PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

SOLVENT-DEPENDENT SPECTROSCOPIC CHARACTERIZATION AND IN VITRO ANTITUMORAL EVALUATION OF 4-METHYLESCULETIN IN COLORECTAL CANCER CELLS

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Coumarins are a class of natural phenolic compounds widely investigated due to their diverse biological properties. Among them, 4-methylesculetin (4ME) stands out for its pharmacological potential, including antioxidant, anti-inflammatory, and antitumoral activities. Considering that the biological activity of a molecule can be strongly influenced by its structural stability and chemical structure in different environments, this study aimed to perform a comprehensive spectroscopic characterization of 4ME and to evaluate its biological effects in an in vitro colorectal cancer model. Spectroscopic

characterization was carried out using UV-Vis absorption spectroscopy and Fourier Transform Infrared (FTIR) spectroscopy. The molecule was analyzed both in solid form (powder) and in solution using different media (DMSO, ultrapure water, and DMEM/F12 culture medium). UV–Vis spectroscopy revealed a clear solvatochromic behavior, indicating that solvent polarity and composition significantly affect the electronic transitions of 4ME. In fact, the maximum absorption band shifted from 342.7 nm (water) to 350.0 nm (DMSO) and 357.7 nm (DMEM F12). This band is attributed to a p-p* transition from the HOMO-LUMO, thus, the polarity and ionic composition of the culture medium likely contribute to a reduction in the band gap energy between these orbitals. FTIR measurements confirmed the structural integrity of the 4ME through the preservation of characteristic vibrational bands (e.g., 744 and 1252 cm?¹, assigned to tCCOC + tCCCC + ?CCH + tCCCO and ?CC + ?CO + dCCC + dCCH). However, significant shifts were observed in the 1660–1696 cm?¹ region, associated with ?CC vibrations, as well as variations in ?CH and ?OH bands, indicating solvent-dependent interactions and changes in hydrogen bonds induced by DMEM/F12 culture medium. In parallel, in vitro assays were performed using colorectal adenocarcinoma (Caco-2) cells as a tumor model. Cells were treated with 4ME sat concentrations from 10-6 to 10-3 M for 24 h, 48 h, and 72 h. Cell viability was assessed by flow cytometry to evaluate potential cytotoxic effects and treatment response. Overall, the results demonstrate that the chemical behavior of 4ME is highly dependent on the surrounding environment, emphasizing the importance of solvent and medium composition in determining its stability and interaction in biological systems. These findings provide essential insights for interpreting the cellular effects of 4ME and support its further investigation as a potential anticancer candidate.

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Palavras-chave: 4-methylesculetin (4me); spectroscopy characterization; colorectal adenocarcinoma cells (caco-2); anticancer candidate.