Selective Excitation Experiments

Take a proton spectrum in experiment 1.

Go to the top menu Edit and drag to Move FID. Move the FID from experiment 1 to experiment 2, and join experiment 2. In the Process tab click Transform to get a copy of the spectrum in experiment 1.

In the top menu Experiments drag to Convert current parameters to do.. - Selective Excitation – 1D z TOCSY. The TOCSY experiment reveals the signals of protons in the same coupling network as the excited one. Alternately, NOESY or ROESY will show the signals of the protons which have an nOE with the excited one, or exchange with it.

In the Acquire – Default tab put two cursors around the signal you want to excite, then click Select. Adjust the spinlock time. With increasing mixing time, the TOCSY spectrum will show signals for the protons more remote from the excited one. Check out Run a mix=0 spectrum, adjust the number of transients and the block size, to be a multiple of 16.

Check the autogain on, then Acquire.

To plot the selective excitation spectrum on top of the proton spectrum, in experiment 2 save the display you want with s1, then change the vertical position vp=90 and plot: pl pscale. Move the saved display parameters: md(2,1) jexp1 r1 ds then in CS plot click plot Spectrum and scale, then click make .pdf.
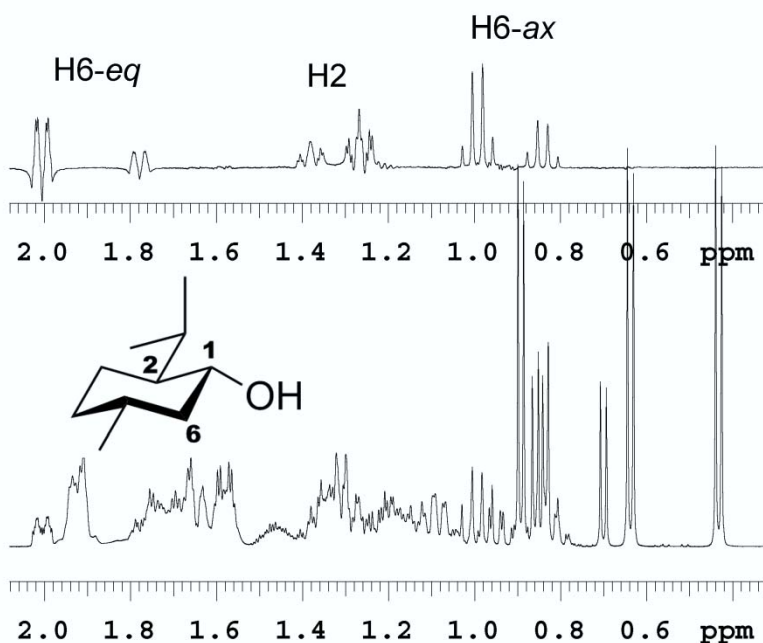
From Ghiviriga, I. *J. Org. Chem.* **2012**, *77*, 3978−3985.

Bottom: Proton spectrum of the reaction mixture of menthol with 2*R*+1*S*-MPA, DCC and DMAP. Top: TOCSY1D spectrum with selective excitation of H1 in the MPA esters.