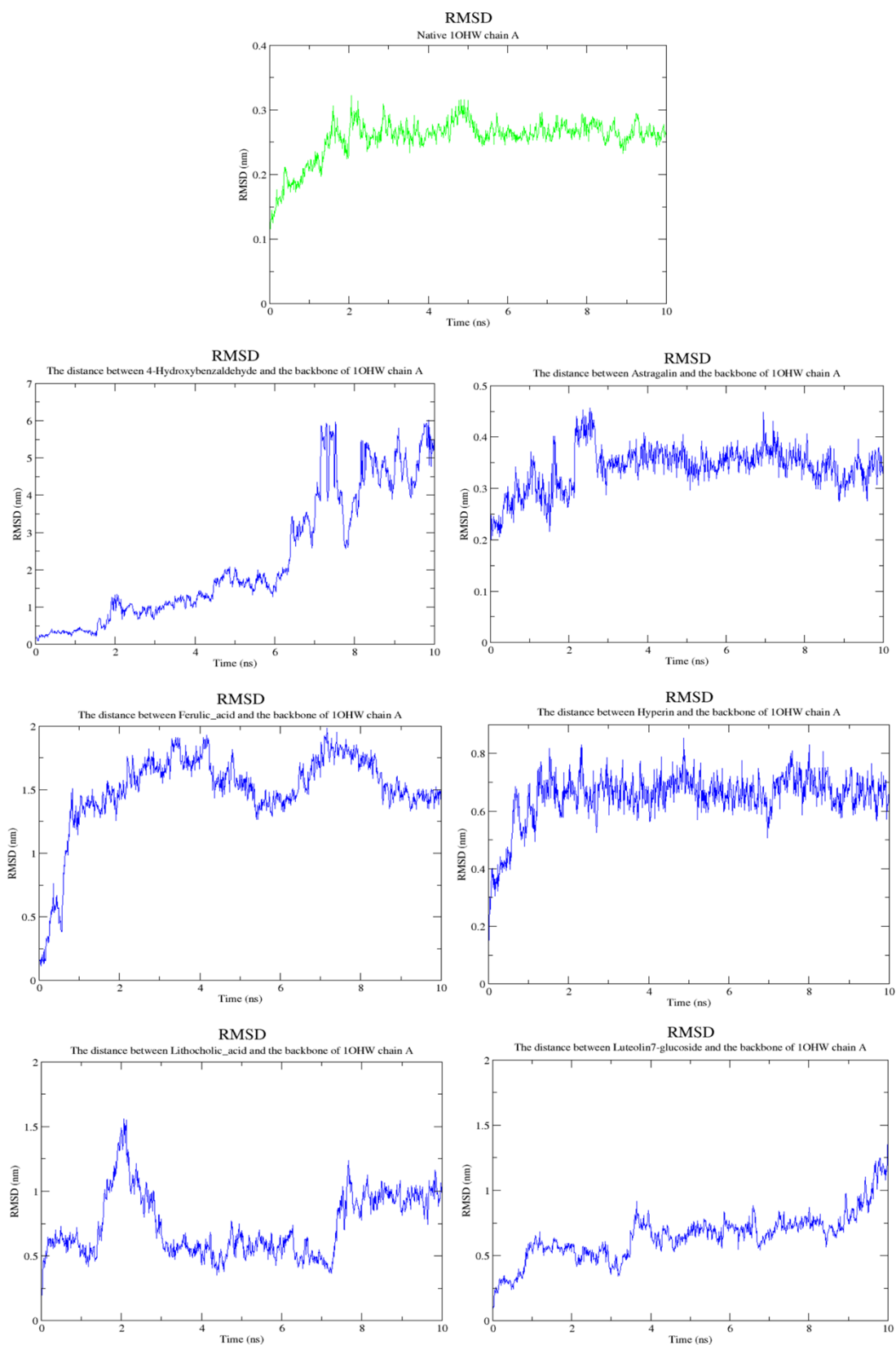
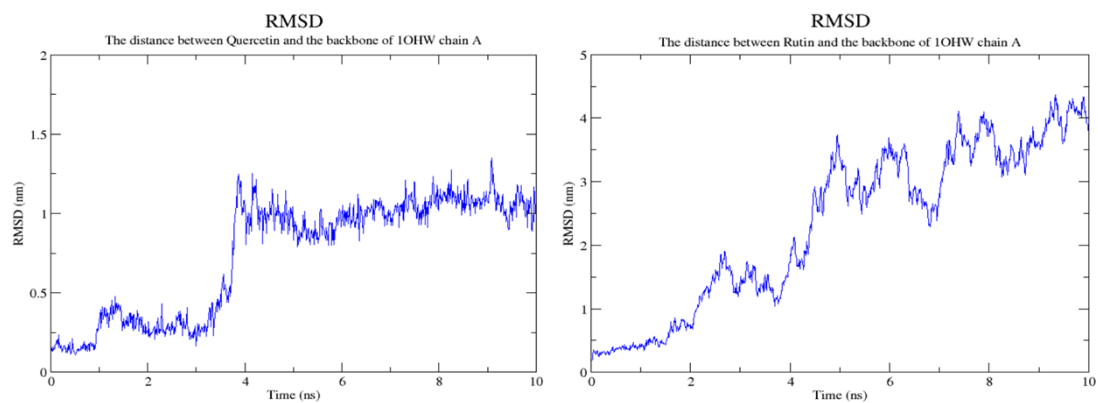
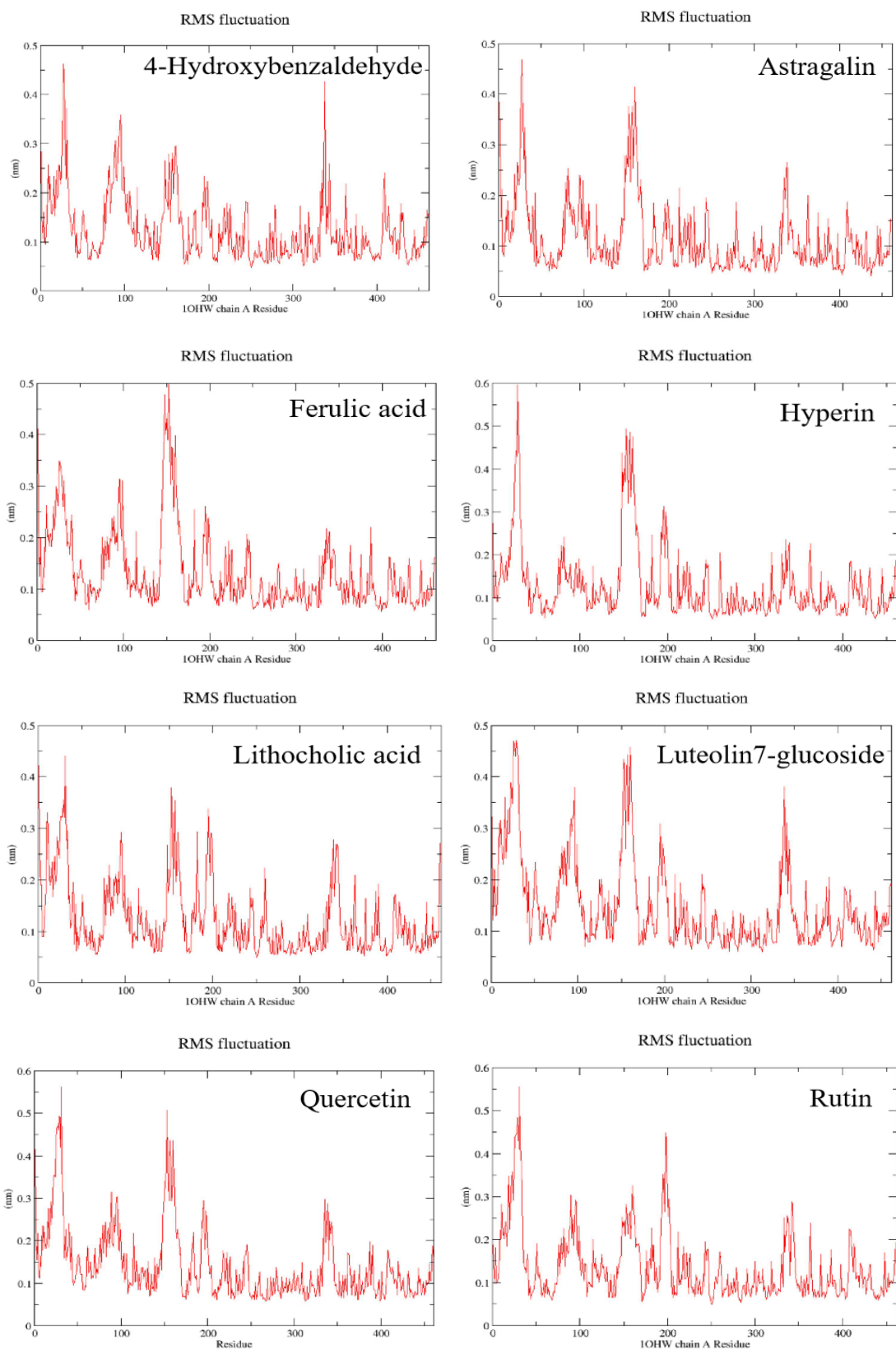


## Supplement Figures

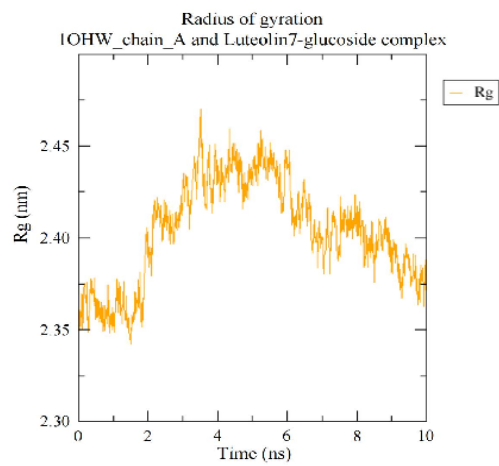
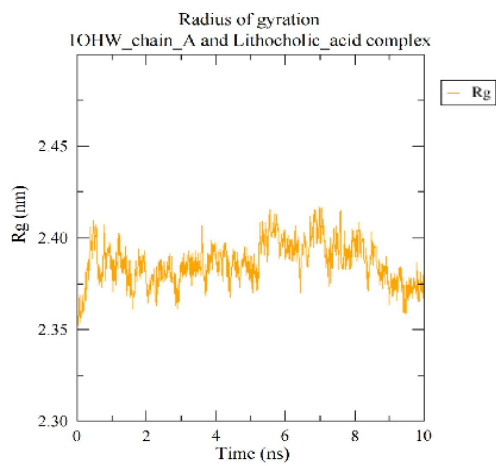
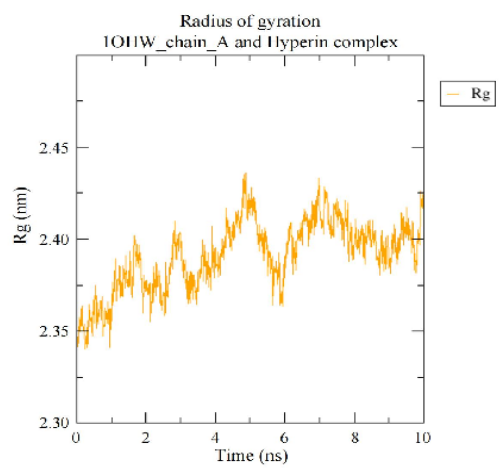
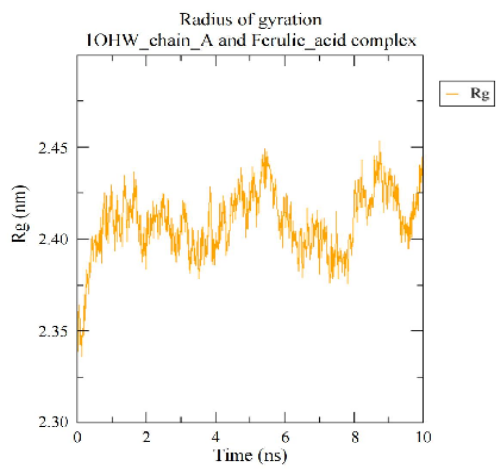
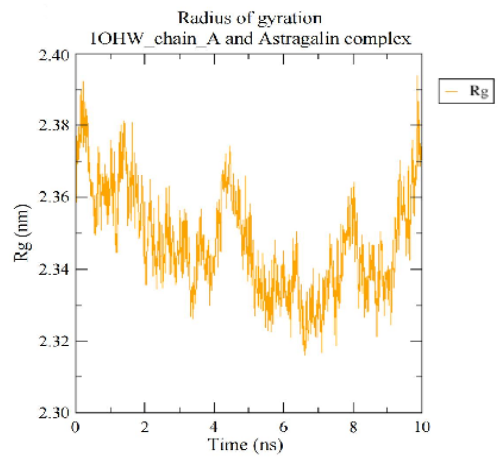
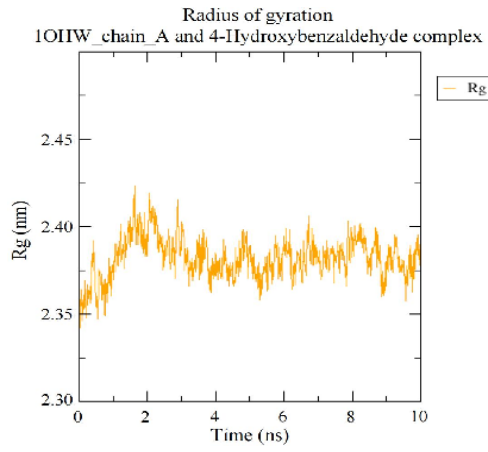


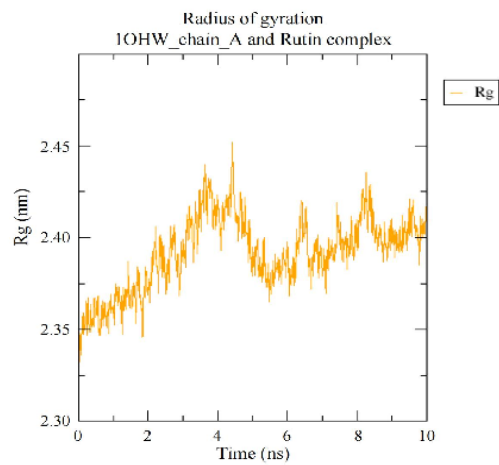
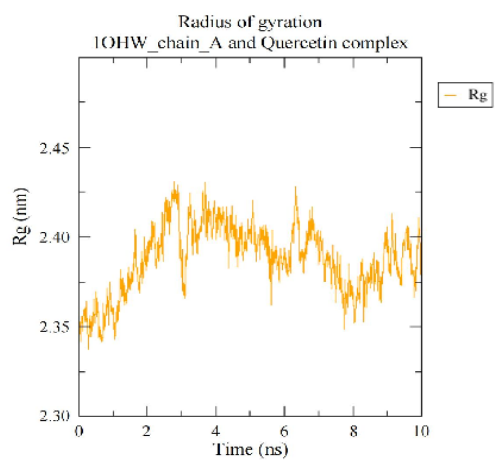


Supplement fig.1 Root Mean Square Deviation (RMSD) analysis of native 1OHW chain A and the complexes of 1OHW chain A with several compounds for 10 ns molecular dynamics simulation.



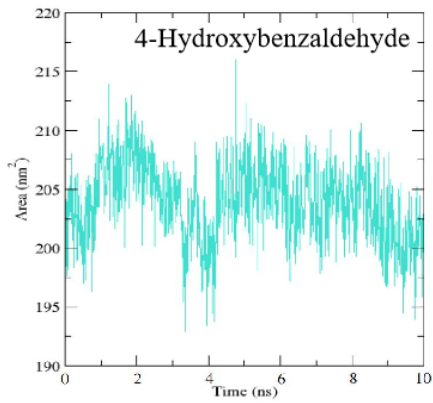
Supplement fig.2 RMS fluctuation (RMSF) analysis of residues of 1OHW chain A for 10 ns molecular dynamics simulation.



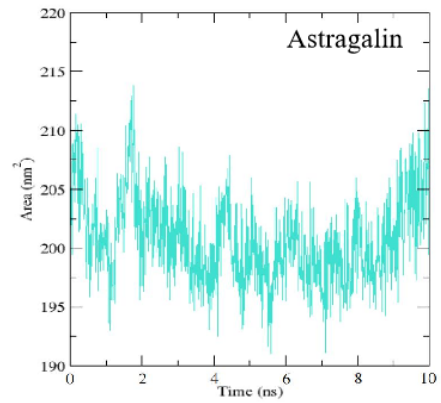


Supplement fig.3 Radius of gyration (Rg) analysis of the complexes of 1OHW chain A with several compounds for 10 ns molecular dynamics simulation.

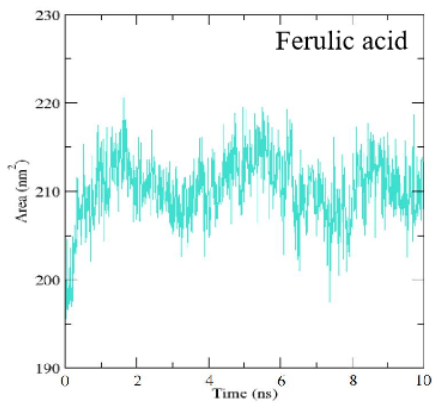
Solvent Accessible Surface Area



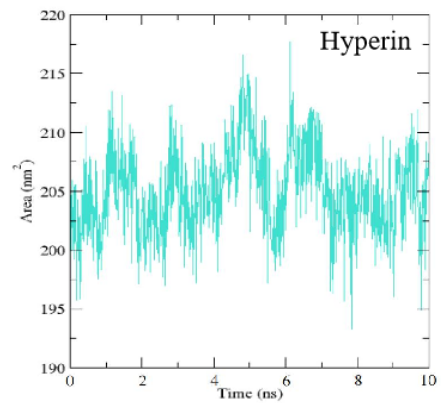
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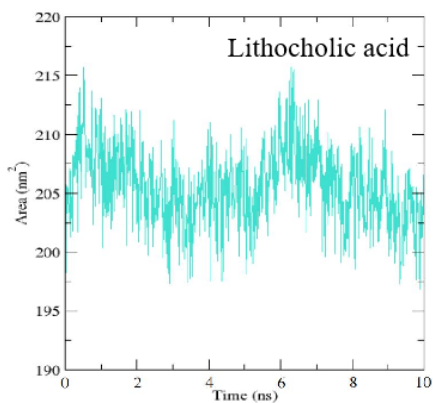
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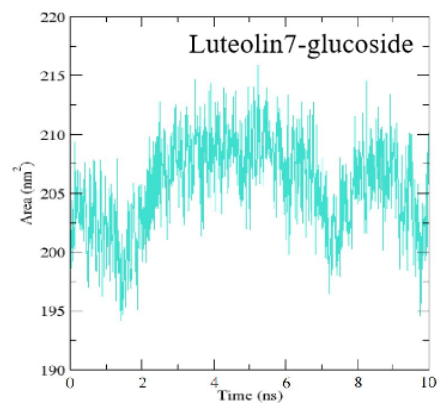
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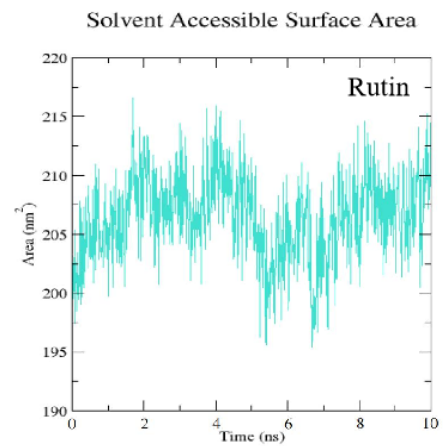
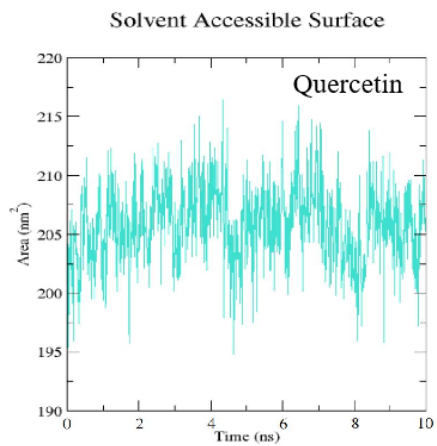


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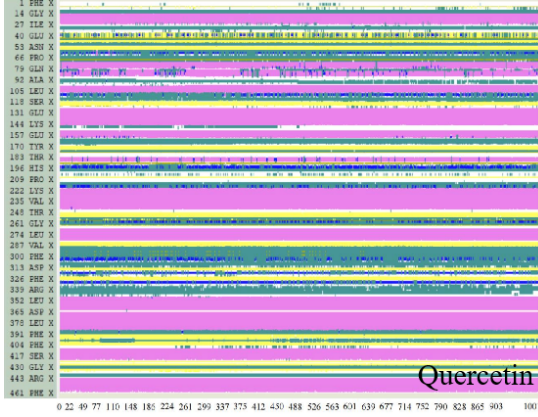
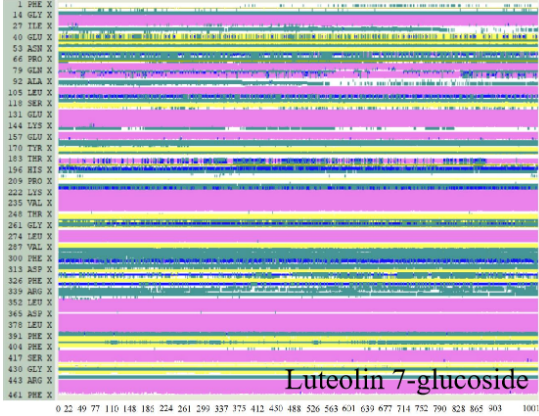
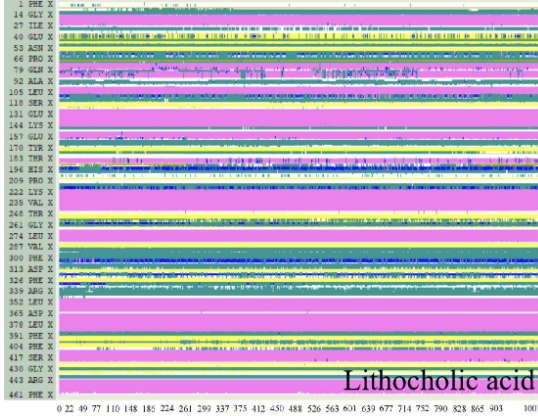
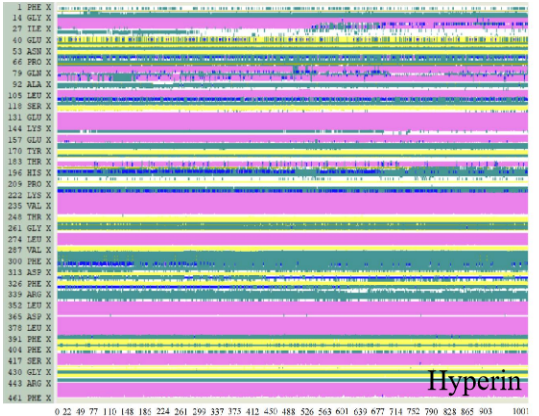
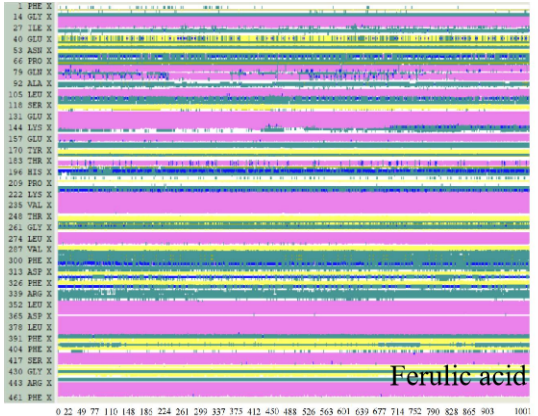
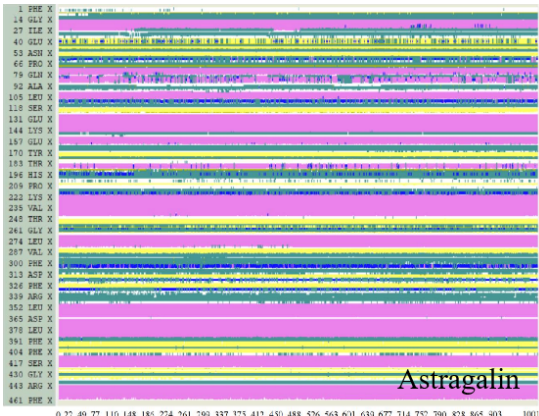
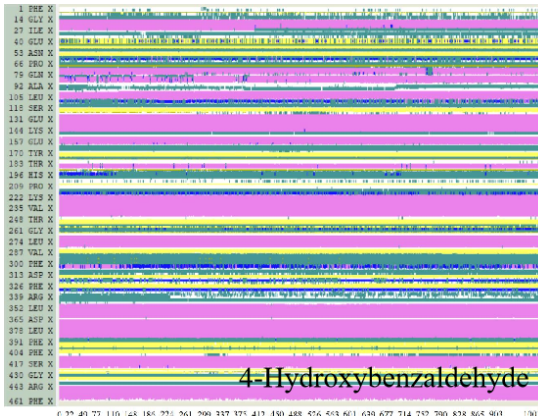


Solvent Accessible Surface Area





Supplement fig.4 Solvent Accessible Surface Area (SASA) analysis of 1OHW chain A interacting with several compounds for 10 ns molecular dynamics simulation.





Supplement fig.5 Dictionary of Secondary Structures of Proteins (DSSP) analysis of 1OHW chain A interacting with several compounds for 10 ns molecular dynamics simulation.