Supplementary Information for Inhibition of the early-stage cross-amyloid aggregation of amyloid-β and IAPP via EGCG: insights from molecular dynamics simulations

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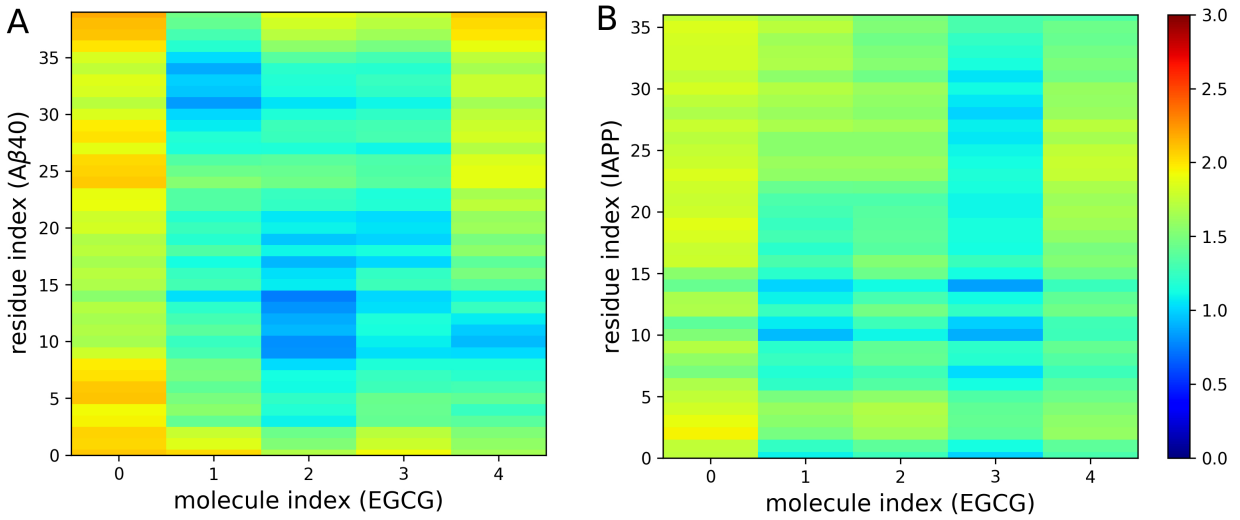

Figure S1: The distance matrices illustrating inter-molecular contacts between EGCG molecule and Aβ40 (**A**), and IAPP and (**B**). The inter-molecular contacts are shown for the whole simulation time. The color bar on the right indicates average inter-molecular distances (in nanometers)

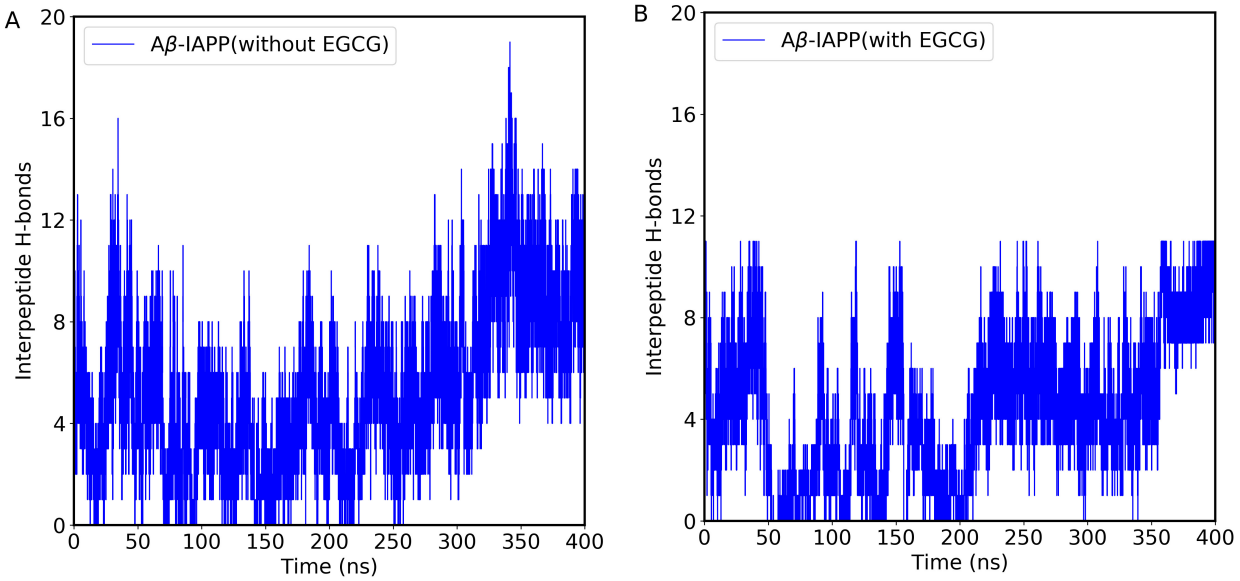

Figure S2: Time evolution of inter-peptide hydrogen bonds formed between Aβ40 and IAPP (**A**) in the absence of EGCG (**B**) in the presence of EGCG of hetero-dimer system.

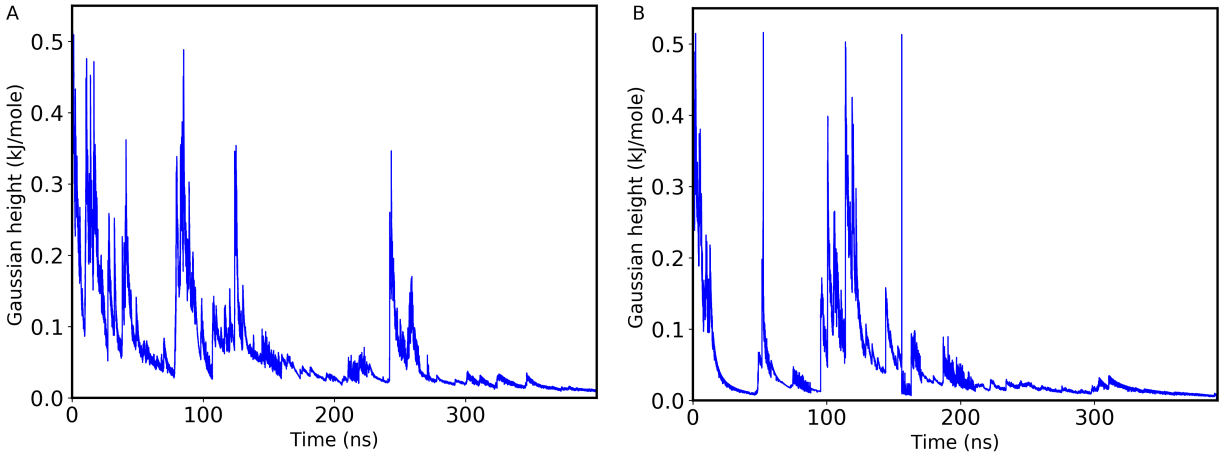

Figure S3: Time evolution of Gaussian hills of heterodimer system during the metadynamics simulation (**A**) in the absence of EGCG, and (**B**) in the presence of EGCG.