CHAPTER 6

CONCLUSION AND RECOMMENDATION

6.1 CONCLUSION

Yearly there are hundreds of thousands of deaths are reported globally due to flaviviruses infection. The rate of morbidity is not preventable due to lack of availability of appropriate vaccines and/or antiviral drugs. This study focused on using computational tools to identify the possible anti viral target binding sites of flaviviruses which can be used for further research of docking models for these viruses and thus aid inhibitor design. The following are the findings of the present study:

1. Anti viral binding sites of Dengue Virus are His 51, Asp 75, Ser 135
2. Anti viral binding sites of West Niles Virus are His 51, Asp 75, Ser 135
3. Anti viral binding sites of Hepatitis C Virus are His 57, Asp 81, Ser 139
4. Anti viral binding sites of Japanese Encephalitis Virus are His 107, Asp 131, Ser 191
5. Anti viral binding sites of Yellow Fever Virus are His 109, Asp 133, Ser 194

Prior to this study several theories suggested that the flaviviruses protease family should be susceptible for allosteric inhibition. The trypsin-like serine protease domain of NS3 contains the functional catalytic triad Histidine, Aspartate, and Serine in the N-terminal region. Inhibition of the NS3 protease activity is expected to prevent the propagation of flaviviruses.

6.2 RECOMMENDATION

Allosteric inhibition of flaviviruses proteases is of potential interest due to the lack of clinically available inhibitors that target the NS2B- NS3pro active site. Therefore, this study has to be extended in order to find the answer to the remaining questions that has arisen. Additional studies are required to determine the role of the residues that confers resistance to flaviviruses infection. Besides that, drug efficacy trial which requires a large sample should be conducted to obtain more accurate information on the resistance of anti viral resistance associated with the presence of NS2B-NS3 protease active site.

Further studies are required to validate and determine the best drug regime for flaviviruses infection. As more studies are conducted, the role and underlying mechanism of Flaviviruses infection and treatment will be clearer.