# Absolute configuration of tropane alkaloids bearing two ?,?-unsaturated ester functions using electronic CD spectroscopy: Application to (R,R)-trans-3-hydroxysenecioyloxy-6-senecioyloxytropane

Humam, Munir

Christen, Philippe

Munoz, Orlando

Hostettmann, Kurt

Jeannerat, Damien

The absolute configuration of heterocyclic natural products substituted with two mobile ?,?-unsaturated esters was studied using electronic circular dichroism (CD) spectroscopy. The conformational flexibility of the side chains imposed the use of density functional theory calculation to determine the set of the most probable conformations in solution. The electronic CD and UV spectra were calculated by Boltzmann-weighted average of the simulated spectra using the results of the excited states calculation of a set of simplified structures. Comparison with the experimental CD spectrum allowed to determine whether the calculations were made with the right enantiomer. The method was applied to the determination of the absolute configuration of (R,R)-trans-3-hydroxysenecioyloxy-6-senecioyloxytropane. 