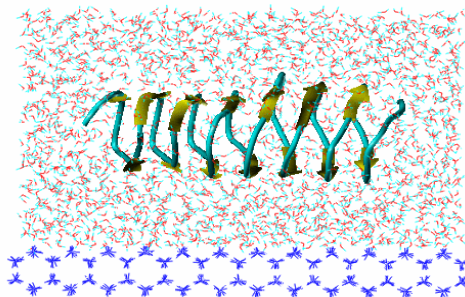


Molecular Modelling of *Deschampsia antarctica* Antifreeze Proteins



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Research Objective

The aim of the project is to model the various isoforms of Antifreeze proteins (AFPs) found in *Deschampsia antarctica* with both molecular modelling and bioinformatical techniques and its relevance for the freezing survival strategy of the grass. Also, to identify potential AFP sequences within the *D. antarctica* and other plant genomes using scripting languages such as PERL. The project is done in collaboration with Plant Biotechnology Centre, Latrobe University, who provided us the primary sequences of DaIRIP (*Deschampsia antarctica* Ice Recrystallization Inhibition Protein) orthologues.

Motivation/Significance

Deschampsia antarctica, an Antarctic hairgrass produces antifreeze proteins to resist to chilling and freezing temperatures. In plants the main function of the antifreeze proteins is to inhibit ice recrystallization rather than depressing the freezing point of plant fluids. Modelling of AFPs will provide an insight to study the residues that bind to the ice surface.

Antifreeze proteins have many internal sequence repeats correspond to functional and structural units. In order to identify the novel AFP sequences in *D. antarctica* and other plant genomes which have repeats, PERL scripts are written to run RADAR program which segments protein query sequence into repeats for all the sequences present in a file and to filter and sort the results to identify any potential antifreeze proteins. By identifying more AFPs in plants, the activity of AFPs can be studied which will lead to the better understanding of function of AFPs in plants.

Results

The three-dimensional structures of DaIRIP orthologues are constructed using the comparative modelling.

Comparative/homology modelling requires a related template structure. Antifreeze protein (AFP) of *Lolium perenne* has shown very good (>60%) homology to the *Deschampsia antarctica* AFP sequences. And hence the theoretical 3-D β -roll model of AFP of *Lolium perenne* is used as a template model for homology modelling.

Aligning each sequence of the IRIP orthologues from *D. antarctica* in two columns revealed approximately 7-amino acid repetitive motifs.

DaIRIP	Total Amino acids	Length of repeating motif	Consensus sequence
DaIRIPa	79	7	S X N X V S G
DaIRIPc	100	7	X X N X V X G
DaIRIPd	135	7	X X N X V X G
DaIRIPe	152	7	X X N X V X G
DaIRIPf	159	7	X N N X V X G

A solvated Molecular Dynamics (MD) simulation was performed to examine the stability of the *Lolium perenne* AFP theoretical structure. It has shown that the left-handed model is more stable than the right-handed one. Using the left handed theoretical 3-D β -roll model of *L. perenne* AFP as a template, DaIRIP models have been built.

Conclusion

The three-dimensional structures of the *Deschampsia antarctica* IRIP orthologues (except DaIRIPb) have been built by homology modelling using the left handed theoretical 3-D β -roll model of *L. perenne* AFP as a template model. PERL scripts are written which finds the repeats in protein sequences and filters and sorts the results in order to identify potential AFPs in plant genomes.