

Supporting Information

Unravelling the destabilization potential of Ellagic acid on α -Synuclein fibrils using molecular dynamics simulations

Opinder Kaur Mankoo,^[a] Anupamjeet Kaur,^{[a]#} Deepti Goyal^{*[b]} and Bhupesh Goyal^{*[c]}

[a] Department of Chemistry, Faculty of Basic and Applied Sciences, Sri Guru Granth Sahib World University, Fatehgarh Sahib–140406, Punjab, India

[b] Department of Chemistry, DAV College, Sector 10, Chandigarh–160011, India

[c] School of Chemistry & Biochemistry, Thapar Institute of Engineering & Technology, Patiala–147004, Punjab, India

*Corresponding author

Email address: deeptig@iitbombay.org; bhupesh@iitbombay.org

#Present address

National Institute of Immunology, Aruna Asaf Ali Marg, New Delhi–110067, India

Table of contents

Figure S1: The input conformation of α -Syn fibril and EA for the docking studies is shown in the left panel. The best-docked pose of EA with α -Syn fibril (right panel). The α -Syn fibril is shown in cartoon and EA is displayed in the stick representation.	S3
Figure S2: The top ten docked conformations of EA with α -Syn fibril.	S4
Figure S3: The 2D interaction maps displaying hydrogen bonds and hydrophobic contacts in the top ten docked conformations of EA with α -Syn fibril. The green dashed line depicts hydrogen bonds between α -Syn fibril and EA.	S5
Figure S4: The conformational snapshots of MD trajectory of α -Syn fibril at different time points in the absence and presence of EA are shown in panel a, and b, respectively.	S6
sFigure S5: The RMSD of α -Syn fibril alone (panel a) and α -Syn fibril + EA (panel b) as a function of simulation time for the repeat simulations with different initial velocities. The RMSF of the residues of α -Syn fibril in the absence and presence of EA for the repeat simulations are shown in panel c, and d, respectively.	S7
Figure S6: The time-dependent evolution of number of contacts between α -Syn fibril and EA.	S8
Figure S7: The 2D interaction map displaying the hydrophobic contacts and hydrogen bonds in the representative conformations of the three most-populated conformational clusters C1', C2' and C3' of α -Syn fibril + EA are displayed in panel a, b, and c, respectively.	S9
Figure S8: The RMSD of chain H and chain J of α -Syn fibril in the absence and presence of EA during simulation are shown in panel a, and b, respectively.	S10

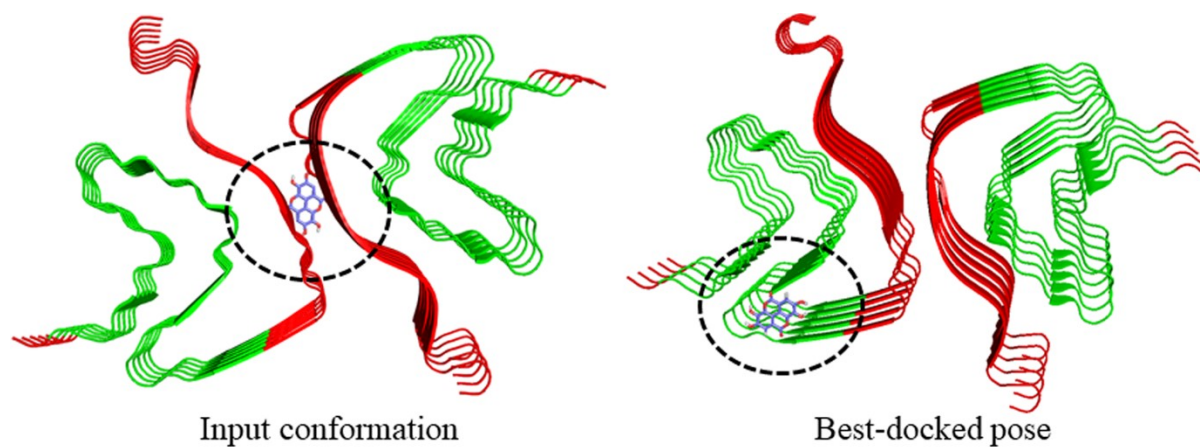


Figure S1: The input conformation of α -Syn fibril and EA for the docking studies is shown in the left panel. The best-docked pose of EA with α -Syn fibril (right panel). The α -Syn fibril is shown in cartoon and EA is displayed in the stick representation.

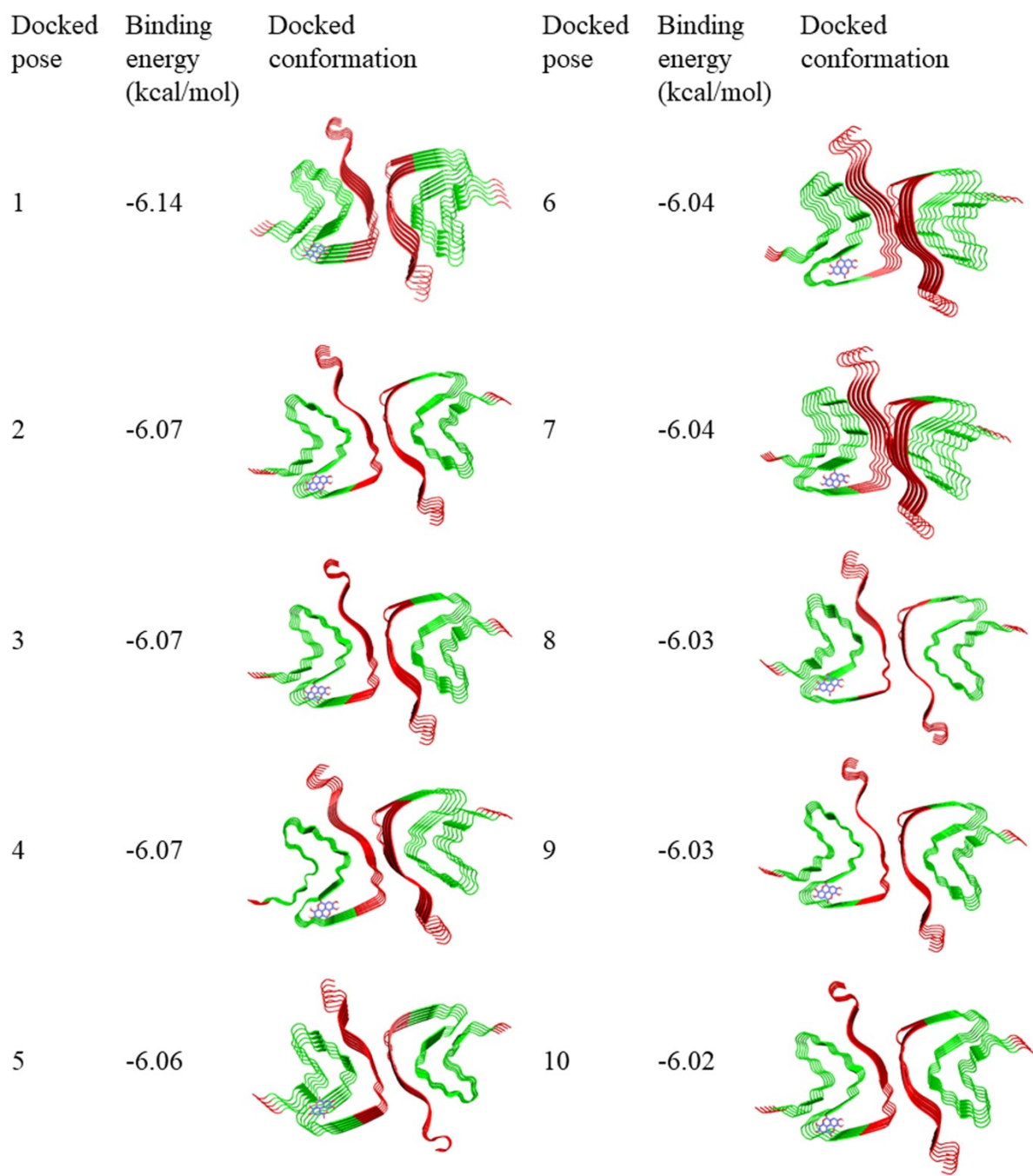


Figure S2: The top ten docked conformations of EA with α -Syn fibril.

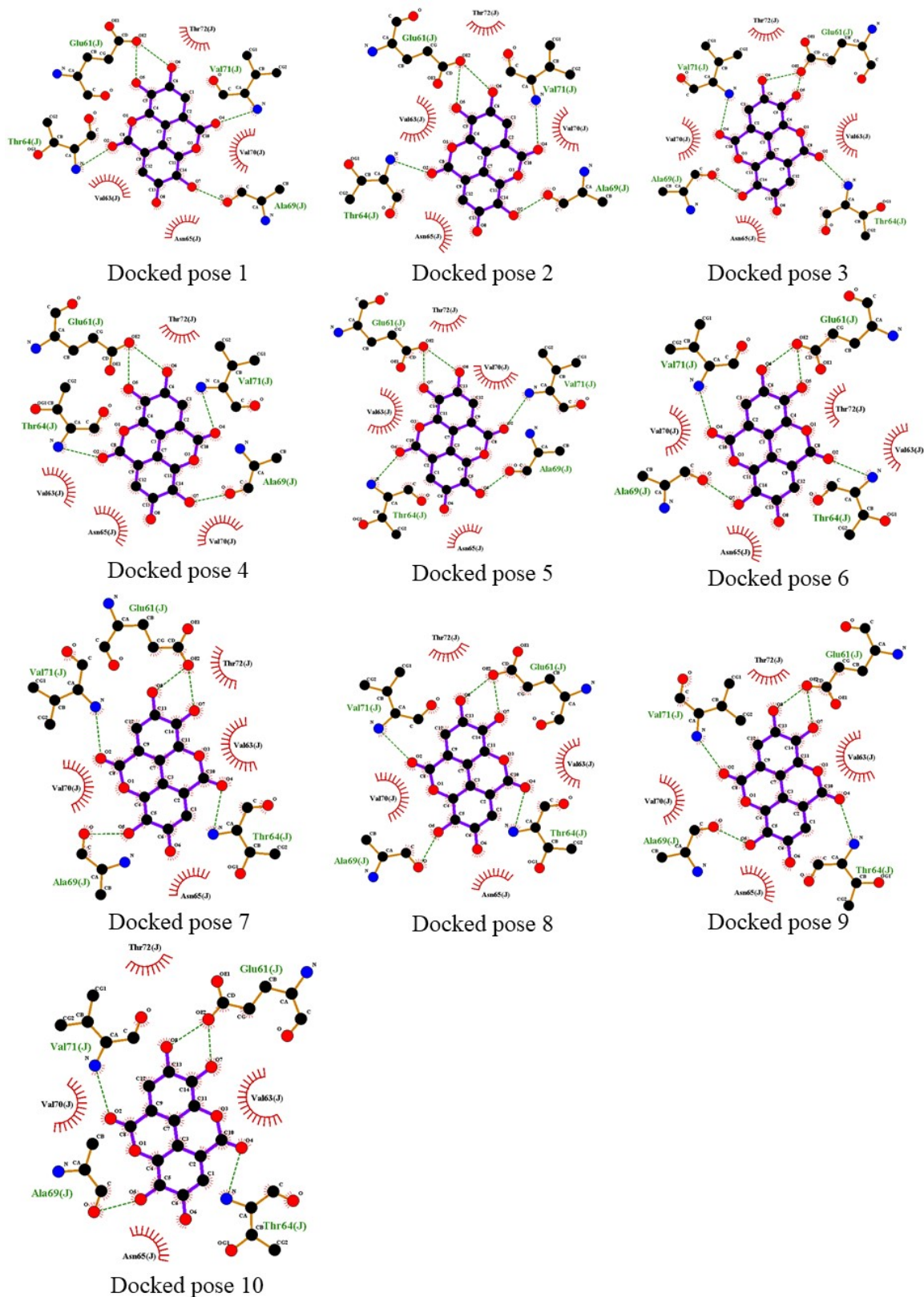


Figure S3: The 2D interaction maps displaying hydrogen bonds and hydrophobic contacts in the top ten docked conformations of EA with α -Syn fibril. The green dashed line depicts hydrogen bonds between α -Syn fibril and EA.

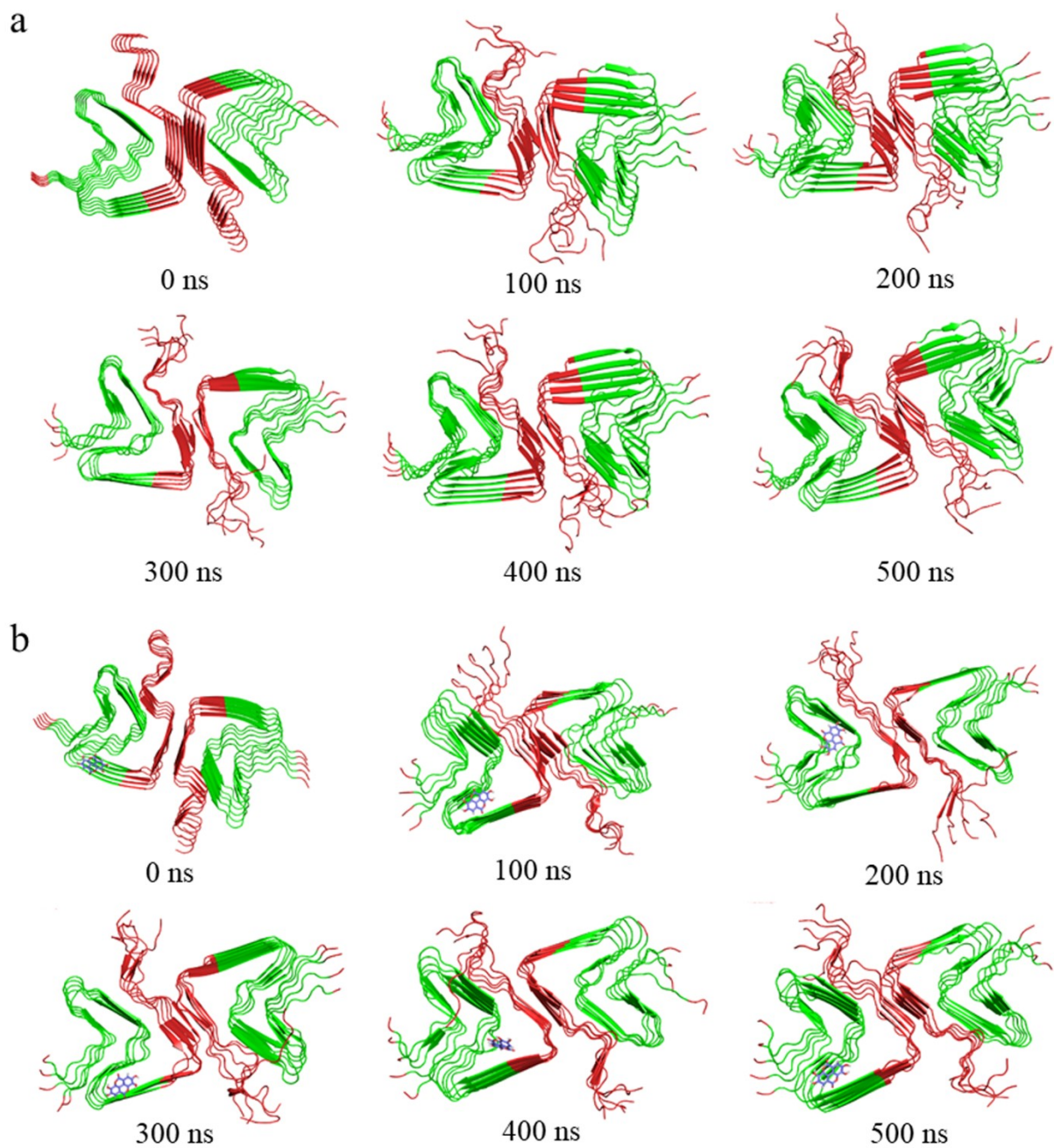


Figure S4: The conformational snapshots of MD trajectory of α -Syn fibril at different time points in the absence and presence of EA are shown in panel a, and b, respectively.

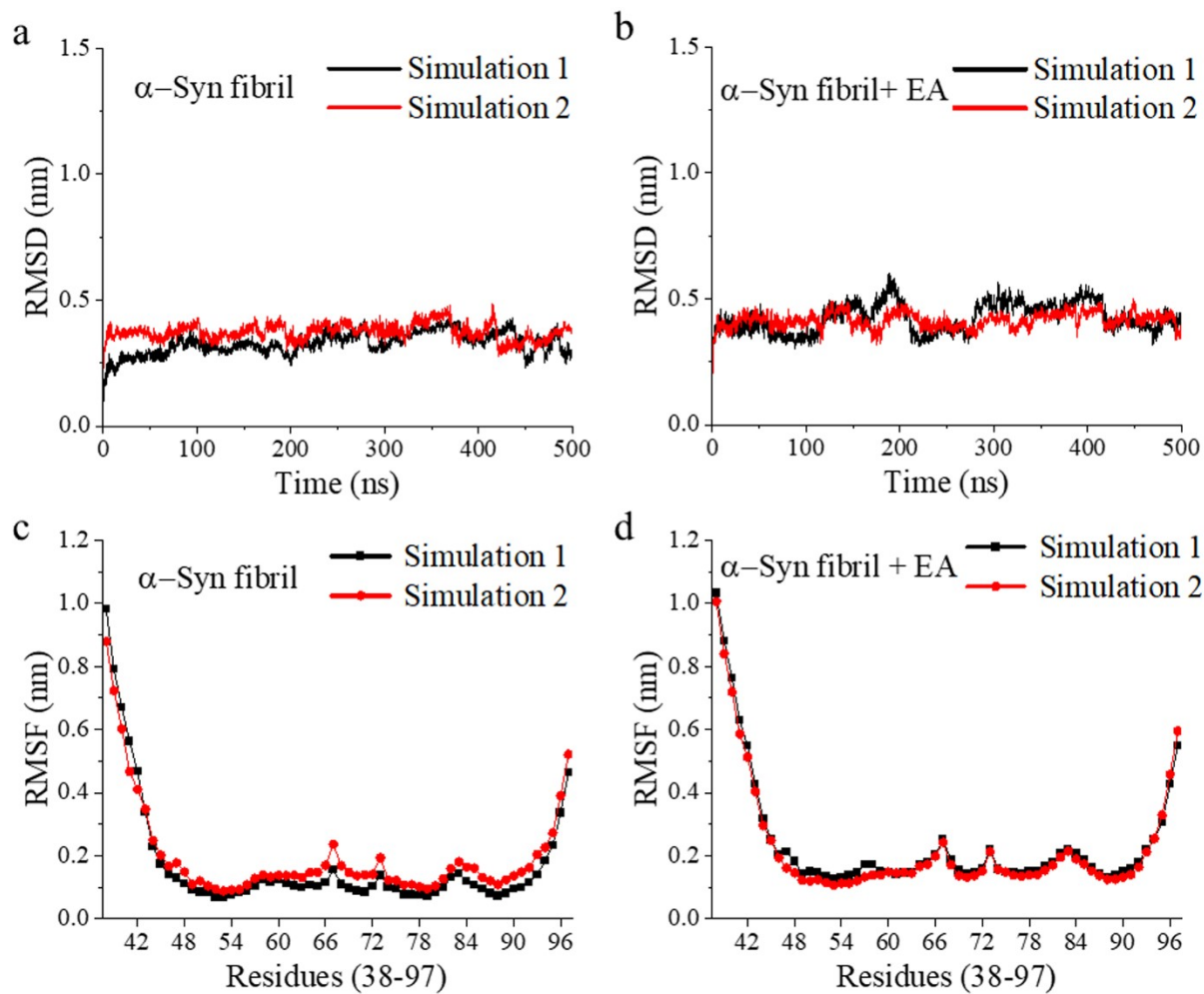


Figure S5: The RMSD of α -Syn fibril alone (panel a) and α -Syn fibril + EA (panel b) as a function of simulation time for the repeat simulations with different initial velocities. The RMSF of the residues of α -Syn fibril in the absence and presence of EA for the repeat simulations are shown in panel c, and d, respectively.

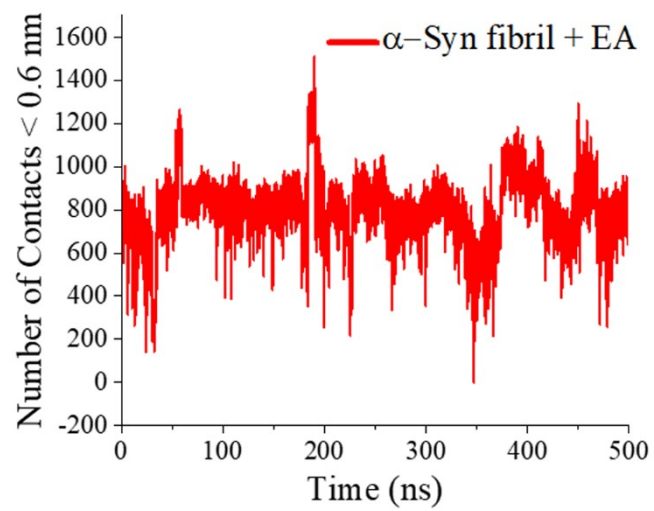


Figure S6: The time-dependent evolution of number of contacts between α -Syn fibril and EA.

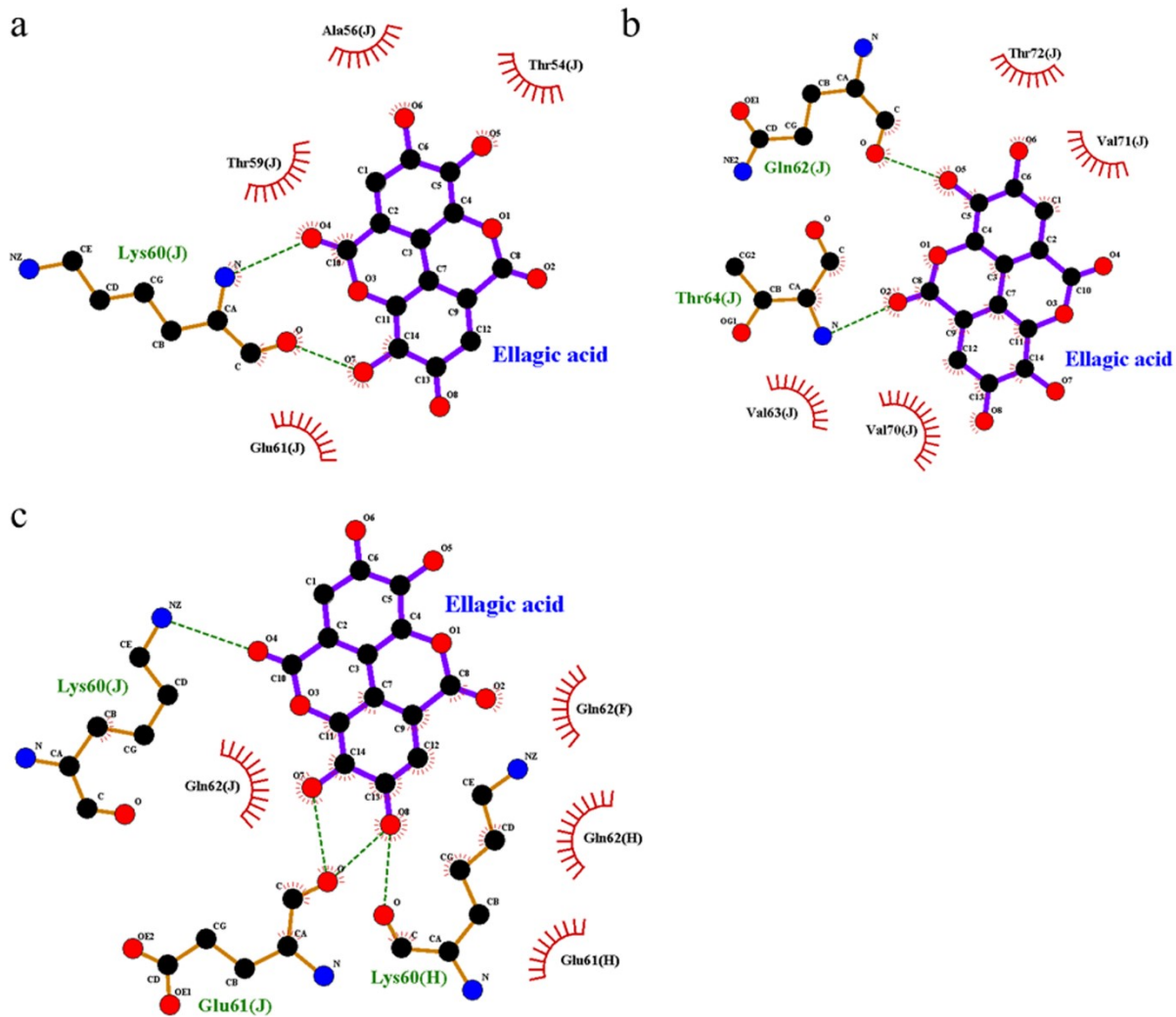


Figure S7: The 2D interaction map displaying the hydrophobic contacts and hydrogen bonds in the representative conformations of the three most-populated conformational clusters C1', C2' and C3' of α -Syn fibril + EA are displayed in panel a, b, and c, respectively.

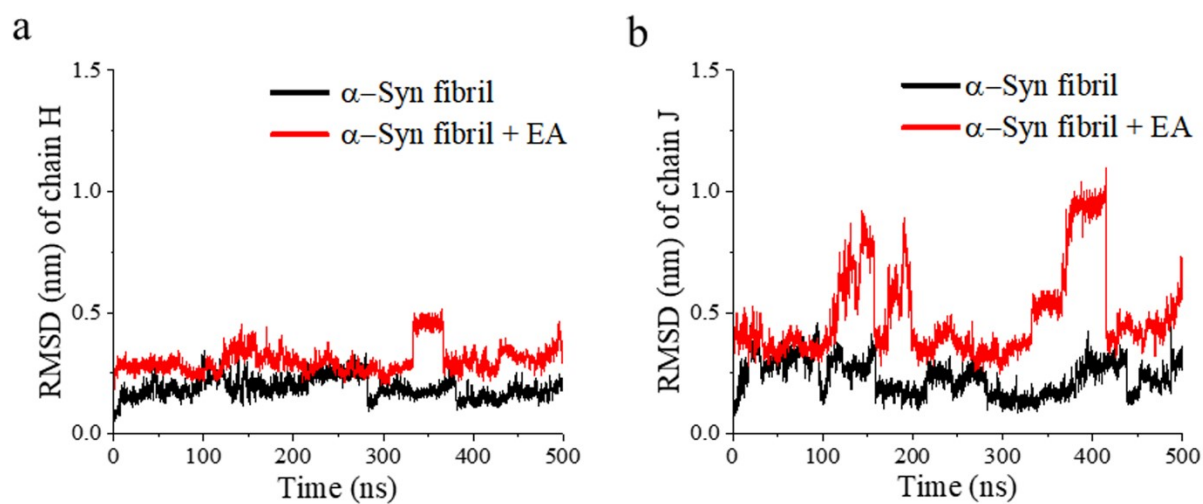


Figure S8: The RMSD of chain H and chain J of α -Syn fibril in the absence and presence of EA during simulation are shown in panel a, and b, respectively.