# Destructive Mechanism of $A\beta_{1-42}$ Protofibril by Norepinephrine revealed via Molecular Dynamics Simulations

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This material contains four figures: the correlations between $A\beta_{1-42}$ protofibril experimental NMR chemical shift ($C_\alpha/C_\beta$ atoms) and simulated chemical shift data (Figure S1), the J-coupling ($^3J(H_N,H_\alpha)$) constants values of $A\beta_{42}$ residues calculated from 5OQV and those from simulation-generated conformational ensembles of $A\beta_{1-42}$ protofibril system (Figure S2), the secondary structure probabilities of $A\beta_{1-42}$ protofibril in the Aβ and Aβ+$NE^0$ systems (Figure S3), the average number of π-π stacking between the aromatic residues of $A\beta_{1-42}$ protofibril and $NE^+/NE^0$ (Figure S4), and the interchain contact number of $A\beta_{1-42}$ protofibril in the absence and presence of NE (in protonated and deprotonated states) (Figure S5).

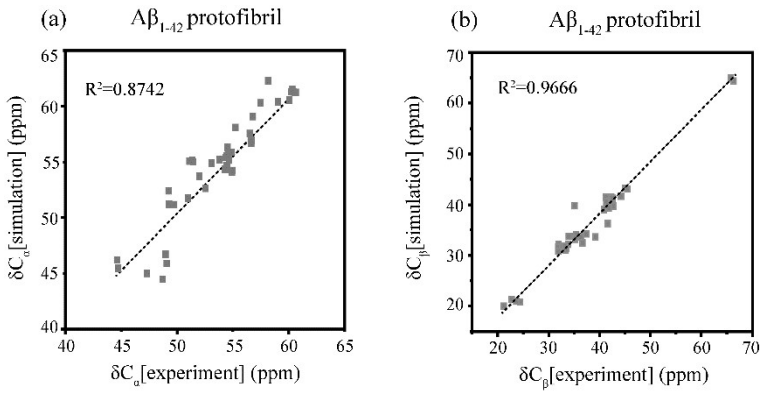


**Figure S1.** Conformational comparison between experimental data and simulated data. (a–b) Correlations between experimental NMR chemical shift data for $C_\alpha$ and $C_\beta$ atoms and simulated chemical shift data for the $A\beta_{1\text{-}42}$ protofibril system.

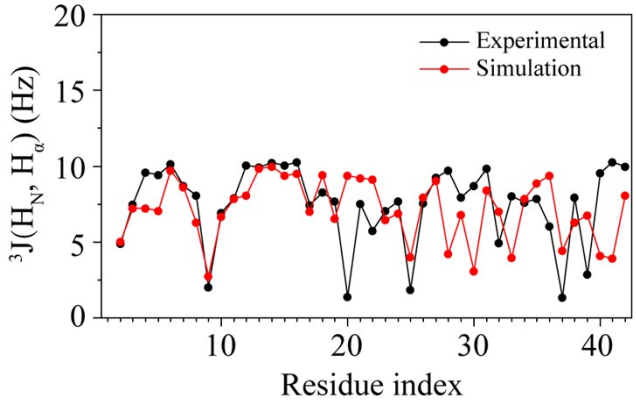


**Figure S2.** The J-coupling ($^3J(H_N,H_\alpha)$) constants values of $A\beta_{42}$ residues calculated from 5OQV and those from simulation-generated conformational ensembles of $A\beta_{1\text{-}42}$ protofibril system.

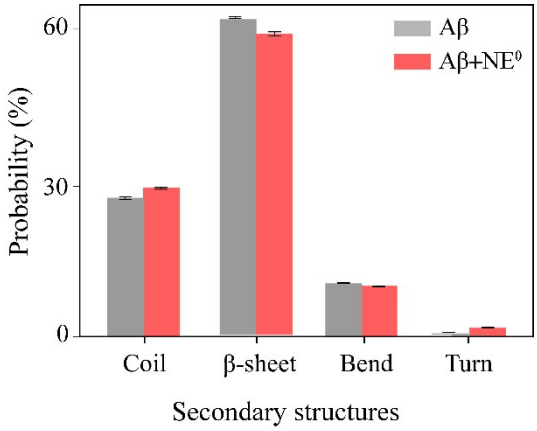


**Figure S3.** Secondary structure probabilities of $A\beta_{1\text{-}42}$ protofibril in the Aβ and Aβ+$NE^0$ systems.

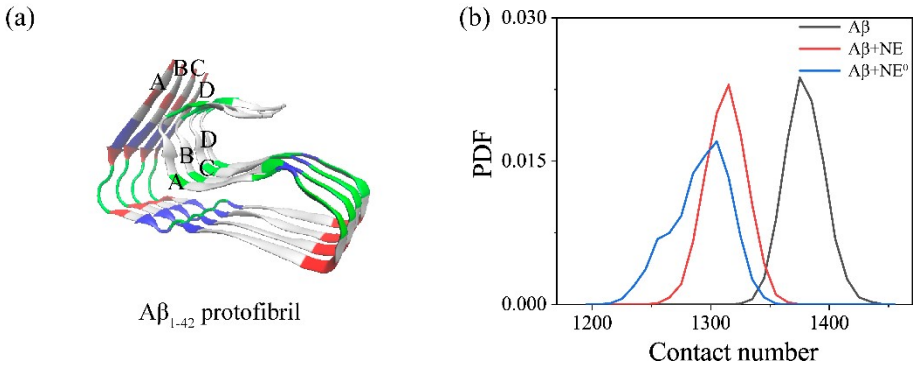


**Figure S4.** The LS-shaped configuration of $A\beta_{1\text{-}42}$ protofibril shown in (a). The ABCD is used to indicate four chains of $A\beta_{1\text{-}42}$ protofibril. (b) The interchain contact number of $A\beta_{1\text{-}42}$ protofibril in the absence and presence of NE (in protonated and deprotonated states). The interchain contact were averaged over the three pairs of neighboring chains (i.e. chain A-chain B, chain B-chain C and chain C-chain D).

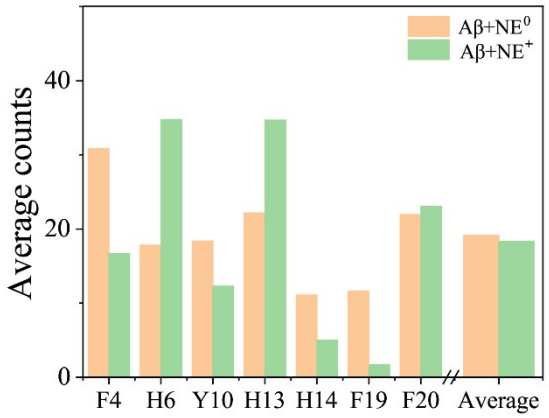


**Figure S5.** Average number of π-π stacking between the aromatic residues of $A\beta_{1\text{-}42}$ protofibril and $NE^{+}/NE^{0}$.