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Molecular complexes of L-phenylalanine with substituted 1,4-benzoquinones in aqueous medium: Spectral and theoretical investigations

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Abstract

Various spectral techniques such as UV-Vis, FT-IR, and fluorescence have been employed to investigate the charge transfer interaction of L-phenylalanine (LPA) with substituted 1,4-benzoquinones (MQ_{1-4}). Kinetic and thermodynamic properties of the complexes were determined in aqueous medium at physiological condition (pH =7). The interaction of MQ_{1-4} with L-phenylalanine (LPA) was found to proceed through the formation of donor-acceptor complex, yielding a radical anion. The stoichiometry of the complexes was determined by Jobs continuous variation method and was found to be 1:1 in all the cases. Fluorescence quenching studies showed that the interaction between the donor and the acceptors is spontaneous. The results indicated that the progressive replacement of chlorine atom (-I effect) by methoxy group (+M effect) in the quinone decreased the electron acceptor property of the quinone. The order of the experimentally measured association constant of these complexes was well supported by DFT/B3LYP calculations.