Supplement of

ssNMRLib: a comprehensive library and tool box for acquisition of solid-state nuclear magnetic resonance experiments on Bruker spectrometers

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Listing S1: parameter naming convention in ssNMRlib

General naming conventions for CPs, plw, spw, cnst
CP power levels are entered in kHz and are generally assigned to the three channels as:

30-39 : 13C
40-49 : 1H
50-56 : 15N
57-63 : Midpoint ramp

Examples:
13C RF field for HC CP → cnst 31
1H RF field for HC CP → cnst 41

Hard Pulses

if 1H detection
p1 : H 90 degree pulse (us) @ plw1
p2 : C 90 degree pulse (us) @ plw2
p3 : N 90 degree pulse (us) @ plw3
p4 : 2H 90 degree pulse (us) @ plw4

if 13C detection
p1 : C 90 degree pulse (us) @ plw1
p2 : H 90 degree pulse (us) @ plw2
p3 : N 90 degree pulse (us) @ plw3
p4 : 2H 90 degree pulse (us) @ plw4

if 15N detection
p1 : N 90 degree pulse (us) @ plw1
p2 : H 90 degree pulse (us) @ plw2
p3 : C 90 degree pulse (us) @ plw3

CP constants

HN CP
cnst 42 : RF field on 1H (kHz)
cnst 52 : RF field on 15N (kHz)
cnst 62 : Midpoint of the ramp
spnam 42 : File name for the ramp
p 45 : CP duration (us)

N-CO CP

cnst 33 : RF field on 13C (kHz)
cnst 43 : RF field on 1H for decoupling (kHz)
cnst 53 : RF field on 15N (kHz)
cnst 63 : Midpoint of the ramp
spnam 53 : File name for the ramp
p 53 : CP duration (us)

Simultaneous HCN CP

cnst 31 : RF field on 13C (kHz)
cnst 41 : RF field on 1H (kHz)
cnst 51 : RF field on 15N (kHz)
cnst 61 : Midpoint of the ramp
spnam 41 : File name for the ramp
p 43 : CP duration (us)

HC/HCA/HCO CP

cnst 31 : RF field on 13C (kHz)
cnst 41 : RF field on 1H (kHz)
cnst 61 : Midpoint of the ramp
spnam 41 : File name for the ramp
p 43 : CP duration (us)

N-CA CP

cnst 34 : RF field on 13C (kHz)
cnst 44 : RF field on 1H for decoupling

cnst 54 : RF field on 15N (kHz)
cnst 60 : Midpoint of the ramp
spnam 54 : File name for the ramp
p 35 : CP duration (us)

HA-CA CP

cnst 35 : RF field on 13C (kHz)
cnst 45 : RF field on 1H (kHz)
cnst 57 : Midpoint of the ramp
spnam 45 : File name for the ramp
p 34 : CP duration (us)
INEPT
d 13 : INEPT delay HC (sec)
d 14 : INEPT delay HN (sec)
d 15 : INPET delay CA-CB (sec)
d 16 : INEPT delay CO-CA, CO transverse (sec)
d 17 : INEPT delay CO-CA, CA transverse (sec)
d 53 : INEPT delay N-CO (sec)
d 54 : INEPT delay N-CA (sec)

Transfer 13C-13C
13C RFDR
cnst 20 : Spinning rate (Hz)
cnst 37 : 13C offset during RFDR
d 8 : Mixing time
p 37 : RFDR duration (us)

DREAM CA-CB
cnst 6 : RF field on 1H (kHz)
cnst 7 : RF of the DREAM (kHz)
cnst 17 : 13C offset for DREAM
cnst 59 : Midpoint of the ramp
p 17 : DREAM duration (us)
snam 7 : DREAM ramp

TOCSY / DIPSI
cnst 15 : RF field on 13C (kHz)
d 15 : Mixing duration (sec)
cpdpd 8 : Mixing sequence
pcpd 5 : Pulse length for the mixing sequence

Transfer 1H-1H
Bass-SD
cnst 48 : 1H carrier during Bass-SD
cnst 49 : RF Bass-SD at midpoint (kHz)
cnst 59 : Midpoint of the Bass-SD shape
spnam 49 : Bass-SD element
p 49 : Bass-SD duration (us)
d 8 : z-filter delay (sec)

1H RFDR
cnst 20 : Spinning rate (Hz)
cnst 37 : 1H offset during RFDR
d 8 : Mixing time (sec)
p 37 : RFDR duration (us)
L0 : RFDR loop

Z-mix
d 8 : Z-mix delay (sec)

Transfer 15N-13C
TEDOR
L1 : Loop number for TEDOR experiment

Transfer 15N-15N
PDSD
d 5 : PDSD mixing time (sec)
**Dynamics**

**REDOR**
- p 18 : 1H pulse 180° (us)
- p 19 : 13C pulse 180° (us)
- cnst 20 : Spinning rate (Hz)
- d 7 : Redor shift delay (sec)
- L0=0 : Redor loop (2 rotor period min)
- L1=0 : Reference

**R1rho**
- cnst 25 : R1rho field strength (kHz)
- p 18 : heat compensation pulse
- p 25 : spinlock
- p 26 : 13C/15N degree pulse (us)
- d 24 : R1rho max delay

**T2**
- d 25 : T2 delay

**CEST**
- cnst 17 : 1H decoupling (kHz) @ plw17
- cnst 27 : 15N RF field (Hz)
- cnst 29 : Set to 0 for reference experiment
- p 17 : Decoupling pulse length (us)
- d 31 : CEST delay (sec)
- cpdprg 5 : 1H decoupling sequence
- cpdprg 6 : CEST 15N sequence

**T1**
- d 25 : T1 delay (sec)

**EXSY**
- d 31 : EXSY mixing time (sec)

**Selective 13C pulses**
- spnam 10 : EBURP2 on-resonance CO according to p11 for the pulse duration
- spnam 11 : EBURP2-TR on-resonance CO according to p12 for the pulse duration
- spnam 13 : ISNOB 2 off-resonance CO according to p13 for the pulse duration
- spnam 14 : REBURP on-resonance CA according to p14 for the pulse duration
- spnam 15 : REBURP on-resonance CA-CB according to p15 for the pulse duration
- spnam 16 : EBURP2 off-resonance CO according to p16 for the pulse duration
- spnam 17 : EBRURP2 off-resonance CO according to p17 for the pulse duration
- spnam 18 : ISNOB2 off-resonance CA according to p18 for the pulse duration
- spnam 19 : REBURP on-resonance CO according to p19 for the pulse duration

**Decoupling**

**13C decoupling during 1H detection**
- cpdprg 1 : sequence used for the 13C decoupling during 1H detection
- pcpd 1 : pulse length in decoupling sequence (us)
- cnst 11 : 13C decoupling power (kHz) @ plw11

**1H decoupling during 13C/15N evolution/detection**
- cpdprg 2 : sequence used for the 1H decoupling during evolution/detection time
- pcpd 2 : pulse length in decoupling sequence (us)
- cnst 12 : 1H decoupling power (kHz) @ plw12

**15N decoupling during 1H detection**
- cpdprg 3 : sequence used for the 15N decoupling during 1H detection
- pcpd 3 : pulse length in decoupling sequence (us)
- cnst 13 : 15N decoupling power (kHz) @ plw13
2H decoupling

cpdprg 5 : sequence used for the 15N decoupling during 1H detection
cpdpd 5 : pulse length in decoupling sequence (us)
cnst 14 : 2H decoupling power (kHz) @ plw14

Solvent suppression

cnst 24 : 1H RF field for solvent suppression (kHz)
d 30 : duration for the solvent suppression (sec)
cpdprg 4 : decoupling sequence
cpdpd 7 : pulse length for the solvent suppression (us)

Other constants

cnst 1 : 13C reference RF field (kHz), from p 21 (for calculation)
cnst 2 : 1H reference RF field (kHz), from p 22 (for calculation)
cnst 3 : 15N reference RF field (kHz), from p 23 (for calculation)
cnst 4 : 2H reference RF field (kHz), from p 24 (for calculation)
cnst 10 : Multiplier for acqt=cnst10*1u set to 1
cnst 15 : Center of CB (39 ppm)
cnst 16 : Center of CO (175 ppm)
cnst 17 : Center of CA (54 ppm)
cnst 18 : Carrier between CA and CO (100 ppm)
cnst 20 : Spinning rate (Hz)

Other delays

d 20 : rotor period (calculated from cnst 20)
d 21 : half rotor-period
Listing S2: currently implemented experiments

NMRlib tools
   Template maker → Implement the current experiment to the library
   Export → Export the loaded template to a folder for sharing
   Import → Import an experiment from your folder to your library
   Delete → Delete the loaded template from the library

Set-up experiments
   KBr
   Adamantane

Set pulse lengths → Set 90° pulse widths

Security → Control your experiment before to launch it

Remove → Remove all the best ramp in order to start a new optimization or user default constants
Recap file → Create or charge a recap file of your optimizations
Load your contents → Load selectively transfer parameters
Save your pulse program → Save your pulse program inside your experiment (not compiled version)

Proteins
   Proton detection

   Set user default parameters: Water suppression parameters, D1 & RG

Calibrations
   O1 Calibration

   Hard Pulse
      1H Calibration based on hNH CP experiment
      1H Calibration based on hCH CP experiment
      15N Calibration based on hNH CP experiment
      13C Calibration based on hCH CP experiment
      1H Direct calibration
      1H Calibration based on hNH INEPT experiment
      1H Calibration based on hCH INEPT experiment
      15N Calibration based on hNH INEPT experiment
      13C Calibration based on hNH INEPT experiment

   Cross Polarization
      CP HN optimization
      CP HC optimization
      CP HCO optimization
      CP HCA optimization
      CP HACA optimization
CP NCO optimization
CP NCA optimization
CP simultaneous hCH hNH optimization
BSH CO-CA optimization

**INEPT**
- hNH
- hCH
INNEPT delay COCA, CO transverse
INEPT delay COCA, CA transverse

**1D spectra**
- Basic 1D experiment
- 1H R1

**Hetero 2Ds HN/HC CP/INEPT**

**Experiments without 2H decoupling**
- hNH CP
- hNH refINEPT
- hCH CP
- hCH refINEPT
Simultaneous CH and NH CP

**Experiments with 2H decoupling**
- hCH CP
- hCH refINEPT
Simultaneous CH and NH CP

**Backbone assignment**

**3D Experiments**

**Experiments without 2H decoupling**
- **hCOcaNH → HN(i)-N(i)-CO(i)**
  - Scalar CO-ca
  - Scalar CO-ca semi constant-time
  - Dipolar CO-ca
- **hCONH → HN(i)-N(i)-CO(i-1)**
- **hCANH → HN(i)-N(i)-CA(i)**
- **hcoCAcoNH → HN(i)-N(i)-CA(i-1)**
- **hCAcoNH → HN(i)-N(i)-CA(i-1)**
  - Dipolar CA-co
- **hcaCBcaNH → HN(i)-N(i)-CB(i)**
- **hcaCBcacoNH → HN(i)-N(i)-CB(i-1)**
  - Scalar ca-co
  - Dipolar ca-co
- **hNcocaNH → HN(i)-N(i)-N(i+1)**
  - Scalar co-ca
  - Dipolar co-ca
- **hNcacoNH → HN(i)-N(i)-N(i-1)**
  - Dipolar ca-co
Experiments with 2H decoupling

\[ \text{hCOcaNH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CO}(i) \]
Scalar \ CO-ca

\[ \text{hcaCBcaNH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CB}(i) \]
\[ \text{hcaCBcacoNH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CB}(i-1) \]

4D Experiments

Experiments without 2H decoupling

\[ \text{hCOCANH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CO}(i)-\text{CA}(i) \]
Scalar \ CO-CA
Scalar \ CO-CA \ semi constant-time
Scalar \ CO-CA \ with \ double \ semi \ constant-time
Dipolar \ CO-CA

\[ \text{hCOCAcoNH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CO}(i)-\text{CA}(i-1) \]
Scalar \ CO-CA
Scalar \ CO-CA-co semi constant-time

\[ \text{hCACONH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CA}(i-1)-\text{CO}(i-1) \]
Dipolar \ CA-CO

\[ \text{hcaCBcaCONH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CB}(i)-\text{CO}(i) \]
Scalar \ ca-CO
Scalar \ ca-CO \ semi constant-time
Dipolar \ ca-CO

\[ \text{hcaCBCANH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CB}(i-1)-\text{CO}(i-1) \]
Scalar \ ca-CO
Scalar \ ca-CO \ semi constant-time
Dipolar \ ca-CO

\[ \text{hcaCBCAcoNH} \rightarrow \text{CB}(i)-\text{CA}(i)-\text{N}(i)-\text{HN}(i) \]
Scalar \ CA-co
Scalar \ CA-co \ semi constant-time
Dipolar \ CA-co

\[ \text{hCONCAHA} \rightarrow \text{CO}(i)-\text{N}(i)-\text{CA}(i)-\text{HA}(i) \]

\[ \text{hNCOcaNH} \rightarrow \text{N}(i+1)-\text{CO}(i)-\text{N}(i)-\text{HN}(i) \]
Scalar \ CO-ca
Dipolar \ CO-ca

\[ \text{hNcoCANH} \rightarrow \text{N}(i+1)-\text{CA}(i)-\text{N}(i)-\text{HN}(i) \]
Scalar \ co-CA
Dipolar \ co-CA

\[ \text{HNcoaNH} \rightarrow \text{HN}(i+1)-\text{N}(i+1)-\text{N}(i)-\text{HN}(i) \]
Scalar \ co-ca

Experiments with 2H decoupling

\[ \text{hCOCANH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CO}(i)-\text{CA}(i) \]

\[ \text{hcaCBcaCONH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CB}(i)-\text{CO}(i-1) \]

\[ \text{hcaCBCANH} \rightarrow \text{HN}(i)-\text{N}(i)-\text{CB}(i-1)-\text{CO}(i-1) \]

\[ \text{hcaCBCAcoNH} \rightarrow \text{CB}(i)-\text{CA}(i)-\text{N}(i)-\text{HN}(i) \]

\[ \text{hNCOcaNH} \rightarrow \text{N}(i+1)-\text{CO}(i)-\text{N}(i)-\text{HN}(i) \]

\[ \text{hNcoCANH} \rightarrow \text{N}(i+1)-\text{CA}(i)-\text{N}(i)-\text{HN}(i) \]

Side-chain assignment

Experiments without 2H decoupling

\[ \text{hCCH TOCSY} \]
\[ \text{hCCH refINEPT TOCSY} \]
Experiment with 2H decoupling

Dynamics

Experiments without deuterium decoupling

Dipolar couplings

- hCH REDOR
- hNH REDOR
- hCH INEPT REDOR
- hNH INEPT REDOR

Longitudinal Relaxation

- R1 hCH 13C → CP
- R1 hCONH 13CO → CP
- R1 hCANH 15N → CP
- R1 hNH 15N → CP
- R1 hCH 13C → INEPT
- T1 hCH 1H → CP
- T1 hCH 1H → INEPT

Transverse Relaxation

- R1rho hCH 1H → CP
- R1rho hCH 13C → CP
- R1rho hCONH 13CO → CP
- R1rho hCANH 15N → CP
- R1rho hNH 15N → CP
- T2 hNH 1H → CP
- T2 hCH 1H → CP

Transverse Relaxation

- hCH EXSY → CP
- hNH EXSY → CP
- Simultaneous hNH hCH EXSY → CP
- CEST hNH → CP

Experiments with deuterium decoupling

- hCH EXSY → CP
- Simultaneous hCH hNH EXSY → CP
- REDOR hCH → CP
- R1rho hCH → CP

Distance Measurements

Experiments with deuterium decoupling

- HhNH HHRFDR
- Simultaneous h(C/N)h(C/N)H HHRFDR
- Simultaneous Hh(C/N)H HHRFDR
- Bass-SD HhCH
Experiments with deuterium decoupling
Simultaneous h(C/N)hh(C/N)H HHRFDR
Simultaneous Hh(C/N)H HHRFDR

Carbon detection

Set user default parameters: D1 & RG

Calibrations

Hard Pulse
13C Calibration based on hC CP experiment
1H Calibration based on hC CP experiment
13C Direct calibration

Cross Polarization
CP HC optimization
CP HCO optimization
CP HCA optimization
CP NCO optimization
CP NCA optimization

INEPT
hC
NCO INEPT
NCA INEPT
CC INEPT

C-C transfer
CC INEPT
DREAM
DARR CO-CX duration
DARR CA-CO duration
RFDR CO-CX duration
RFDR CA-CO duration
CO-CA BSH CP
CA-CO BSH CP

1D Experiments
13C direct
CP HC
INEPT HC
hNCA → double CP
hNCO → double CP
1D Relaxation Experiments

- $^1$H $T_1 \rightarrow$ via CP or INEPT
- $^1$H $T_2 \rightarrow$ via CP or INEPT
- $^{13}$C $T_1 \rightarrow$ via CP
- $^{13}$CA $T_2 \rightarrow$ via CP
- $^{13}$CO $T_2 \rightarrow$ via CP

2D Experiments

CC experiments

- $h^{13}$C $\rightarrow$ CP DARR
- $h^{13}$C $\rightarrow$ CP DREAM
- $h^{13}$C $\rightarrow$ CP RFDR
- $h^{13}$C $\rightarrow$ CP Alfresco
- $h^{13}$C $\rightarrow$ CP BSH
- $h^{13}$C $\rightarrow$ CP HHmixing $h^{13}$C $\rightarrow$ CP INEPT
- CC $\rightarrow$ Direct INEPT
- $h^{13}$C $\rightarrow$ INEPT

HC experiments

- HC HETCOR $\rightarrow$ CP
- HC HETCOR $\rightarrow$ INEPT

NC experiments

- $h^{15}$N $h^{13}$C $\rightarrow$ CP HHmixing
- $h^{15}$N $h^{1}$C $\rightarrow$ Double CP
- $h^{15}$N $h^{1}$C $\rightarrow$ Double CP
- $h^{15}$N $h^{1}$C $\rightarrow$ INEPT
- $h^{15}$N $h^{1}$C $\rightarrow$ INEPT
- $h^{15}$N $h^{1}$C $\rightarrow$ CP BSH
- $h^{15}$N $h^{1}$C $\rightarrow$ INEPT
- $h^{15}$N $h^{1}$C $\rightarrow$ CP BSH
- $h^{15}$N $h^{1}$C $\rightarrow$ INEPT

3D Experiments

- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP /CP /CP
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP /CP /CP
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP /CP /DREAM
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP/CP/CP/DREAM
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP/CP/BSH
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP/CP/BSH
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP /CP /DARR
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP /CP /DARR
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP /CP /RFDR
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP /CP /RFDR
- $h^{15}$N $h^{1}$C $h^{1}$C $\rightarrow$ CP/BSH/DREAM
4D Experiments

\[ \text{hCANCOCX} \rightarrow \text{CP/CP/CP/DARR} \]
\[ \text{hCONCACX} \rightarrow \text{CP/CP/CP/DARR} \]
\[ \text{hCONCACB} \rightarrow \text{CP/CP/CP/DREAM} \]

Nitrogen detection

Set user default parameters: D1 & RG

Calibrations

Hard Pulse

15N Calibration based on hN CP experiment
15N Direct calibration

Cross Polarization

CP HN optimization

INEPT

hN

1D

HN \rightarrow \text{CP or INEPT}
15N T1 \rightarrow \text{CP}
15N T2 \rightarrow \text{CP}

2D

HN HETCOR \rightarrow \text{CP or INEPT}
hNN \rightarrow \text{CP PDSD}
hNhN \rightarrow \text{CP}
Listing S3: Example of parameter file (“recap file”), which can be saved (and retrieved) from the ssNMRlib window

# System: Avance III HD 600 NMR spectrometer

MAS Probe used : B6292_00230 (PH MASDVT 600S3 TL2 CNDH 1.3mm)
Probe diameter: 1.3 mm
Spinning rate: 55.006 (kHz)
Temperature : 258.0 (K) with Gas Flow measured : 1300.000000 (lph)
Topspin data location : /home/avallet/nmrsolids/2020-06-22_PythonTest_13mm/2
Sample id in sample database : 516

1Hcal  Hard_Pulse_on_1H : 3.28 (us)  @ 2020-06-24 10:04:05
1H_CPdefcal Hard_Pulse_for_CP_on_1H : 3.28 (us)  @ 2020-06-24 10:04:05
13Ccal Hard_Pulse_on_13C : 2.85 (us)  @ 2020-06-24 10:07:09
13C_CPdefcal Hard_Pulse_for_CP_on_13C : 2.85 (us)  @ 2020-06-24 10:07:09
15Ncal Hard_Pulse_on_15N : 3.40 (us)  @ 2020-06-24 10:10:45
15N_CPdefcal Hard_Pulse_for_CP_on_15N : 3.40 (us)  @ 2020-06-24 10:10:45

O1_calibration O1p : 4560 (Hz)  @ 2020-06-24 10:03:58

Water_Suppression_Delay D 30 : 0.15 (sec)  @ 2020-06-24 10:11:07
RFField_for_Water_Suppression CNST 24 : 12 (kHz)  @ 2020-06-24 10:11:07

CP_HN_BestRamp Ramp used: ramp90100.100  @ 2020-06-24 10:18:05
TargetField_1H_CP_HN_ramp90100_cal CNST 42 : 84 (kHz)  @ 2020-06-24 10:12:05
TargetField_15N_CP_HN_ramp90100_cal CNST 52 : 35.001 (kHz)  @ 2020-06-24 10:14:21
CP_HN_duration P 45 : 800 (us)  @ 2020-06-24 10:16:35

CP_HCA_BestRamp Ramp used: ramp50100.100  @ 2020-06-24 10:23:45
CP_HCA_duration P 43 : 3000 (us)  @ 2020-06-24 10:18:32
TargetField_1H_CP_HCA_ramp50100_cal CNST 41 : 14.454545 (kHz)  @ 2020-06-24 10:20:05
TargetField_13C_CP_HCA_ramp50100_cal CNST 31 : 39.998 (kHz)  @ 2020-06-24 10:22:25

CP_HCO_BestRamp Ramp used: ramp70100.100  @ 2020-06-24 10:28:26
TargetField_1H_CP_HCO_ramp70100_cal CNST 41 : 84.000000 (kHz)  @ 2020-06-24 10:23:58
CP_HCO_duration P 43 : 4750.000000 (us)  @ 2020-06-24 10:25:35
TargetField_13C_CP_HCO_ramp70100_cal CNST 31 : 35.002 (kHz)  @ 2020-06-24 10:27:05

CP_CN_BestRamp Ramp used: ramp90100.100  @ 2020-06-24 10:33:00
TargetField_15N_CP_CN_ramp90100_cal CNST 53 : 36.363636 (kHz)  @ 2020-06-24 10:28:48
CP_CN_duration P 53 : 9368.421053 (us)  @ 2020-06-24 10:30:02
TargetField_13C_CP_CN_ramp90100_cal CNST 33 : 16.999 (kHz)  @ 2020-06-24 10:31:31

CP_NCA_BestRamp Ramp used: ramp90100.100  @ 2020-06-24 10:39:14
TargetField_15N_CP_NCA_ramp90100_cal CNST 54 : 38 (kHz)  @ 2020-06-24 10:33:17
CP_NCA_duration P 35 : 9000.0 (us)  @ 2020-06-24 10:35:09
TargetField_13C_CP_NCA_ramp90100_cal CNST 34 : 15.362636 (kHz)  @ 2020-06-24 10:37:28

INEPT_delay_HN D 14 : 0.001 (sec)  @ 2020-06-24 10:42:08
INEPT_delay_HC  D 13 : 0.001 (sec)  @ 2020-06-24 10:43:35
INEPT_delay_NCO  D 53 : 0.010 (sec)  @ 2020-06-24 10:45:45
INEPT_delay_NCA  D 54 : 0.01 (sec)  @ 2020-06-24 10:47:27
TargetField_BSH_CP_cal  CNST 38 : 21.741217 (kHz)  @ 2020-06-24 10:50:01
TargetField_BSH_CP_duration_cal  P 38 : 4500 (us)  @ 2020-06-24 10:51:52
DARR_COCX_duration  D 5 : 0.2 (sec)  @ 2020-06-24 10:54:02
CP_DREAM_duration  P 17 : 5000 (us)  @ 2020-06-24 10:56:05
TargetField_DREAM  CNST 7 : 6.103091 (kHz)  @ 2020-06-24 10:57:58
RFDR_COCX_duration  D 8 : 0.004 (sec)  @ 2020-06-24 10:59:24
Each pulse sequence within the solid-state NMRlib module is associated with a jython script named as “experiment_p.py”. This script allows the user to define selectively which parameters will be verified for this specific experiment.

In order to perform the safety checks, the safety script will compare the parameter value within the topspin experiment with the safety table adapted by the user for his probes.

This safety table, so-called “Security_table_SSNMRlib.txt”, is located in “/NMRlib/py” and contains all the maximum values authorized for each probe.

An extract of this file is shown below.

| SIZE | PULSE TYPE | ELEMENT | DEFINITION | CSTN NAME | MAX. KHZ | PULSE | DURATION | UNIT | SPWN | MIDPOINT | RAPP | SEQ DETECTION |
|------|------------|---------|------------|-----------|----------|-------|----------|------|------|----------|------|---------------|
| 8.7  | HP         | 1H      | 1H HP      | CNST1     | 15       | P1    | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST2     | 15       | P2    | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST3     | 15       | P3    | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST4     | 15       | P4    | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST5     | 15       | P5    | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST6     | 15       | P6    | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST7     | 15       | P7    | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST8     | 15       | P8    | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST9     | 15       | P9    | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST10    | 15       | P10   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST11    | 15       | P11   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST12    | 15       | P12   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST13    | 15       | P13   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST14    | 15       | P14   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST15    | 15       | P15   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST16    | 15       | P16   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST17    | 15       | P17   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST18    | 15       | P18   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST19    | 15       | P19   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST20    | 15       | P20   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST21    | 15       | P21   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST22    | 15       | P22   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST23    | 15       | P23   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST24    | 15       | P24   | 15 us    |      |      |          |      |               |
| 8.7  | HP         | 1H      | 1H HP      | CNST25    | 15       | P25   | 15 us    |      |      |          |      |               |

The security check is automatically performed when an experiment is loaded from NMRlib. Moreover, if the user wants to change a parameter inside topspin, a “security button” can be hit, at any time, in order to re-do all the checks.

If a problem appears, a pop-up is generated showing the actual problematic topspin value and the specification in order to alert the user. This warning is also written in the topspin terminal.
In this way, each pulse sequence has its own personalized security which is adapted for its use and to the probe specification:

For each pulse sequence:
- All the parameters (water suppression elements, pulse, duration & RF power) within the pulse sequence are checked according to the probe.
- In a ramped RF shape, for CP or DREAM/BSH, the maximum value of the ramp is taken into account. To this end, the maximum value in the shape file is extracted, and the corresponding kHz value is calculated.
- The safety check verifies that midpoint of the ramp that is stored in a constant (e.g. cnst62 = 95 for a 90-to-100 ramp) and used for calculating the power level of the ramp, is indeed the mean of that ramp. This is done by explicitly verifying the ramp in the shape file.
- In CP experiments, the values of the two corresponding RF fields is checked. If the values are too far from Hartmann-Hahn conditions a popup window informs the user. This may point to mis-calibration of the reference pulses, as the CP power levels are calculated from them.
- If a list is used in the pulse sequence (e.g. the spin-lock duration in an $R_{1\rho}$ experiment), the safety check retrieves all the values within this list and determines the maximal value. This ensures that all values are within the safety limits.
- If an element is repeated multiple times, the safety check will verify the total duration, i.e. the duration of the unit element times the number of repeats.
- The decoupling times are retrieved automatically for the whole direct and indirect dimensions, i.e. the maximum evolution time ($t_{1\text{max}}$) is considered.

In addition, for the calibrations:
- As the parameter optimization array is define within the python script, negative values are automatically discarded.
- In a parameter optimization, the safety check verifies that none of the experiments of the array exceeds the allowed safety limits.
- Clicking the button of a calibration experiment generally starts the acquisition automatically. However, if a safety problem is detected, the calibration is not launched automatically.
Listing S4 : Security checks – How does it work?

Each pulse sequence within the solid-state NMRlib module is associated with a jython script named as “experiment_p.py”. This script allows the user to define selectively which parameters will be verified for this specific experiment.

In order to perform the safety checks, the safety script will compare the parameter value within the topspin experiment with the safety table adapted by the user for his probes. This safety table, so-called “Security_table_SSNMRlib.txt”, is located in “/NMRlib/py” and contains all the maximum values authorized for each probe.

An extract of this file is shown below.

| SIZE | PULSE TYPE | ELEMENT | DEFINITION | CSTN NAME | MAX. Hz | PULSE | DURATION | UNIT | SPIN | MIDPOINT | PARM | SEQ | DETECTION |
|------|------------|---------|------------|-----------|--------|-------|----------|------|------|----------|------|-----|------------|
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P1    | 15 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P2    | 15 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P3    | 15 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P4    | 25 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P5    | 25 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P6    | 25 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P7    | 25 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P8    | 25 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P9    | 25 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P10   | 25 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P11   | 25 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P12   | 25 us    |      |      |          |      |     |            |
| 8.7  | HP         | 3H      | 3H HP      | CSTN42    | 100    | P13   | 25 us    |      |      |          |      |     |            |

The security check is automatically performed when an experiment is loaded from NMRlib. Moreover, if the user wants to change a parameter inside topspin, a “security button” can be hit, at any time, in order to re-do all the checks.

If a problem appears, a pop-up is generated showing the actual problematic topspin value and the specification in order to alert the user. This warning is also written in the topspin terminal.
In this way, each pulse sequence has its own personalized security which is adapted for its use and to the probe specification:

For each pulse sequence:
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- In CP experiments, the values of the two corresponding RF fields is checked. If the values are too far from Hartmann-Hahn conditions a popup window informs the user. This may point to mis-calibration of the reference pulses, as the CP power levels are calculated from them.
- If a list is used in the pulse sequence (e.g. the spin-lock duration in an $R_{1p}$ experiment), the safety check retrieves all the values within this list and determines the maximal value. This ensures that all values are within the safety limits.
- If an element is repeated multiple times, the safety check will verify the total duration, i.e. the duration of the unit element times the number of repeats.
- The decoupling times are retrieved automatically for the whole direct and indirect dimensions, i.e. the maximum evolution time ($t_{1\text{max}}$) is considered.

In addition, for the calibrations:
- As the parameter optimization array is define within the python script, negative values are automatically discarded.
- In a parameter optimization, the safety check verifies that none of the experiments of the array exceeds the allowed safety limits.
- Clicking the button of a calibration experiment generally starts the acquisition automatically. However, if a safety problem is detected, the calibration is not launched automatically.
Listing S5: Adding an experiment in NMRLib

Routing file:
- If 1H detection experiment -> 1Hdetection
- If 13C detection experiment -> 13COnCaCx4D
- If 15N detection experiment -> 15Ndetection

Experiment name:  Experiment name, reference

Important parameters:
Parameters that can be popup for checking during the set-up of the experiment