Pharmacophore Recognition Study for HIV(I) Entry-Inhibition Drugs

Jyoti Sharma & Neelima Gupta\*

Design Innovation Centre (DIC-RU), Centre for Converging Technologies

University of Rajasthan, Jaipur

Email: jyoticct31@gmail.com, guptaniilima@gmail.com

Human Immunodeficiency Virus (HIV) is the reason for Acquired Immuno-Deficiency Syndrome (AIDS), whose treatment always remain as a hot topic in pharma research. Virus glycoproteins are the most enormous structural units responsible for initial binding to host cells leading to infection. For Human Immunodeficiency Virus, the protein gp120 plays the same role and binds with host CD4+ T cells [1]. HAART (Highly Active Anti-Retroviral Therapy) is a multiple antiretroviral drug therapy currently used to improve the treatment of HIV-positive and AIDS patients at different stages. HAART plays a decent role in early treatment of patients but shows some unfavourable results in the long-term consumption of selected drugs due to constant modifications in gp120. Entry inhibitor drugs are also used to deactivate the association of the gp120 viral protein with CD4 host cell [2]. Pharmacophore study is one of the effective ways to predict the biological activity pattern of the most efficient entry-inhibitor market drugs. Pharmacophore models represent chemical functions, valid not only for the bonding with currently known targets but also unknown molecules may be resultant from viral protein mutation [3]. BMS-488043, BMS-378806, BMS-626529, and BMS-663068 have been used in this study to predict the common features of drug molecules. The results focus on the identification of the main structural features of drugs responsible for interaction with the specific active site of HIV (type I) and alter their biological responses.

References

1. Yu F, Lu L, Du L, Zhu X, Debnath AK, Jiang S. Approaches for Identification of HIV-1 Entry Inhibitors Targeting gp41 Pocket. *Viruses*. 2013;5(1):127-149. doi:10.3390/v5010127.
2. Pandey D., Podder A., Pandit M., Latha N. (2016): CD4-gp120 Interaction Interface - A Gateway for HIV-1 Infection in Human: Molecular Network, Modeling and Docking Studies, *Journal of Biomolecular Structure and Dynamics*, DOI: 10.1080/07391102.2016.1227722
3. Yadav D, Paliwal S, Yadav R, Pal M, Pandey A. Identification of novel HIV 1--protease inhibitors: application of ligand and structure based pharmacophore mapping and virtual screening. *PLoS One*. 2012;7(11):e48942. doi: [10.1371/journal.pone.0048942](https://dx.doi.org/10.1371/journal.pone.0048942)