

Poster I-61

Expected packing density allows to predict both amyloidogenic and unfolded regions in protein chain



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Short Abstract: It has been shown that regions with strong expected packing of residues would be responsible for the amyloid formation, at the same time regions with weak expected packing of residues would be responsible for the appearance of unfolded regions.

Long Abstract:

Identification of potentially amyloidogenic and unfolded regions in polypeptide chains is very important because such regions are essential for protein function. In our work we introduce a new parameter, namely mean packing of residues (packing density) to detect amyloidogenic and unfolded regions in a protein sequence. It has been shown that regions with strong expected packing of residues would be responsible for the amyloid formation. Our predictions are consistent with known disease-related amyloidogenic regions for 8 of 11 amyloid-forming proteins and peptides in which the positions of amyloidogenic regions have been revealed experimentally. Our findings support the concept that the mechanism of amyloid fibril formation is similar for different peptides and proteins. Moreover, we have demonstrated that regions with weak expected packing of residues would be responsible for the appearance of unfolded regions. Our method has been tested on datasets of globular proteins and long disordered protein segments, and showed improved performance over other widely used methods.

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