

In silico analysis and homology modelling of antioxidant proteins of barley

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SUMMARY

Barley (*Hordeum vulgare* L.) is an important major cereal grain. It is used as animal fodder, as a source of fermentable material for beer and certain distilled beverages, and as a component of various health foods and often associated with beneficial health effects. In this paper, a bioinformatics and molecular modeling approach was adopted to explore properties and structure of barley antioxidant proteins by studying the antioxidative proteins *viz.*, ascorbate peroxidase (APX), phospholipid hydroperoxide glutathione peroxidase-like protein (PHGPX) and 2-Cys peroxiredoxin BAS1 (2-CPs). The properties of these proteins have been interpreted by physico-chemical characterization including pI, EC, AI, GRAVY and instability index. Functional characterization was done by predicting motifs, patterns, disulfide bridges and secondary structure. Three dimensional structures for these proteins were not available as yet at PDB. Therefore, homology models for these antioxidant proteins were developed by using SWISS MODEL server. The model was analyzed for its fold reliability by using server ProSA, ERRAT server was used for analyzes the statistics of non-bonded interactions between different atom types. The model was validated using protein structure checking tool WHAT IF. These structures will provide a good foundation for functional analysis of experimentally derived crystal structures.

Key Words : Homology modeling, Antioxidant

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