Mechanistic insight into the disruption of Tau R3-R4 protofibril by curcumin and epinephrine: an all-atom molecular dynamics study
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\begin{itemize}
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\end{itemize}

This material contains seven supplemental figures.

(a) \hspace{1cm} \hspace{1cm} \hspace{1cm} \hspace{1cm} \hspace{1cm}
\begin{align*}
\text{Dimer} & \quad \text{Trimer} & \quad \text{Tetramer} & \quad \text{Pentamer} & \quad \text{Hexamer}
\end{align*}

(b) \hspace{1cm} \hspace{1cm} \hspace{1cm} \hspace{1cm} (c)
\begin{align*}
\text{Pentamer(5mer)+Cur} & \hspace{1cm} \text{Pentamer(5mer)+EP} & \quad \text{Curcumin (Cur)} & \quad \text{Epinephrine (EP)}
\end{align*}

Fig. S1 Initial states of each Tau oligomer (a), 5mer+Cur system (b) and 5mer+EP system (c), and the chemical structures of Cur (d) and EP (e).
Fig. S2 Time evolution of average RMSD values of Tau oligomers over five MD runs for each system (a). RMSD values of different sizes of Tau oligomers (b-f) as a function of simulation time.

Fig. S3 Time evolution of average β-sheet probabilities of Tau oligomers over five MD runs for each system (a). β-sheet probabilities of different sizes of Tau oligomers (b-f) as a function of simulation time.
Fig. S4 PDF of the distance between the positively charged group of the side chain and two rings of Cur (a, b).

Fig. S5 The residue-based contact number and fraction of reduced β-sheet in 5mer+Cur (a) and 5mer+EP (b) systems. The probabilities of reduced β-sheet were calculated using the residue-based β-sheet probabilities of Tau pentamer in 5mer system minus those in 5mer+Cur and 5mer+EP systems.
Fig. S6 Representative conformations of the first two most-populated clusters of Tau pentamer in 5mer+Cur system in five MD runs.

Fig. S7 Representative conformations of the first two most-populated clusters of Tau pentamer in 5mer+EP system in five MD runs.