

Absolute configuration of sargaol acetate using DFT calculations and vibrational circular dichroism

Muñoz, Marcelo A.

Areche, Carlos

Rovirosa, Juana

San-Martín, Aurelio

Joseph-Nathan, Pedro

The absolute configuration (AC) of sargaol acetate (2), isolated from the brown alga *Styopodium flabelliforme*, was determined using vibrational circular dichroism (VCD) measurements and density functional theory (DFT) calculations. Conformational searches using the Monte Carlo stochastic algorithm for 2 and three model compounds with a smaller side chain (diisoprenyl, isoprenyl and ethyl) provided 2172, 596, 82 and 12 conformations, respectively. In the last two cases the moderate number of conformations allowed conformational distributions assessment using single point energy calculations and considering a Boltzmann behavior. In the larger model molecules a prior selection from the original conformational set was done based on structure diversity as implemented in the Spartan'04 modeling software, keeping only 100 conformations in each case. All final conformers were further subjected to geometry optimizations and vibrational calculations providing weighted theoretical IR and VCD sp