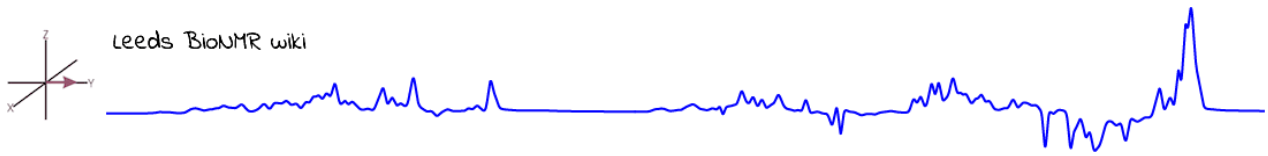
THIS IS A PDF VERSION OF THE CORRESPONDING WIKI PAGES



RelaxLib /

RelaxLib

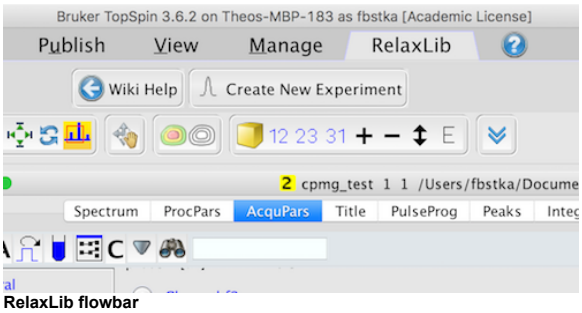
This is a Leeds topspin library for the automatic setup of 15N relaxation experiments

Currently installed on the 600. Please read this page before using,
a link to the wiki is provided in topspin.

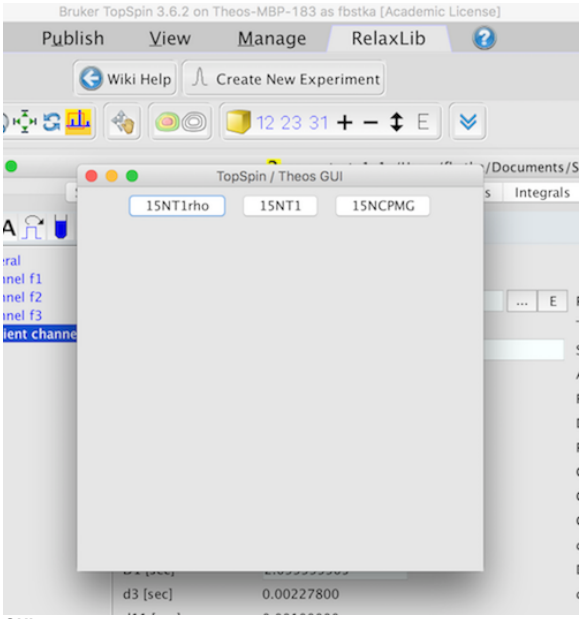
VERY IMPORTANT, check that the hard power levels are what you expect from pulse calibrations

Click the RelaxLib tab in topspin. This will bring up a flowbar with two options:

- Wiki Help. Provides a link to the wiki page
- CreateNewExperiment. This will bring up a window with buttons for the setup of the equivalent experiment.
  Look at the corresponding subpage for instructions.



RelaxLib flowbar

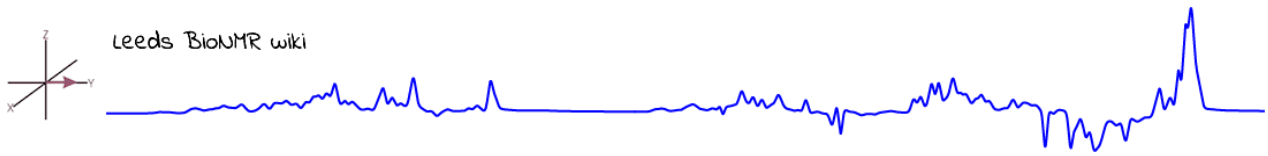


GUI

These experiments all measure the relaxation of the inphase 15N coherence and can be used in combination in fitting of NMR relaxation data. Examples:

1. Karamanos, Tugarinov, Clore, PNAS, 2020
2. Karamanos, Tugarinov, Clore, PNAS, 2019

Any questions ask Theo.



15NT1rho /

15NT1rho

Set **cnst28** to the spin lock field strength you want
eg. 1000 to 2500 Hz
The pulse lengths and power levels used in the parameter set are noted in the title.

1H channel:
Adjust your p1 to the calibrated value and
make sure pl1 is the correct proton hard power

13C channel:
Adjust your p2 to the calibrated value
make sure pl2 is the correct carbon hard power

15N channel:
Adjust your p7 to the calibrated value
make sure pl7 is the correct nitrogen hard power

Update the vplist with your spin lock delays (0 - 200 ms). (Always save as a new file)
Important Set **p18** to the maximum delay in us (eg 80000).
Set **TD1** to the number of delays
Set **TD2** to the number of 15N t1 points

For processing and analysis to extract R1rho rates see
15N T1rho
(Second half of the page)

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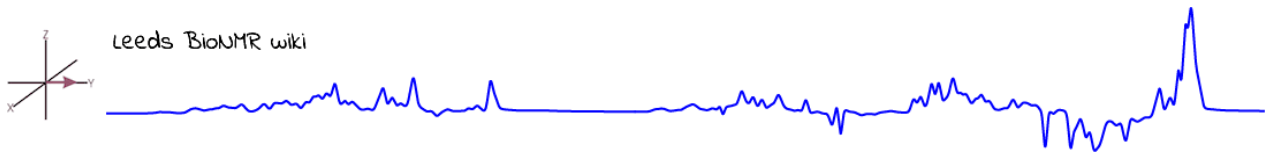

15NT1 /

15NT1

Normally used in combination with a T1rho experiment.
The pulse lengths and power levels used in the parameter set are noted in the title.

Heat compensation: Set **cnst28** to the spin lock field strength you used in the coresponding T1rho experiment
Important Set **p18** to the maximum delay in us (eg 80000).

1H channel:
Adjust your p1 to the calibrated value and
make sure pl1 is the correct proton hard power

13C channel:
Adjust your p2 to the calibrated value
make sure pl2 is the correct carbon hard power

15N channel:
Adjust your p7 to the calibrated value
make sure pl7 is the correct nitrogen hard power

Update the vclist with the ncyc (number of cycles) values. (Always save as a new file)
The T1 delay given by:

delay=ncyc*2*20ms (1)

Set **TD1** to the number of delays
Set **TD2** to the number of 15N t1 points

Processing and Analysis
You can use the scripts and the general procedure described in 15N T1rho
In the procX.com script change the tauList variable to the relaxation delays calculated from (1) **in ms**
Make sure that the number of points and SW in X, Y are correct (as you would normally do in fid.com)
*Use the product of TD2*TD1 (eg 256*3) as the total number of Y points.*

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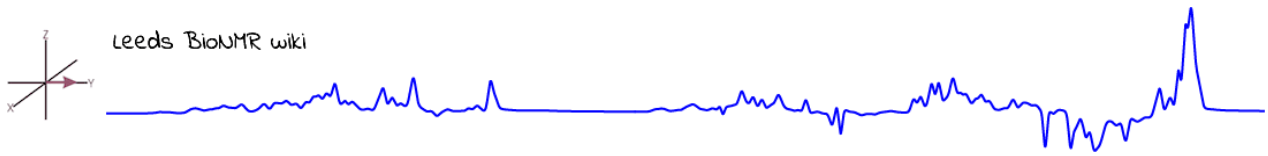

15NCPMG /

15NCPMG

This is the 15N CPMG experiment of Hansen et al, that uses 1H saturation during the CPMG period to keep the 15N magnetization inphase.

Clicking the 15N CPMG button in RelaxLib sets up a dataset which we use to setup our sample dependent parameters.
Specifically:
Set **d24** to the desired relaxation time (20 - 100 ms)
Set your desired **vclist**. Make sure that the max cpmg frequency is not higher than 1000 Hz
Set **TD1** to the number of cpmg points
Set **TD2** to the number of 15N t1 points
Use at least 8 scans

1H channel:
Adjust your **p1** to the calibrated value and
make sure pl1 is the correct proton hard power

13C channel:
Adjust your **p2** to the calibrated value
make sure pl2 is the correct carbon hard power

15N channel:
Adjust your **p7** to the calibrated value
make sure pl7 is the correct nitrogen hard power

After all these parameters are set we need to setup the power levels for the 1H decoupling. These depend on the value of ncyc, p1, pldb1, d24 (time_T2). To calculate them automatically type:

```
cpmg.py
```

This will append a line in the pulse program with the correct values of the 1H cw power levels.
The new pulse program is now called `auto_cpmg.ppy`.
You can now start the acquisition.

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