Supplementary material

A Computational–Experimental Investigation of the Molecular Mechanism of Interleukin-6−Piperine Interaction

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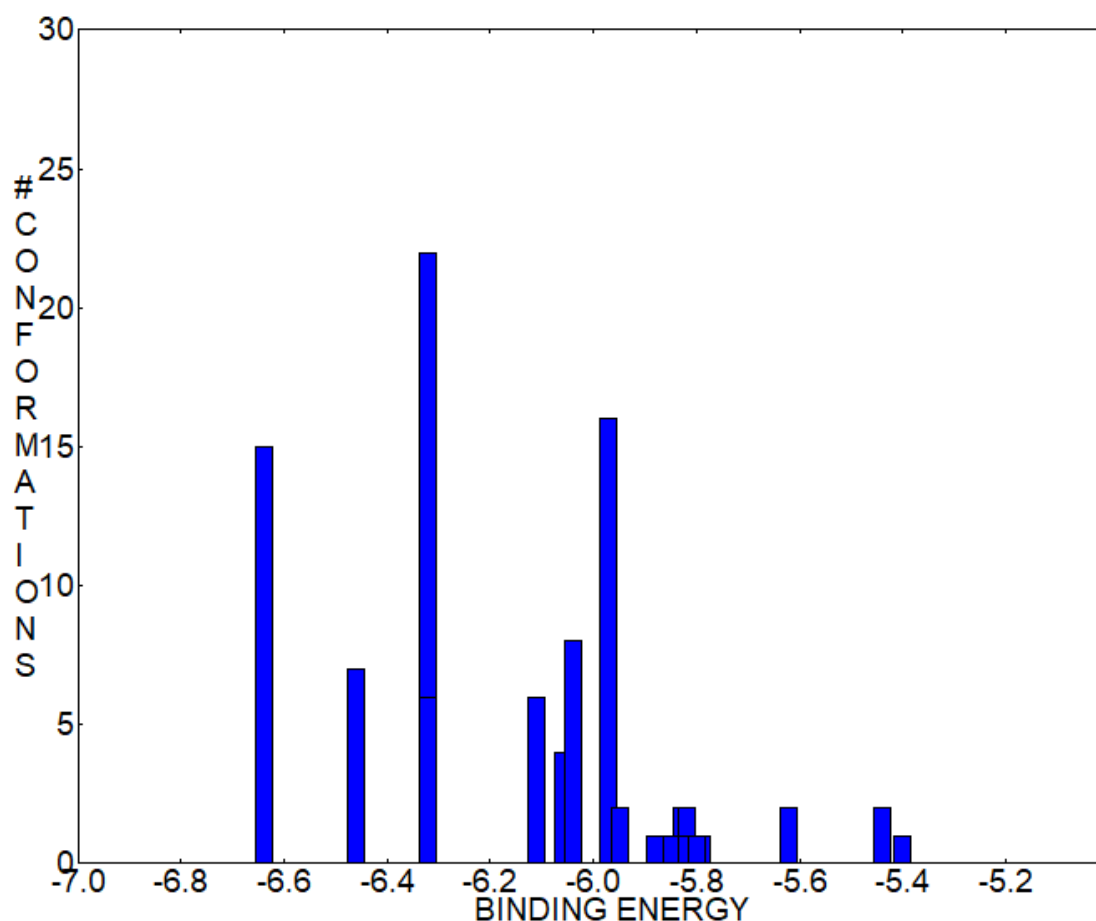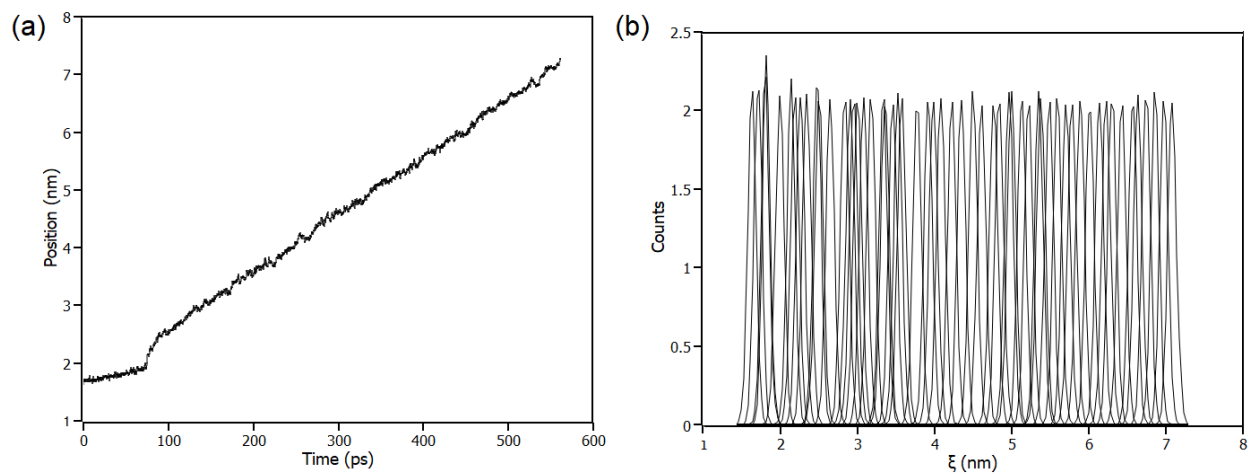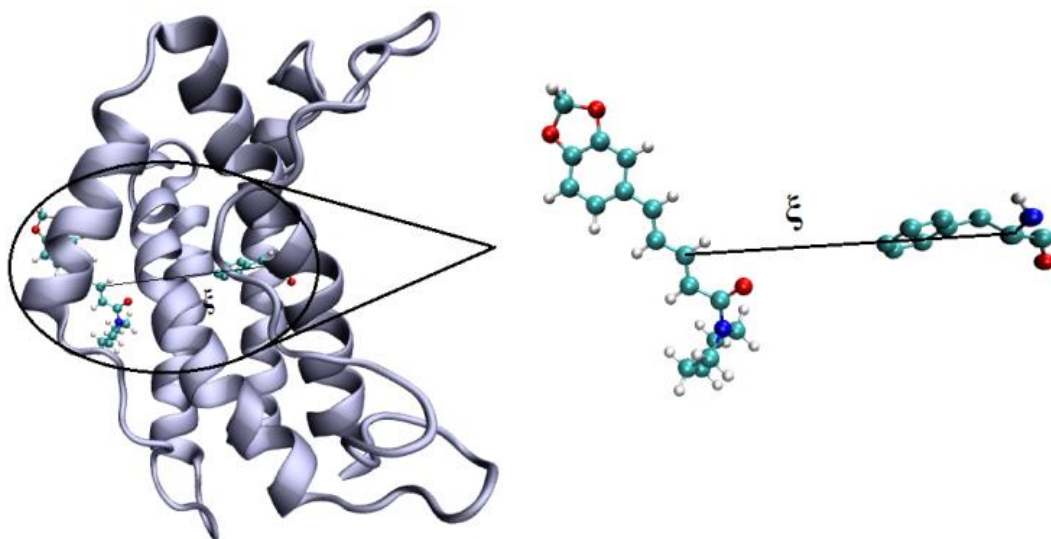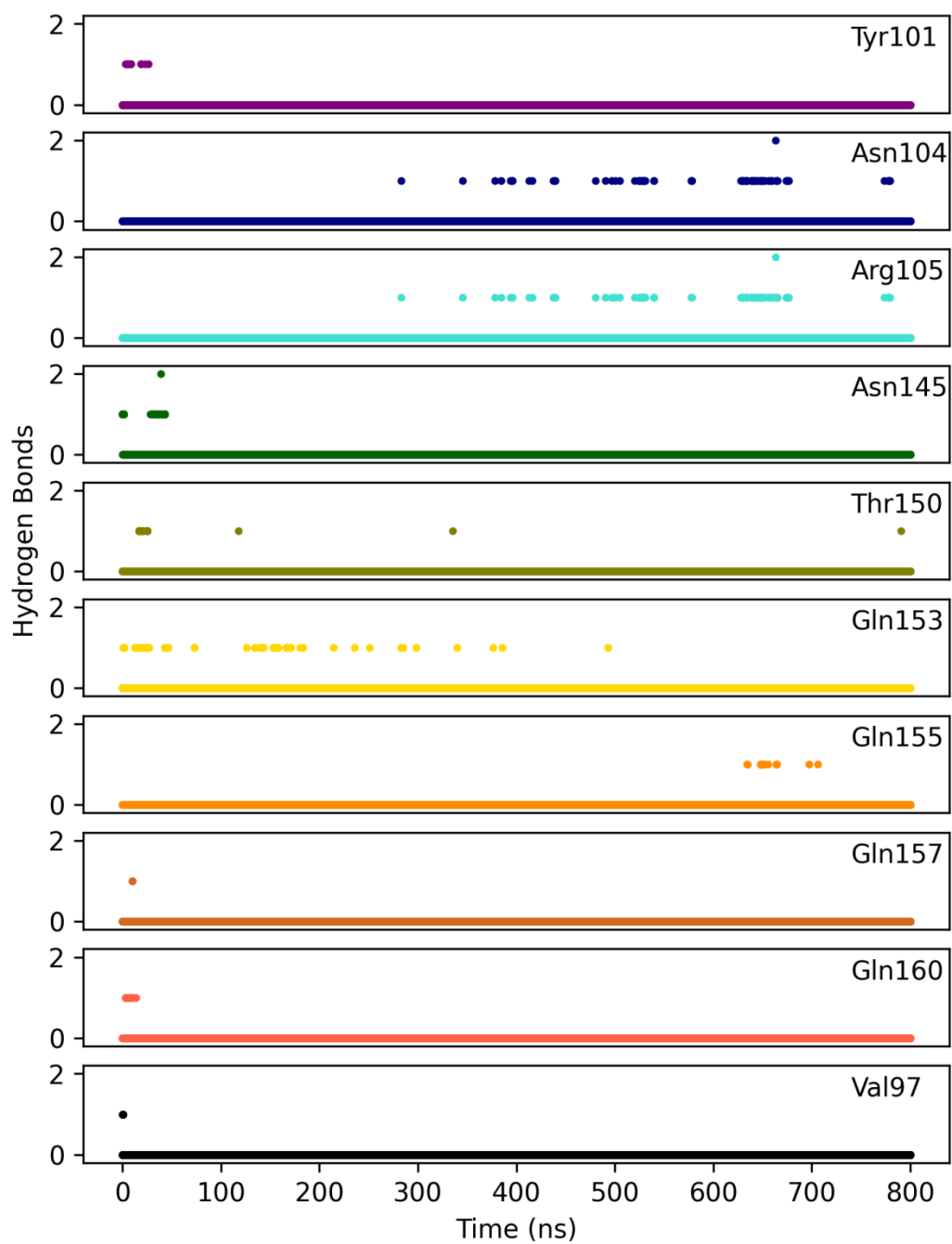
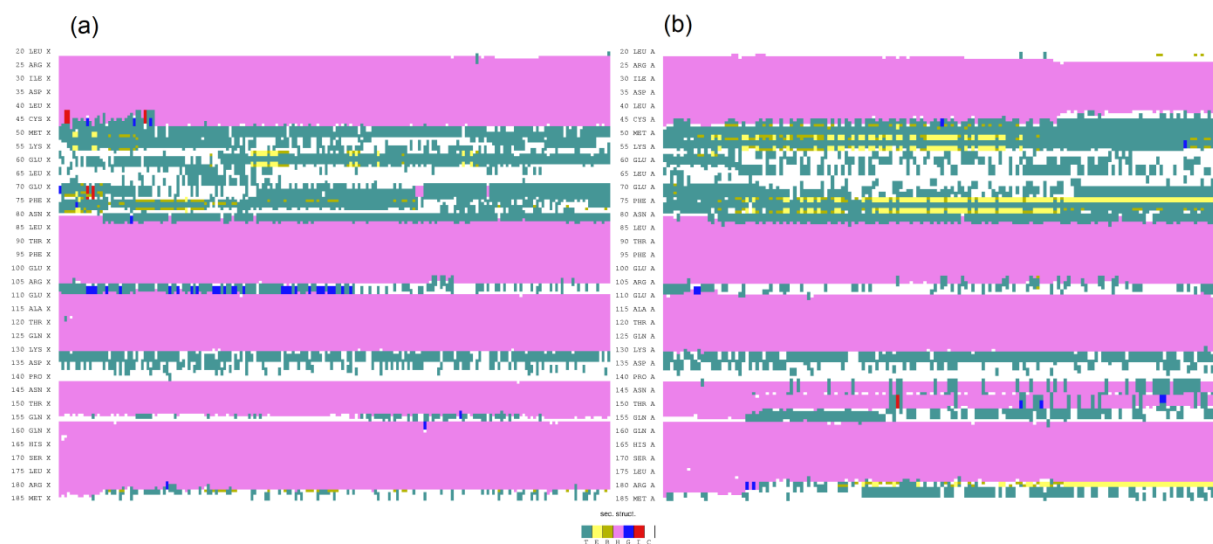**Figure S1:** Molecular docking clusters with their respective energy scores

Figure S2: (a) Pulling profile during the pulling simulation. Y-axis is the value of reaction coordinate (ξ) and x-axis is the time of simulation. **(b)** Configuration histograms of the pulling in z-axis with the windows distance = 0.1 nm.

Figure S3: The atoms picked to define the reaction coordinate (ξ) in umbrella sampling calculations. Zoomed in view of piperine and Phe171.

Figure S4: Hydrogen bonds performed during 800 ns of simulation.

Figure S5: Global secondary structures of IL6 calculated during the molecular dynamics simulations in **(a)** the absence of piperine and **(b)** piperine inside the binding pocket.