

Accepted Manuscript

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

Samima Khatun, Riyazuddeen, Faizan Abul Qais



PII: S0167-7322(18)30916-4
DOI: doi:[10.1016/j.molliq.2018.08.040](https://doi.org/10.1016/j.molliq.2018.08.040)
Reference: MOLLIQ 9485
To appear in: *Journal of Molecular Liquids*
Received date: 21 February 2018
Revised date: 1 August 2018
Accepted date: 6 August 2018

Please cite this article as: Samima Khatun, Riyazuddeen, Faizan Abul Qais , Characterization of the binding of triprolidine hydrochloride to hen egg white lysozyme by multi-spectroscopic and molecular docking techniques. Molliq (2018), doi:[10.1016/j.molliq.2018.08.040](https://doi.org/10.1016/j.molliq.2018.08.040)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

Samima Khatun¹, Riyazuddeen^{1*} and Faizan Abul Qais²

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

²Department 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 investigated 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 is also supported by UV-vis absorption study. The binding constant K_b was $2.31 \times 10^4 \text{ M}^{-1}$ 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.

Download English Version:

<https://daneshyari.com/en/article/7841661>

Download Persian Version:

<https://daneshyari.com/article/7841661>

[Daneshyari.com](https://daneshyari.com)