

Supporting Information

Action of Caffeine as an Amyloid Inhibitor in the Aggregation of $A\beta_{16-22}$ Peptide

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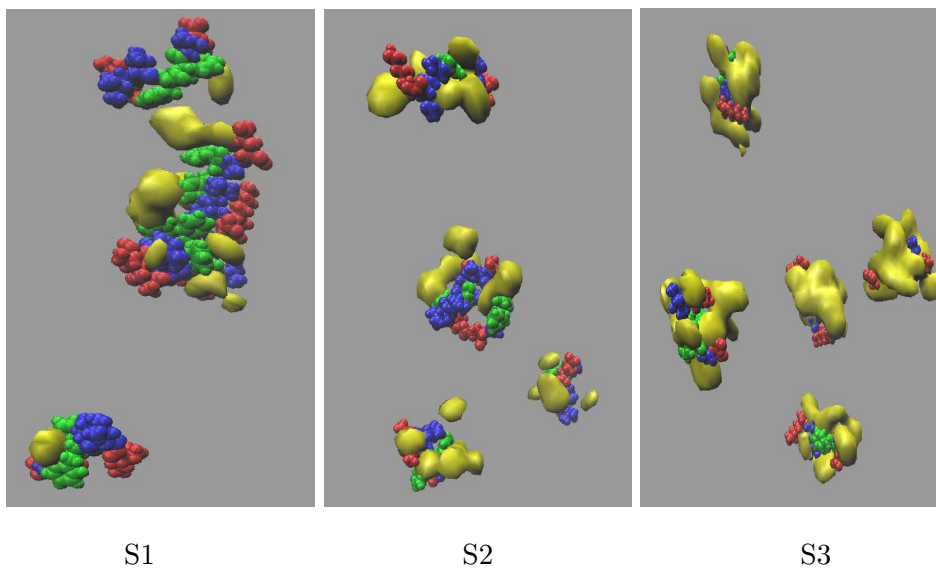
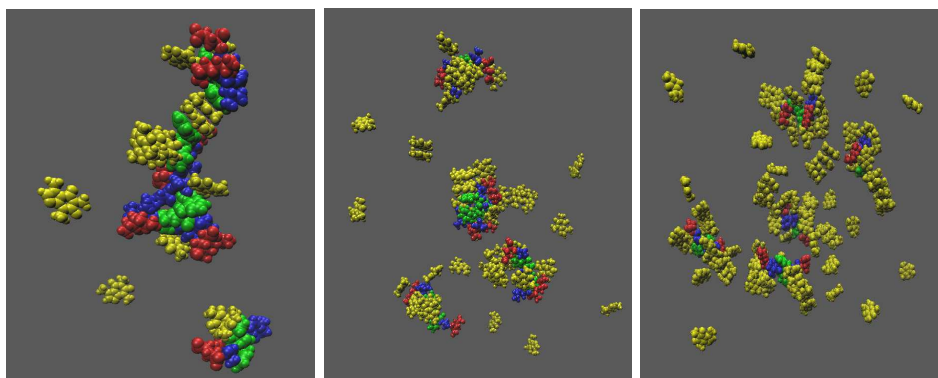


FIG. S1: Contour density plots for caffeine around A β_{16-22} peptides within 7.5 Å of peptide for the last 10 ns of simulation. Yellow color represents caffeine density, and other colors represent peptide. Hydrophobic parts are represented in blue, hydrophilic parts in red, and Phe residues are represented in green color.



S1

S2

S3

FIG. S2: Snapshots of the last state of simulation for different systems. Yellow color represents caffeine molecules, and other colors represent peptide. Hydrophobic parts are represented in blue, hydrophilic parts in red, and Phe residues are represented in green color.

S3

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