

Processing and analysis of ^{15}N R_1 , ^{15}N $R_{1\rho}$ relaxation and ^{15}N - $\{^1\text{H}\}$ HetNoe experiments

Spectra have been recorded on a Bruker Avance I system in an inter-leaved manner.

To split and process ^{15}N R_1 spectra with NMR Pipe, execute the following scripts and routines:

1. Execute *fid.com*
2. *split.com* (For R_1 , the Bruker vclist must be converted into vplist with ms entries beforehand.)
3. *nmrproc.com*
4. Peak pick with NMR Draw
5. Assign the spectra with *ass.com*
6. Execute *selectTab.com* which will collect all assigned peaks in the file relax.tab
7. Copy+paste the header of sum.ass.tab into the header of relax.tab
8. *relax.com*
9. *model.com*
10. *summary.tcl -in relax.tab > t1.tab*
11. Copy t1.tab into a newly created directory data
12. R_1 rates will be calculated together with the $R_{1\rho}$ and R_2 using: *crtR1p.tcl | sort -n > ouput.tab*
(Beforehand the $R_{1\rho}$ data should be evaluated.)

^{15}N $R_{1\rho}$ spectra

- 1.-11. Steps 1 to 11 are identical to the processing of the R_1 spectra, generate the table t1rho.tab
12. Copy the following entry in the header of the t1rho.tab file and adjust spectrometer and ^{15}N carrier frequency as used in experiment

```
REMARK 600MHz for T1rho
REMARK -yOBS = 60.818
REMARK -yCAR = 119.06
```

13. *extract_PPM.com* will generate a table called fusionOffset.tab that contains the offset of the peak ^{15}N frequency relative to the carrier frequency (which will be needed to calculate the angle θ for the extraction of R_2 data from the R_1 and $R_{1\rho}$ data).

14. Copy the files `t1rho.tab` and `fusionOffset.tab` to the directory *data*.
15. Adjust spectrometer frequency, spin-lock power, in the script `crtR1p.tcl` and execute:
crtR1p.tcl | sort -n > R1R2.tab
16. `R1R2.tab` will contain the fitted $R_{1\rho}$ rates, theta angle, R_2 rates and R_1 rates.

$^{15}\text{N}\{-^1\text{H}\}$ Noe spectra

$^{15}\text{N}\{-^1\text{H}\}$ Noe spectra have been recorded in an inter-leaved manner.

1. To split the spectra create a vplist (0 1).
 2. *fid.com*
 2. *split.com*
 3. *ft2.com*
 4. Peak pick the spectra.
 5. *ass.com*
 6. *selectTab.com*
 7. Copy header of `sum.ass.tab` to `relax.tab`
 8. *script.com*
 9. *autoFit.com*
 10. Determine the noise in the spectra and enter in the script *error_hetnoe.tcl*
 11. Execute *error_hetnoe.tcl | sort -n > hetnoe.tab*
- Hetnoe.tab contains the $^{15}\text{N}\{-^1\text{H}\}$ Noe values.