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Structural Analysis of *Arabidopsis* NADPH-dependent Thioredoxin Reductase between Isotype A and C using Molecular Dynamics Simulations

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2-Cys peroxiredoxins (Prxs) play important roles in the protection of chloroplast proteins from oxidative damage. *Arabidopsis* NADPH-dependent thioredoxin reductase (NTR) isotype C (AtNTRC) was identified as efficient electron donor for chloroplastic 2-Cys Prx-A. There are three isotypes (A,B,C) of thioredoxin reductase (TR) in *Arabidopsis*. AtNTRA contains only TR domain, but AtNTRC consists of N-terminal TR domain and C-terminal thioredoxin (Trx) domain. AtNTRC has various oligomer structures, and it is known that the Trx domain is important for chaperone activity. To confirm the role of Trx domain in AtNTRA, the AtNTRA was connected with Trx domain from AtNTRC. After that, the hybrid has formed variety of structures and shown strong chaperone activity. But, it has not shown the disulfide reductase activity at all. Expectedly, AtNTRC and AtNTRA-(Trx-D) will have same forms but it cannot transfer electron. To understand this situation in the structural basis, we performed two different molecular dynamics (MD) simulations on AtNTRC protein and AtNTRA-(Trx-D) protein with same substrates such as NADPH and flavin adenine dinucleotide (FAD) during 4ns. In results, structural difference for the two proteins was compared and the main reason that AtNTRA-(Trx-D) cannot transfer the electron from TR domain to Trx domain was proposed and discussed.