Supplementary File S7

Molecular Dynamics (MD) Simulation of Top Ligand-Receptor Complexes

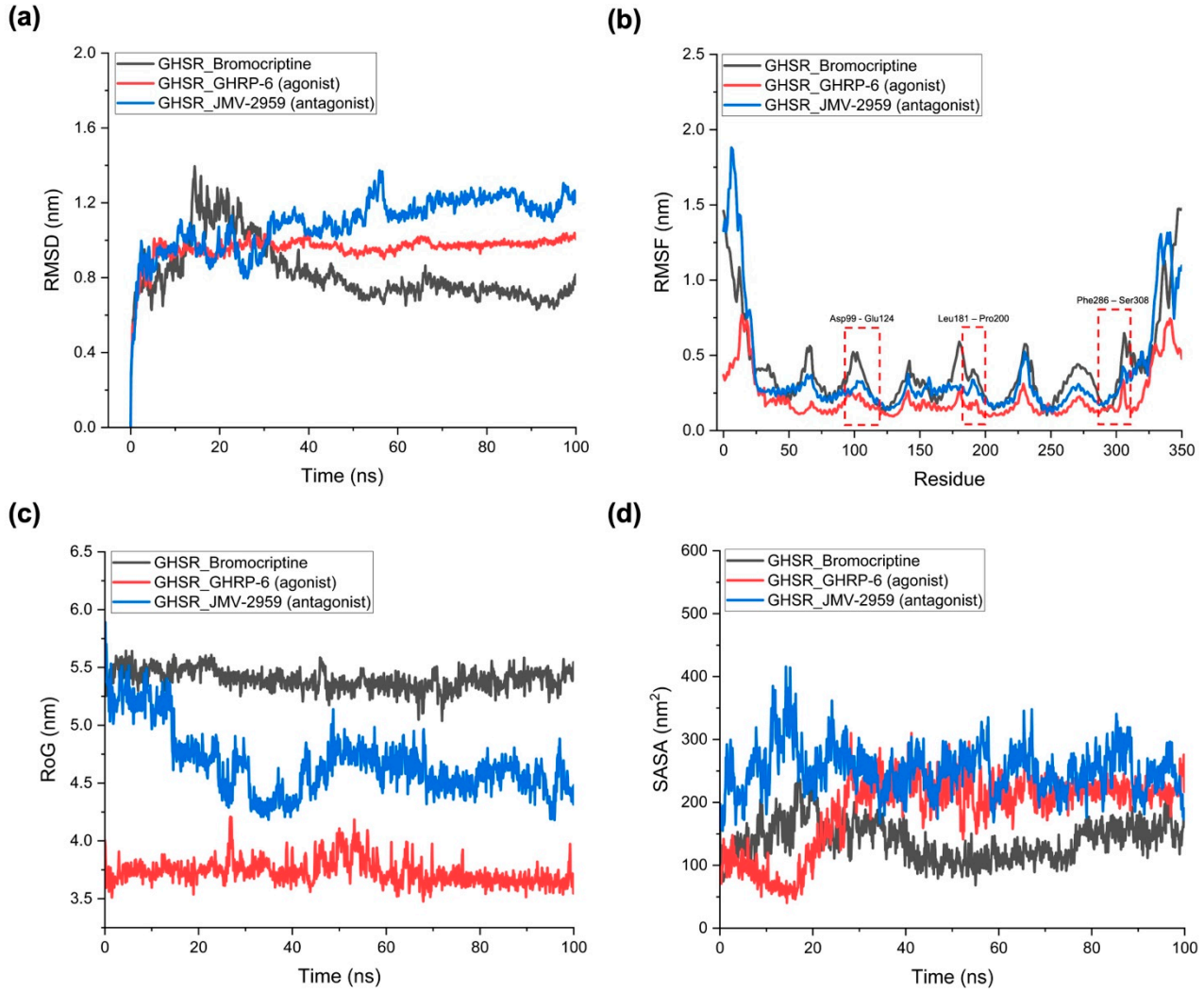


Figure S5. MD simulation profiles of bromocriptine, standard agonists, and antagonists bound to the GHSR LBD. (**a**) Root mean square deviation (RMSD). (**b**) Root mean square fluctuation (RMSF). (**c**) Radius of gyration (RoG). (**d**) Solvent-accessible surface area (SASA).

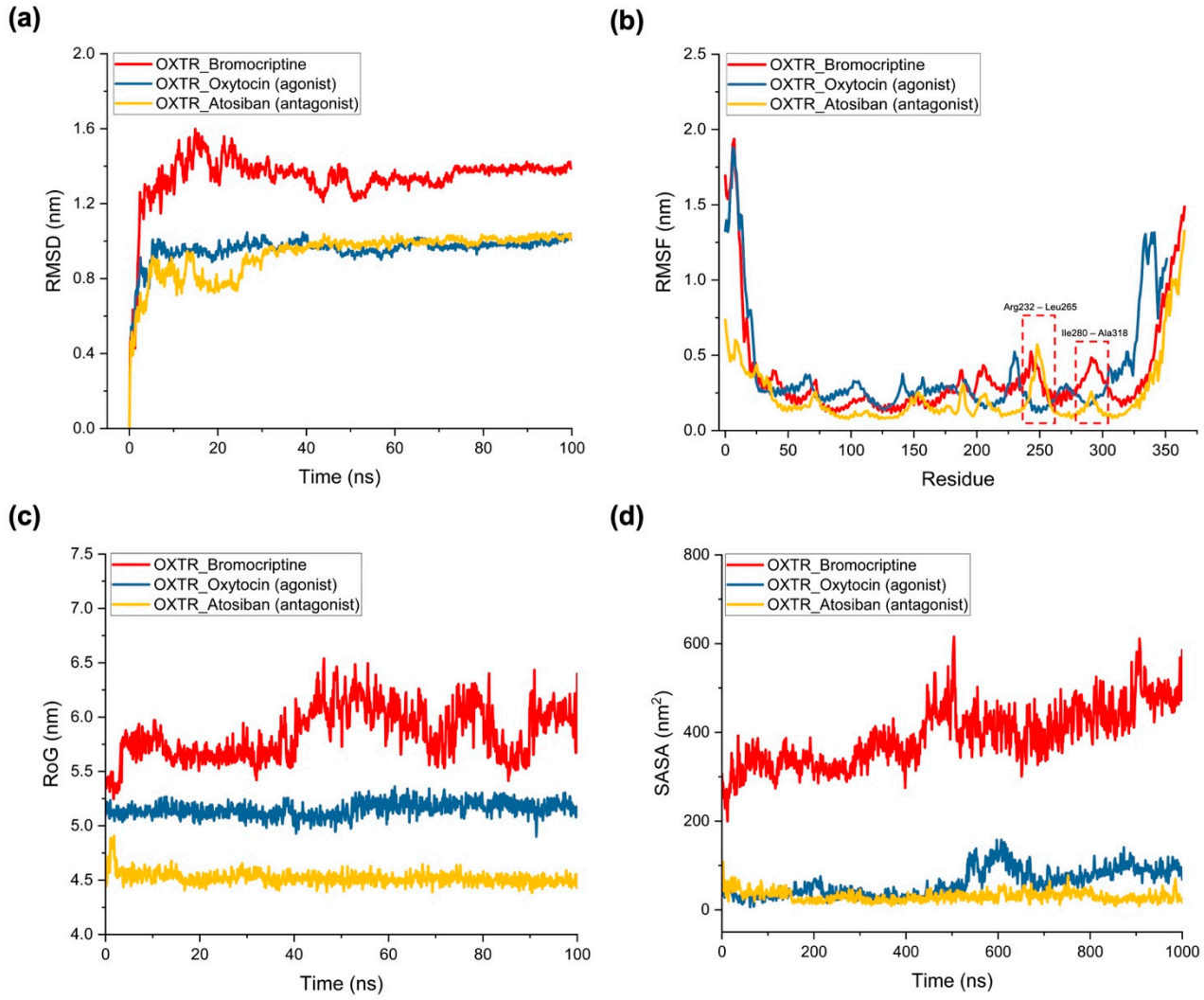


Figure S6. MD simulation profiles of bromocriptine, standard agonists, and antagonists bound to the OXTR LBD. (**a**) Root mean square deviation (RMSD). (**b**) Root mean square fluctuation (RMSF). (**c**) Radius of gyration (RoG). (**d**) Solvent-accessible surface area (SASA).