Supporting information

How Does the P7C3-Series of Neuroprotective Small Molecules Prevent Membrane Disruption?

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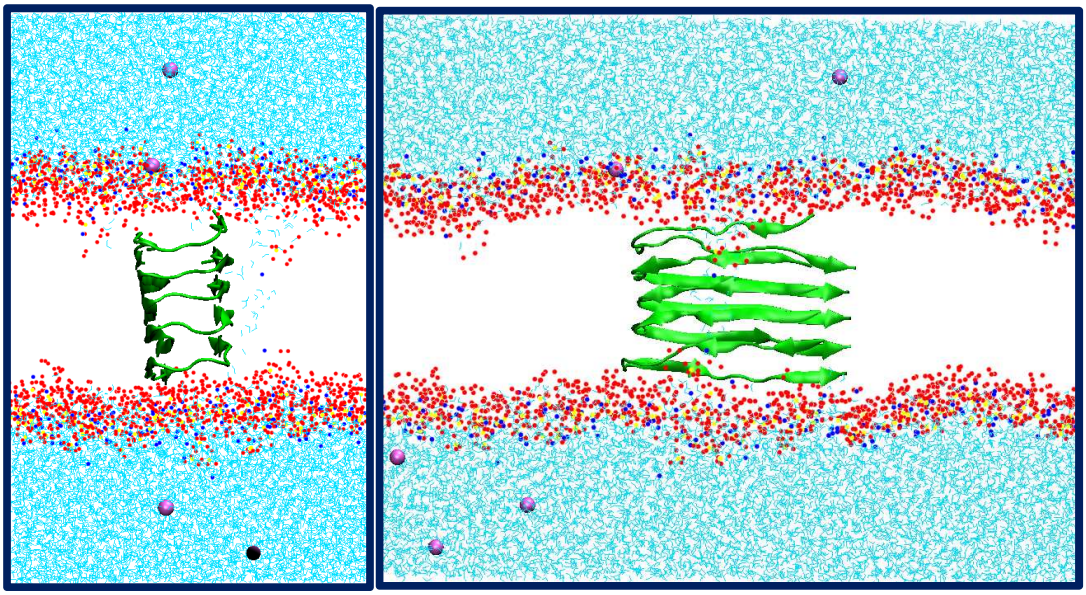

Figure S1. Snapshots of the Aβ stack interacting with membrane/aqueous ionic solutions (larger system with 256 molecules). The Aβ stack is colored green (using a cartoon representation), and for the lipid bilayer, the red, blue and yellow points represent the oxygen, nitrogen and phosphorous atoms of headgroups, respectively. The acyl chains are removed for clarity. Water and ions are shown with blue lines and purple spheres.

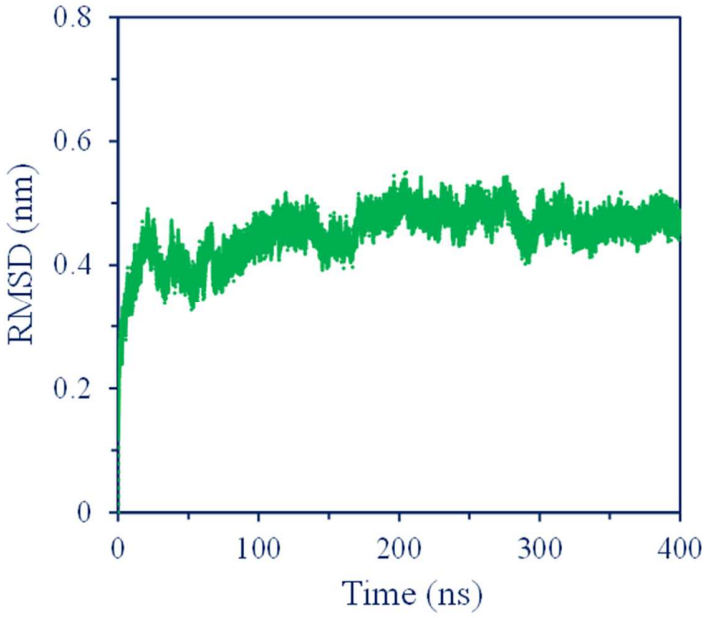

Figure S2. The RMSD of fibrils, followed over 400 ns.

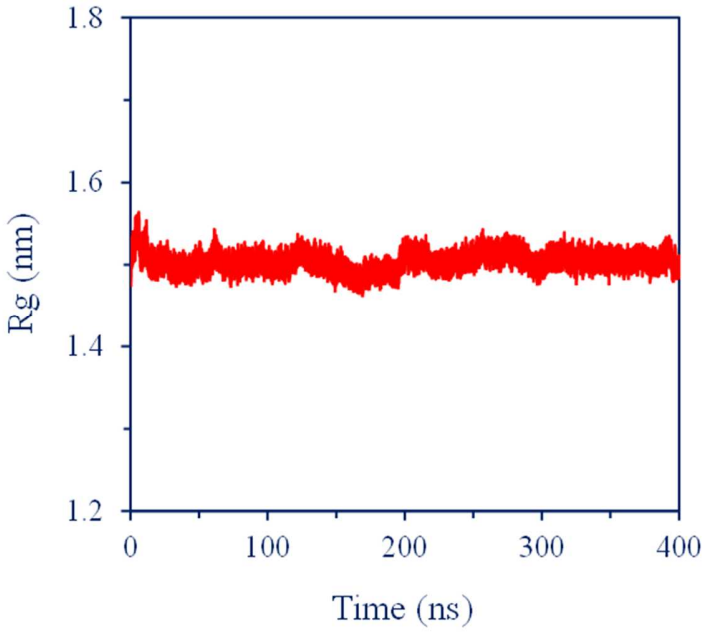

Figure S3. The R_g of fibrils, followed over 400 ns.

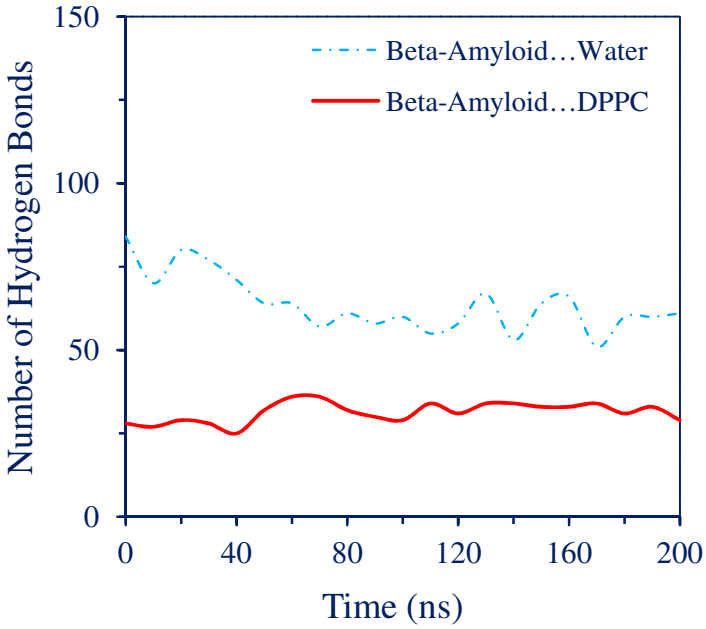

Figure S4. Number of hydrogen bonds over last 200 ns of simulations for system II.

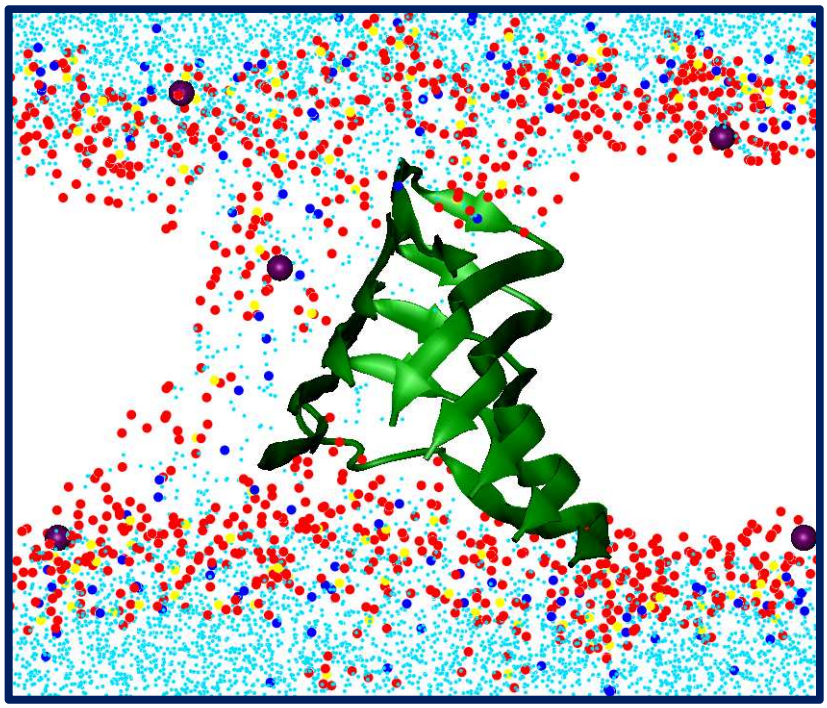

Figure S5. Another perspective of system II after 400 ns of simulation. (Acyl chains are removed for clarity)

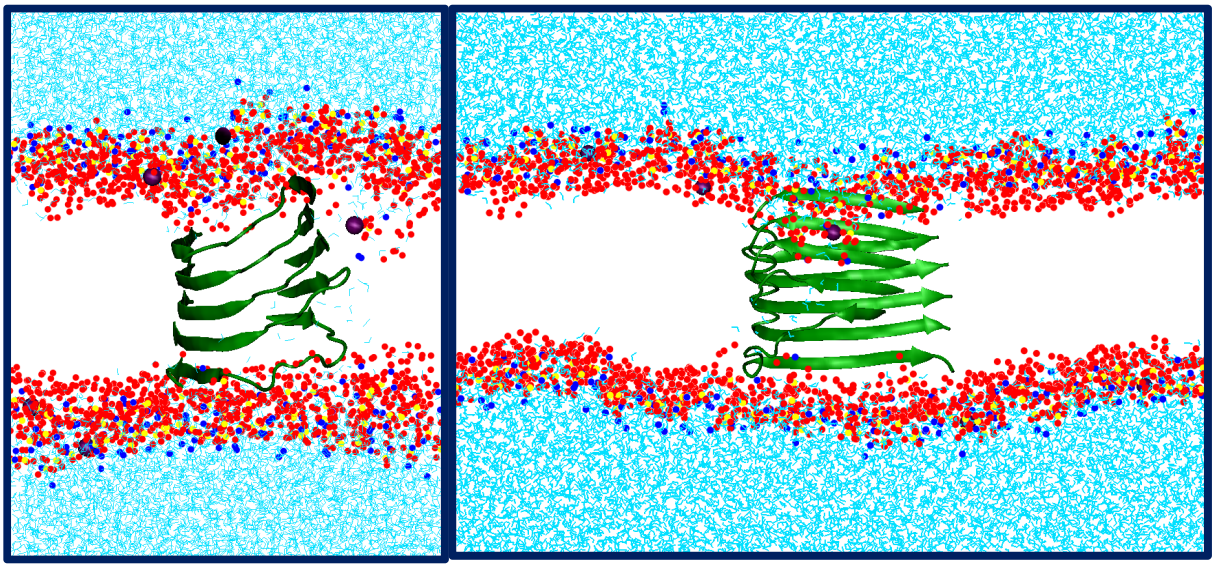

Figure S6. Snapshots of the Aβ stack interacting with POPC membrane/aqueous ionic solutions. The Aβ stack is colored green (using a cartoon representation), and for the lipid bilayer, the red, blue and yellow points represent the oxygen, nitrogen and phosphorous atoms of headgroups, respectively. The acyl chains are removed for clarity. Water and ions are shown with blue lines and purple spheres.

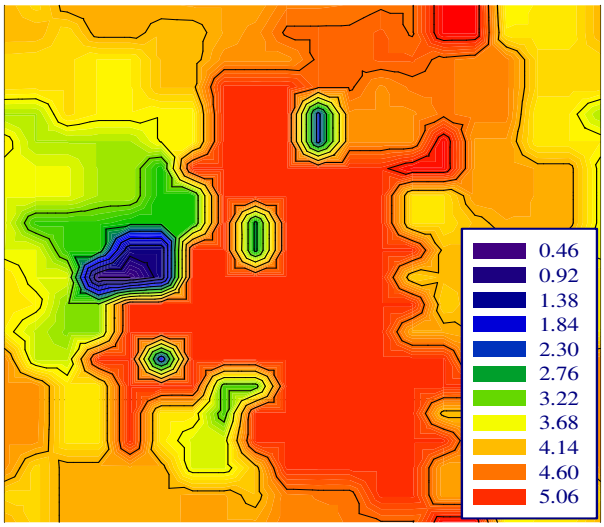

Figure S7. The time averaged local bilayer thickness around the embedded peptides. The legend shows bilayer thickness (nm), mapped to the corresponding colors.

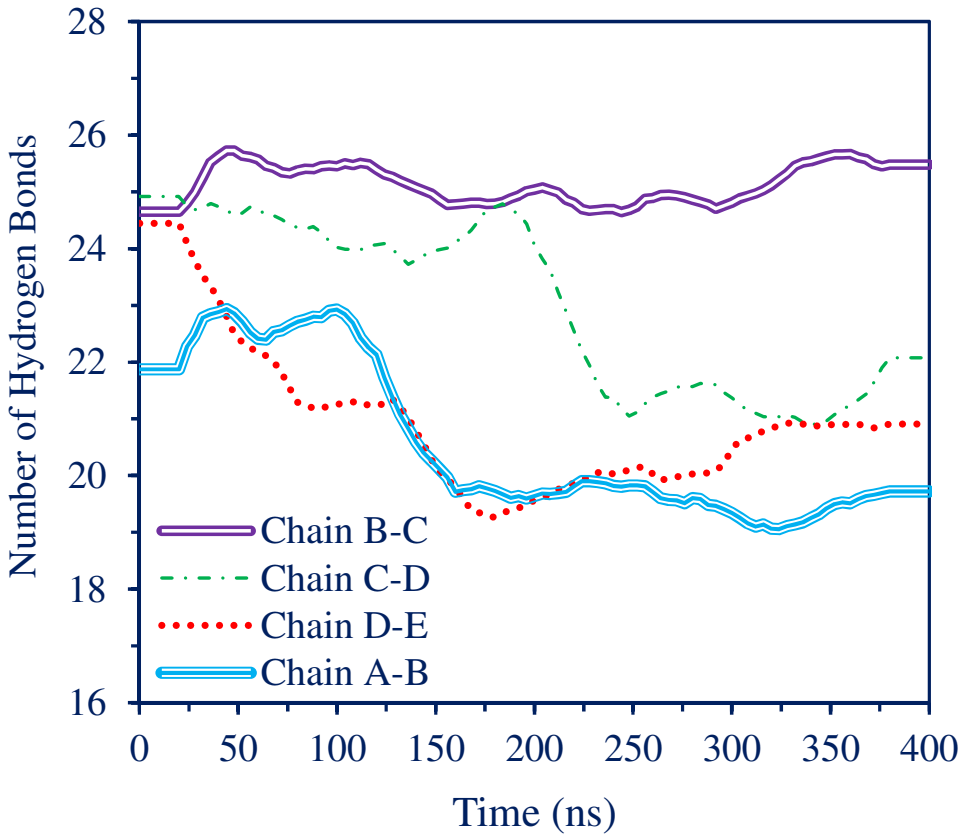

Figure S8. Number of interchain backbone hydrogen bonds over time.

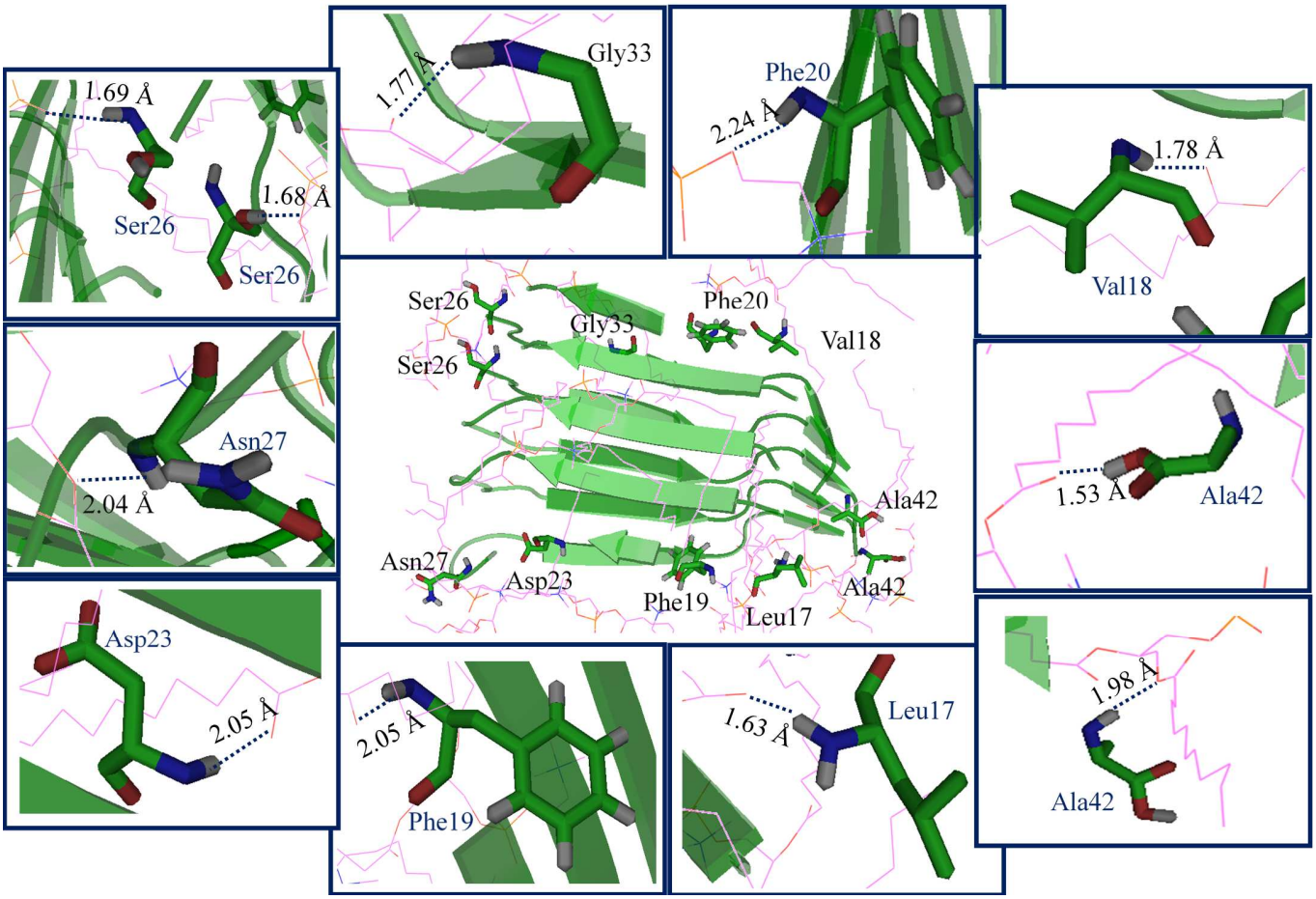

Figure S9. The main interaction of lipids with Aβ fibril.

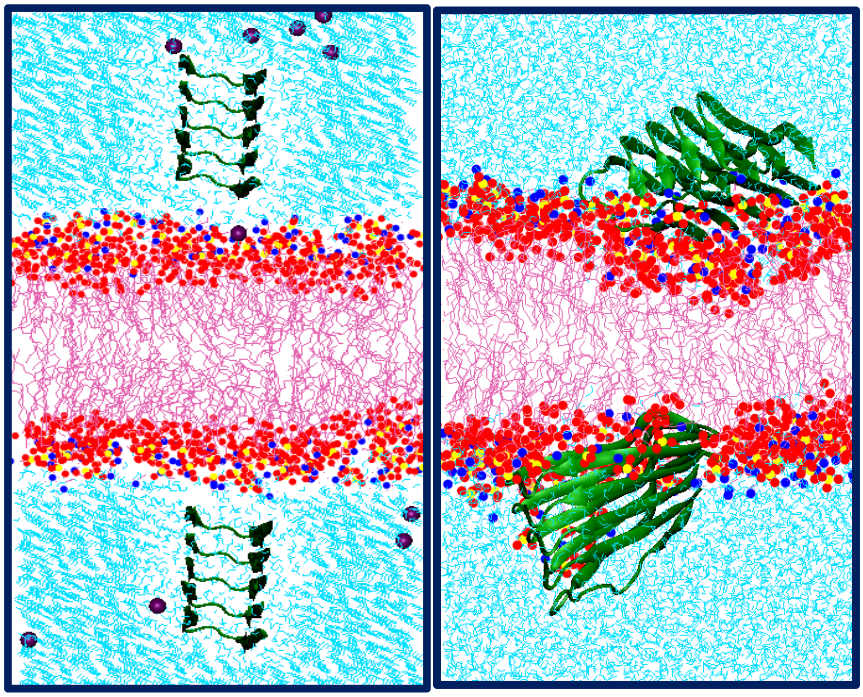

Figure S10. Snapshots of the membrane/aqueous ionic solutions and Aβ stack at the start of simulation (left) and after 400 ns of simulation (right).

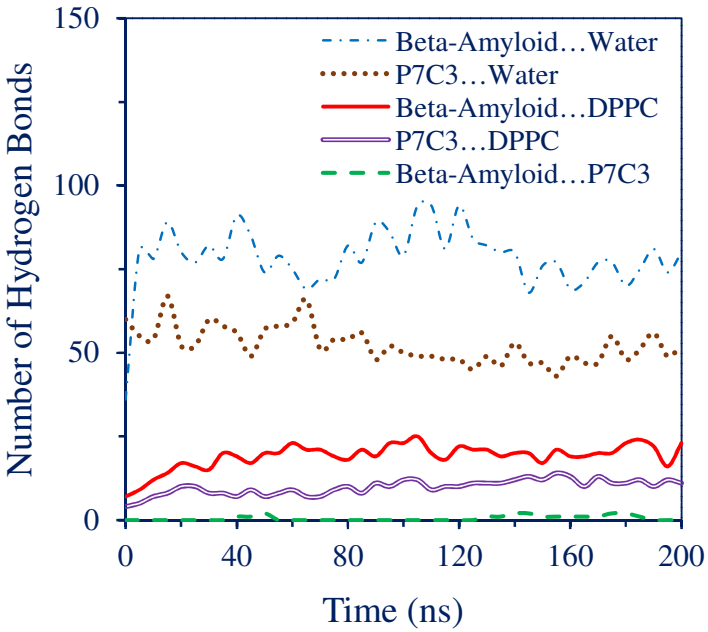

Figure S11. Number of hydrogen bonds over last 200 ns of simulations for system III.

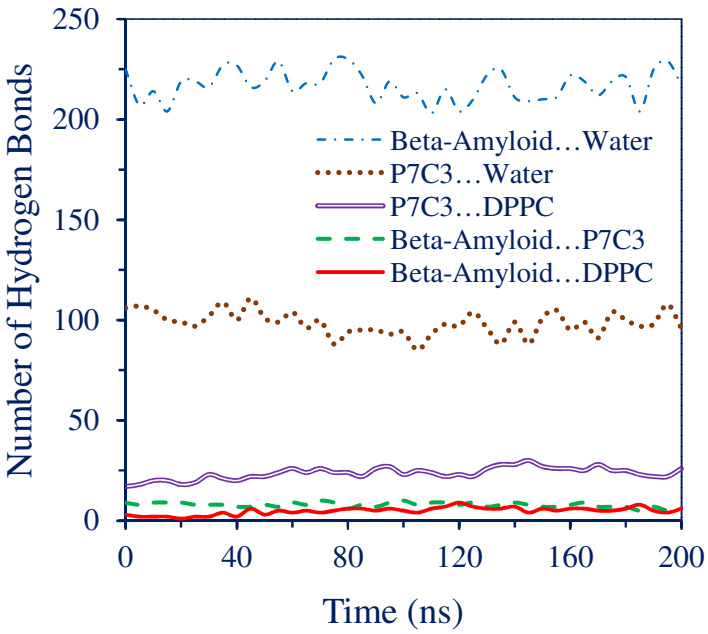

Figure S12. Number of hydrogen bonds over last 200 ns of simulations for system IV.