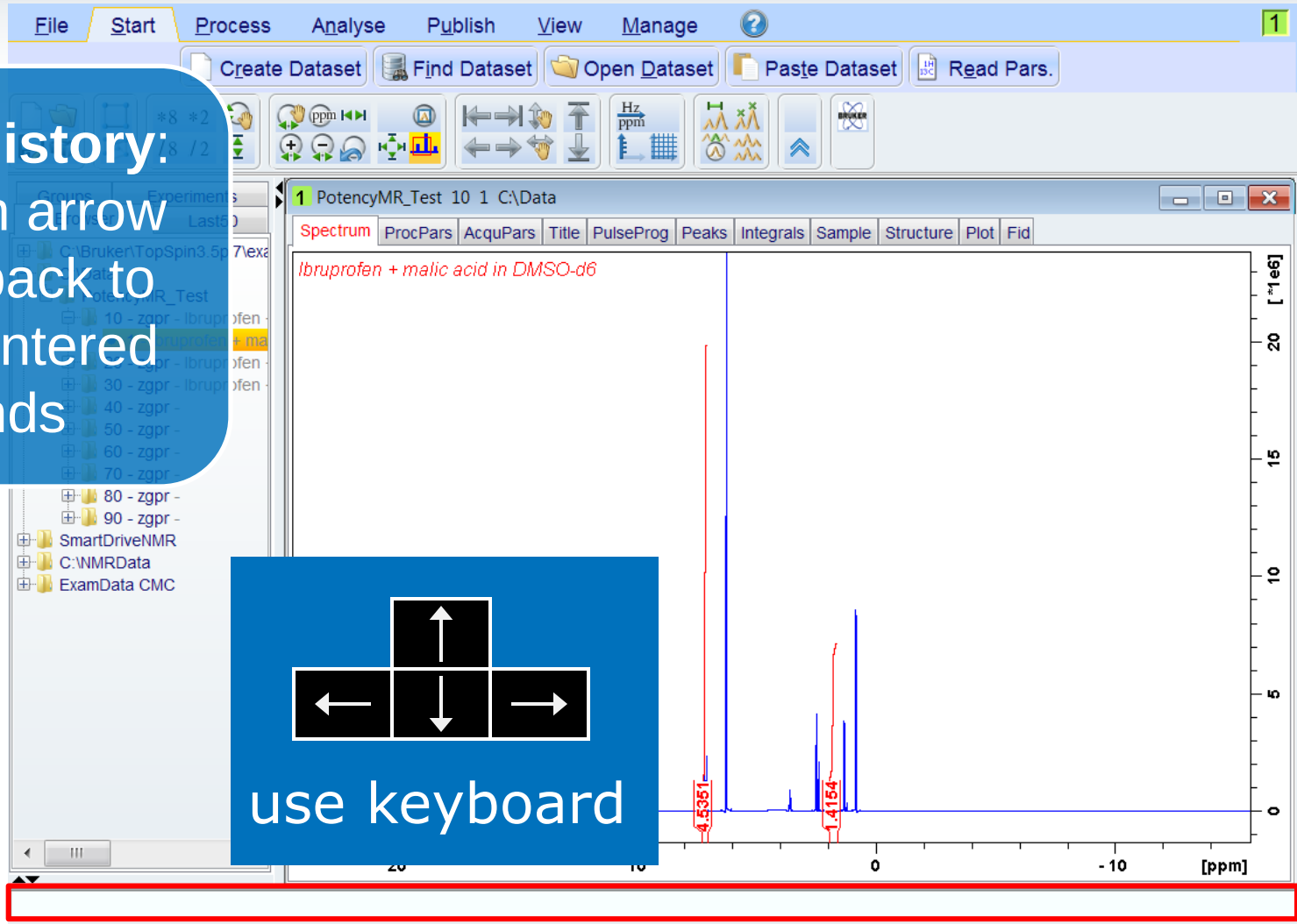
Useful commands – **expl help**

expl help:
lists all available options



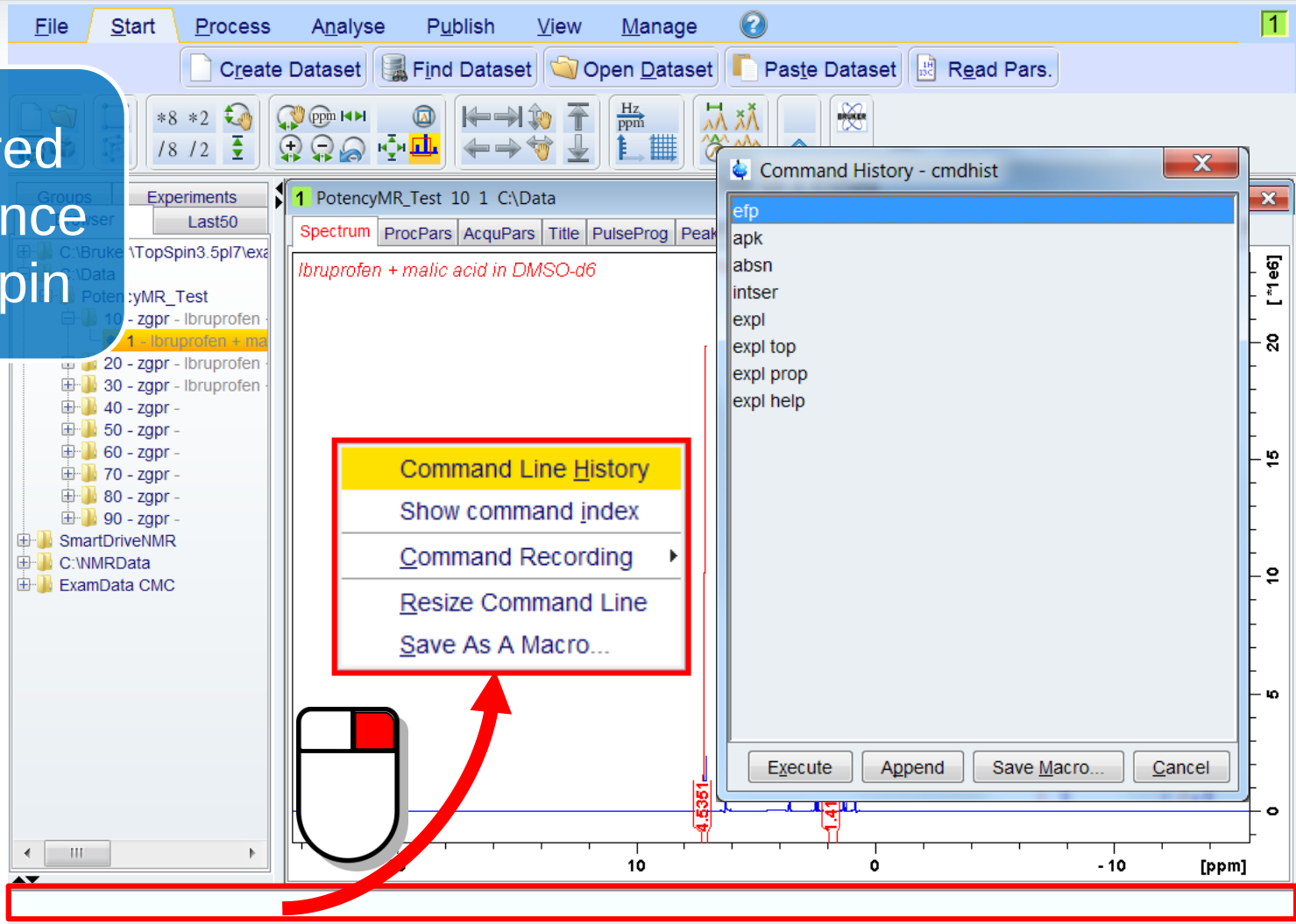
Useful commands – command history

command history: use up/down arrow keys to go back to previously entered commands

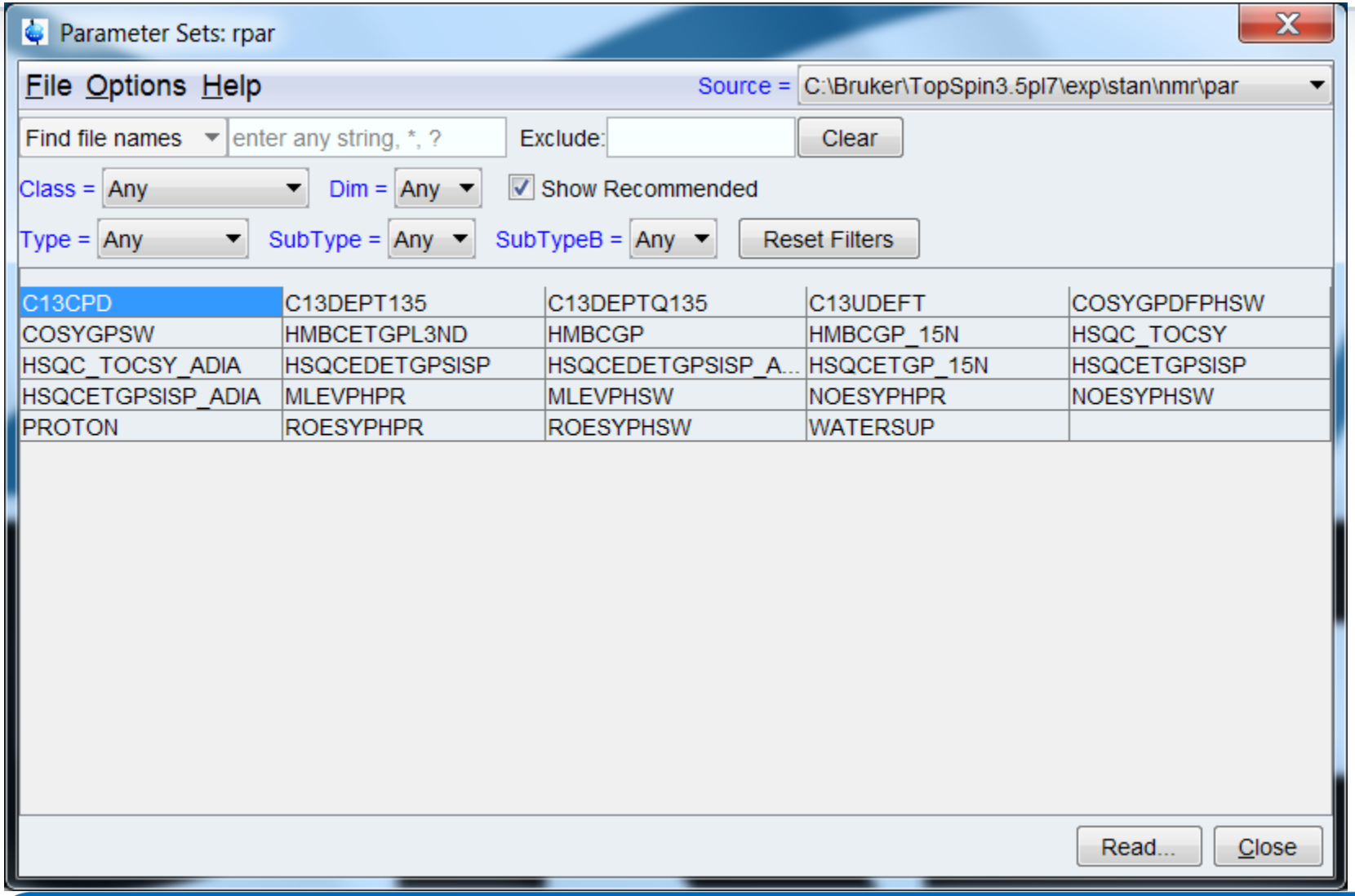


Useful commands – command line history **cmdhist**

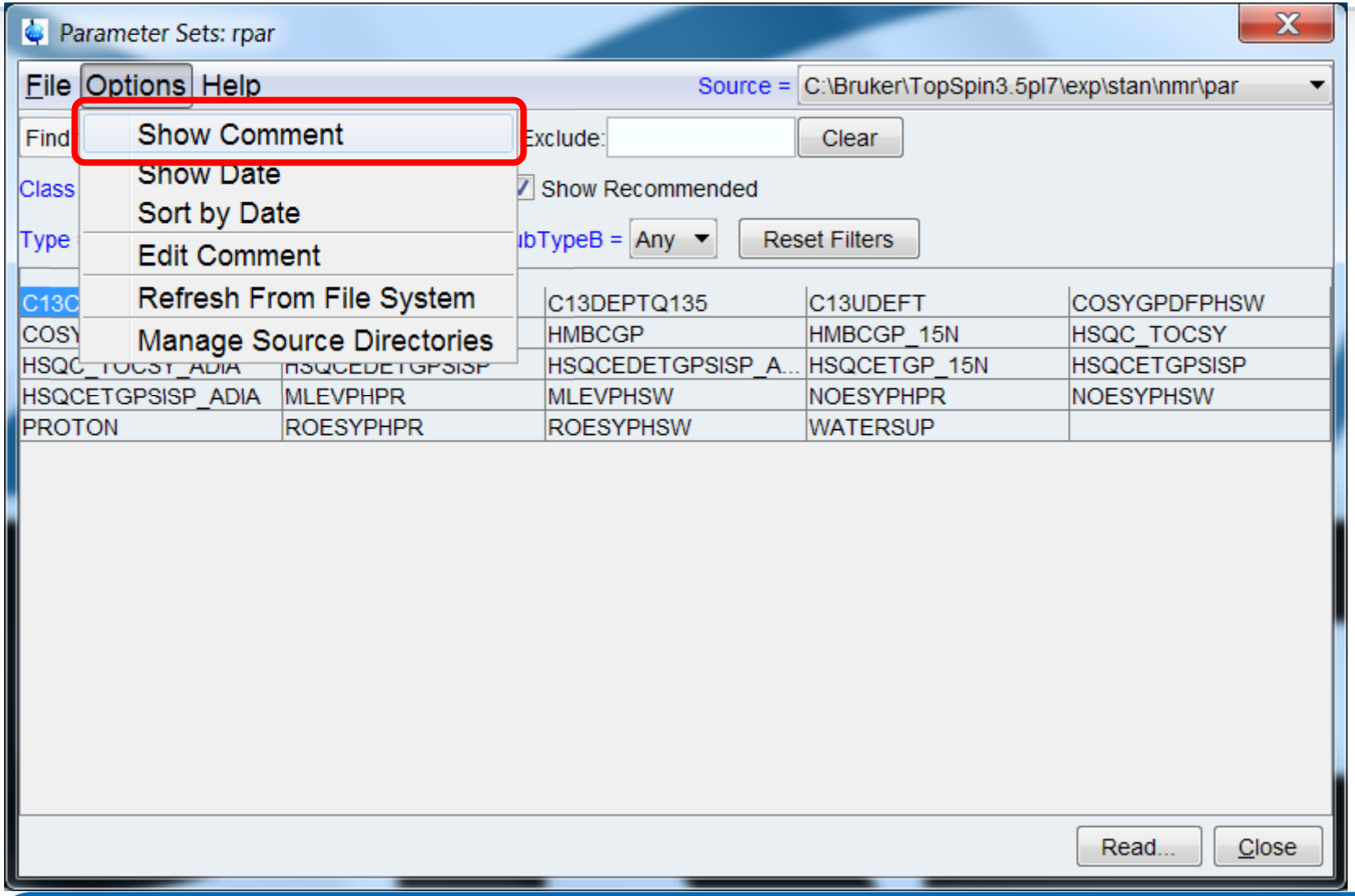
lists all entered commands since start of TopSpin



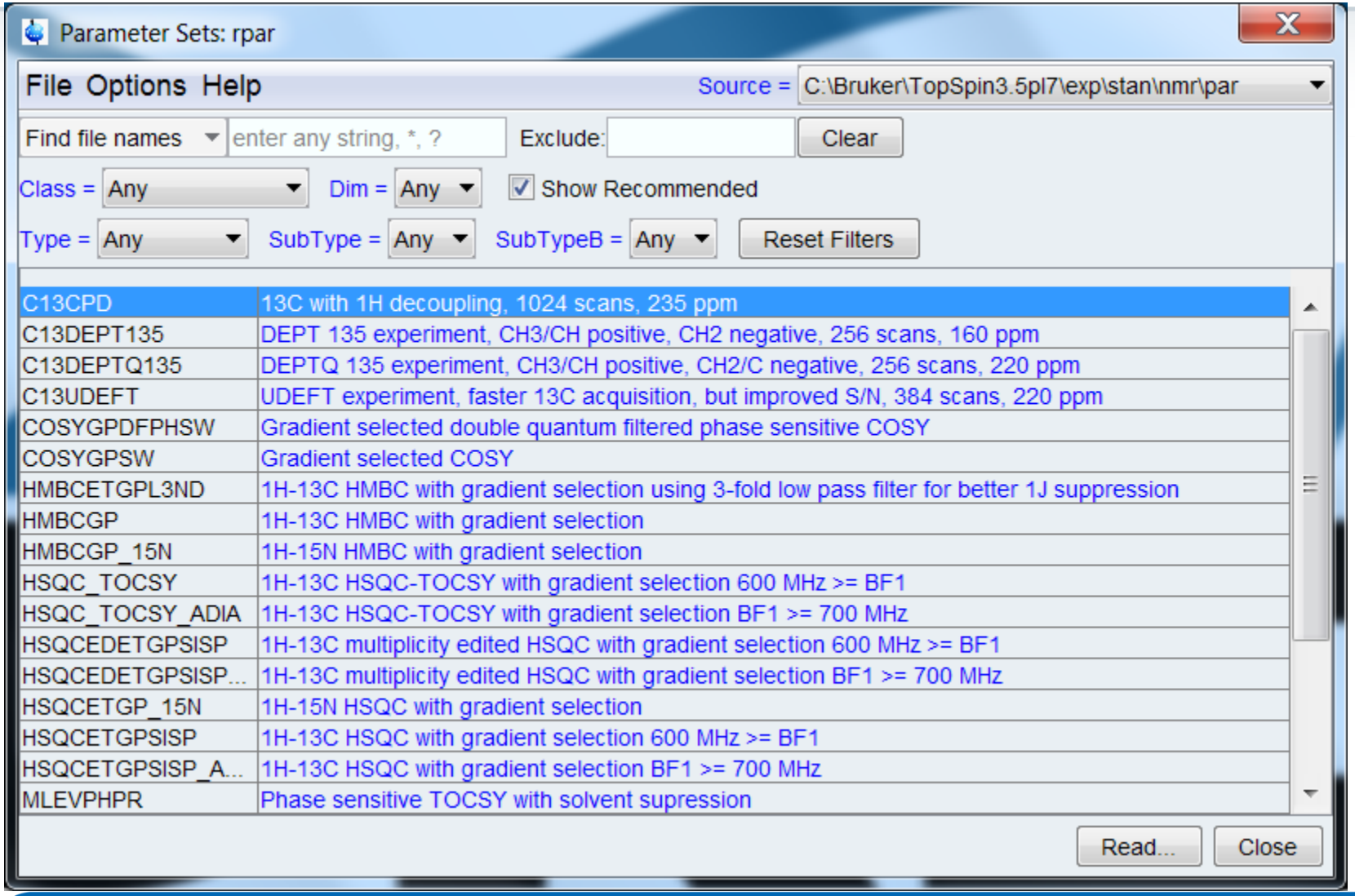
How to identify parameter sets?



How to identify parameter sets? Comments!



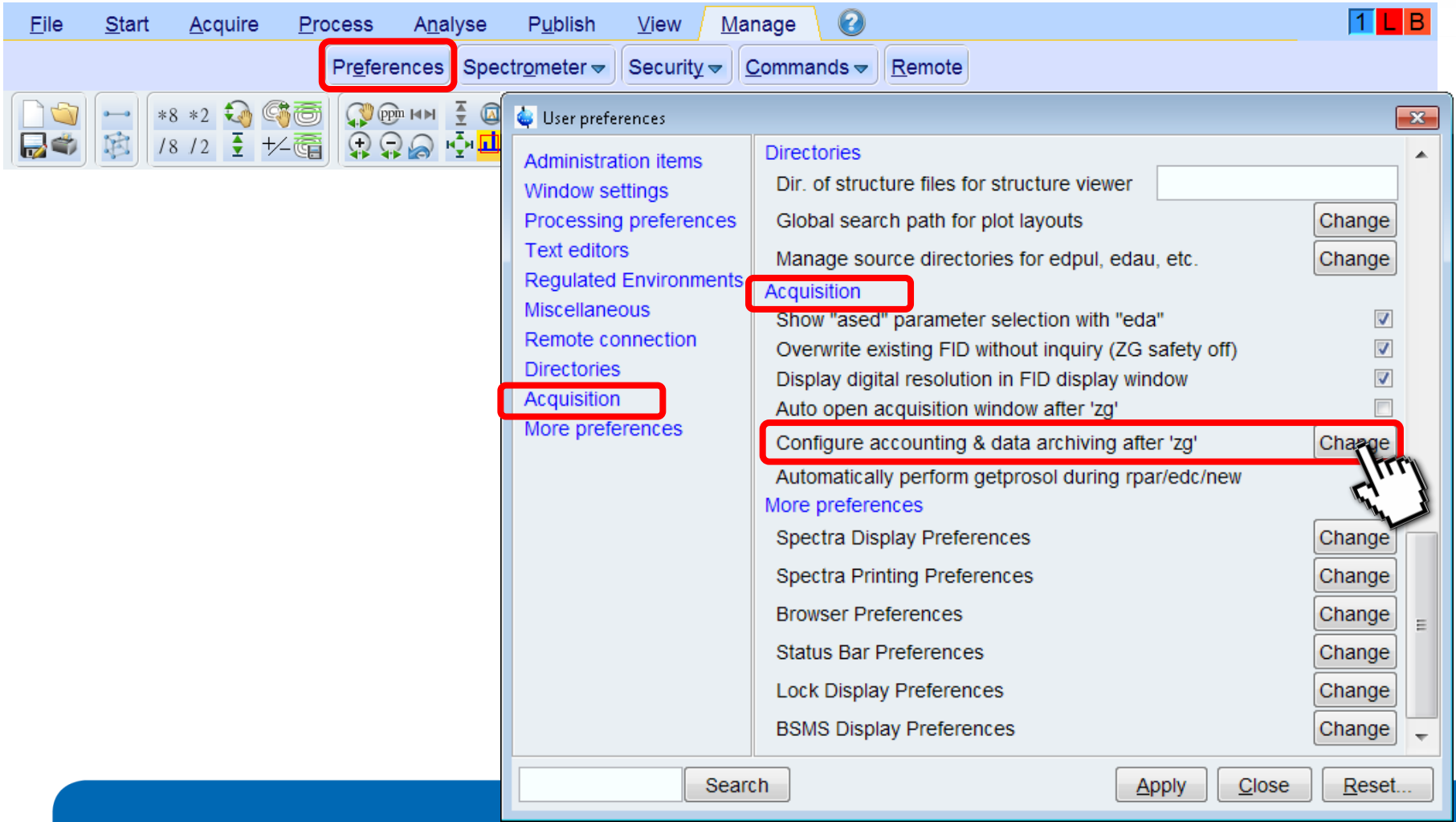
Comments


Parameter Sets: rpar
File Options Help
Source = C:\Bruker\TopSpin3.5pl7\exp\stan\nmr\par
Find file names
enter any string, *, ?
Exclude:
Clear
Class = Any
Dim = Any
Show Recommended
Type = Any
SubType = Any
SubTypeB = Any
Reset Filters
C13CPD 13C with 1H decoupling, 1024 scans, 235 ppm
C13DEPT135 DEPT 135 experiment, CH3/CH positive, CH2 negative, 256 scans, 160 ppm
C13DEPTQ135 DEPTQ 135 experiment, CH3/CH positive, CH2/C negative, 256 scans, 220 ppm
C13UDEFT UDEFT experiment, faster 13C acquisition, but improved S/N, 384 scans, 220 ppm
COSYGPDFPHSW Gradient selected double quantum filtered phase sensitive COSY
COSYGPSW Gradient selected COSY
HMBCETGPL3ND 1H-13C HMBC with gradient selection using 3-fold low pass filter for better 1J suppression
HMBCGP 1H-13C HMBC with gradient selection
HMBCGP_15N 1H-15N HMBC with gradient selection
HSQC_TOCSY 1H-13C HSQC-TOCSY with gradient selection 600 MHz >= BF1
HSQC_TOCSY_ADIA 1H-13C HSQC-TOCSY with gradient selection BF1 >= 700 MHz
HSQCEDETGPSISP 1H-13C multiplicity edited HSQC with gradient selection 600 MHz >= BF1
HSQCEDETGPSISP... 1H-13C multiplicity edited HSQC with gradient selection BF1 >= 700 MHz
HSQCETGP_15N 1H-15N HSQC with gradient selection
HSQCETGPSISP 1H-13C HSQC with gradient selection 600 MHz >= BF1
HSQCETGPSISP_A... 1H-13C HSQC with gradient selection BF1 >= 700 MHz
MLEVPHPR Phase sensitive TOCSY with solvent supression
Read...
Close

- **Archiving & Accounting**

Accounting in TopSpin

- Accounting in TopSpin has to be activated manually once

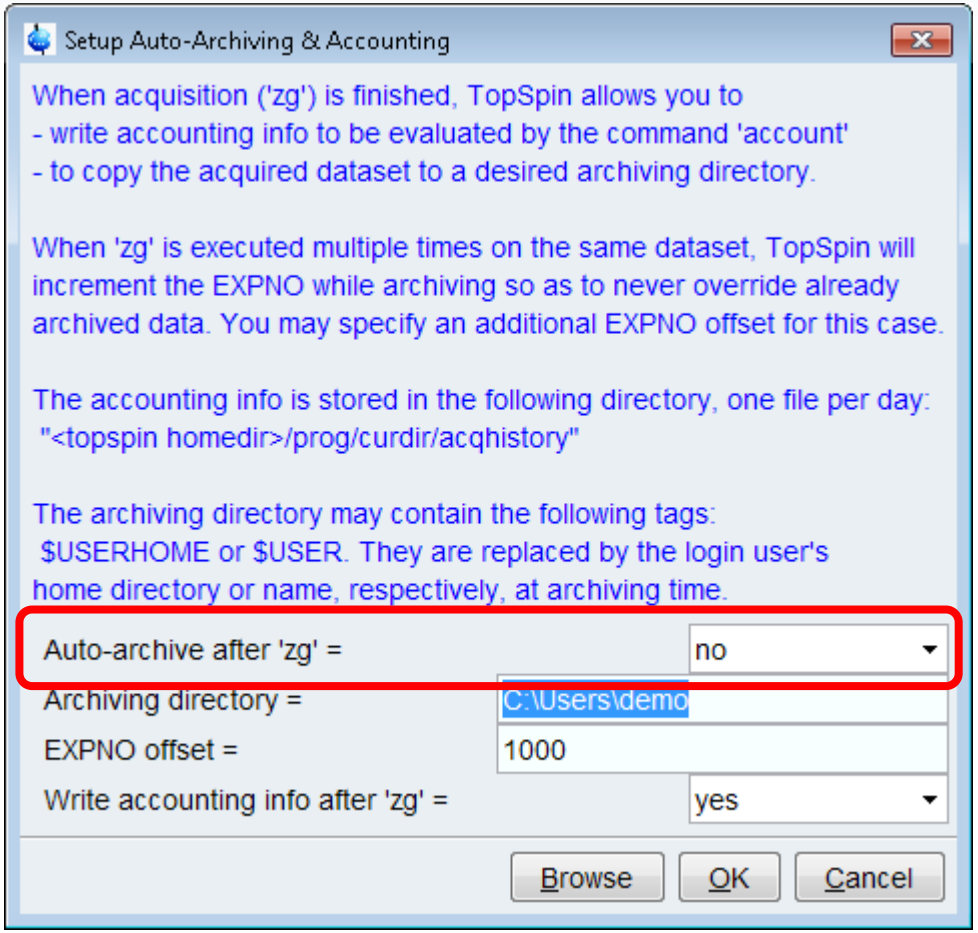


Archiving configuration

Like archive option in ICON-NMR

will archive each acquisition which has been started from within TopSpin GUI

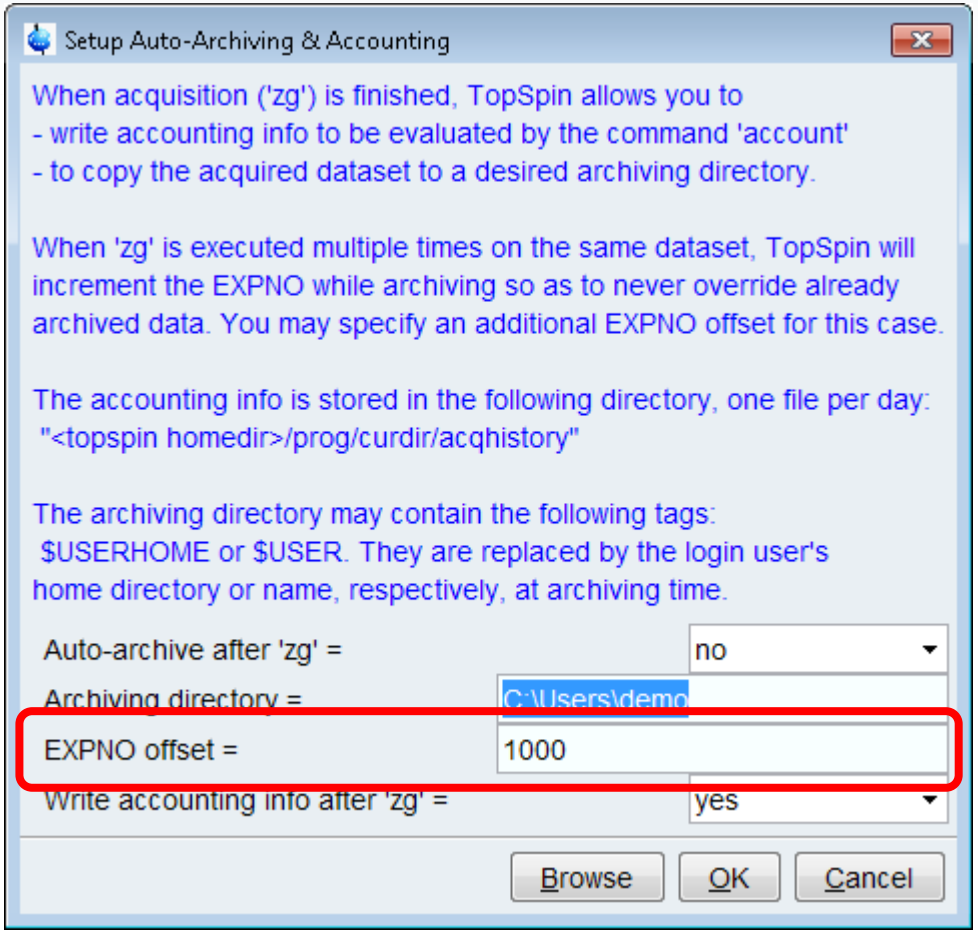
(for AU programs: use '**XCMD("sendgui zg")**'



Archiving configuration

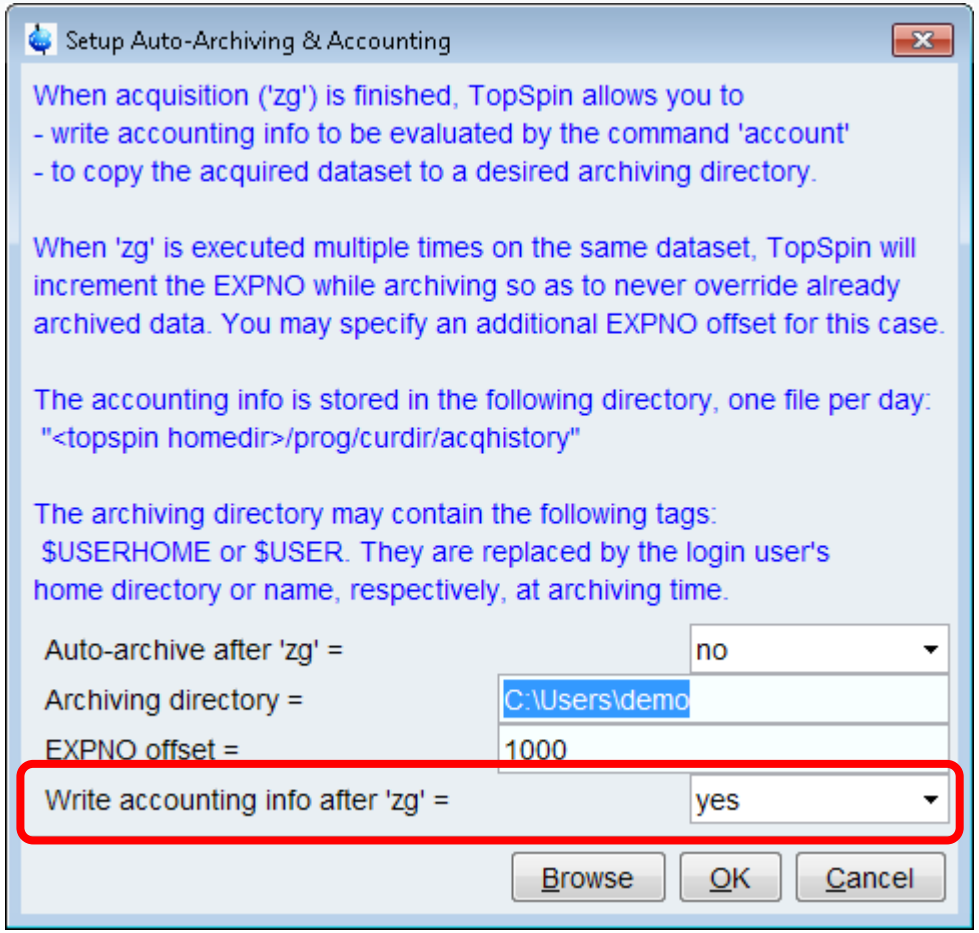
If an experiment is executed a second time, the dataset is added to the archive as a new expno

Increment is user-specific.



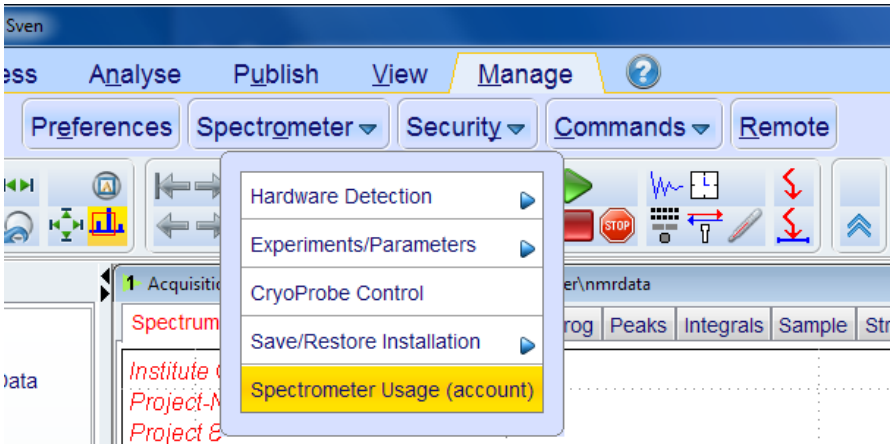
Archiving configuration

A new accounting possibility is implemented.



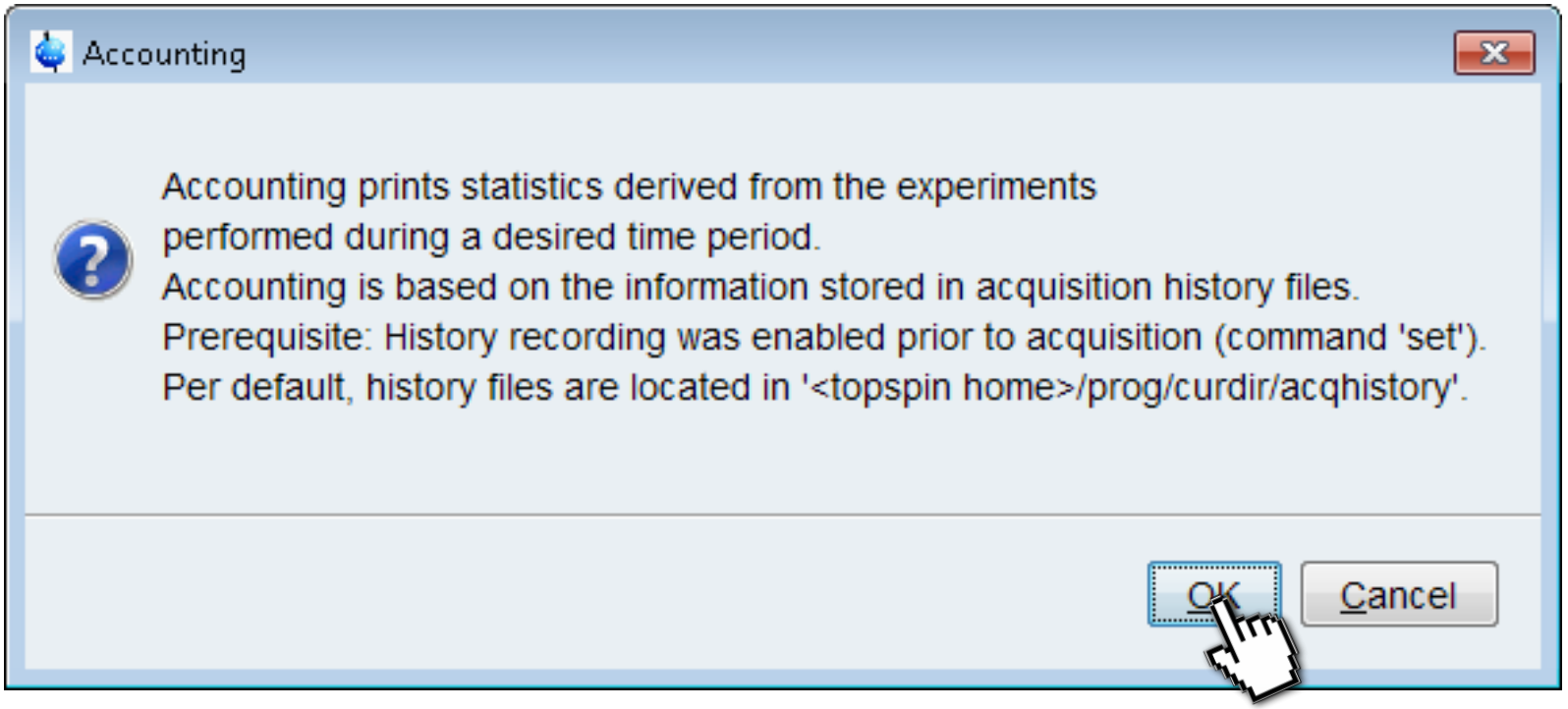
Accounting in TopSpin

- The accounting file (a file per day; XML format) will be stored in: <topspinhome>/prog/curdir/acqhistory
- The accounting file can be opened via
  Manage → Spectrometer → Spectrometer Usage (account)

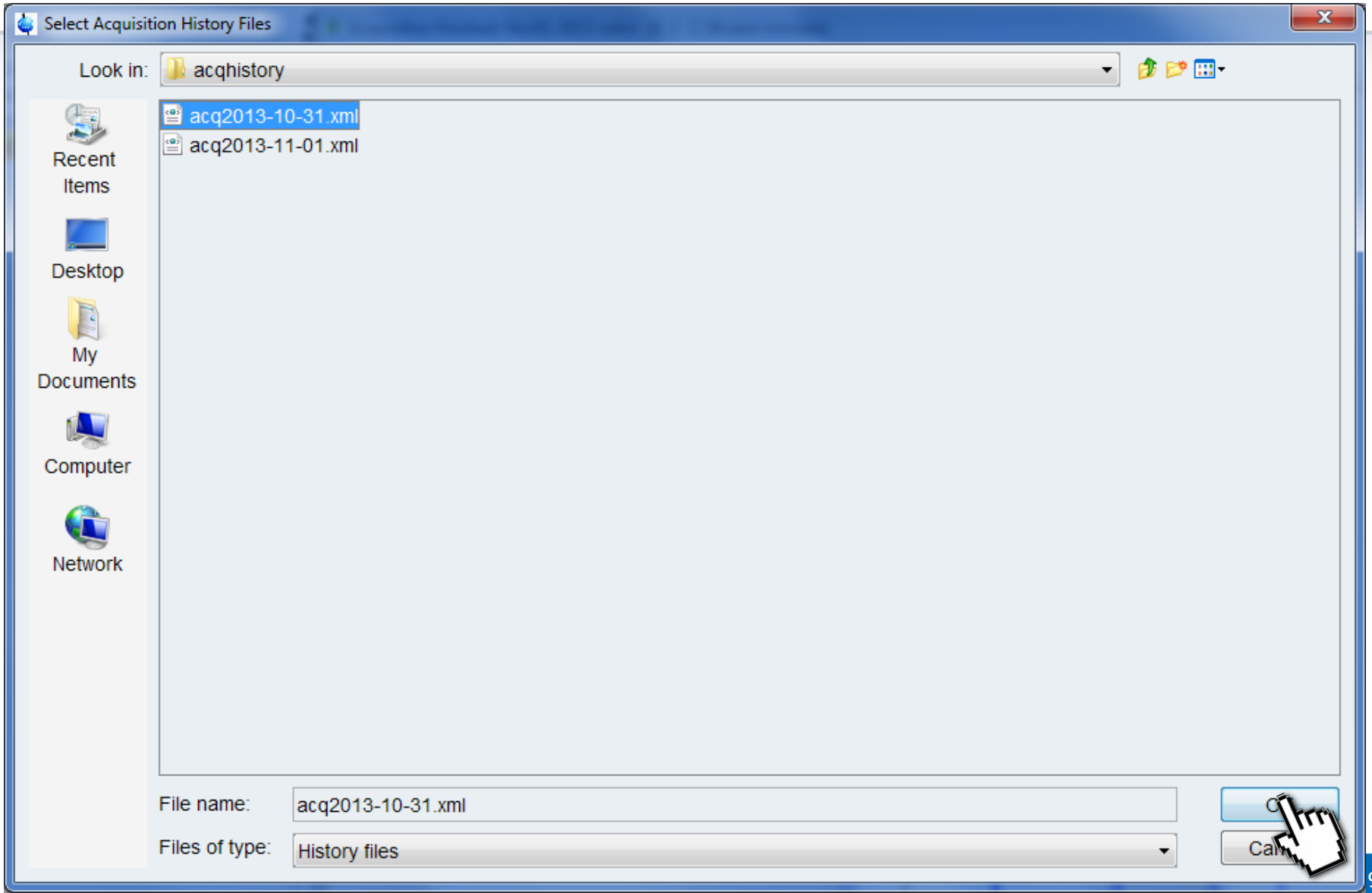


- or the TopSpin command **account**

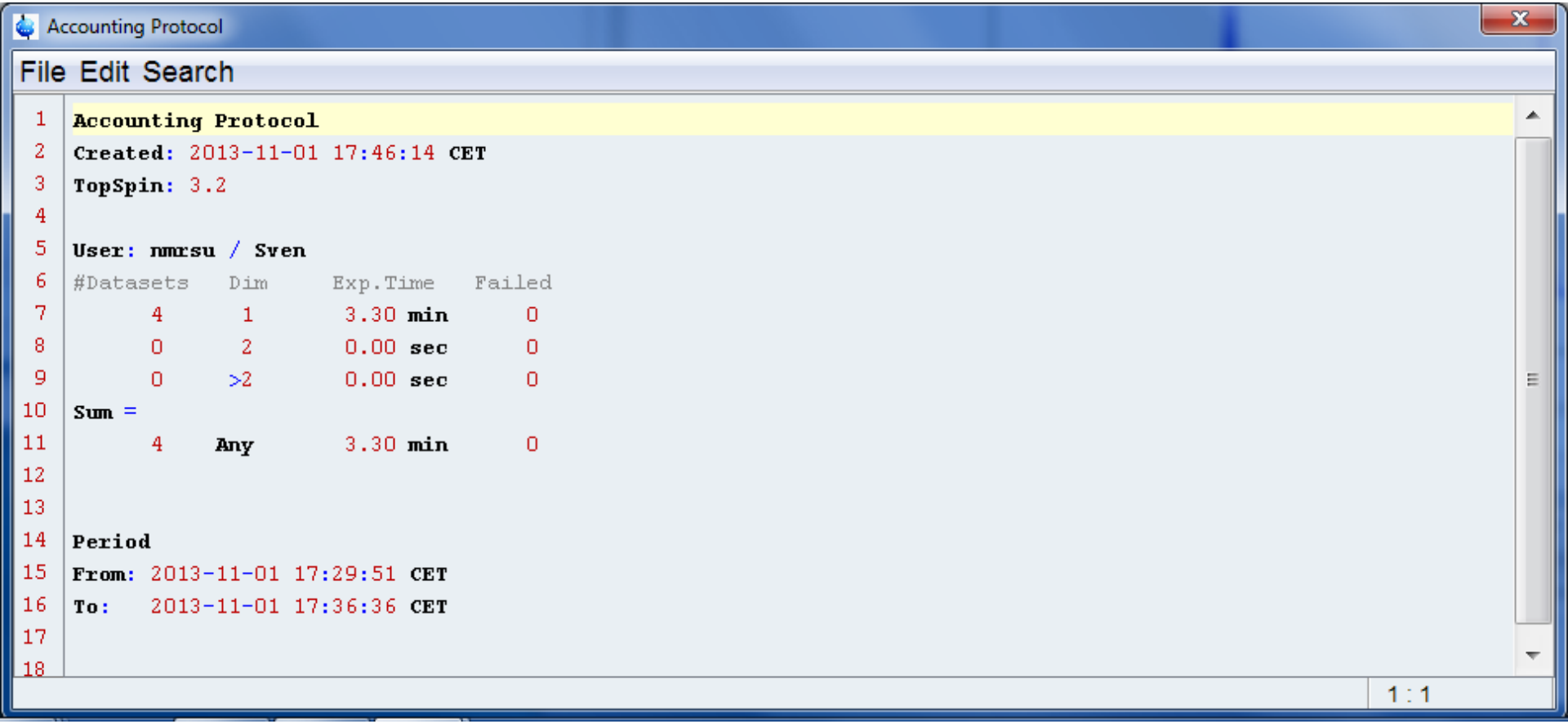
Accounting in TopSpin



Accounting in TopSpin

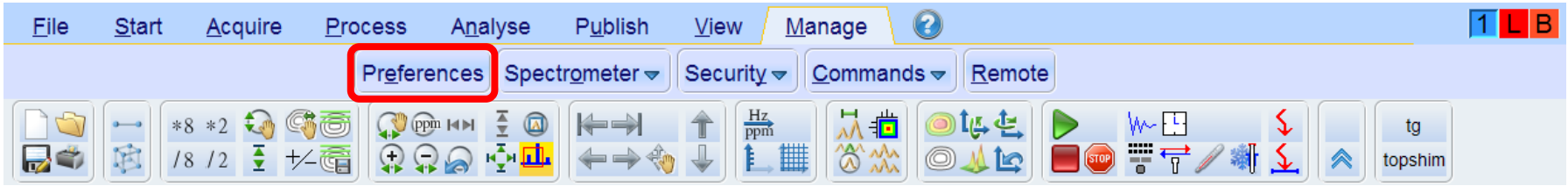


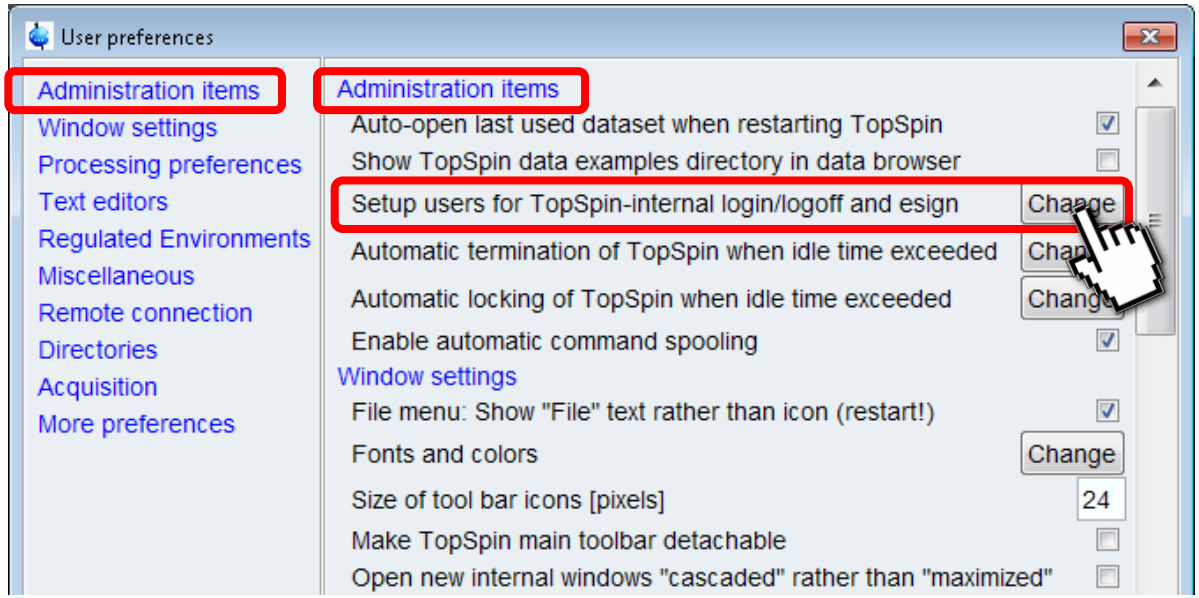
Accounting in TopSpin



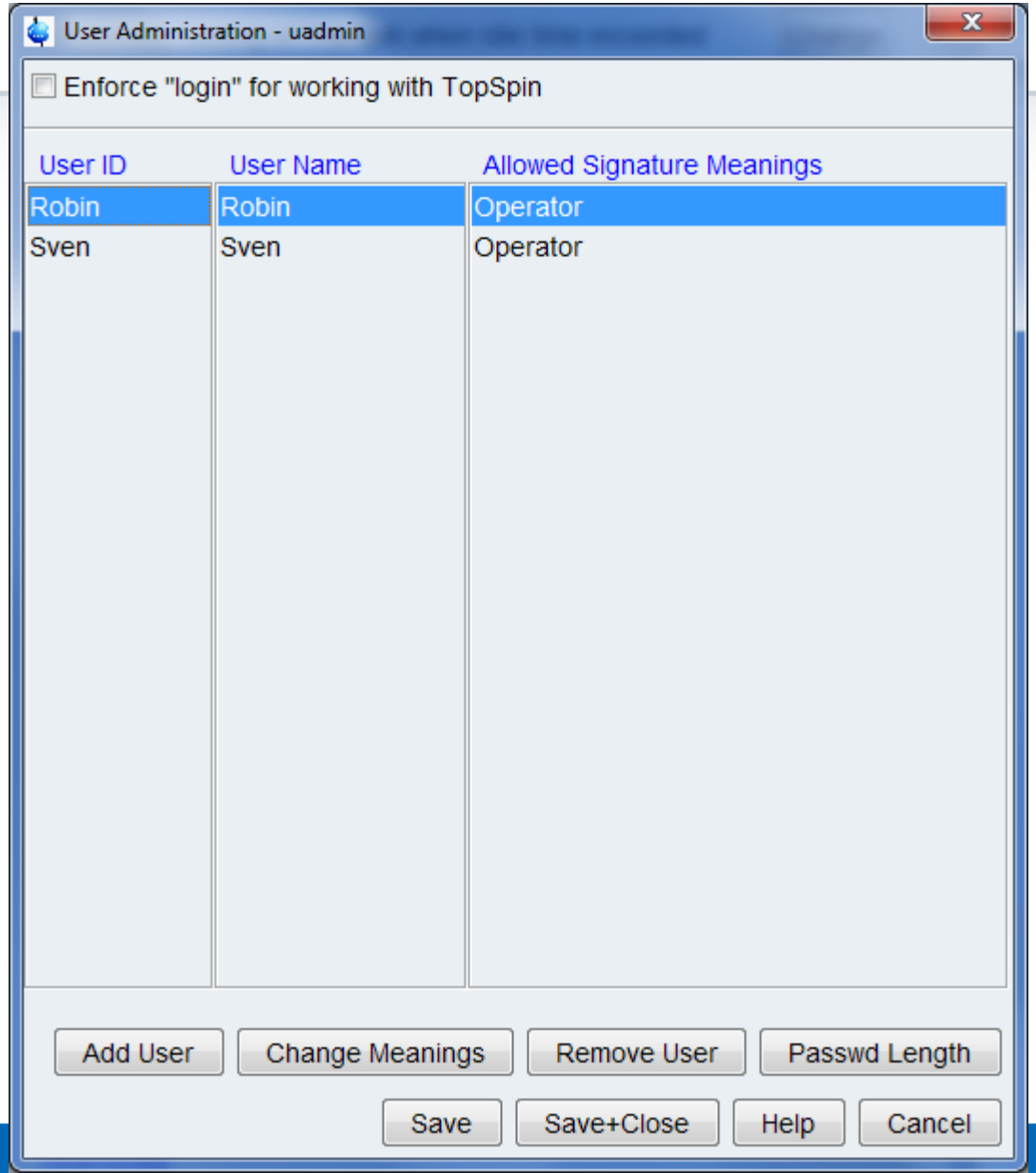
Accounting in TopSpin

- User-specific accounting with TopSpin-internal users



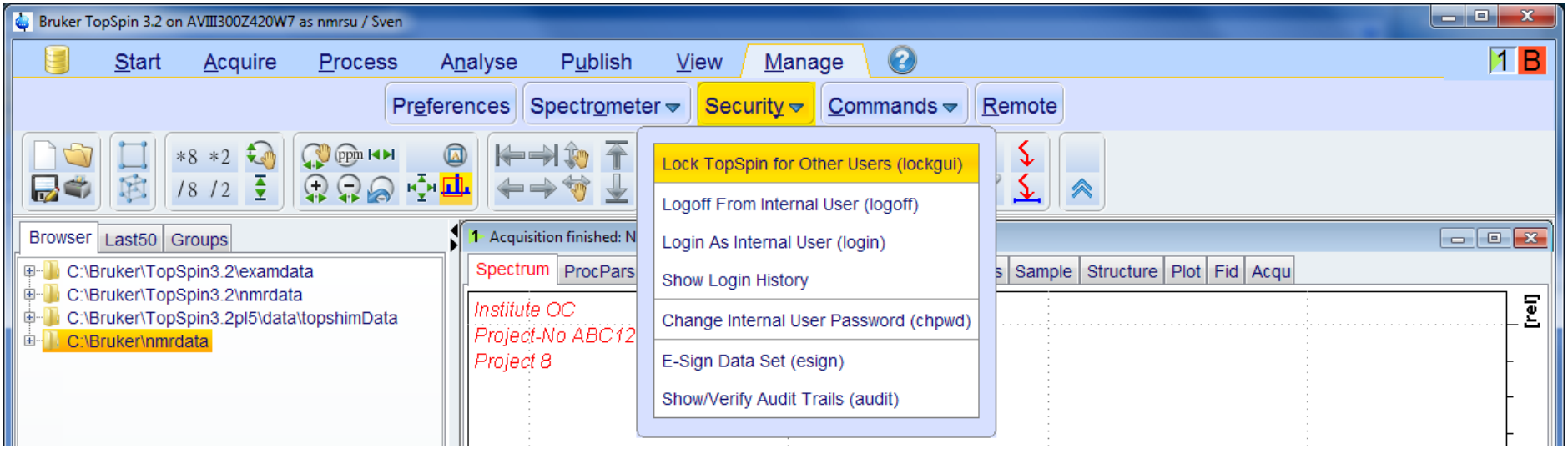


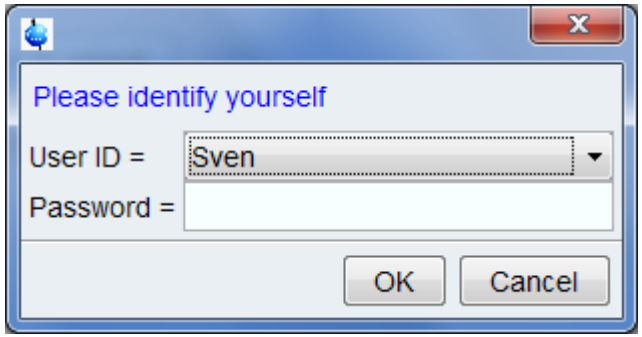
TopSpin-internal users



Accounting in TopSpin

- Switching the user can be executed with the commands **login** / **logoff**





User-specific accounting in TopSpin

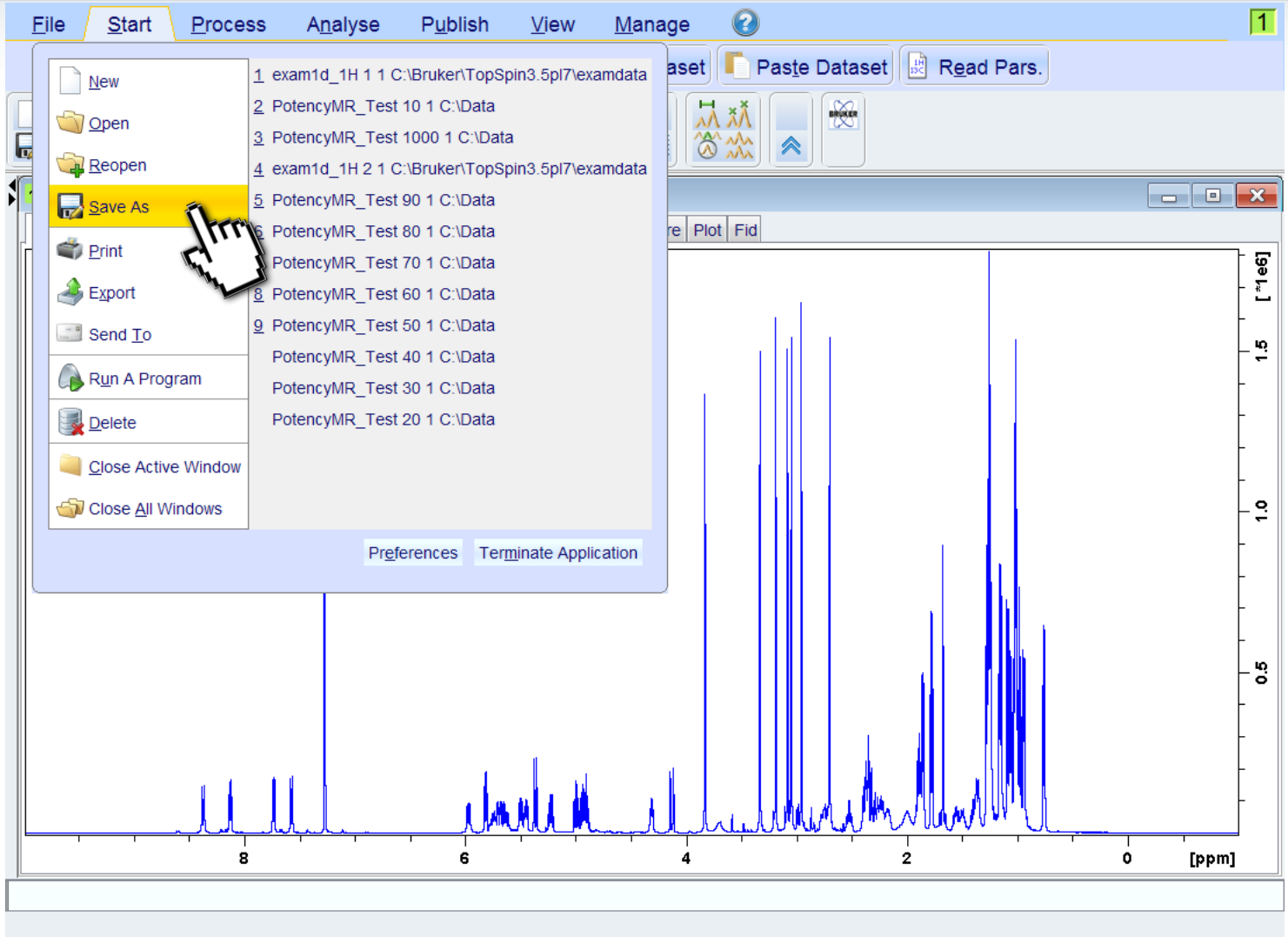
Accounting Protocol

File Edit Search

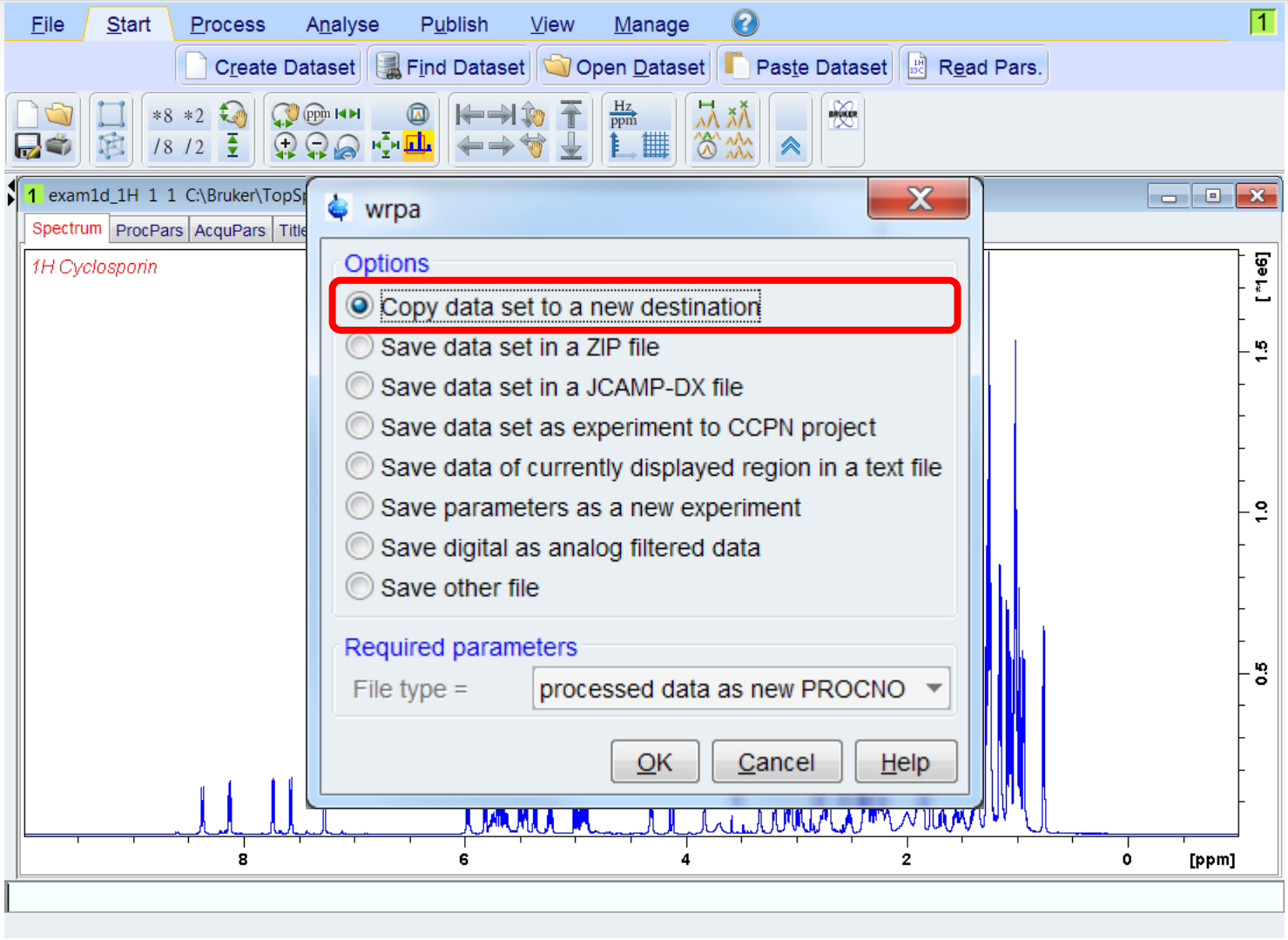
```
Accounting Protocol
Created: 2013-11-01 17:44:16 CET
TopSpin: 3.2

User: nmrsu
#Datasets    Dim      Exp.Time    Failed
       2       1       1.07 min       0
       0       2       0.00 sec       0
       0      >2       0.00 sec       0
Sum =
       2     Any       1.07 min       0


Period
From: 2013-10-31 16:44:10 CET
To:   2013-10-31 16:48:33 CET


------------------------------------------------------------


User: nmrsu / Robin
#Datasets    Dim      Exp.Time    Failed
       4       1       1.59 min       1
       0       2       0.00 sec       0
       0      >2       0.00 sec       0
Sum =
       4     Any       1.59 min       1


Period
From: 2013-10-31 16:50:28 CET
To:   2013-10-31 16:51:44 CET

The following datasets had "acquisition failed" status:

C:\Bruker\nmrdata\Oct31-2013-robin\16\pdata\1
  failed: Raw data file 'fid' not found: No such file or directory Oct31-2013-robin  16  1  C:\Bruker\nmrdata

------------------------------------------------------------
```

- **Save/Convert Data Sets**

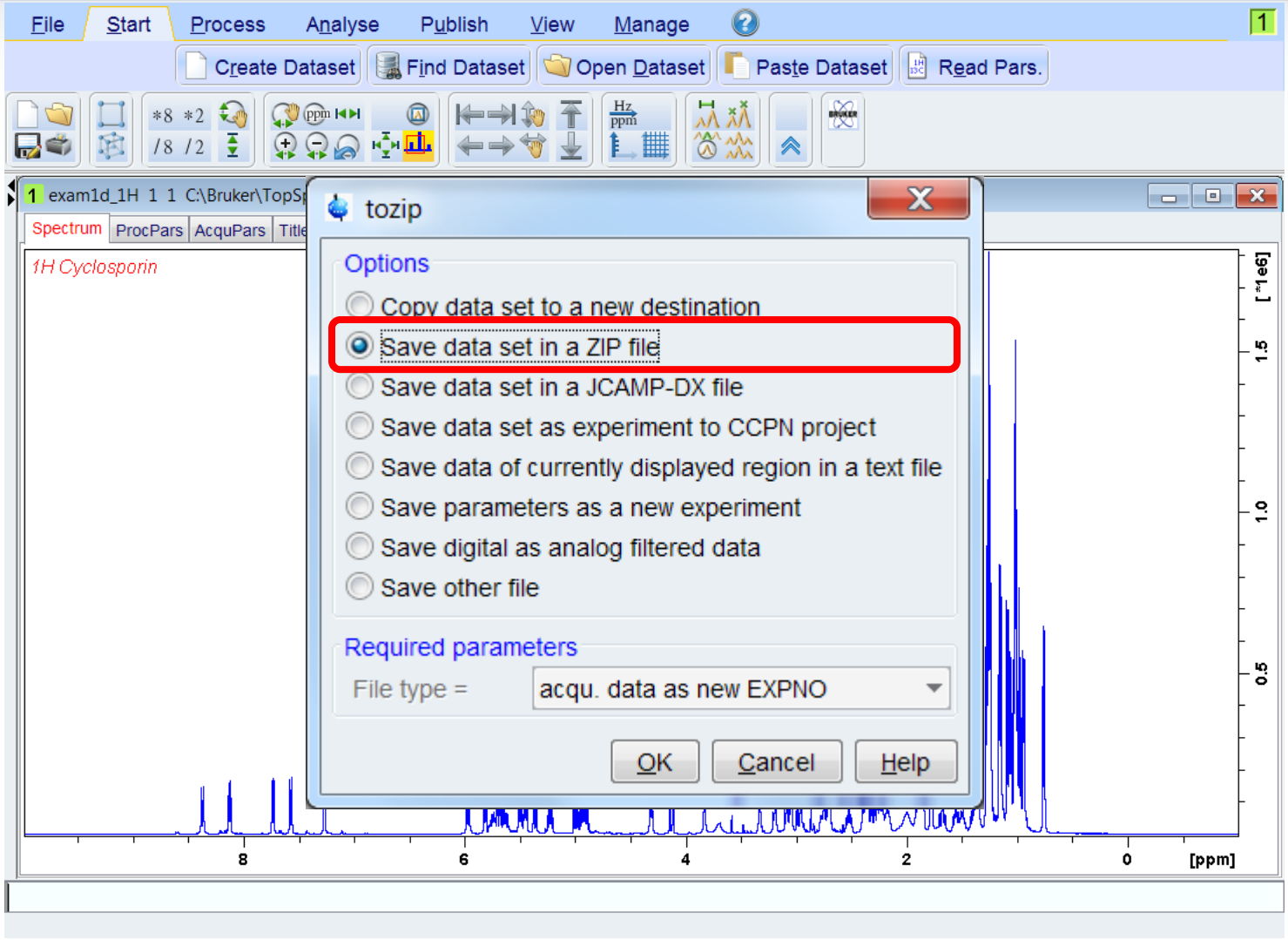
Save data as…


File
Start
Process
Analyse
Publish
View
Manage
Paste Dataset
Read Pars.
New
Open
Reopen
Save As
Print
Export
Send To
Run A Program
Delete
Close Active Window
Close All Windows
1 exam1d_1H 1 1 C:\Bruker\TopSpin3.5pl7\examdata
2 PotencyMR_Test 10 1 C:\Data
3 PotencyMR_Test 1000 1 C:\Data
4 exam1d_1H 2 1 C:\Bruker\TopSpin3.5pl7\examdata
5 PotencyMR_Test 90 1 C:\Data
6 PotencyMR_Test 80 1 C:\Data
7 PotencyMR_Test 70 1 C:\Data
8 PotencyMR_Test 60 1 C:\Data
9 PotencyMR_Test 50 1 C:\Data
PotencyMR_Test 40 1 C:\Data
PotencyMR_Test 30 1 C:\Data
PotencyMR_Test 20 1 C:\Data
Preferences
Terminate Application
Plot
Fid
[*1e6]
1.5
1.0
0.5
8
6
4
2
0
[ppm]

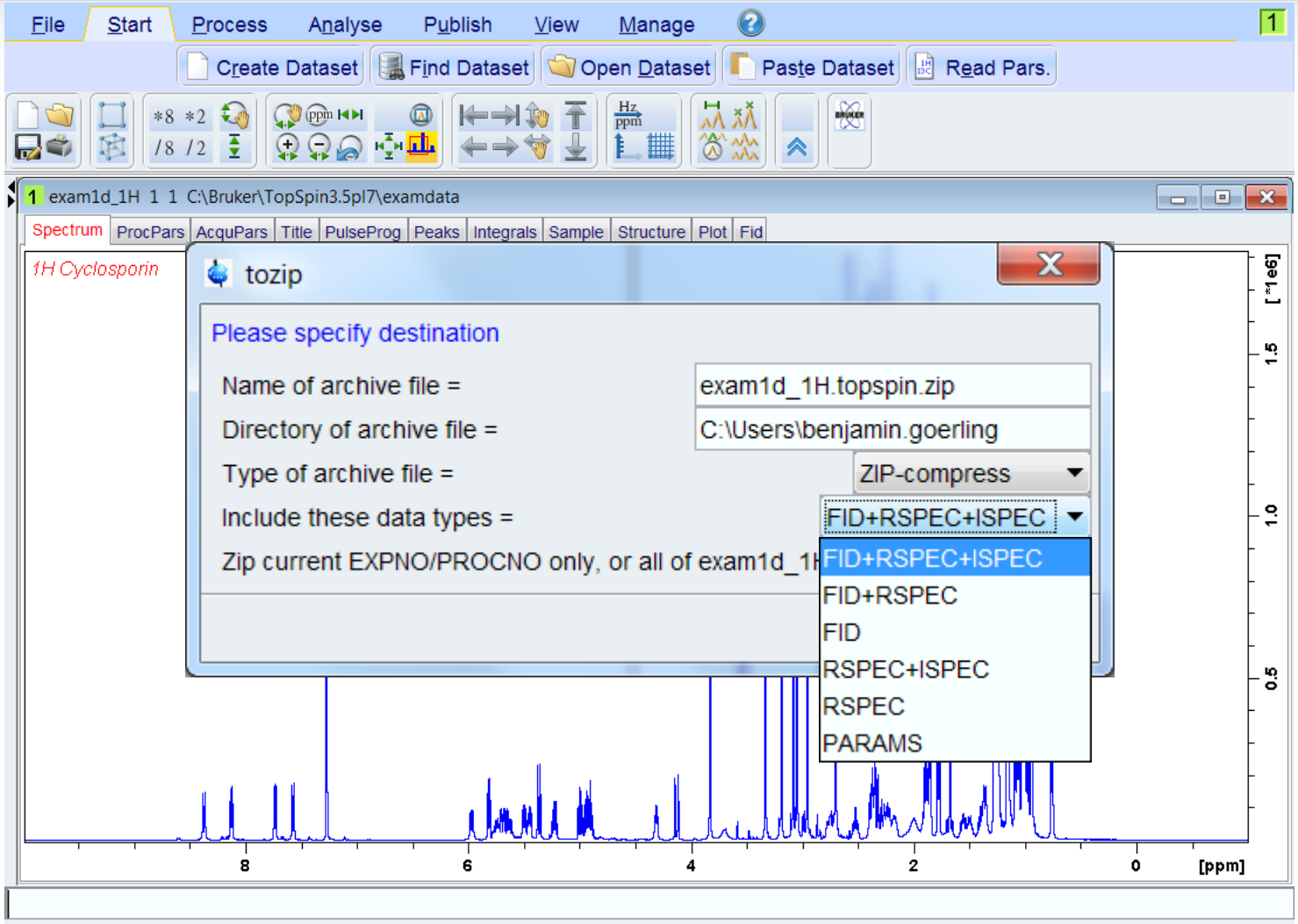
Copy data set to new destination



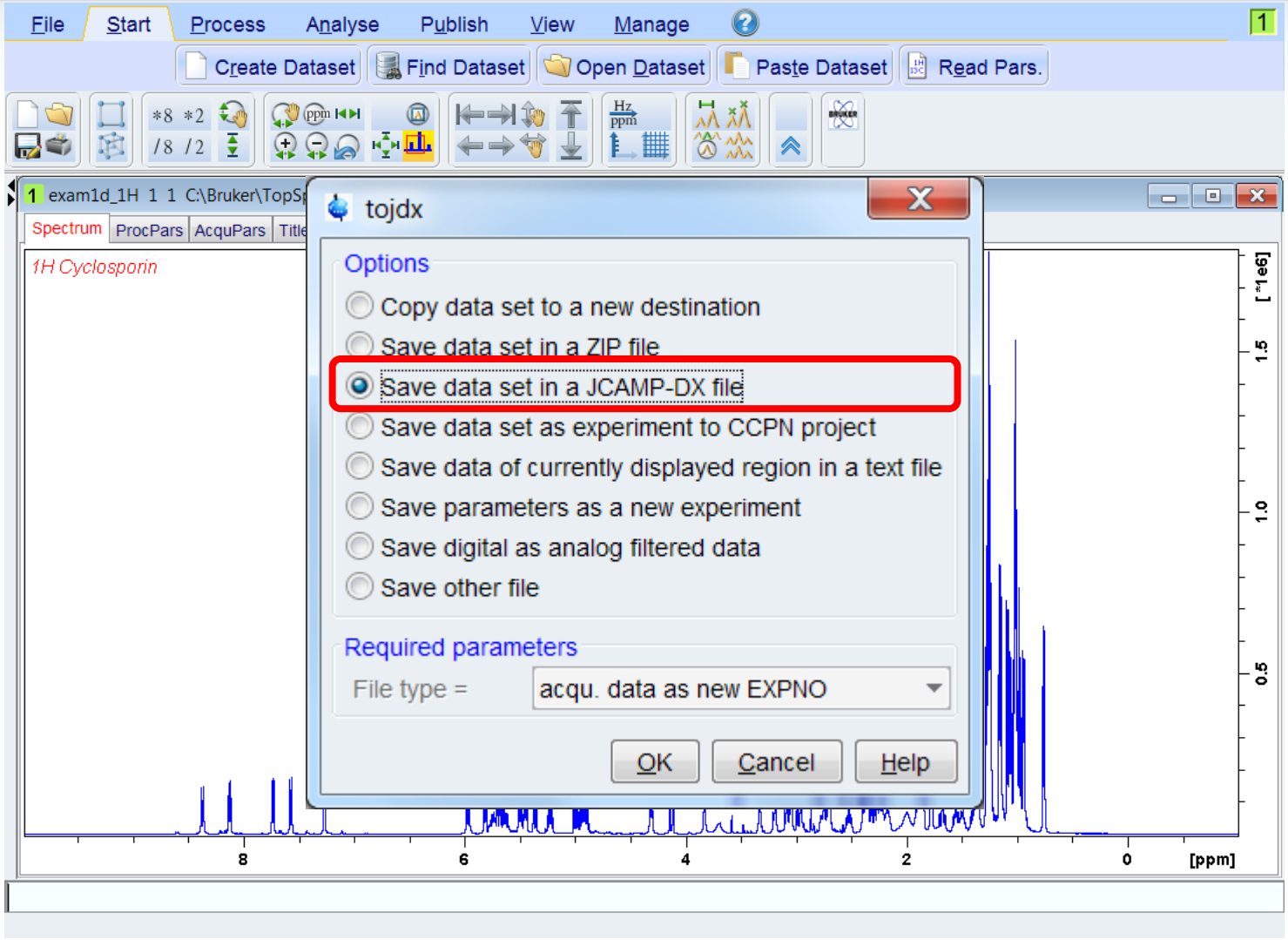
Save data set as ZIP file



Save data set as ZIP file



Save data set in a JCAMP-DX file

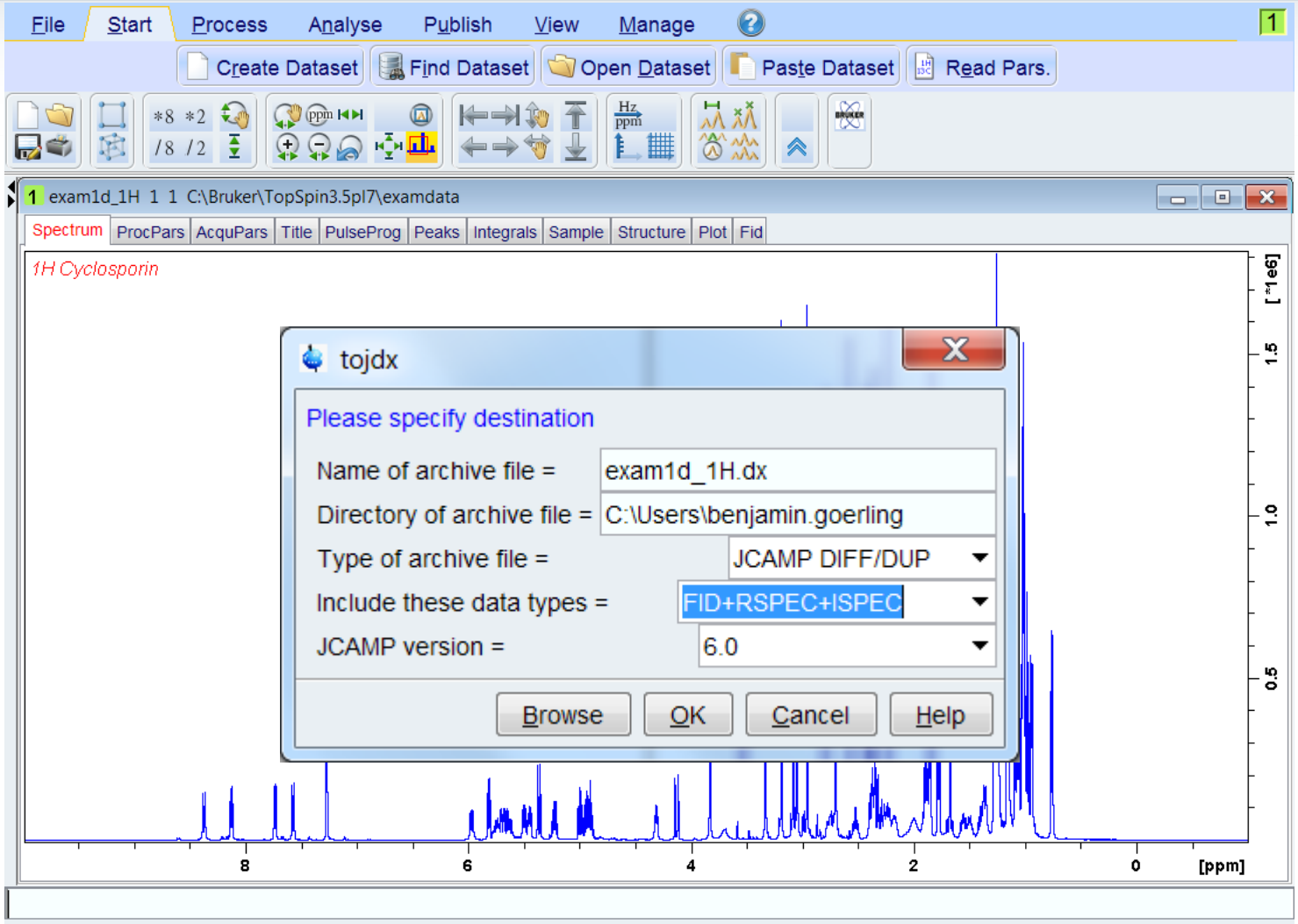


JCAMP???

What is a JCAMP file?

JCAMP is a IUPAC standard format!
It is an ASCII file that contains all necessary information of the spectrum/FID.

Save data set in a JCAMP-DX file



JCAMP-DX: TopSpin

For JCAMP format, you can choose between the following compression mode:

- FIX (=0) : table format
- PACKED (=1) : no spaces between the intensity values
- SQUEEZED (=2) : the sign of the intensity values is encoded in the first digit
- DIFF/DUP (=3) : the difference between successive values is encoded, suppressing repetition of successive equal values (default = DIFF/DUP)

JCAMP-DX: TopSpin

For the included data types, you have the following choices:

- FID: raw data
- RSPEC+ISPEC: real and imaginary processed data
- RSPEC: real processed data
- PARAMS: parameter files
- FID+RSPEC+ISPEC: raw data, real and imaginary processed data
- FID+ALL_PROCNOS: raw data and all processed data
- ALL_EXPNOS_DIM_1_2: all EXPNOS of the dimensions 1D and 2D under this <NAME>

exam1d_1H.dx - Editor

Datei Bearbeiten Format Ansicht ?

```
##TITLE=1H Cyclosporin
##JCAMPDX= 6.0          $$ Bruker NMR JCAMP-DX V2.0
##DATA TYPE= NMR FID
##DATA CLASS= NTUPLES
##ORIGIN= UXNMR, Bruker Analytische Messtechnik GmbH
##OWNER= root
$$ TOPSPIN                Version 1.2
$$ 2004-09-21 23:17:47.879 +0200  gaty@SVEN
$$ Compression mode = diff/dup
##.OBSERVE FREQUENCY= 500.13250065
##.OBSERVE NUCLEUS= ^1H
##.DELAY= (6, 6)
##.ACQUISITION MODE= SIMULTANEOUS (DQD)
##.ACQUISITION SCHEME= undefined
##.AVERAGES= 16
##.DIGITISER RES= 18
##SPECTROMETER/DATA SYSTEM= spect
##.PULSE SEQUENCE= zg
##.SOLVENT NAME= CDCl3
##.SHIFT REFERENCE= (INTERNAL, CDCl3, 0, 11.008)
##AUDIT TRAIL= $$ (NUMBER, WHEN, WHO, WHERE, WHAT)
$$ ##TITLE= Audit trail, TOPSPIN                Version 1.2.b.15
$$ ##JCAMPDX= 5.01
$$ ##ORIGIN= Bruker BioSpin GmbH
$$ ##OWNER= nmrsu
$$ $$ d:/data/nmrsu/nmr/exam1d_1H/1/audita.txt
$$ ##AUDIT TRAIL=  $$ (NUMBER, WHEN, WHO, WHERE, WHAT)
(   1,<2004-03-30 16:00:49.843 +0200>,<nmrsu>,<KASTOR>,
      <created by zg, POWCHK disabled, PULCHK disabled
       configuration hash MD5:
       91 84 CA F9 28 91 F3 2D B7 D4 7D 96 EC CF 24 FE
       data hash MD5: 64K
       92 8A 14 05 B3 09 B1 4C 6C 7A AD 10 96 4D A5 B8>)
$$ ##END=
$$
$$ $$ hash MD5
$$ $$ 75 DB 0B A0 EF A6 51 CA 3C 5D 36 1B 0A 21 AE EB
##$RELAX=
##$BRUKER FILE EXP=format.temp
$$ EDIT_PAR COMMAND FILE
$$
$$ DI_MODE          LONG
$$ ED_ENTRY         ACQU
$$ ORDER            FILE
$$
$$
$$ HEADER                "F2 - Acquisition Parameters"
$$ T_NAME                Date_
$$              TYPE     R64
$$              CLASS    ACQU
$$              SUBRANGE 0.0 50000000
$$              REL      "Date_=itodate(DATE)"
$$              INV_REL  "DATE=datetoi(Date_,DATE)"
```

Some examples about the content of JCAMP:

Parameters

Acquisition audit trail

Parameter on the plot

exam1d_1H.dx - Editor

Datei Bearbeiten Format Ansicht ?

```
$$ ;$Id: Avance2.incl,v 1.10 2003/02/25 14:46:08 ber Exp $
$$ # 6 "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg" 2
$$
$$
$$
$$ # 1 "mc_line 9 file C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg expanding definition of mc command after ze"
$$ define delay MCWRK
$$ define delay MCREST
$$ "MCWRK = 0.500000*30m"
$$ "MCREST = 30m - 30m"
$$ # 9 "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg"
$$ 1 ze
$$ # 1 "mc_line 9 file C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg expanding definition of mc command after ze"
$$ # 10 "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg"
$$ # 1 "mc_line 10 file C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg expanding start label for mc command"
$$ 2 MCWRK  * 2
$$ LBLF0, MCREST
$$ # 11 "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg"
$$   d1
$$   p1 ph1
$$   go=2 ph31
$$ # 1 "mc_line 14 file C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg expanding mc command in line"
$$   MCWRK wr #0
$$   MCWRK zd
$$   lo to LBLF0 times td0
$$
$$ # 15 "C:/Bruker/TOPSPIN/exp/stan/nmr/lists/pp/zg"
$$ exit
$$
$$
$$ ph1=0 2 2 0 1 3 3 1
$$ ph31=0 2 2 0 1 3 3 1
$$
$$
$$ ;pl1 : f1 channel - power level for pulse (default)
$$ ;p1 : f1 channel -  high power pulse
$$ ;d1 : relaxation delay; 1-5 * T1
$$ ;NS: 1 * n, total number of scans: NS * TD0
$$
$$
$$
$$ ;$Id: zg,v 1.7 2002/06/12 09:05:19 ber Exp $
##$RELAX=
##$BRUKER FILE EXP=uxnmr.par
$$ ##TITLE= Parameter file, TOPSPIN            Version 1.2.b.15
$$ ##JCAMPDX= 5.0
$$ ##DATATYPE= Parameter Values
$$ ##ORIGIN= Bruker BioSpin GmbH
$$ ##OWNER= nmrsu
$$ $$ 2004-03-24 09:47:27.794 +0100  nmrsu@KASTOR
$$ $$ D:/Bruker/ts12b15/conf/instr/spect/uxnmr.par
$$ ##$ACB= 0
$$ ##$ACBTAT= (0..15)
```

Some examples about the content of JCAMP:

Spectrometer configuration

exam1d_1H.dx - Editor

Datei Bearbeiten Format Ansicht ?

```
##$SI= 32768
##$SIGF1= 0
##$SIGF2= 0
##$SINO= 400
##$SIOLD= 32768
##$SREGLST= <1H.CDCl3>
##$SSB= 0
##$STSI= 0
##$STSR= 0
##$SW_p= 6009.6153846154
##$SYMM= 0
##$S_DEV= 0
##$TDeff= 0
##$TDoff= 0
##$TI= <>
##$TILT= no
##$TM1= 0
##$TM2= 0
##$TOPLEV= 0
##$USERP1= <user>
##$USERP2= <user>
##$USERP3= <user>
##$USERP4= <user>
##$USERP5= <user>
##$WDW= 1
##$XDIM= 8192
##$YMAX_p= 0
##$YMIN_p= 0
$$ End of Bruker specific parameters
$$ --------------------------------
##NTUPLES= NMR FID
##VAR_NAME=  TIME,           FID/REAL,        FID/IMAG
##SYMBOL=    X,              R,               I
##VAR_TYPE=  INDEPENDENT,    DEPENDENT,       DEPENDENT
##VAR_FORM=  AFFN,           ASDF,            ASDF
##VAR_DIM=   32768,          32768,           32768
##UNITS=     SECONDS,        ARBITRARY UNITS, ARBITRARY UNITS
##FACTOR=    0.0001664,      1,               1
##FIRST=     0,              0,               0
##LAST=      5.4524288,      0,               0
##MIN=       0,              -1582073,        0
##MAX=       5.4524288,      1314760,         0
$$ Real data points
##PAGE= N=1
##DATA TABLE= (X++(R..R)), XYDATA
0@%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%Nj4K5m0N6o4P2q8J04j28J52j76K08k40K73l10L56
40A91l99M48n12N83o60P40q26R21j029J140j256J388j535J691j853K027k220K425
58A264k637K868l103L334l557L743l850L786l356K129J032r650L8944k54830j358190
73a582073J854586M11558j302000J226544L6290j273191P96721J73042q89244
82e47767Q85271J45978j133348M44279M72009o35168M01170M84267o82213j71544
92c37066M33522j38221j43080J49054K9818l61o3958k5415K47905m7122l02574
103a97498M2830J5182L7174L23007j95939k51125L66947j45751k03962N14158
113C05023l20019m99378O40266j11166n52803O80611R8671n48724M78064J4400
```

Some examples about the content of JCAMP:

Parameters

Spektrum/FID

Datasets as text file

The command **tojdx** converts NMR dataset into JCAMP format. It contains also peak information, audit trail, pulse program etc.
Works on 1D and 2D data, raw/real/imaginary data.

The command **totxt** has been implemented to store the data of the displayed region in text format.
Works on 1D and 2D data.

A new AU program **convbin2asc** has been implemented. It writes a 1D spectrum, with or without imaginary data points, into a file in ASCII table format.

Datasets as text file

totxt

tojdx

exam1d_1H-3.5pl6-fix-1r_1i.dx - Notepad

File Edit Format View Help

```
##TITLE=1H Cyclosporin
##JCAMPDX= 6.0          $$ Bruker NMR JCAMP-DX V2.0
##DATA TYPE= NMR SPECTRUM
##DATA CLASS= NTUPLES
##ORIGIN= UXNMR, Bruker Analytische Messtechnik GmbH
##OWNER= root
$$ XWIN-NMR                Version 3.5
$$ Tue Sep 21 02:15:35 2004 W. Europe Daylight Time (UT+2h)  BRUKER\svcu@XENIA
##.OBSERVE FREQUENCY= 500.13250065
##.OBSERVE NUCLEUS= ^1H
##.ACQUISITION MODE= SIMULTANEOUS (DQD)
ION SCHEME= undefined
= 16
R RES= 18
TER/DATA SYSTEM= spect
QUENCE= zg
NAME= CDCl3
FERENCE= (INTERNAL, CDCl3, 0, 11.008)
IL= $$ (NUMBER, WHEN, WHO, WHERE, WHAT)
 Audit trail, TOPSPIN                Version 1.3.b.7
X= 5.01
= Bruker BioSpin GmbH
 svcu
r/topspin1.3/data/guest/nmr/exam1d_1H/1/pdata/1/auditp.txt
```

exam1d_1H.txt - WordPad

File Edit View Insert Format Help

```
# File created = Saturday, April 16, 2005 6:27:36 AM CEST
# Data set = a-009
# Spectral Region:
# LEFT = 11.008049964904785 ppm. RIGHT = -1.0080566166148195 ppm.
#
# SIZE = 32768 ( = number of points)
#
# In the following ordering is from the 'left' to the 'right'
# Lines beginning with '#' must be considered as comment lines
#
-156545.53125
-156179.59375
-156036.96875
-155695.25
-155015.3125
-154496.34375
-154347.34375
-153882.15625
-153178.4375
-152669.3125
-152399.71875
```

For Help, press F1

ascii-spec.txt - WordPad

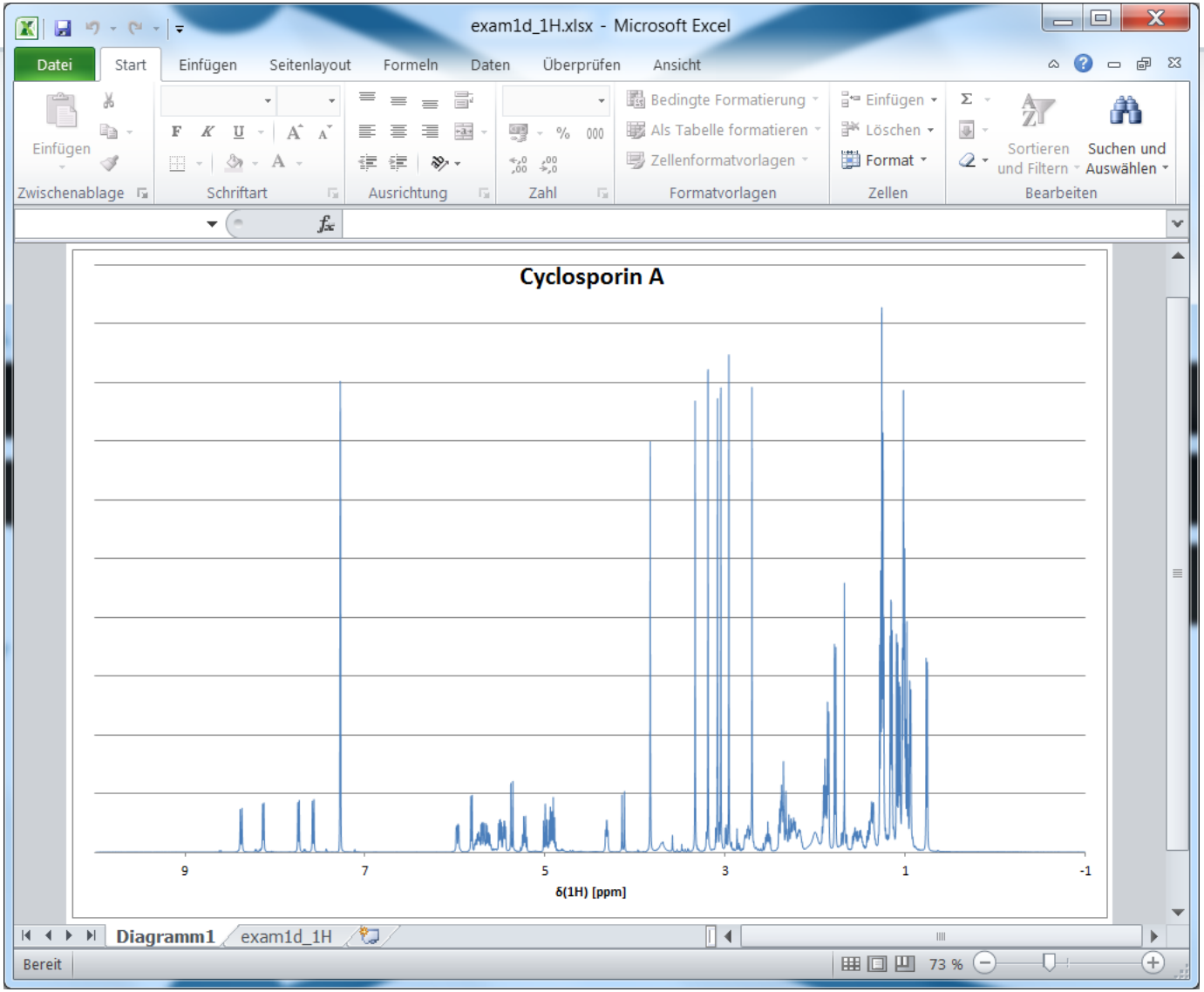
File Edit View Insert Format Help

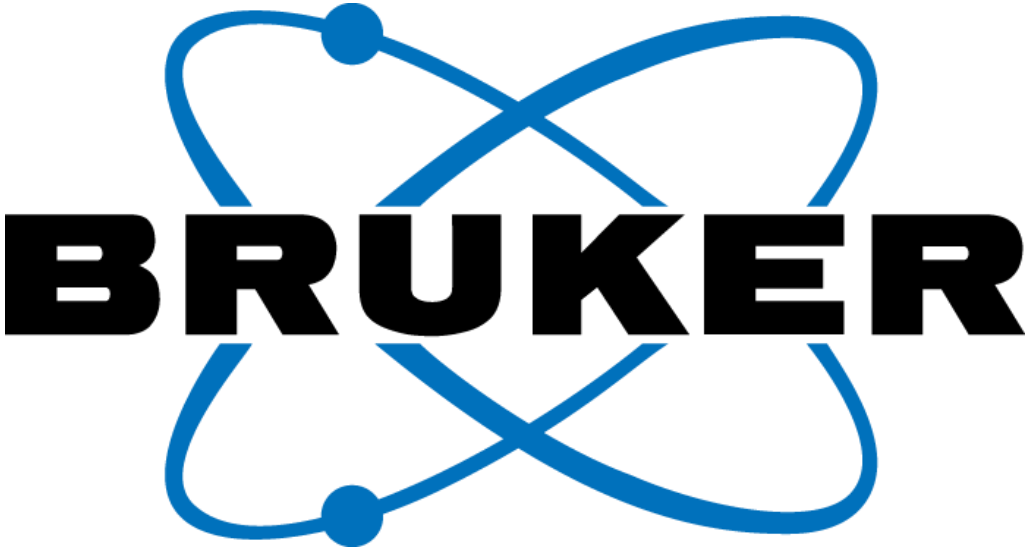
```
 1, -5009457, 5505.364, 11.0079
 2, -4997747, 5505.181, 11.0075
 3, -4993183, 5504.998, 11.0071
 4, -4982248, 5504.814, 11.0068
 5, -4960490, 5504.631, 11.0064
 6, -4943883, 5504.447, 11.0060
 7, -4939115, 5504.264, 11.0057
 8, -4924229, 5504.081, 11.0053
 9, -4901710, 5503.897, 11.0049
10, -4885418, 5503.714, 11.0046
11, -4876791, 5503.530, 11.0042
12, -4871369, 5503.347, 11.0038
13, -4856147, 5503.164, 11.0035
14, -4842060, 5502.980, 11.0031
15, -4831028, 5502.797, 11.0027
16, -4820532, 5502.613, 11.0024
17, -4807014, 5502.430, 11.0020
18, -4791021, 5502.247, 11.0016
19, -4780020, 5502.063, 11.0013
20, -4765746, 5501.880, 11.0009
21, -4750765, 5501.696, 11.0005
```

For Help, press F1

convbin2asc

NMR meets Excel





www.bruker.com