

Supplementary Information:

**Modeling of the hydrophobic microenvironment of water-soluble
molybdoenzymes in an aqueous micellar solution**

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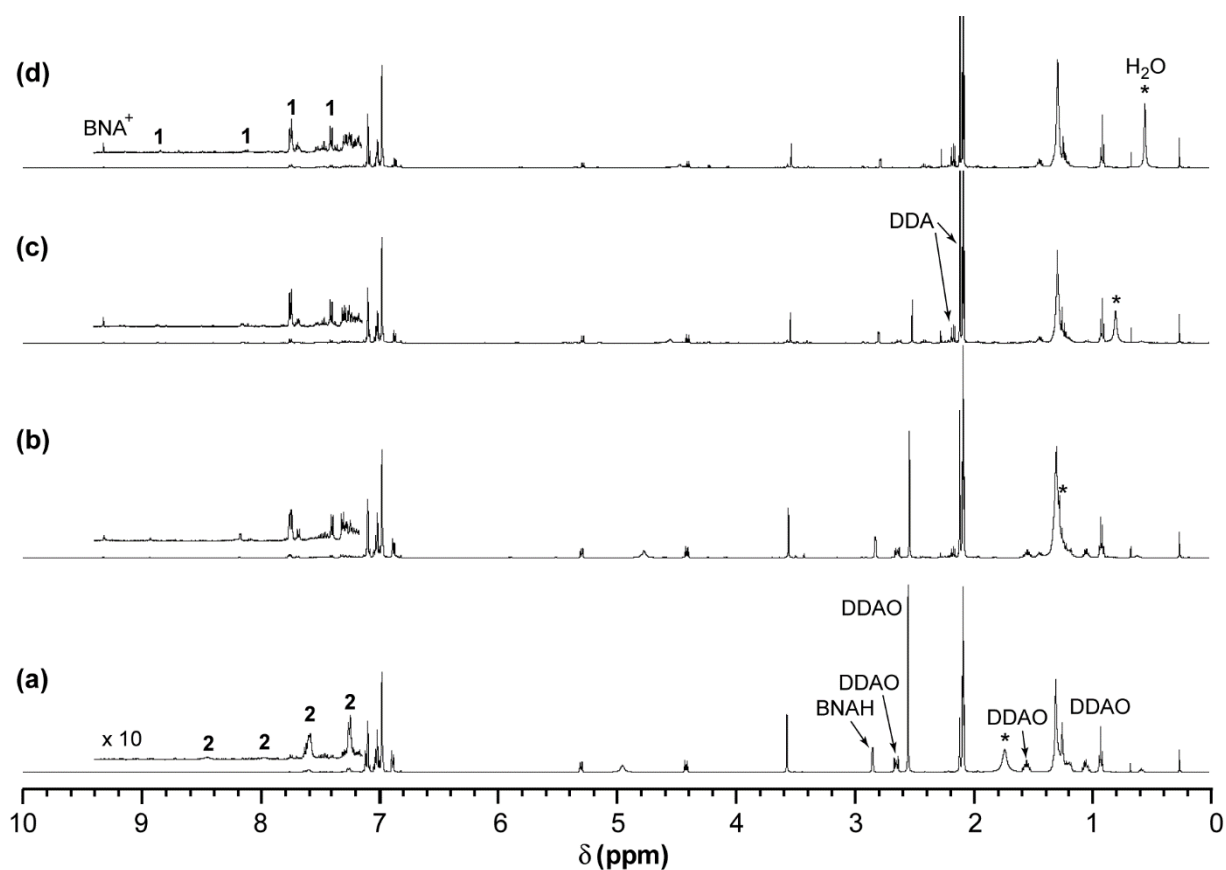


Fig. S1 ^1H NMR spectral change in water-containing toluene- d_8 during the catalytic reduction of DDAO by BNAH with 2 mol% of **2** at 27 °C after (a) 0.5 h, (b) 96 h, (c) 373 h, and (d) 887 h.

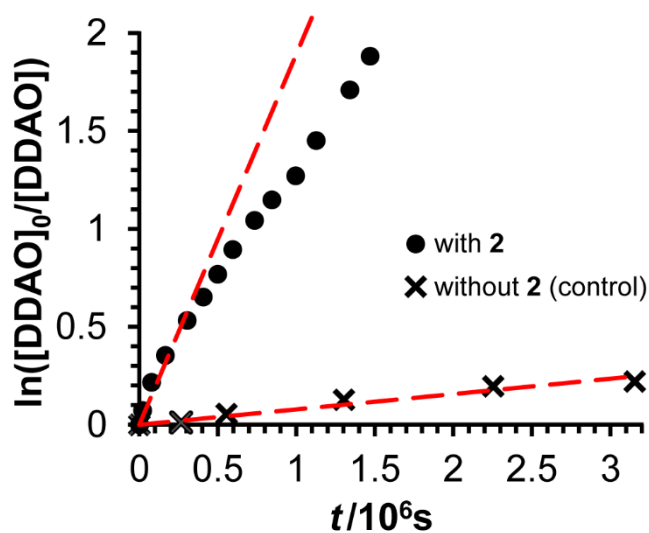


Fig. S2 Kinetic plots of the catalytic reduction of DDAO by BNAH with **2** and the control experiment in water-containing toluene- d_8 .