

Binding Interface of PrxQ to the Membrane Probed by Molecular Simulation

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During photosynthesis, hydrogen peroxide is frequently produced as a byproduct in chloroplasts of photosynthetic organisms and must be detoxified. The Peroxiredoxin family of proteins is involved in the cellular defense of reactive oxygen and nitrogen species such as hydrogen peroxide. Through its catalytic process in which it binds to a phospholipid bilayer, proteins in the Peroxiredoxin family can reduce phospholipid hydroperoxides produced by oxidative stress from elevated levels of hydrogen peroxide. However, the binding site in Peroxiredoxin proteins found in *Arabidopsis thaliana* and *Chlamydomonas reinhardtii* is unknown. Using molecular simulations, we found that the binding position of AtPrxQ and CrPrx6 involves an important pair of cystine residues in close contact to the lipid bilayer. This binding position was the only consistent pose for both proteins across all replicates of the simulations. These results help us understand how exactly proteins in the Peroxiredoxin family bind to membranes and potentially reveal residues involved in reducing phospholipid hydroperoxides. We expect these early simulations to be the beginning of further molecular simulations investigating how this family of proteins interact with phospholipid hydroperoxides to maintain homeostasis. In the future, simulations could be run with different concentrations of these phospholipid hydroperoxides to investigate whether they aggregate near the protein binding position to investigate how the mechanism of these proteins work as well as how differing levels of oxidative stress impact their function.