



Mechanisms of secondary structure breakers in soluble proteins

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Breaking signals of secondary structure put strong limitations on the tertiary structures of proteins. In addition to proline and glycine cl usters, which are well-known secondary structure breakers, clusters of amphiphilic residues were found to be a novel type of secondary structure breaker. These secondary structure breakers were found to depend on specific environmental factors. Such conditions included the a verage hydrophobicity, the helical periodicity, the density of serine and threonine residues, and the presence of tryptophan and tyrosine cluste rs. Principal component analysis of environmental factors was conducted in order to identify candidate breakers in the secondary structure b reaking regions. Predicted breakers were located in breaking regions with an accuracy of 72%. Taking the loop core into consideration, almo st 90% of the predicted breakers were located in the loop segments. When the migration effect of the breaking point was taken into accoun t, the loop segments with the predicted breakers covered two thirds of all loop segments. Herein, the possibility of secondary structure prediction based on secondary structure breakers is discussed. The system of the present method is available at the URL: http://bp.nuap.nagoya-u.ac.jp/sosui/sosuibreaker/sosuibreaker_submit.html.

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