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Solution structures of native photosystems revealed by small-angle neutron scattering

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Photosystems I (PSI) and II (PSII) are pigment-protein complexes capable of performing the light-induced charge separation necessary to convert solar energy into a biochemically storable form, an essential step in photosynthesis. Small-angle neutron scattering (SANS) is unique in providing structural information on PSI and PSII in solution under nearly physiological conditions without the need for crystallization or temperature decrease [1-4]. We show that the reliability of the solution structure critically depends on proper contrast matching of the detergent belt surrounding the protein. Especially, "invisible" specifically deuterated detergents are shown to be properly matched out in SANS experiments by a direct, quantitative comparison with conventional matching strategies. In contrast, protonated detergents necessarily exhibit incomplete matching, so that related SANS results systematically overestimate the size of the membrane protein under study. While the solution structures obtained are close to corresponding high-resolution structures, we show that temperature and solution state lead to individual structural differences compared with high-resolution structures. We attribute these differences to the presence of a manifold of conformational substates accessible by protein dynamics under physiological conditions.

1.) M. Golub et al., J. Phys. Chem. B 2022, 126, 2824-2833.

- 2.) A. Kölsch et al., Current Research in Structural Biology 2 (2020) 171-179.
- 3.) M. Golub et al., J. Phys. Chem. B 2022, 124, 8583-8592.
- 4.) M. Golub et al., Crystals 2021, 11, 203.

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