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Bioinformatic Design of a Non-toxic Modified Adjuvant from the Native A1 Structure of Cholera Toxin with Membrane Synthetic Peptide of Naegleria fowleri

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Abstract : Naegleria fowleri is the causative agent of primary amebic meningoencephalitis, this disease is acute and fulminant that affects humans. It has been reported that despite the existence of therapeutic options against this disease, its mortality rate is 97%. Therefore, the need arises to have vaccines that confer protection against this disease and, in addition to developing adjuvants to enhance the immune response. In this regard, in our work group, we obtained a peptide designed from the membrane protein MP2CL5 of Naegleria fowleri called Smp145 that was shown to be immunogenic; however, it would be of great importance to enhance its immunological response, being able to co-administer it with a non-toxic adjuvant. Therefore, the objective of this work was to carry out the bioinformatic design of a peptide of the Naegleria fowleri membrane protein MP2CL5 conjugated with a non-toxic modified adjuvant from the native A1 structure of Cholera Toxin. For which different bioinformatics tools were used to obtain a model with a modification in amino acid 61 of the A1 subunit of the CT (CTA1), to which the Smp145 peptide was added and both molecules were joined with a 13-glycine linker. As for the results obtained, the modification in CTA1 bound to the peptide produces a reduction in the toxicity of the molecule in in silico experiments, likewise, the prediction in the binding of Smp145 to the receptor of B cells suggests that the molecule is directed in specifically to the BCR receptor, decreasing its native enzymatic activity. The stereochemical evaluation showed that the generated model has a high number of adequately predicted residues. In the ERRAT test, the confidence with which it is possible to reject regions that exceed the error values was evaluated, in the generated model, a high score was obtained, which determines that the model has a good structural resolution. Therefore, the design of the conjugated peptide in this work will allow us to proceed with its chemical synthesis and subsequently be able to use it in the mouse meningitis protection model caused by N. fowleri.

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