Computational Identification of Putative Viral Epitopes for Vaccine Development

S. W. Njuki[1], V.O, Adunga[1,2] and E. K. Murungi[3]

[1]Department of Biochemistry and Molecular Biology, P.O Box 536-20115
Egerton, Kenya
[2]International Center of Insect Physiology and Ecology,
P.O. Box 30772-00100 Nairobi, Kenya
[3]Department of Biochemistry, School of Health Sciences,
Kisii University, P.O. Box 408 – 40200 Kisii, Kenya
***Corresponding Author**: suzannenjuki@gmail.com*

Infectious diseases (IDs) account for 90% of the health problems worldwide, killing about 14 million people annually, 90% of who are from the developing world. Viruses, mostly as zoonoses, account for most of the EIDs and re-EIDs and consequently account for most of the IDs fatalities. Currently, control and management of EIDs and re-EIDs involves vector control, vaccination and chemotherapeutics. These approaches are suboptimal, therefore, improvement of current and/or development of novel control approaches is necessary. One possible solution of huge potential for control of EIDs of viral origin is vaccines. Here, 24 viruses were selected, genome and protein sequences analysed. Using antigen and epitope predicting tools, protein homology modeling and molecular dynamic simulations, 22 potential vaccine candidates were identified. These proteins are found in viruses of international public health importance without licensed vaccines. Epitope prediction, protein structure analyses and MD simulation revealed the identified epitopes as highly immunogenic, highly antigenic, non-allergenic, surface exposed and solvent accessible on the respective proteins and hence most likely accessible to host immune molecules. Additionally, conformational flexibility analyses revealed that the viral proteins are stable to allow epitopes interaction with host immune molecules. Together, these indicate good candidates for further validation and vaccine development. Notably, the *in silico* approach applied is faster and cheaper for potential use in identification of vaccine and diagnostic candidates for viruses.

Key words: Computational tools, emerging infectious diseases, epitopes, re-emerging infectious diseases, vaccine candidates, viruses.