

Absolute Configurations of Brominated Sesquiterpenes Determined by Vibrational Circular Dichroism. Chirality 18:335

Abstrak

Two brominated sesquiterpenes, majapolene B (1) and acetylmajapolene B (2), isolated from the red algal genus *Laurencia* were investigated using vibrational circular dichroism (VCD). The ab initio theoretical VCD and IR calculations of 1 and 2 were performed by density functional theory (DFT) using the B3PW91/6-31G(d,p) basis set. The experimental VCD spectra and corresponding population-weighted theoretical VCD spectra were found to be in excellent agreement in CCl₄ solution in the 1800-850 cm⁻¹ region, which allowed unambiguous determination of the absolute configurations of (-)-1 and (-)-2 as 7S,10S and 7S,10S, respectively.