ABSTRACT

Spectroscopic and theoretical studies on the charge transfer complexes of chosen drugs viz. ketoconazole, oxatomide, trimethoprim, cimetidine, azacyclonol and iron phthalocyanines with substituted 1,4-benzoquinones have been investigated. Various spectral techniques such as UV-Vis, FT-IR, emission, elemental, $^1$H NMR and LC-MS etc. were used to investigate the interaction between the donors and acceptors. The spectral, kinetic, thermodynamic studies and DFT calculations revealed the nature of the interaction between donor and acceptor. The rate of the interaction was observed to increase with an increase in the relative permittivity of the medium. The physico-chemical properties like oscillator strength, dipole moment, ionization potential and dissociation energy of the CT complexes indicated that the formed complexes are of strong type. The charge transfer complexes of two series of novel electron acceptors, 1,4-benzoquinones possessing variable number of methoxy/chloro groups and different alkoxy substitutents with azacyclonol and cimetidine drug molecules have been investigated. The charge transfer properties of these acceptors are investigated, for that first time, in aqueous medium. The stability constant of these interactions were obtained from electronic and emission spectral methods which are well correlated with theoretically obtained HOMO-LUMO energy gap values. The mechanism of the interaction of these biologically significant molecules studied may be useful in understanding the binding of these molecules in real pharmacokinetic study. A preliminary attempt was also made to use selected charge transfer adducts in colorimetric sensing of amino acids, amines and fluoride and acetate ions.