



# IV ASBioSim – Advanced School on Biomolecular Simulation: Protein Engineering with Rosetta, from fundamental principles to tutorials

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## **Title: Computational Design of Neutralizing Aptamer Bind Epitopes on CHIKV E2 protein**

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### **Abstract:**

Millions of cases of Chikungunya (CHIKV) virus infections have been reported worldwide and transmission of the virus remains active in several American countries including Brazil, thus signaling the risk of an impending global CHIKV epidemic. The virus causes a serious febrile illness and is characterized mainly by a debilitating polyarthrits, which can be chronic and thus persist for years causing a significant morbidity. Currently, there is no specific chemotherapy or chemoprophylaxis and no licensed vaccine against CHIKV. Surface glycoproteins E1 and E2 form heterodimers that allow interaction with cell receptors and fusion of the virus with the cell membrane to initiate infection. These proteins are highly immunogenic, and most patients infected with CHIKV develop antibodies against structural proteins (particularly E2). In a study, using human anti-CHIKV monoclonal antibodies, a screening of epitopes on the CHIKV E2 protein was done. The study showed that monoclonal antibodies used against this protein inhibited infection at various stages in the viral life cycle and protected *in vivo* against the pathogenesis of the disease in mice. Thus, neutralizing antibodies produced against B-domain epitopes of E2 protein may be a strategic target for the development of vaccines and immunotherapies against CHIKV. The present work proposes to use the engineering of proteins for the planning of aptamers (synthetic antibodies) that are capable of specifically recognizing target epitopes and thus can be used for therapeutic and / or vaccine purposes. With the set of computational techniques in this study it was possible to produce and analyze thousands of possible candidates for CHIKV aptamers in a short time and in a rational way. In the subsequent steps, experimental evaluations of the aptamers that have been energetically viable will be made.

### **Keywords:**

Chikungunya Vrus (CHIKV), Aptamers, Synthetic antibody, Disease diagnosis, Therapeutic, Prophylactic