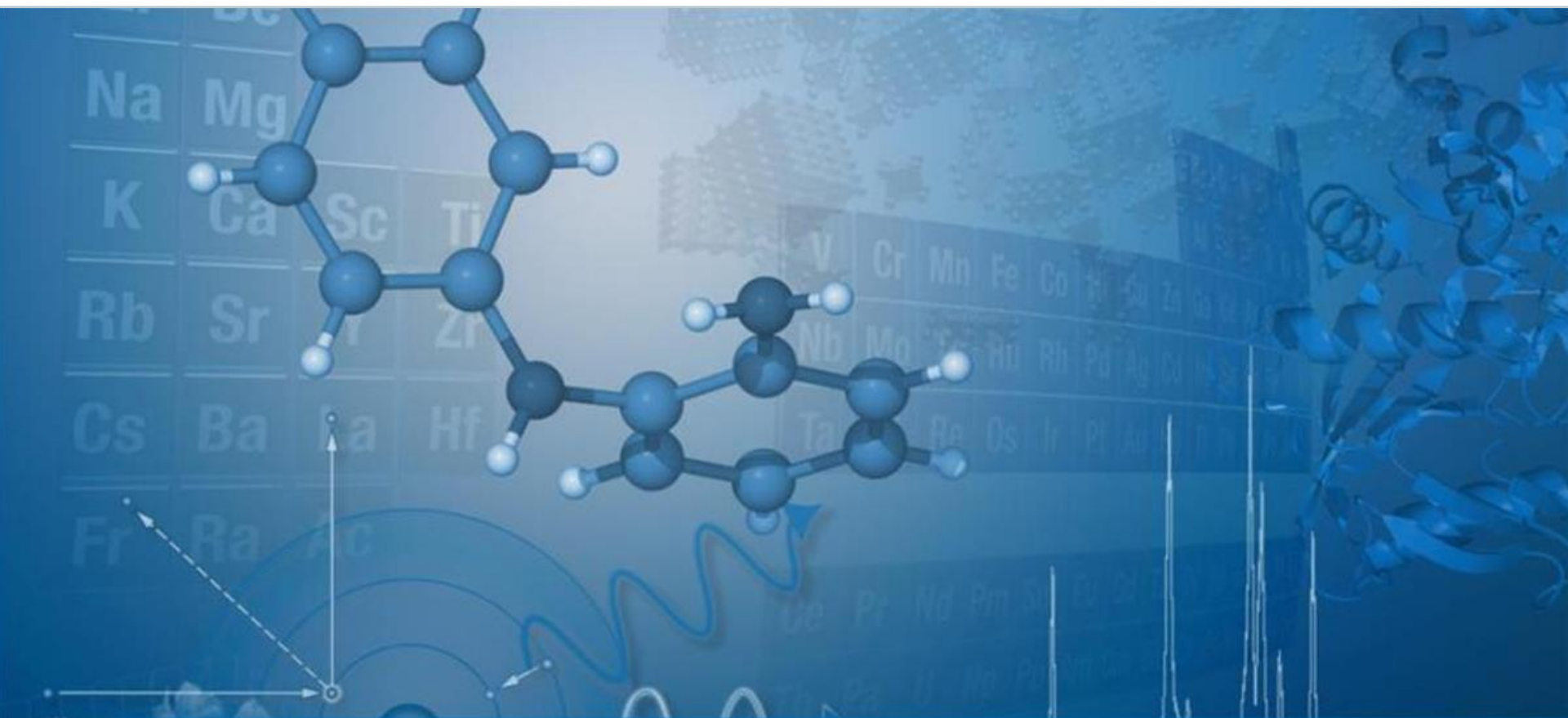
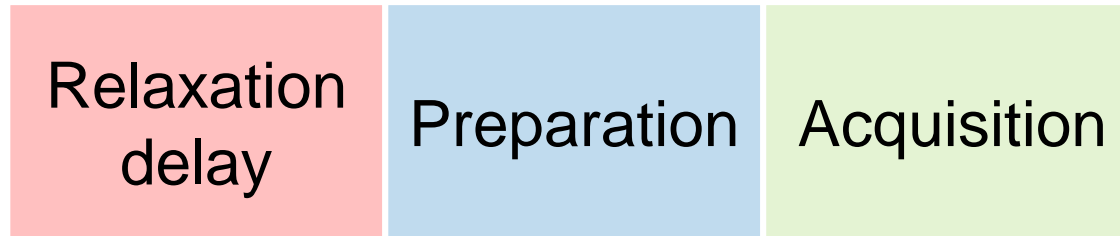


2D Acquisition and Processing

Dr. Benjamin Görling





- **Relaxation delay**: time needed for relaxation
- **Preparation**: spins are excited by one or more pulses
- **Acquisition**: Signal is detected as a function of time t_2

Relaxation
delay

Preparation

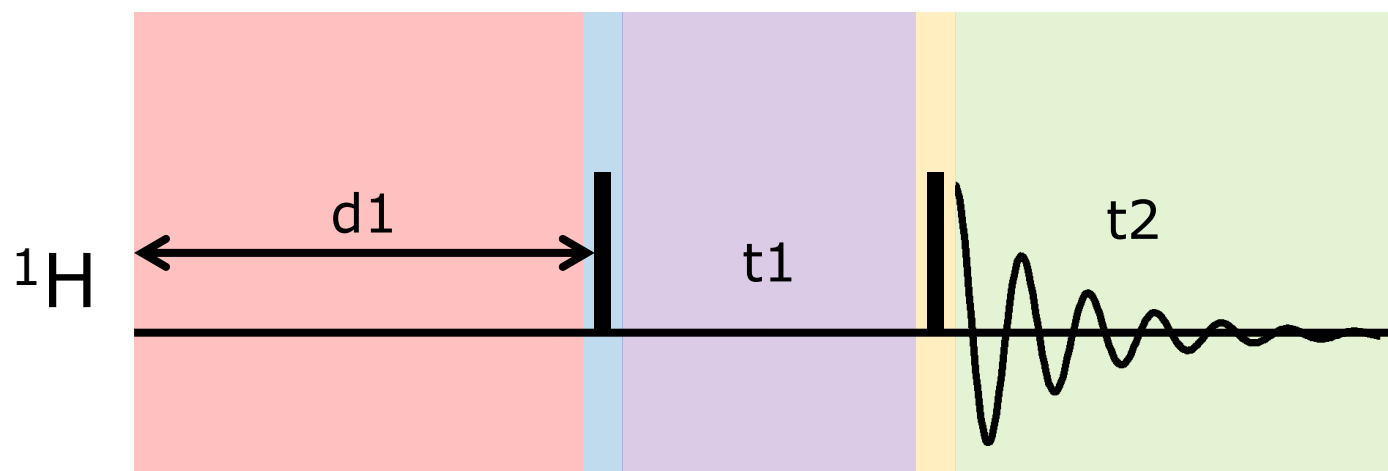
Evolution

Mixing

Acquisition

- **Relaxation delay**: time needed for relaxation
- **Preparation**: spins are excited by one or more pulses
- **Evolution**: evolution of the spins during a time t_1
- **Mixing**: one or more pulses to select desired correlations
- **Acquisition**: Signal is detected as a function of time t_2

2D Experiments



Relaxation
delay

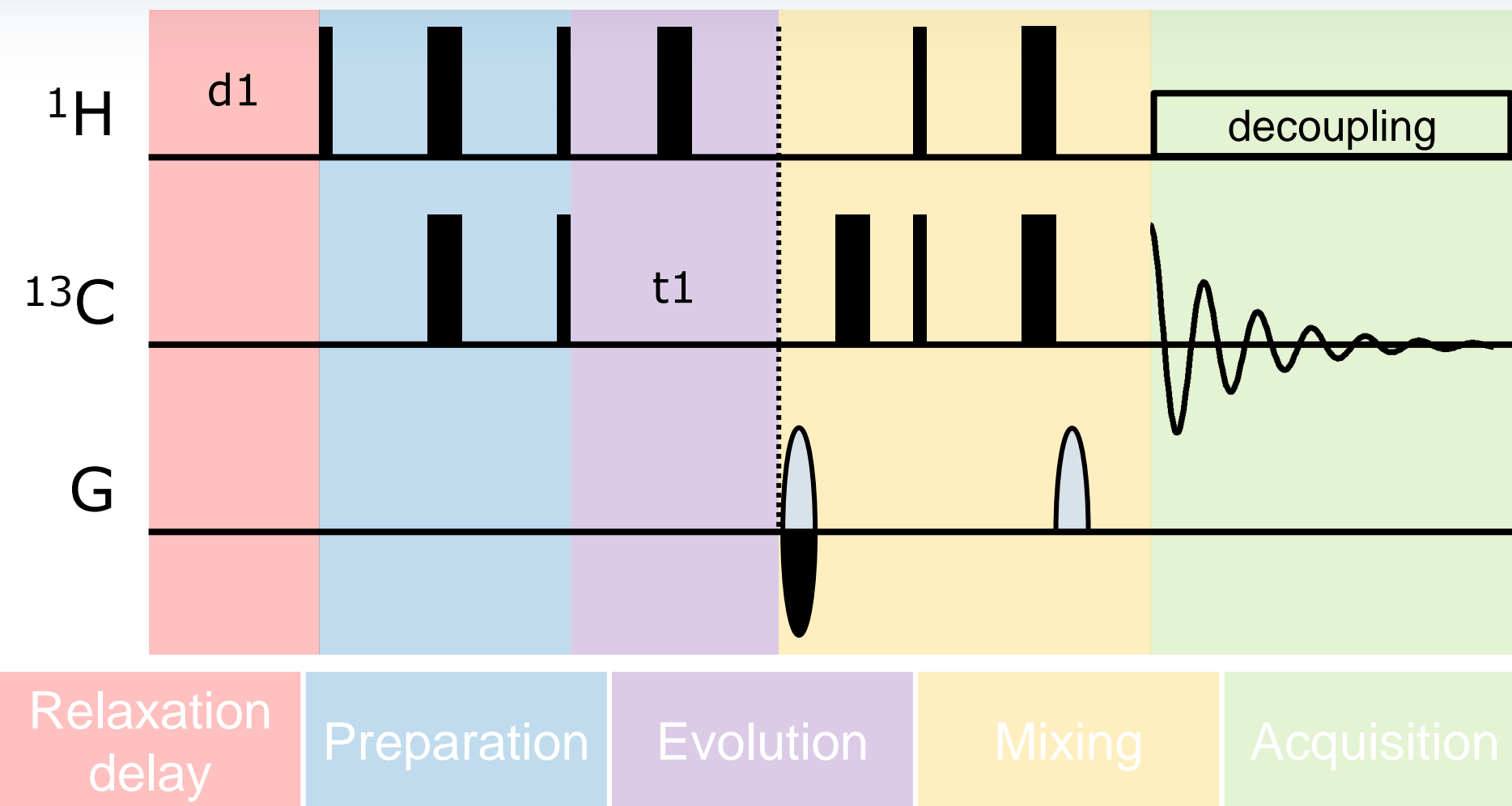
Preparation

Evolution

Mixing

Acquisition

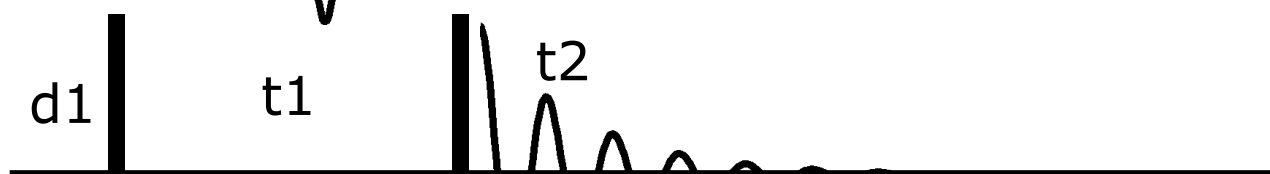
2D Experiments



2D Experiments



$$t1 = d0$$



$$t1 = d0 + in0$$

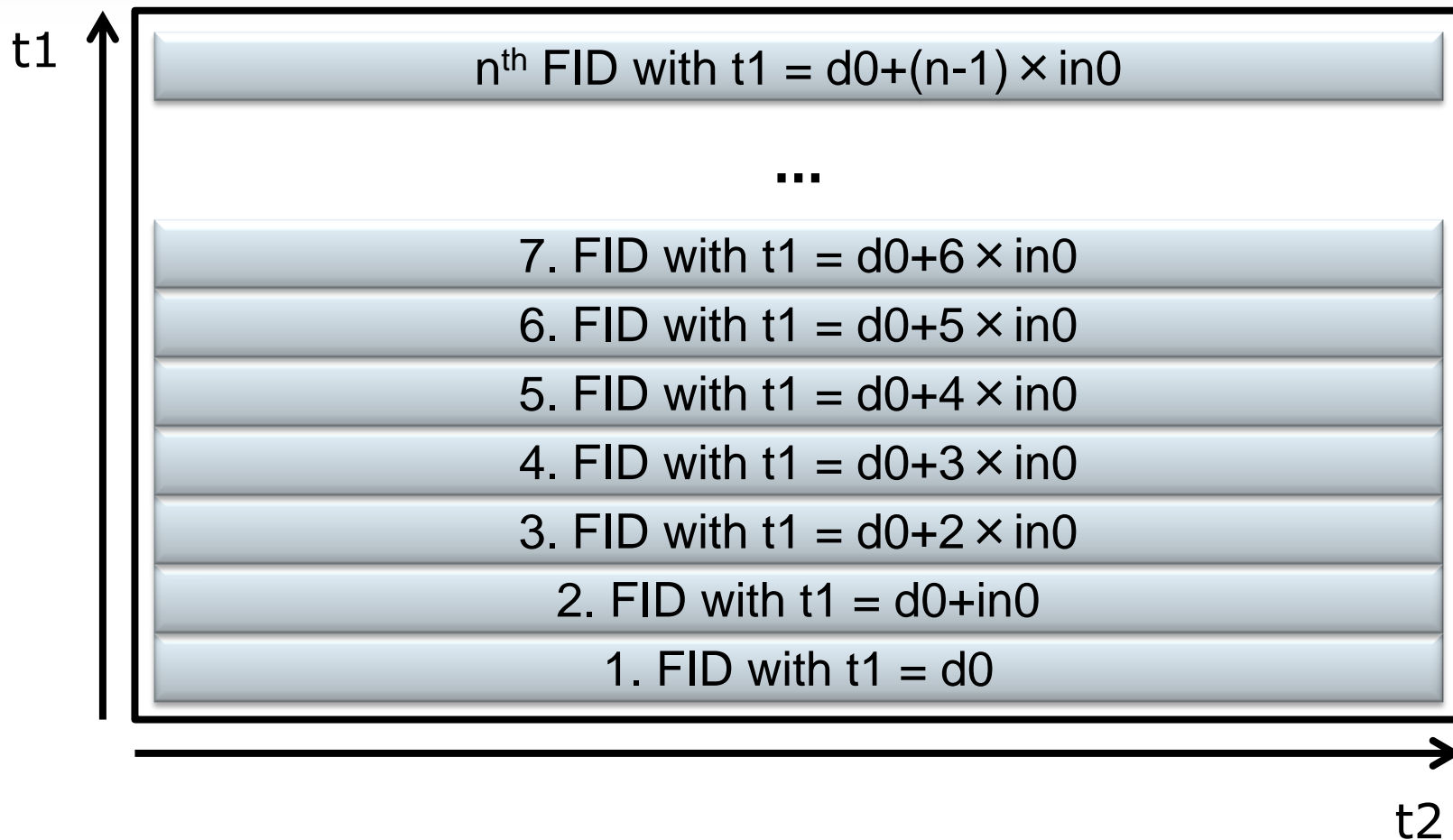


$$t1 = d0 + 2 \times in0$$

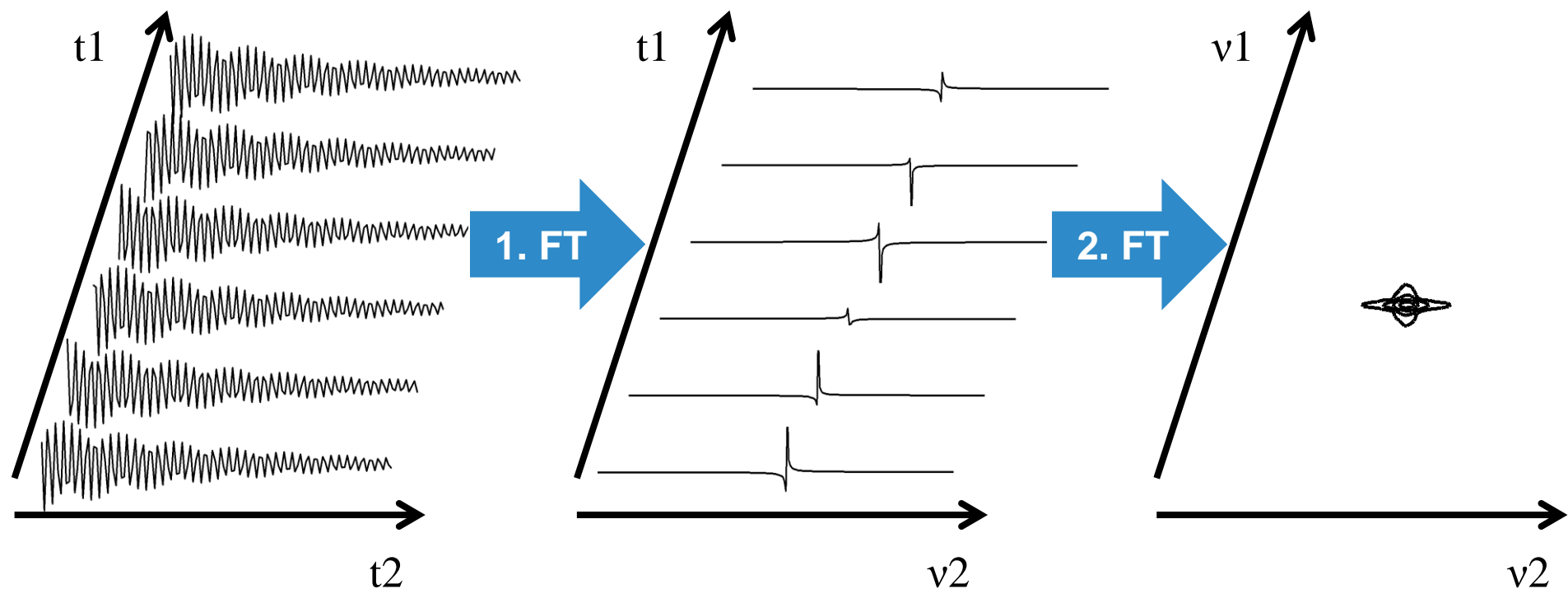


$$t1 = d0 + 3 \times in0$$

2D Experiments



Fourier Transformation



- Parameters are :
 - time domain **TD**
 - spectral width **SW/SWH**
 - dwel time **DW**
 - incremented delay **INO**
 - acquisition time **AQ**
- **Some parameters are needed twice!**
 - **TD** (TD(F2), TD(F1))
 - **SW/SWH** (SW(F2), SW(F1))
- **INO** is the equivalent to **DW** for the second dimension.

Spectral width



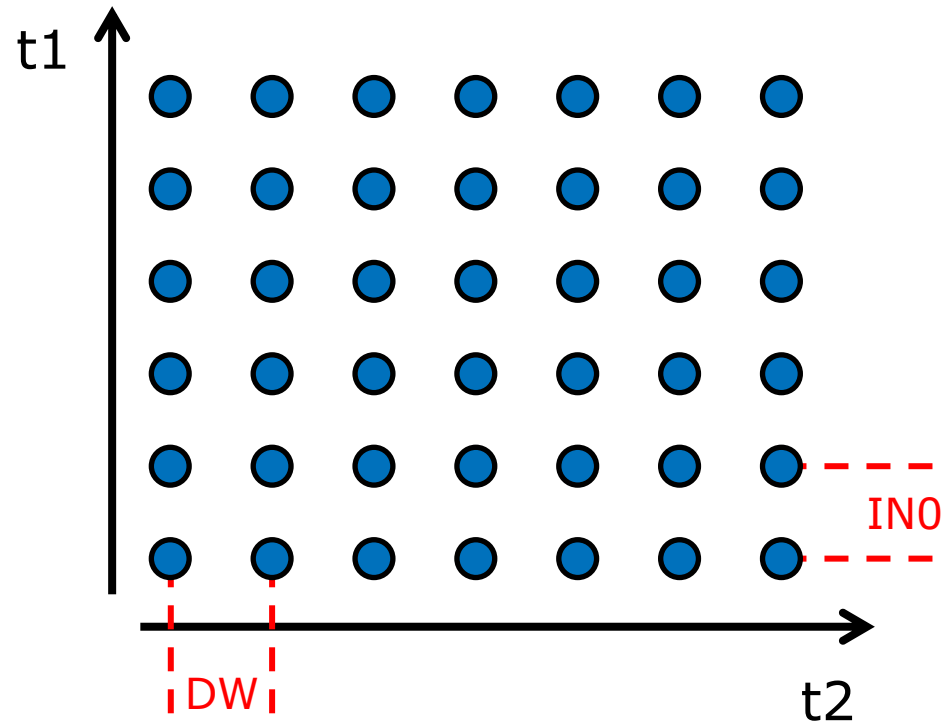
- Spectral width in 1D (now F2) was:

$$SWH(F2) = \frac{1}{2 \cdot DW}$$

- Corresponding to **DW** in F1 is **IN0**

- Spectral width in F1:

$$SWH(F1) = \frac{1}{2 \cdot IN0}$$



- Resolution in 1D (now F2) was:

$$HzpPt(F2) = \frac{1}{AQ(F2)} = \frac{1}{DW \cdot TD(F2)}$$

- Now for F1:

$$HzpPt(F1) = \frac{1}{AQ(F1)} = \frac{1}{IN0 \cdot TD(F1)}$$

To get a good resolution, many points need to be acquired.

If a good resolution in F1 is needed, experiment time will get very long!

- **How to setup a 2D data set?**

Create new experiment [new/edc]



The screenshot shows the Bruker software interface with the 'Create New Dataset - new' dialog box open. The background shows a menu bar with 'File', 'Start', 'Acquire', and 'Process' tabs, and a toolbar with 'Create Dataset' and 'Read Pars.' buttons. The dialog box contains the following fields and options:

- NAME:** Avance_Training
- EXPNO:** 1
- PROCNO:** 1
- Use current parameters
- Experiment **Select** (highlighted with a red box)
- Options:**
 - Set solvent: DMSO
 - Execute 'getprosol'
 - Keep parameters: P 1, PLW 1 **Change**
 - DIR:** C:\NMRData
 - Show new dataset in new window
 - Number of additional datasets: (1,2, ...16) 1
- TITLE:**

At the bottom of the dialog box are buttons for **OK**, **Cancel**, **More Info...**, and **Help**.

Create new experiment [new/edc]



File Start Acquire Process

Create D

dataset Read Pars.

Create New Dataset - new

Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

NAME Avance_Training

EXPNO 1

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

C13CPD	C13DEPT135	C13DEPTQ135	C13UDEFT	COSYGPDPHPSW
COSYGPSW	HMBCETGPL3ND	HMBCGP	HMBCGP_15N	HSQC_TOCSY
HSQC_TOCSY_ADIA	HSQCEDETGPSISP	HSQCEDETGPSISP_ADIA	HSQCETGP_15N	HSQCETGPSISP
HSQCETGPSISP_ADIA	MLEVPHPR	MLEVPHSW	NOESYPHPR	NOESYPHPSW
PROTON	ROESYPHPR	ROESYPHPSW	WATERSUP	

Set selected item in editor Close

Create new experiment [new/edc]



The screenshot shows the Bruker software interface with the 'Create New Dataset - new' dialog box open. The dialog box contains the following fields and options:

- NAME:** Avance_Training
- EXPNO:** 60
- PROCNO:** 1
- Use current parameters
- Experiment: COSYGPSW (with a 'Select' button)
- Options:**
 - Set solvent: H2O+D20
 - Execute 'getprosol'
 - Keep parameters: P 1, PLW 1 (with a 'Change' button)
- DIR:** C:\NMRData\data\bgoe\nmr
- Show new dataset in new window
- Number of additional datasets: (1,2, ...16):** 1
- TITLE:** (empty text box)

At the bottom of the dialog box, the 'OK' button is highlighted with a red square. Other buttons include 'Cancel', 'More Info...', and 'Help'.

Acquisition parameters [ased]



Avance_Training 60 1 C:\NMRData\data\bgoe\nmr

Spectrum ProcPars **AcquPars** Title PulseProg Peaks Integrals Sample Structure Plot Fid Acqu

Probe: BBFOSP

General
Channel f1
Gradient channel

General

PULPROG	cosygpppqf	E	Pulse program for acquisition
TD	2048		Time domain size
SWH [Hz, ppm]	5197.51	12.9895	Sweep width
AQ [sec]	0.1970176		Acquisition time
RG	64		Receiver gain
DW [µsec]	96.200		Dwell time
DE [µsec]	6.50		Pre-scan-delay
d0 [sec]	0.00000300		Incremented delay (2D) [3 usec]
D1 [sec]	2.000000000		Relaxation delay; 1-5 * T1
d11 [sec]	0.03000000		Delay for disk I/O [30 msec]
d12 [sec]	0.00002000		Delay for power switching [20 usec]
d13 [sec]	0.00000400		Short delay [4 usec]
D16 [sec]	0.000200000		Delay for homospoil/gradient recovery
DS	16		16
in0 [sec]	0.00019240		1/(1 * SW) = 2 * DW
INF1 [µsec]	192.40		1/SW = 2 * DW
NS	1		1 * n
TDav	0		Number of averages in nD
SFO1 [MHz]	400.1324008		Frequency of ch. 1
O1 [Hz, ppm]	2400.78	6.000	Frequency of ch. 1

Several parameters needed for a 2D data set are only shown in the complete list.

Acquisition parameters [eda]



Probe: BBFOSP

Frequency axis: F2, F1

Parameter	Value	Value	Description
PULPROG	cosyppppqf	E	Current pulse program
AQ_mod	DQD		Acquisition mode
FnTYPE	traditional(planes)		nD acquisition mode for 3D etc.
FnMODE	QF		Acquisition mode for 2D, 3D etc.
TD	2048	128	Size of fid
DS	16		Number of dummy scans
NS	1		Number of scans
TD0	1		Loop count for 'td0'
TDav	0		Average loop counter for nD experiments
SW [ppm]	12.9895	12.9895	Spectral width
SWH [Hz]	5197.505	5197.505	Spectral width
IN_F [µsec]		192.40	Increment for delay
AQ [sec]	0.1970176	0.0123136	Acquisition time
FIDRES [Hz]	5.075689	81.211021	Fid resolution
FW [Hz]	4032000.000		Filter width
RG	64		Receiver gain
DW [µsec]	96.200		Dwell time

Homonuclear 2D experiment.

Acquisition parameters [eda]



Probe: BBFOSP

Category	Parameter	Value	Unit	Description
Nucleus 1	NUC1	1H	1H	Observe nucleus
	O1 [Hz]	2400.78		Transmitter frequency offset
	O1P [ppm]	6.000		Transmitter frequency offset
	SFO1 [MHz]	400.1324008	400.1324008	Transmitter frequency
Nucleus 2	BF1 [MHz]	400.1300000	400.1300000	Basic transmitter frequency
	NUC2	off		2nd nucleus
	O2 [Hz]	2400.78		Frequency offset of 2nd nucleus
	O2P [ppm]	6.000		Frequency offset of 2nd nucleus
	SFO2 [MHz]	400.1324008		Frequency of 2nd nucleus
	BF2 [MHz]	400.1300000		Basic frequency of 2nd nucleus

Homonuclear 2D experiment.

Channel Routing

[edasp]



The screenshot shows the 'Channel Routing' window with the following table:

Frequency	Logical Channel	Amplifier	Preamplifier	Receiver	Observe Channel
BF1 400.13 MHz	NUC1				NIUC1
SFO1 400.132401 MHz	F1	SGU1	X 300 W	1H	
OFS1 2400.78 Hz	1H				
BF2 400.13 MHz	NUC2				
SFO2 400.132401 MHz	F2	SGU2	1H 100 W	2H	
OFS2 2400.78 Hz	off				
BF3 400.13 MHz	NUC3				
SFO3 400.132401 MHz	F3	SGU3	X 300 W	19F	
OFS3 2400.78 Hz	off				
			2H 150 W	XBB19F 2HS	
				XBB19F 2HP	
				XBB19F 2HS	

Legend:

- : cable wiring
- - - : possible RF routing
- : cortab available

settings

- show selected routing
- show receiver wiring
- show probe wiring
- show RF routing
- show receiver routing
- show power at probe in

Buttons: Save and Close, Switch F1/F2, Switch F1/F3, Add logical channel, Remove logical channel, Default, Info, Param, Close

Routing of the spectrometer is saved in each parameter set.

Can be opened with [edasp] or

Acquisition parameters [eda]



Avance_Training 61 1 C:\NMRData\data\bgoe\nmr

Spectrum ProcPars **AcquPars** Title PulseProg Peaks Integrals Sample Structure Plot Fid Acqu

Probe: BBFOSP

F2 F1 Frequency axis

Experiment
Width
Receiver
Nucleus
Durations
Power
Program
Probe
Lists
NUS
Wobble
Lock
Automation
Miscellaneous
User
Routing

Experiment

PULPROG hsqcetdgpsisp2.3 E Current pulse program

AQ_mod DQD Acquisition mode

FnTYPE traditional(planes) nD acquisition mode for 3D etc.

FnMODE Echo-Antiecho Acquisition mode for 2D, 3D etc.

TD 2048 256 Size of fid

DS 32 Number of dummy scans

NS 4 Number of scans

TD0 1 Loop count for 'td0'

TDav 0 Average loop counter for nD experiments

Width

SW [ppm] 12.9895 165.0000 Spectral width

SWH [Hz] 5197.505 16602.352 Spectral width

IN_F [µsec] 60.23 Increment for delay

AQ [sec] 0.1970176 0.0077098 Acquisition time

FIDRES [Hz] 5.075689 129.705872 Fid resolution

FW [Hz] 4032000.000 Filter width

Receiver

RG 203 Receiver gain

DW [µsec] 96.200 Dwell time

Heteronuclear 2D experiment.

Acquisition parameters [eda]



Probe: BBFOSP

Parameter	Value 1	Value 2	Description
Observe nucleus	1H	13C	Observe nucleus
Transmitter frequency offset	O1 [Hz]	1880.61	7545.96
Transmitter frequency offset	O1P [ppm]	4.700	75.000
Transmitter frequency	SFO1 [MHz]	400.1318806	100.6203145
Basic transmitter frequency	BF1 [MHz]	400.1300000	100.6127685
2nd nucleus	NUC2	13C	2nd nucleus
Frequency offset of 2nd nucleus	O2 [Hz]	7545.96	
Frequency offset of 2nd nucleus	O2P [ppm]	75.000	
Frequency of 2nd nucleus	SFO2 [MHz]	100.6203145	
Basic frequency of 2nd nucleus	BF2 [MHz]	100.6127685	

Heteronuclear 2D experiment.

Channel Routing

[edasp]



Channel Routing

Frequency	Logical Channel	Amplifier	Preamplifier	Receiver	Observe Channel
BF1 400.13 MHz	NUC1				NUC1
SFO1 400.131881 MHz	F1	SGU1	X 300 W	1H	SGU1 F1
OFS1 1880.61 Hz	1H				
BF2 100.612769 MHz	NUC2				NUC2
SFO2 100.620314 MHz	F2	SGU2	1H 100 W	19F	SGU2 F2
OFS2 7545.96 Hz	13C				
BF3 400.13 MHz	NUC3				NUC3
SFO3 400.131881 MHz	F3	SGU3	X 300 W	XBB19F 2HS	SGU3 F3
OFS3 1880.61 Hz	off				off

— : cable wiring
 - - : possible RF routing
 ● : cortab available


settings

show selected routing show receiver routing
 show receiver wiring
 show probe wiring
 show RF routing show power at probe in

Save and Close Switch F1/F2 Switch F1/F3 Add logical channel Remove logical channel Default Info Param Close

Routing of the spectrometer is saved in each parameter set.

Can be opened with [edasp] or



Channels and spectral axis



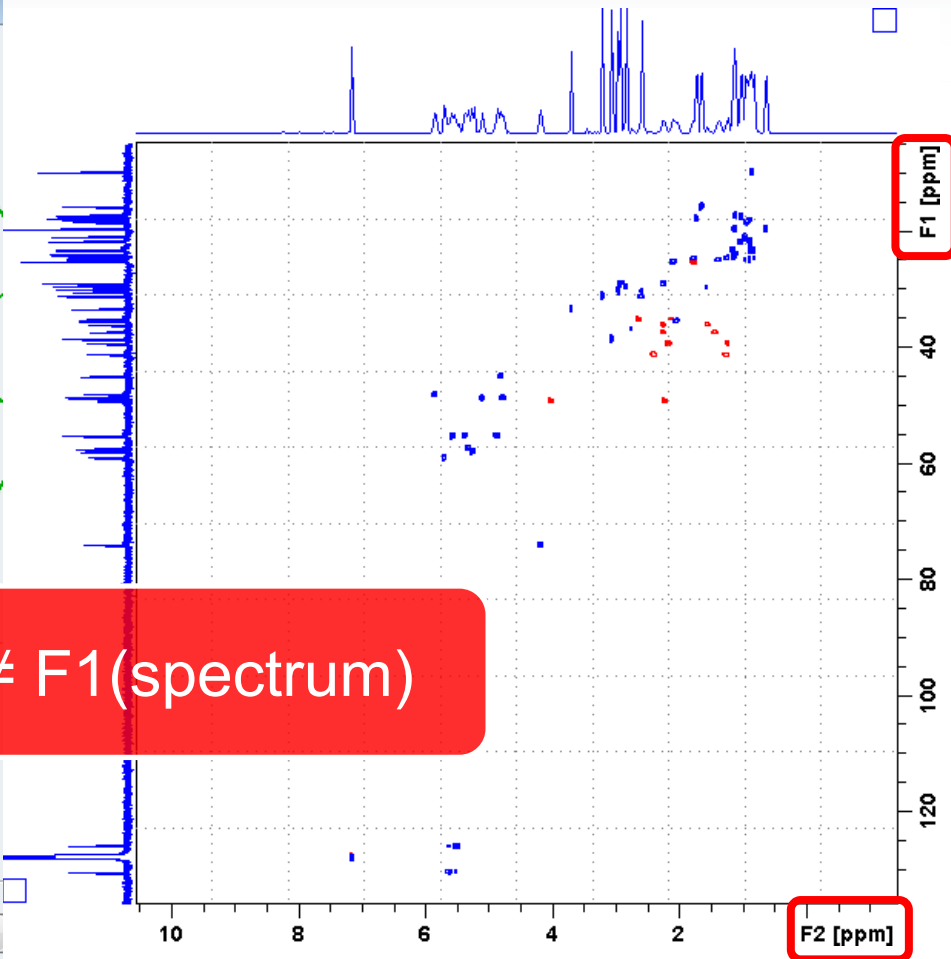
Channel Routing

Frequency	Logical Channel	Amplifier
BF1 400.13 MHz	NUC1	
SFO1 400.131881 MHz	F1	SGU1 X 300 W
OFS1 1880.61 Hz	1H	
BF2 100.612769 MHz	NUC2	
SFO2 100.620314 MHz	F2	SGU2 1H 100 W
OFS2 7545.96 Hz	13C	X 300 W
BF3 400.13 MHz	NUC3	
SFO3 400.131881 MHz	F3	SGU3 2H 150 W
OFS3 1880.61 Hz	off	

— : cable wiring
- - : possible RF routing
● : cortab available

settings
 show receiver wiring
 show probe wiring
 show RF routing

Save and Close Switch F1/F2 Switch F1/F3 Add logical channel



F1(routing) ≠ F1(spectrum)

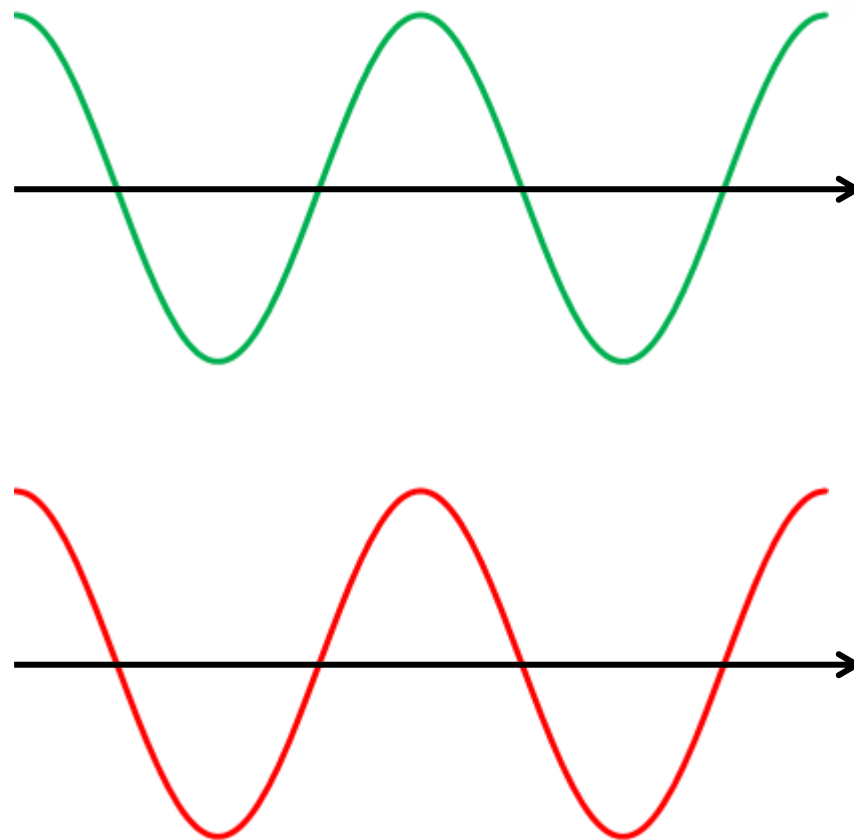
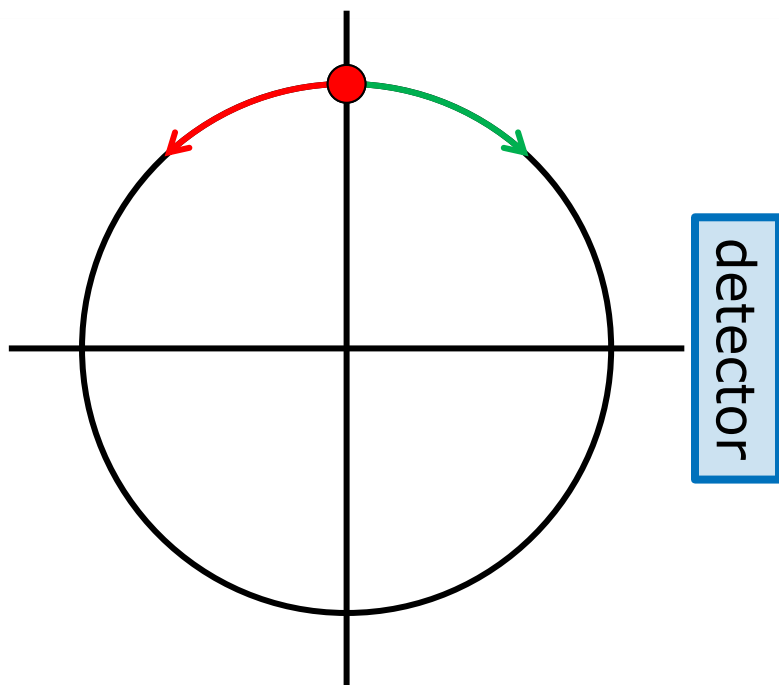
- **Acquisition Mode**

Acquisition mode

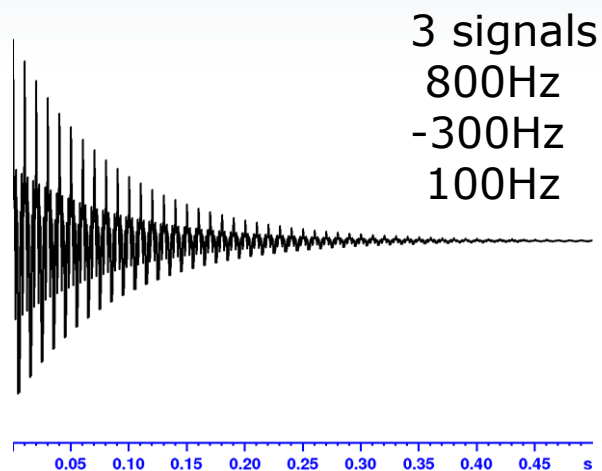


- Defines how the data is acquired.
- Acquisition mode for F1 and F2 are defined by **FnMODE** and **AQ_mod**, respectively.
- Necessary to get correct signal position and phase.
- **AQ_mod** is always DQD (digital quadrature detection)

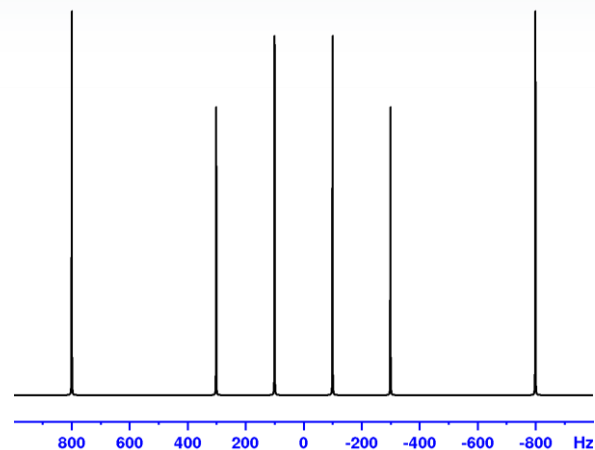
Quadrature detection



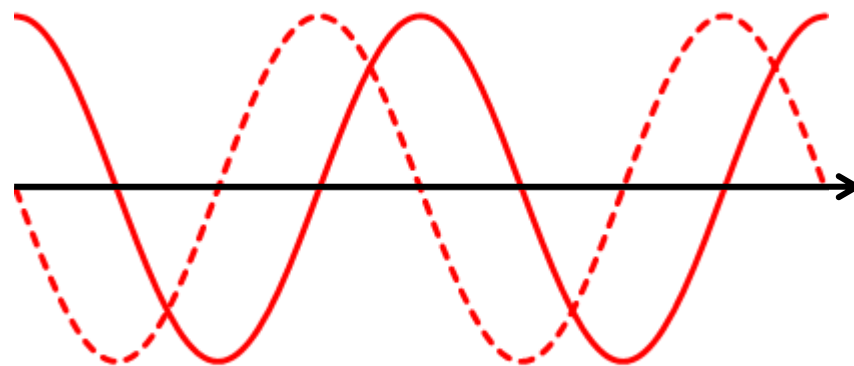
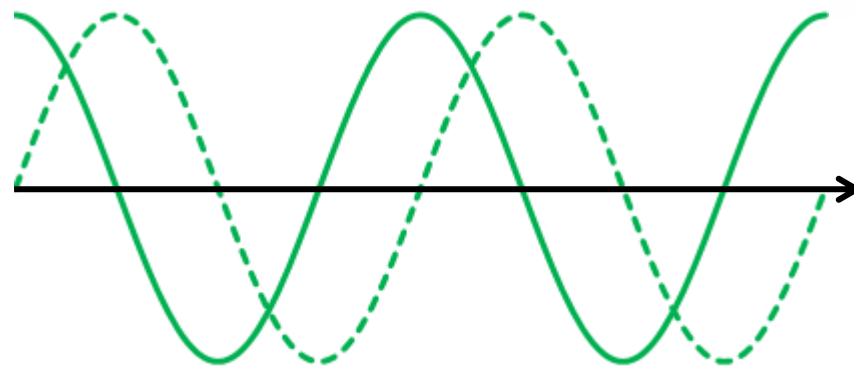
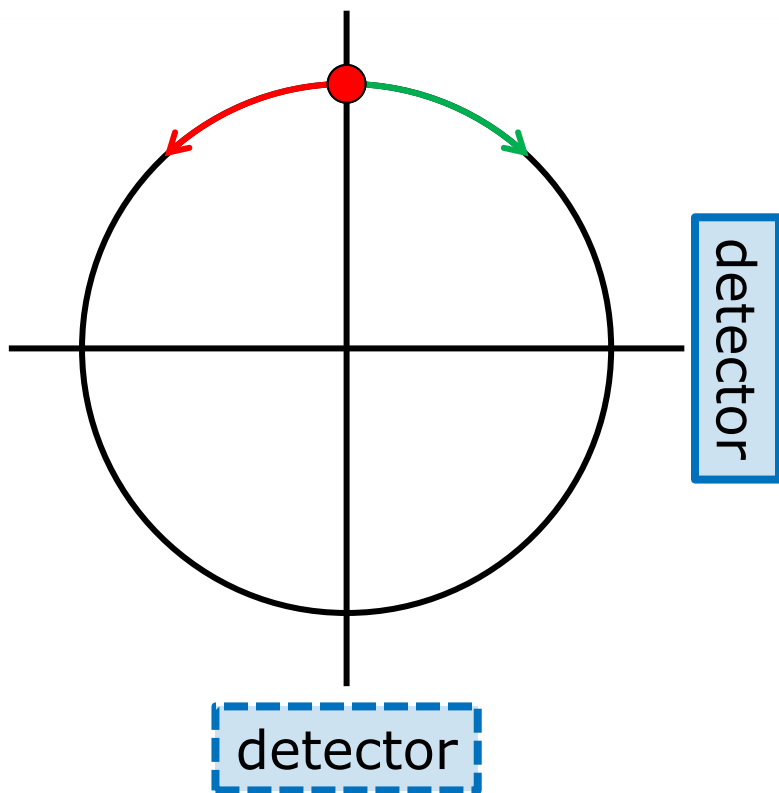
Quadrature detection



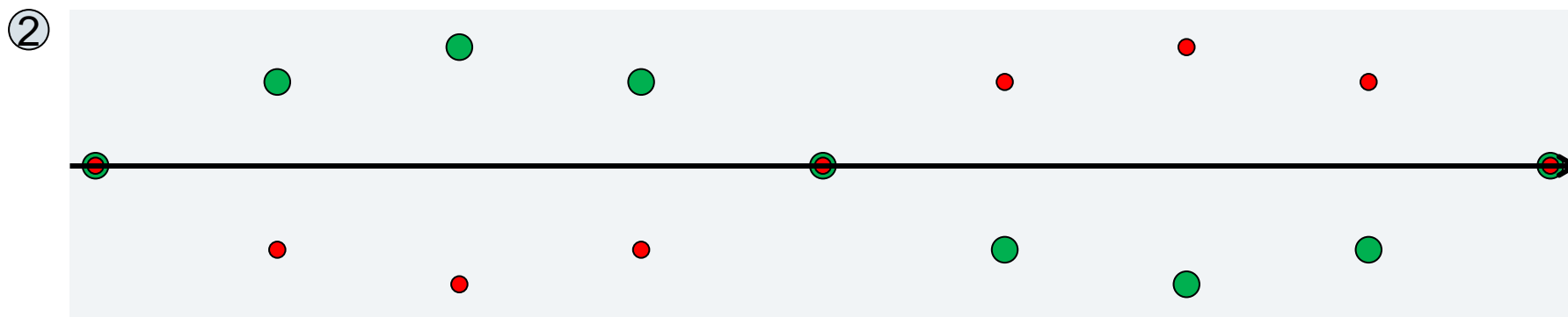
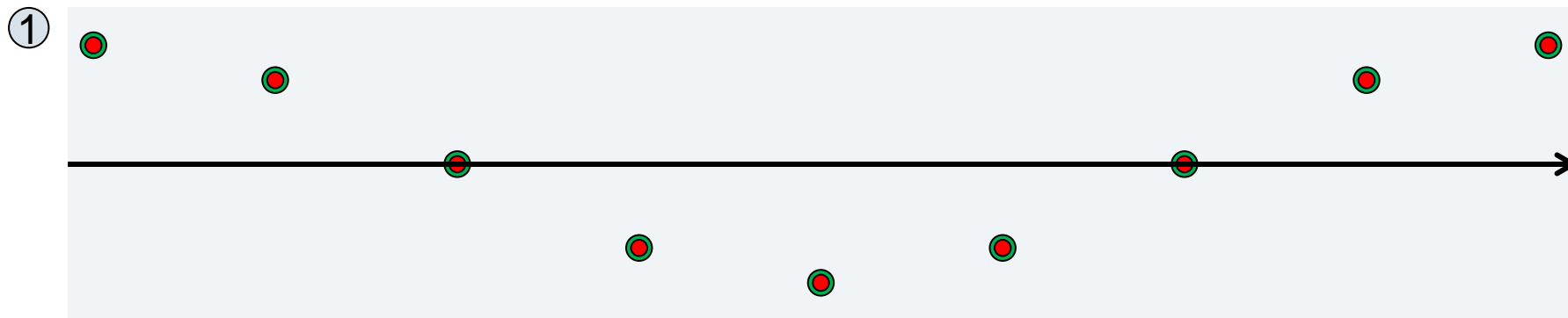
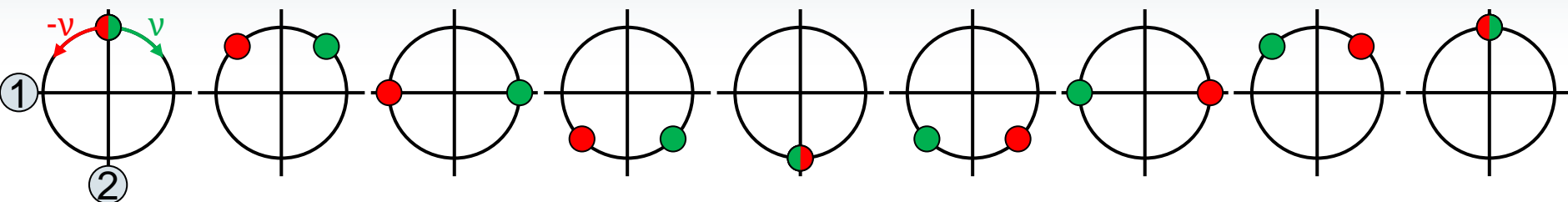
FT
→
only cos



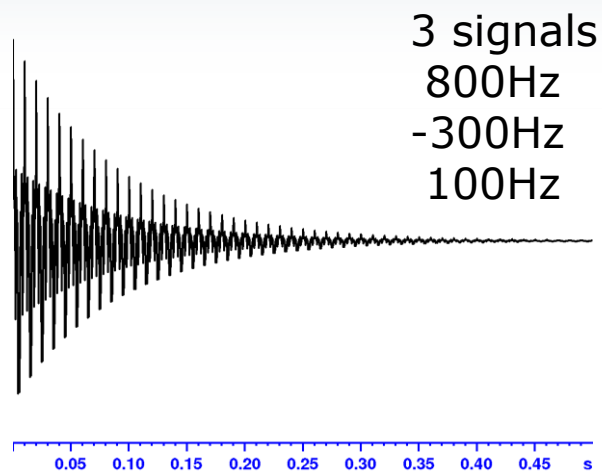
Quadrature detection



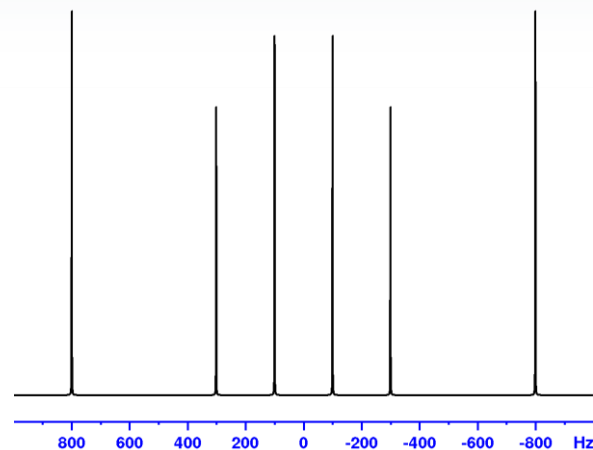
Quadrature detection



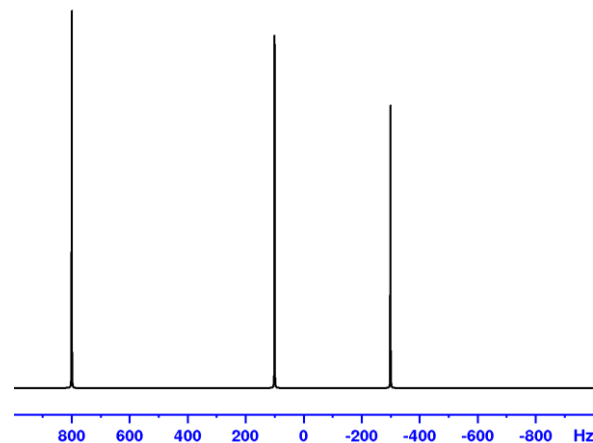
Quadrature detection



FT
→
only cos



FT
→
sin & cos





- Quadrature detection in the F1 Dimension in 2D experiments is not possible!
- Frequency discrimination is done by phase cycling/gradient selection
- **not phase sensitive experiments:**
storage of the cosine and sine component not separately
- **phase sensitive experiments:**
storage of the cosine and sine component separately

Acquisition modes



FnMODE

not phase sensitive

QF

cosygpppqf

hmbcgplpndqf

FnMODE

phase sensitive

TPPI

States

States-TPPI

cosygpphpp

mlevphpp

noesygpphpp

FnMODE

phase sensitive

Echo-Antiecho

hsqcetgpsisp2.2

hmbcetgpl3nd

Recommended 2D Experiments



H-H

COSY

cosygpmf`phpp`, cosygppp`qf`

TOCSY

mlev`phpp`, mlev`phpr.2`

NOESY

noesygp`phpp`, noesygp`phpr`

ROESY

roesy`phpp.2`, roesy`phpr.2`

H-X

¹³C-HSQC

hsqcdi`etgpsisp.2`,
hsqced`etgpsisp2.3`, hsqc`etgpsisp2.2`

¹³C-HMBC

hmbc`etgpl3nd`, hmbc`gplpndqf`

¹⁵N-HSQC/HMBC

hsqc`etgpsi2/hmbcgpndqf`

JRES

jres`qf`, jres`prqf`

Recommended 2D Parameter Sets



H-H

COSY

COSYGPDPHSW, COSYGPSW

TOCSY

MLEVPHSW, MLEVPHPR

NOESY

NOESYPHSW, NOESYPHPR

ROESY

ROESYPHSW, ROESYPHPR

H-X

¹³C-HSQC

HSQC_TOCSY
HSQCEDETGPSISP, HSQCETGPSISP

¹³C-HMBC

HMBCETGPL3ND, HMBCGP

¹⁵N-HSQC/HMBC

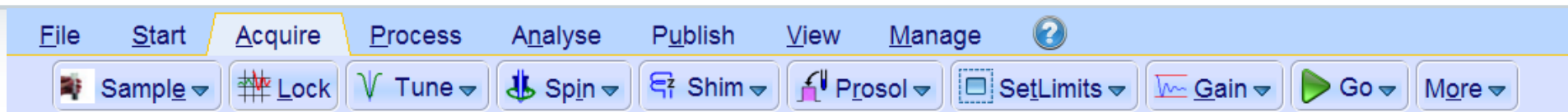
HSQCETGP_15N/HMBCGP_15N

JRES

PROF_JRES (presat)

- **How to acquire a spectrum?**

Acquire Toolbar



Very similar to 1D acquisition.

Acquire Toolbar - SetLimits



- Helps to set limits for 2D spectra from 1D data sets
- Interactive mode to define spectral width (**SW**) and transmitter frequency (**O1P/O2P**)
- [**copypars**] will be discussed in Tips & Tricks session

Acquire Toolbar - SetLimits



The screenshot shows the Bruker software interface. On the left is a 'Browser' pane with a tree view of datasets. The main window displays a 'Spectrum' plot. A 'setlimits' dialog box is open in the center, containing the following text:

Close this dialog box after setting frequencies.

1. Open 1D dataset from Browser.
2. Zoom into region of interest.
3. Click OK to set frequencies and return to original dataset.

At the bottom of the dialog are 'OK' and 'Cancel' buttons.

Below the dialog, a red rounded rectangle contains the text: **Do not click OK until you are finished!**

The 'Structure' pane at the bottom left shows 'No structure available.'

Acquire Toolbar - SetLimits



The screenshot displays the Bruker software interface. On the left is a 'Browser' pane with a list of experiments, including '18 - zg0 - Influence o', '19 - zg0 - Influence o', '20 - zg0 - Influence o', '21 - zg0 - Influence o', '22 - zg0 - Influence o', '23 - zg0 - Influence o', '24 - zg0 - Influence o', '25 - zg0 - Influence o', '26 - zg0 - Influence o', '27 - zg0 - Influence o', '28 - zg0 - Influence o', '30 - zg2d - Lock off', '31 - zg2d - Lock on', '40 - zg', '41 - Shim', '42 - Shim', '43 - Shim', '44 - Shim', '45 - Shim', '46 - Shim', '47 - Shim', '48 - Shim', '49 - Shim', '50 - zg', '51 - zg30', '52 - zgpg', '53 - cosygpppqf', '60 - cosygpppqf', '61 - hsqcedetgpsisp2'. A blue arrow points from the '50 - zg' entry to the 'setlimits' dialog box. The main window shows an NMR spectrum plot with a y-axis labeled '14 [rel]' and an x-axis labeled '15 [ppm]'. A 'setlimits' dialog box is open in the center, containing the following text:

Close this dialog box after setting frequencies.

1. Open 1D dataset from Browser.
2. Zoom into region of interest.
3. Click OK to set frequencies and return to original dataset.

Buttons for 'OK' and 'Cancel' are visible at the bottom of the dialog box. A blue callout box on the right side of the plot contains the text: 'Drag and drop 1D data set.'

Acquire Toolbar - SetLimits



The screenshot shows the Bruker software interface. On the left is a 'Browser' pane with a list of experiments, including '50 - zg' which is highlighted. The main window displays a spectrum plot with a red zoomed-in region. A 'setlimits' dialog box is open in the center, containing the following text:

Close this dialog box after setting frequencies.

1. Open 1D dataset from Browser.
2. Zoom into region of interest.
3. Click OK to set frequencies and return to original dataset.

The 'OK' button in the dialog box is highlighted with a red rectangle. A blue callout box on the right contains the following text:

Zoom into desired region and click OK.

This SW and corresponding O1P/O2P will be set in the 2D data set.

Acquire Toolbar - SetLimits

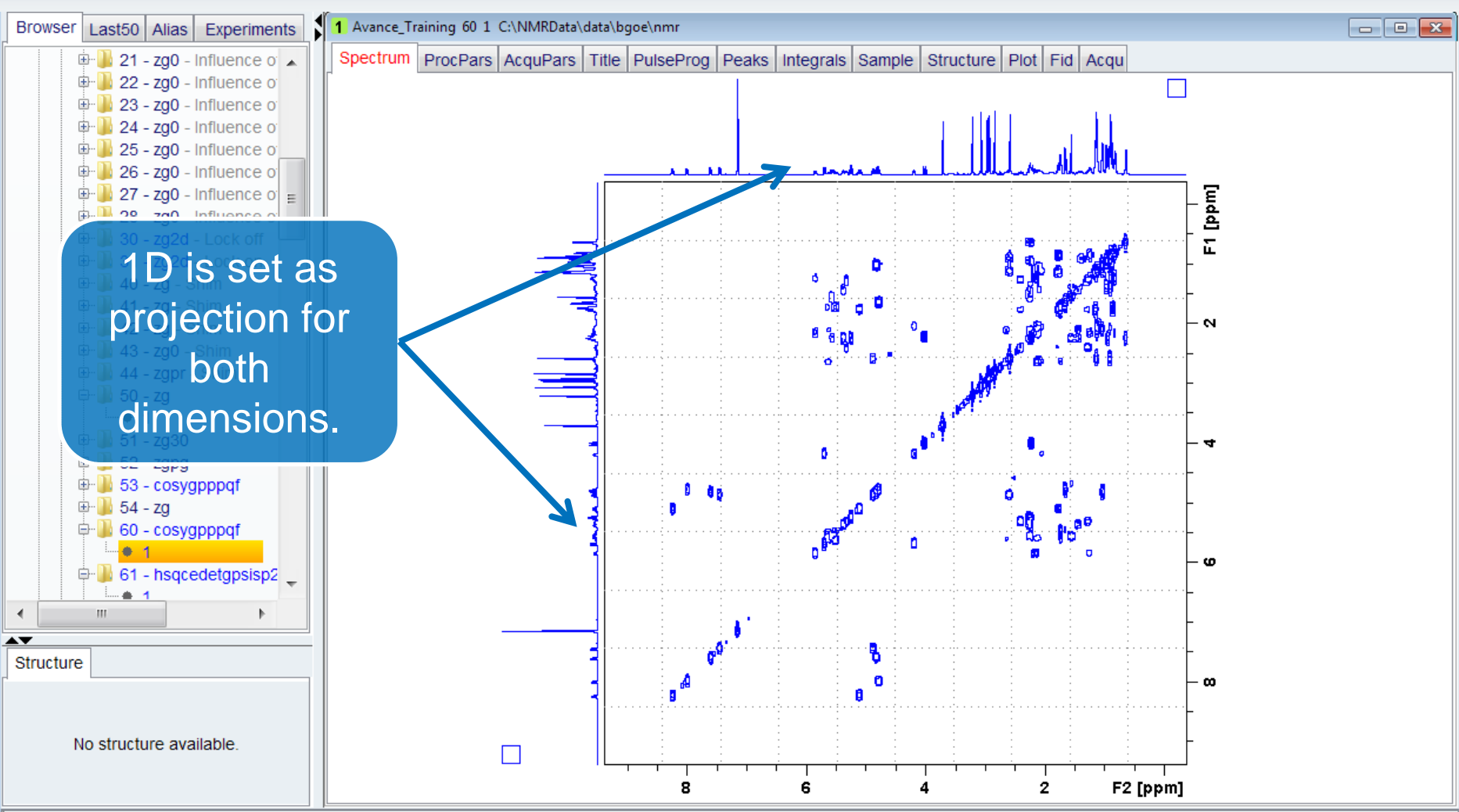


The screenshot shows the Bruker software interface. On the left is a 'Browser' pane with tabs for 'Last50', 'Alias', and 'Experiments'. It lists various experiment files, with '50 - zg' selected. Below the browser is a 'Structure' pane displaying 'No structure available.' The main window title is '1 Avance_Training 60 1 C:\NMRData\data\bgoe\nmr'. The toolbar includes 'Spectrum', 'ProcPars', 'AcquPars', 'Title', 'PulseProg', 'Peaks', 'Integrals', 'Sample', 'Structure', 'Plot', 'Fid', and 'Acqu'. A message dialog box is open in the center, containing the following text:

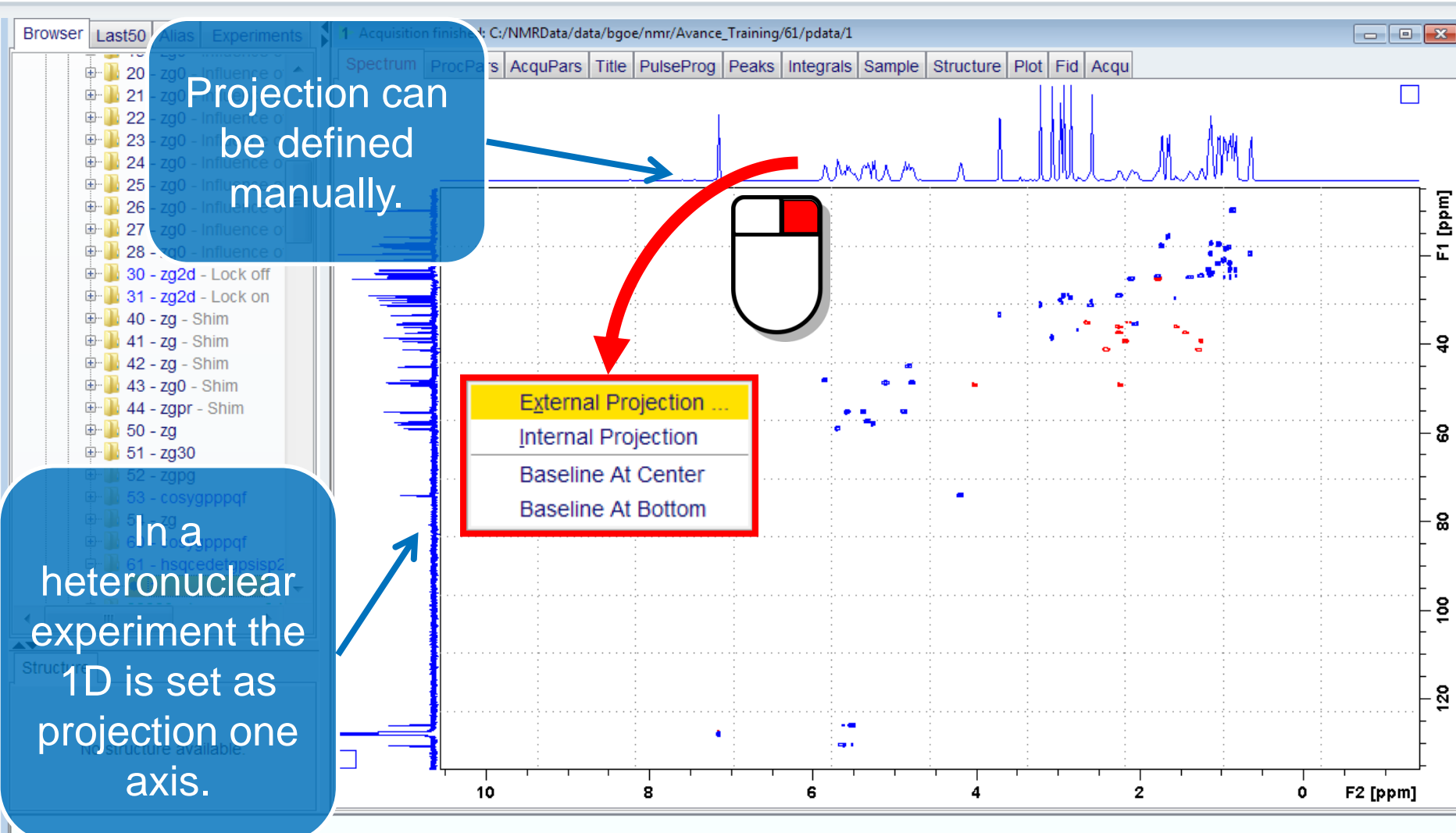
1H spectral limits copied for F1 and F2 dimensions.
SW: 9.7624 ppm
O1P: 4.511 ppm

The dialog box has a 'Close' button at the bottom right.

Projections



Projections



Projection can be defined manually.

In a heteronuclear experiment the 1D is set as projection one axis.

Projections



The screenshot displays the Bruker NMR software interface. On the left, a 'Browser' pane lists various experiments, with '61 - hsqcedetgpsisp2' selected. The main window shows a 2D spectrum with F2 [ppm] on the x-axis (ranging from 10 to 0) and F1 [ppm] on the y-axis (ranging from 40 to 120). A 'Data set for F2 projection' dialog box is open, allowing the user to select a 1D data set. The dialog box contains the following information:

Data set for F2 projection

Options

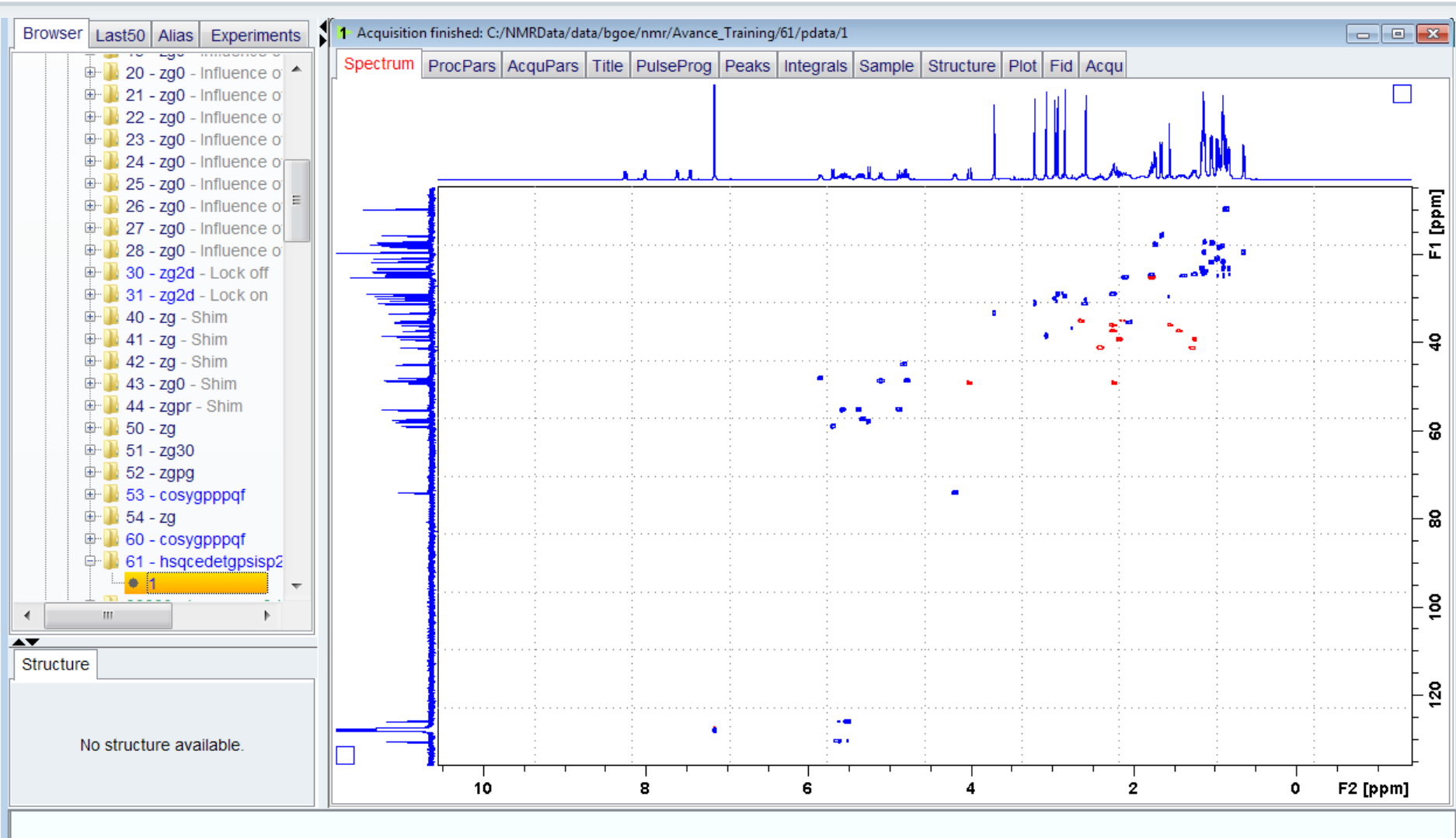
- Display data in same window
- Display data in new window

NAME = Avance_Training
EXPNO = 50
PROCNO = 1
DIR = C:\NMRData\data\bgoe\nmr

Buttons: OK, Cancel, Browse, Find..., Help

A blue callout box with white text is overlaid on the 2D spectrum, stating: "Select appropriate 1D data set."

Projections



From 1D to 2D



1 Avance_Training 1 1 C:\NMRData

Spectrum ProcPars **Acq** Title PulseProg Peaks Integrals Sample Structure Plot Fid Acqu

Probe: BBFOSP

Experiment
Width
Receiver
Nucleus
Durations
Power
Program
Probe
Lists
Wobble
Lock
Automation
Miscellaneous
User
Routing

Experiment

PULPROG zg30 Current pulse program
AQ_mod DQD Acquisition mode
TD 65536 Size of fid
DS 2 Number of dummy scans
NS
TD0

Warning!

You are about to change the dimension of the current dataset.
As a consequence an existing FID will be deleted!

Change acquisition dimension of dataset from 1D to 2D

OK Cancel

Receiver

RG
DW [µsec]
DWOV [µsec] 0.025 Oversampling dwell time
DECIM 2496 Decimation rate of digital filter
DSPFIRM sharp(standard) DSP firmware filter
DIGTYP DRU Digitizer type
DIGMOD digital Digitization mode

If you want to make a 2D data set from a 1D data set you have to change dimensionality.

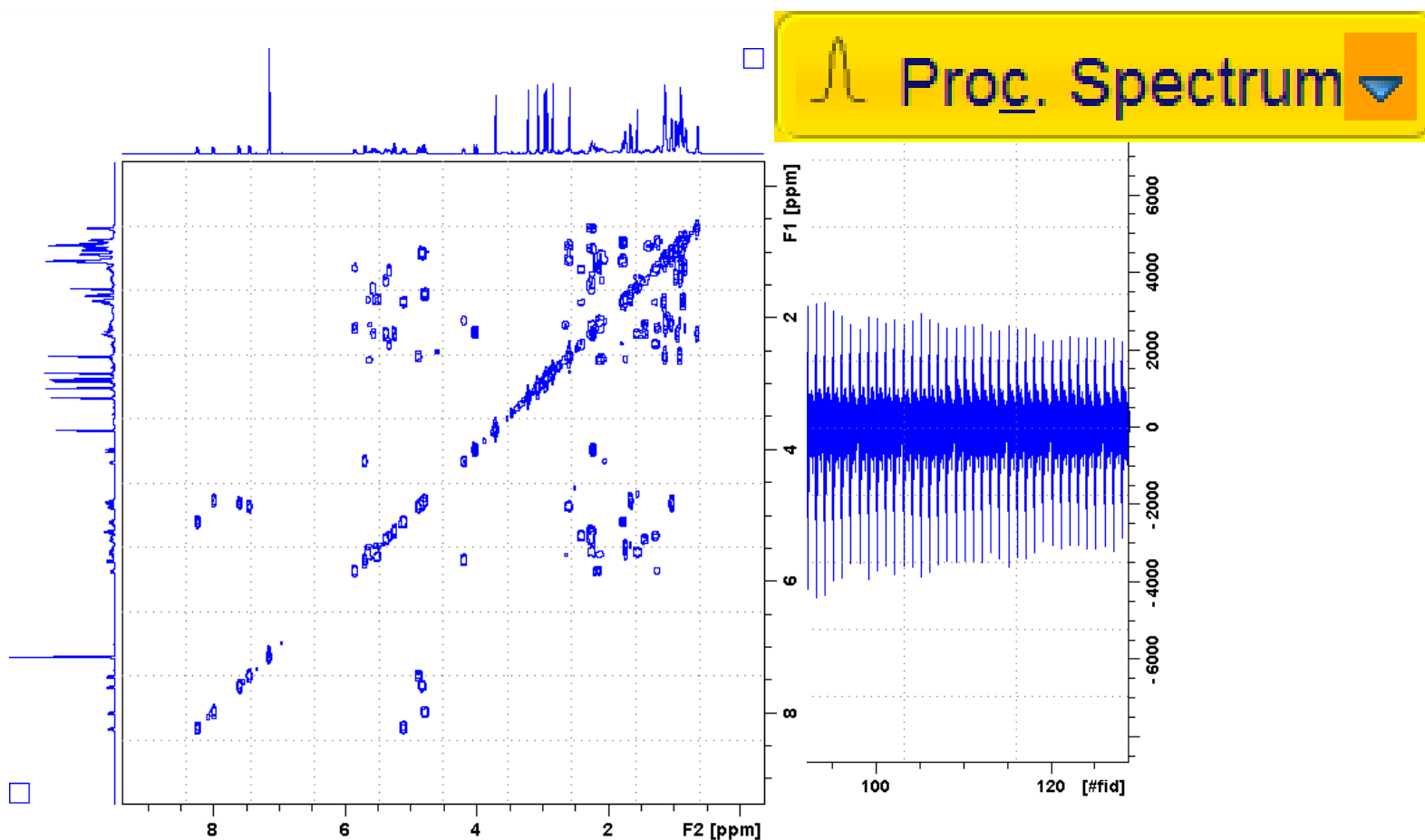
- **2D Processing**

1-Click processing

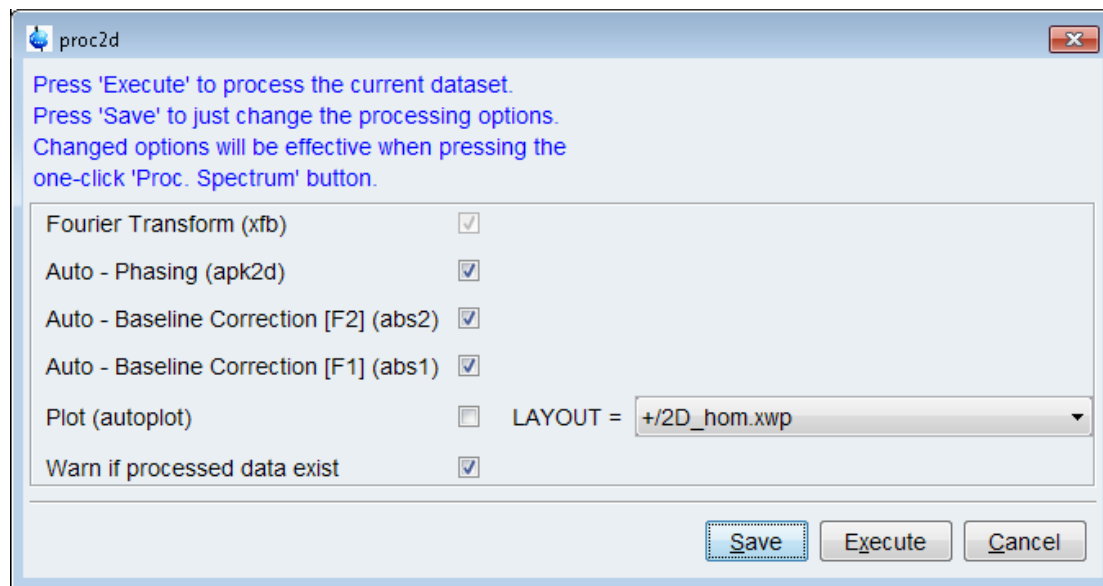
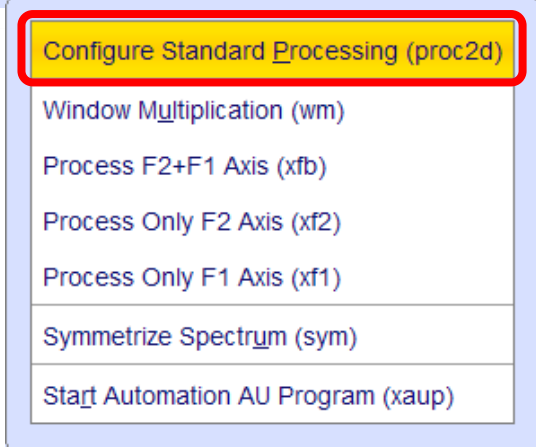
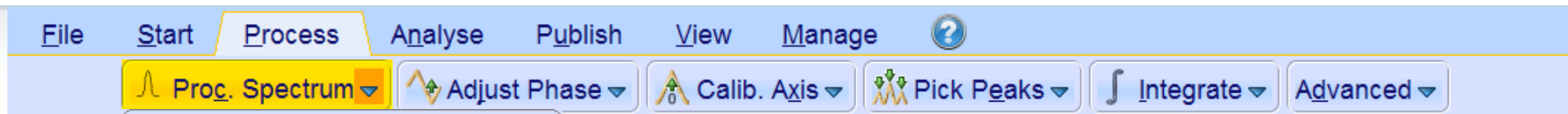


File Start **Process** Analyse Publish View Manage ?

Proc. Spectrum Adjust Phase Calib. Axis Pick Peaks Integrate Advanced



1-Click processing options



- [**xfb**] processes data in both dimensions with the following steps:
 - Baseline correction
 - Linear prediction
 - Window multiplication
 - Fourier transformation
 - Phase correction
- [**xf2**] processes data only in F2
- [**xf1**] processes data only in F1

- Parameters are :
 - size **SI**
 - spectrum reference frequency **SR**
 - spectral resolution **HzpPt**
 - window function **WDW**
 - sine bell shift **SSB**
 - phase mode **PH_mod**
 - 0th order correction **PHC0**
 - 1st order correction **PHC1**
- **All of these processing parameters are needed twice!**

Processing parameters [edp]



Avance_Training 60 1 C:\NMRData\data\bgoe\nmr

Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Plot Fid Acqu

S 1,2... M

Reference Window Phase Baseline Fourier NUS Peak Automation Miscellaneous User

Reference

F2 F1 Frequency axis

SI	1024	1024	Size of real spectrum
SF [MHz]	400.1300000	400.1300000	Spectrometer frequency
OFFSET [ppm]	9.39188	9.39188	Low field limit of spectrum
SR [Hz]	0	0	Spectrum reference frequency
HZpPT [Hz]	3.814697	3.814697	Spectral resolution
SPECTYP	UNDEFINED		Type of spectrum e.g. COSY, HMQC, ...

Window function

WDW	QSINE	QSINE	Window functions for trf, xfb, ...
LB [Hz]	1.00	0.30	Line broadening for em
GB	0	0.1	Gaussian max. position for gm, 0<GB<1
SSB	0	0	Sine bell shift SSB (0,1,2,...)
TM1	0	0.1	Left limit for tm 0<TM1<1
TM2	0	0.9	Right limit for tm 0<TM2<1

Phase correction

PHC0 [degrees]	0	0	0th order correction for pk
PHC1 [degrees]	0	0	1st order correction for pk
PH_mod	no	mc	Phasing modes for trf, xfb, ...

Baseline correction

ABSC	5	5	Degree of polynomial for abs (0..5)
------	---	---	-------------------------------------

Typical processing parameters



	F2 dimension	F1 dimension
SI	TD(F2)	4(8)×TD(F1)
WDW	QSIN	QSIN
SSB	0	0
PH_mod	no	mc
PHC0	0	-
PHC1	0	-

For FnMODE: QF

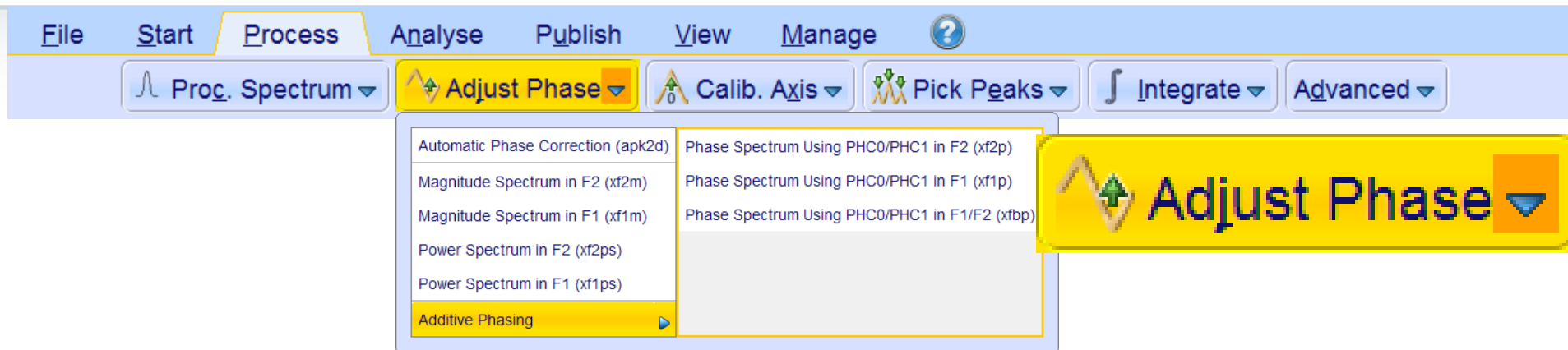
Typical processing parameters



	F2 dimension	F1 dimension
SI	TD(F2)	4(8)×TD(F1)
WDW	QSIN	QSIN
SSB	2	2
PH_mod	pk	pk
PHC0	0	Depends on
PHC1	0	experiment

For FnMODE: States, TPPI, States-TPPI, Echo-Antiecho

Adjust Phase



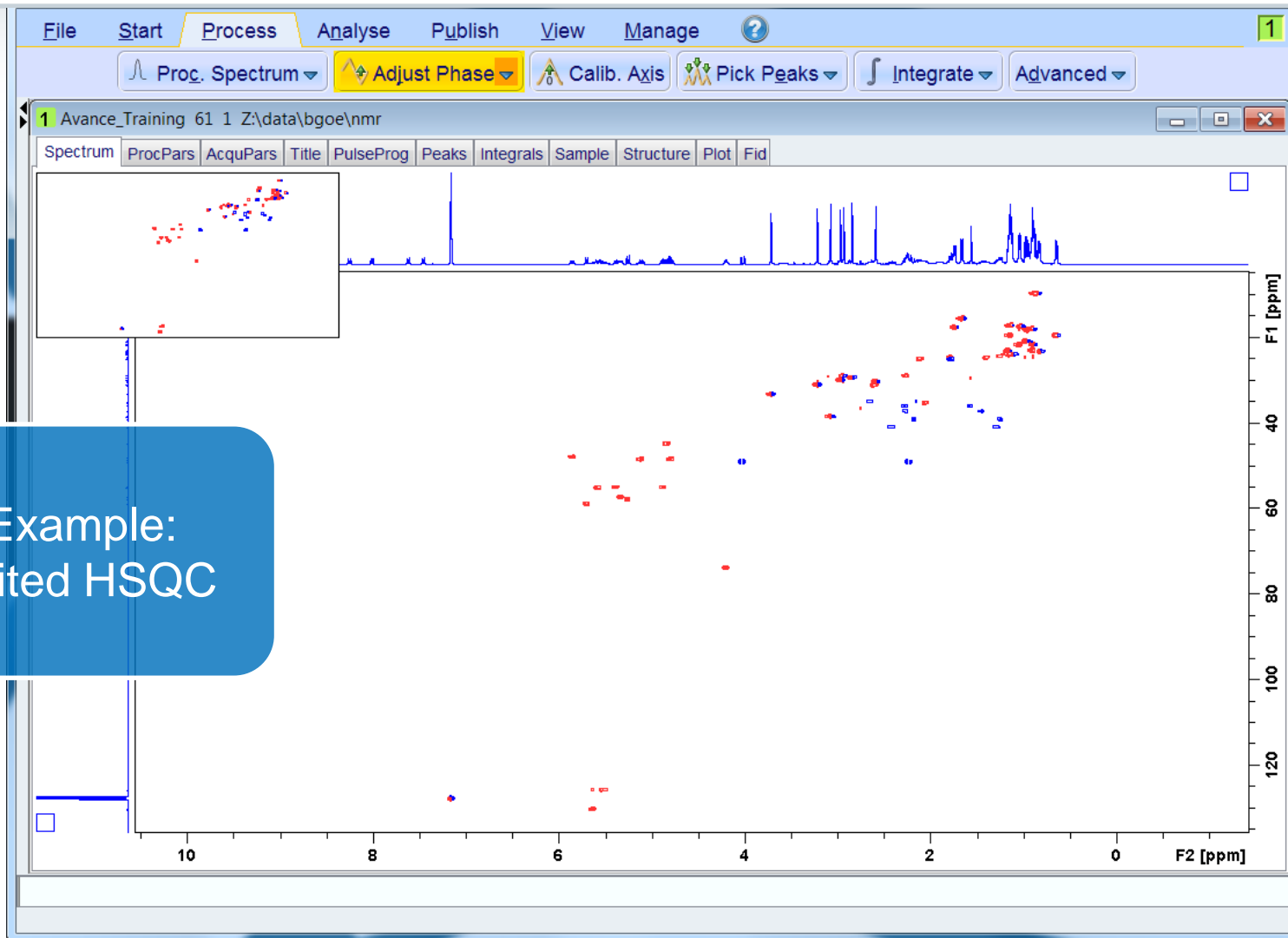
- Manual phase correction with **[.ph]**
- Automatic phase correction with **[apk2d]**
- **[xfb]** uses values of **PHC0(F1/F2)** and **PHC1(F1/F2)**



No phase correction is necessary for not phase sensitive experiments!

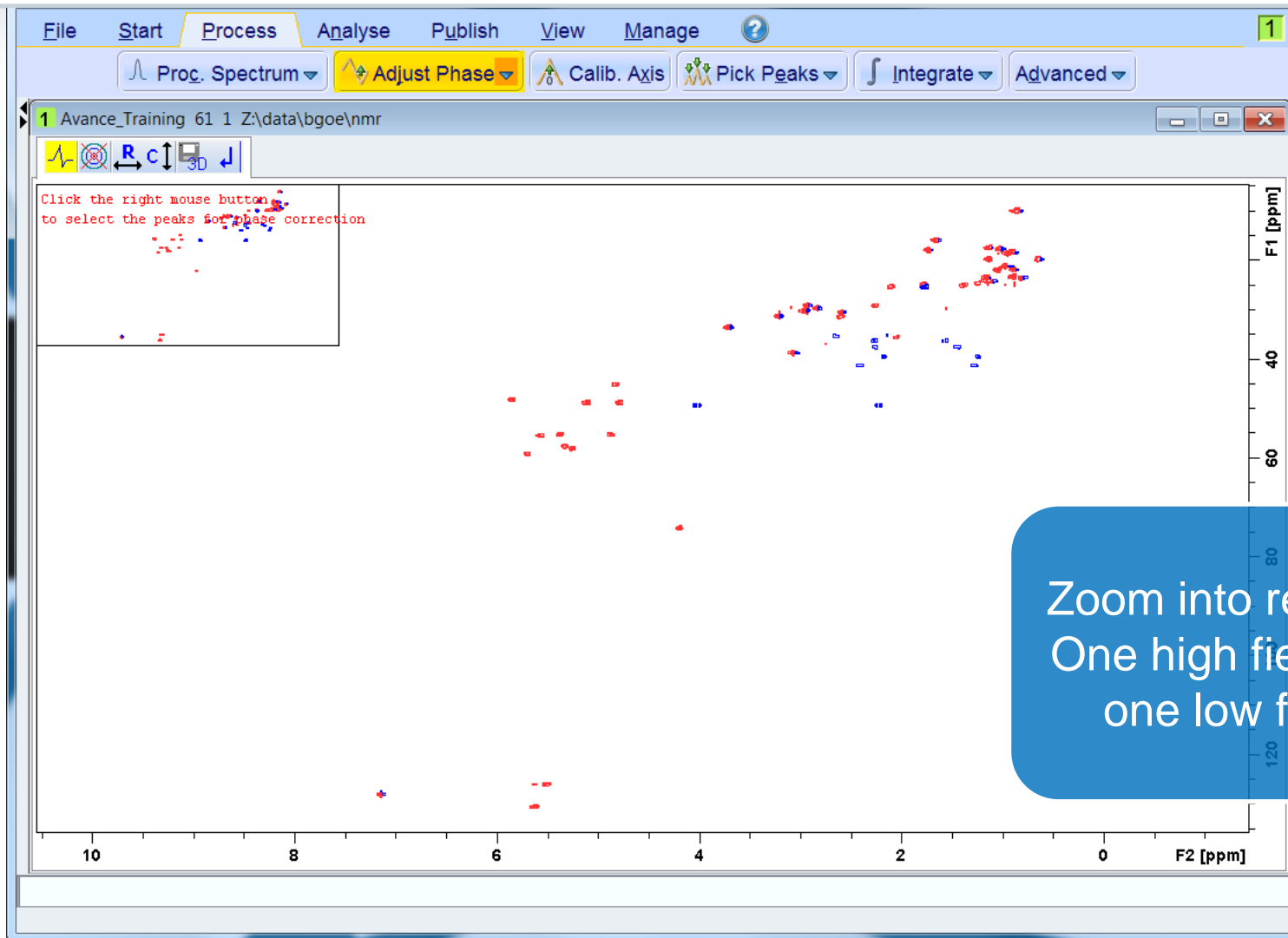
- Phase correction for phase sensitive experiments are typically only necessary for the F2-dimension.
- The values for homonuclear experiments for F1 are mentioned in the pulse program.
- Heteronuclear experiments are automatically corrected in F1.

Phasing



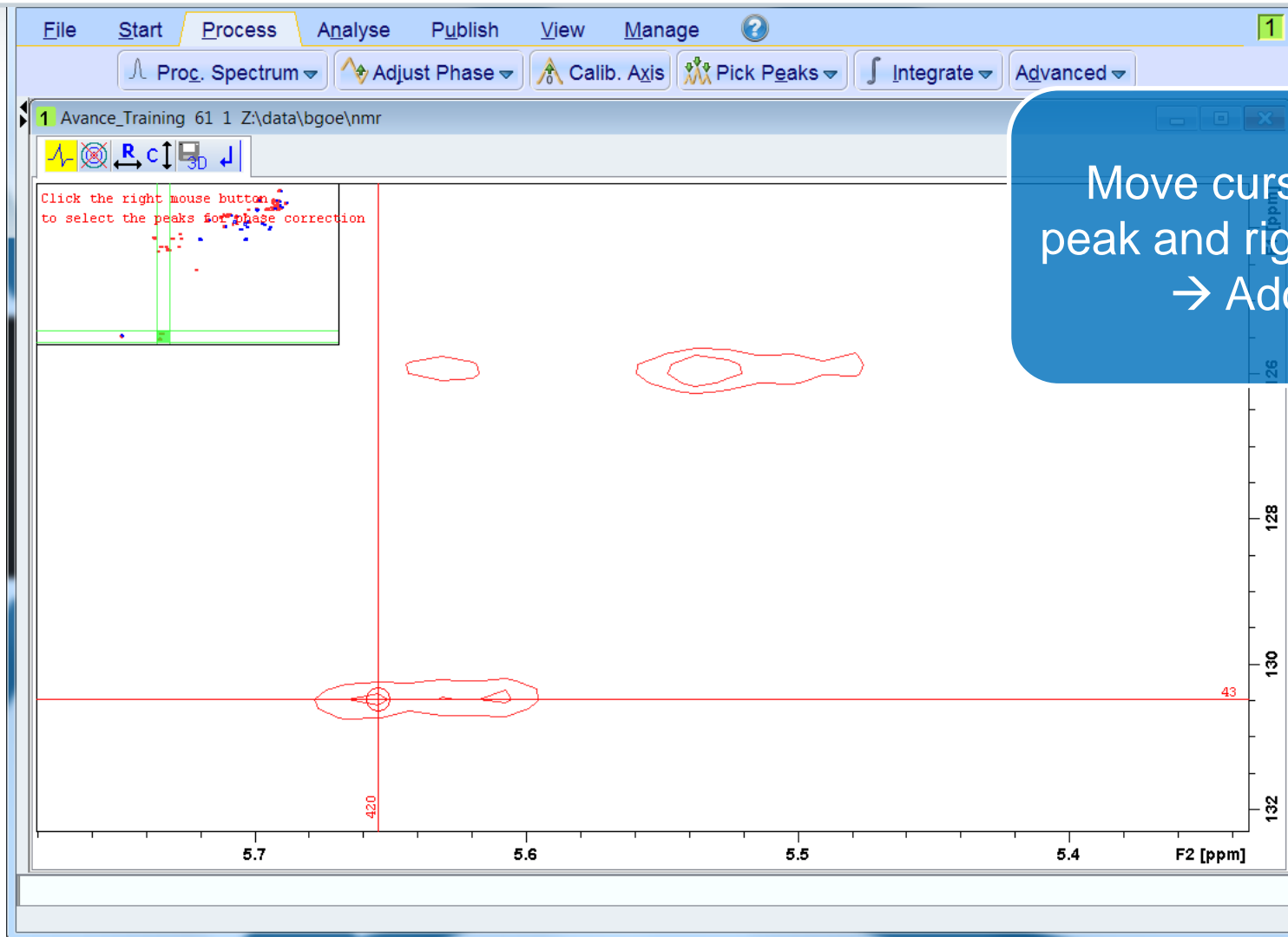
Example:
edited HSQC

Phasing



Zoom into regions.
One high field and
one low field.

Phasing

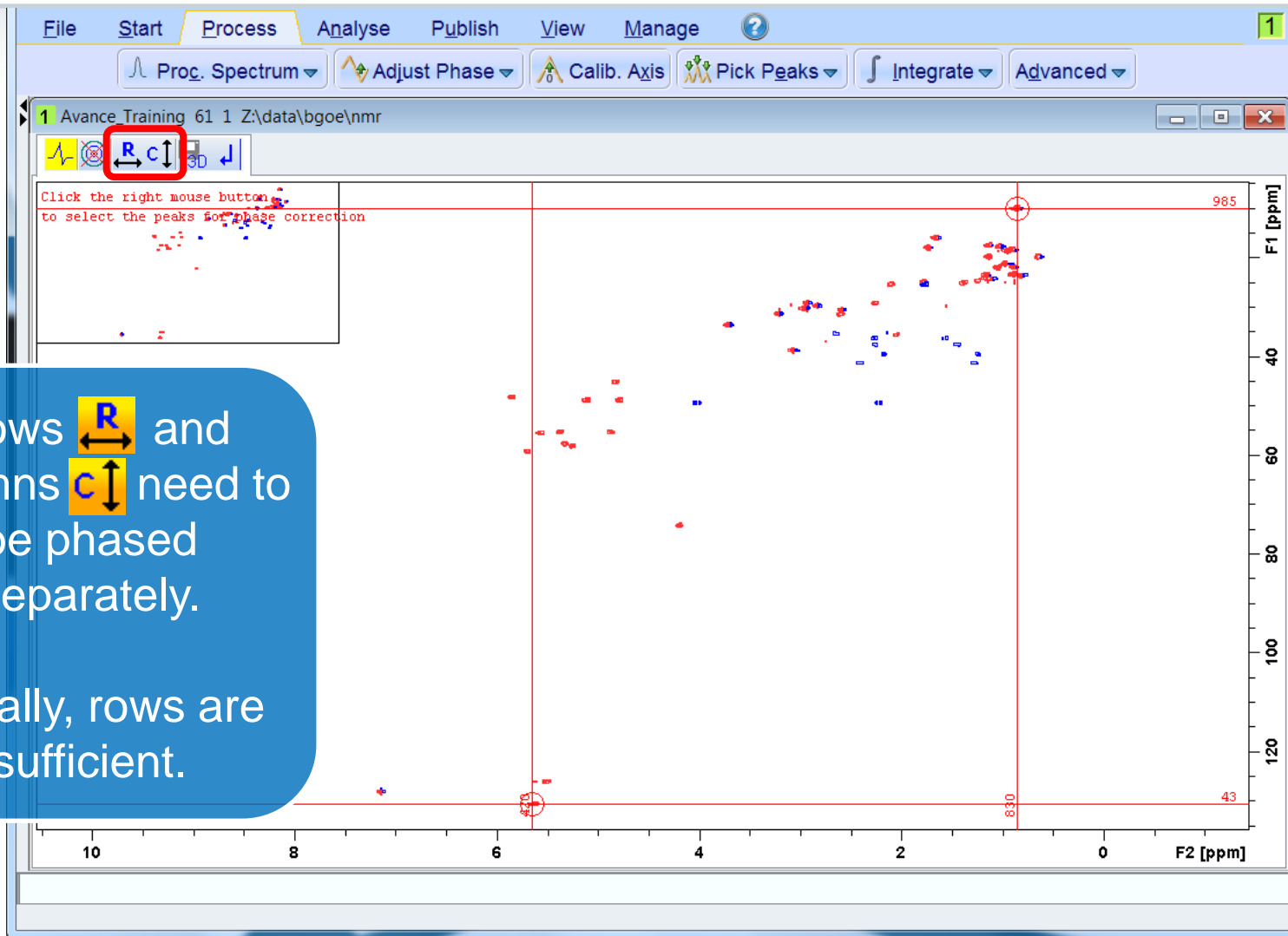


Move cursor to
peak and right click
→ Add

Phasing



Phasing



Rows **R** and columns **C** need to be phased separately.

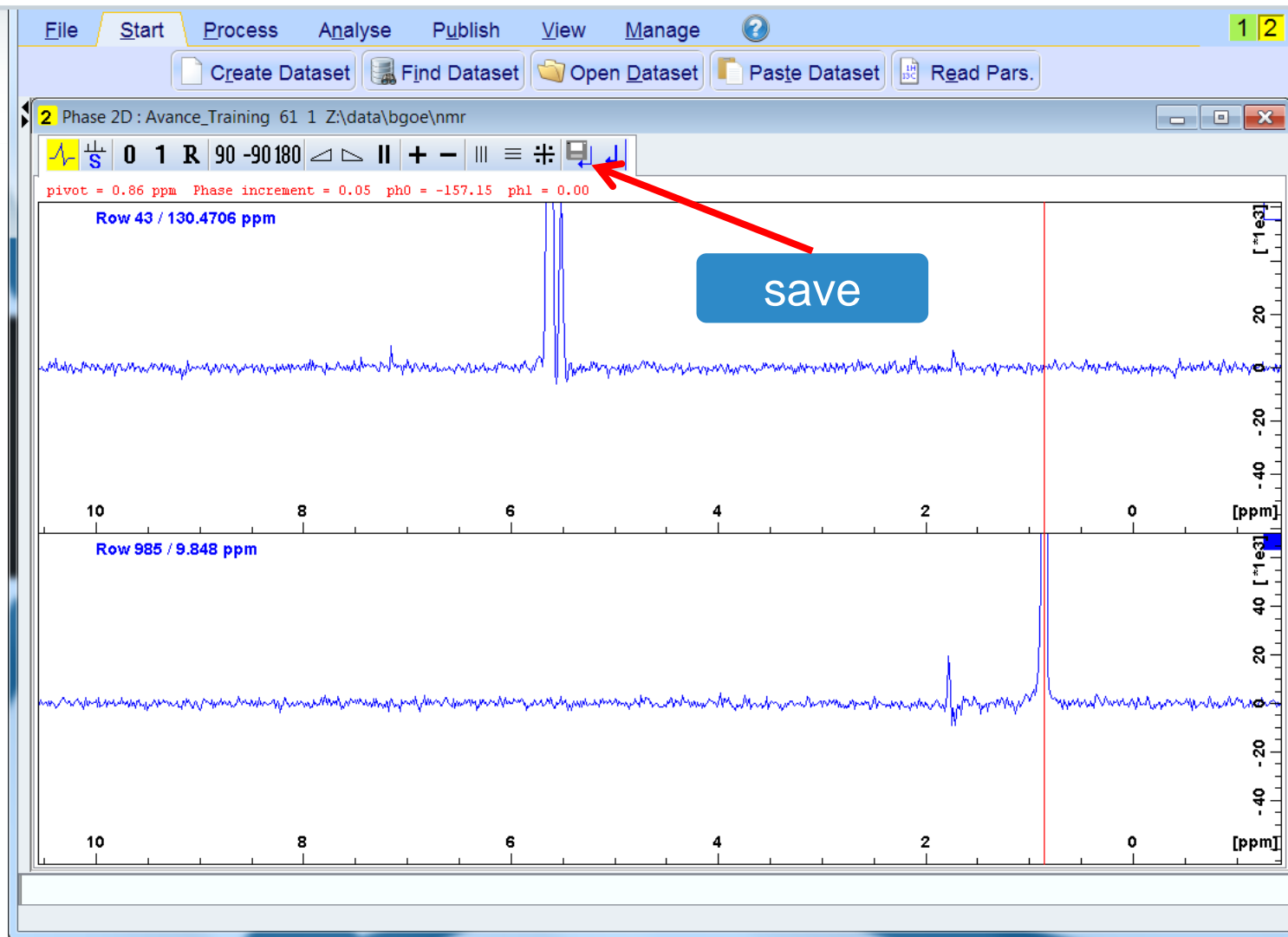
Usually, rows are sufficient.

Phasing

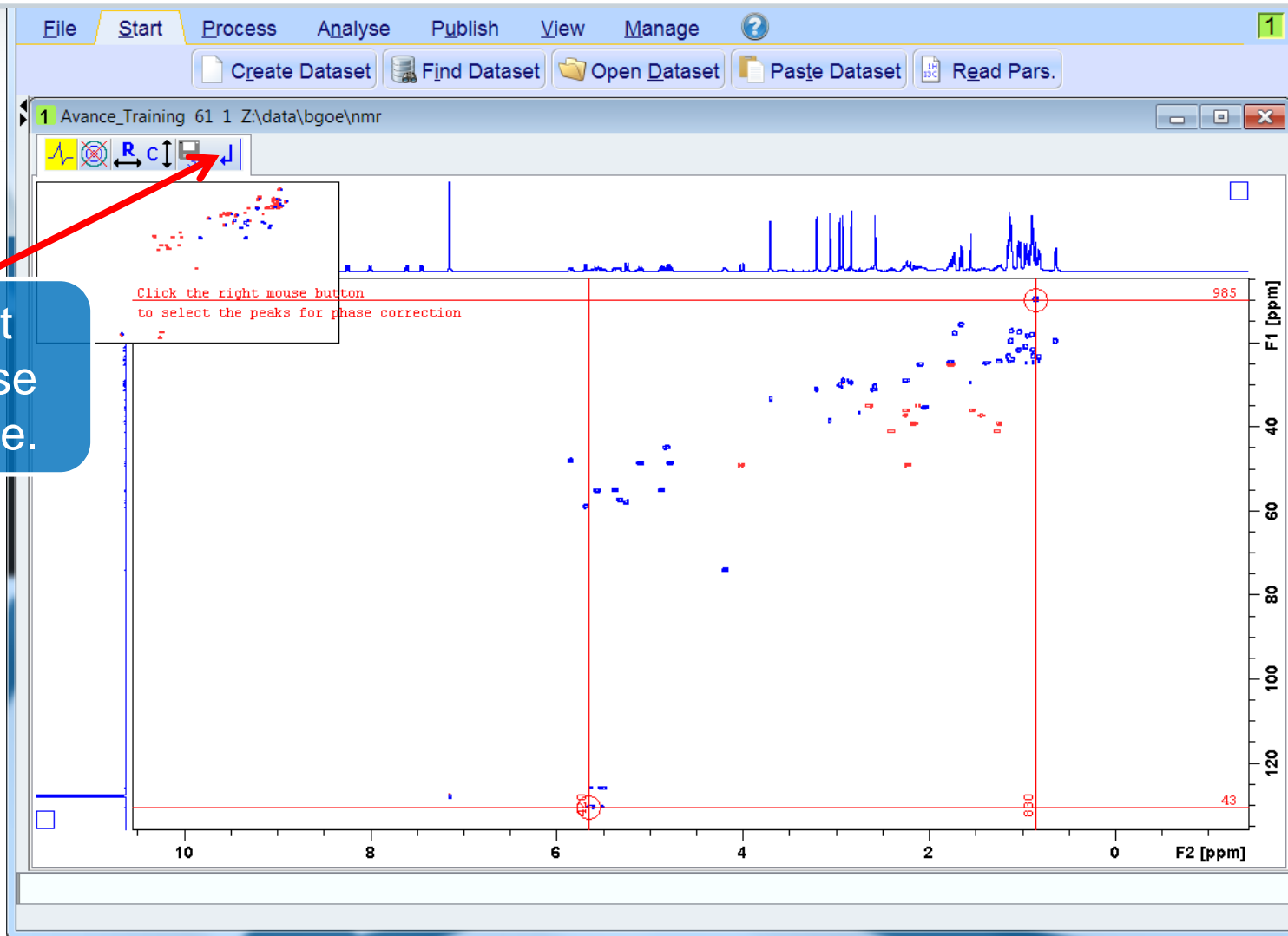


Push and hold
buttons to phase.
First 0th order **0**
Then 1st order **1**.

Phasing

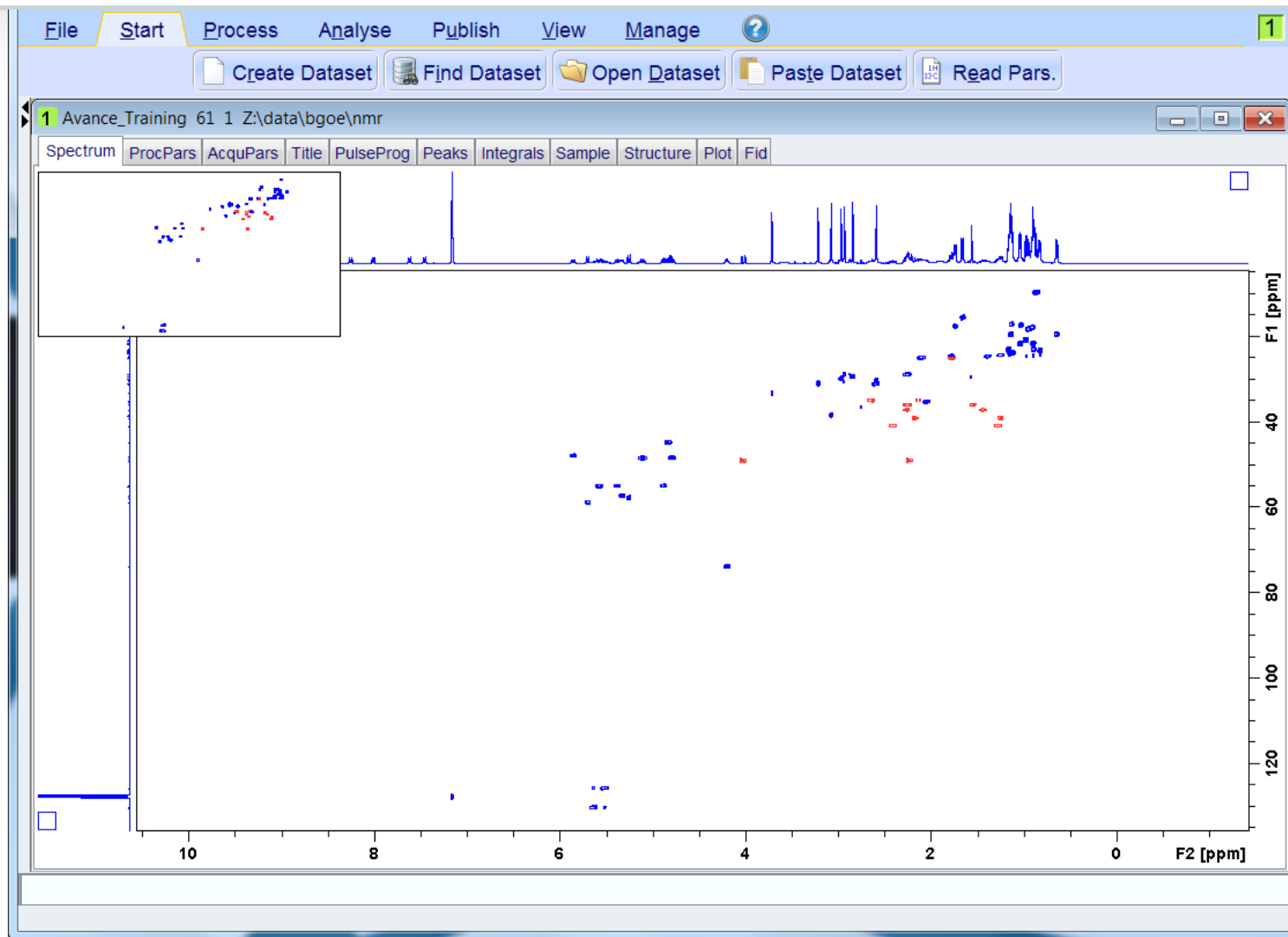


Phasing

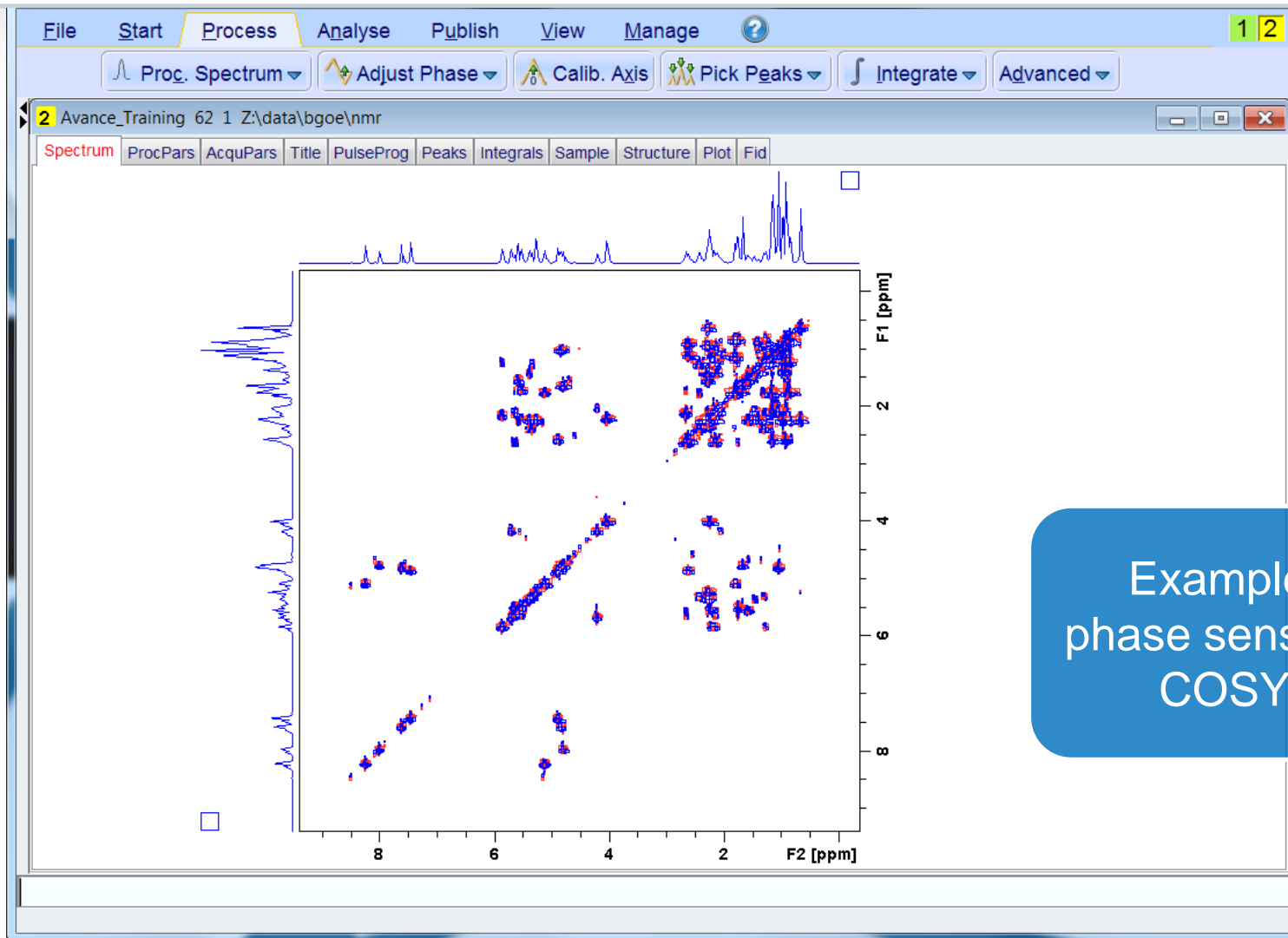


Exit
phase
mode.

Phasing

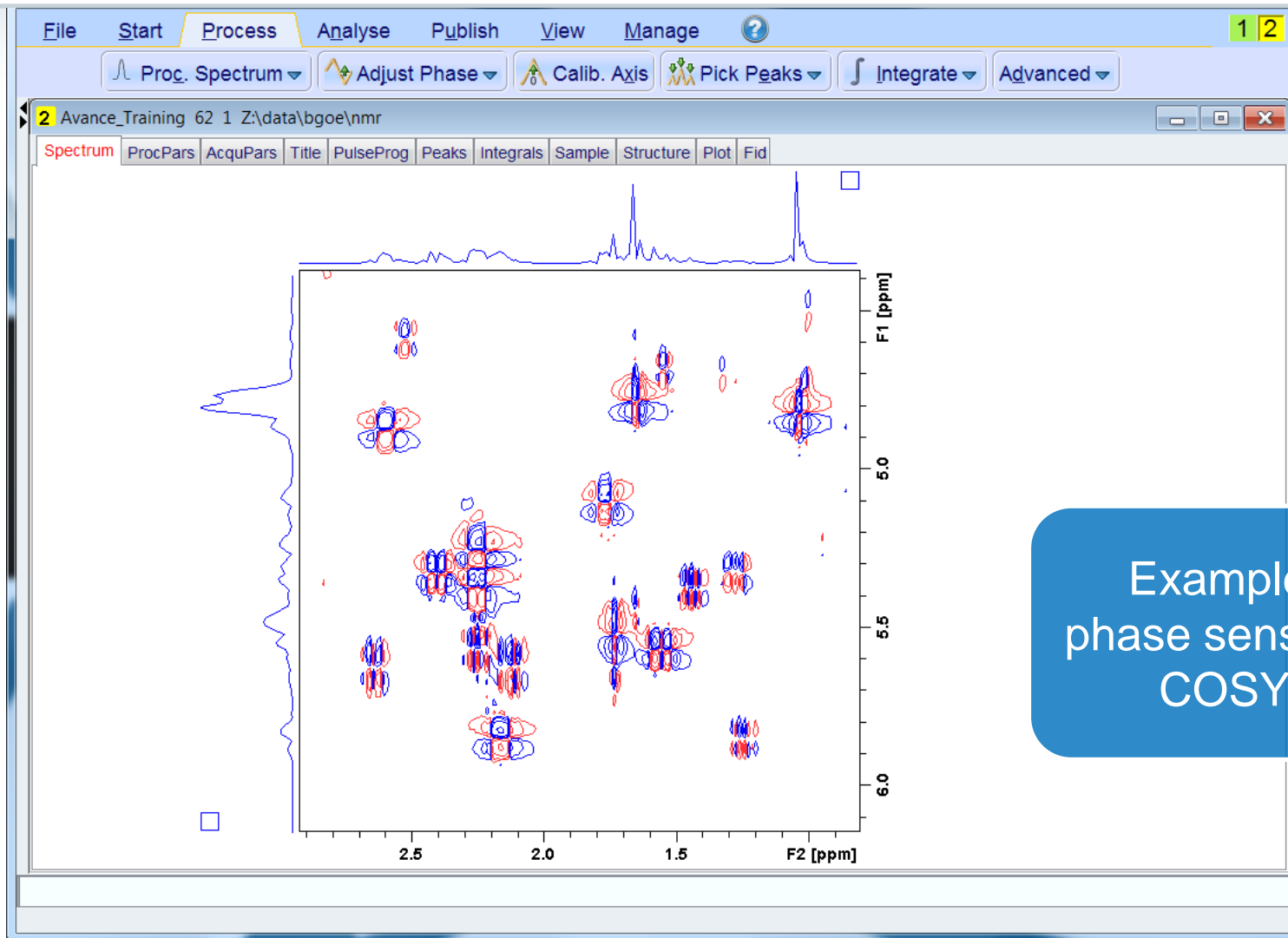


Phasing DQF-COSY



Example:
phase sensitive
COSY

Phasing DQF-COSY



Example:
phase sensitive
COSY

Phasing DQF-COSY



Phase correction
for F1 is
mentioned in
pulse program.

```
cosygpmpfphp (C:\Bruker\TopSpin3.5pl7\exp\stan\nmr\lists\pp)
File Edit Search
Graphical_Edit Set PULPROG
72 ;p110: f1 channel - power level for TOCSY-spinlock
73 ;p1 : f1 channel - 90 degree high power pulse
74 ;p2 : f1 channel - 180 degree high power pulse
75 ;p16: homospoil/gradient pulse
76 ;p17: f1 channel - trim pulse [2.5 msec]
77 ;d0 : incremented delay (2D)
78 ;d1 : relaxation delay; 1-5 * T1
79 ;d11: delay for disk I/O [30 msec]
80 ;d12: delay for power switching [20 usec]
81 ;d16: delay for homospoil/gradient recovery
82 ;inf1: 1/SW = 2 * DW
83 ;in0: 1/(1 * SW) = 2 * DW
84 ;nd0: 1
85 ;ns: 1 * n
86 ;ds: 16
87 ;td1: number of experiments
88 ;FnMODE: States-TPPI, TPPI, States or QSEQ
89
90 ;use gradient ratio: gp 1 : gp 2
91 ; 10 : 20 for double quantum filter
92 ; 10 : 30 for triple quantum filter
93
94 ;for z-only gradients:
95 ;gpz1: 10%
96 ;gpz2: 20% for DQF, 30% for TQF
97
98 ;use gradient files:
99 ;gpnam1: SMSQ10.100
100 ;gpnam2: SMSQ10.100
101
102
103 ;Processing
104
105 ;PHC0(F1): 90
106 ;PHC1(F1): -180
107 ;FCOR(F1): 1
108
109
110
111 ;$Id: cosygpmpfphp,v 1.3 2012/01/31 17:49:22 ber Exp $
112
```

Phasing DQF-COSY



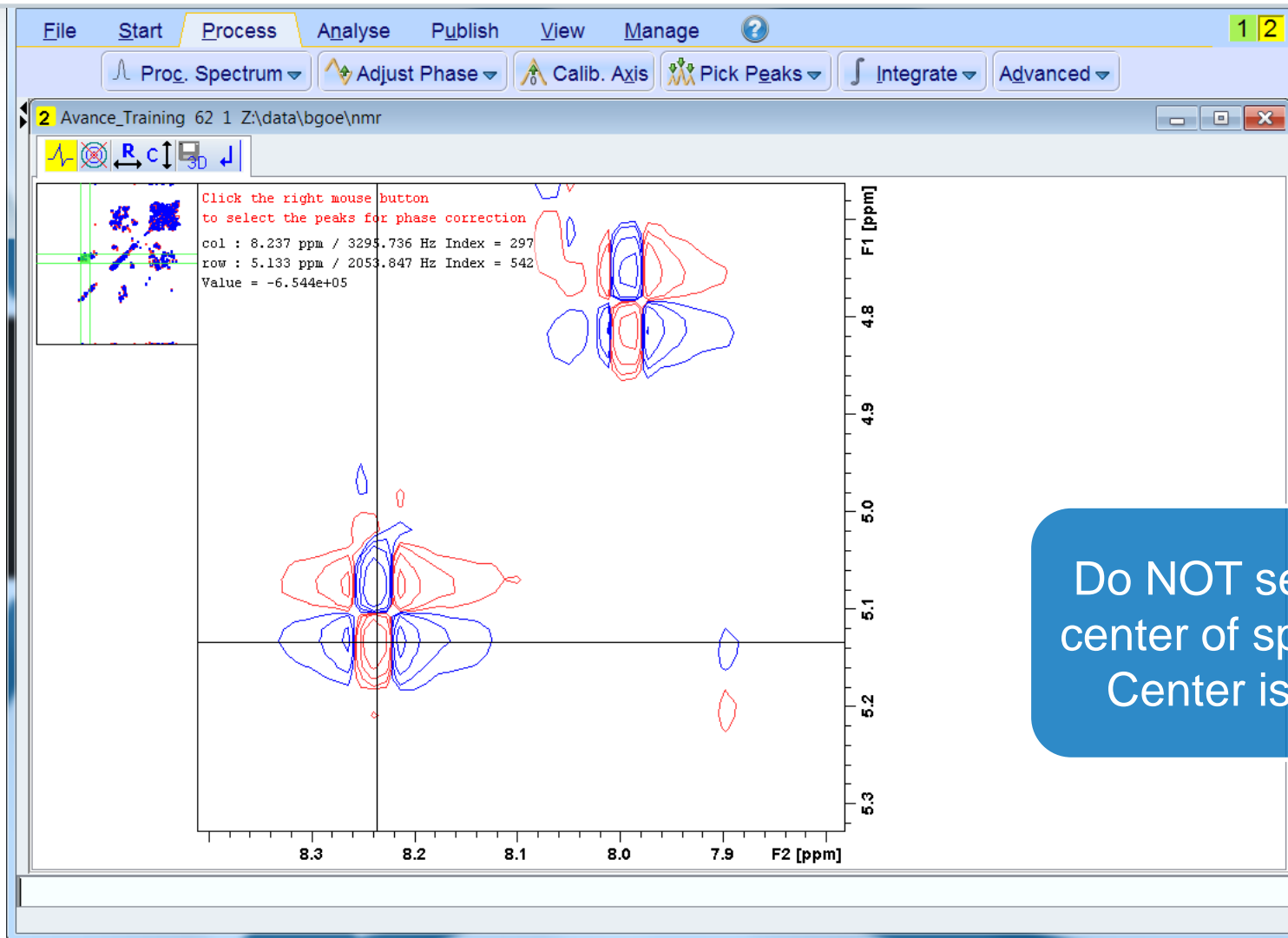
1 Avance_Training 62 1 Z:\data\bgoe\nmr

Spectrum ProcPars AcqParS Title PulseProg Peaks Integrals Sample Structure Plot Fid

PHC0 [degrees]	0	90.000	0th order correction for pk
PHC1 [degrees]	0	-180.000	1st order correction for pk
PK_Mod	pk	pk	Phasing modes for trf, xfb, ...
Baseline correction			
ABSG	5	5	Degree of polynomial for abs (0..5)
ABSF1 [ppm]	1000.00000	1000.00000	Left limit for absf
ABSF2 [ppm]	-1000.00000	-1000.00000	Right limit for absf, abs1, abs2
LCFW [ppm]	1.00000	1.00000	Filter width for bc (sfil/qfil)
COROFFS [Hz]	0	0	Correction offset for BC_MOD=spol etc.
BC_Mod	quad	no	Fid baseline modes for em, ft, xfb,...
Fourier transform			
TDeff	0	0	Number of fid data points used by ft
STSR	0	0	First output point of strip transform
STSI	0	0	Total number of output points of strip transform
ME_mod	no	LPfc	Linear prediction for ft, xfb, ...
NCOEF	0	32	Number of LP coefficients
LPBIN	0	0	Number of output points for LP
TDoff	0	0	Number of back-predicted points
REVERSE	FALSE	FALSE	Reverse spectrum during transform
FCOR	0.5	1	Weighting factor for first fid point
PKNL	TRUE		Group delay compensation

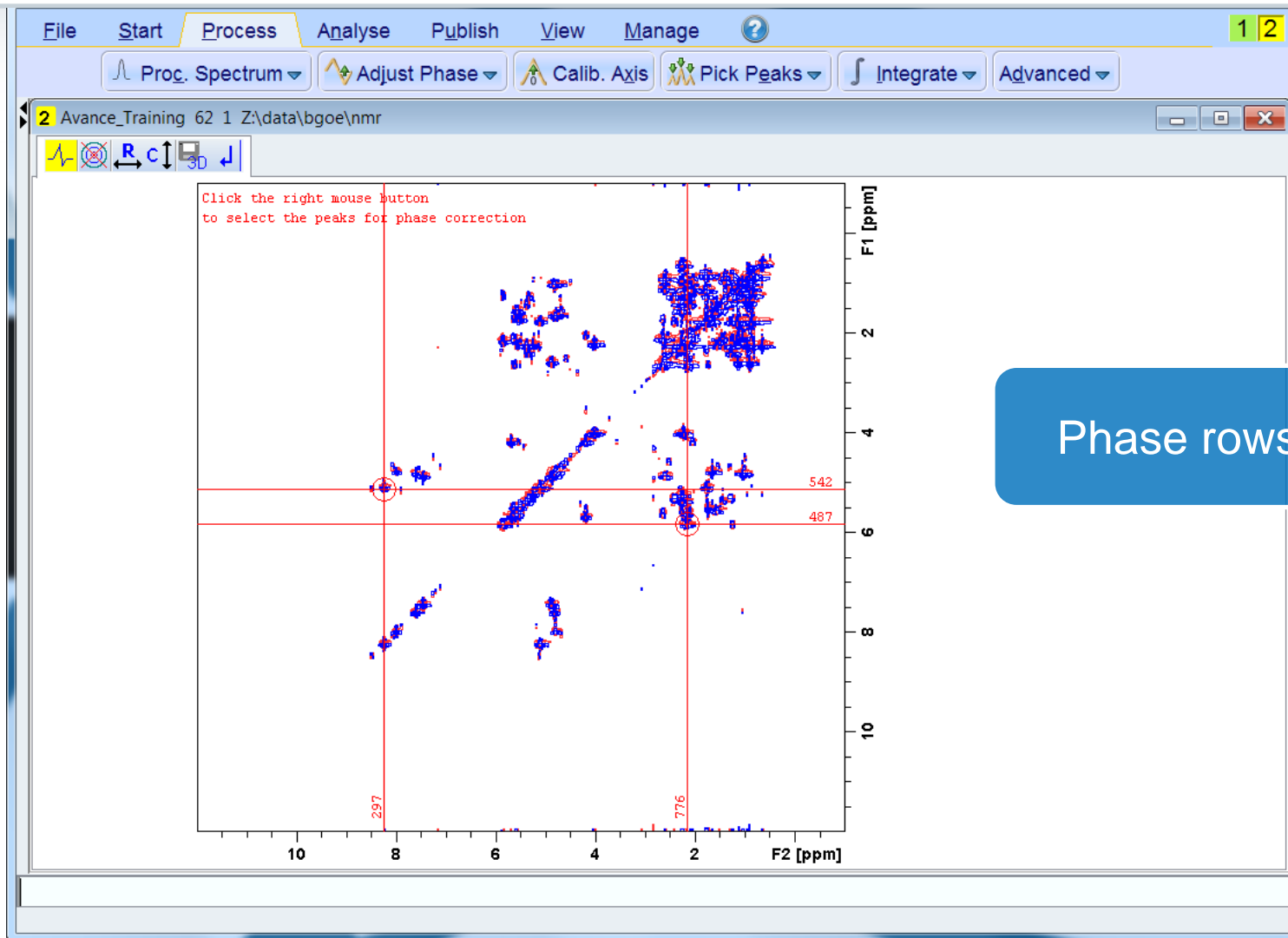
Phase correction for F1 is mentioned in pulse program.


Phasing DQF-COSY



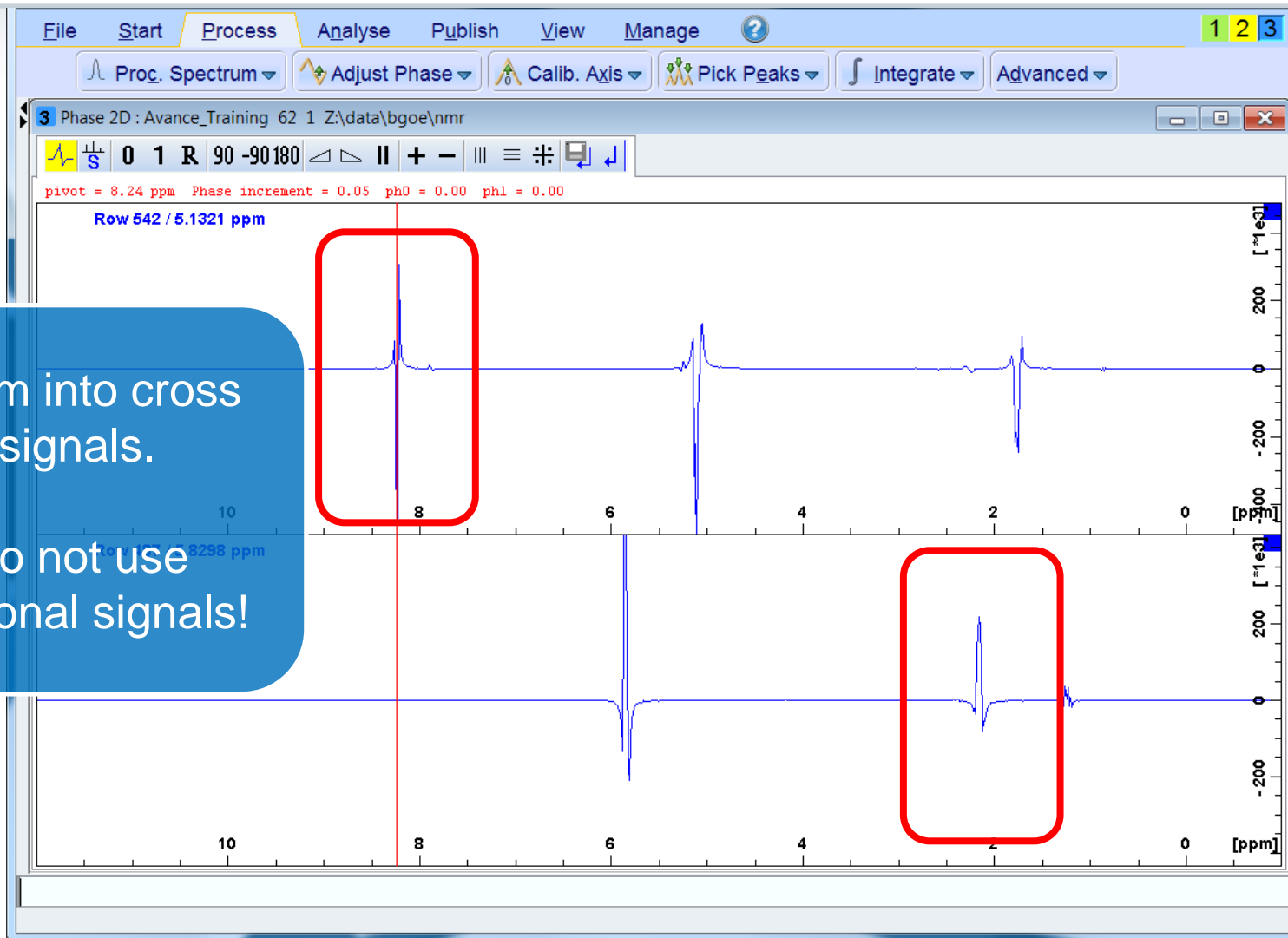
Do NOT select
center of speak.
Center is 0.

Phasing DQF-COSY



Phase rows  .

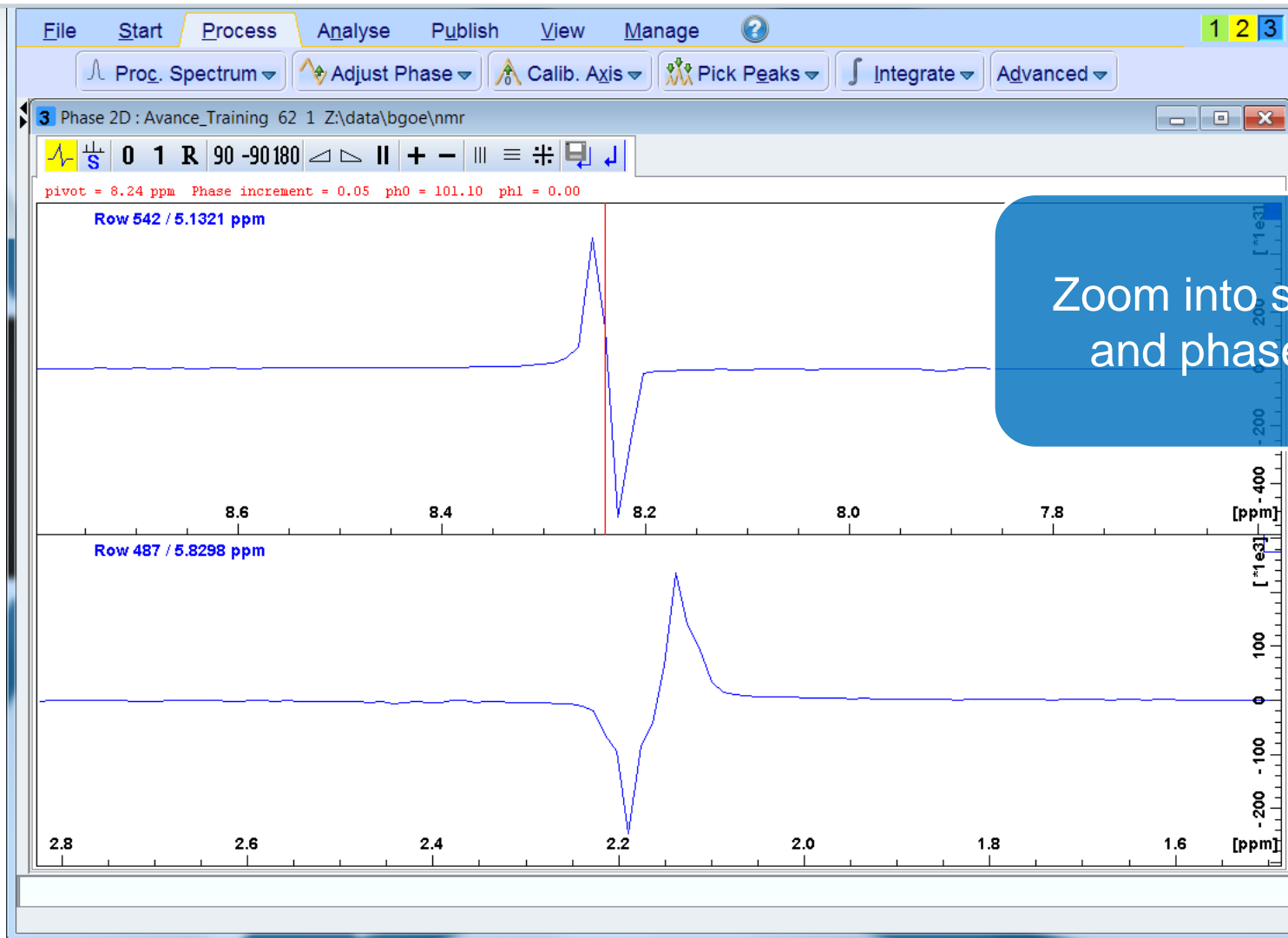
Phasing DQF-COSY



Zoom into cross
signals.

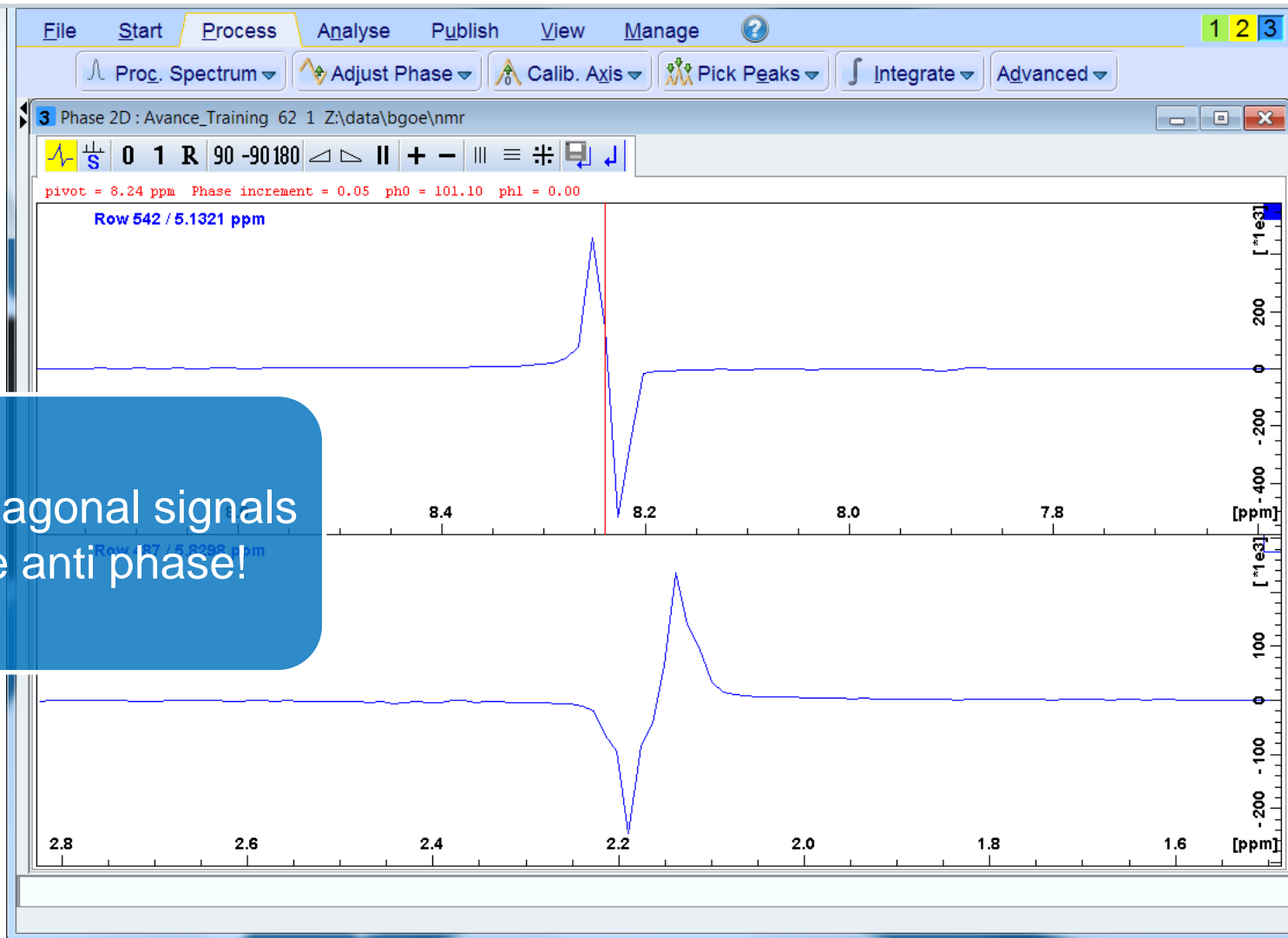
Do not use
diagonal signals!

Phasing DQF-COSY



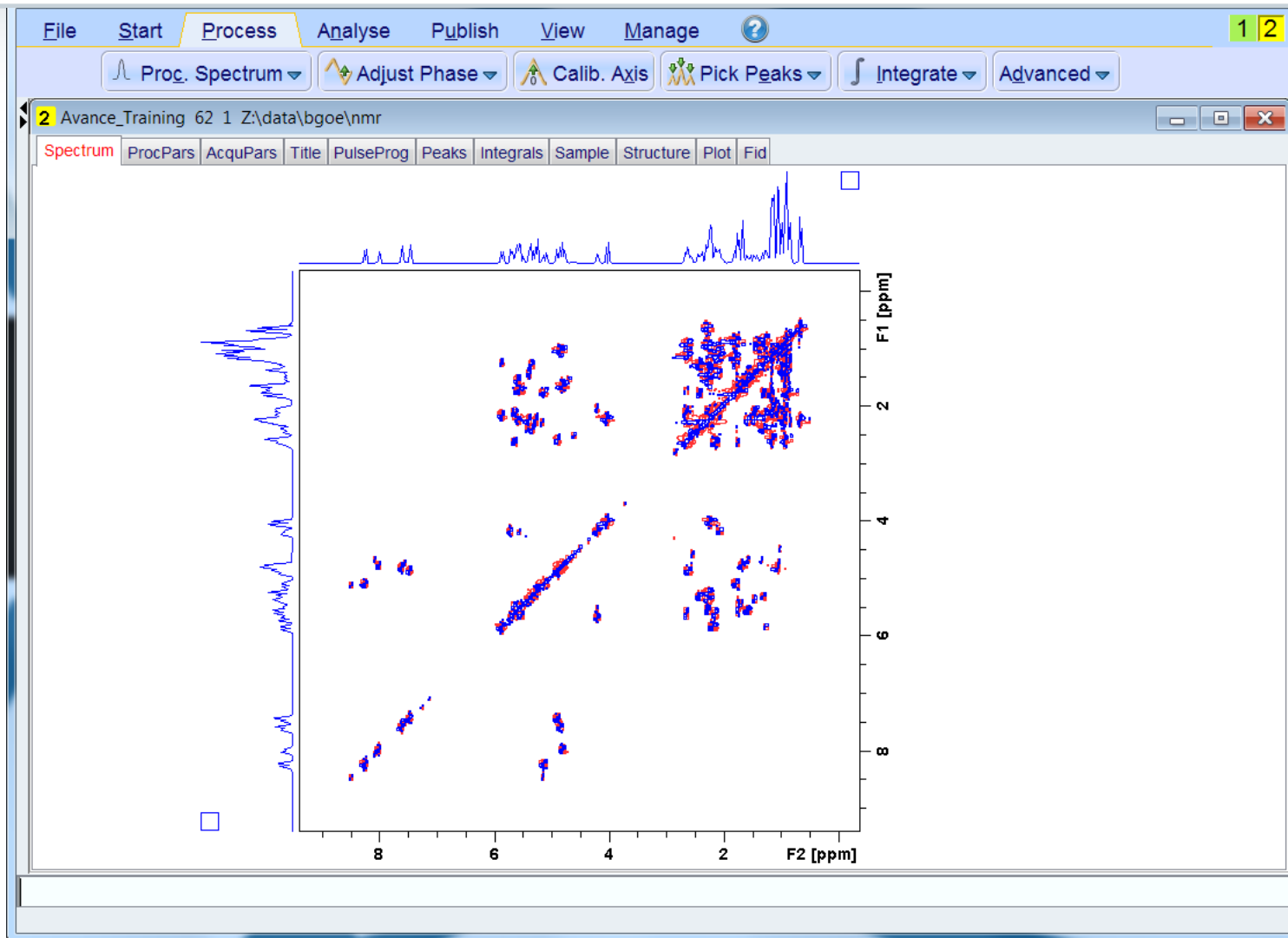
Zoom into signal
and phase it.

Phasing DQF-COSY

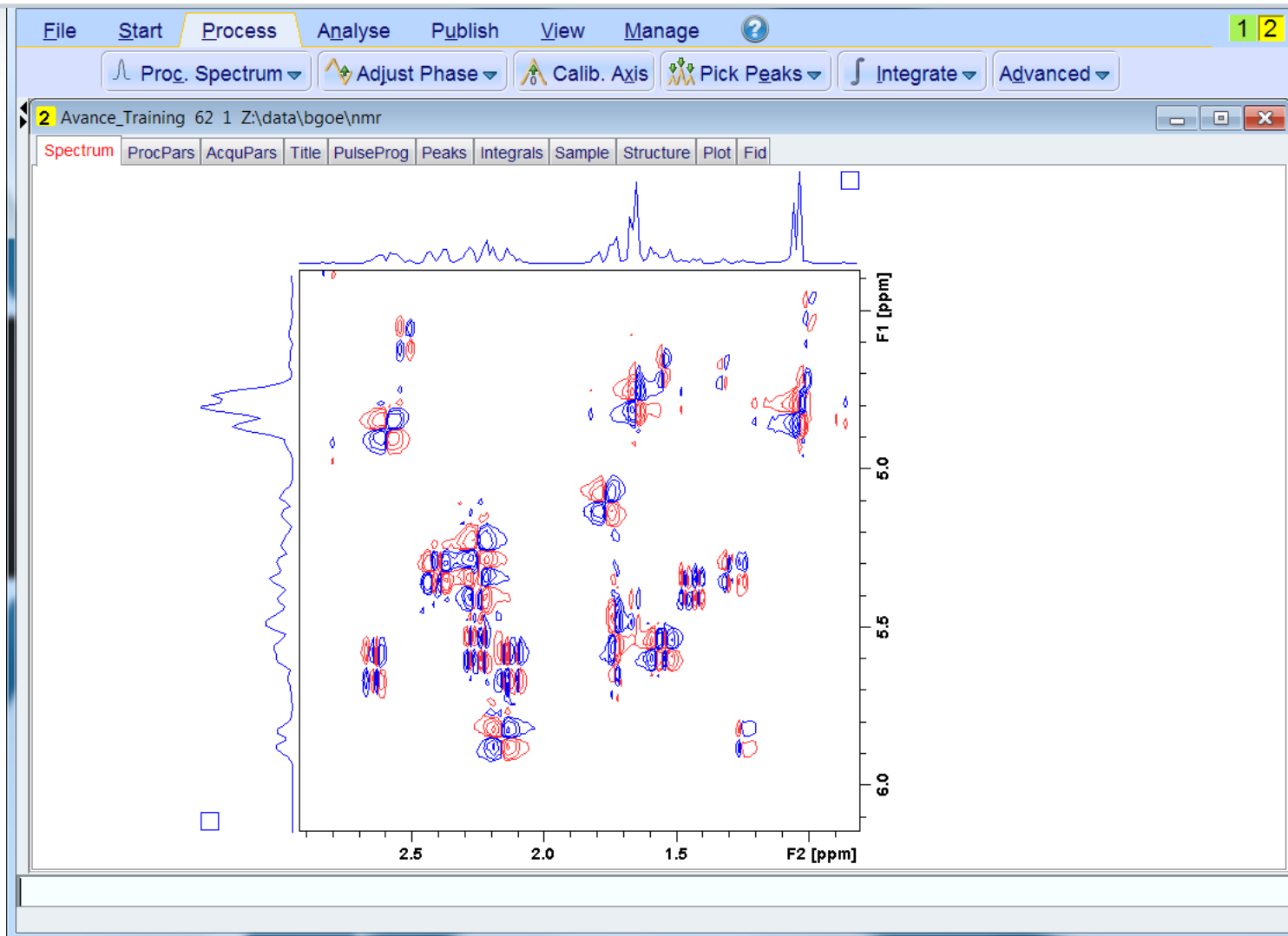


Off diagonal signals
are anti phase!

Phasing DQF-COSY



Phasing DQF-COSY

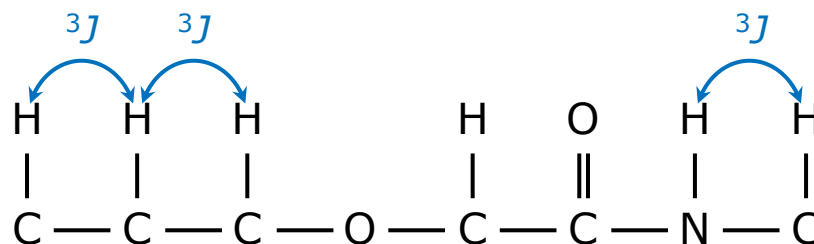


- **Basic 2D experiments**

COSY COrrrelation SPECTROSCOPY



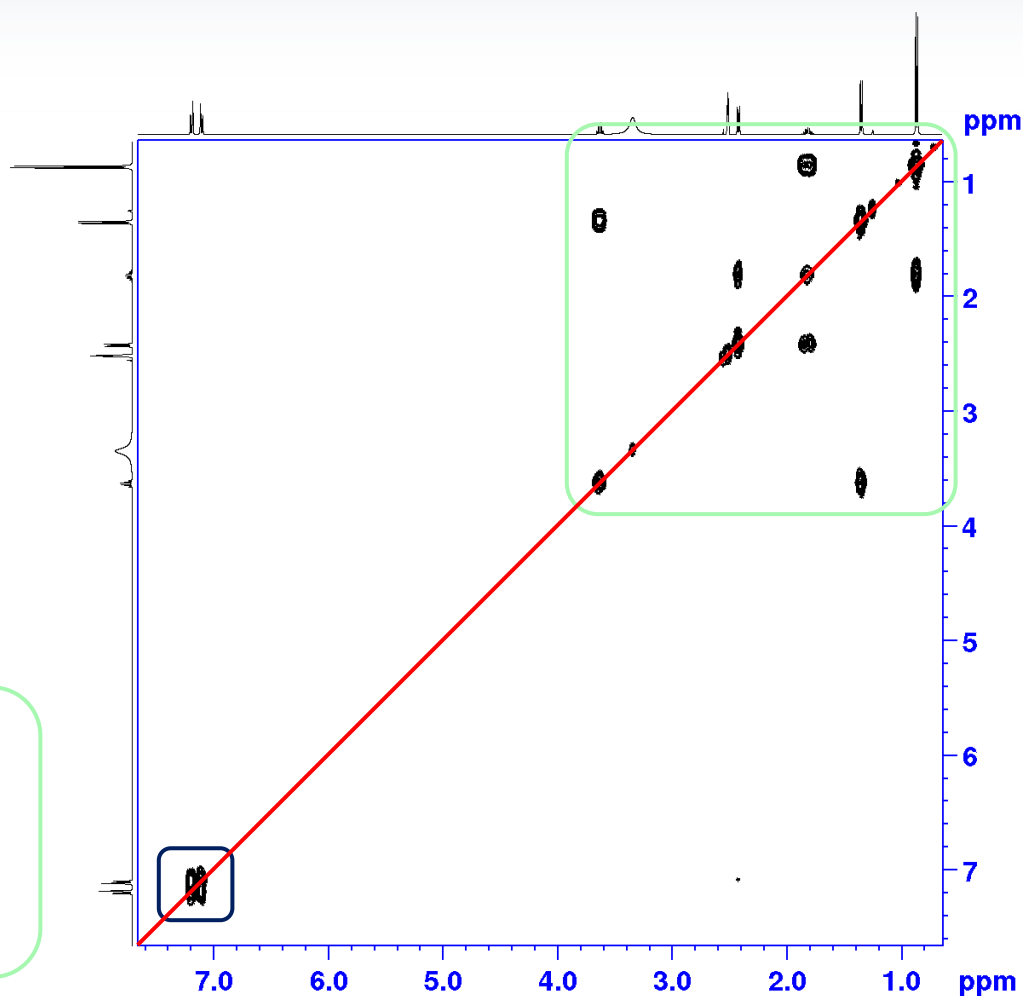
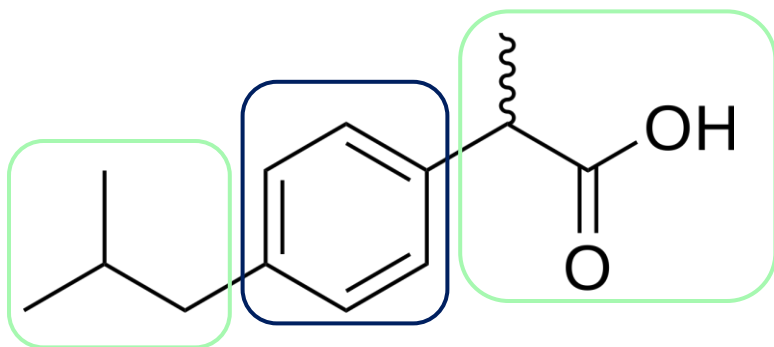
- Correlation between directly coupled protons
- Via scalar couplings



COSY COrrrelation SpectroscopyY



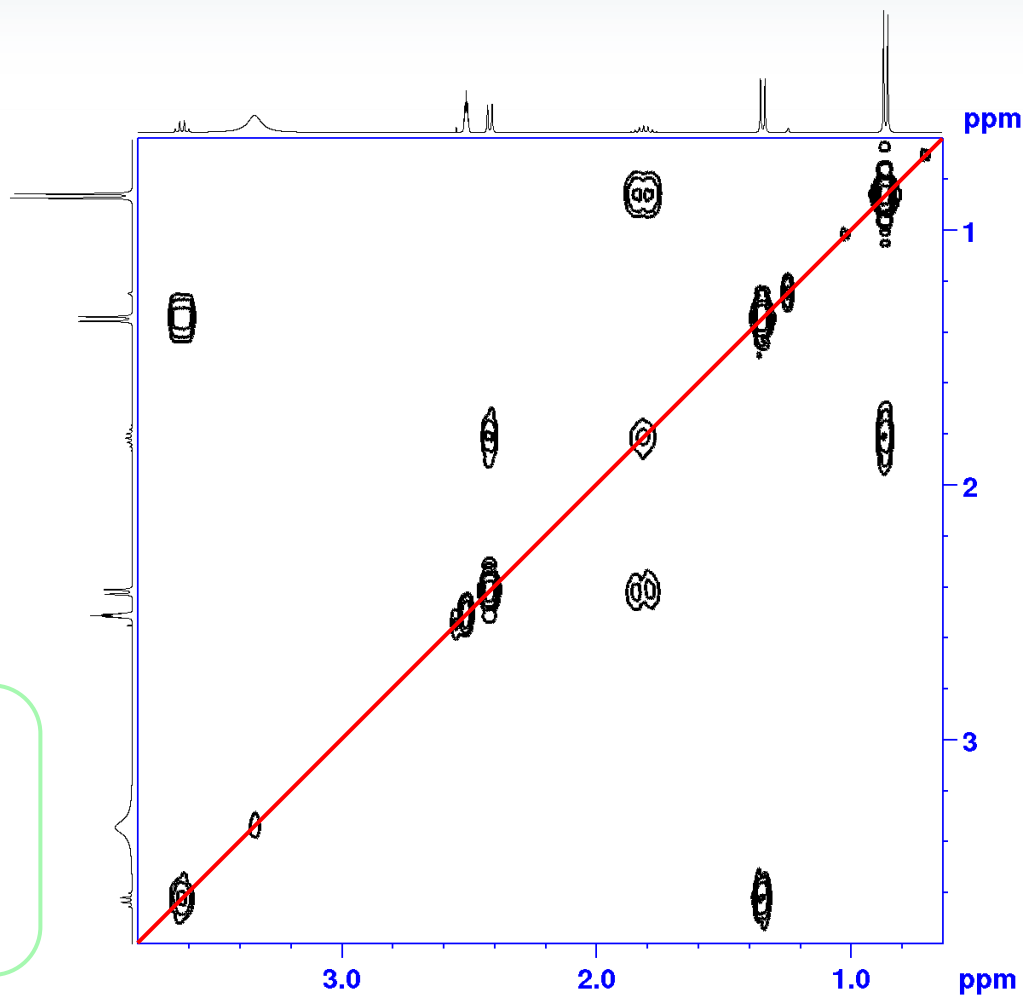
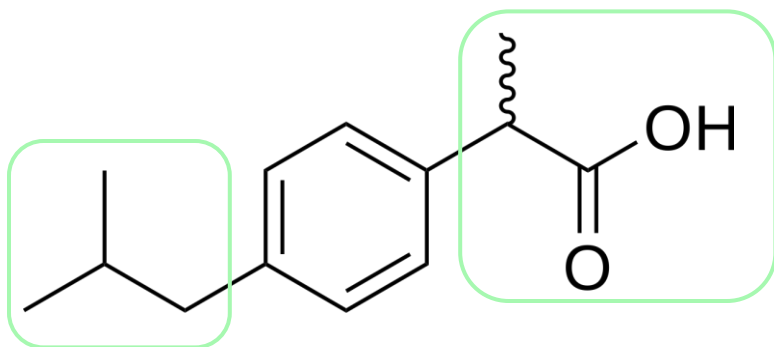
- Correlation between directly coupled protons
- Diagonal \triangleq 1D spectrum
- No new information



COSY CORrelation SPECTROSCOPY



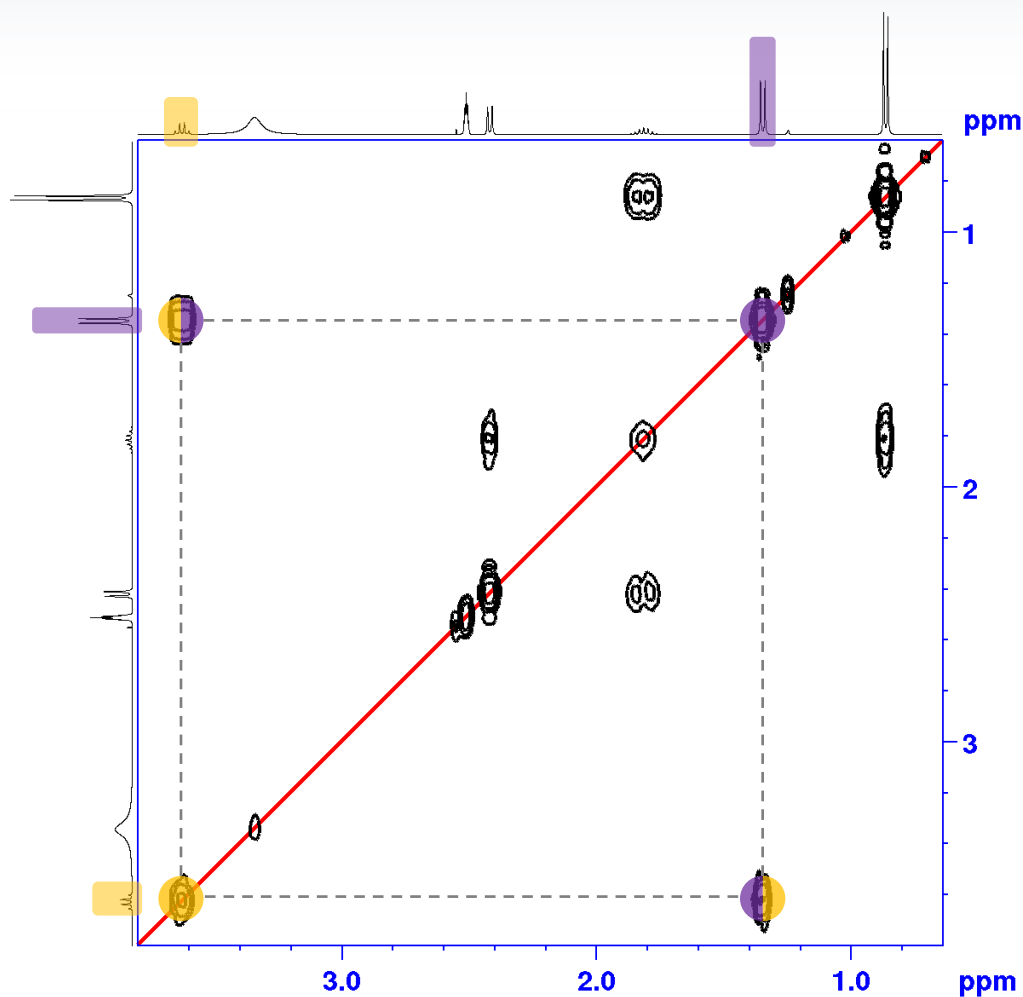
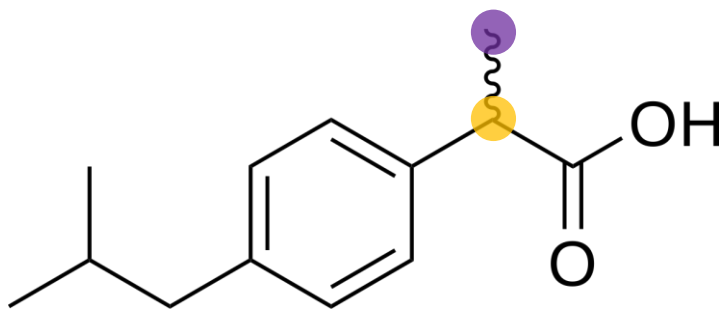
- Correlation between directly coupled protons
- Diagonal \triangleq 1D spectrum
- No new information



COSY COrrrelation Spectroscopy



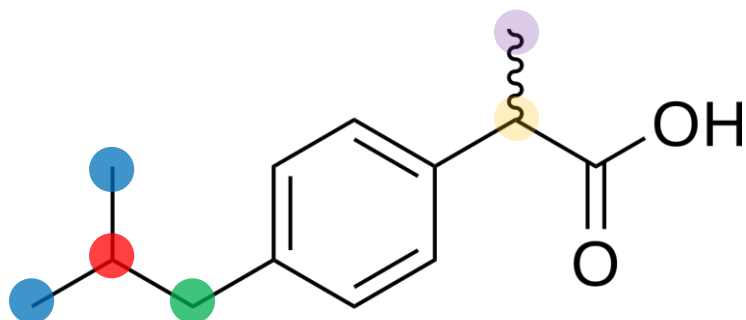
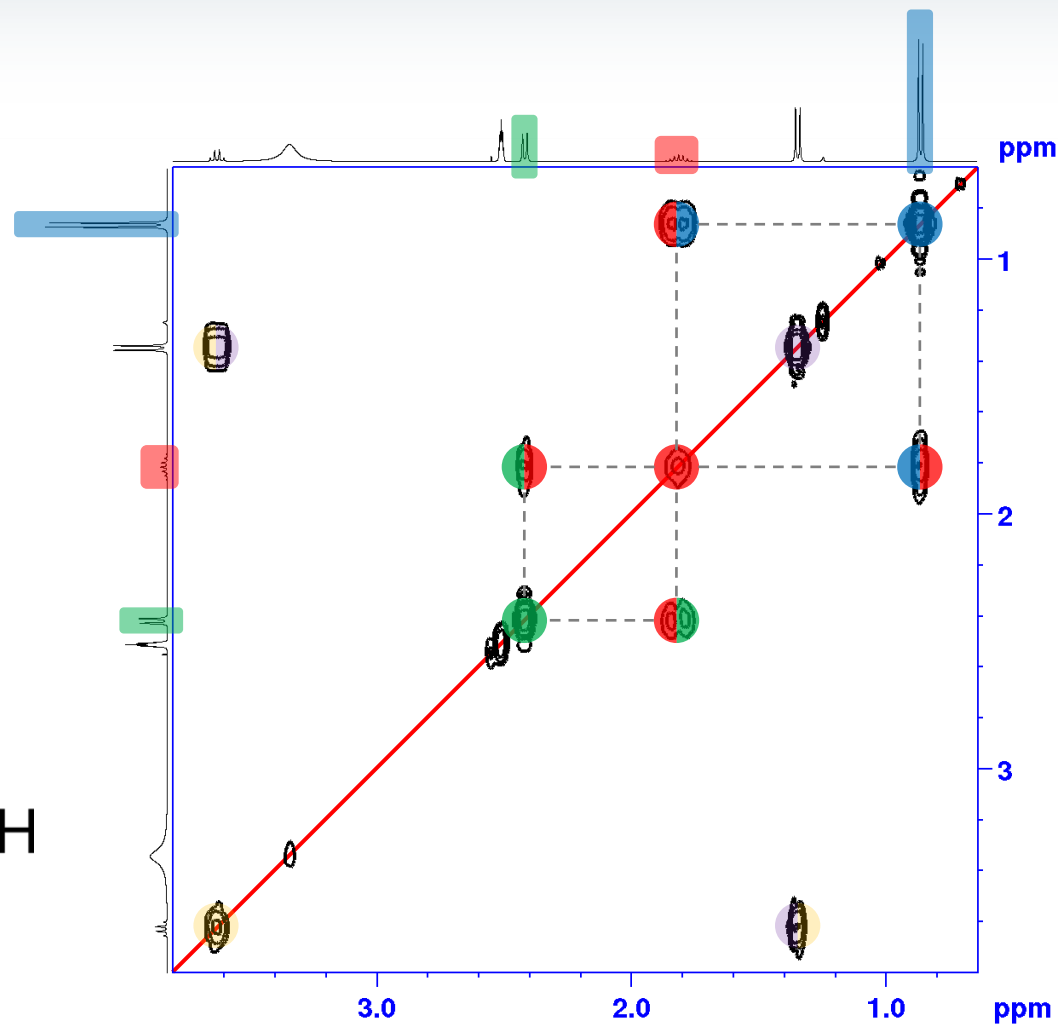
- Off diagonal peaks from coupled spins
- Typically 2J and 3J couplings



COSY COrrrelation Spectroscopy



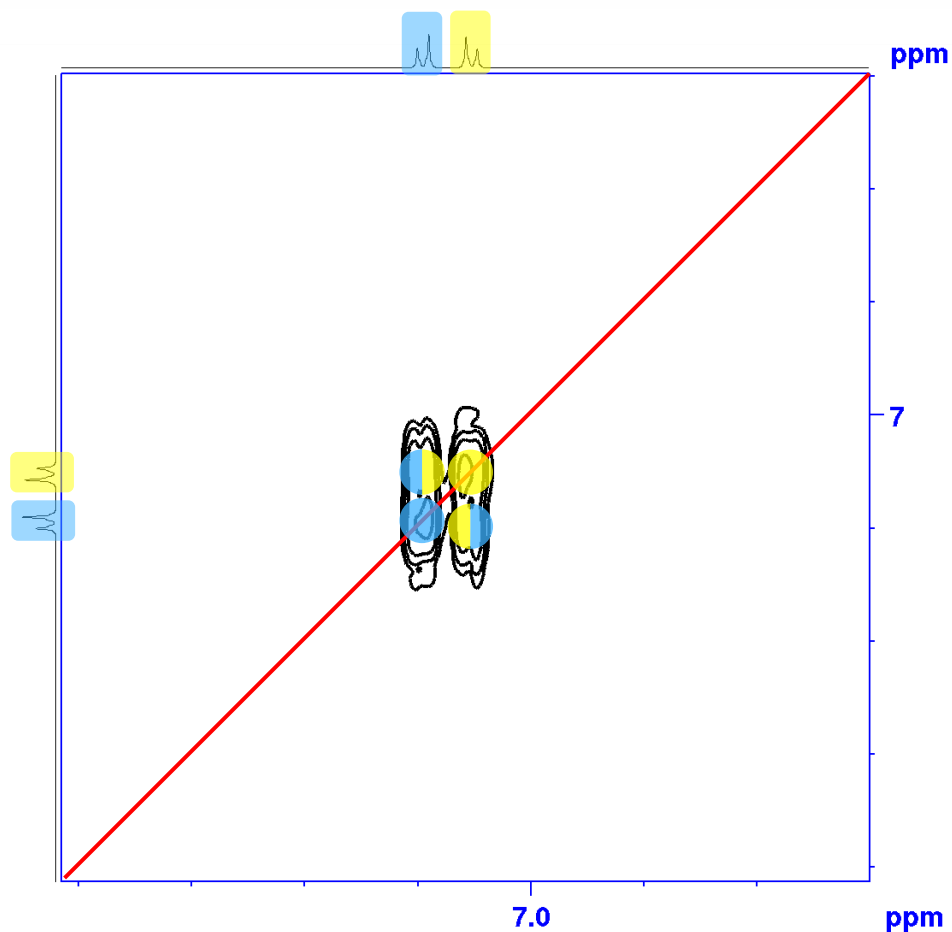
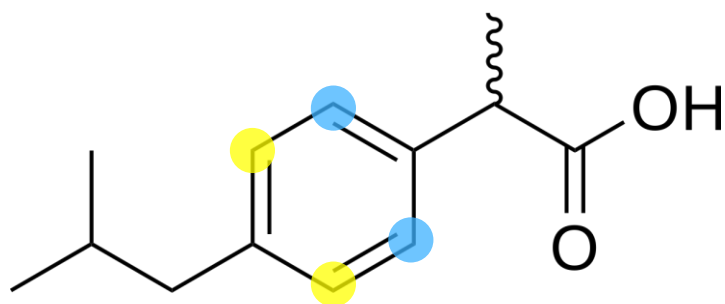
- Off diagonal peaks from coupled spins
- Typically 2J and 3J couplings



COSY COrrrelation Spectroscopy



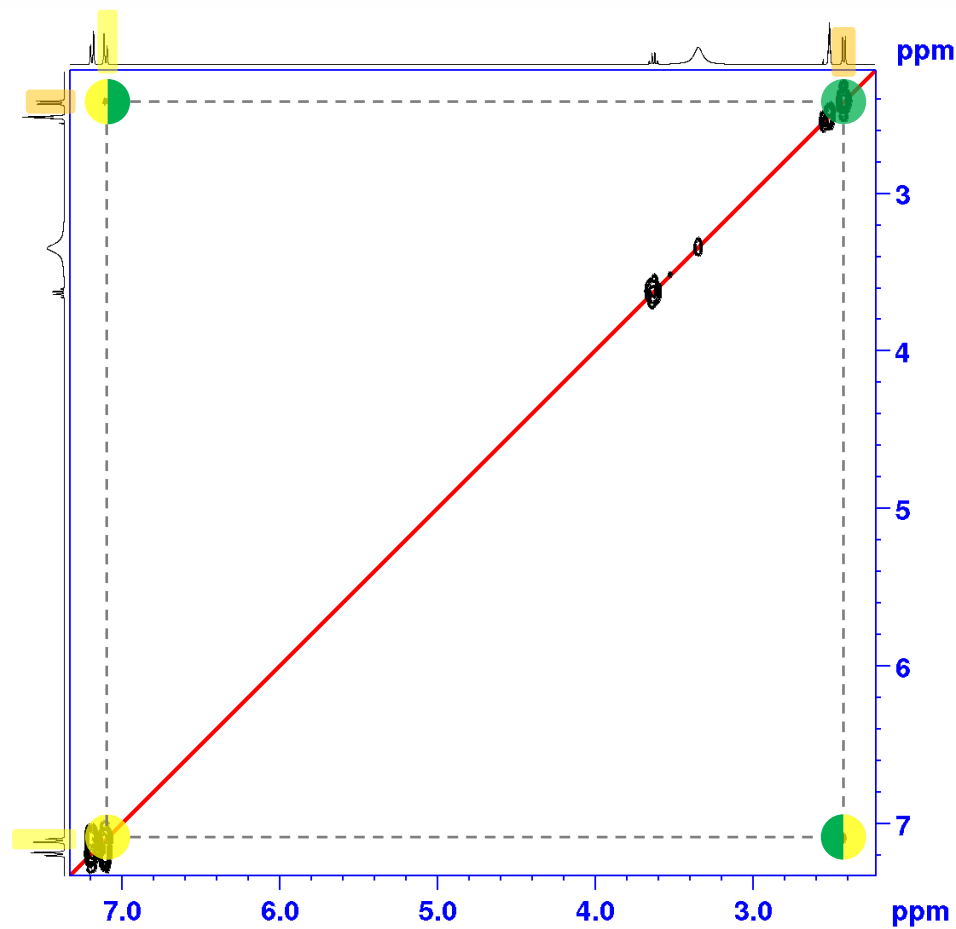
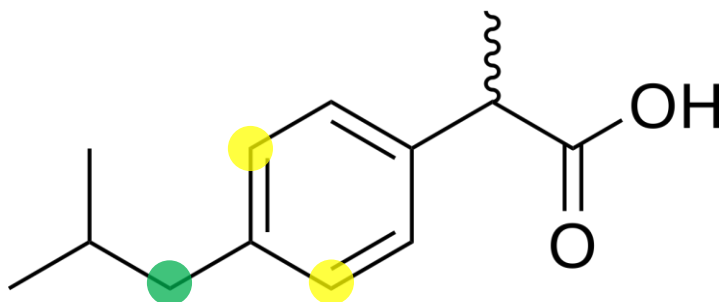
- Off diagonal peaks from coupled spins
- Typically 2J and 3J couplings



COSY CORrelation Spectroscopy



- Off diagonal peaks from coupled spins
- Typically 2J and 3J couplings
- 4J can be visible as well

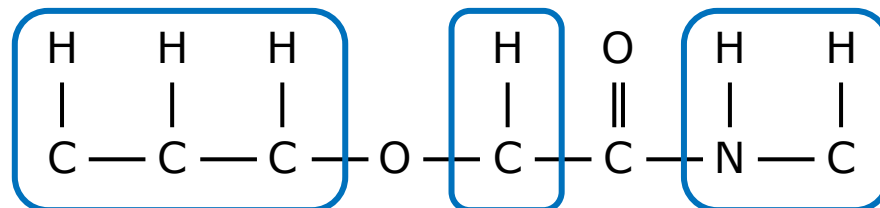


TOCSY

Total **C**orrelation **S**pectroscopy



- Correlation between all spins within one spin system
- Spin system: all spins that are connected via scalar couplings

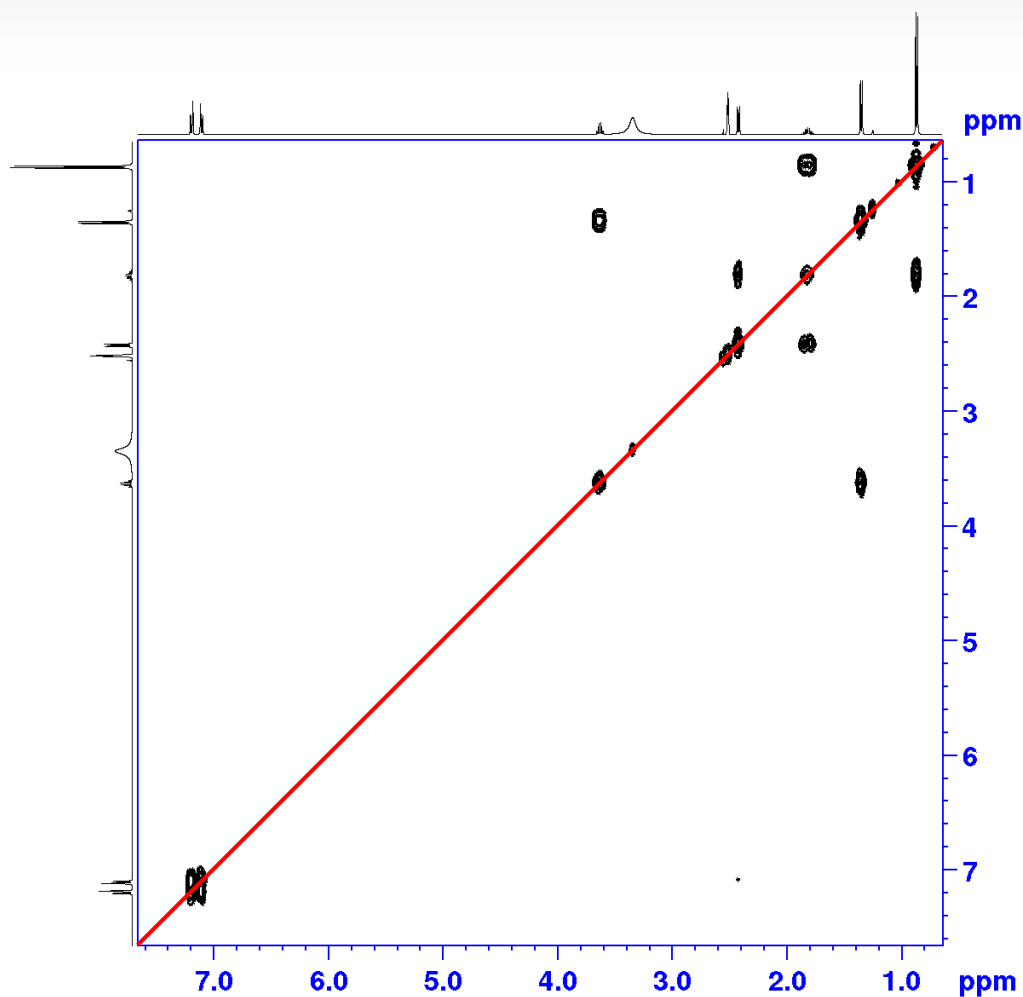
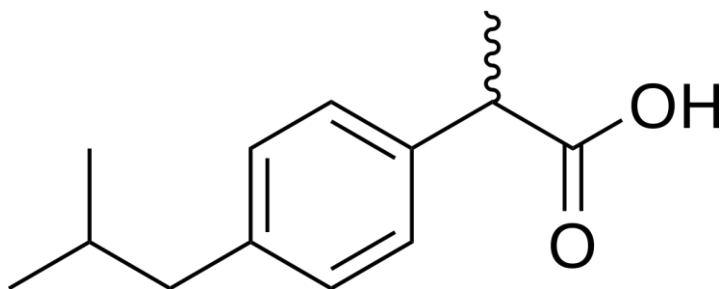


TOCSY

Total **C**orrelation **S**pectroscopy



- Correlation between all spins within one spin system
- Spin system: all spins that are connected via scalar couplings

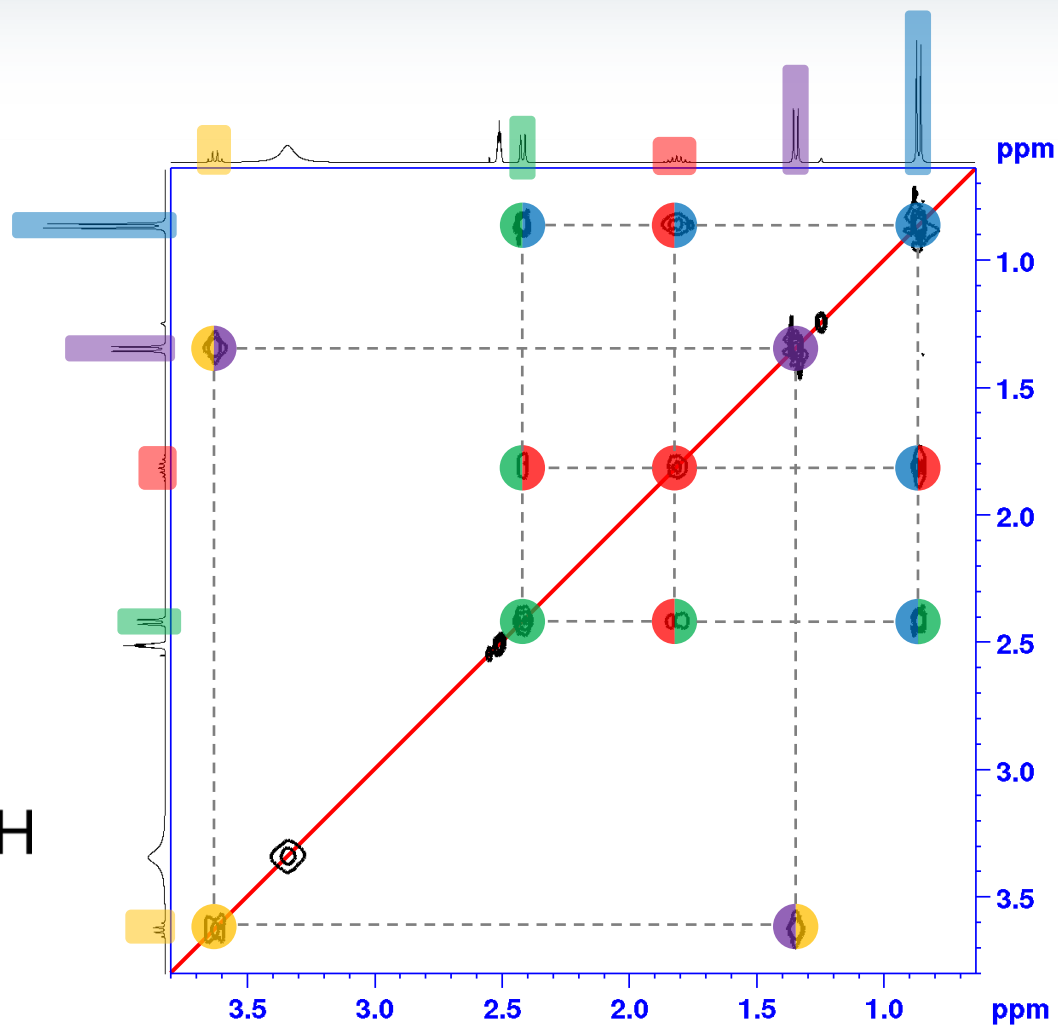
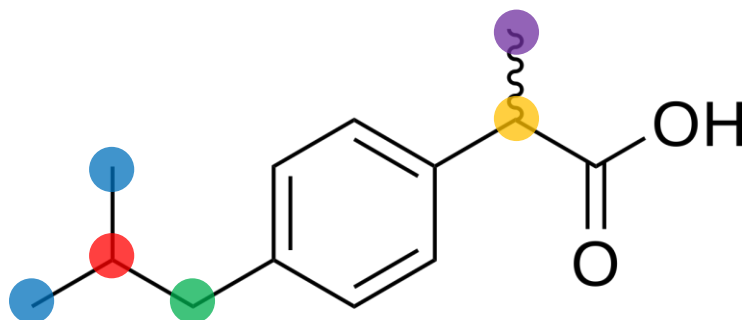


TOCSY

Total **C**orrelation **S**pectroscopy



- Correlation between all spins within one spin system
- Spin system: all spins that are connected via scalar couplings

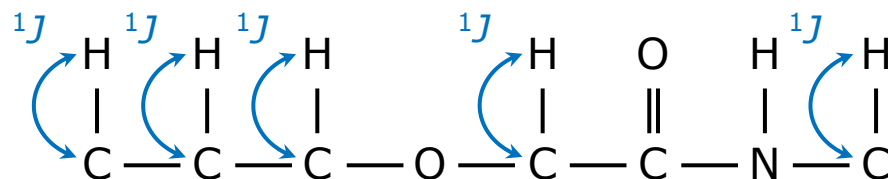


HSQC

Heteronuclear **S**ingle **Q**uantum **C**oherence spectroscopy



- Correlation between protons and directly coupled carbons
- Only carbons with attached protons are visible

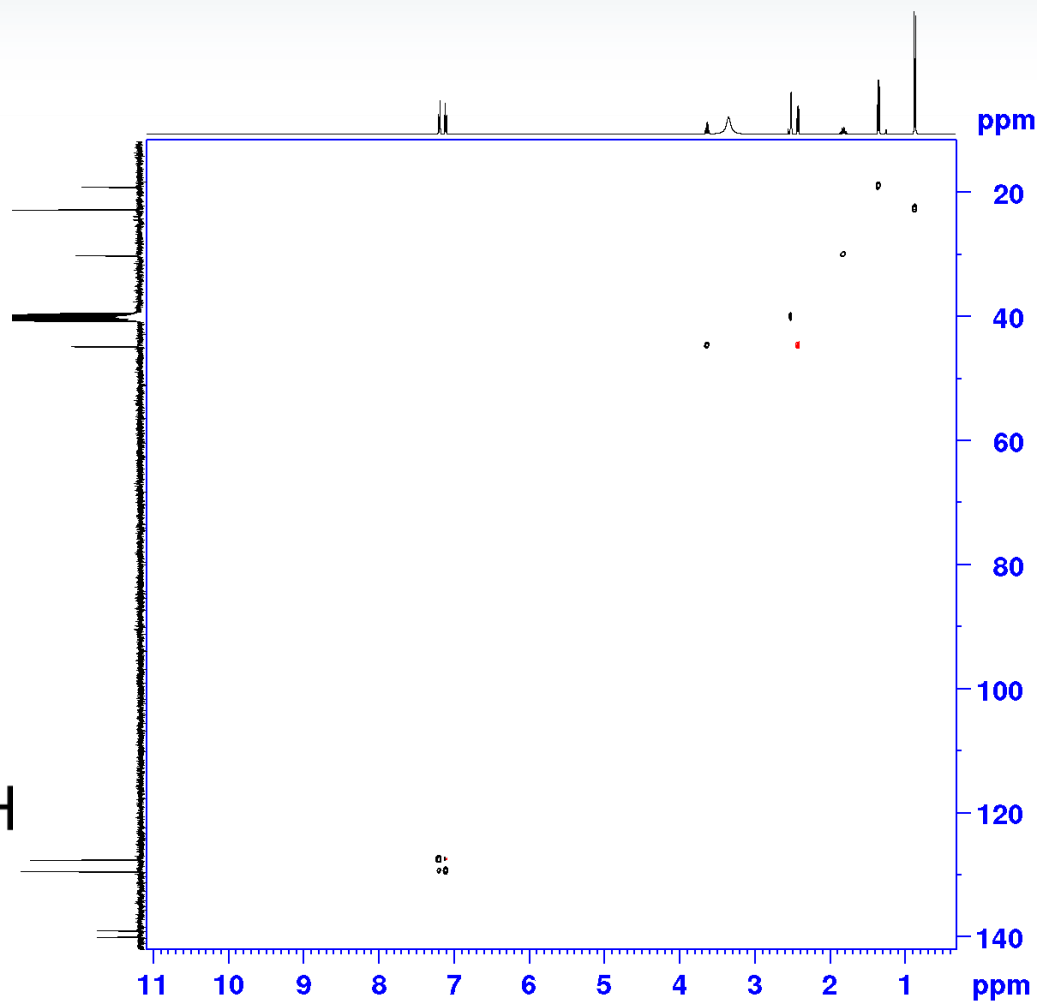
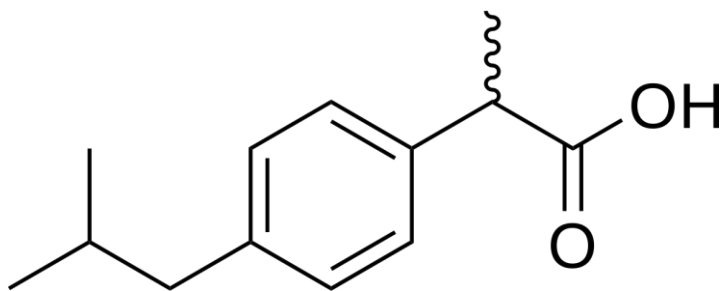


HSQC

Heteronuclear **S**ingle **Q**uantum **C**oherence spectroscopy



- Correlation between protons and directly coupled carbons
- Only carbons with attached protons are visible

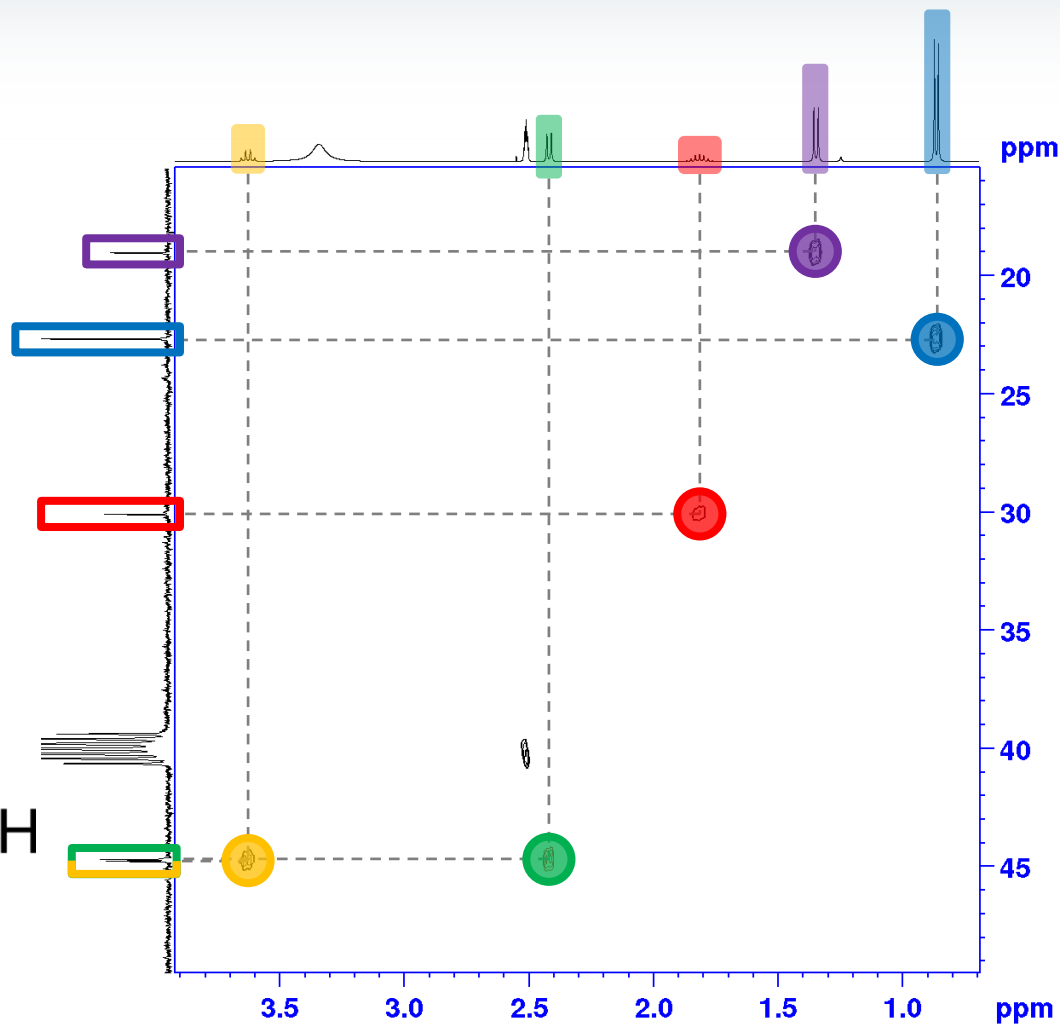
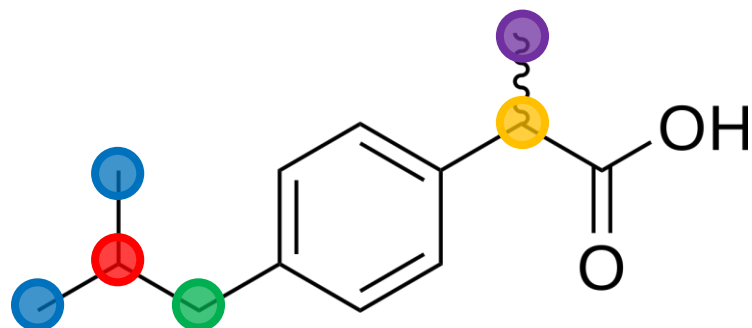


HSQC

Heteronuclear Single Quantum Coherence spectroscopy



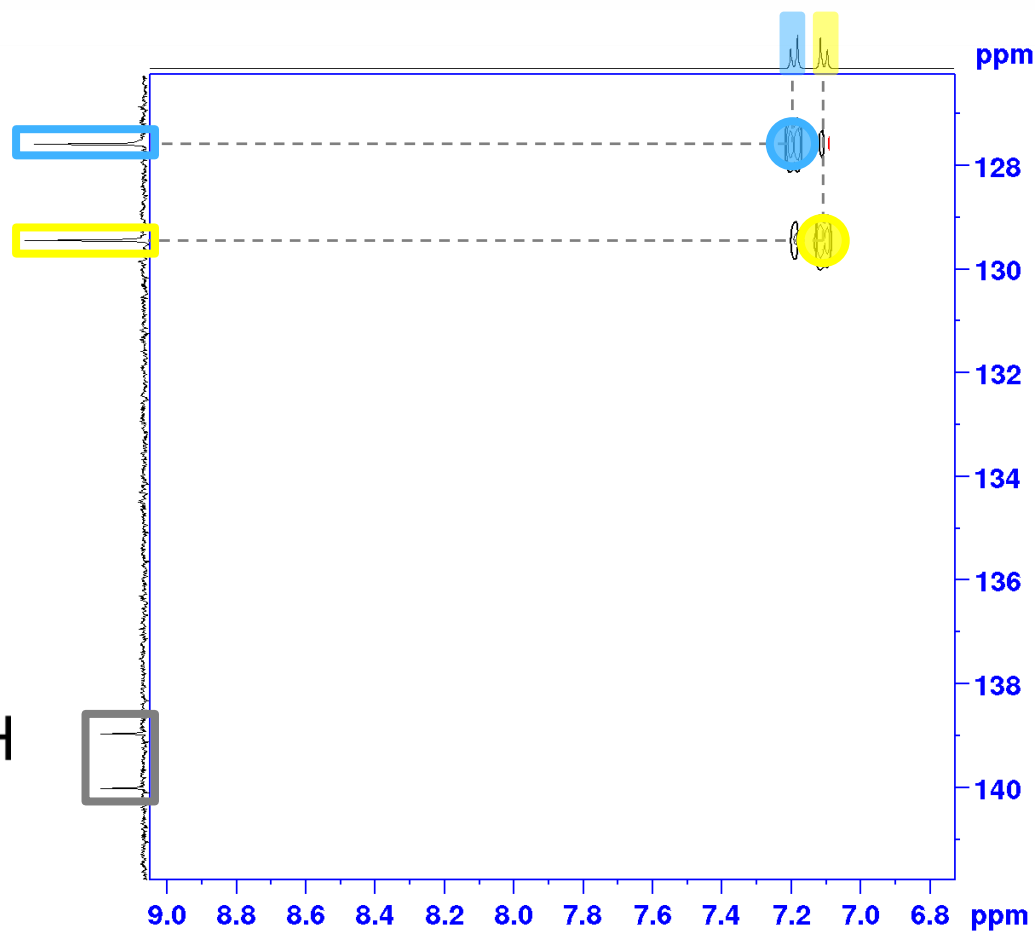
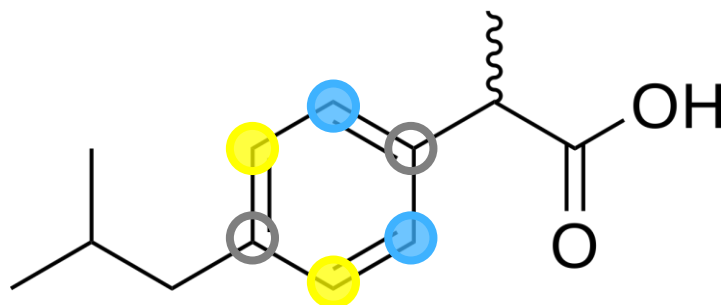
- Correlation between protons and directly coupled carbons
- Only carbons with attached protons are visible



HSQC Heteronuclear **S**ingle **Q**uantum **C**oherence spectroscopy



- Correlation between protons and directly coupled carbons
- Only carbons with attached protons are visible

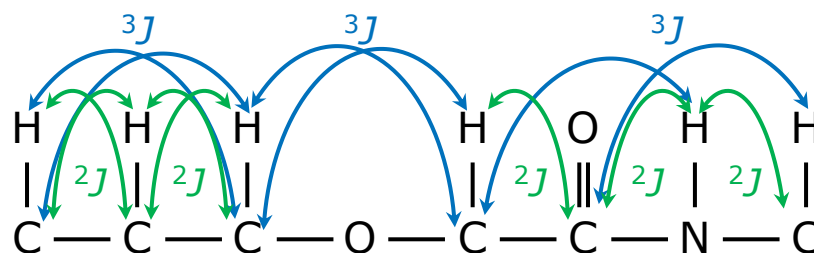


HMBC

Heteronuclear Multiple Bond Correlation spectroscopy



- Correlation between protons and carbons that are two or three bonds away
- Coupling to quaternary carbons possible

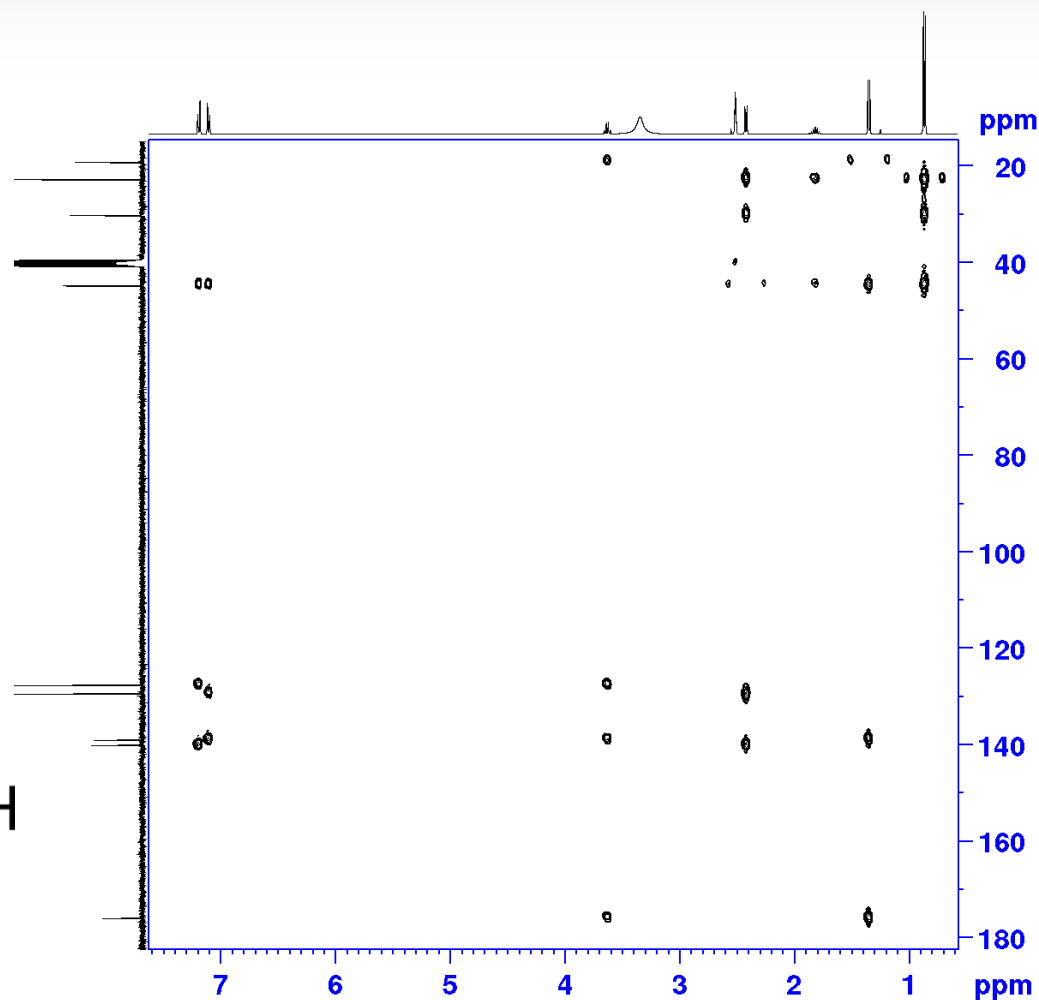
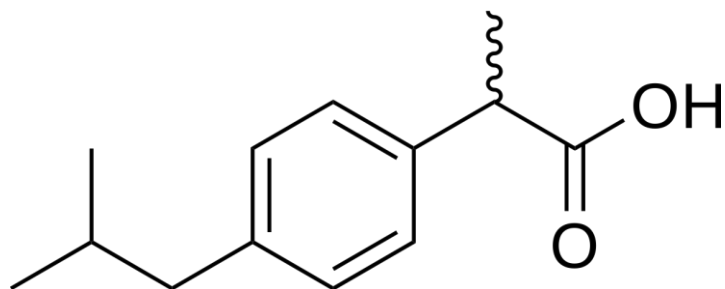


HMBC

Heteronuclear Multiple Bond Correlation spectroscopy

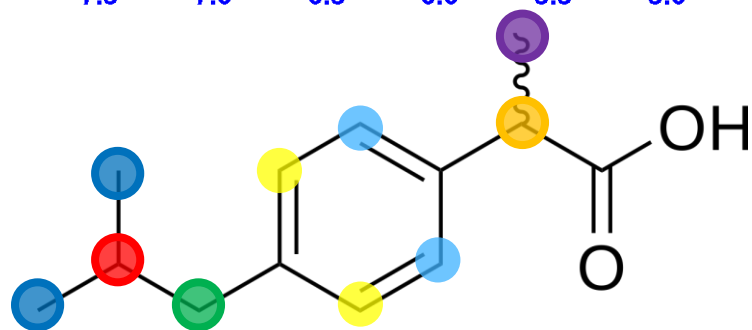
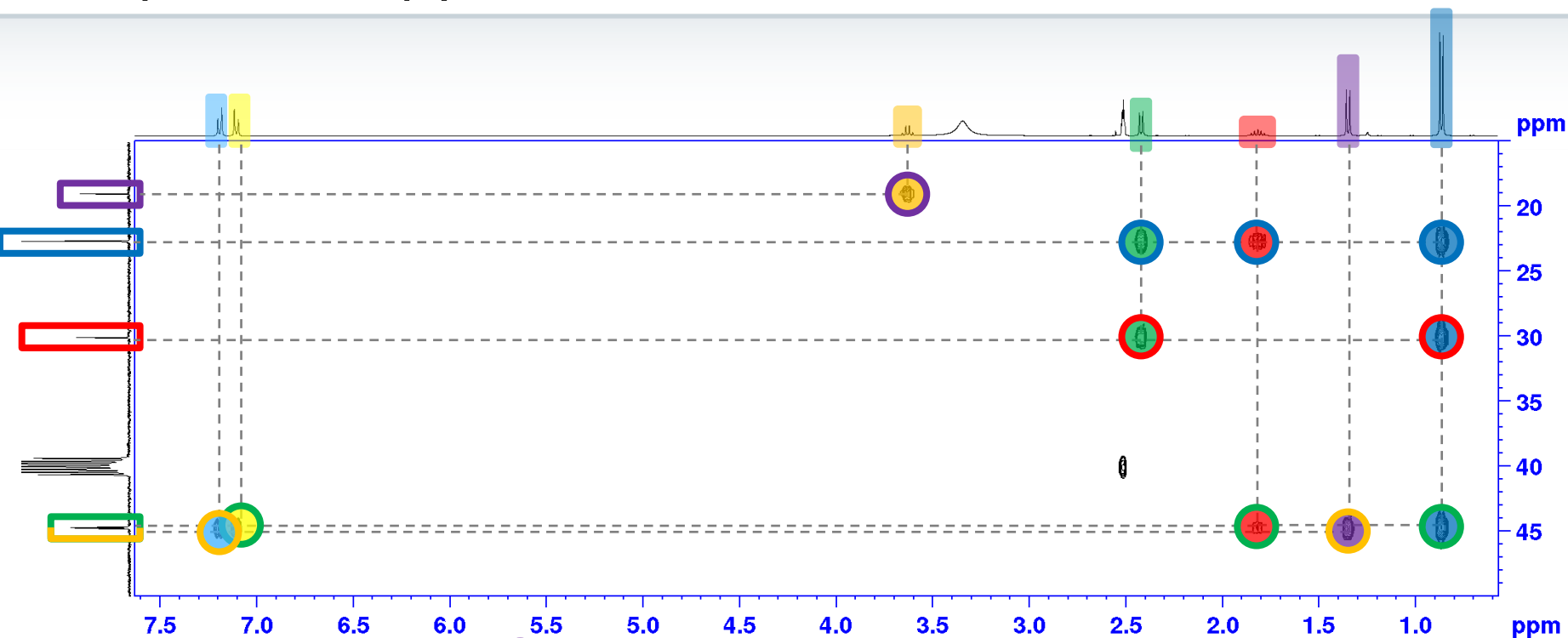


- Correlation between protons and carbons that are two or three bonds away
- Coupling to quaternary carbons possible



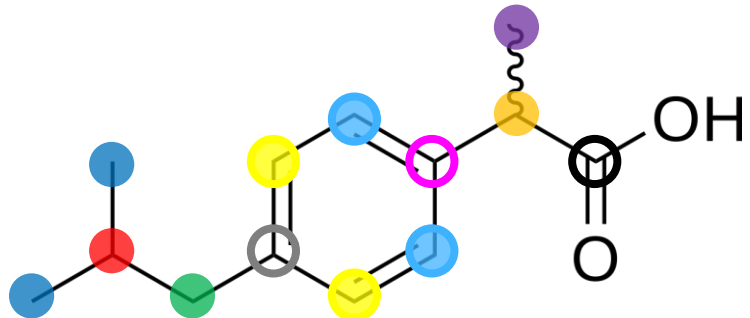
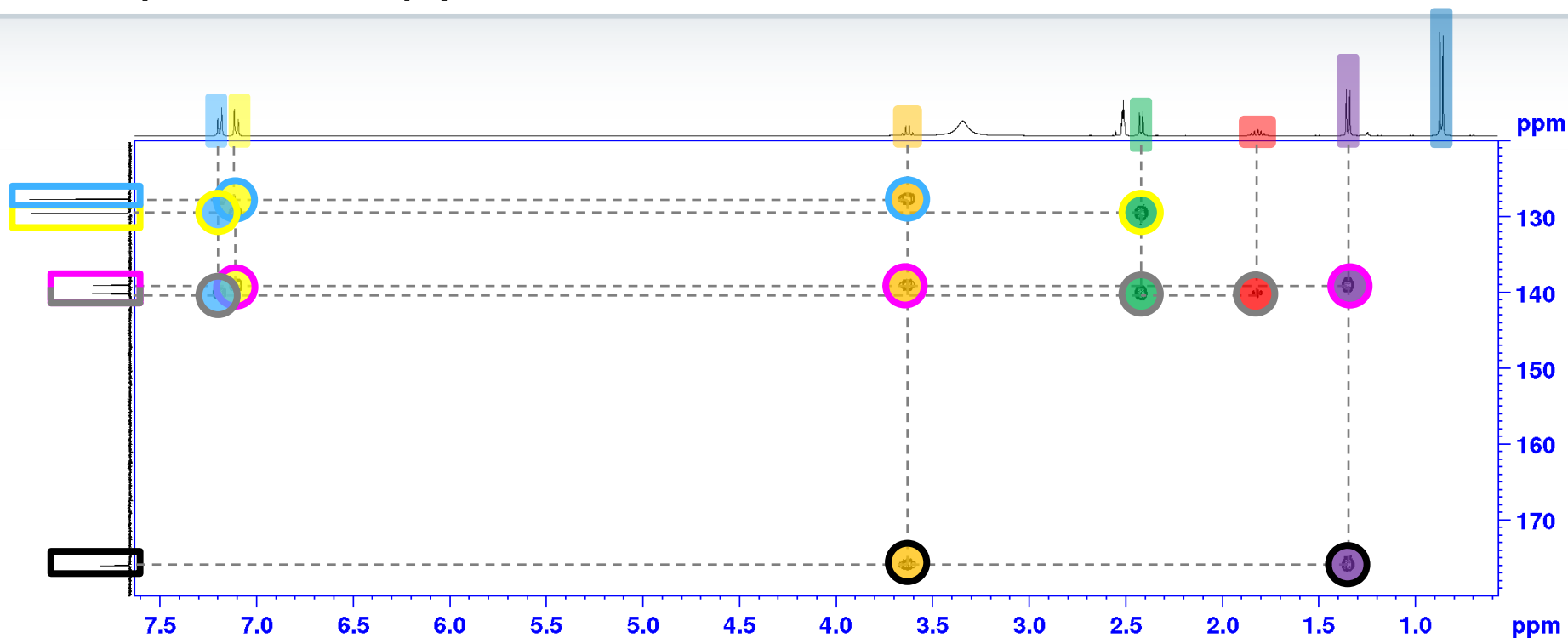
HMBC

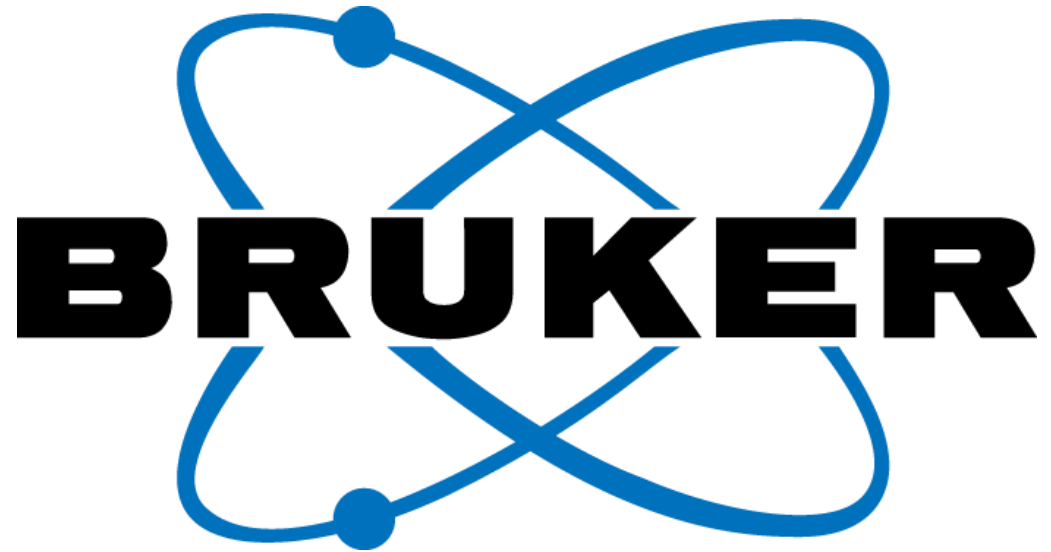
Heteronuclear Multiple Bond Correlation spectroscopy



HMBC

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