

# TopSpin

*Data Display &  
Processing*

**Data Display Modes**

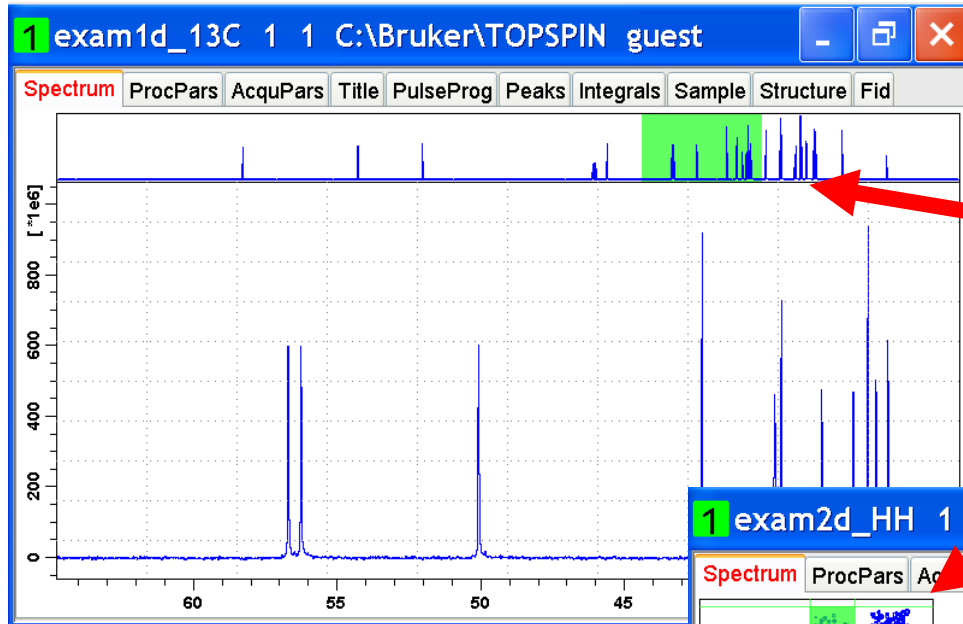
**Processing Guide**

**Interactive Processing Examples**

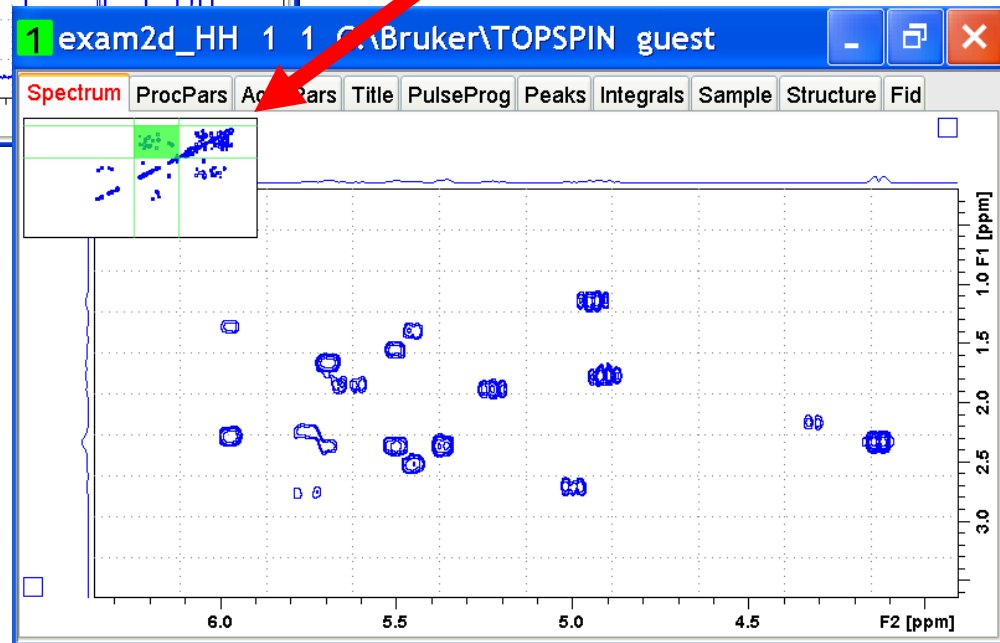
**Data Processing Functionalities**

**Serial Processing**

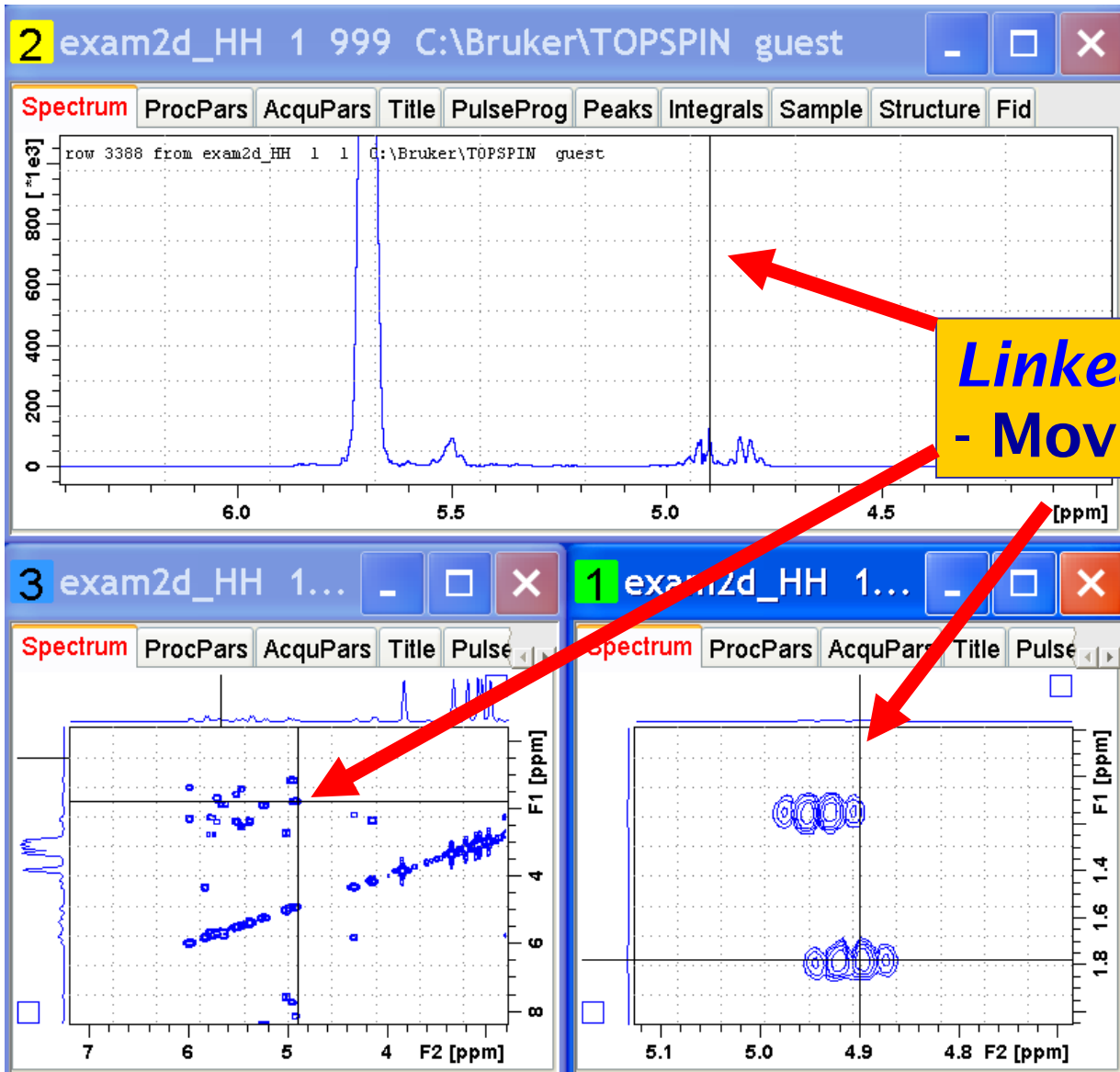
# Data Display Modes



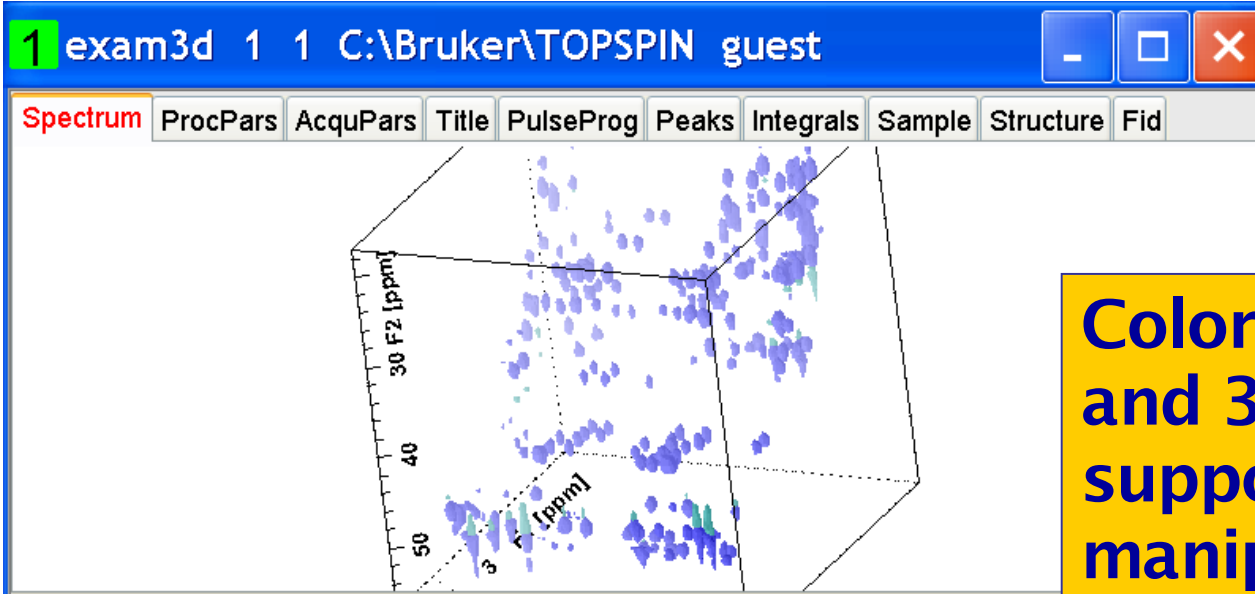
- Overview spectrum display
- Expanded region highlighted and draggable



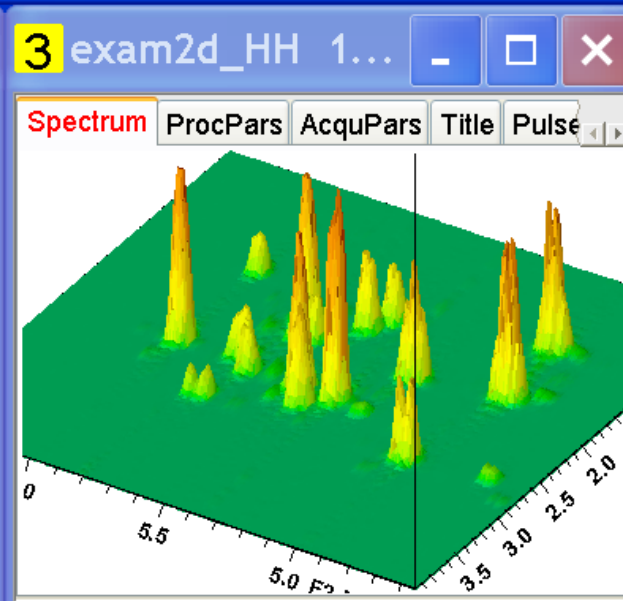
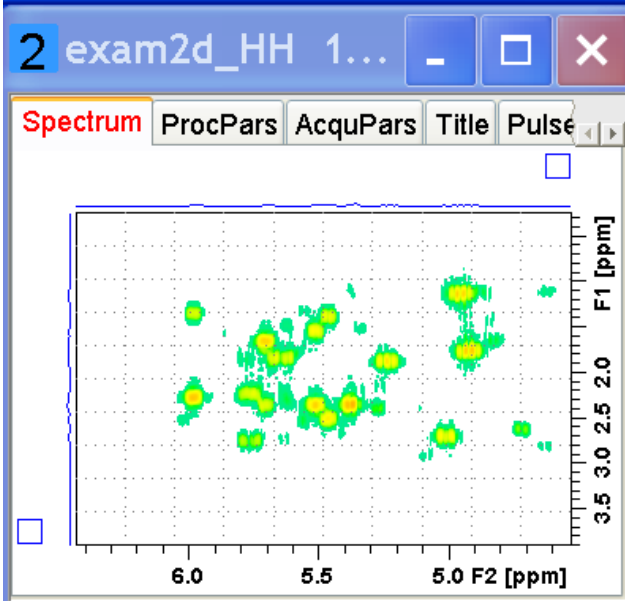
# Data Display Modes



# Data Display Modes



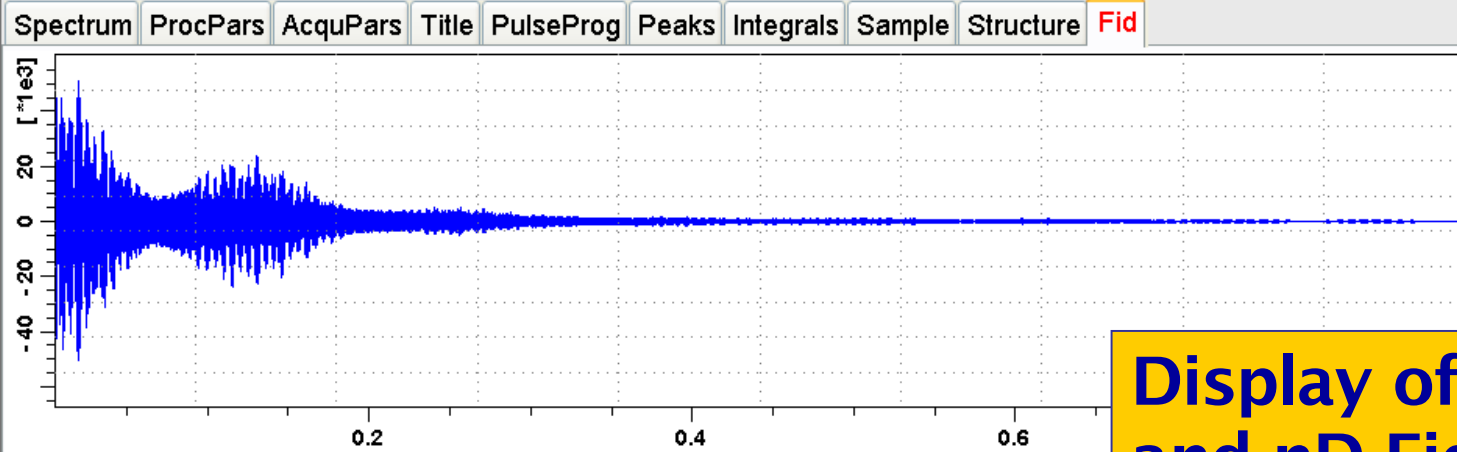
**Color display of 2D and 3D spectra, supports interactive manipulations**



# Data Display Modes

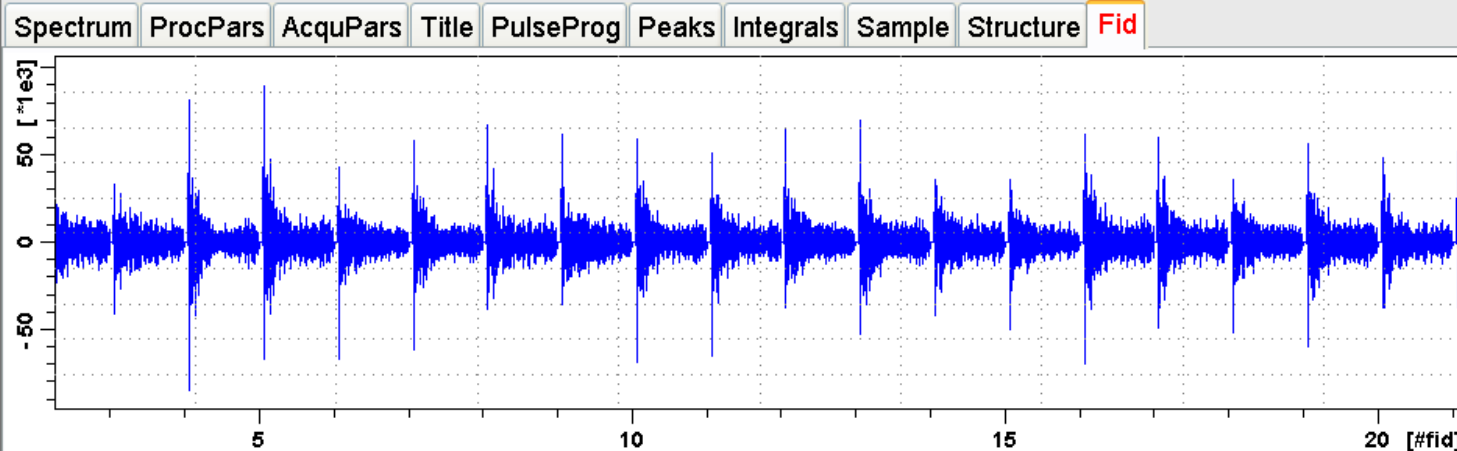


2 Benzaldehyde 240 1 C:\Bruker\TOPSPIN guest



Display of 1D and nD Fids

1 exam2d\_HH 3 1 C:\Bruker\TOPSPIN guest



# Data Display Modes



4 Benzaldehyde 240 ...

Spectrum ProcPars AcqPars Title PulseProg Pe

3 Benzaldehyde 240 ...

PulseProg Peaks Integrals Sample Structure Fid

2 Benzaldehyde 240 ...

Spectrum ProcPars AcqPars Title PulseProg Peaks

Peak	v(F1) [ppm]	v(F1) [Hz]	Intensity
1	10.1636	6096.8387	0.10
2	10.0386	6021.8550	0.20
3	10.0200	6010.6974	15.00
4	9.9992	5998.2201	0.23
5	9.8691	5920.1770	0.09
6	8.0438	4825.2343	0.06
7	8.0311	4817.6160	0.07
8	7.9887	4792.1815	0.43

1 Benzaldehyde 240 ...

Spectrum ProcPars AcqPars Title

Experiment

Width

Receiver

Nucleus

Durations

Power

Program

Probe

Lists

Experiment

PULPROG zg30

AQ\_mod DQD

TD 65536

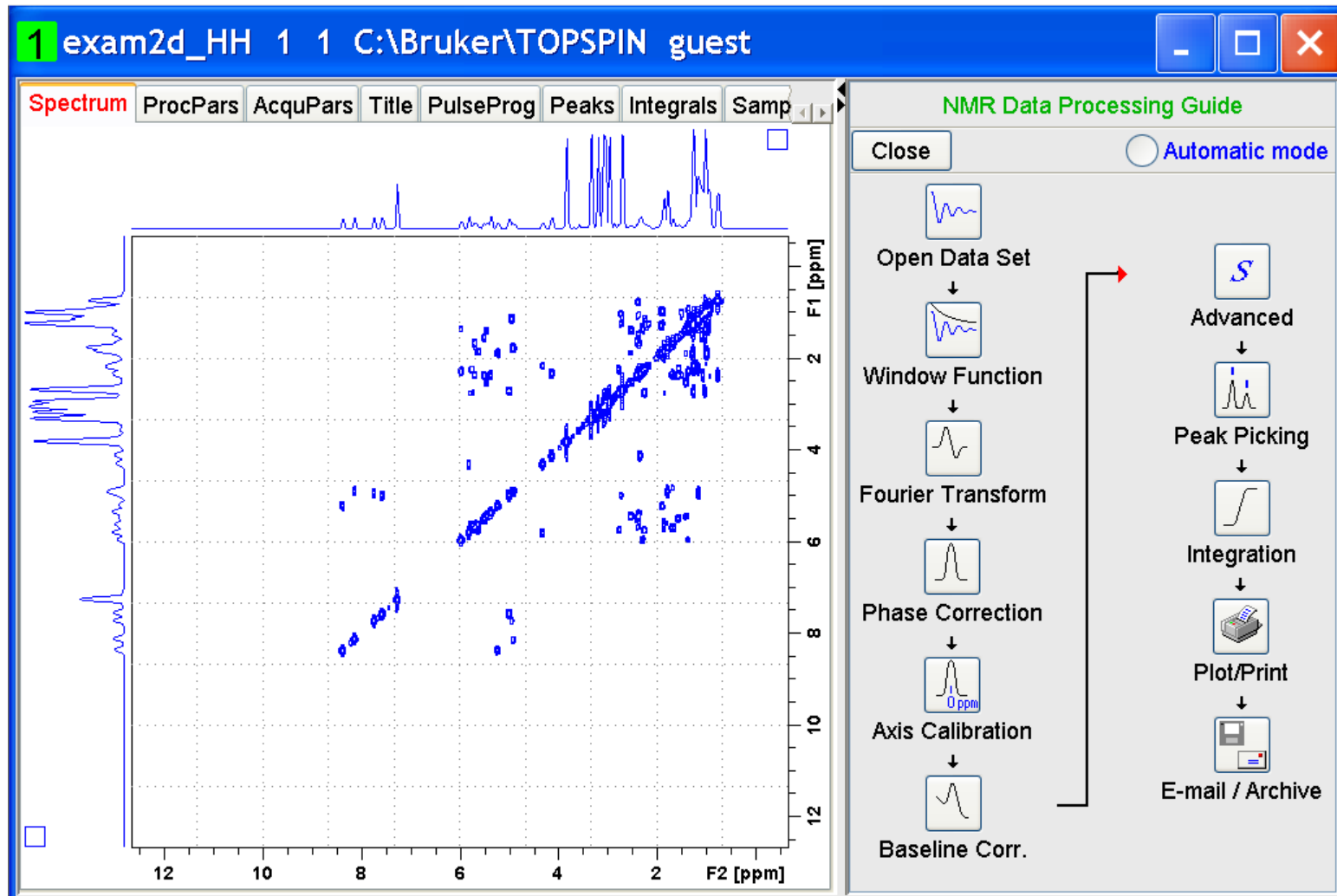
NS 8

DS 2

TD0 1

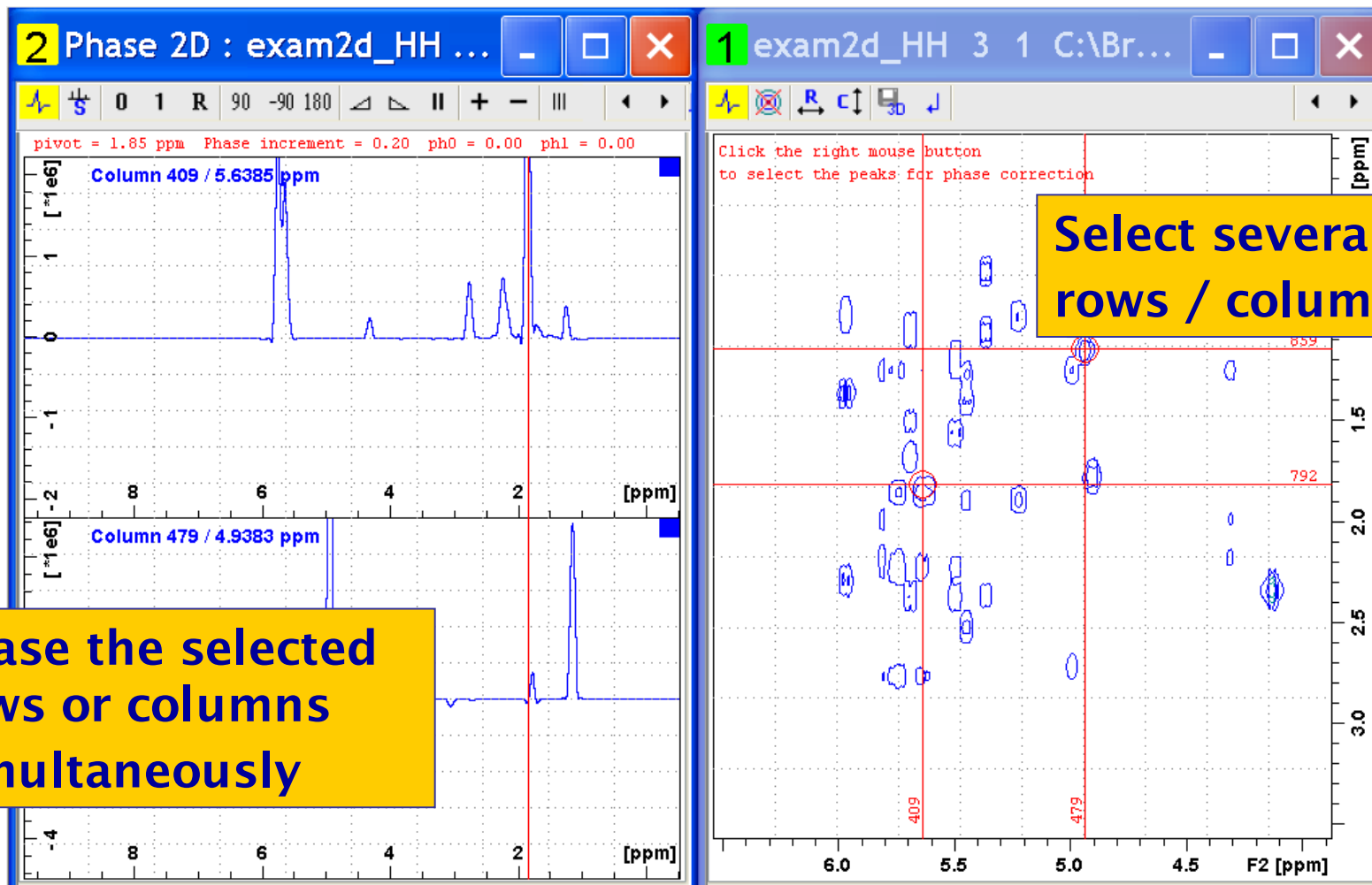
Simultaneous display of spectrum, fid, parameters, peak table (and/or other spectrum components)

Guides novel users through the data processing workflow



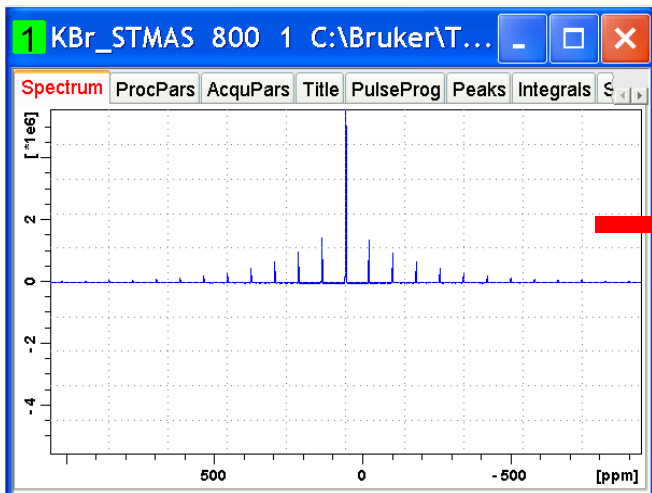


## Manual 2D phase correction

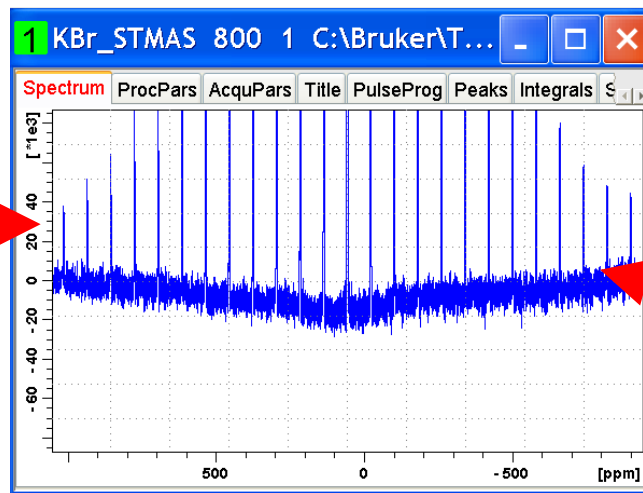


Phase the selected rows or columns simultaneously

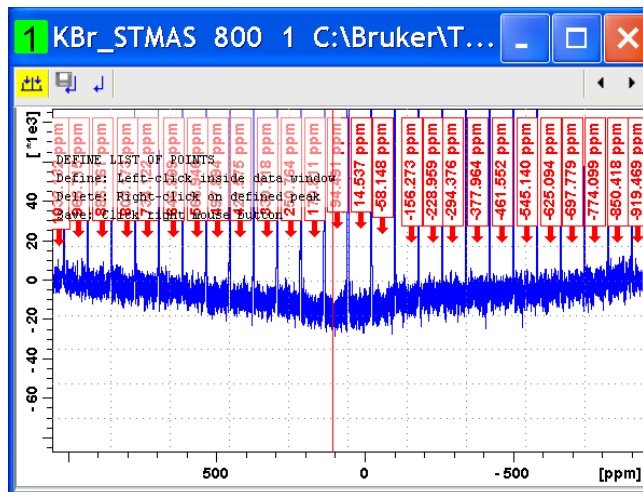
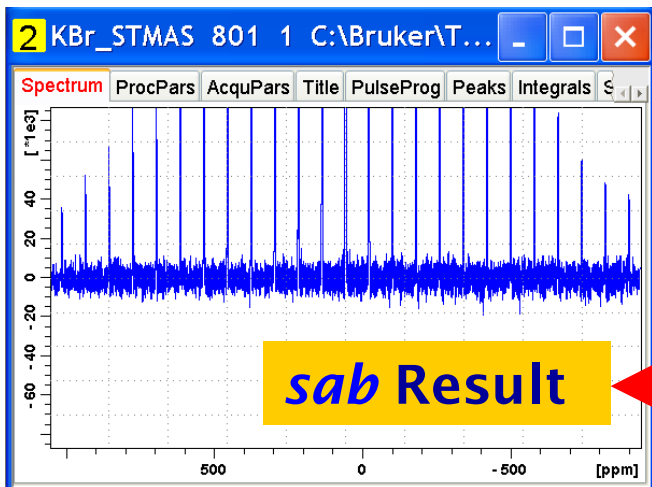
## Cubic spline baseline correction (*sab*)



\*64



Click to define baseline points



All baseline points defined, type *sab*

**Up to 5D processing supported**

**Strip Fourier Transform**

**Inverse Fourier Transform**

**Hilbert Transform**

**Linear Prediction forward / backward / “delayed”**

**Add / Subtract**

**Extraction, display and processing of rows, columns, planes, sub-cubes of 1D-5D data**

# Serial Processing



**Purpose: Process a list of datasets using the same command, macro, AU or Python program**

The diagram illustrates a two-step workflow for serial processing:

- Create list:** This step involves using the 'Find data' dialog to search for datasets. The search results are displayed in a list, showing details such as the dataset name (Benzaldehyde), experiment number (EXPNO), and file path. A yellow box labeled 'Create list' is positioned over the search results.
- Process list:** This step involves using the 'Serial Processing' dialog to configure the processing options. The dialog includes options for processing specified data set lists, browsing for data set lists or serial scripts, and creating new lists or scripts. A yellow box labeled 'Process list' is positioned over the 'Serial Processing' dialog.

A red arrow points from the 'Create list' step to the 'Process list' step, indicating the flow of the process.

**Find data dialog details:**

- NAME: Benz
- EXPNO: [ ]
- PROCNO: [ ]
- USER: [ ]
- Title: [ ]
- Pulse Prog.: [ ]
- Dimension: [ ]
- Data type: [ ]
- Date, from: mm/dd/yy: [ ]
- Date, till: mm/dd/yy: [ ]
- Data directories: C:\Bruker\TOPSPIN, \hera\pub

**Search result: 12 Data Sets.**

Benzaldehyde	240	1	C:\Bruker\TOPSPIN	guest
Benzaldehyde	240	2	C:\Bruker\TOPSPIN	guest
Benzaldehyde	240	100	C:\Bruker\TOPSPIN	guest
Benzaldehyde	240	200	C:\Bruker\TOPSPIN	guest
Benzaldehyde	240	300	C:\Bruker\TOPSPIN	guest
Benzaldehyde	240	400	C:\Bruker\TOPSPIN	guest
Benzaldehyde	240	500	C:\Bruker\TOPSPIN	guest
Benzaldehyde	240	999	C:\Bruker\TOPSPIN	guest
Benzaldehyde	241	1	C:\Bruker\TOPSPIN	guest
Benzaldehyde	241	999	C:\Bruker\TOPSPIN	guest
Benzaldehyde	242	1	C:\Bruker\TOPSPIN	guest
Benzaldehyde	243	1	C:\Bruker\TOPSPIN	guest

**Serial Processing dialog details:**

- Options:
  - Process specified data set list with specified script
  - Browse for a data set list
  - Browse for a serial script
  - Edit specified data set list
  - Edit specified serial script
  - Create new data set list
  - Create new serial script
- Required parameters:
  - Data set list (full path) = mylist.txt
  - Serial script name = efp
  - Show data sets during script execution = yes
  - Script type = Macro