BARE BONES GUIDE TO gradientCOSY
on the Varian Inova-400&500 (with PFG probe) VNMRJ 3.2

This guide is written assuming proficiency in basic operation of the Varian NMR instrument. You should be experienced in performing basic 1-dimensional NMR experiments before attempting to perform 2D experiments on your own. Please ask for help the first time you perform this, to minimize your frustration.

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These instructions represent one way to setup this experiment and acquire the data using the VNMRj 3.2 software. The GUI interface allows all of this to be done with little or no typing, but this guide is intended as a self-start guide for users who have previously used the older, VNMR 6.1C software.

These instructions leave your ^{1}H spectrum in Exp:1, and acquire your 2D in Exp:2, (or another experiment number), alloweing the same ^{1}H spectrum to be used for setting up multiple 2D experiments if desired. If you are not familiar with the Varian/Agilent "Experiment Number" workspace concept, please be sure to ask for an explanation from Dr. Shoemaker or NMR Facility Staff before proceeding.

Note: All **commands** in boldface assume that you press **<Return>** afterwards.

1) Make sure you are working in Exp:1 (type **jexp1**, and verify you are working in Exp:1).
2) Acquire a normal ^{1}H NMR spectrum, and save it to be used as a 1D-Trace for the 2D-plots.
3) *Type* **mf(1,2) <space> jexp2 <Enter>** (this means: "move fid" … meaning, "copy" your FID and parameters from Exp:1 to Exp:2, then join Exp:2) – *Note, that you could substitute "3" for "2" in the above line if you have already setup another experiment in Exp:2… i.e., mf(1,3) jexp3 … would copy the 1H NMR located in Exp:1 to Exp:3, and then join Exp:3 for further setup.*
4) Place the red-cursors around the region of interest – DO NOT ZOOM IN. (Note: if you select a region with peaks outside that region, you will have *folded* peaks in your spectrum...this can be OK, or it can be a problem; depending upon where the folded peaks land).
5) Type **movesw** , (or *click* on [MoveSW] in the [Acquire] panel. and this will set the spectral width and offset to match your selected window – ignore the apparent change to the shift scale at this point – go to the next step.
6) Go to the [Experiments] Pull-Down menu, via [*Convert Current Experiment to Do…*], [Homonuclear Correlations], [gradient COSY].
7) Set NT (# transients) in the [Acquire]/[Defaults] panel, or just type in the command line…
   a) If your sample is very concentrated, you can use **nt=1** (this takes the minimum amount of time).
   b) For the best spectrum with minimal artifacts, use **nt=2**.
   c) Use **nt=4** for more dilute samples (will take 2x as long as (b)).
8) Set the number if increments in the *t1* dimension:
   a) Under [Acquire]/[Defaults], you can select the number of increments in the second dimension ("ni").
   b) ni should be 128 by default, You select or type **ni=256** . This improves resolution, but it takes longer.
9) Type **time** (or *click* on [Show Time]) to see how long the experiment will take (*optional*).
10) *Click* on [Acquire] **(**or type **cpgo**) to start the experiment.
    a) You can process the data while it is acquiring via the [Process][Default] panel.
11) If you must stop the acquisition before it is done (i.e., you run out of time), always stop the 2D experiment by typing: **sa('nt')** . This will stop the experiment at the end of the current FID.

12) Save the data using "Save As…", navigate to your Directory in /nmrdata/rgroups/group/user, the same as you would with a 1D spectrum. Verify that the data is saved properly.

13) Type **jexp1** , eject your sample, and re-insert the reference. Lock on the reference as usual.