

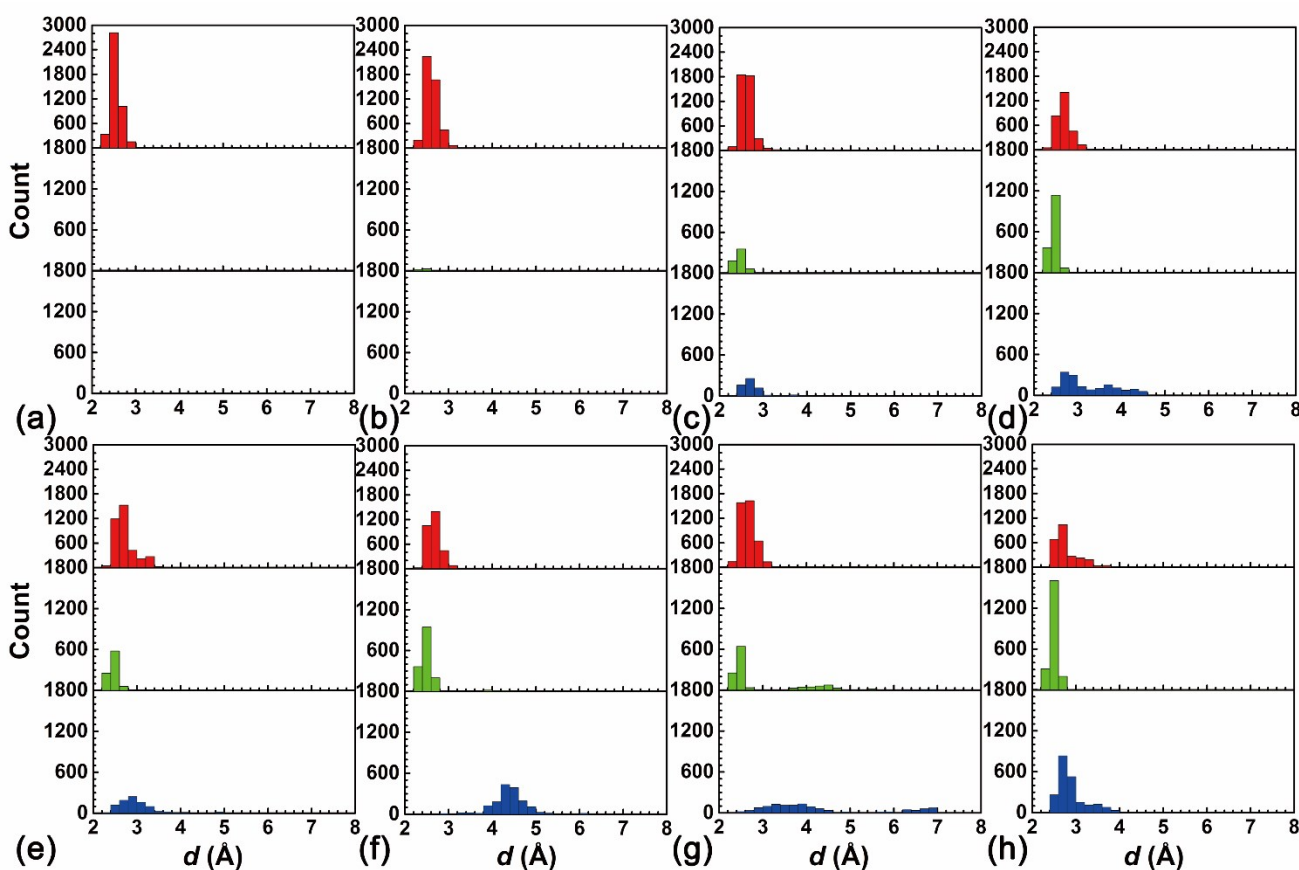
## Electronic Supplementary Information

# Insights into Protonation for Cyclohexanol/Water Mixtures at the Zeolitic Brønsted Acid Site

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**Fig. S1** Distributions of the minimum  $O_{OH}-O_{Al}$  distance (red) in frames containing the protonated cyclohexanol and the minimum  $O_W-O_{OH}$  distance (green) and minimum  $O_W-O_{Al}$  distance (blue) in frames containing the protonated water. All data was extracted from the 10 ps equilibrium AIMD simulation of (a) H-BEA-CyOH-1W, (b) H-BEA-CyOH-2W, (c) H-BEA-CyOH-3W, (d) H-BEA-CyOH-4W, (e) H-BEA-CyOH-5W, (f) H-BEA-CyOH-6W, (g) H-BEA-CyOH-7W, and (h) H-BEA-CyOH-8W.