

Supplementary Materials

Deciphering the Effect of Lysine Acetylation on the Misfolding and Aggregation of Human Tau Fragment $^{171}\text{IPAKTPPAPK}^{180}$ Using Molecular Dynamic Simulation and the Markov State Model

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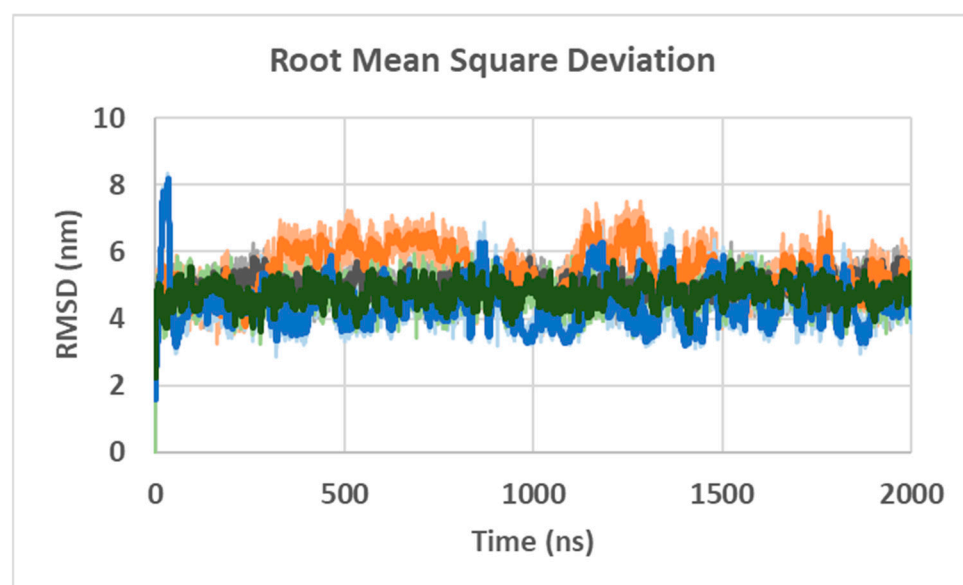


Figure S1. RMSD profile of Differently Modified 16-mer of $^{171}\text{IPAKTPPAPK}^{180}$. The WT non-modified peptides, acetylated K174, acetyl-mimic KQ peptides and deacetyl-mimic KR is shown in grey, red, blue, and green color respectively.

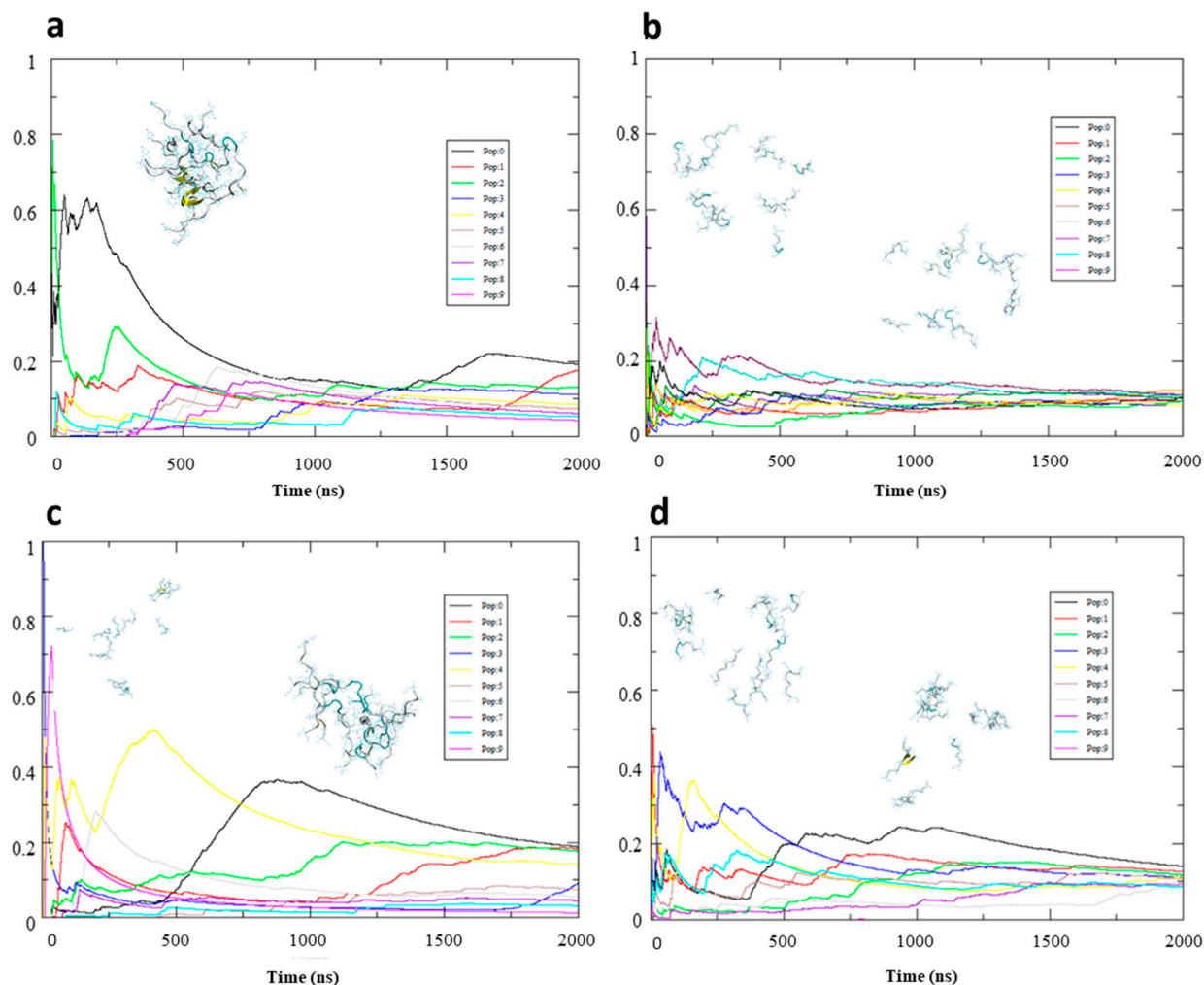


Figure S2. Time-lapse Cluster Analysis of Differently Modified 16-mer of $^{171}\text{IPAKTPPAPK}^{180}$. (a) acetylated K174 16-mers, (b) non-modified WT 16-mers, (c) The acetyl-mimic KQ mutated 16-mers and (d) the deacetyl-mimic KR mutated 16-mers. Different Cluster populations are shown in different colors.

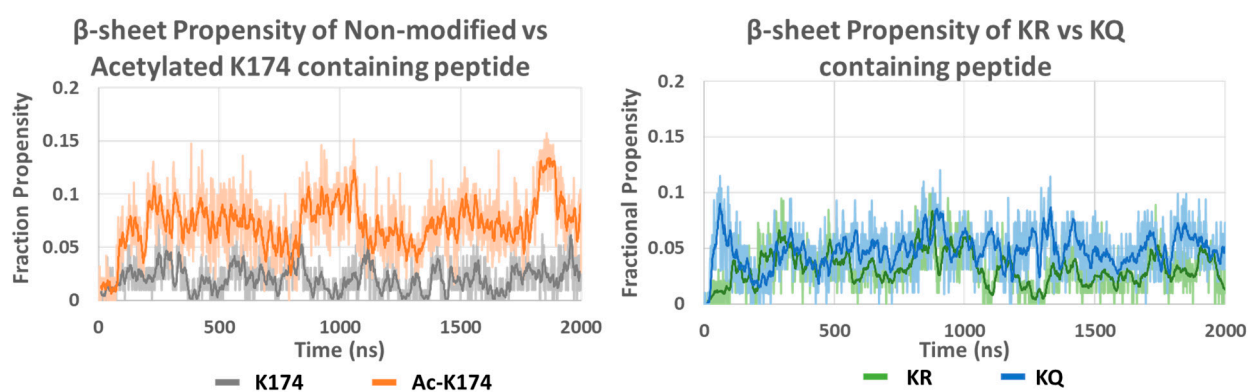


Figure S3. β -sheets propensity of differently modified $^{171}\text{IPAKTPPAPK}^{180}$ tau fragments as predicted by DSSP analysis. The non-modified WT, ac-K174, KQ and KR is shown in grey, orange, blue and green color, respectively.

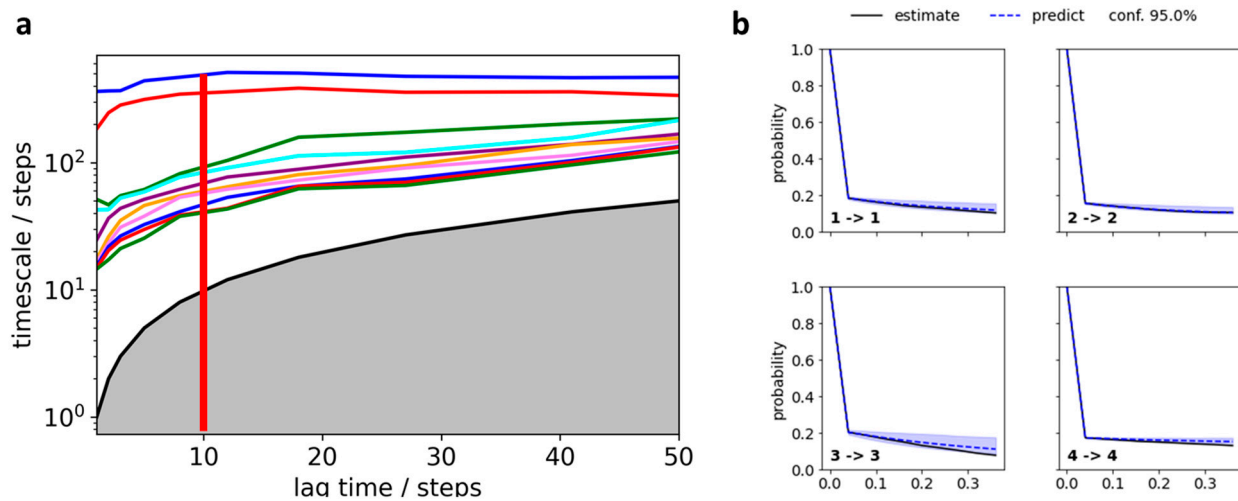


Figure S4. Markov state model validation for C3-C13 Dimer. (a) Implied relaxation timescale as a function of lag time $\tau = 10$ ns (10 steps) is appropriate and (b) Chapman-Kolmogorov test curves obtained by lumping 300 microstates into 5 macrostates.