- Run a 1H Experiment First
    - Run with Narrowest possible sweep width
        - run 1H experiment
        - expand around spectrum
            - click on spectrum with left button
            - define left cursor with middle button
            - define right cursor with middle button
            - display will expand around the cursors.
        - click "utilities", then "sw-sfo1"
            - write down "sw" and "O1"
            - click "return"
    - type "rg"
        - write down number
        - DOT NOT CHANGE VALUE
        - hit carrage return on keyboard
- type "dir" and choose "cosy"
- type "acqu" to go to acquisition window
- type "eda"
    - You will see 2 columns of numbers: F2 and F1
        - F2 is the directly detected dimension (normal 1D) (this is t2 in my notes)
        - F1 is the indirectly detected dimension (this is t1 in my notes)
    - You only need to change a few parameters
        - TD in F2 column
            - this is the number of points that will be collected in t2
            - if this number is too large (like what is normally used in 1D H NMR) the data files will be too large for the computer to handle.
            - try 1k -> 2k (k = 1024)
        - TD in F1 column
            - this is the number experiments performed in 2D or equivalently the number of points in t1.
            - if this is too large, not only will the data set be too large to handle, the experiment will take a long time to do.
            - try 512 -> 1k
        - NS (number of scans). Needs to be a multiple of 8.
        - DS (number of dummy scans: scans without acquistion used to create a steady state magnetization for the experiment) try 0, 2, or 4
        - SW F1 and F2. (sweep widths for 1st and 2nd dimensions) enter the value determined in your 1D H NMR experiment (see above)
        - rg (receiver gain) set to value used in 1D H NMR experiment (see above)
        - O1 (center frequency of spectrum) You will need to scroll down a little to find this parameter. Use the value that you used in the 1D H NMR experiment (see above)
        - click on "save"
- Other parameters
    - D1 (recycle delay) set to (1-5)*T1 (longitudinal relaxation time)
    - P1 (H 90 pulse) about 10us
- type "expt"
    - This will give you the experiment time
    - If the experiment will take too long, you can either change NS or TD{F1} (in eda)
    - You should expect the experiment to take 3-12 hours.
- Type "zg" to run the experiment.
- Come back when the experiment is finished.

- Set up processing parameters. Type "edp".
    - SI{F2} = TD{F2}
    - SI{F1} = 2*TD{F1}
    - wdw{F2} = wdw{F1} = GM
    - To set lb and gb for F1 and F2
        - use my defaults of lb = -1.0 and gb = 0.1
        - or find good values for your experiment
            - click "save"
            - type "rser 1"
            - click "process", then "manuel window adjust"
                - will get a duel display
                    - Top: damped FID with window function
                    - Bottom: Fourier Transform of this FID
                - click "gm"
                - click "+" or "-" next to "lb" and "gb" to adjust the values
                - adjust "lb" and "gb" until FID goes to zero at end and the spectrum looks good to you
                - write down values of "lb" and "gb"
                - click "return"
            - Click "file", then "recall last", then "last 2D data set"
            - type "edp"
            - enter valuse of "lb" and "gb" into the proper fields
            - click "save"
- type "xfb" to Fourier Transform both dimensions
- 2D spectrum will be displayed
- Phase 2D
    - click "phase"
    - click "row"
        - Will now get cross hairs in 2D spectrum
        - click on a peak with the middle mouse button
        - click with right mouse button to remove cross hairs
        - can change the chosen slice by clicking "+" and "-"
        - when you have the slice that you want, click "mov:1"
            - will move slice to window 1
            - you can change the height of spectrum with "*2" and "/2" buttons below the "mov:1:2:3" buttons
    - choose 2 other rows and move them to windows 2 and 3 with the "mov:2" and the "mov:3" buttons. Choose the to sample entire spectrum (peaks near both edges and in the middle)
    - phase with "PH0" and "PH1" (remember that the peaks in this experiment are not all positive)
    - click "column" and follow the same procedure (steps 2-4 above) to phase the columns.
    - click "return", then "save and return"
      the program will ask: "start xfbp?" (perform phasing in both dimensions)
      click "OK"
- Plot 2D
    - Define Plot Region
        - click on the box (upper left of xwinnmr window)
        - outline the region of interest
            - hold right mouse button to draw box around peaks
            - click right button to define region
    - Define Intensity of Spectrum

        - click "+/-" twice (until gauge on right side of xwinnmr window shows both red and purple region. This shows both positive and negative peaks)
        - click on "*8", "/8", "*2", "/2" until the spectrum intensity is as you want it.
    - Open "output", then "Define/Show Plot region", then "According to screen limits". Program will ask:
        - "change levels?" answer "Y"
        - "Please enter number of pos. levels" enter the number of positive levels that you want. try 5
        - "Please enter number of neg. levels" enter the number of negative levels that you want. try 5
        - "Display contours?" answer "N"
    - To see what will be plotted
        - type "view"
        - quit view window by clicking on "quit"
    - Plot by typing "plot"

II. NOESY

- Run a 1H Experiment First

    - Run with Narrowest possible sweep width
        - run 1H experiment
        - expand around spectrum
            - click on spectrum with left button
            - define left cursor with middle button
            - define right cursor with middle button
            - display will expand around the cursors.
        - click "utilities", then "sw-sfo1"
            - write down "sw" and "O1"
            - click "return"
    - type "rg"
        - write down number
        - DOT NOT CHANGE VALUE
        - hit carrage return on keyboard
- type "dir" and choose "noesy"
- type "acqu" to go to acquisition window
- type "eda"
    - You will see 2 columns of numbers: F2 and F1
        - F2 is the directly detected dimension (normal 1D) (this is t2 in my notes)
        - F1 is the indirectly detected dimension (this is t1 in my notes)
    - You only need to change a few parameters
        - TD in F2 column
            - this is the number of points that will be collected in t2
            - if this number is too large (like what is normally used in 1D H NMR) the data files will be too large for the computer to handle.
            - try 1k -> 2k (k = 1024)
        - TD in F1 column
            - this is the number experiments performed in 2D or equivalently the number of points in t1.
            - if this is too large, not only will the data set be too large to handle, the experiment will take a long time to do.

        - try 512 -> 1k
    - NS (number of scans). Needs to be a multiple of 8.
    - DS (number of dummy scans: scans without acquistion used to create a steady state magnetization for the experiment) try 0, 2, or 4
    - SW F1 and F2. (sweep widths for 1st and 2nd dimensions) enter the value determined in your 1D H NMR experiment (see above)
    - rg (receiver gain) set to value used in 1D H NMR experiment (see above)
    - O1 (center frequency of spectrum) You will need to scroll down a little to find this parameter. Use the value that you used in the 1D H NMR experiment (see above)
    - click on "save"
- Other parameters
    - D1 (recycle delay) set to (1-5)*T1 (longitudinal relaxation time)
    - P1 (H 90 pulse) about 10us
    - D8 (mixing time for cross relaxation) try (0.01->1.0)*T1 (longitudinal relaxation time) you might need to do a series of NOESY experiment as a function of D8
- type "expt"
    - This will give you the experiment time
    - If the experiment will take too long, you can either change NS or TD{F1} (in eda)
    - You should expect the experiment to take 3-12 hours.
- Type "zg" to run the experiment.
- Come back when the experiment is finished.
- Set up processing parameters. type "edp"
    - SI{F2} = TD{F2}
    - SI{F1} = 2*TD{F1}
    - wdw{F2} = wdw{F1} = GM
    - To set lb and gb for F1 and F2
        - use my defaults of lb = -1.0 and gb = 0.1
        - or find good values for your experiment
            - click "save"
            - type "rser 1"
            - click "process", then "manuel window adjust"
                - will get a duel display
                    - Top: damped FID with window function
                    - Bottom: Fourier Transform of this FID
                - click "gm"
                - click "+" or "-" next to "lb" and "gb" to adjust the values
                - adjust "lb" and "gb" until FID goes to zero at end and the spectrum looks good to you
                - write down values of "lb" and "gb"
                - click "return"
            - Click "file", then "recall last", then "last 2D data set"
            - type "edp"
            - enter valuse of "lb" and "gb" into the proper fields
            - click "save"
- type "xfb" to Fourier Transform both dimensions
- 2D spectrum will be displayed
- Phase 2D
    - click "phase"
    - click "row"
        - Will now get cross hairs in 2D spectrum
        - click on a peak with the middle mouse button

        - click with right mouse button to remove cross hairs
        - can change the chosen slice by clicking "+" and "-"
        - when you have the slice that you want, click "mov:1"
            - will move slice to window 1
            - you can change the height of spectrum with "*2" and "/2" buttons below the "mov:1:2:3" buttons
    - choose 2 other rows and move them to windows 2 and 3 withe the "mov:2" and "mov:3" buttons. Choose the slices to sample entire spectrum (peaks near both edges and in the middle)
    - phase with "PH0" and "PH1" (remember that the peaks in this experiment are not all positive)
    - click "column" and follow the same procedure (steps 2-4 above) to phase the columns.
    - click "return", then "save and return"
      the program will ask: "start xfbp?" (perform phasing in both dimensions)
      click "OK"
- Plot 2D
    - Define Plot Region
        - click on the box (upper left of xwinnmr window)
        - outline the region of interest
            - hold right mouse button to draw box around peaks
            - click right button to define region
    - Define Intensity of Spectrum
        - click "+/-" twice (until gauge on right side of xwinnmr window shows both red and purple region. This shows both positive and negative peaks)
        - click on "*8", "/8", "*2", "/2" until the spectrum intensity is as you want it.
    - Open "output", then "Define/Show Plot region", then "According to screen limits". Program will ask
        - "change levels?" answer "Y"
        - "Please enter number of pos. levels" enter the number of positive levels that you want. try 5
        - "Please enter number of neg. levels" enter the number of negative levels that you want. try 5
        - "Display contours?" answer "N"
    - To see what will be plotted
        - type "view"
        - quit view window by clicking on "quit"
    - Plot by typing "plot"

III. H C 2D Correlation Experiment (2D HC INEPT)

- Run a 1H and 13C Experiments First

    - Run with both spectra with the narrowest possible sweep widths
        - run 1H experiment
        - expand around spectrum
            - click on spectrum with left button
            - define left cursor with middle button
            - define right cursor with middle button
            - display will expand around the cursors.
        - click "utilities", then "sw-sfo1"
            - write down "sw" and "O1"
            - click "return"

        - repeat steps b and c with 13C experiment
- type "dir" and choose "HC_inept_2d"
- type "acqu" to go to acquisition window
- type "eda"
    - You will see 2 columns of numbers: F2 and F1
        - F2 is the directly detected dimension (normal 1D) (this is t2 in my notes)
        - F1 is the indirectly detected dimension (this is t1 in my notes)
    - You only need to change a few parameters
        - TD in F2 column
            - this is the number of points that will be collected in t2
            - if this number is too large (like what is normally used in 1D H NMR) the data files will be too large for the computer to handle.
            - try 1k -> 2k (k = 1024)
        - TD in F1 column
            - this is the number experiments performed in 2D or equivalently the number of points in t1.
            - if this is too large, not only will the data set be too large to handle, the experiment will take a long time to do.
            - try 512 -> 1k
        - NS (number of scans). Needs to be a multiple of 16.
        - DS (number of dummy scans: scans without acquistion used to create a steady state magnetization for the experiment) try 0, 2, or 4
        - SW F1 and F2. (sweep widths for 1st and 2nd dimensions)
            - SW{F2} = sweep width from your 13C NMR experiment (see above)
            - SW{F1} = sweep width form your 1H NMR experiment (see above)
        - O1 (center frequency of 13C spectrum) You will need to scroll down a little to find this parameter. Use the value that you used in the 13C experiment (see above)
        - O2 (center frequency of 1H spectrum) You will need to scroll down a little to find this parameter. Use the value that you used in the 1H experiment (see above)
        - click on "save"
- Other parameters
    - D1 (recycle delay) set to (1-5)*T1 (longitudinal relaxation time)
    - P1 (H 90 pulse) about 10us
    - type "rga" to set receiver gain.
- type "expt"
    - This will give you the experiment time
    - If the experiment will take too long, you can either change NS or TD{F1} (in eda)
    - You should expect the experiment to take 3-12 hours. THIS TENDS TO BE A LONG EXPERIMENT.
- Type "zg" to run the experiment.
- Come back when the experiment is finished.
- Set up processing parameters. type "edp"
    - SI{F2} = TD{F2}
    - SI{F1} = 2*TD{F1}
    - wdw{F2} = EM wdw{F1} = GM
    - To set lb and gb for F1 and F2
        - use my defaults of
            - for F2 lb = 5
            - for F1 lb = -1.0 and gb = 0.1
        - or find good values for the lb{F2}

- click "save"
- type "rser 1"
- click "process", then "manuel window adjust"
  - will get a duel display
    - Top: damped FID with window function
    - Bottom: Fourier Transform of this FID
  - click "em"
  - click "+" or "-" next to "lb"" to adjust the values
  - adjust "lb"" until FID goes to zero at end and the spectrum looks good to you
  - write down values of "lb"
  - click "return"
- Click "file", then "recall last", then "last 2D data set"
- type "edp"
- enter valuse of "lb"" into the proper fields
- click "save"

- to find values for lb{F1} and gb{f1} take a 1H spectrum with TD = TD{F1} and use the manuel window adjust to find good values. Enter the values in the proper fields in edp.

- type "xfb" to Fourier Transform both dimensions
- 2D spectrum will be displayed
- Phase 2D
  - click "phase"
  - click "row"
    - Will now get cross hairs in 2D spectrum
    - click on a peak with the middle mouse button
    - click with right mouse button to remove cross hairs
    - can change the chosen slice by clicking "+" and "-"
    - when you have the slice that you want, click "mov:1"
      - will move slice to window 1
      - you can change the height of spectrum with "*2" and "/2" buttons below the "mov:1:2:3" buttons
  - choose 2 other rows and move them to windows 2 and 3. Choose the slices to sample entire spectrum (peaks near both edges and in the middle)
  - phase with "PH0" and "PH1" (remember that the peaks in this experiment are ALL POSITIVE)
  - click "column" and follow the same procedure (steps 2-4 above) to phase the columns.
  - click "return", then "save and return"
    the program will ask: "start xfbp?" (perform phasing in both dimensions)
    click "OK"
- Plot 2D
  - Define Plot Region
    - click on thebox (upper left of xwinnmr window)
    - outline the region of interest
      - hold right mouse button to draw box around peaks
      - click right button to define region
  - Define Intensity of Spectrum
    - click "+/-" twice (until gauge on right side of xwinnmr window shows both red and purple region. This shows both positive and negative peaks)
    - click on "*8", "/8", "*2", "/2" until the spectrum intensity is as you want it.
  - Open "output", then "Define/Show Plot region", then "According to screen limits".
    Program will ask

        - "change levels?" answer "Y"
        - "Please enter number of pos. levels" enter the number of positive levels that you want. try 5
        - "Please enter number of neg. levels" enter the number of negative levels that you want. use 0 (there should be no negative peaks in this experiment)
        - "Display contours?" answer "N"
- To see what will be plotted
    - type "view"
    - quit view window by clicking on "quit"
- Plot by typing "plot"