Supporting Information

for

Molecular Dynamics Simulation Studies of Caffeine Aggregation in Aqueous Solution

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Supplementary Material

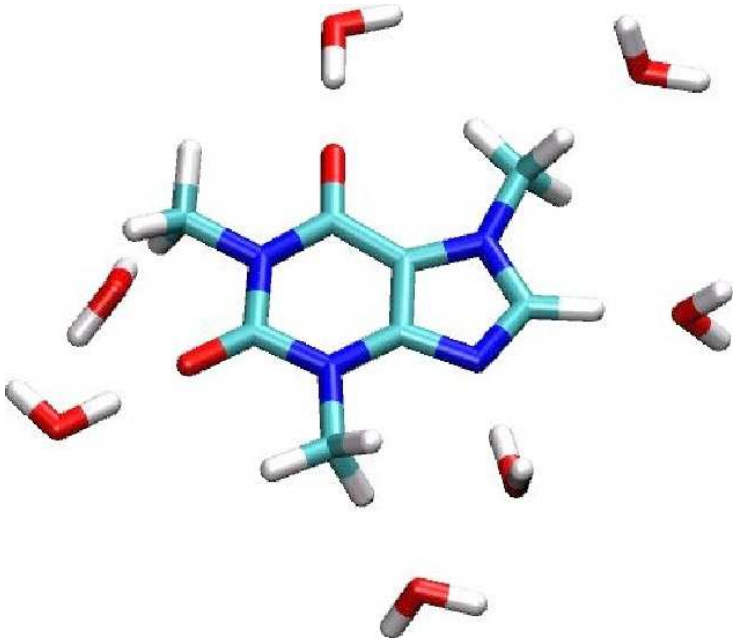

Figure S1. The positions for water molecules used in the charge optimization.

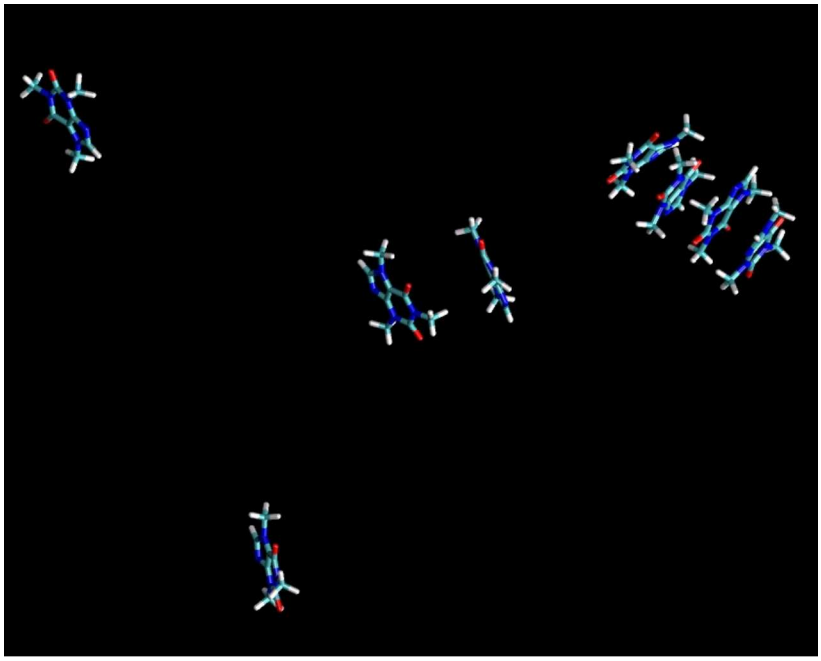

Figure S2. A representative snapshot from the simulation showing monomers and clusters of two different sizes.