



**Virtual symposium celebrating
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Protein Data Bank**

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Day 1 Abstracts



Worldwide
Protein Data Bank
Foundation

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In silico structural survey of newly identified late embryogenesis abundant proteins (LEAPs) from *R. serbica* and their structure - function relationship

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Desiccation or extreme water loss leads to protein denaturation, aggregation, and degradation and impairs membrane lipid fluidity, resulting in loss of membrane integrity at the cellular level. The induction of late embryogenesis abundant proteins (LEAPs) is considered an essential component of desiccation tolerance strategy in so-called resurrection plants. This heterogeneous group of hydrophilic, non-globular proteins is characterized by a high structural plasticity that allows them to adopt a random conformation in aqueous solutions that transforms into α -helices during dehydration [1]. Therefore, LEAPs can interact with various ligands and partners, including ion sequestration and stabilization of membranes and enzymes during freezing or drying [2].

Our new transcriptome database of an endemic resurrection species *Ramonda serbica* allowed us to identify 153 members of the LEA gene family. LEAPs of this sample data have an average primary sequence similarity and identity of 10% and 6%, respectively, but with a high variance (141 and 108), which means that the sample proteins can be classified based on domain homology. The averaging is based on multiple sequence alignment and the variance is estimated using pairwise sequence alignment scores. Accordingly, all identified LEAPs were clustered into six groups based on protein families (PFAM). Among these groups, LEAPs differ significantly in their secondary structure, disorder propensity and aggregation potential. Furthermore, we built homology models using Protein Data Bank structure information as templates. For each group, an ensemble of superimposed 3D homology models was analyzed.

The information obtained from the representative structural models is key to understanding the function of LEAPs and the regulation of their intrinsic structural disorder-to-order transition during desiccation. This will pave the way for the identification of LEAPs endogenous partners and their targets in the cell and provide further insights into the protective mechanisms of desiccation tolerance.

References:

1. Hundertmark M, Hincha DK (2008). *BMC Genom* 9:1.
2. Chakrabortee S, Tripathi R, Watson M, Schierle GSK, Kurniawan DP, Kaminski CF, ..., Tunnacliffe A (2012). *Mol. Biosyst.* 8:210-19.

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