

## 1D PSYCHE:

Generate a new 2D experiment and proceed as follows. In the acquisition parameter set, by typing *eda*, set the acquisition parameters. The pulse sequence should be stored in the main directory of topspin program, under:

*~TopSpin.xplx/exp/stan/nmr/lists/pp/user*

Experiment			
PULPROG	UoM_1d_if_psyche_ts4x	Pulse sequence	
AQ_mod	DQD	Acquisition mode	
FnTYPE	traditional(planes)	nD acquisition mode for 3D etc.	
FnMODE	QF	Acquisition mode for 2D. 3D etc.	
TD	32768	20	Number of chunks
DS	2		Number of dummy scans
NS	2		Number of scans
TD0	1		Loop count for 'td0'
TDav	0		Average loop counter for nD experiments
Width			
SW [ppm]	19.9947	0.1000	
SWH [Hz]	10000.000	50.000	Spectral window ( $1/\tau_{\text{chunk}}$ )
IN_F [ $\mu\text{sec}$ ]		20000.00	Chunk duration ( $\tau_{\text{chunk}}$ )
AQ [sec]	1.6384000	0.2000000	Acquisition time
FIDRES [Hz]	0.610352	5.000000	Fid resolution
FW [Hz]	4032000.000		Filter width

Set DIGMOD to *baseopt*.

DSPFIRM	rectangle	DSP firmware filter
DIGTYP	DRX	Digitizer type
DIGMOD	baseopt	Digitization mode
DR	32	Digitizer resolution
DDR	0	Digital digitizer resolution

Type *ased* in the topspin command-line and set the rest of pulse sequence dependent parameters. Set drop-points and gradient recovery delay. Use at least 1 ms for the gradient recovery delay. (*d16*)

PULPROG	UoM_1d_if_psyche_ts4x	...	E	Pulse program for acquisition
TD	32768			Time domain size
SWH [Hz, ppm]	10000.00	19.9947		Sweep width
AQ [sec]	1.6384000			Acquisition time
RG	32			Receiver gain
DW [μsec]	50.000			Dwell time
DE [μsec]	6.50			Pre-scan-delay
CNST4	4.0000000			Number of drop points
D0 [sec]	0			Incremented delay
D1 [sec]	2.000000000			Relaxation delay
D16 [sec]	0.001000000			Recovery delay for gradients
DS	2			Number of dummy scans
in0 [sec]	0.01000000			1/(2 * SW) = DW
INF1 [μsec]	20000.00			Increment for F1

The parameters set so far are common in all 1D interferogram experiments (BIRD, ZS, BS, and PSYCHE). The followings are specific to the PSYCHE experiment.

Set the appropriate flip angle and the bandwidth (according to the waveform) for the PSYCHE pulse element. The pulse sequence uses these parameters to calculate the corresponding r.f. amplitude of the pulse.

SFO1 [MHz]	500.1325006		Frequency of ch. 1	PSYCHE pulse parameters
O1 [Hz, ppm]	2500.65	5.000	Frequency of ch. 1	
NUC1	1H	Edit...	Nucleus for channel 1	
CNST20	15.0000000		Desired flip angle for PSYCHE pulse element (degree) (normally 10-25)	
CNST21	10000.0000000		Bandwidth of each chirp in PSYCHE pulse element (Hz) (normally 10000)	
cnst31	270000.000000		cnst31= (p30/p1) * (p30/p1)	
cnst50	48.112522		cnst50=(cnst20/360)*sqrt((2*cnst21)/(p40/2000000))	

Set the PSYCHE pulse shape and its duration. The rf power will be calculated automatically based on the parameters bandwidth, flip angle, and the pulse duration. The wave should be stored in the main directory of topspin program, under: *~TopSpin.xpl/x/exp/stan/nmr/lists/wave/user*

P40 [μsec]	30000.000		Duration of double-chirp PSYCHE pulse element	
PLW0 [W, dB]	0	1000.00	Zero power (120 dB)	
PLW1 [W, dB]	25.267	-14.03	High power (dB)	
SPNAM 40	PSYCHE_Saltire_10kHz_30m	...	E	File name for PSYCHE pulse element
SPOAL40	0.500			Phase alignment of freq. offset in SP40
SPOFFS40 [Hz]	0			Offset frequency for SP40
spw40 [W, -dBW]	9.3581e-05	40.29		RF power of double-chirp PSYCHE pulse element

Set the gradient shapes and amplitudes for PSYCHE and CTP selection.

GPNAM 1	SINE.100	...	E	SINE.100	
GPZ1 [%]	77.00			CTP gradient (77%)	CTP selection
GPNAM 2	SINE.100	...	E	SINE.100	
GPZ2 [%]	49.00			CTP gradient (49%)	
GPNAM 10	RECT.1	...	E	RECT.1	
GPZ10 [%]	3.00			Weak gradient during PSYCHE element (1-3%)	
p10 [μsec]	30000.00			Duration of weak gradient during PSYCHE pulse element	
P16 [μsec]	1000.000			Duration of CTP gradients (1m)	

## 1D TSE-PSYCHE:

The general setup of 1D TSE-PSYCHE is the same as 1D PSYCHE, but two more chirp pulses and two more weak gradients are needed.

PULPROG	UoM_1d_if_tsepsyche_ts4x	...	E	Pulse sequence
AQ_mod	DQD			Acquisition mode
FnTYPE	traditional(planes)			nD acquisition mode for 3D etc.
FnMODE		QF		Acquisition mode for 2D, 3D etc.
TD	32768	20		Size of fid <b>Number of chunks</b>
DS	2			Number of dummy scans
NS	2			Number of scans
TD0	1			Loop count for 'td0'
TDav	0			Average loop counter for nD experiments
Width				
SW [ppm]	19.9947	0.1000		Spectral width
SWH [Hz]	10000.000	50.000		Spectral window ( $1/\tau_{\text{chunk}}$ )
IN_F [μsec]		20000.00		Chunk duration ( $\tau_{\text{chunk}}$ )
AQ [sec]	1.6384000	0.2000000		Acquisition time
FIDRES [Hz]	0.610352	5.000000		Fid resolution
FW [Hz]	240000000.000			Filter width

Set the appropriate flip angle and the bandwidth (according to the waveform) for the PSYCHE pulse element. The pulse sequence uses these parameters to calculate the corresponding r.f. amplitude of the pulse. Set the r.f. amplitude for the 180-degree chirp pulses. This information can be found in the name of the shape.

CNST20	15.0000000	Desired flip angle for PSYCHE pulse element (degree) (normally 10-25)
CNST21	10000.0000000	Bandwidth of each chirp in PSYCHE pulse element (Hz) (normally 10000)
cnst31	270000.000000	cnst31= (p30/p1) * (p30/p1)
cnst32	3127.987305	cnst32= (p31/p1) * (p31/p1)
cnst50	48.112522	cnst50=(cnst20/360)*sqrt((2*cnst21)/(p40/2000000))
CNST51	447.0000000	RF amplitude for 180-degree chirp pulses (Hz)

Set the PSYCHE pulse shape and two 180-degree chirps and their durations. The rf power will be calculated automatically based on the parameters bandwidth, flip angle, and the pulse duration for PSYCHE pulse, and based on the pulse duration and the provided r.f. amplitude for the 180-degree chirps. All waves should be stored in the main directory of topspin program, under `~TopSpin.xplx/exp/stan/nmr/lists/wave/user`

P40 [μsec]	30000.000		Duration of double-chirp PSYCHE pulse element
P41 [μsec]	40000.000		Duration of 1st 180-degree swept-frequency pulse
P42 [μsec]	40000.000		Duration of 2nd 180-degree swept-frequency pulse
PLW0 [W, dB]	0	1000.00	Zero power
PLW1 [W, dB]	25.267	-14.03	High power
SPNAM 40	PSYCHE_Saltire_10kHz_30m	... E	File name for PSYCHE pulse element
SPOAL40	0.500		Phase alignment of freq. offset in SP40
SPOFFS40 [Hz]	0		Offset frequency for SP40
spw40 [W, -dBW]	9.3581e-05	40.29	RF power of double-chirp PSYCHE pulse element
SPNAM 41	Chirp10kHz40m20s447Hz10000LH	... E	File name for 1st 180-degree swept-frequency pulse
SPOAL41	0.500		Phase alignment of freq. offset in SP41
SPOFFS41 [Hz]	0		Offset frequency for SP41
spw41 [W, -dBW]	0.0080777	20.93	RF power of 1st 180-degree swept-frequency pulse
SPNAM 42	Chirp10kHz40m20s447Hz10000HL	... E	File name for 2nd 180-degree swept-frequency pulse
SPOAL42	0.500		Phase alignment of freq. offset in SP42
SPOFFS42 [Hz]	0		Offset frequency for SP42
spw42 [W, -dBW]	0.0080777	20.93	RF power of 2nd 180-degree swept-frequency pulse

Set the gradient shapes and amplitudes for PSYCHE and CTP selection.

GPNAM 1	SINE.100	... E	SINE.100	CTP selection
GPZ1 [%]	35.00		CTP gradient (35%)	
GPNAM 2	SINE.100	... E	SINE.100	
GPZ2 [%]	49.00		CTP gradient (49%)	CTP selection
GPNAM 3	SINE.100	... E	SINE.100	
GPZ3 [%]	77.00		CTP gradient (77%)	
GPNAM 10	RECT.1	... E	RECT.1	CTP selection
GPZ10 [%]	3.00		Weak gradient during PSYCHE element (1-3%)	
GPNAM 11	RECT.1	... E	RECT.1	
GPZ11 [%]	2.00		Weak gradient during 1st 180-degree chirp (1-3%)	CTP selection
GPNAM 12	RECT.1	... E	RECT.1	
GPZ12 [%]	2.00		Weak gradient during 2nd 180-degree chirp (1-3%)	
P16 [μsec]	1000.000		Duration of CTP gradients (1m)	

## Covariance processing for $F_1$ PSYCHE-TOCSY:

In the topspin command-line type *covariance man* and proceed as follows.

