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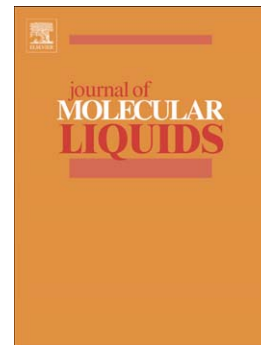
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Assessment of non-covalent interaction between insulin and some antibiotics in aqueous solution through ultrasonic studies and *in silico* docking analysis

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Abstract

The molecular interaction studies are carried out on ternary systems of human mixtard insulin (HMI) and four commonly used antibiotics in aqueous medium at four different temperatures (including physiological temperature of 310K) to assess the non-covalent interaction between the drug and insulin. Ultrasonic and refractometric investigations are extensively done to probe solute-solute interaction in the four ternary mixtures at different temperatures. Ultrasonic velocity (u), density (ρ) and viscosity (η) are measured at different temperatures and from these measured properties; thermo-acoustic parameters such as isentropic compressibility (κ_s), free length (L_f) and acoustic impedance (Z) are computed. The existence of solute-solute interaction in aqueous solutions of the ternary mixtures is established from the variation in ultrasonic velocity and other acoustical parameters with blend composition. Refractive indices are determined for the pure and blend solutions of antibiotics with HMI at the four temperatures. Molar (R_M) and relative molar refractive indices (ΔR_M) are reported for the four systems at four different temperatures. The trend in R_M and ΔR_M with blend composition is used to establish the composition at which the HMI-antibiotic interaction is strong. *In silico* docking analysis is carried out to assess the strength of interaction between HMI and different antibiotics.

Keywords : Human mixtard insulin; antibiotics; molecular interactions; ultrasonic, docking methods; H-bonding.

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