the Qo site. We show that removal of chlorophyll does not impair the overall structure of the b6f complex, but perturbs in vivo and in vitro plastoquinol oxidation in the Qo site, disproving a simple structural role for the chlorophyll. In addition, this compromised activity can be correlated with conformational changes, which comprises the same polypeptide segments that are also subject to conformational changes in the related Qo sites of the bc1 and b6f complexes upon inhibitor binding. This common flexibility might be involved in the gating of the Qo site to avoid short circuits, introducing a double gating.

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S11.P1

Lutein as a mediator of effective yet ‘economic’ regulator of light-harvesting in photosystem II of plants
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The antenna of photosystem II (PSII) in plants possesses an intrinsic photoprotective switch that allows for rapid adaptation to changing light intensity. The essence of this switch is the formation of energy-quenching sites within the antenna that trap and dissipate excess excitation energy, thereby mitigating the photoinhibitory damage associated with high light \cite{1}. The molecular mechanisms at the heart of this process, known as Non-Photochemical Quenching, are well debated and there are several competing models \cite{1}. One such model, based on time-resolved fluorescence measurements, suggests that NPQ occurs via the incoherent transfer of energy from chlorophyll to the xanthophyll lutein 1, followed by rapid (~10 ps) non-radiative decay, in the major PSII antenna complex LHCII \cite{2}. Our recent theoretical model of chlorophyll–xanthophyll energy transfer in LHCII indicates that this mechanism is sufficient to explain the fluorescence quenching in LHCII crystals \cite{3}. Additionally we reported that a combination of solid-state NMR and theoretical modelling implies that aggregation-induced quenching in LHCII may be controlled by fine tuning of chlorophyll–xanthophyll distances \cite{4}. We here present the incorporation of this lutein-mediated quenching mechanism into coarse-grained models of energy transfer in PSII-antenna superstructures and show that lutein is an effective NPQ site in the photosynthetic membrane. Additionally, we show that this model is consistent with our recent fluorescence induction measurements \cite{5}. We show that lutein in the PSII antenna can function as an ‘economic’ quencher, offering protection to closed reaction centres whilst simultaneously preserving photosynthetic productivity in a broad range of light intensities.

References

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S11.P2

Inter-monomer electron transfer in asymmetrically mutated fusion hybrid cytochrome bc1-like complex supports the enzyme function in vivo
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Cytochrome $bc_{1}$ is one of the key catalytic complexes involved in the bioenergetic processes. This dimeric enzyme operates according to the Q cycle functionally linking quinone catalytic sites on the opposite sides of the membrane. While recent studies indicate that this link can be achieved by intra- or inter-monomer electron transfer, the physiological relevance of the latter remains unclear. To address this issue we used a system based on a fusion hybrid protein build of cytochrome $b$ subunits from two different species: $Rhodobacter capsulatus$ and $Rhodobacter sphaeroides$. It assembles into a functional $bc_{1}$-like complex and allows introduction of mutations in an asymmetric manner \cite{1}. We report that the cross-inactivated $bc_{1}$ constructs, enforcing the inter-monomer transfer as the only way to electronically connect the opposite catalytic sites, supported the cytochrome $bc_{1}$-dependent photoheterotrophic growth of bacteria. This indicates that inter-monomer route for electrons is able to sustain the function of the enzyme in vivo. Moreover, given the differences in amino acid composition between the fused cytochromes $b$, we suggest that the minimal requirement for the enzyme bioenergetic efficiency is to provide the uninterrupted electron connection of the quinone catalytic sites on the opposite sides of the membrane in a manner robustly tolerant to structural alterations.

Reference

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S11.P3

Role of electrostatic and hydrophobic interactions in the encounter complex formation of plastocyanin and cytochrome f
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Cytochrome f (cyt f) and plastocyanin (pc) are electron transfer proteins forming a transient complex. During complex formation, an initial encounter complex rearranges into an active complex. Both, electrostatic and non-covalent short-range forces have been reported to be important for the complex in Phormidium laminosum or Nostoc \cite{1}. In this work, the association of cyt f and pc were studied using paramagnetic NMR spectroscopy, Monte Carlo simulations \cite{2} and ensemble docking in order to get deeper insights into the dynamics of the electron transfer complexes. For this purpose, spin labels were attached to cyt f, and relaxation enhancements of pc nuclei were measured, demonstrating that a large part of the cyt f surface area is sampled by pc. The distribution of the encounter complex