

2D-*J* Spectroscopy

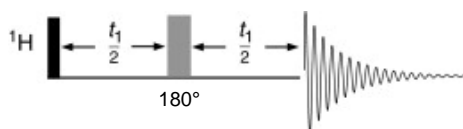
- Displays 1D splitting on second axis.
- Can be applied to any nucleus; most useful for deconvoluting overlapping resonances.

2D Total Correlation Spectroscopy (2D TOCSY)

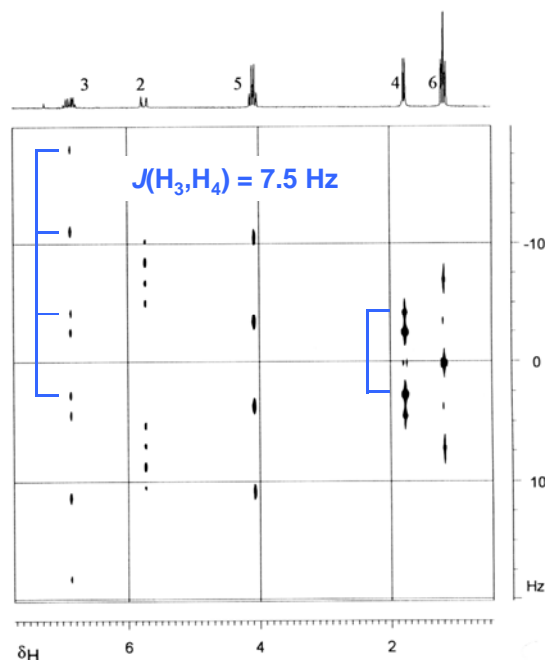
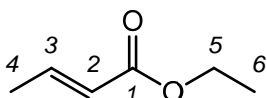
- Typically ^1H - ^1H homonuclear.
- All protons in a continuous coupled set (connected by 2J or 3J) show crosspeaks.
- Often used to characterize biomolecule oligomers.

2D-*J* Spectroscopy

Displays 1D splitting on second axis.

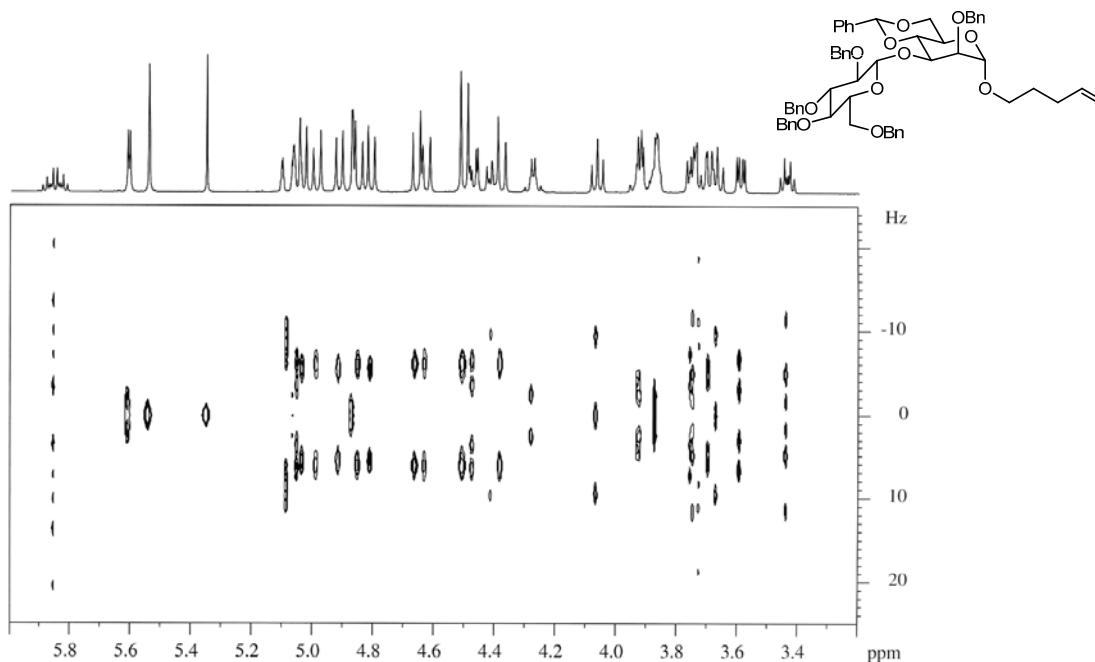


Method is like spin-echo, except w/ t_1 on second axis.



2D-*J* Spectroscopy

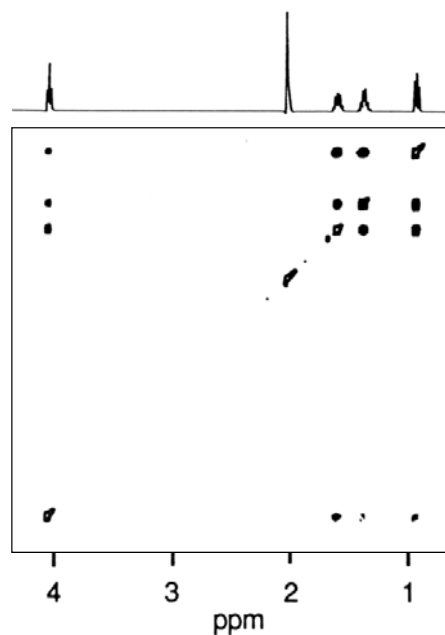
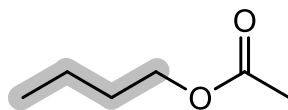
Good for deconvoluting overlapping multiplets.



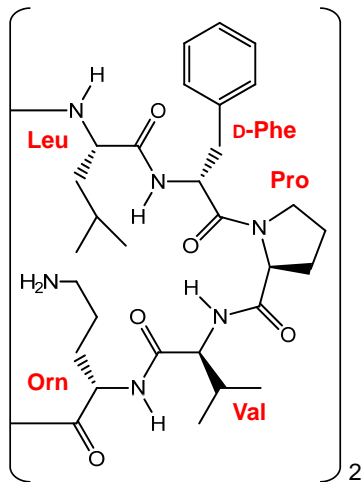
2D Total Correlation Spectroscopy (2D TOCSY)

- Typically ¹H-¹H homonuclear.
- All protons in a continuous coupled set (connected by ²*J* or ³*J*) show crosspeaks.

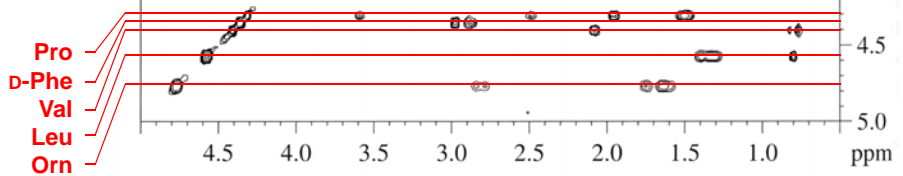
All four protons in chain correlate.



2D TOCSY

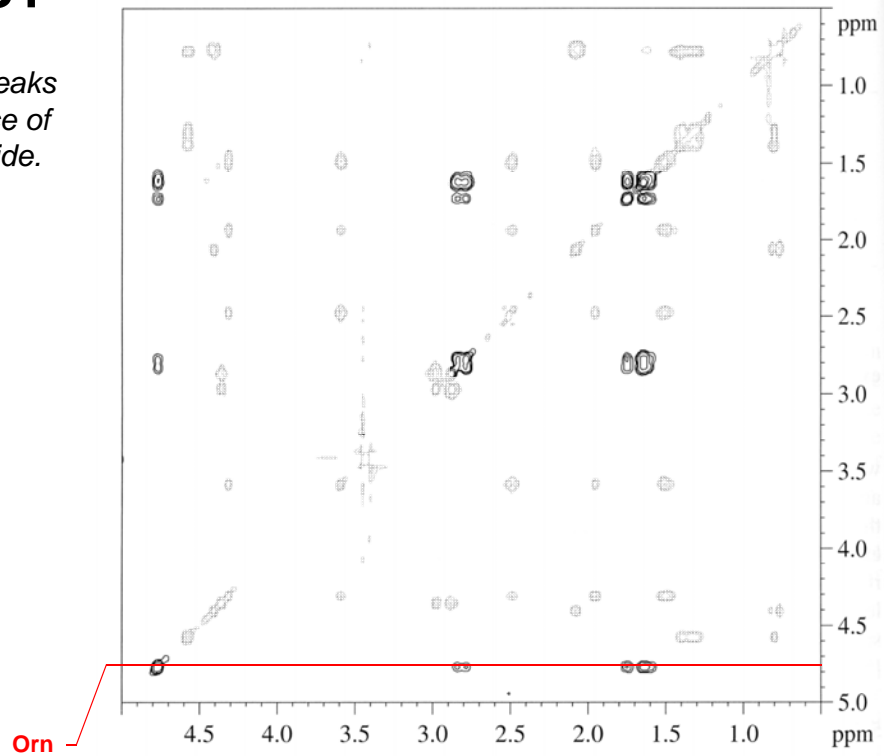
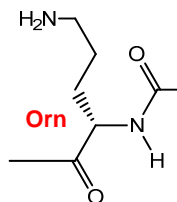


gramicidin S (in $CDCl_3$)



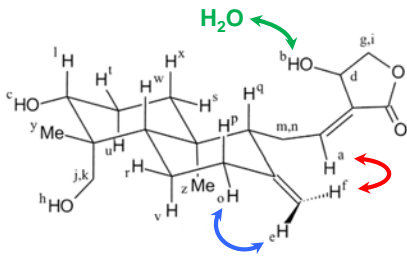
2D TOCSY

Pattern of crosspeaks confirms presence of ornithine in peptide.

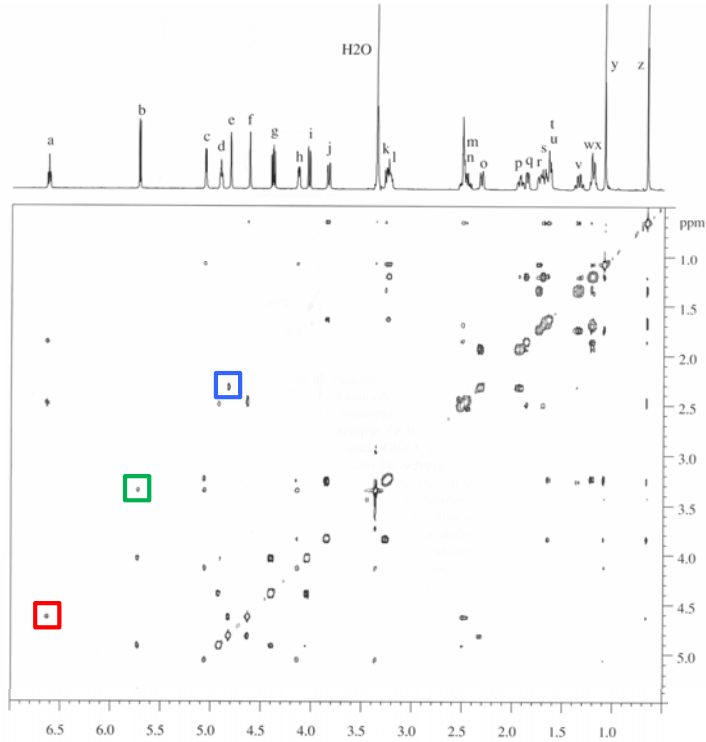


2D NOE Correlation (NOESY)

Measures through-space NOE correlations, shows them as off-diagonal peaks. Magnitude related to $\sim 1/r^6$ (as with 1D NOE).

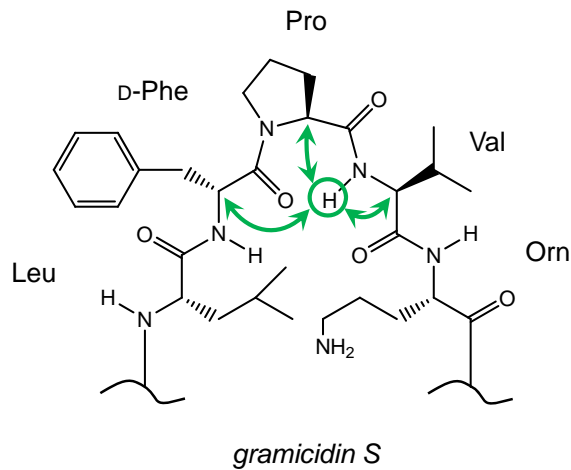
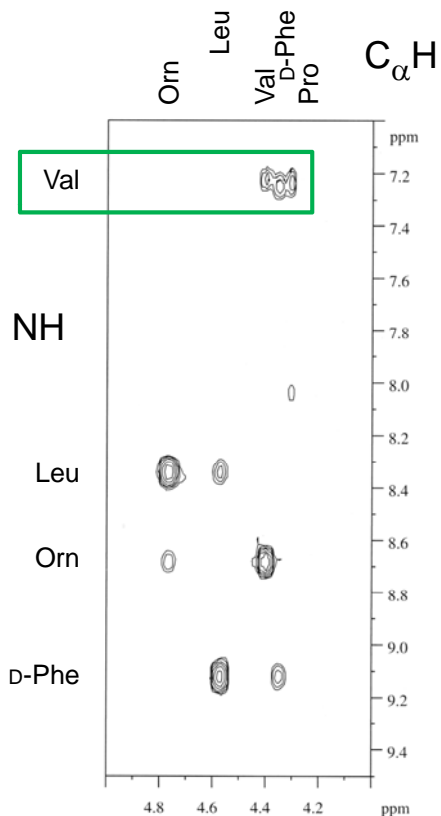


Warning: Rapid chemical exchange also shows crosspeaks.



2D NOESY

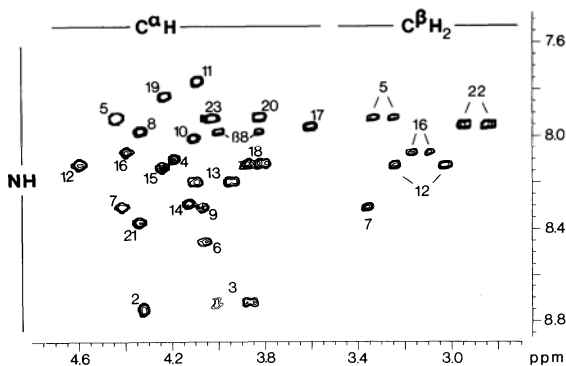
Great for analyzing spatial relationships in large molecules.



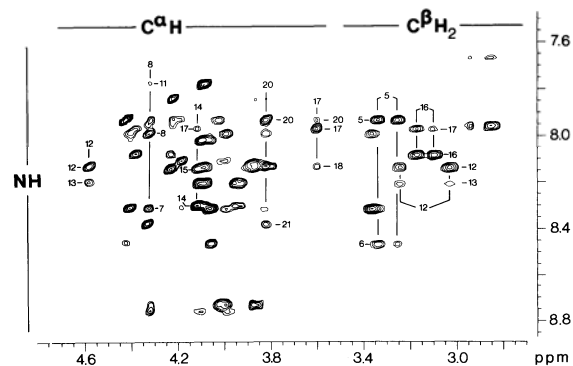
Three correlations with Val NH indicates that it is part of a Pro turn.

Scalar Crosspeaks in 2D NOESY

2D TOCSY



2D NOESY



both of magainin, a 23-amino-acid peptide.

NOESY spectra will sometimes contain scalar coupling (2J , 3J) artifacts.
Running NOESY with zero-quantum filtering (and pulsed-field gradients)
eliminates these artifacts.

Users can also collect a TOCSY spectrum to rule out these peaks.