Structure and Absolute Configuration of Ginkgolide B Characterized by IR- and VCD Spectroscopy

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Experimental and calculated (B3LYP/6-31G(d)) vibrational Circular dichroism (VCD) and IR spectra are compared, illustrating that the structure and absolute configuration of ginkgolide B (GB) may be characterized directly in solution. A conformational search for GB using MacroModel and subsequent DFT optimizations (B3LYP/6-31G(d)) provides a structure for the lowest energy conformer which agrees well with the structure determined by X-ray diffraction. In addition, a conformer at all energy of 7 kJ mol(-1) (B3LYP/6-311+G(2d,2p)) with respect to the lowest energy conformer is predicted, displaying different intramolecular hydrogen bonding. Differences between measured and calculated IR and VCD spectra for GB at certain wavenumbers are rationalized in terms of interactions with solvent, intermolecular GB-GB interactions, and the potential presence of more than one conformer. This is the first detailed investigation of the spectroscopic fingerprint region (850-1300 cm(-1)) of the natural product GB employing infrared absorption and VCD spectroscopy. Chirality 22:217-223, 2010.

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