

Lab #3 Problem Set:

As usual, if you have any problem getting time on DRX300, logging-in, finding the Menthol sample, collecting data, processing data, analyzing data, or plotting data, please see either Mark Girvin or Sean Cahill.

1. Run and process the following 2D experiments on the DRX300 using the Menthol sample:

2D ^1H - ^{13}C HSQC
2D ^1H - ^1H COSY

Plot out the 2D spectra obtained. Indicate on the 2D ^1H - ^1H COSY spectrum the -CHOH proton signal (as diagonal peak) and proton signals that are coupled to it (as cross peaks) – is this data consistent with the results obtained from the homonuclear decoupling experiment done in Lab#2?

Assign on the 2D ^1H - ^{13}C HSQC spectrum the -CHOH cross peak – is this assignment consistent with the results obtained from the 1D ^{13}C spectrum with selective proton decoupling experiment done in Lab#2?

2. Assign all of the proton chemical shifts and carbon chemical shifts of Menthol (use the attached sheet) - there is no need to distinguish the chemical shifts of the methyls in the $(\text{CH}_3)_2\text{CH}$ - group and the protons of methylene groups.

If needed, use the following data under dataset name “LAB3” on the “nmr0” server:

expno 1 2D ^1H - ^{13}C HSQC
expno 2 2D ^1H - ^{13}C HMBC
expno 3 2D ^{13}C - ^{13}C INADEQUATE
expno 4 2D ^1H - ^1H DQF-COSY

Access the data by running xwinnmr on nmr0; the data is located on the “unmr0” drive under user “class” and dataset name “LAB3”. Use the “browse” command to go to desired dataset, then use “wrđ” command to copy data to your username, then use the “browse” command again to go to dataset in your directory. The data is unprocessed so you will need to process it first before you can analyze it.

