Supplementary Materials: Effect of Water Clustering on the Activity of *Candida antarctica* Lipase B in Organic Medium

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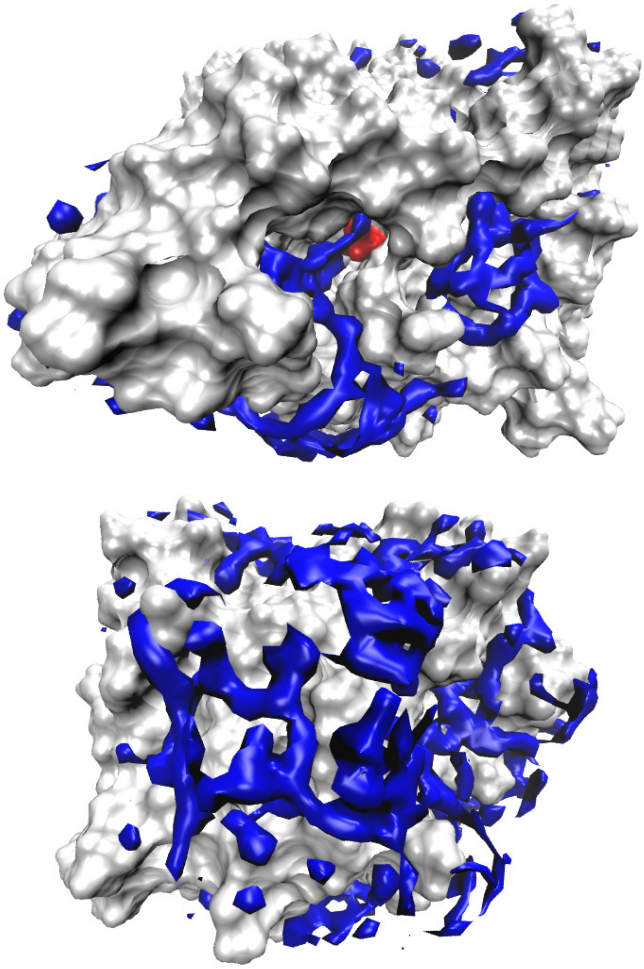

Figure S1. The spatial distribution of water occupancy at the molecular surface of CALB in MTBE at high water percentage (16.62%) averaged over the last 10 ns of simulation. The contours are shown for the isovalue 0.5. The enzyme is shown as a surface representation and colored white; the active site residue, Ser105, is shown in red, and the spatial distribution of water molecules are shown in blue. In order to give a complete view of the surface, two sides (front and back sides) of the enzyme are shown.

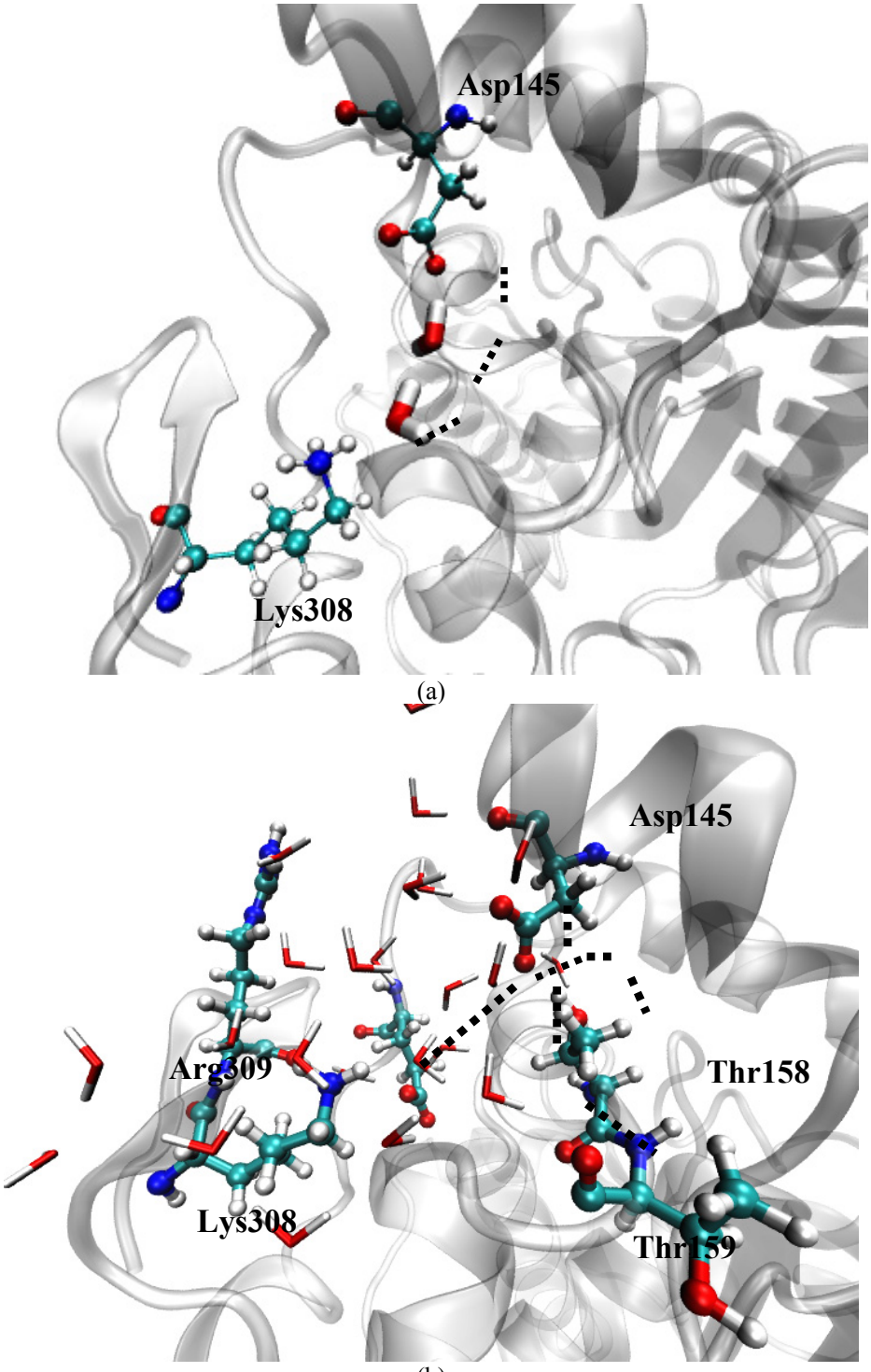

Figure S2. Selected part of the hydrogen-bonding network of the hot spot region IV located close to the active site pocket of CALB at water activities (a) 0.18 and (b) 0.54. The network gradually increases with increasing water activity. At low water activity, there are two water molecules, while with increasing water activity more water molecules bind to that hot spot region leading to an increase in cluster size.

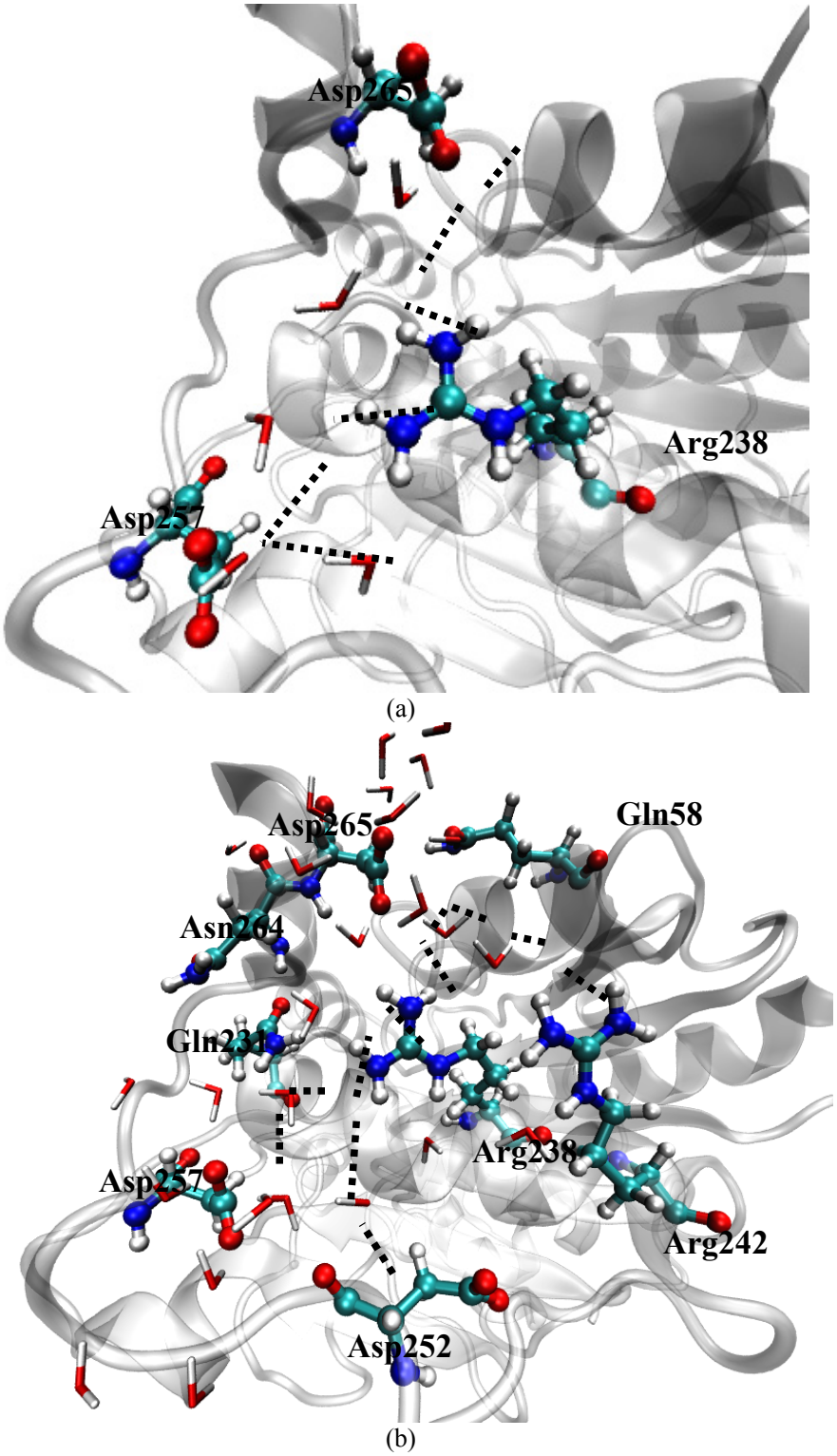

Figure S3. Selected part of the hydrogen-bonding network of the hot spot region II distal from the active site pocket of CALB at water activities (a) 0.18 and (b) 0.54. The network gradually increases with increasing water activity. At low water activity, there are relatively few water molecules, while with increasing water activity more water molecules bind to that hot spot region leading to an increase in cluster size.

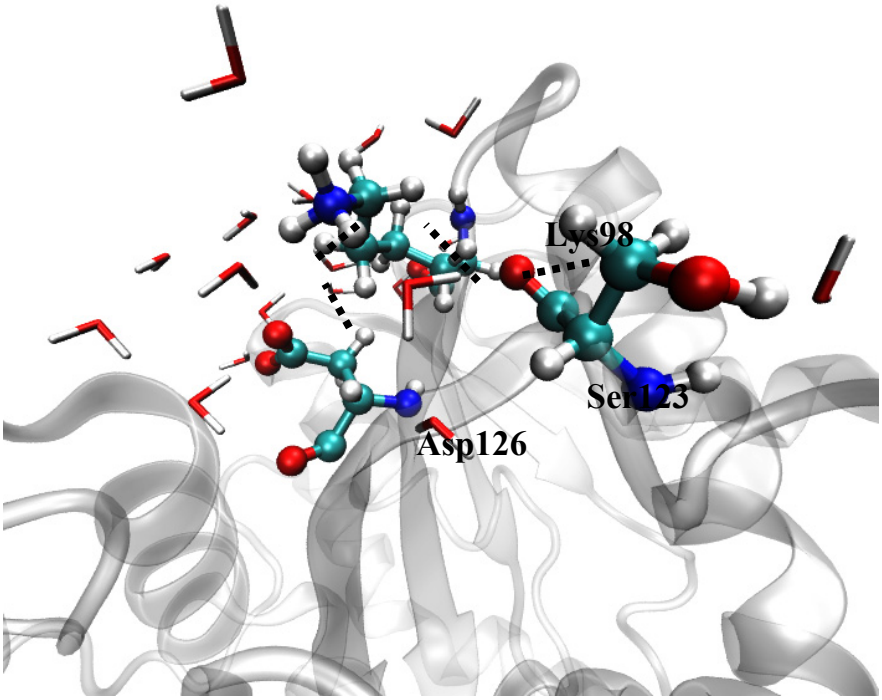

Figure S4. The hydrogen-bonding network of the hot spot region I of CALB at water activity 0.54.