Instructions for extended Hadamard MT 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 protons' peaks from 1D (Watergate or 11-echo spectrum) using peak picking – and save it (note that up to 4 and 8 peaks will be encoded into eH4 and eH8 matrix, respectively)

2. Create new HMT experiment (use parameter set, not prosol compatible)

3. Use command "had_pl"

4. Type the experiment number with 1D spectrum where peaks are saved

5. "had_pl" will automatically create peak list inside HMT experiment

6. Type the experiment number with 1D spectrum where peaks are saved

7. Based on spectral resolution and broadness of the peaks – choose appropriate saturation B1 field in cnst23

8. Choose p28, duration of cw saturation – standard option is 600-800ms

9. For 15N labeled samples, in order to allow long saturation in the presence of 15N decoupling, without damaging the probe and heating up the sample, very soft decoupling should be used and applied in the middle of imino 15N chemical shift (for example pcpd7=500 us, cnst18 = 153ppm)

10. 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

11. Use au program "wvm -a" to create all the pulses and update acquisition parameters

12. 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)

13. Start the experiment

14. 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_pl", 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 cnst23