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Structure Dynamics of the Energy Conversion Proteins ATP-Synthase and F1ATPase: From SANS at ILL-D11 to time resolved SAXS during reaction cycle at ESRF-ID02

Bio-energy converting membrane proteins couple the transport of material across a membrane, e.g. protons, with the reversible formation or cleavage of an energy rich chemical bond (ATP). Thus local energy is stored and available in the cell lumen or tissue, by temporal energized protein state.
The most common energy transfer protein ATP-Synthase (M = 500 000) and its catalytic head F1ATPase was studied by SANS at ILL-D11, -D22 and FZ Jülich, and SAXS at DESY Hamburg, ELETTRA Trieste and ESRF-ID02 and –ID01. Already the SANS of bacterial F1ATPase starting 1978 at ILL-D11 (fig. a) and DESY-EMBL depicted a highly organized but flexible hollow structure of segregated subunits, which results in SANS and SAXS side maxima. The structure is dynamic, as the side maxima change position and height by functional changes of the enzyme. Details were resolved by crystallography of resting F1ATPase by Walker (Noble award 1997). But the mechanism of reversible energy conversion in the ATP reaction cycle remains unknown.
Our studies of the flexible structure of F1ATPase and ATP-Synthase in detergent solution with SANS at ILL-D11 and D22, and SAXS at DESY, ELETTRA and ESRF depicted rearrangements of the subunit complex upon regulatory states and inhibition, e.g. by temperature, pH and azide. ATP-Synthase was reconstituted into liposomes, and with Bacteriorhodopsin or caged acids for light-induced energization. After the very first SANS of D-contrast matched proteo-liposomes with ATP-Synthase at FZ Jülich, our studies in energized liposomes, at membrane ⊠pH>1 by time-resolved SANS at ILL-D22 depicted temporal energetic structure changes by Rg-changes.
The structure dynamics of the F1ATPase in the reaction cycle was investigated by time resolved SAXS upon ATP activation by stopped-flow, and flash photolysis (caged ATP). A tour through EU-synchrotrons lead from first success at ELETTRA Trieste to ESRF-ID02, and contributed later to the DESY-PETRA P12 setup. Fig.c depicts cyclic dynamics of working F1ATPase in subsequent ATP reaction cycles at 1013 ph/s with He-jet cooling, triggered by stopped-flow mixing (Rg-changes T-depended). The results could trigger the development of novel energy conversion materials with improved efficiency, e.g. chimeric polymer-protein systems.

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