

# NMRlib for liquids

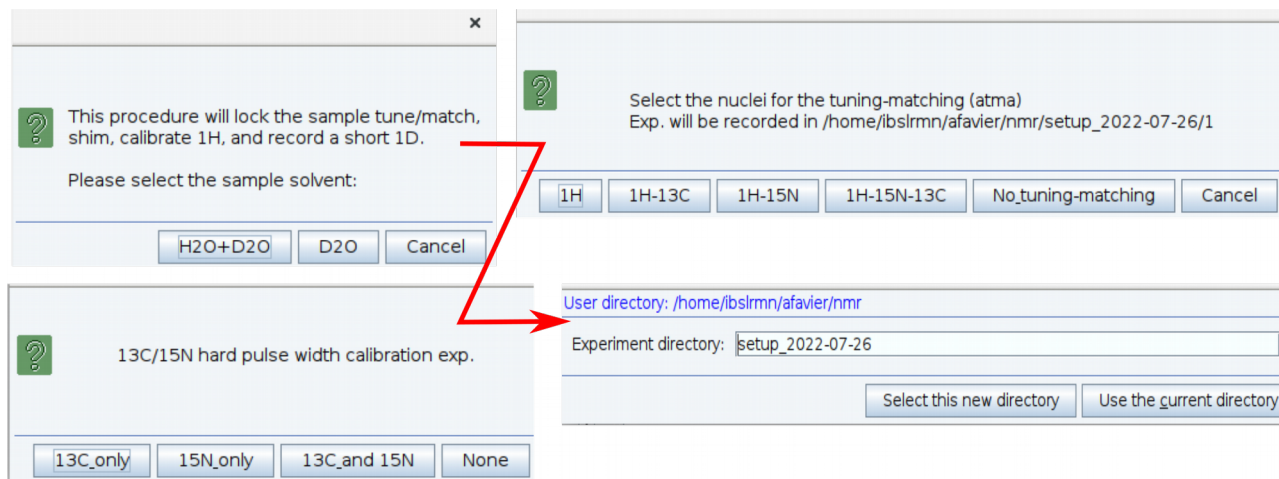
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# Proteins

## *Spectrometer setup liquids*

### Experiments Comments

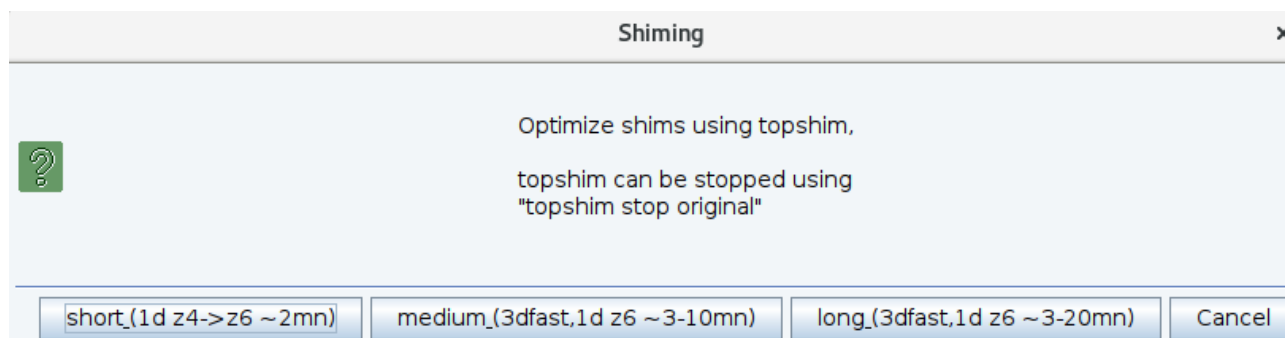
Setup lock Tune shim (1H-13C-15N) pulse calibration



Stop setup run Allows to stop setup experiments

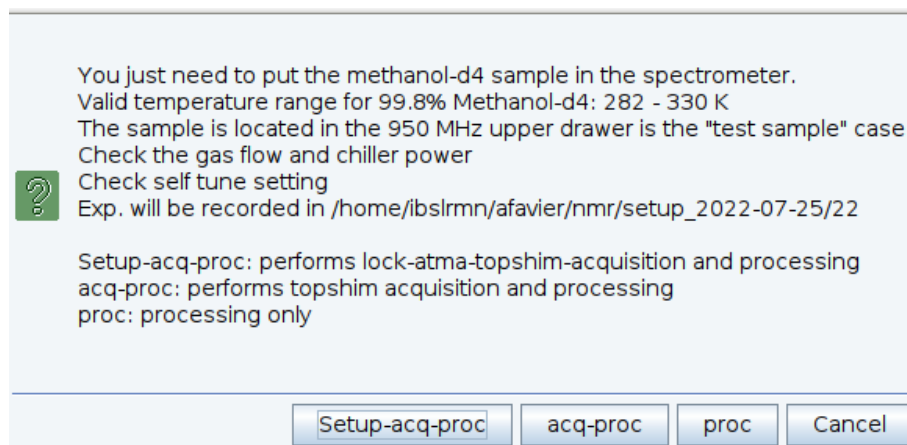
## Experiments Comments

Optimize shims      run different flavours of topshim



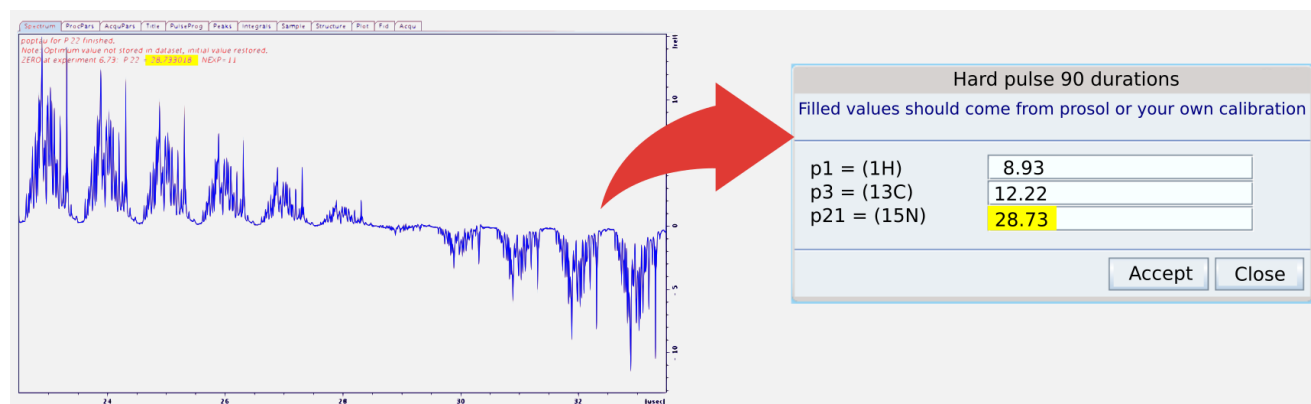
Check Shims      Measure the deuterium line width

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
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## Experiments

## Comments

nD popt

varying a parameter  
in nD expt

×

Execute popt on nD experiments

Arrayed parameter	<input type="text" value="O1"/>	ex: CNST 22, P 1, GPZ 3, PLdB 9, PLW 9
Center of the array	<input type="text" value="O1"/>	ex: 4566.5, CNST 22, P 1, GPZ 1
fit target	<input type="text" value="MAGMIN"/>	ZERO POSMAX NEGMAX MAGMAX MAGMIN
Width of the array	<input type="text" value="200"/>	ex: O1min = O1-100; O1max = O1+100
Number of exp.	<input type="text" value="10"/>	Number of steps
F2P	<input type="text" value="4.5"/>	right limit of the spectrum
F1P	<input type="text" value="5.5"/>	left limit of the spectrum
NS	<input type="text" value="1"/>	0: uses the actual NS
RG	<input type="text" value="1"/>	0: uses the actual RG
DS	<input type="text" value="0"/>	-1: uses the actual DS
auto phase	<input type="text" value="0"/>	no: 0, yes: 1
serfile	<input type="text" value="0"/>	no: 0, yes: 1

Accept

Close

## QualityControl liquids

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

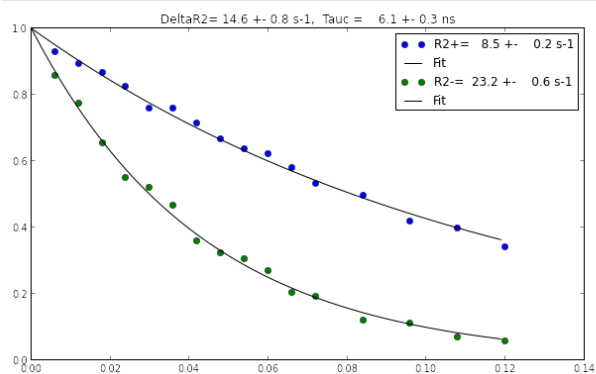
### 1 Ubiquitin

```

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 d2l = 0.003
7 min_val = 9.5
8 max_val = 8.6
9

1 tractAna(filename1, filename2, vclist_file_nl, vclist_file_nl, d2l, 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

```

1 libLoc = '/hosts/ibs1300/nmrdata/nmr/lib/'
2 filename1 = '/hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/pdata/1'
3 difflist_file = '/hosts/950neo/ibslrmn/afavier/nmr/2019-12-11_S21-LSFubi/2/difflist'
4 min_val = 2
5 max_val = -1.0

```

```

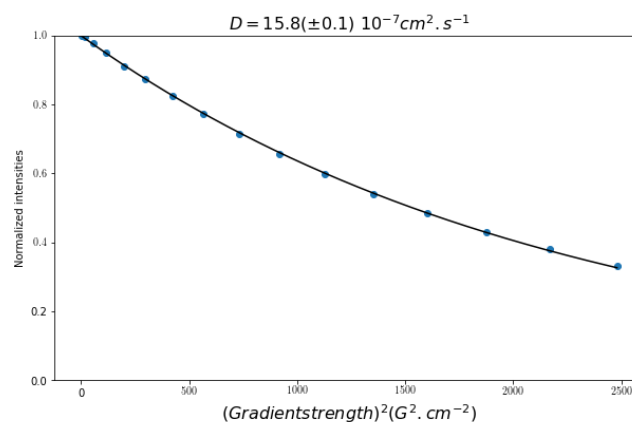
1 dosyAna(libLoc, filename1, difflist_file, min_val, max_val)

```

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	<i>Analysis tool provided</i>
2D HETSOFAST	Local structural compactness	
HAD SOFAST amides	1D SOFAST with additional 15N filter	<i>Analysis tool provided</i>

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

<b>Experiments</b>	<b>Comments</b>
ALIPHATICS	2D 1H-13C
AROMATICS	2D 1H-13C
METHYLS	2D 1H-13C

## **Amides**

<b>Experiments</b>	<b>Comments</b>
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

<sup>13</sup>C SE HSQC

### Comments

<sup>1</sup>H-<sup>13</sup>C HSQC with sens-enhancement and CO decoupling

## Aromatics

### Experiments

<sup>13</sup>C BEST-HSQC

### Comments

2D <sup>1</sup>H-<sup>13</sup>C BEST-HSQC with CT option

<sup>13</sup>C BEST-TROSY

2D <sup>1</sup>H-<sup>13</sup>C BEST-TROSY with CT option

## Methyls

### Experiments

methyl SOFAST selective

### Comments

for proteins in H<sub>2</sub>O

CT methyl SOFAST sel

same with CT editing

methyl SOFAST BIP

for proteins in D<sub>2</sub>O

AA-type edited methyl SOFAST

Amio-acid-type edited CT SOFAST

## ***BackboneAssignment***

<b>Experiments</b>	<b>Comments</b>
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**

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

<b>Experiments</b>	<b>Comments</b>
Hconhtocsy	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***

<b>Experiments</b>	<b>Comments</b>
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

<b>Experiments</b>	<b>Comments</b>
TyrHECD	HE-CD correlations in Tyr side chains
IBSTyrHECZ	HE-CZ correlations in Tyr side chains

## ***NOESYs***

<b>Experiments</b>	<b>Comments</b>
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-methylSOFAST
13C methyl SOFAST-NOESY-SOFAST	3D 13C-13C-1H NOESY (methyls only)
15N NOESY-HSQC	3D 15N-edited NOESY-SEHSQC

## ***RDC***

<b>Experiments</b>	<b>Comments</b>
15N BEST TROSY	15N TROSY peak selection
15N BEST semiTROSY	15N semi_TROSY peak selection
BEST HNC0 JNH	J(NH) from splitting in CO dim

**Experiments**

BEST HNCO JCOCA

BEST HNCO JCOH

BEST HNCOCA JCAHA

**Comments**

J(COCA) from splitting in CO dim

J(CO-HN) from splitting in CO dim

J(CA-HA) from splitting in CA dim

***Hbonds*****Experiments**

Best HNCO hbonds

BT HNCO hbonds

**Comments**

Best-HNCO with a transfer delay of 135ms

BestTrosy-HNCO with a transfer delay of 135ms

***Relaxation liquids*****Experiments**

15N RELAXATION

13C RELAXATION

**Comments**

15N T1, T2 , HetNOE, CPMG, EXSY

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 number 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

3D methyl SQ-CPMG

## Comments

SQ (13C)CPMG-RD (pseudo-3D)

## *Kinetics*

## Experiments

pseudo3D H-N SOFAST

## Comments

repeats SOFAST (pseudo 3D)

pseudo3D H-N BTROSY

repeats BTROSY (pseudo 3D)

## Macros

## Scripts

Acquisition

## Comments

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

×

Decoupling calibration tool  
uses wavemaker: Decoupling scheme available in  
[\\$TOPSPINDIR/exp/star/nmr/wavemaker/shapes/decoupling | spinlock](#)  
  
WARNING: The adiabatic decoupling (wurst2\_d) uses SP15

cpd parameter	15N	cpd3(s), cpd2(s), cpd(s), '15N', '13C', '1H'
decoupling scheme	garp16	waltz16 garp16 wurst2_d dipsi2 ...
spectral width	40 ppm	40 ppm, 2000 Hz

OK

Cancel

setup carrier frequencies vs DSS  
 changes carrier frequencies (o1p, o2p, ...) so that

## Scripts

## Comments

Temperature  
ramp

Acquire the current  
experiment at  
different  
temperatures

Select the temperature range

Check the temperature correction settings  
Values must be integers

temp. array(K)	300 302 304
stabilisation duration	60
rga	yes
topshim	yes
atma	yes
pulsecal	yes
Spectro already setup for the first exp. (topshim, atma, pulsecal)?	no
First exp.	3
Number of exp	1

Accept

Close

Repeat a set  
of exp

Acquire several times  
a set of experiments

Select the experiments to be repeated

Repeats experiments several times,  
for example, experiments "1 4 6" will be copied 2 times  
and setup in exp. 10001 10004 10006 20001 20004 20006

Selected exp.	1 4 6
Number of repeats	2
Exp. shift	10000
Run also selected exp.	no

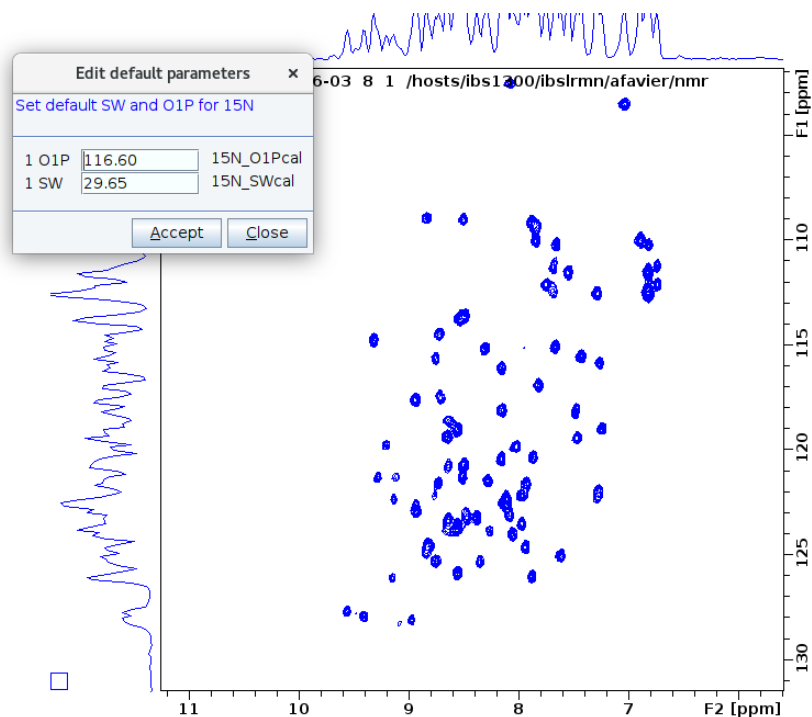
no: sele

## 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)

The figure shows a dialog box titled 'Select the temperature range'. It contains the text 'Nucleus 15N in dim 1, number of points: 256'. Below this, there are two rows of input fields: 'O1P' with the value '116.600' and 'SW' with the value '29.650'. To the right of these fields are labels 'Current value: 118.000' and 'Current value: 36.000'. At the bottom of the dialog are 'Accept' and 'Close' buttons.

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  
be identical (number of  
points...)

Linear combination of several identical Exp.	
added dataset = coef1 * data1 + coef2 * data2 for 2 exp. coef1 and coef2 are not used for more than 2 datasets	
Root path to the exp. to be added	/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03
Expnum of the exp. to be added separated by "," or "firstExp-lastExp"	8,9,10
Path to add exp.	/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03/9876
coeff of exp1 (not used for more than 2 datasets)	1.0
coeff of exp2 (not used for more than 2 datasets)	1.0

Scripts

Comments

Add 2 proc  
data (1D to  
nD)

Experiments should  
identical (number of  
points...)

Linear combination of 2 identical processed nD data Exp. ×

added dataset = coef1 \* data1 + coef2 \* data2

Path to the expdir 1	/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03
Exp num 1	8
procnum 1	1
Path to expdir 2	/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03
Exp num 2	8
procnum 2	1
Path to expdir add	/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03
Exp num add	8
procnum add	1
coeff of exp1	1.0
coeff of exp2	1.0

Accept

Close

3D rephasing

extract a plane of  
the 3D and  
reconstruct the  
imaginaries for  
phasing

3D rephasing macro ×

Extract 13 or 23 planes of the matrix  
option 1: autophase the plane  
option 2: reprocess the matrix  
  
note: in case of NUS, you can recreate the imaginary part  
with tht3 tht2 tht1 and rephase with tf1p tf2p tf3p (very very long!)

direction (13 12 or 23)	13	0: both direction in auto mode
plane number	0	0: Calculate the projection plane
autophase	0	0: manual 1110: adjust phase phc0 and phc1 for F3 and only phc0 for F1 1010: adjust only zero-order for F3 and F1 1111: adjust zero and first order for F3 and F1

Accept

Close

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
------------------	--

Drift correction for nD experiments ✕

Drift expressed in Hz/hour  
numpy and nmrglue package nedded

Path to the exp to be shifted	<input type="text" value="/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03/8"/>
Path to shifted exp	<input type="text" value="/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03/2000"/>
drift in Hz/hour	<input type="text" value="20"/>
exp Duration (s)	<input type="text" value="0"/>

Circular shift	shift indirect dimension of 2D spectra
----------------	--

Circular shift for 2D experiments in indirect dimension ✕

Shift expressed in points

Path to the exp to be shifted	<input type="text" value="/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03/8"/>
Path to shifted exp	<input type="text" value="/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03/2000"/>
shift in points	<input type="text" value="20"/>

## ***Display***

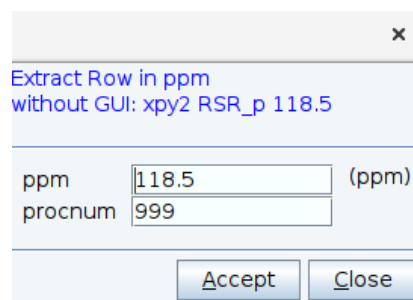
### **Scripts**

### **Comments**

Save levels

Get levels

Extract Row in  
ppm



Extract Row in ppm

without GUI: xpy2 RSR\_p 118.5

ppm 118.5 (ppm)

procnum 999

Accept Close

Extract Col in  
ppm

Scripts

Plot spectra  
using  
Matplotlib

Comments

1D and 2D (and  
overlays) allows  
absolute comparison

Plotting spectra with matplotlib

For spectra overlays, define specific spectrum parameters with strings of values separated by semicolumns:  
To define the threshold of 3 overlaid spectra use 3e6:4e5:8e8

dataset1	/hosts/ibs1300/ibslrmn/afavier/nmr/CEST_ubi_2022-06-03/8/pdata/1	Empty field will plot all 2Ds present in the directory
dataset2		
dataset3		
dataset4		
dataset5		
dataset6		
dataset7		
Contour number	16	
Scaling factor between contour levels	1.3	
line widths	1.0	
Negative contour colors	k	
Positive contour colors	b:r:g:c	
+/- contours	1	1 plot both +/- contours, 0 + only
F1 label	0	13C(ppm)
F1 limits	101.85:131.50	100:130
F2 label	1H (ppm)	1H(ppm)
F2 limits	5.58:11.25	6:11
Threshold	9514	3e7:4e8
legend	none	spectrum1:spectrum2, none for no legend
Save plot	0	file.png file.svg or file.pdf
PSB	0	1: set standart plotting limits

AcceptClose

Open the  
spectrum with  
sparky

RNA

Experiments

CALIBRATIONS

Imino 1D

Comments

13C Calibration

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**

1H-15N BTROSY

#### **Comments**

### ***RNA 1H-13C***

#### **Experiments**

1H-13C arom-BTROSY

1H-13C arom-BTROSY CT

#### **Comments**

1H-13C BTROSY

1H-13C BTROSY CT

### ***RNA CPMG***

#### **Experiments**

3D 13C arom-CPMG

2D 13C arom-CPMG

#### **Comments**

### ***RNA HCNN***

#### **Experiments**

2D BEST HCNN COSY

#### **Comments**

H-bond expt for A-U

## ***RNA NOESYs***

### **Experiments**

2D imino NOESY

### **Comments**

## **Spectro tests**

### **Experiments**

1D library run

2D library run

Full library run

### **Comments**

25 1D BEST-SOFAST exp. in 5 mn

60 BEST-SOFAST exp. in 1h25

1D to 3D runs (using ASCOM)

## **LibTools**

### **Experiments**

Template Maker

Export

Import

### **Comments**

Implement the current experiment to the library

Export the loaded template to a folder for sharing

Import an experiment from a folder to your library

## Experiments

Delete

## Comments

Delete the loaded template from the library