ABSTRACT

BanLec, a carbohydrate binding protein, possessing anti-HIV activity was used in this research for understanding its interactions with the gp120 responsible for the binding of HIV with the $CD4^+$ cells. Non-antigenic Oligo-peptides and variants of the BanLec were also designed and analysed for their anti-HIV activity. Among all the variants of BanLec, Lectin B formed by removing 17 amino acids from the N-terminal of BanLec, showed 10 Hydrogen bonds when was interacted with the HIV gp120. Whereas a total of 9, 11 and 9 Hydrogen bonds were formed by Oligo-peptide 2 (CCNDCEQGHILKMFPSTWYV), Oligo-peptide 11 (RRNDCKKGHALKMMP SWWYT) and Oligo-peptide 16 (ARNDCETGGYMLWWPSTWYV), respectively. There was an increase in H-bonds both for the variants and Oligo-peptides as compared to BanLec which had only 5 H-bonds in interactions with HIV glycoprotein. This increased H- bonding could thus prevent the $CD4^+$ cells and gp120 attachment ultimately inhibiting the viral entry into the cells. These variants and Oligo-peptides can serve as an anti-HIV drug candidate. However there is need to synthesize and analyze these drug candidates in in-vivo conditions.