Electronic Supplementary Information

Molecular basis for turnover inefficiencies (misses) during water oxidation in Photosystem II

Guangye Han^{a,b}, Petko Chernev^a, Stenbjörn Styring^a, Johannes Messinger^{a,c} and Fikret Mamedov^a

^a Molecular Biomimetics, Department of Chemistry, Ångström Laboratory, Box 523, Uppsala University, 751 20 Uppsala, Sweden. ^b Current address: Photosynthesis Research Center, Key Laboratory of Photobiology, Institute of Botany, Chinese Academy of Sciences, No. 20, Nanxincun, Xiangshan, Beijing, 100093, China. ^c Department of Chemistry, Umeå University, 901 87 Umeå, Sweden.



Supplementary Figure 1. EPR spectra used to quantify the fraction of PSII centers in the different S states after 0–6 saturating flashes with at 1 °C with 5 (orange) and 10 Hz flash frequency °C (blue). (A) Flash-dependent oscillation of the Split S_1 , Split S_3 and Split S_0 EPR signals. EPR signals were induced by illumination by visible light for 4 min at 5 K. The spectra are light minus dark difference spectra. (B) Flash-dependent oscillation of the S_2 multiline EPR signal. The large intensity from Y_D^{\bullet} in the center has been removed for clarity (dashed line). (C) Flash-dependent oscillation of the Split S_3 (stars) EPR signal induced by illumination by NIR light for 10 min at 5 K. The spectra presented are light minus dark difference spectra. Peaks used to quantify the EPR signals are indicated by arrows (S_1 , A), bars (S_0 , A and S_2 , B) and stars (S_3 , A and C). EPR conditions: for A and C: microwave power 25 mW, microwave frequency 9.27 GHz, modulation amplitude 10 G, temperature T 5 K; for B: microwave power 10 mW, microwave frequency 9.27 GHz, modulation amplitude 20 G, T 10 K.



Supplementary figure 2. EPR spectra used to quantify the fraction of PSII centers in the different S states after 0–6 saturating flashes with at 20 °C with 5 (orange) and 10 Hz flash frequency °C (blue). (A) Flash-dependent oscillation of the Split S_1 , Split S_3 and Split S_0 EPR signals. EPR signals were induced by illumination by visible light for 4 min at 5 K. The spectra are light minus dark difference spectra. (B) Flash-dependent oscillation of the S_2 multiline EPR signal. The large intensity from Y_D^{\bullet} in the center has been removed for clarity (dashed line). (C) Flash-dependent oscillation of the Split S_3 (stars) EPR signal induced by illumination by NIR light for 10 min at 5 K. The spectra presented are light minus dark difference spectra. Peaks used to quantify the EPR signals are indicated by arrows (S_1 , A), bars (S_0 , A and S_2 , B) and stars (S_3 , A and C). EPR conditions: for A and C: microwave power 25 mW, microwave frequency 9.27 GHz, modulation amplitude 10 G, temperature T 5 K; for B: microwave power 10 mW, microwave frequency 9.27 GHz, modulation amplitude 20 G, T 10 K.

Accuracy in our miss parameter determination

The standard error in our EPR measurement include possible differences during sample preparation (175 μ L of PSII membranes in the calibrated 4 mm quartz EPR tubes, acceptor addition (10 μ L), flashing/freezing and EPR measurements. Standard errors for each flash series are show in the corresponding tables (Table 1, 4, 5). Taken all together, the precision in estimation of the miss parameter shown in Table 2 is estimated to be less than 5%.