

## Processing and analysis of $^{15}\text{N}$ $\text{R}_1$ , $^{15}\text{N}$ $\text{R}_{1\rho}$ relaxation and $^{15}\text{N}\{-^1\text{H}\}$ HetNoe experiments

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

To split and process  $^{15}\text{N}$   $\text{R}_1$  spectra with NMR Pipe, execute the following scripts and routines:

1. Execute *fid.com*
2. *split.com* (For  $\text{R}_1$ , 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.  $\text{R}_1$  rates will be calculated together with the  $\text{R}_{1\rho}$  and  $\text{R}_2$  using: *crtR1p.tcl | sort -n > ouput.tab*  
(Beforehand the  $\text{R}_{1\rho}$  data should be evaluated.)

## $^{15}\text{N}$ $\text{R}_{1\rho}$ spectra

- 1.-11. Steps 1 to 11 are identical to the processing of the  $\text{R}_1$  spectra, generate the table t1rho.tab
12. Copy the following entry in the header of the t1rho.tab file and adjust spectrometer and  $^{15}\text{N}$  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  $^{15}\text{N}$  frequency relative to the carrier frequency (which will be needed to calculate the angle  $\theta$  for the extraction of  $\text{R}_2$  data from the  $\text{R}_1$  and  $\text{R}_{1\rho}$  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.