

P-075: DETERMINATION OF THE ABSOLUTE CONFIGURATION OF TERTIARY ALCOHOLS BY ^{13}C NMR SPECTROSCOPY USING CHIRAL LANTHANIDE SHIFT REAGENT

Wai Sheung Ma, Bill J. Baker

Department of Chemistry, University of South Florida 4202 Fowler Avenue CHE 205, Tampa, FL 33620

Tertiary alcohol **1** has been synthesized by Grignard reaction and has been studied on its absolute configuration by ^{13}C NMR using chiral lanthanide shift reagent (R)- and (S)-Pr(tfc)₃. The ^{13}C chemical shift of **1** in the presence of (R)- and (S)-Pr(tfc)₃ causes a upfield and downfield shift, respectively, with respect to that with no shift reagent. Absolute configuration of the hydroxyl stereocenter can be determined by the $\Delta\Delta\delta$ value, which can be calculated by the chemical shifts of the α -carbons of the tertiary alcohol with (R)- and (S)-Pr(tfc)₃. The technique will be applied to determining the absolute configuration of chiral centers of more complex molecules containing the tertiary hydroxyl functionality such as norsellic acid **2**, a marine natural product.

