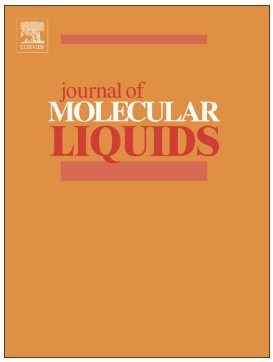


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Samima Khatun, Riyazuddeen, Faizan Abul Qais

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# Characterization of the binding of triprolidine hydrochloride to hen egg white lysozyme by multi-spectroscopic and molecular docking techniques

**Samima Khatun[1], Riyazuddeen[1]* and Faizan Abul Qais[2]**

[1]Department of Chemistry, Aligarh Muslim University, Aligarh, 202002, U.P, India

[2]Department of Agricultural Microbiology, Aligarh Muslim University, Aligarh 202002, U.P, India

Email: rz1@rediffmail.com

***Corresponding Author**

## ABSTRACT

The interaction between triprolidine hydrochloride (TRP), a strong histamine H1-receptor antagonist and hen egg white lysozyme (HEWL) was investigation by UV-vis, fluorescence, Förster's resonance energy transfer (FRET), circular dichroism (CD), fourier transform infrared (FTIR) and molecular docking studies. The steady state fluorescence study shows that TRP quenches the intrinsic fluorescence of HEWL through a static quenching mode which also supported by UV-vis absorption study. The binding constant $K_b$ was $2.31 \times 10^4$ $M^{-1}$ and binding stoichiometry (n) was approximately one. The synchronous fluorescence spectroscopy showed that the binding of TRP changed the microenvironment around Trp and Tyr residue to a more hydrophilic region. The FRET analysis established that there is energy transfer from HEWL to TRP. The decreased α-helical content of HEWL on interaction with TRP indicated that TRP destabilized the native structure of HEWL. The alterations in the secondary structure of HEWL in presence of TRP is also revealed by 3D fluorescence and FTIR spectroscopic studies. In addition, molecular docking was performed to confirm the binding site of TRP on HEWL, mode of binding and amino acids involved in this binding. This study will provide an insight into the molecular basis of the interaction between HEWL and TRP at pharmacological level and highlights its significance in the clinical medicine.

**Keywords:** Hen egg white lysozyme; Triprolidine hydrochloride; Fluorescence spectroscopy; Circular dichroism; Fourier transform infrared; Molecular docking.