

Supporting information

Destabilization mechanism of R3-R4 tau protofilament by purpurin: a molecular dynamics study

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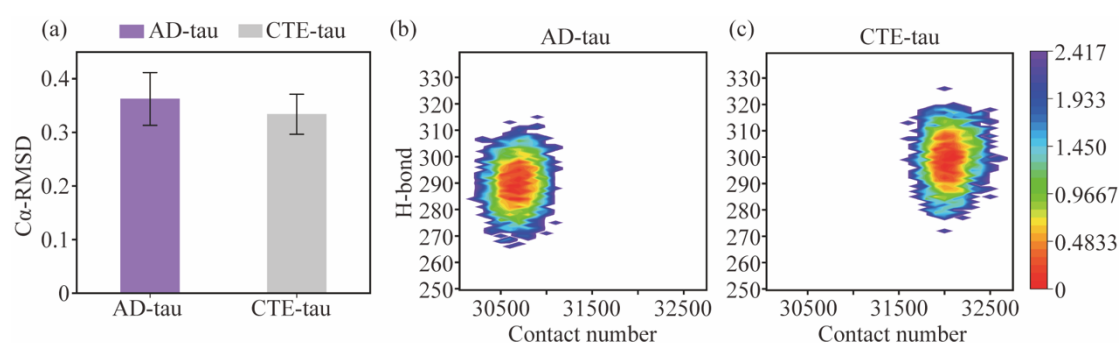


Figure S1. Statistics analysis of Cα-RMSD of AD-tau and CTE-tau(a). Potential mean force (in kcal/mol) of AD-tau(b) and CTE-tau(c) as functions of the H-bond number and contact number. The Cα-RMSD, contact number and H-bond was calculated using 250–450 ns data of three MD runs in AD-tau and CTE-tau system, respectively.

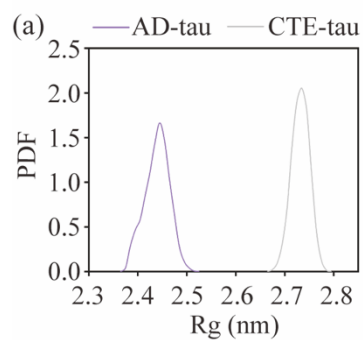


Figure S2. The PDF of radius of gyration (R_g) of AD-tau (purple) and CTE-tau (grey).

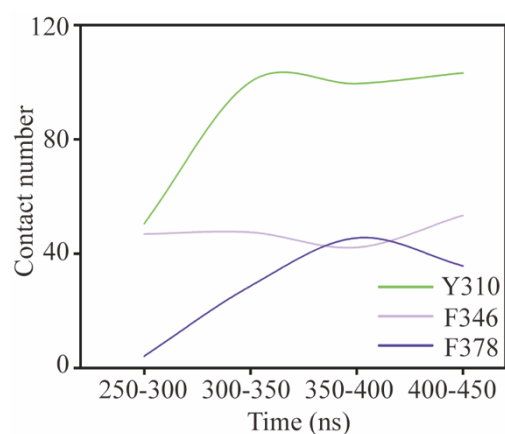


Figure S3. The contact number between Y310, F346, F378 and purpurin molecules at 250-300, 300-350, 350-400 and 400-450 ns.

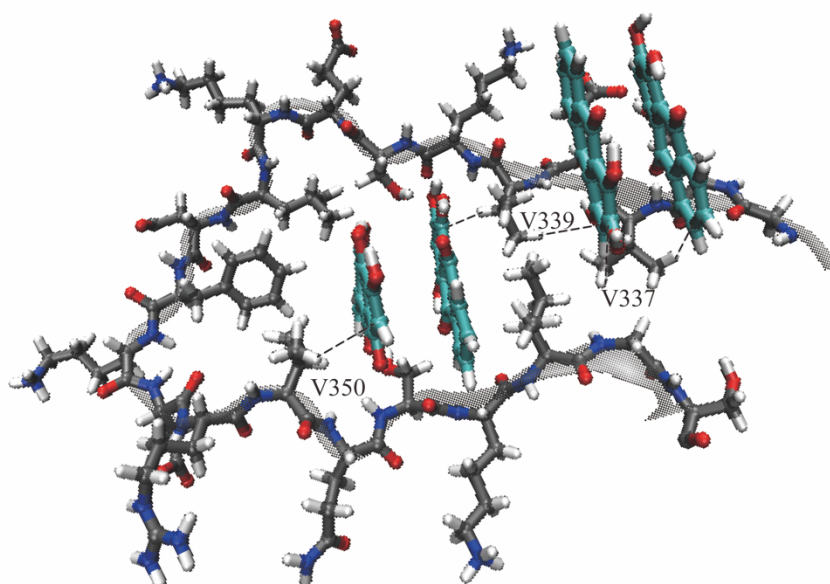


Figure S4. A snapshot of the hydrophobic contacts between purpurin and V337, V339, V350. The black dashed lines represent hydrophobic contacts.

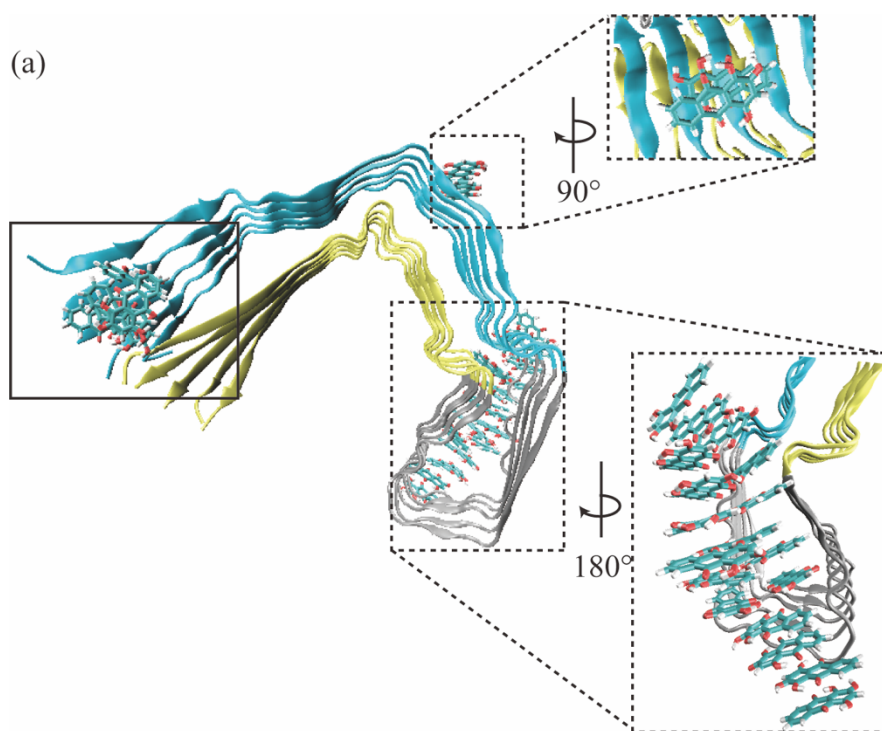


Figure S5. A respective snapshot showing the distribution of purpurin molecules on CTE-tau protofilament. Three squares are highlight the three regions where purpurin molecules contact with CTE-tau. The two dashed line squares are enlarged and shifted tp show the spatial distribution of purpurin and CTE-tau protofilament. Tau protofilament are divided to three regions. S305-G335 (blue), Q336-G355 (gray) and N356-R379 (yellow).