12. HOMODEC on AM/AC Spectrometers

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I. Setting Up

- Obtain a normal ^1H NMR spectrum. Save file using **WR** command.
- Choose **all irradiation frequencies** that you want to irradiate, e.g., you have two such frequencies (*vide infra*).
- Frequencies can be selected by moving the cursor in EP mode to a desired position in the spectrum, followed by **O2** and **L**. On the first frequency, the spectrometer will offer FQLIST.001 as a default list name: you may hit **<ret>** to accept this name, or enter a new name of your own. All other frequencies, require just **O2** and **L**. Repeat this until you have chosen all the irradiation frequencies.
- **<ret>** to exit EP to Command Interpreter.
- **AS HOMODEC.AU <ret>**

  D1 = 1 (sec)
  O2 FQLIST.001
  1 = (first irradition frequency) **<ret>**
  2 = (second irradiation frequency) **<ret>**
  ...and so on, if you have more irradiation frequencies.
  3 = END

  (Note that this frequency list is automatically set if you have chosen the frequencies with **O2** and **L** commands in EP subroutine.)

  S3 = 20L (decoupler power; use **20L** to **10L**; the lower the number is, the higher the power)
  RD = 2.0 (0 can be used, but better if 1 or 2 sec is used)
  PW = 2.5 (whatever is used in job file)
  DE = (dead time: set automatically by the spectrometer)
  NS = 8 (number of scans)
  DS = 2 (number of dummy scans; **0** works fine in most cases)
  NE = 2 (number of experiments = number of irradiation frequencies)

II. Taking ^{1}H NMR Decoupling Spectrum

- **EXPT** does not work!! Calculate the experimental time as (RD+AQ)*(NS+DS)*NE*(~1.2). The factor 1.2 estimates the amount of disk access time spent. Use a larger number like 1.5 if RD+AQ<2 s, or 1.0 if RD+AQ>10 s. If the experiment is too long, adjust NS, DS, AQ or RD accordingly.
- **ZE**; **AU <ret>**

  INPUT FREQ. LIST FILENAME #1: **FQLIST <ret>**
  INPUT FID FILENAME #2: **KL** (any filename with no extension) **<ret>**
- FIDs are now collected and stored automatically into FILENAME #2's with extensions 1 through the total number of frequencies (i.e., KL.1 and KL.2).

III. Processing FIDs

- Work up the first irradiation spectrum as follows:

  LB = 0; **RE KL.1** (to read FILENAME #2.1); **EF** (do EM plus FT); **EP**; **<ctrl> R**; **BP**; **<ctrl> B**; phase the spectrum with **C**- and **D**-knobs; **M**; **<ret>**.

- Save the resulting irradiation spectrum, e.g., **WR SKL.1**.

- Process other irradiation spectra using EFP (EM + FT + PK) as follows:

  RE KL.2 (to read FILENAME #2.2); **EFP**; **WR SKL.2** (the second irradiation spectrum; any filename can be used).

  Or set **NE** = # files, and use **AU FT.AU** to automatically process all the files.

- To plot these spectra, set DPO, CX, and CY. Then, **PX**. In WP console, **USR FASTU** to send the stored spectrum to the PC data stations.

- **PO** (decoupler power off) before leaving the spectrometer.

IV. Listing of Automation Routine

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;  HOMODEC.AU
;  HOMONUCLEAR DECOUPLING USING ONE FREQ. LIST AND ONE POWER SETTING.

   1  FL #1   / INPUT FREQ. LIST  ; READ IN FREQ. LIST AND INITIALIZE POINTER
   2  ZE
   3  D1 HD O2 S3    ; TURN ON HOMODEC. WITH POWER S3 AND SET
                     ; O2 FREQ. FROM CURRENT FL LIST, INCREMENT
                     ; FREQ. POINTER.
   4  GO = 4         ; ACQUIRE DATA
   5  WR #2          ; INPUT FID
                     ; STORE FID
   6  IF #2          ; INCREMENT FILE EXTENSION
   7  IN = 2         ; LOOP FOR NEXT EXPERIMENT
   8  D1 DO
      EXIT           ; EXIT WITH DEC. OFF

;  PROGRAM REQUESTS A FILENAME FOR FREQ. LIST AND FID STORAGE
;  D1 = 1 SEC TO SET FREQ.
;  S3 = DESIRED DEC. POWER
;  NE DEFINES NUMBER OF ITEMS IN FL LIST = NO. OF EXPERIMENTS
;  USE RD AS DESIRED AND AT LEAST 2 DUMMY SCANS.
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