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Abstract

A simple, accurate and fast spectrophotometric method for the quantitative determination of melatonin (ML) drug in its pure and pharmaceutical forms was developed based on the formation of its charge transfer complex with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) as an electron acceptor. The different conditions for this method were optimized accurately. The Lambert-Beer's law was found to be valid over the concentration range of 4-100 µg mL^{-1} ML. The solid form of the CT complex was structurally characterized by means of different spectral methods. Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations were carried out. The different quantum chemical parameters of the CT complex were calculated. Thermal properties of the CT complex and its kinetic thermodynamic parameters were studied, as well as its antimicrobial and antifungal activities were investigated. Molecular docking studies were performed to predict the binding modes of the CT complex components towards *E. coli* bacterial RNA and the receptor of breast cancer mutant oxidoreductase.

Keywords: Melatonin, DDQ, Charge transfer, TD-DFT, Molecular electrostatic potential, Spectrophotometry, Thermal analyses, Molecular docking.