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STEREOCHEMISTRY OF FUROFURAN LIGNANS BY OPTICAL ROTATORY DISPERSION: INTERPLAY BETWEEN THEORY AND EXPERIMENT

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Furofuran lignans are important bioactive secondary metabolites widely distributed in the plant kingdom. Even though their biosynthesis is described from the enantioselective dimerization of two phenylpropanoid units, varying enantiomeric compositions have been reported in different plant species. Additionally, their absolute configuration assignments are mostly based on empirical comparisons of optical rotation values and electronic circular dichroism spectra obtained for structurally related molecules. Since the main structural differences among furofuran lignans reside on the substitution patterns of the aromatic moieties, as well as their relative orientations, this approach is risky and prone to error propagation. Currently, the most reliable procedure to use chiroptical spectroscopy involves the comparison of experimental data with those obtained by quantum chemical calculations. Thus, in the present work, we describe the use of optical rotatory dispersion (ORD) at 589, 578, 546, 436, 405 and 365 nm, associated with density functional theory (DFT) calculations, for the stereochemical analysis of the furofuran lignans sesamin, episesamin, eudesmin, epieudesmin, kobusin and phillygenin isolated from Aristolochiaceae species. The chiroptical properties of the target compounds were evaluated in methanol, acetonitrile and chloroform solutions. The results obtained allowed for an independent verification of the absolute configurations reported in the literature, besides providing information about the influence of different structural features and solvent effects for the specific rotation of this class of secondary metabolites.

Keywords: *ORD, DFT, natural products, absolute configuration, conformational analysis, chiroptical methods*

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