

NOE Difference on the DRX-400

XWINNMR vers. 3.1

Applicable to other Bruker Avance systems also

- Change Samples
- Wobb
- Shim
- Acquire 1D ^1H Spectra

Click on Utilities

Click on O2

Write down the Mhz values of the ^1H signals to irradiate

400.1324754 (look in the small info display box near top of display area)

400.1317992

400.1314016 (one of these values will be for the control..region of no peaks)

File....New

{create expno 11, 12, 13, 14, etc}

(Do not acquire any data in this new file dataset. We want this file to not contain any data until we start the AU program)

rpar

AA_noe.diff.BBO

click on all the parameter boxes *acqu, proc, plot, outd*

click on copy

eda

FQ1LIST (scroll down to near the bottom to locate)

click on **down-arrow** to right of filename **noe1**

click on **"EDIT CURRENT"**

O 400.13
2475.4
1799.2
1401.6

Do not modify first line in file

2nd line...this value in Hz + 400.13Mhz = O2 value that you wrote down earlier. Control freq.

$$400.1324754 = 2475.4$$

$$\{400.13 \text{ Mhz} + 2475.4 \text{ hz} = 400.1324754 \text{ Mhz}\}$$

3rd line....enter next O2 value

4th line....enter next O2 value

NS 16 or more

DS 4

xau noediff

program will ask to verify a few parameters

4 interleaves or more

Process & Phase the **"Control"** Spectra

(**re 11** **re control#**)

edc

create new **expno** (20), (21), (22), etc

edp

DC = -1
Datmod = raw

edc2

data #2 = expno of irradiated 1H
data #3 = expno of control

NAME2 *filename*

EXPNO2 **12**

PROCNO2 **1**

NAME3 *filename*

EXPNO3 **11** "control"

PROCNO3 **1**

Process.....Special Processing.....File Algebra.....addfid

efp

irradiated peak should be negative
anti-phase peaks are subtraction errors
look for peaks with proper phase

Now process & plot & list values from all experiments
for use in calculating % NOE enhancement

Read in the **“Control”** data (re 11 re *control#*)

cy = 1000

wpar john {*parameters to save, proc & plot & title*}

basl

integrate {*calibrate integral that remains constant for scaling*}

save as reg **wmisc** → integ → john

lipp

rpar john

rmisc → integ → john

efp

basl

intscl = -1

cy = -1

lipp ===== *this output will be scaled relative to your 1st listing*