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Fig. S1The salt-bridge was formed between the CO₂⁻ moiety of Asp²³ and the NH₃⁺ in Lys²⁸ residue as a function of time.



а

b.

Fig. S2The salt-bridge was formed between the CO_2^- moiety of Glu^{22} and the NH_3^+ in Lys²⁸ residue as a function of time.



b

а



Fig. S3 Distance between C α (Val24) and C α (Asn27) as a function of time.









Fig. S6 Difference in SASA values for $A\beta_{1-40}$ -Zn²⁺ and $A\beta_{1-40}$.



a.

Fig. S7 Convergence of trajectories for different conformations of a) $A\beta_{1-40}$ and b) $A\beta_{1-42}$ peptides in the presence of metal ions (Cu^{2+} and Zn^{2+}).

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