

2-D gradient DQCOSY

IU NMR Facility – August 31, 2004

Summary:

COSY or its gradient version gCOSY are easy to run and useful 2-D NMR experiments. Resolution is limited in absolute value mode however, and large singlets (i.e. from solvents) can dominate these experiments. Absolute value DQCOSY provides the COSY information with singlets removed and no relay peaks but at lower S/N. The phase sensitive DQCOSY offers excellent resolution to extract coupling constants for example, has the diagonal in-phase and ideally singlets are completely suppressed. The gradient version gDQCOSY is especially attractive as it is free from subtraction errors and nt can be 1 to provide fast results.

Experiment Overview:

- 1) Set up is similar to other phase sensitive 2-D homonuclear experiments.
- 2) Do not spin the sample. Lock, shim and acquire a ¹H spectrum with a 90 degree pulse width. Phase and reference it. Use **movesw** to narrow the observation width if desired. Optionally copy the parameters to another experiment with for example **mp(1,2)**.
- 3) Type **iugdqcpsy** or use the Other/2D menu and select **gdqcpsy**. For a longer or shorter experiment vary any of **ni**, **nt** and **d1**. **nt** can be 1!

Processing:

- 1) No separate processing macro is currently provided for gDQCOSY. After acquiring the data, process with **wft2da** optionally preceded with linear prediction setup, for example: **lp2d(1024)**.
- 2) The macros **plot2d** or **iuplcosy** can be used to plot the 2-D data with the 1-D spectrum on the sides. Type **plot2d** and follow the prompts. Typical inputs for **iuplcosy** are something like **iuplcosy(12,1.4,1,3,3) iupage** which will plot up to 12 positive contour levels (1 negative level by default) with a spacing of 1.4 and plot the spectrum in EXP1 on the sides with a scaling factor of 3. Learn more about either with **man('cosy')** or **man('plot2d')** help files.

Notes:

It is often useful to save your data again after processing (overwrite the original data) to save the processing parameters so that the next time you call up the data you can simply type **wft2da** to view it.

See other guides for more information on processing and displaying 2-D experiments!