The role of a plant-specific binding pocket in information transfer pathways in profilins

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Profilins are small proteins that participate in regulating actin polymerization, with binding surfaces for actin, phospholipids, and regulatory proteins with poly-L-proline (PLP) moieties. Plant profilins include a binding pocket that is absent from animal and fungal profilins, and it is suspected to be the binding site for an endogenous ligand. A comprehensive docking experiment with plant-derived molecules revealed that myricetin and similar polyphenols can fit in the pocket. To explore the connections of this pocket with the binding sites for other effectors, we carried out molecular dynamics simulations of profilins from plants, yeast and animals, with and without myricetin. From these simulations we calculated the degree of coupling between binding sites using network theory. Curiously, plant profilins display better coupling between the pocket and the PLP binding site, both with and without the ligand, than yeast and animal profilins, suggesting that the site is functional in plants. On the other hand, the coupling between the PLP and actin binding sites is better in animal and yeast profilins than in plant profilins, which appear to tune this coupling with the binding of myricetin. These information transfer differences may be related to the presence of only one profilin in animals and yeast, and many in plants, and to the distinct physiological roles each plays.