

***In silico* DESIGNING OF A PROSPECTIVE DRUG
AGAINST HUMAN HERPES VIRUS GROUP**



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SESSION: 2015-2017

**DEPARTMENT OF LIFE SCIENCES
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LAHORE, PAKISTAN.**

DECLARATION

I **Rabiya Nisar** d/o **Rana Nisar Ahmed** ID: **15001254012**, Session 2015-2017 hereby declare that the matter printed in the thesis titled “*In silico* Designing of a **Prospective Drug Against Human Herpes Virus Group**” is my own work and has not yet been printed, published and submitted as research work, thesis or publication in any form in any university, research institution etc. in Pakistan or abroad.

Dated:

Rabiya Nisar

DEDICATION

I dedicate this thesis

to

*my Parents, my Brothers Zubair Nisar Rana, Talha Nisar
Rana and my Sister Dr. Nida Nisar Rana*

without their prayers

I would never be able

to

work hard and gain this achievement.

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Rabiya Nisar

Abstract

The infection associated with Human Herpes Virus Group leads to long term effects in terms of various diseases, specifically neurological ones. The Herpes infection is an emerging threat and no clinically approved antiviral treatment is discovered yet to cure the disease. Computational approaches for drug development are proven to be effective and time efficient as these are not based on costly and hectic laborious works. In drug discovery, the molecular dynamics simulations help in the study of the motions of biological macromolecules such as proteins and nucleic acids. Computational mechanisms of biological targets and their related small-molecule ligands are useful in drug discovery; these include identifying the binding sites, virtual screening of numerous compounds libraries and estimation of ligand binding energies. The binding process of the tegument proteins with the inhibitors illuminates the process of inhibition with efficiency and specificity of that inhibitor. It was aim of the present study to identify potential inhibitors of the virus replication and the tegument proteins were targeted in this study using 2053 plant derived compounds. The successfully docked compounds with high binding affinity and reactivity are reported against the proteins. These are all effective drug like compounds. Due to higher affinities and reactivity of these compounds against the tegument proteins, these compounds can be further analysed using *in vitro* and *in vivo* approach to elucidate their inhibitory mechanism against HHV.

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1. Introduction

Herpesviridae family consists of the three sub-families which include (1) Alphaherpesvirinae, (2) Betaherpesvirinae and (3) Gammaherpesvirinae, their individuals taint a wide scope of creature species which includewarm-blooded creatures, reptiles and winged animals (Davison *et al.*, 2009). As of not long ago, in excess of 130 herpes-infections are found, from those eight are known as human pathogens. These include the Alphaherpesvirinae members varicella zoster infection (VZV), herpes simplex infection compose 1 (HSV-1) and herpes simplex infection write 2 (HSV-2). Betaherpesvirinae individuals human herpesvirus compose 6 (HHV-6) and human herpesvirus write 7 (HHV-7) and human cytomegalovirus (HCMV). Gammaherpesvirinae individuals Kaposi's sarcoma-related herpesvirus (KSHV) and Epstein-Barr infection (EBV). The HSV causes most ordinarily mucocutaneous diseases, bringing about repetitive or genital sores (Roizman *et al.*, 2007). HCMV contamination is in charge of around 8% of irresistible mononuclear-sister cases and is additionally connected with inflammatory ailments (Söderberg-Nauclér, 2006; Steininger, 2007). KSHV and EBV are related to a few malignancies, for example, Kaposi's sarcoma and Burkitt's lymphoma (Chang *et al.*, 1994; Kutok and Wang, 2006).