

## Short Talk 12, Magnus Andersson - Tracking Ca<sup>2+</sup> ATPase Intermediates in Real-Time by X-ray Solution Scattering

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Sarco/endoplasmic reticulum Ca<sup>2+</sup> ATPase (SERCA) transporters regulate calcium signaling by active calcium ion reuptake to internal stores. Several of the structural transitions associated with transport have been characterized

by X-ray crystallography, but critical intermediates of the inward-outward switching are missing.

We combined time-resolved X-ray solution scattering (TR-XSS) experiments and molecular dynamics (MD) simulations for real-time tracking of concerted SERCA reaction-cycle dynamics in the native membrane. The TR-XSS pre-pulse model differed in the domain arrangement compared to Ca<sub>2</sub>E1 crystal structures. A 1.5 ms intermediate showed closure of the cytosolic domains typical of Ca<sup>2+</sup>- and ATP-bound E1 states. A subsequent

transient state with a 13 ms rise-time showed a novel actuator (A) domain arrangement that exposes the ADP-binding site after phosphorylation. Hence, the obtained TR-XSS models determine the relative timing of so-far elusive domain rearrangements in a native environment.

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**Session Classification :** Keynotes and Short talks 8