The original MATLAB fitting script is developed by Chevelkov, *et al.* for 15NH/D-SOLEXSY spectral processing. We did some modifications and created a graphic interface to process the output from Sparky.

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This package includes:

1. Example

Peakheights\_deut\_WTGB3: output from Sparky for the 1N2H build-up profile

Peakheights\_prot\_WTGB3: output from Sparky for the 1N1H decay profile

SOLEXSY\_output : the files output after running the SOLEXSY program in MATLAB

1. MATLAB\_scripts

SOLEXSYFIT.m : master script for fitting SOLEXSY data

parseSparkyDecayList.m : function used to read the residue numbers and intensities from the Sparky data file

getMixingtimes.m : function used to read the mixing time from the Sparky data file

chi2\_simple35.m : function used to calculate SOLEXSY profiles and evaluate the difference (chi2) between the calculated and measured profiles (same with original script)

chi2\_simple35noise.m : same as chi2\_simple35.m, but operates on the profiles with added noise; introduced for purely technical reasons (same with original script)

chi2\_simple\_plot35.m : same chi2\_simple35.m, but prepares the data for plotting of the best-fit SOLEXSY profiles (same with original script)

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In Sparky “Relaxation Fitting” module (go to Extensions, Integration, Relaxation peak heights) output each residues peak heights at different mixing time for the original protonated 15N1H and deuterated 15N2H respectively. The number of residues for each one should be matched.

Open SOLEXSYFIT.m file in MATLAB

Click “Run” in MATLAB, a SOLEXSY-FIT graphic interface will open.

In the SOLEXSY-FIT interface load Deutoron file (e.g. Peakheights\_deut\_WTGB3), Proton files (e.g. Peakheights\_prot\_WTGB3) respectively, and then the number of H and D peaks will be displayed which are required to be matched.

Input the number of Monte Carlo simulations

Input the NMR spectral noise

Click to generate the initial guess

Click FIT& GENERATE PLOTS to start processing

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Finally fit\_dataout35ref, fit\_genout35error, fit\_genout35ref and v35plot\_Res#res.eps are created in the same folder. The format is same with the original output file of Chevelkov et, al.

In fit\_genout35error.dat each column represents:

res : residue

k1H : k(HD) exchange rate from the original experimental data

k1Hav : average k(HD) exchange rate obtained from the spectra with added noise

k1std : standard deviation of k(HD) from the spectra with added noise

k2D k2Dav k2std : k(DH) exchange rate this is not an independent parameter, k1H=1.1\*k2D

R1H R1Hav R1Hstd : nitrogen longitudinal rate R1(NH)

R1D R1Dav R1Dstd : nitrogen longitudinal rate R1(ND)

a0H a0Hav a0Hstd : initial magnetization in protonated amide NzH(0)

a0D a0Dav a0Dstd : initial magnetization in deuterated amide NzD(0)

b0D b0Dav b0Dstd : filter leakage eps(H)

err : sqrt(chi2), rmsd between experimental and best-fit profiles

errk1 : err\*k1H

fit\_dataout35ref.dat : experimental SOLEXSY profiles + best-fit profiles

fit\_genout35ref.dat : reduced version of fit\_genout35error.dat, same notations

\*.eps : plots of the experimental SOLEXSY profiles + best-fit profiles for individual residues (residue number included in the filename)