CALCULATING COSY AND HMBC SPECTRA

While coupling constants are rarely reported, they are of course required to determine splitting patterns in proton spectra and in providing 2D spectra, specifically HH coupling constants for COSY spectra and CH coupling constants for HMBC spectra, both of which are essential tools for assignment of structure. The "raw" experimental data are in presented in the form of contour plots, while calculated results are given in terms of a series of circles on a 2D plot corresponding to large couplings. A large degree of concurrence suggests that they are likely to be referring to the same or a very similar molecule whereas significant differences signals that something is amiss.

Two different display modes for calculated COSY and HMBC spectra are supported. The first displays all couplings ($^{3}J^{HH}$ for COSY and both $^{2}J^{CH}$ and $^{3}J^{CH}$ for HMBC) where the absolute value of the coupling constant is greater than a set magnitude. These take the form of open circles the size of which is independent of the magnitude of the coupling constant, but for HMBC the color of which depends on whether it is 2 or 3-bond. Rather than displaying the contour plot obtained directly from the COSY or HMBC experiment, assigned couplings are entered manually. Matching calculated and experimental data (that is, involving the same atoms) can be "linked" with ellipses drawn connecting the circles and crosses. The second mode, applicable only where experimental data have been provided, displays only calculated couplings for which an experimental coupling has been provided. As it is much less crowded (depending on the threshold set for displaying calculated couplings), it is likely to be the more useful of the two in trying to see if calculated and experimental HMBC spectra closely match.