

Absolute configuration of the meroditerpenoids taondiol and epitaondiol diacetates by vibrational circular dichroism

Muñoz, Marcelo A.

Areche, Carlos

Rovirosa, Juana

Martín, Aurelio San

Gordillo-Román, Bárbara

Joseph-Nathan, Pedro

The absolute configuration of alga meroditerpenoids (-)-taondiol diacetate (1b) and (+)-epitaondiol diacetate (2c) are assigned by vibrational circular dichroism (VCD). The spectra of (2S,3S,6R,7R,10R,11R,14S)-1b and (2S,3S,6S,7S,10R,11R,14S)-2c enantiomers, calculated at the B3LYP/DGDZVP and at the B3LYP/DGDZVP2 levels of theory, respectively, matched confidently with the experimental ones. The numerical approach using neighborhood similarity indexes in the CompareVOA algorithm software supports the assignments with 100% confidence. The X-ray diffraction structures of 1b and 2c were determined to verify their relative stereochemistry and the crystal stereostructure of the meroditerpenoid stypotriol triacetate (5) is also reported. © 2012 The Japan Institute of Heterocyclic Chemistry.