# In silico prediction discontinuous B cell epitope peptide vaccine against leishmaniasis

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## Abstract

**Introduction:** The kinetoplastid protozoan parasites of the genus *Leishmania* cause diseases for which treatment is difficult and there is still no vaccine for use in humans. Leishmanolysin is the major enzymatic protein component of the promastigote surface. Because of its role as a ligand involved in the interaction of the parasite with defensive systems of the host, including components of the complement system and the macrophage surface is an attractive candidate for designing peptide vaccines.

**Methods and Results:** In the current study, PEPOP was used to predict peptides from Leishmanolysin in the form of discontinuous B-cell epitopes. PEPOP identified segments comprised of accessible and sequence continuous amino acids. These segments were clustered according to their spatial distances using method of extensions: Optimized Nearest Neighbor (ONN), Optimized Flanking Nearest Neighbor (OFN), Optimized Patched segments Path (OPP), Traveling Salesman Problem (TSP), and Shortest Path (SHP). Each peptide sequence has been generally comprised of several segments. From 3D structure of Leishmanolysin, PEPOP identified 100 segments gathered in three clusters according to their spatial distances. In this study, we wanted to predict peptides from a specific region of the protein, the residue 264-345 on the active site of Leishmanolysin. It corresponds to the segments S34 to S48. The predicted peptides, which did not relate to this region (264-345) were removed and at last 29 peptides were selected.

**Conclusions:**

These results using bioinformatics analyses could be conducted in vaccine design against Leishmania infections.

**Key words:** Leishmaniolysin, Discontinuous B cell epitope, Bioinformatics, Peptide vaccine

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