The idea of using peptides as cost-effective vaccines, seems a striking approach for the prevention and treatment of many infectious diseases and malignant disorders [1-2]. Such peptides can be designed synthetically [3] to elicit a response in immune system.

Approximately 83% of B-cell epitopes are conformational in nature with discontinuous regions of the sequence coming together in the 3D fold of the protein and it is therefore important to study how well synthetic peptides are able to mimic these conformations.

**Aims:** Characterization of B-cell epitopes to inform improved vaccines and antibody design and allow development of peptide vaccine.

**Advantages:**
- Specificity of Immune Response
- Exclusion of undesirable Immune response
- Improving Immunity
- Cost Effective
- Ease of Storage/Transport

**Epitope Regions’ Shape Analysis**
Shapes of epitopes were analysed as folded, linear and curved because epitopes are more likely to be represented by peptides.

**Molecular Dynamics Simulations of Regions**
Molecular dynamics simulations were performed to determine that whether isolated peptides adopt the same conformation as in the whole (native) protein.

**Future Directions**
- Further molecular dynamics simulations of linear and folded regions will be performed to access their conformational stability.
- For folded peptides, the effect of stapling the peptides on the dynamics will be explored.
- The mutations will be explored to stabilize the conformations.
- Linkers will be designed for epitopes containing 2 or 3 regions followed by their MD simulations.

**Design of automated pipeline**

**Epitope Composition Analysis**
Most epitopes are comprised of 1-4 regions. Regions’ lengths vary from 3 to 30 amino acids.

**Contact Hydrophobic residues**

No thought that the hydrophobic residues (in stick representation) are causing distortion in secondary structure.

What if we replace them with hydrophobic residues?

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