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Investigations of Protein Aggregation Using Sequence and Structure Based Features

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Abstract : The main cause of several neurodegenerative diseases such as Alzhemier, Parkinson, and spongiform encephalopathies is formation of amyloid fibrils and plaques in proteins. We have analyzed different sets of proteins and peptides to understand the influence of sequence-based features on protein aggregation process. The comparison of 373 pairs of homologous mesophilic and thermophilic proteins showed that aggregation-prone regions (APRs) are present in both. But, the thermophilic protein monomers show greater ability to 'stow away' the APRs in their hydrophobic cores and protect them from solvent exposure. The comparison of amyloid forming and amorphous b-aggregating hexapeptides suggested distinct preferences for specific residues at the six positions as well as all possible combinations of nine residue pairs. The compositions of residues at different positions and residue pairs have been converted into energy potentials and utilized for distinguishing between amyloid forming and amorphous b-aggregating peptides. Our method could correctly identify the amyloid forming peptides at an accuracy of 95-100% in different datasets of peptides.

Keywords : aggregation, amyloids, thermophilic proteins, amino acid residues, machine learning techniques
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