Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Critical nucleus of Greek-key-like core of α-synuclein protofibril and its disruption by dopamine and norepinephrine

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This material contains three supplemental figures.

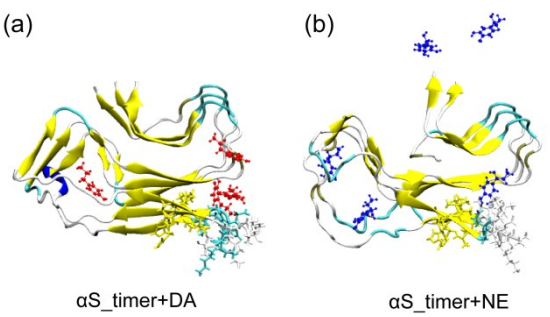

Fig. S1 Snapshots in the αS_trimer+DA and αS_trimer+NE systems, showing that the

smaller size of DA enables more DA molecules to bind to residues 45~52 which are located at the entry of the Greek-key-like core.

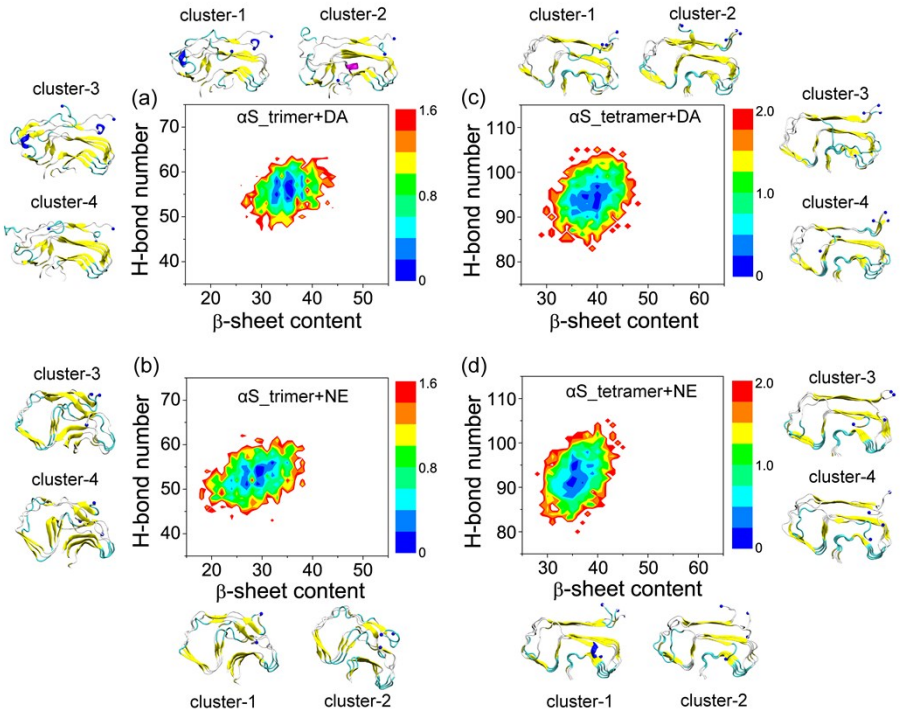

Fig. S2 Potential of mean force (PMF) for αS trimer (a, b) and tetramer (c, d) in the presence of DA/NE molecules. The PMF (in kcal mol^{-1}) of αS oligomers plotted as a function of β-sheet content and the number of H-bonds of αS oligomers. The conformations in the side and bottom of the PMF show the first four most-populated clusters of different systems.

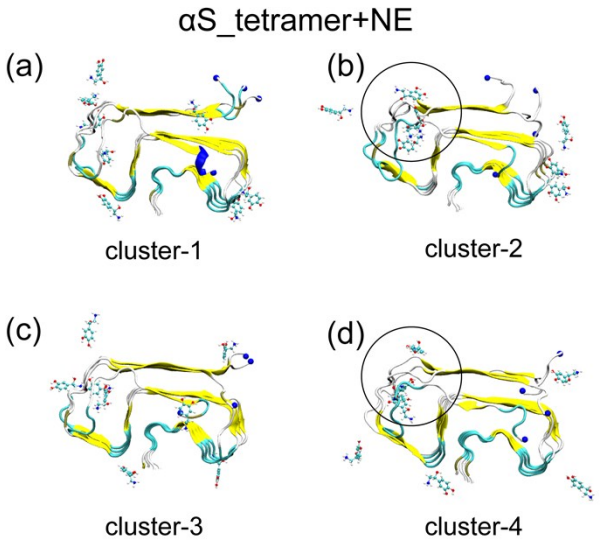

Fig. S3 Representative conformations of the first four most-populated clusters of αS_tetramer+NE system. The Cα atom in the N-terminal of each αS chain is represented by the blue bead.