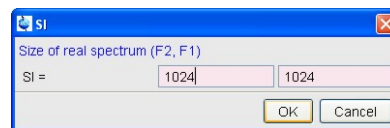


¹H-¹H NOESY Processing Bruker Avance-600 73 & DRX-400 83

on the HP Windows-XP pc computers {73 & 83} Bruker TopSpin © vers. 1.3
Applicable to other Bruker Avance systems also



si



ProcPars

	<u>F2</u>	<u>F1</u>
SI =	1024	1024
SF =	set F1 value equal to F2	
WDW =	QSINE	QSINE
SSB =	2	2
PHCO =	###	90
PHC1 =	###	-180
PH_mod =	pk	pk

Noesy-test 2 1 C:\Bruker\TOPSPIN jas

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

Reference	F2	F1	Frequency axis
Window	1024	1024	Size of real spectrum
Phase	400.1300123	400.1300123	Spectrometer frequency
Baseline	8.760	8.989	Low field limit of spectrum
Fourier	12.32	12.30	Spectrum reference frequency
Peak	3.767602	0.008707	Spectral resolution
Automation	QSINE	QSINE	Window functions for trf, xfb,...
Miscellaneous	0.25	0.98	Line broadening for em
User	0	0.1	Gaussian max. position for gm 0<
	2	2	Sine bell shift SSB (0,1,2,...)
	0	0.1	Left limit for tm 0<TM1<1
	0	0.9	Right limit for tm 0<TM2<1
Phase correction	-130.072	90.000	0th order correction for pk
	-4.800	-180.000	1st order correction for pk
	pk	pk	Phasing modes for trf, xfb, ...

Noesy-test 2 1 C:\Bruker\TOPSPIN jas

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

Reference	ABSG =	5	5	Degree of polynomial for abs (0..5)
Window	ABSF1 [ppm] =	10.000	1000.000	Left limit for absf
Phase	ABSF2 [ppm] =	0.000	-1000.000	Right limit for absf
Baseline	BCFW [ppm] =	1.000	1.000	Filter width for bc (sfil/qfil)
Fourier	COROFFS [Hz] =	0.00	0.00	Correction offset for BC_MOD=spol etc.
Peak	BC_mod =	quad	no	Fid baseline modes for em, ft, xfb,...
Automation	Fourier transform			
Miscellaneous	TDef =	0	0	# of fid data points used by ft
User	STSR =	0	0	First output point of strip transform
	STSI =	0	0	Total # of output points of strip transform
	ME_mod =	no	no	Linear prediction for ft, xfb, ...
	NCOEF =	0	0	# of LP coefficients
	LPBIN =	0	0	# of output points for LP
	TDoff =	0	0	# 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
	FT_mod =	fsc	no	Fourier transform mode for trf, xtrf*
	MC2 =	2F		FT mode 2nd/3rd dim. for no-FnMODE data

	<u>F2</u>	<u>F1</u>
FCOR =	0.5	1

rser 1 99

extract first FID in 2D and write it as EXPNO 99

ProcPars

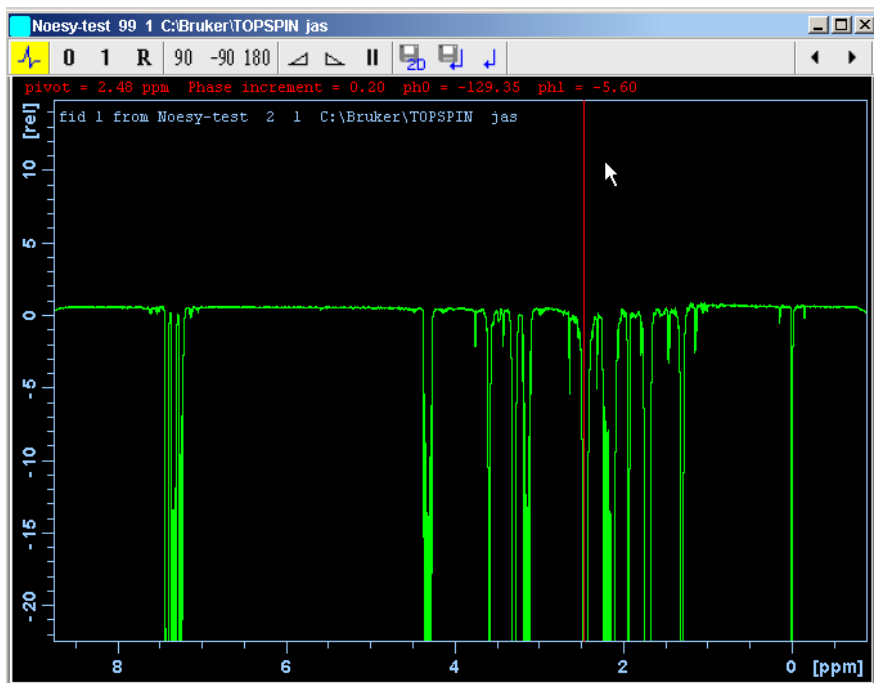
SI = 8192

Parameter	Value	Description
SI	8192	Size of real spectrum
SF [MHz]	400.1300123	Spectrometer frequency
OFFSET [ppm]	8.788	Low field limit of spectrum
SR [Hz]	12.32	Spectrum reference frequency
HZpPT [Hz]	0.470950	Spectral resolution
WDW	QSINE	Window functions for trf, xfb,...
LB [Hz]	0.25	Line broadening for em
GB	0	Gaussian max. position for gm
SSB	2	Sine bell shift SSB (0,1,2,...)
TM1	0	Left limit for tm 0<TM1<1
TM2	0	Right limit for tm 0<TM2<1

qsin

ft

Phase peaks negative



Small Molecule:

Phase peaks negative

**Fast Exchange Molecule:
Peptides:**

Phase peaks positive

ProcPars

Parameter	Value
PHC0 [degree]	-129.351
PHC1 [degree]	-5.600
PH_mod	pk

re 2

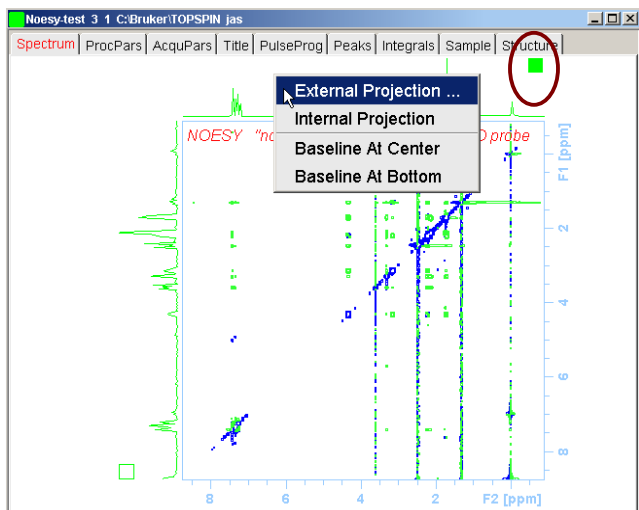
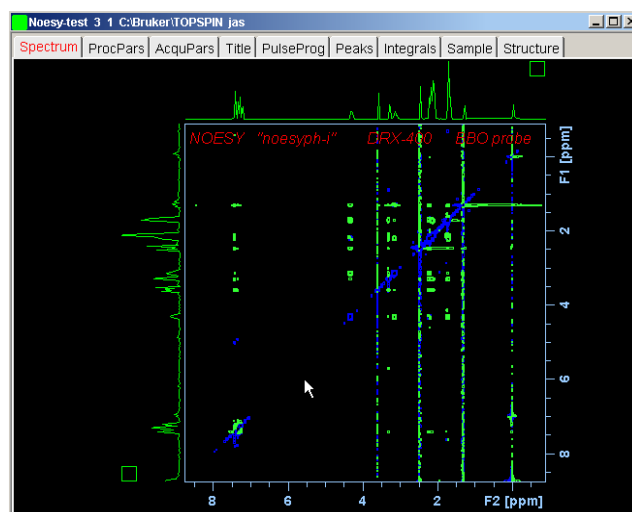
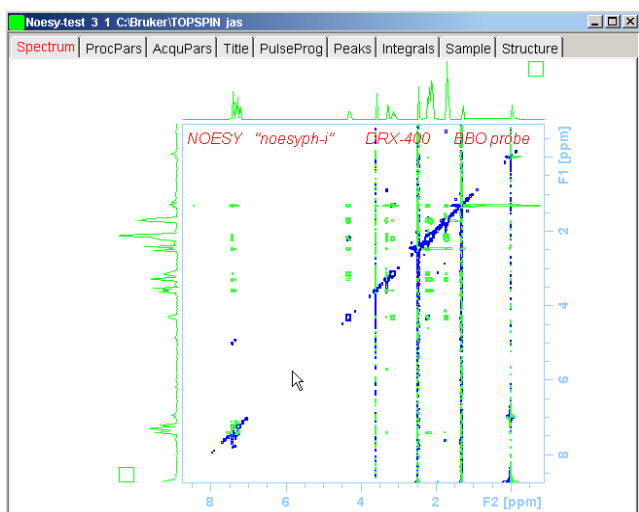
or click on window for 2

2D

ProcPars

Phase correction	
PHC0 [degree] =	-129.351 90.000
PHC1 [degree] =	-5.600 -180.000
PH_mod =	pk pk
Baseline correction	

xfb



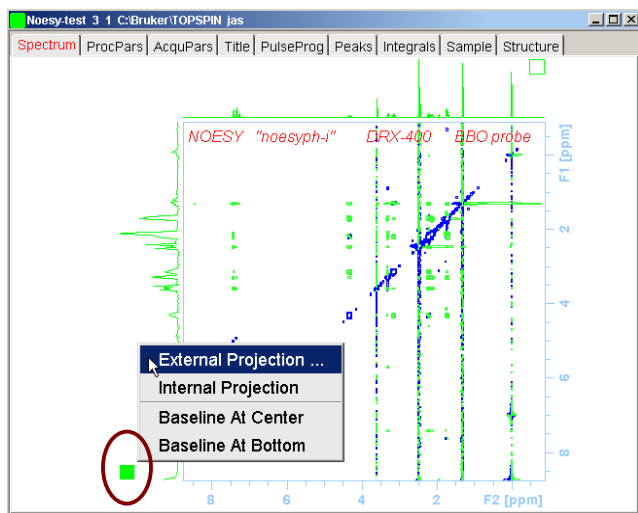
Data set for F2 projection

Options

Display data in same window
 Display data in new window

NAME = Noesy-test
EXPNO = 1
PROCNO = 1
DIR = C:\Bruker\TOPSPIN
USER = jas

OK Cancel Browse Find... Help




1	24220.0	-24220.0
2	33908.0	-33908.0
3	47471.2	-47471.2
4	66459.7	-66459.7
5	93043.6	-93043.6
6	130261.0	-130261.0
7	182365.4	-182365.4
8	255311.5	-255311.5
9	357436.1	-357436.1
10	500410.6	-500410.6

	Positive	Negative
Base level	24220.0	-24220.0
Level increment	1.4	1.4
Number of levels		35

1. Contour level sign
2. Level increment
3. Number of levels
4. Fill
5. Apply
6. OK

