INTRODUCTION

The 2009 outbreak of Influenza A virus subtype H1N1 is a pandemic of a new strain of influenza virus identified in April 2009, commonly referred to as "swine flu." Unusually for a virus genome of Influenza virus contains seven or eight pieces of segmented negative-sense RNA, each piece of RNA containing either one or two genes. The influenza A genome contains 11 genes on eight pieces of RNA, encoding for 11 proteins: hemagglutinin (HA), neuraminidase (NA), nucleoprotein (NP), M1, M2, NS1, NS2(NEP), PA, PB1, PB1-F2 and PB2. According to antigenic properties, influenza virus has two functional surface glycoproteins: HA and NA (Wang et al., 2009 and Payungporn, 2010).

In terms of medication, the two FDA approved antiviral drugs, Tamiflu (oseltamivir) and Relenza (zanamivir) are effective against this new type of virus. Unfortunately, such virus types are known for their quick mutations and gene assortments which enable them to escape the host immune systems and resist drugs. Developing new antiviral drugs for this new H1N1 pdm virus is an extremely urgent matter. The influenza virus RNA-dependent RNA polymerase is a heterotrimeric complex (PA, PB1 and PB2) with multiple enzymatic activities for catalyzing viral RNA transcription and replication. The critical role of the polymerase complex in the influenza virus life cycle and high sequence conservation suggest it should be a major target for therapeutic intervention.

MATERIAL AND METHODS

We have followed the ten basic steps of SBDD for Swine flu, starting from the target identification to structure optimization by using various online and offline tools/software of drug designing.

Computational resources

Target for the drug designing was selected from the literature, target structure was validated from KEGG for pathways and other associated information related to the role of target in disease, sequence alignment was performed using BLAST, 3D target structure were retrieved using PDB, for visualizing 3D structure of protein SPDBV was used, target structure was validated using SAVES.

Ramachandran plots and statistics were generated by
PROCHECK (Singh et al., 2006), active site of the target protein was determined using LIGSITE. [2-amino-1,7-dihydro-6H-purine-6-one (C5H5N2O)] was identified lead molecule, using HEX 4.2 lead molecule was introduced into cavity, LIGBUILD was used for growing lead inside the binding pocket. For the purpose of docking QUANTUM 3.3.0 software was used. Finally for ADME/Tox exploration Molinspiration Cheminformatics, Orisis Property Explore, Molsoft LLC, Pharma algorithm online servers were used.

RESULTS AND DISCUSSION
Our aim was to develop safe drug molecule which is complementary (structurally as well as chemically) enough to inhibit the selected target molecule using computational biology and bioinformatics for the fatal disease H1N1 Swine Flu in short period of time, which recently had resulted in pandemic in several areas and is likely to cause pandemic with new strain of virus in future. After going through all the processes of Structure Based Drug designing (SBDD), we can conclude that the inhibitor molecule has grown successes fully inside the active site of protein molecule (RNA dependent RNA polymerase) and has made protein inhibitor complex with effective binding energy of -30.22KJ/mol. Thus through modifications and improvement, the drug can be used for the effective treatment of H1N1 Swine Flu. Following figures shows the Absorption, Distribution, Metabolism, and Excretion (ADME)/Tox exploration of newly developed drug.

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