

Instructions for extended Hadamard HETMAT experiment

You will need to copy TS/wavemaker/excitation/cw file to TS/wavemaker/inversion/cw_i wvm_x/wvm – Unix executable to be placed in Topspin/ext/stan/nmr/wavemaker/bin folder

1. Select imino ^{15}N - ^1H peaks from 2D HSQC/HMQC spectra using peak picking – and save it – automatic peak picking also works great but mind the threshold (note that up to 4 and 8 peaks will be encoded into eH4 and eH8 matrix, respectively)
2. Create new HETMAT experiment (use parameter set, not prosol compatible)
3. Use command “had_plx”
4. Type the experiment number with 2D spectrum where peaks are saved
5. “had_plx” will automatically create peak list inside HETMAT experiment
6. Based on spectral resolution and broadness of the peaks – choose appropriate γB_1 nutation field in cnst23 and pulse duration in cnst22 (20 Hz and 46 ms were used at 1 GHz NMR)
7. Choose mixing time in d8 – standard options are d8 = 80 – 125 ms
8. Choose the number of loops in L1 - by default use 8-14 loops
9. For using extended Hadamard matrix, copy eH4.had or eH8.had file and paste into the current experiment and then change filename into wvm.had
10. Use au program “wvm -a” to create all the pulses and update acquisition parameters
11. Use au program “wvm_x” to crease Hadamard pulses based on wvm.had file (if wvm.had file is missing, “wvm_x” will generate pulses based on the regular Hadamard matrix)
12. Start the experiment
13. Use “proc_hadx” to process the spectrum – zero filling set up with SI will artificially increase F1 resolution

When setting up experiment for the first time, ased will complain that it doesn't contain necessary pulses – after “had_plx”, do immediately “wvm -a” which will create pulses using default parameters and will allow you to go through pulse parameters. Don't forget to do “wvm -a” and “wvm_x” at the end again if you change cnst22 and cnst23