Title: Sequence analysis and molecular dynamics to decipher the role of C2 domains from plant plasmodesmata MCTP proteins for membrane tethering

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Abstract (upto 300 words)

Intercellular communication is critical for multicellularity. Plants have developed remarkable cellular machines –the plasmodesmata (PD) pores- which interconnect every single cell within the plant body, establishing direct membrane and cytoplasmic continuity, a situation unique to plants. A striking feature of PD organisation, setting them apart from animal cell junctions, is a strand of tightly constricted ER called the desmotubule forming the center of plasmodesmata and connected to the PM by tethering elements which appear like spokes by electron microscopy and are assumed to be proteinaceous. Very recently, it was shown by the team of E. Bayer that highly plasmodesmata-enriched proteins, members of the Multiple C2 domains and Transmembrane region Proteins (MCTPs) were significantly more abundant in PD with tight membrane connections, and exhibit the domain architecture expected of membrane tethering proteins, with multiple lipid-binding C2 domains in the N-terminal, and an ER-anchored transmembrane region in the C-terminal region.

Our work is focused on investigating the potential docking of C2 domains of MCTPs on the plant plasma membrane at a molecular level. We first performed sequence analysis to accurately define the C2 domains from the MCTP and to obtain good 3D models by homology modelling. Then, molecular dynamics is carried out to predict the docking of the different C2 domains onto biomimetic plant plasma membrane and eventually lipid specificity. Based on those results and sequence analysis, specific binding sites in the C2 domains could be predicted. Our preliminary results suggest that the different C2 domains of MCTP proteins could have different roles in lipid tethering, depending or not of calcium.

Biography (upto 150 words)

Dr Laurence Lins (PhD Sciences-Free University of Brussels-Belgium) has completed her PhD at the age of 27 years from Free University of Brussels (Belgium). She is now Senior Research Fellow at the belgian FNRS (Fonds National de la Recherche Scientifique) and Associate Professor at the University of Liège ans she is Head of The Lab of Molecular Biophysics at Interfaces (LBMI). She has over 100 publications that have been cited over 3000 times and her H-index is 31.

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