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## **Supplementary Information**

Hydration of the oxygen-evolving complex of Photosystem II probed in the dark-stable S<sub>1</sub> state by proton NMR dispersion profiles

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**SI Figure S1:** EPR spectra demonstrating the absence of  $Mn^{2+}$  (six-line EPR signal, g = 2) in intact (spectrum a) and in Mn-depleted (spectrum b) PSIIcc samples. Spectrum c: same as spectrum b, but after addition 0.3 M HCl (final concentration) to the Mn-depleted sample, which completely denatures PSII and would thus release any remaining bound Mn into the buffer. EPR spectra were recorded at 10 K; Microwave frequency, 9.39 GHz; Modulation amplitude, 20 G; Microwave power, 10 mW. The chlorophyll concentration was 1.0 mg/ml.

**SI Table S1:** The effective correlation times and the corresponding number of  $\beta$  waters for the best fit of Eq. 1-3 to the R1 NMRD profiles of the Mn-depleted and the native PSIIcc samples collected at 1°C and [PSIIcc] = 60  $\mu$ M.

sample	$q_i$	$\tau_{ci} = 1, 2, 3$
		(ns)
Mn depleted	51	$\tau_{c1=1500}$
	180	$\tau_{c2=75}$
Native sample	45	$\tau_{c1=1300}$
	165	$\tau_{c2=330}$
	160	$\tau_{c3=50}$

**SI Table S2**: The effective correlation times and the corresponding number of  $\beta$  waters for the best fit of Eq. 1-3 to the R1 NMRD profiles of the Mn-depleted and the native PSIIcc samples collected at 20°C and [PSIIcc] = 60  $\mu$ M.

sample	q <sub>i</sub>	$\tau_{ci \ i=1, 2, 3 \ (ns)}$
Mn depleted	46	$\tau_{c1=1500}$
	180	$\tau_{c2=75}$
Native sample	17	$\tau_{c1=1100}$
	165	$\tau_{c2=330}$
	160	$\tau_{c3=50}$