Electronic Supplementary Information

Computational prediction and experimental validation of low-affinity target of triptolide and its analogues

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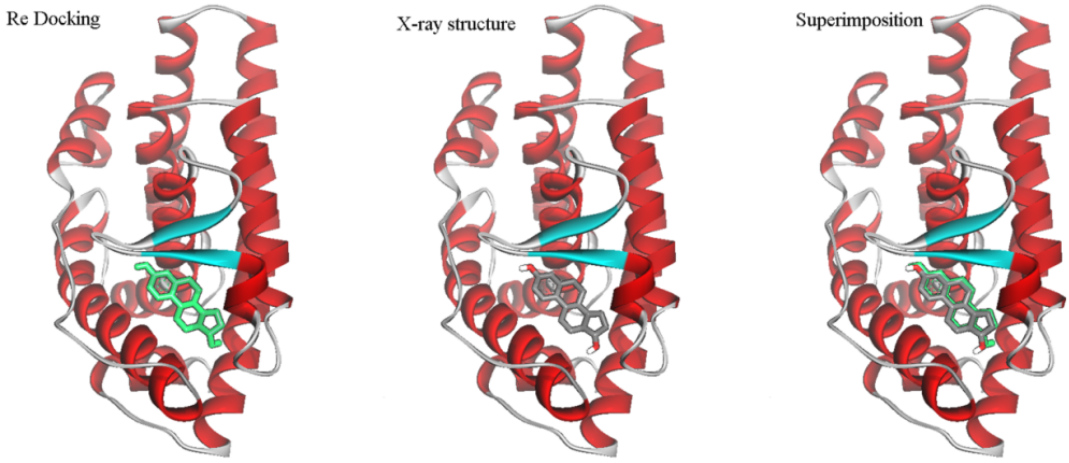

Figure S1. Comparison of autodock poses and X-ray crystallographic pose for estradiol in ERα-LBD. Crystallographic pose is in grey with the redocked pose in green.

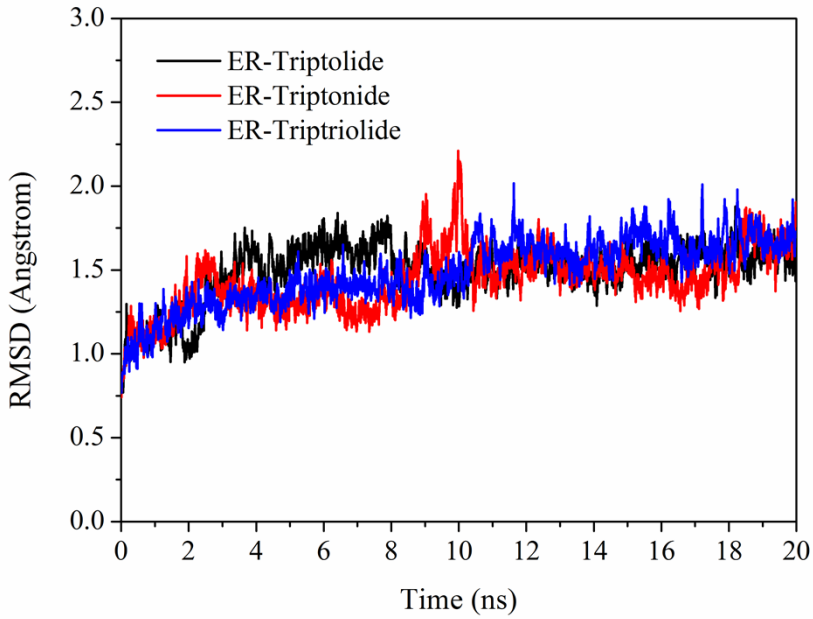

Figure S2. The results of molecular dynamics (MD) simulation. The MD simulation time vs. root mean-square deviation (RMSD) of the backbone atoms for ERα-triptolide complex system (black), ERα-triptonide complex system (red) and ERα-triptriolide complex system (blue).

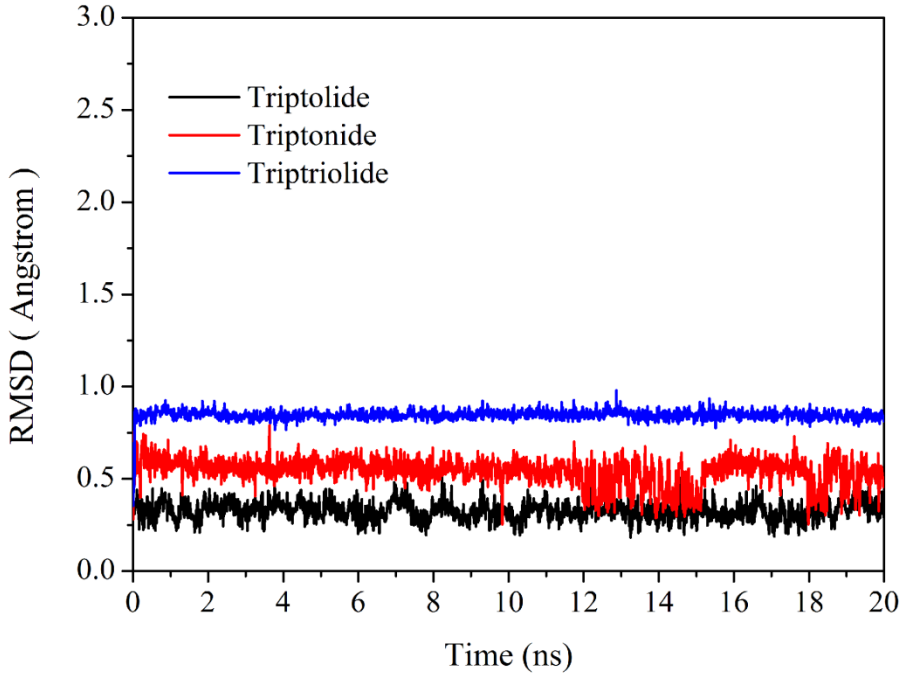

Figure S3. The results of molecular dynamics (MD) simulations. The RMSD values of triptolide (black), triptonide(red) and triptriolide (blue) from protein-ligand complexes during 20 ns of MD simulation period.