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## *In silico* Studies on structures of functional amyloids

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The classical histopathological definition of amyloid is an extracellular proteinaceous deposit exhibiting  $\beta$ -sheet structure usually associated with neuro-degenerative diseases in mammals. Microbial amyloids termed as 'functional amyloids' are reported for functional physiological traits that benefit the producing organism. Functional amyloids have been reported to contribute to biofilm formation, host colonization, immune activation and invasion. In this study, we generated various amyloid protein structures of different microorganisms by homology modelling and analysed *in silico* their attributes. In this *in silico* study, we have analysed the various microbial functional amyloids and their attributes. Using the FASTA sequences available on NCBI GenBank, the protein sequences and their homologous structures (PDB) were constructed using online servers (Swiss model, CPH). GROMACS and MD- simulation were used to check the changes in protein by applying temperature, pressure, potential and density, various result were formed in the form of graph i.e; radius of gyration, RMSD (backbone after Isq fit to backbone) and RMSD(backbone after Isq to system). And VMD was used to see all result and trajectory was also seen. And in PMDB all the protein PDB formats were submitted. The structural differences before and after simulation were significant.

### Biography

Kush K Mehta is a Research student at C.G. Bhakta Institute of Biotechnology, Uka Tarsadia University, Gujarat, India. He completed his integrated Masters in the year 2016. He has been studying protein structure analysis using GROMACS, Gromos and AutoDock including basic bioinformatic tools like ExPASy, Swiss PDB viewer and PyMol, etc.

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