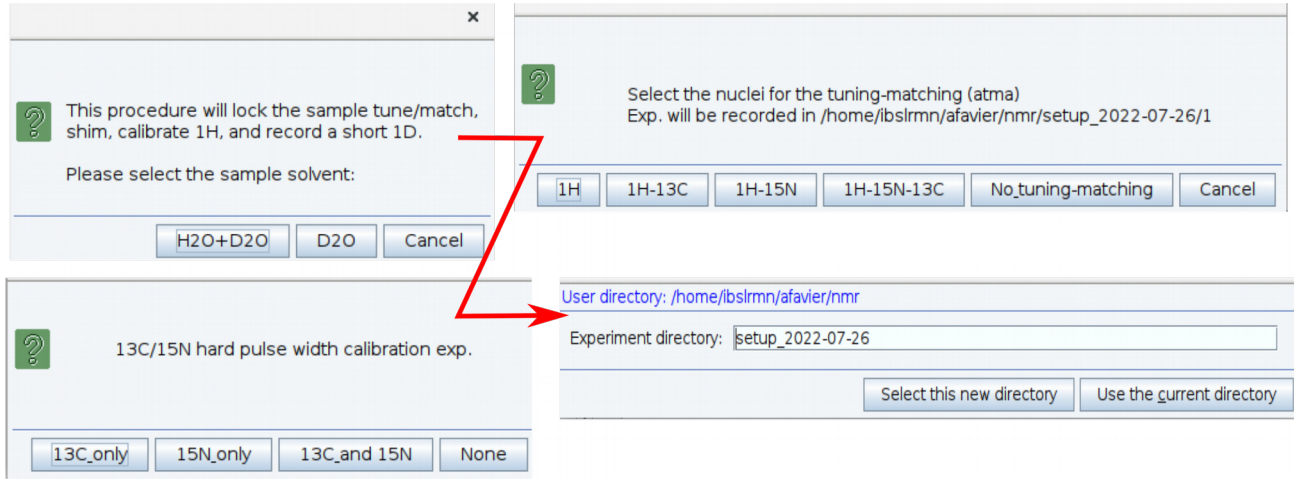
NMRlib for liquids

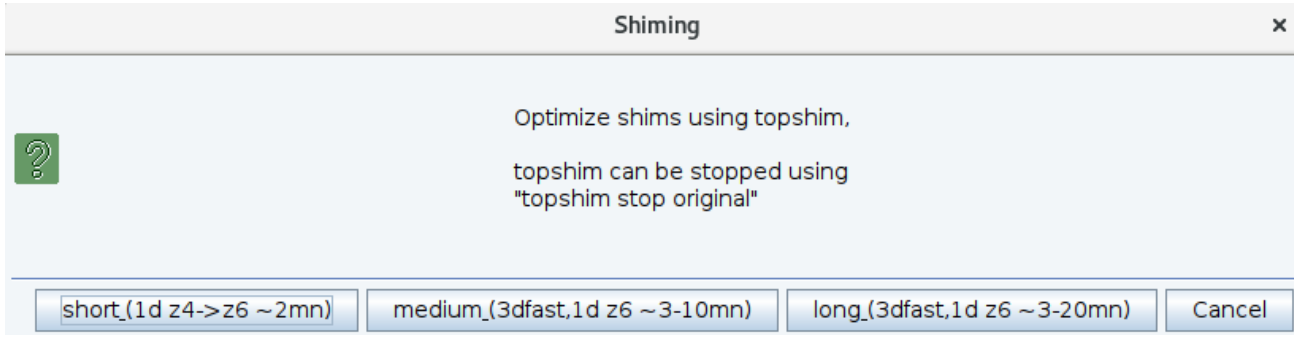
Proteins

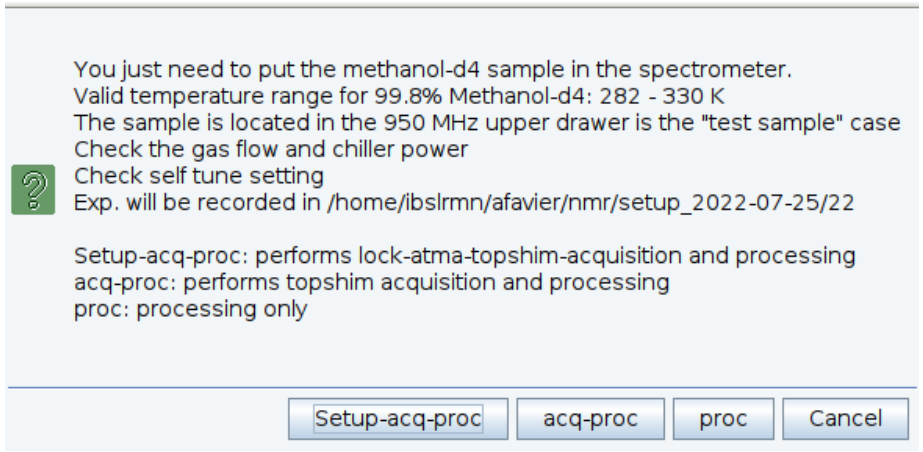
Spectrometer setup liquids

Experiments	Comments
Setup	lock Tune shim (1H-13C-15N) pulse calibration
Stop setup run	Allows to stop setup experiments



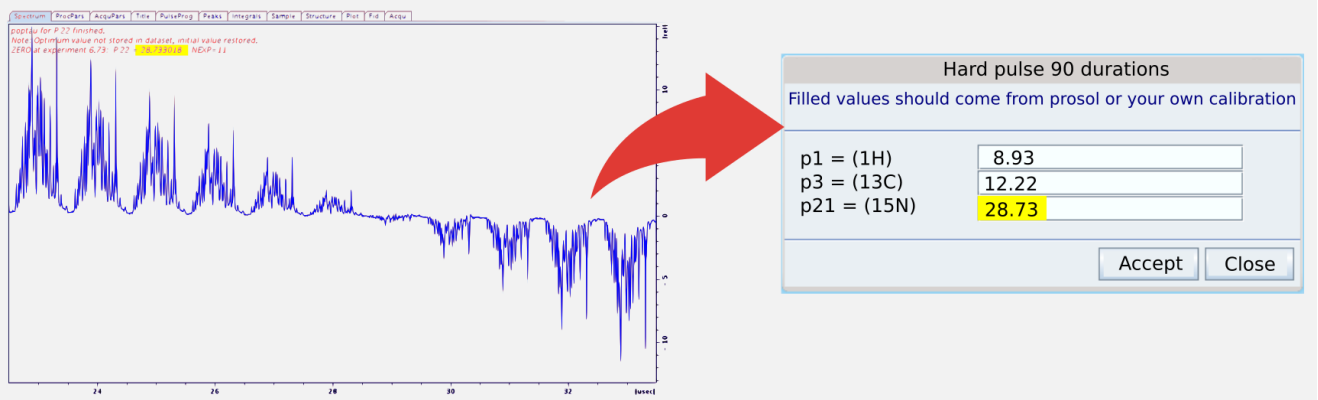
Experiments	Comments
Optimize shims	run different flavours of topshim
Check Shims	Measure the deuterium line width
Check Temperature	Requires a standart thermometer sample Me-d6



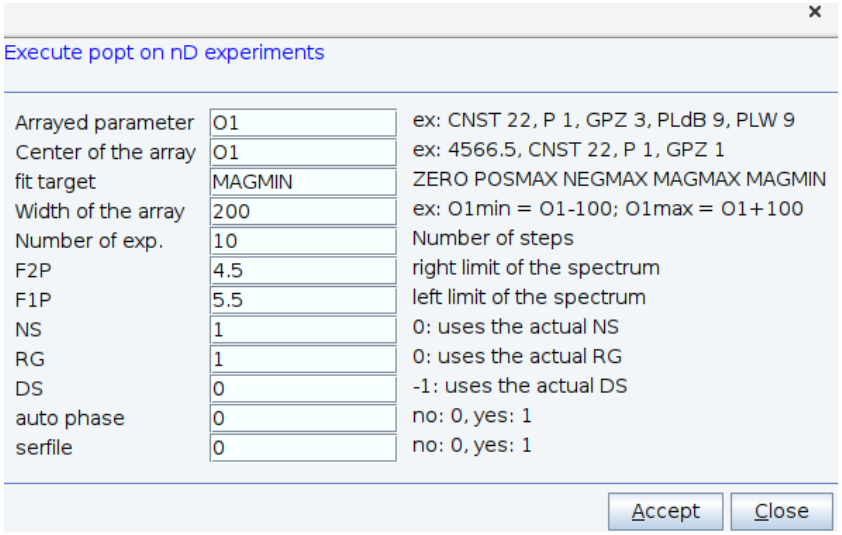


Calibration liquids

Experiments	Comments
1H pulse calibration	Bruker pulsecal tool (p1)
13C pulse calibration	SOFAST based (p3)
15N pulse calibration	SOFAST based (p21)
O1 calibration (using popt)	varying O1 using popt on presat



Experiments	Comments
nD popt	varying a parameter in nD expt



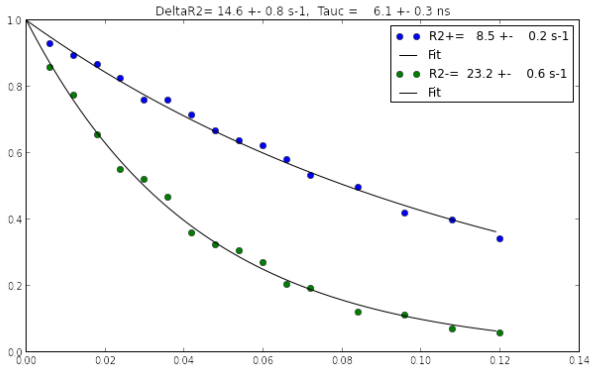
QualityControl liquids

Experiments	Comments
15N TRACT 1D	Estimation of tumbling correlation time

1 Ubiquitin

```
: 1  libLoc = '/hosts/ibs1300/nmrdata/nmrlib/'
  2  filename1 = '/hosts/ibs700/ibslrmn/afavier/nmr/2019-02-04_ubi-S43/15/pdata/1'
  3  filename2 = '/hosts/ibs700/ibslrmn/afavier/nmr/2019-02-04_ubi-S43/16/pdata/1'
  4  vclist_file_nl = '/hosts/ibs700/ibslrmn/afavier/nmr/2019-02-04_ubi-S43/15/vclist'
  5  vclist_file_bl = '/hosts/ibs700/ibslrmn/afavier/nmr/2019-02-04_ubi-S43/16/vclist'
  6  d21 = 0.003
  7  min_val = 9.5
  8  max_val = 8.6
  9
```

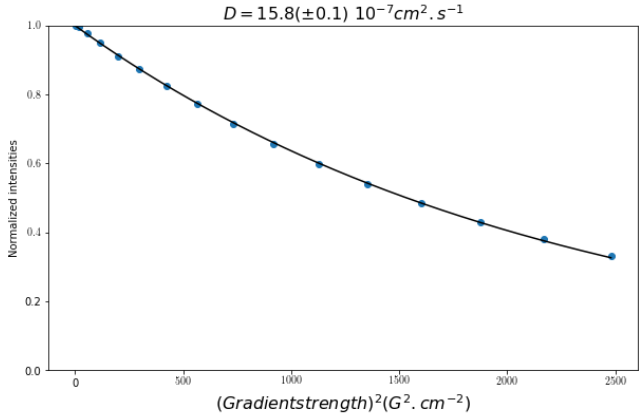
```
: 1  tractAna(filename1, filename2, vclist_file_nl, vclist_file_nl, d21, min_val, max_val )
```



Analysis tool provided

sel 1H DOSY	1H region selected with selective pulse, e.g. methyls
13C-filt 1H DOSY	13C filter for methyl 1H

Experiments	Comments	

15N-filt 1H DOSY	15N filter for amide 1H	**2 Ubiquitin**
		`libLoc = '/hosts/ibs1300/nmrdata/nmrlib/'`
		`filename1 = '/hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/pdata/1'`
		`difflist_file = '/hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/difflist'`
		`min_val = 2`
		`max_val = -1.0`
		`dosyAna(libLoc, filename1, difflist_file, min_val, max_val)`
		`Max: 10581648.267089844`
		`Diffusion fitting values saved in: /hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/pdata/1/DOSY.fit`
		`Normalized intensities saved in: /hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/pdata/1/DOSY.int`
		 
		
		Analysis tool provided

1D HETSOFAST	Global structural compactness	*Analysis tool provided*
2D HETSOFAST	Local structural compactness	
HAD SOFAST amides	1D SOFAST with additional 15N filter	*Analysis tool provided*

Experiments	Comments
ERETIC	Quantitative 1D NMR for concentration measurement

ProtonNMR

Experiments	Comments
1H PRESAT	1D with water presaturation
1D SCULPTING	1D using excit. sculpting for water suppression
1D SCULPTING with 15N/13C dec	1D with 13C/15N decoupling
2D TOCSY	with 13C and 15N decoupling option
	DIPSI mixing / Excitation Sculpting
2D NOESY	with 13C and/or 15N decoupling option
	and Excitation Sculpting

Hetero2D

Experiments	Comments
AMIDES	2D 1H-15N

Experiments	Comments
ALIPHATICS	2D 1H-13C
AROMATICS	2D 1H-13C
METHYLS	2D 1H-13C

Amides

Experiments	Comments
15N fast HSQC	1H-15N HSQC using WATERGATE (3-9-19)
15N SE HSQC	1H-15N HSQC with sens-enhancement
15N TROSY	gradient selected 1H-15N TROSY
15N BEST HSQC	1H-15N BEST-HSQC
15N BEST TROSY	1H-15N BEST-TROSY
2D HETSOFAST	1H-15N with/without saturation of aliphatics/water
15N seqHADAMAC	1H-15N HADAMAC for AA-type editing (pseudo 3D)
15N SOFAST	1H-15N SOFAST-HMQC
15N ST SOFAST	1H-15N single-transition SOFAST-HMQC

Aliphatics

Experiments	Comments
13C SE HSQC	1H-13C HSQC with sens-enhancement and CO decoupling

Aromatics

Experiments	Comments
13C BEST-HSQC	2D 1H-13C BEST-HSQC with CT option
13C BEST-TROSY	2D 1H-13C BEST-TROSY with CT option

Methyls

Experiments	Comments
methyl SOFAST selective	for proteins in H2O
CT methyl SOFAST sel	same with CT editing
methyl SOFAST BIP	for proteins in D2O
AA-type edited methyl SOFAST	Amio-acid-type edited CT SOFAST

BackboneAssignment

Experiments	Comments
BEST HNC	3D BEST H-C-N expts
BTROSY HNC & HNN	3D BEST-TROSY H-C-N and H-N-N expts
BTROSY HNC for Deuterated proteins	3D BEST-TROSY H-C-N with 2H decoupling

BEST HNC

Experiments	Comments
BEST HNCO SE	HN(i)-N(i)-CO(i-1)
BEST HNCO INEPT	HN(i)-N(i)-CO(i-1)
BEST HNCA	HN(i)-N(i)-CA(i)/CA(i-1) INEPT/SE versions
BEST HNcoCA	HN(i)-N(i)-CA(i-1) INEPT/SE versions
BEST HNCACB	HN(i)-N(i)-CA(i)/CA(i-1)/CB(i)/CB(i-1) INEPT/SE versions
BEST HNcoCACB	HN(i)-N(i)-CA(i-1)/CB(i-1) INEPT/SE versions

BEST TROSY HNC

Experiments	Comments
BT HNCO	HN(i)-N(i)-CO(i-1)
BT HNcaCO	HN(i)-N(i)-CO(i)/CO(i-1)
BT HNCO+	improved HN(i)-N(i)-CO(i)/CO(i-1)
BT HNCA	HN(i)-N(i)-CA(i)/CA(i-1)
BT iHNCA	HN(i)-N(i)-CA(i)
BT HNcoCA	HN(i)-N(i)-CA(i-1)
BT HNCA+	improved HN(i)-N(i)-CA(i)/CA(i-1)
BT HNCACB	HN(i)-N(i)-CA(i)/CA(i-1)/CB(i)/CB(i-1)
BT iHNCACB	HN(i)-N(i)-CA(i)/CB(i)
BT HNCACB+	improved HN(i)-N(i)-CA(i)/CA(i-1)/CB(i)/CB(i-1)
BT HNcoCACB	HN(i)-N(i)-CA(i-1)/CB(i-1)
BT hNcocaNH	HN(i)-N(i)-N(i+1)
BT hNcaNH	HN(i)-N(i)-N(i+1)/N(i-1)

Experiments	Comments
BT hNcacoNH	HN(i)-N(i)-N(i-1)
1D run	runs first FID of the main bb exp

Deuterated

Experiments	Comments
BT HNCACB 2H	HN(i)-N(i)-CA(i)/CA(i-1)/CB(i)/CB(i-1) + 2H decoupling
BT HNcoCACB 2H	HN(i)-N(i)-CA(i-1)/CB(i-1) + 2H decoupling
BT HNCA 2H	HN(i)-N(i)-CA(i)/CA(i-1) + 2H decoupling
BT HNcoCA 2H	HN(i)-N(i)-CA(i-1) + 2H decoupling
BT HNcaCO 2H	HN(i)-N(i)-CO(i)/CO(i-1) + 2H decoupling

SideChains

Experiments	Comments
hCCH	double 13C-edited 3D hCCH-TOCSY
HCcH	double 1H-edited 3D HCcH-TOCSY
Cconhtocsy	Caliph-backbone N-H (Semi-CT in 15N)

Experiments	Comments
Hcconhtocsy	Haliph-backbone N-H (Semi-CT in 15N)
HBHAcoNH	3D HBHA(i-1)-NH(i) correlation expt
2D planes	record all 2D planes of the expts. above

Aromatics assign

Experiments	Comments
HisHDCB	HD-CB correlation in His side chains
HisHDCG	HD-CG correlation in His side chains
HisHNSOFAST	H-N one-bond correlations in His side chains
HISHCSOFAST	H(C)-N correlations (transfer via 2J and 3J HN couplings)
HisHCN	H(C)-N correlations (option for NH and N moieties)
AROMBESTHSQCsel	1H-13C correlations with sign inversion for Tyr CE-HE
TyrHDCG	HD-DG correlations in Tyr side chains
TyrHDCB	HD-CB correlations in Tyr side chains
TyrHECG	HE-CG correlations in Tyr side chains

Experiments	Comments
TyrHECD	HE-CD correlations in Tyr side chains
IBSTyrHECZ	HE-CZ correlations in Tyr side chains

NOESYs

Experiments	Comments
13C aliph NOESY-HSQC	3D 13C-edited NOESY-SEHSQC
13C arom NOESY-HSQC	3D 13C-edited NOESY-HSQC
13C methyl NOESY-SOFAST	3D 13C-edited NOESY-metylSOFAST
13C meythyl SOFAST-NOESY-SOFAST	3D 13C-13C-1H NOESY (methyls only)
15N NOESY-HSQC	3D 15N-edited NOESY-SEHSQC

RDC

Experiments	Comments
15N BEST TROSY	15N TROSY peak selection
15N BEST semiTROSY	15N semi_TROSY peak selection
BEST HNCO JNH	J(NH) from splitting in CO dim

Experiments	Comments
BEST HNCO JCOCA	J(COCA) from splitting in CO dim
BEST HNCO JCOH	J(CO-HN) from splitting in CO dim
BEST HNCOCA JCAHA	J(CA-HA) from splitting in CA dim

Hbonds

Experiments	Comments
Best HNCO hbonds	Best-HNCO with a transfer delay of 135ms
BT HNCO hbonds	BestTrosy-HNCO with a transfer delay of 135ms

Relaxation liquids

Experiments	Comments
15N RELAXATION	15N T1, T2 , HetNOE, CPMG, EXSY
13C RELAXATION	methyl 13C CPMG-RD

15N Relaxation

Experiments	Comments
15N T1	15N T1 (pseudo 3D)
15N T2	15N T2 (pseudo 3D)
15N T1 rho	15N T1 rho (pseudo 3D)
15N HETNOE 3D	heteronuclear NOE (interleaved)
15N Best HETNOE	het-NOE “sat” or “ref” plane (with BEST scheme)
15N Best HETNOE 3D	heteronuclear NOE (BEST, interleaved)
BT CPMG RD 2D	15N CPMG-RD (2D, fixed numer of 180)
BT CPMG RD 3D	15N CPMG-RD with CPMG (vd) list (3D)
15N BEST EXSY	3D H-N-N EXSY: Nz exchange expt

13C Relaxation

Experiments	Comments
2D methyl MQ-CPMG	MQ (1H-13C)CPMG-RD
3D methyl MQ-CPMG	MQ (1H-13C)CPMG-RD (pseudo-3D)

Experiments	Comments
3D methyl SQ-CPMG	SQ (13C)CPMG-RD (pseudo-3D)

Kinetics

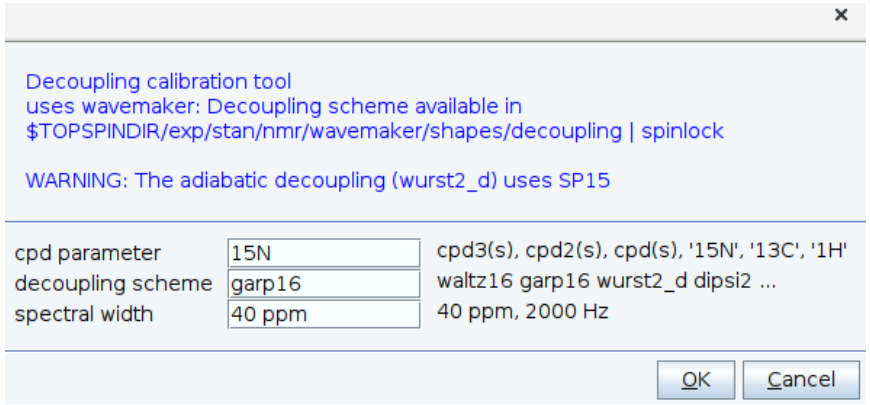
Experiments	Comments
pseudo3D H-N SOFAST	repeats SOFAST (pseudo 3D)
pseudo3D H-N BTROSY	repeats BTROSY (pseudo 3D)

Macros

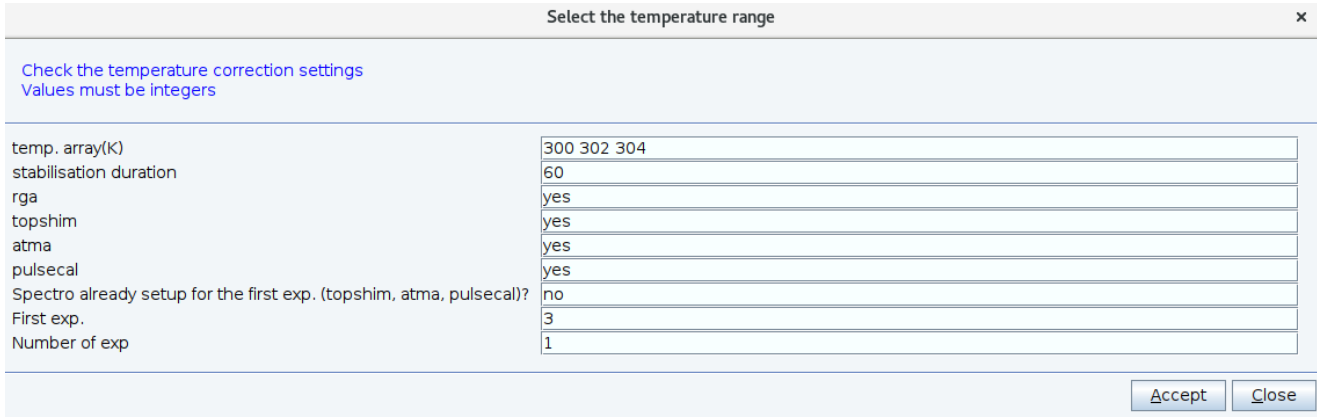
Scripts	Comments
Acquisition	Decoupling setup, temperature ramps…
Display	Save/set contour levels, plot using matplotlib
Processing	Save/set processing, reference spectra

Acquisition

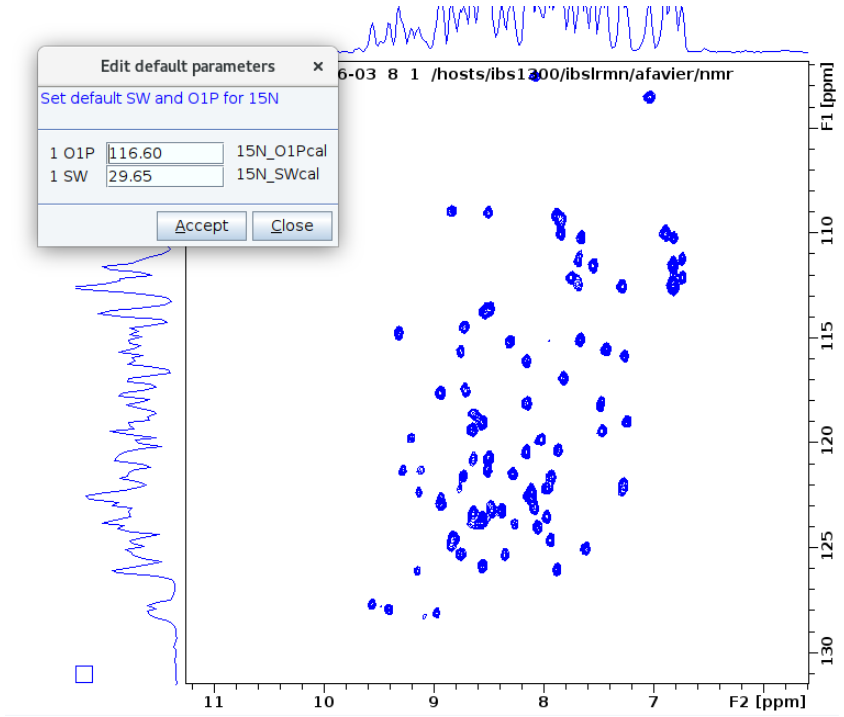
Scripts	Comments
Decoupling Setup	Choose 15N/13C composite decoupling and frequency range
setup carrier frequencies vs DSS	changes carrier frequencies (o1p, o2p, …) so that

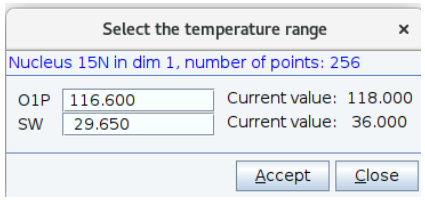


Scripts	Comments
Temperature ramp	Acquire the current experiment at different temperatures
Repeat a set of exp	Acquire several times a set of experiments



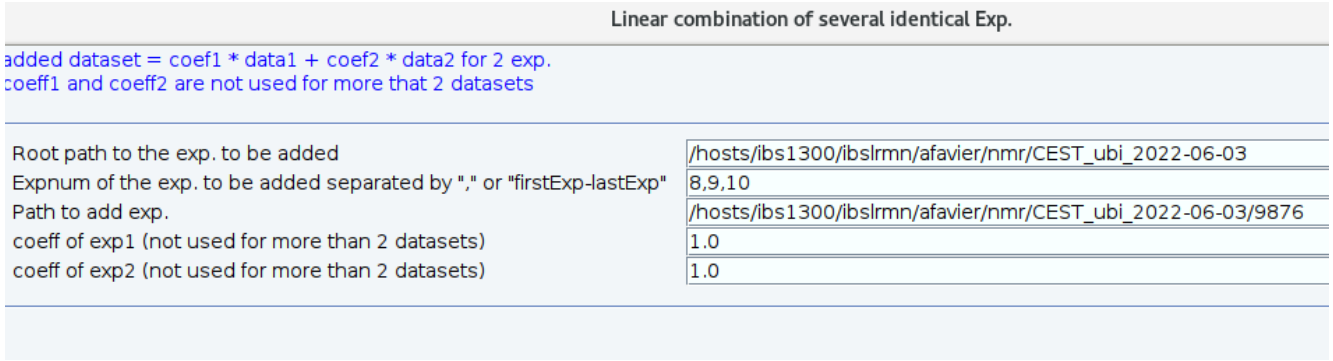
Scripts	Comments
Get indirect SW and O1p	Store values from the displayed region (only 2D)
Set indirect SW and O1p	Load the stored values (2D to nD)
2D-ASCOM	Minimal SW1 by spectral aliasing

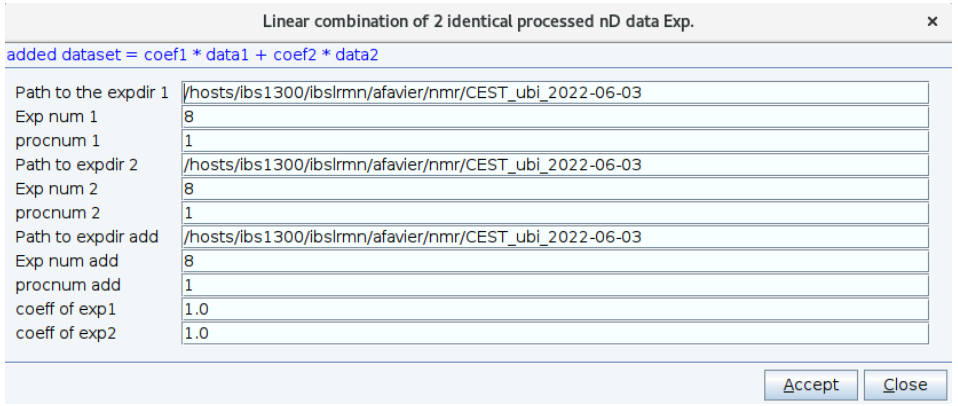
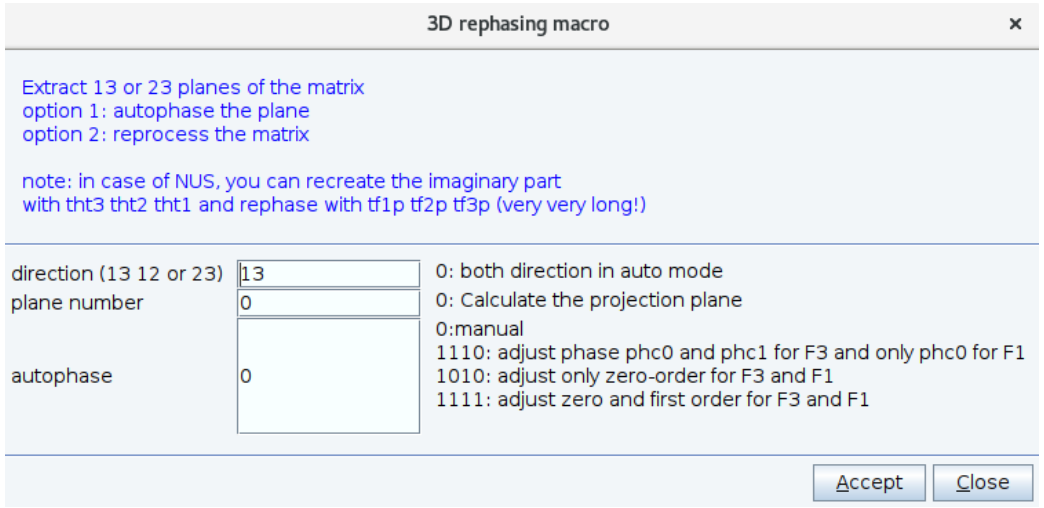




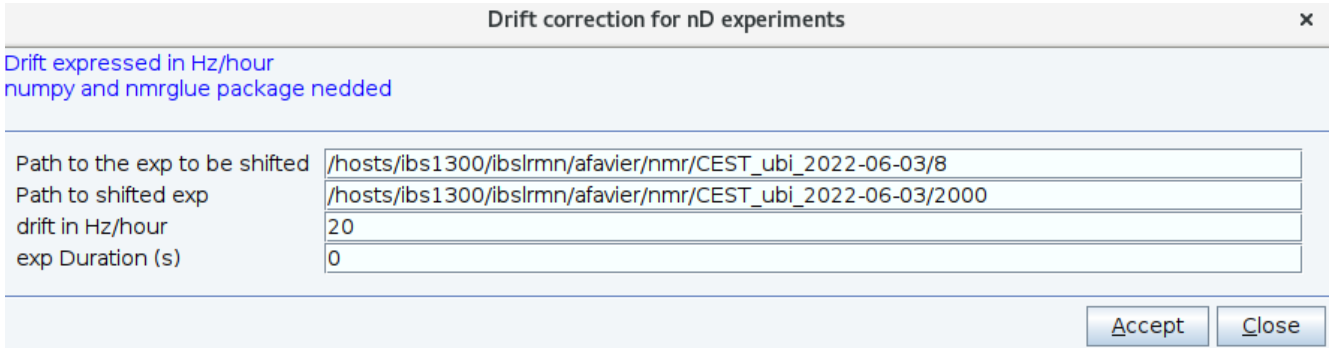
Processing

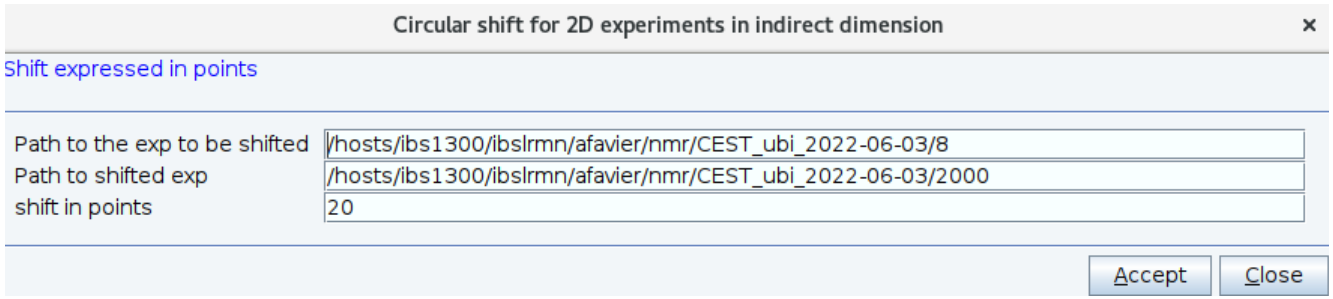
Scripts	Comments
Save processing	
Get processing	
Reference spectra vs DSS	Uses empirical water CS determined from the temperature
Add 2 or more fid/ser (1D to nD)	Experiments should identical (number of points…)



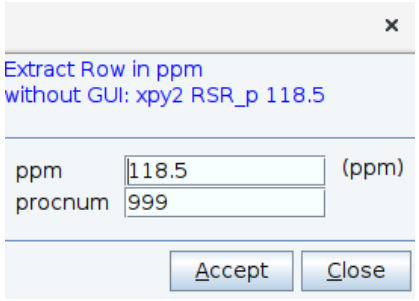
Scripts	Comments	
Add 2 proc data (1D to nD)	Experiments should identical (number of points…)	
3D rephasing	extract a plane of the 3D and reconstruct the imaginaries for phasing	
Remove bad FIDs	set bad FIDs to zero	

Scripts	Comments
Auto Make nmrPipe scripts	Generate automatically nmrPipe processing macros
Drift correction	shift the fids according to the magnet drift
Circular shift	shift indirect dimension of 2D spectra

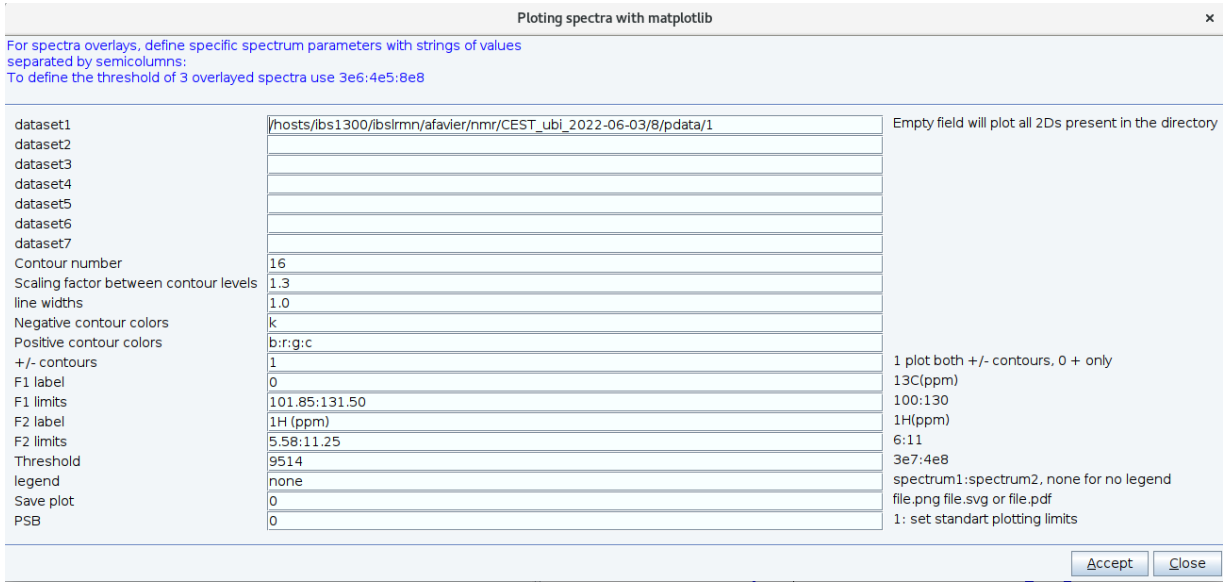




Display

Scripts	Comments
Save levels	
Get levels	
Extract Row in ppm	
Extract Col in ppm	

Scripts	Comments
Plot spectra using Matplotlib	1D and 2D (and overlays) allows absolute comparison



Open the spectrum with sparky

RNA

Experiments	Comments
CALIBRATIONS	13C Calibration
Imino 1D	standart and Hadamac

Experiments	Comments
1H-15N	BTROSY
1H-13C	BTROSY, with/without CT
CMPG	2D/3D 13C aromatic CPMG
HCNN	BEST CNN COSY
Imino NOESY	BEST 1H-1H NOESY

RNA Calibrations

Experiments	Comments
13C pulse calibration	SOFAST based calibration (p3)

RNA 1Ds

Experiments	Comments
1D imino 1H	
HAD-imino-1H	

RNA 1H-15N

Experiments	Comments
1H-15N BTROSY	

RNA 1H-13C

Experiments	Comments
1H-13C arom-BTROSY	1H-13C BTROSY
1H-13C arom-BTROSY CT	1H-13C BTROSY CT

RNA CPMG

Experiments	Comments
3D 13C arom-CPMG	
2D 13C arom-CPMG	

RNA HCNN

Experiments	Comments
2D BEST HCNN COSY	H-bond expt for A-U

RNA NOESYs

Experiments	Comments
2D imino NOESY	

Spectro tests

Experiments	Comments
1D library run	25 1D BEST-SOFAST exp. in 5 mn
2D library run	60 BEST-SOFAST exp. in 1h25
Full library run	1D to 3D runs (using ASCOM)

LibTools

Experiments	Comments
Template Maker	Implement the current experiment to the library
Export	Export the loaded template to a folder for sharing
Import	Import an experiment from a folder to your library

Experiments	Comments
Delete	Delete the loaded template from the library