# Supporting Information

# "Invisible" Detergents Enable a Reliable Determination of Solution Structures of Native Photosystems by Small-Angle Neutron Scattering

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**Figure S1:** SANS data of PSI obtained using deuterated and protonated detergent are shown for the PSI-dDDM complex in 100% D2O (red points), the PSI-hDDM complex in 18% D2O (green), and the PSI-hDDM complex in 5% D2O (green). The black line represents the fit curve obtained using Dammif [1](#_ENREF_1). The data of PSI at 5% D2O (green) are shown for comparison and taken from Kölsch et al., 2020 [2](#_ENREF_2). Note that Dammif fits are technically restricted to the low Q-range.



**Figure S2:** SANS data of dimeric PSII obtained using dDDM at 100% D2O (cyan points). The black line represents the fit curve obtained using Dammif [1](#_ENREF_1). Note that Dammif fits are technically restricted to the low Q-range.

**Table S1.** Parameters of the SANS measurements of PSII/PSI-dDDM in 100% D2O contrast

|  |  |  |
| --- | --- | --- |
| Sample | PSII-dDDM | PSI-dDDM |
| Organism | *Thermosynechococcus elongatus* | |
| Instrument | D22 | |
| Wavelength (Å) | 6 | |
| Aperture (mm) | 11 | |
| Sample to detector distance (m) | 2 and 8 | |
| Q measured range | 0.0075 – 0.04538 | |
| Normalization | To empty beam flux | |
| Exposure time (s) | 30 | |
| Sample thickness (mm) | 1 | |
| SEC mode | online | |
| Sample temperature | Room temperature | |
| Guinier analysis |  |  |
| I(0) (cm-1) | 1.73±0.5 | 2.42±0.5 |
| Rg (Å) | 57.23±1 | 69.7±1 |
| Porod volume (Å3) | 795000 | 1180000 |
| Qmin (Å-1) | 0.000861 | 0.000751 |
| QRg max | 1.26 | 0.52 |
| P(r) analysis (Gnom) |  |  |
| I(0) (cm-1) | 1.73±0.5 | 2.164 |
| Rg (Å) | 57.25±1 | 70.5±1 |
| Dmax (Å) | 187.7±10 | 206.52±10 |
| Q range for fitting (Å-1) | 0.000861 – 0.08823  (only 8m data was used) | 0.000751 – 0.10707  (only 8m data was used) |
| Porod volume (Å3) | 792000 | 1250000 |
| Total Estimate | 0.91 | 0.9082 |
| Dammif |  |  |
| Number of calculations | 20 (fast mode) | 20 (fast mode) |
| Q range for fitting (Å-1) | 0.000861 – 0.08823  (only 8m data was used) | 0.000751 – 0.10707  (only 8m data was used) |
| Symmetry, anisotropy assumptions | P2, no anisotropy assumptions | P3, oblate anisotropy assumption |
| Chi2 against raw data | 1.22 | 1.059 |
| Pepsi |  |  |
| Q range for fitting (Å-1) | Full range | Full range |
| pdb structure | 5kaf[3](#_ENREF_3) | 6rtd[2](#_ENREF_2) |
| Chi2 | 6.936 | 6.52 |

**References:**

1. Franke, D.; Svergun, D. I. Dammif, a Program for Rapid Ab-Initio Shape Determination in Small-Angle Scattering. *J. Appl. Crystallogr.* **2009,** *42*, 342-346.

2. Kölsch, A.; Radon, C.; Golub, M.; Baumert, A.; Bürger, J.; Mielke, T.; Lisdat, F.; Feoktystov, A.; Pieper, J.; Zouni, A., et al. Current Limits of Structural Biology: The Transient Interaction between Cytochrome C6 and Photosystem I. *Curr. Res. Struct. Biol.* **2020,** *2*, 171-179.

3. Young, I. D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Fuller, F.; Koroidov, S.; Brewster, A. S.; Tran, R.; Alonso-Mori, R.; Kroll, T., et al. Structure of Photosystem Ii and Substrate Binding at Room Temperature. *Nature* **2016,** *540*, 453-457.