

Supporting Information

Glycerol binding at the narrow channel of photosystem II stabilizes the low-spin S₂ state of the oxygen-evolving complex

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Figure S1: QM/MM optimized models for LS-S₂ and HS-S₂ states

Figure S2: Umena et al. (2011) model of the proposed glycerol binding site in the 1.90 Å structure (3WU2).

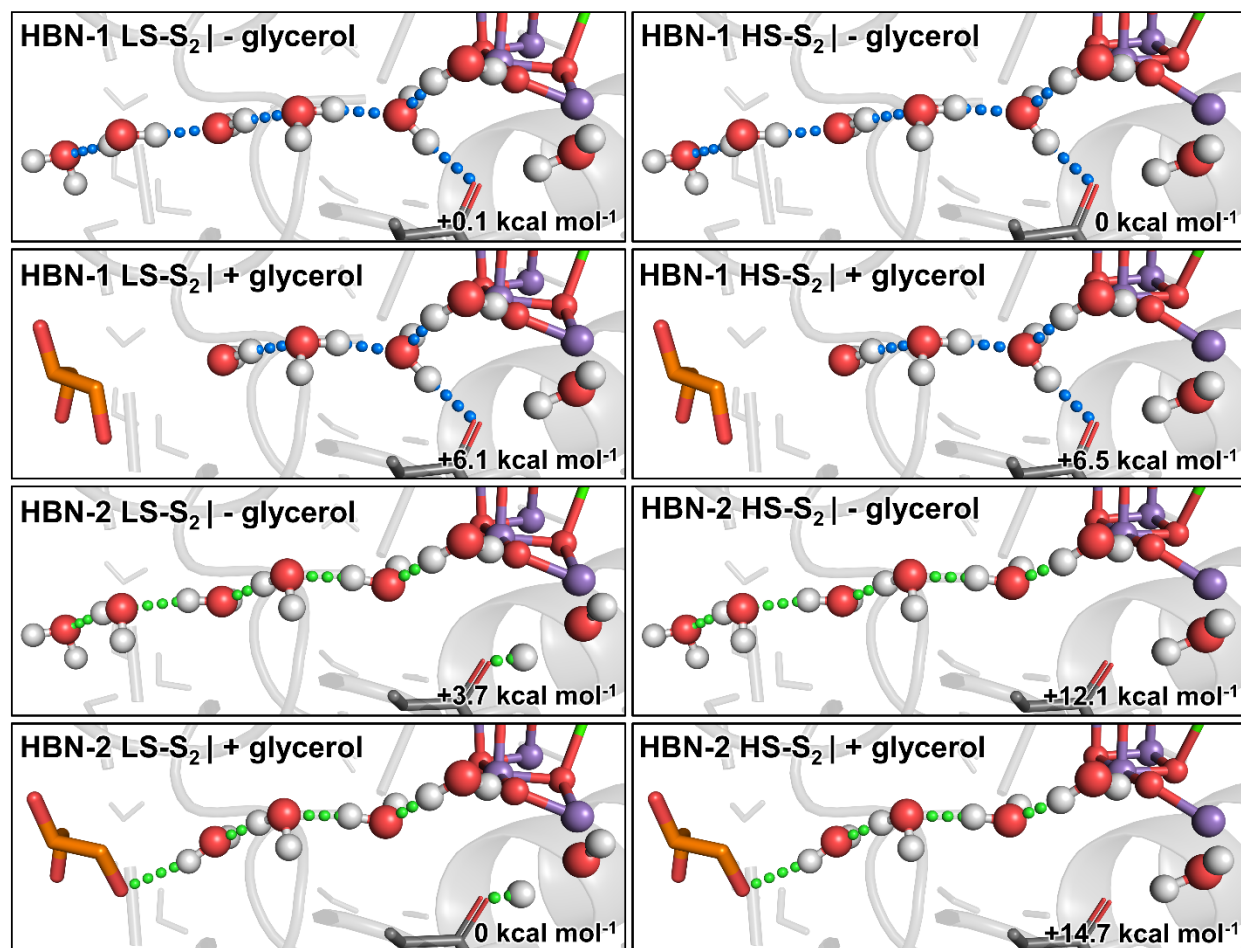


Figure S1. QM/MM optimized models for LS-S₂ and HS-S₂ states in HBN-1 and HBN-2 with glycerol (+ glycerol) and without glycerol (- glycerol). Waters and the OEC are shown as ball and stick models. Glycerol and D1-Asp61 are shown as stick models. Hydrogen-bonding interactions are shown as dotted lines where HBN-1 is depicted in blue and HBN-2 is depicted in green. The models are labeled in the top left and the DFT-QM/MM energy differences, scaled to the lowest energy model per structure, are labeled in the bottom right.

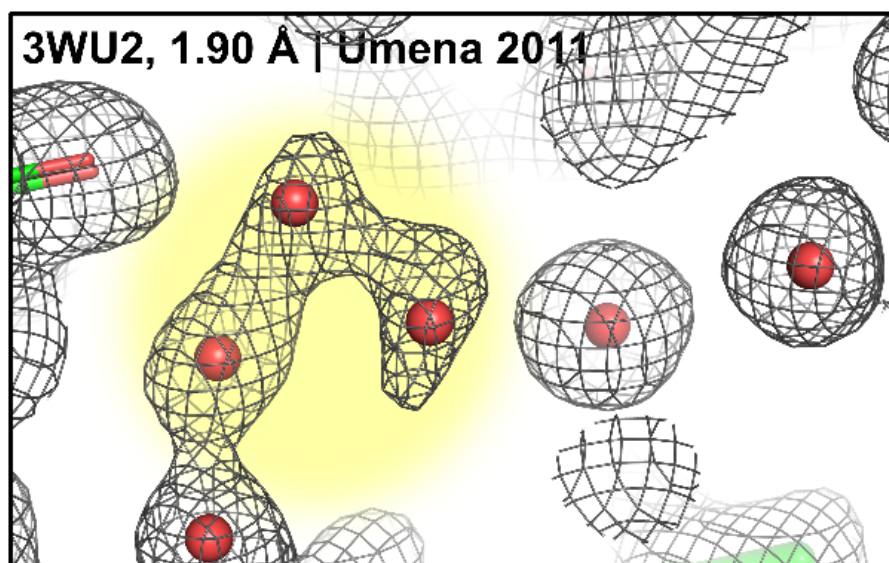


Figure S2. Visualization of the glycerol binding site proposed by Wiwczar et al. (2017) in the original model by Umena et al. (2011). The proposed glycerol binding site is highlighted in yellow. The grey mesh represents the structure map at 0.5σ . The mesh density has been increased to assist in visualization. Modeled waters are depicted using red spheres.

References

- Umena Y, Kawakami K, Shen J-R, Kamiya N (2011) Crystal structure of oxygen-evolving photosystem II at a resolution of 1.9 Å. *Nature* 473:55–60.
<https://doi.org/10.1038/nature09913>
- Wiwczar JM, LaFountain AM, Wang J, et al (2017) Chlorophyll *a* with a farnesyl tail in thermophilic cyanobacteria. *Photosynth Res* 134:175–182.
<https://doi.org/10.1007/s11120-017-0425-4>