snapToCarbonHSQC

Introduction

This tool is used when the HSQC peaks are picked manually. When this occurs, the carbon coordinates of the HSQC peaks may be different from the values in the 1-D carbon spectrum. This can lead to problems when the simpleNMR program attempts to harmonise all the different spectra and assign the carbons to their CHn group and to specific atoms in the molecule.

This tool attempts to move the carbon coordinates in the HSQC spectrum to the 1-D carbon spectrum values.

Using the Tool.

Peak pick the HSQC spectrum manually using the standard tools in MNOVA. Try to be as precise as possible by aligning the position of the peak over the carbon 1-D projection and the center of the proton peak or multiplet.

A screen shot of a graph

AI-generated content may be incorrect.

Figure 1 Manually peak pick the HSQC spectrum making sure the position is close to the carbon 1-D resonance as possible and at the center of the proton multiplet, not on the peak maximum.

Once all the peaks have been picked, integrate the peaks using the impleNMR 2-D integrate button. Then click on the Snap to Carbon button adjust the carbon coordinates of the HSQC peaks so that match the 1-D carbon values.

In the figure 2. A below one can see that the two diastereo-isomer peaks have been picked slightly above and below the position of the carbon resonance displayed at the side.

