

Side Chain navigation

Macro is based on "Browse resonances" popup. It is designed primarily to facilitate side chain display and assignments using strip plots, but can also be used for general resonance navigation. There are two modes of operation.

In the first mode, controlled by the top row buttons, user selects one or two resonances and navigates to the position defined by the chemical shifts. If only one resonance is selected the chemical shift defines the plane or the position in the plane depending on the spectra. If two resonances are selected they will define the strip. The resonances have to be assigned to different atom types, such as 1H and 13C.

In the second mode one proton or carbon resonance is selected and the whole side chain is displayed in the strip plot. The resonances are displayed in alphabetical order which is printed in the console window. If several strips are set in the 2D HSQC window, the vertical dimension will be centred on the last 13C resonance.

Spectra window selection. The spectra are selected through pull-down lists on the left. The first two correspond to 3D windows and the third is for a 2D HSQC. Only windows compatible with the selected resonances are displayed.

Buttons

Goto position. Display strips corresponding to one/two selected resonances.

Nxt/Prv/0 strip. Increment/decrement/zero active strip in all selected windows.

Mark Res. Mark all selected resonances. Can be any number of resonances.

Shw All Rs. Display strips corresponding to all CH groups from a residue identified by the selected resonance.

Mrk All Rs. Mark all CH resonances from a residue.

Del Marks. Delete all marks.

Please note. Although the popup looks like the Resonance popup, it currently does not have the full functionality. If you need to manipulate resonances you have to start the Resonance popup proper.

Suggested use in the side chain assignments. Get C^α/H^α , C^β/H^β from triple resonance spectra.

Display corresponding strips in HCH- and CCH-TOCSYs. Identify cross-peaks corresponding to other side chain resonances and assign them to the most likely positions in the side chain.

Confirm/refine assignments by navigating to the strips corresponding to new assignments.

Installation. Import ResTblScGui from ResTbl_igb.py using Macro->Edit macros.



