

Supporting Information

The A₋₁ Pigment Photosystem I Contributes to (P700⁺ – P700) FTIR Difference Spectra: Cyanobacterial PSI.

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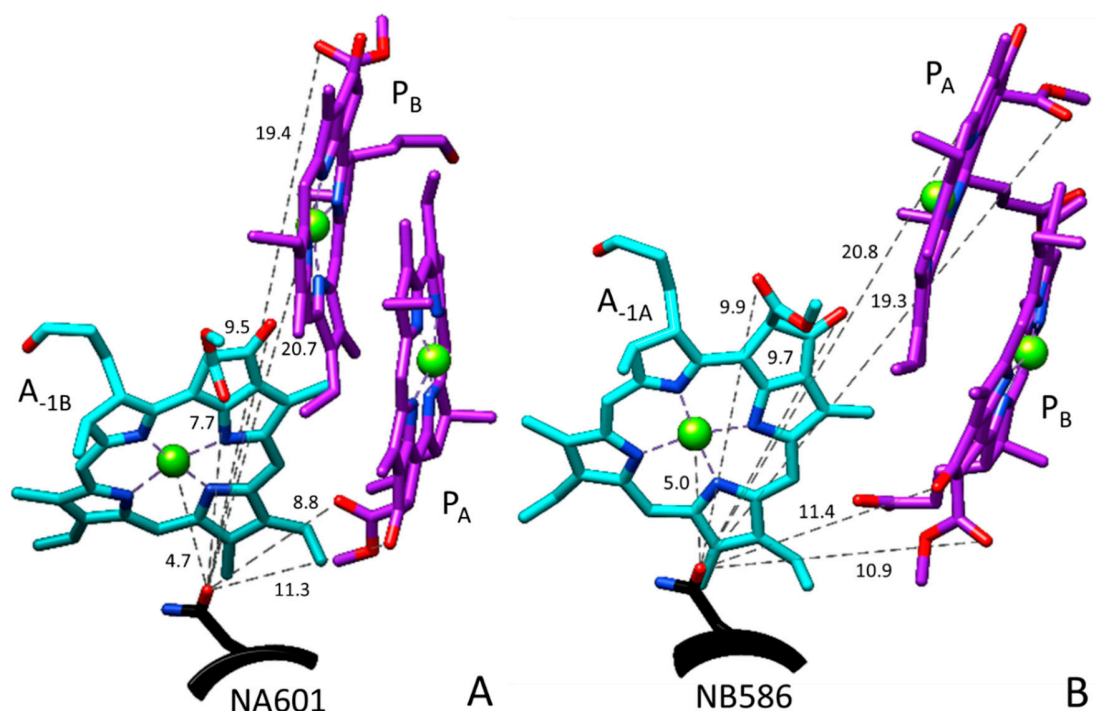


Figure S1. Structural organization of the (A) A-1B, and (B) A-1A pigments. The P_A and P_B pigments are also shown. P_A and P_B are in purple and A-1A/B are in cyan. Structure obtained using the cryo-electron microscopy structure of PSI from *C. reinhardtii* at 2.90 Å resolution (PDB file 6JO5) [1]. Asn at A601 and B586 are also shown (*backbone in black*). Distances from the Asn carbonyl oxygen atoms are shown (*dashed lines*). Distances are in Å and are also listed in Table S1.

Table S1. Distances (in Å) between the C=O oxygen atom of Asn and various atoms of molecular groups of the P_A and P_B pigments in PSI from *C. reinhardtii* (6JO5).

	Asn carbonyl oxygen atom (NB586) SEE FIGURE S1B	Asn carbonyl oxygen atom (NA601) SEE FIGURE S1A
H ₂ O oxygen atom	-	-
Mg atom	5.0	4.7
13 ¹ -keto carbonyl oxygen atom of P _A	20.8	11.3
13 ³ -ester carbonyl oxygen atom of P _A	19.3	8.8
13 ¹ -keto carbonyl oxygen atom of P _B	11.4	20.7
13 ³ -ester carbonyl oxygen atom of P _B	10.9	19.4
13 ¹ -keto carbonyl oxygen atom of A-1A	9.7	15.2 (not in Fig.2)
13 ³ -ester carbonyl oxygen atom of A-1A	9.9	18.4 (not in Fig.2)
13 ¹ -keto carbonyl oxygen atom of A-1B	15.2 (not in Fig.2)	9.5
13 ³ -ester carbonyl oxygen atom of A-1B	18.3 (not in Fig.2)	7.7

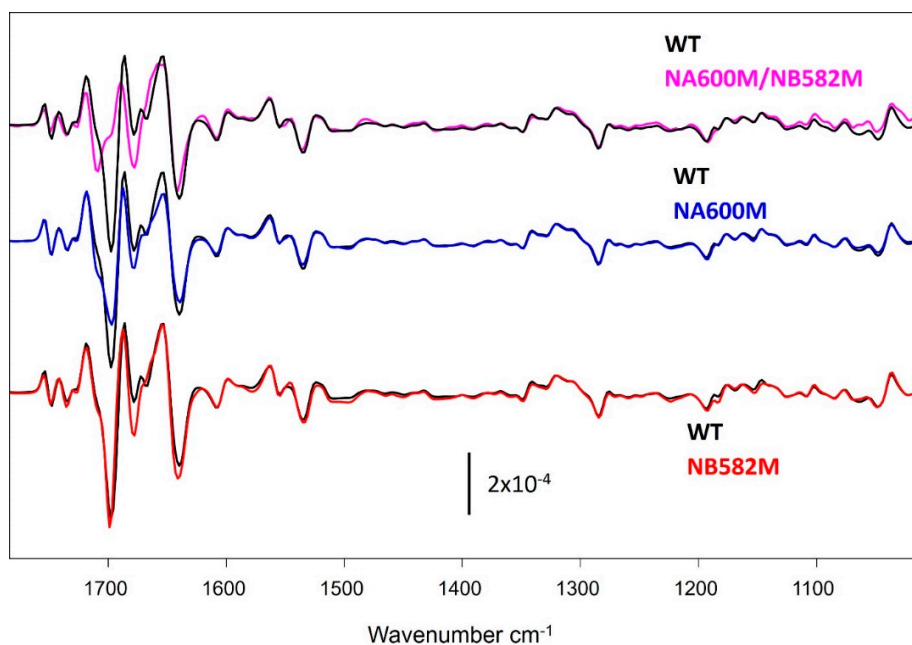


Figure S2. RT ($P700^+ - P700$) FTIR DS for WT and mutant PSI samples in the 1800-1050 cm^{-1} region. The same WT FTIR DS (black) is shown overlaid with each mutant FTIR DS. FTIR DS are the average of three measurements. The WT and mutant spectra were scaled so the 1748(-)/1754(+) cm^{-1} difference bands were similar. The data in the figure indicate that such a scaling minimizes the differences between the DS over the entire spectral region. Absorbance difference of 2×10^{-4} (in OD units) is indicated by the black bar.

REFERENCES

1. Suga, M., et al., *Structure of the green algal photosystem I supercomplex with a decameric light-harvesting complex I*. Nature Plants, 2019. **5**(6): p. 626-636.