# Processing and analysis of $^{15}N$ $R_1$, $^{15}N$ $R_{1\rho}$ relaxation experiments

Spectra has been recorded on a Bruker system

**$^{15}N$ $R_1$**

1. Copy the files from the attached folder T1 to the working directory (experiment folder).
2. *$ chmod u+x *.com*
3. *$ bruker* to open the NMRPipe Conversion Utility and generate the *fid.com* file.
4. *$ fid.com*
5. *$ split.com* (For R1 the Bruker *vclist* must be converted into a *vplist* with ms entries beforehand: *$ mv vclist vplist* and edit the *vplist*).
6. *$ nmrproc.com* (Edit the tauValues [*vplist* values] beforehand).
7. *$ nmrDraw* to draw the spectrum and pick the peaks. If the phase is not correct press v for vertical 1D-signal projection and h for horizontal 1D-signal projection. With P0 you can adjust the phase, remember the phase difference and correct the phase in the *nmrproc.com* file.
8. *$ ass.com* (copy a peak list in your working directory beforehand) to assign the spectra. Left mouse button to assign, right mouse button to deassign peaks.
9. *$ python3 NoneDeleter.py* to create *relax.tab*.
10. *$ relax.com*
11. *$ autoFit.com*
12. *$ model.com*
13. *$ modelExp.com*
14. *$ bash summary.tcl -in relax.tab > t1.tab*
15. Copy *t1.tab* into a newly created directory *data*.

**$^{15}N$ $R_{1rho}$**

1. Copy the files attached from the folder T1rho to the working directory (experiment folder).
2. *$ chmod u+x *.com*
3. *$ bruker* to open the NMRPipe Conversion Utility and generate the *fid.com* file.
4. *$ fid.com*
5. *$ split.com*
6. *$ nmrproc.com* (Edit the tauValues [*vplist* values] beforehand).
7. *$ nmrDraw* to draw the spectrum and pick the peaks. If the phase is not correct press v for vertical 1D-signal projection and h for horizontal 1D-signal projection. With P0 you can adjust the phase, remember the phase difference and correct the phase in the *nmrproc.com* file.
8. *$ ass.com* (copy a peak list in your working directory beforehand) to assign the spectra. Left mouse button to assign, right mouse button to deassign peaks.
9. *$ python3 NoneDeleter.py* to create *relax.tab.*
10. *$ relax.com*
11. *$ autoFit.com*
12. *$ model.com*
13. *$ modelExp.com*
14. *$ bash summary.tcl -in relax.tab > t1rho.tab*

15. $ Copy the following header in the *t1rho.tab* file (you get the values from the *fid.com* file):

    REMARK 600MHz for T1rho

    REMARK -yOBS = 60.818

    REMARK -yCAR = 119.06

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