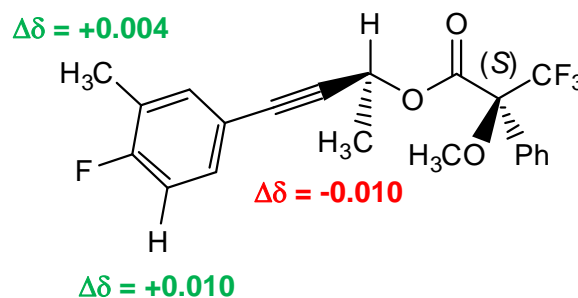
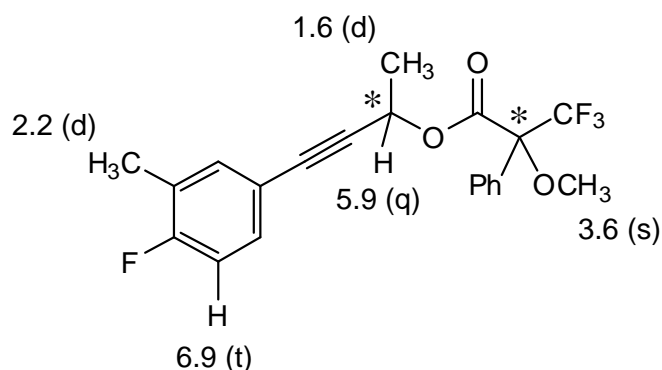


In-Class Exercise Solutions: Resolving Stereochemistry with Mosher Esters

- a. The first thing we need to do is assign at least some of the resonances in the spectrum to protons in the Mosher ester structure. For simplicity, I'll assign only the clearest resonances—I'll leave most of the aryl region alone. Something neat about this molecule are its fairly large proton-fluorine coupling constants; For the $\delta = 6.9$ ppm triplet, $^3J_{\text{HF}} = 9$ Hz (in addition to the $^3J_{\text{HH}} = 9$ Hz), and for the arylmethyl group, $^4J_{\text{HF}} = 2$ Hz.

Next, we ask, for each of these resonances, comparing the bottom spectrum to the top spectrum, did the peak move right ($\delta_S - \delta_R > 0$) or left ($\delta_S - \delta_R < 0$)? I always think of these issues in terms of the most stable conformation of the (S)-ester (shown at right). If $\Delta\delta < 0$, that means in the (S)-ester the resonance was pushed upfield (to lower δ values) by the face of the phenyl group. Here, the α -methyl group follows this pattern. On the other hand, if $\Delta\delta > 0$, that means in the (S)-ester the resonance is pushed downfield by the electronegative oxygen atom. Here, that is true of the alkynylphenyl group.



- b. So, the stereochemistry must be that shown above, (S) at the alcohol center.