Instructions for Conducting NMR-Based Kinetics Measurements

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I. Setting Up the Experiment
   A. Optimize lock and shim at desired temperature with representative sample in NMR (ie. proper concentrations for actual NMR run)
   B. Load one-dimensional NMR experiment, typically ^{1}H
   C. Set spectral parameters (nt, np, sw, ss, etc.), appropriately
   D. Set **pad** equal to zero (pad=0)
   E. Type **time** <return> to obtain time for one experiment (e.g. ~347 s for one pulse sequence for a 20 mM sample)
   F. Decide the overall length of the kinetics run (e.g. 4 hrs (2400s)) and at what increments you would like to record spectra (e.g. every 10 mins (600s)) with 24 increments (2400s/600s)
   G. Determine preaquisition delay (pad) according to the length of one pulse sequence and increment size (e.g. 600s-347s=253s=pad)

II. To create array
   A. Type **array** <return>
   B. Instrument prompts *param to array*, type **pad** <return>
   C. Instrument prompts *# steps in array*, type **24** <return>
   D. Instrument prompts *starting value*, type **253** <return>
   E. Instrument prompts *array increment*, type **0** <return>
   F. Need to adjust first delay
      i. Type **pad[1]=0** <return>
   G. Type **time** <return> to get (approximate) total time for arrayed experiment
   H. Type **ga** <return> to begin experiment

III. Processing Spectra
   A. Type **ai** to set display in absolute intensity mode. for course baseline correction
   B. Type **cdc dc** for a coarse baseline correction (see application note on baseline correction for a better way to do this – if necessary)
   C. Viewing Spectra
      i. Type **ds(1)** to load first spectrum
      ii. Type **vsadj** to scale first spectrum (note that the integral intensity does not depend on vs, but it is useful to review the data set)
      iii. Type **dssh** to see comparison of spectra (inspect relative intensities)
   D. Printing
      i. To print one spectrum, type normal print commands
      ii. To print all spectra in a horizontal fashion, type **pl('all') page**

E. Saving
    i. To save fids, use normal save commands
    ii. To save display array of spectra, type **pl('all') page('filename.ps')**
    iii. To move saved array to archive
        1. Type **cp** ***filename*** **/archive/*your archive name*** <return>