

Figure S1. RMSD values for each 100 ns MD trajectory in the G-SM and G-DM system with three replicates.

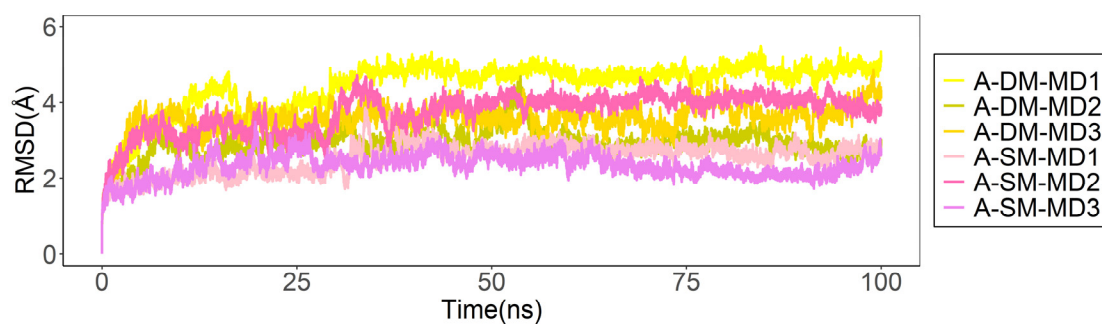


Figure S2. RMSD values for each 100 ns MD trajectory in the A-SM and A-DM system with three replicates.

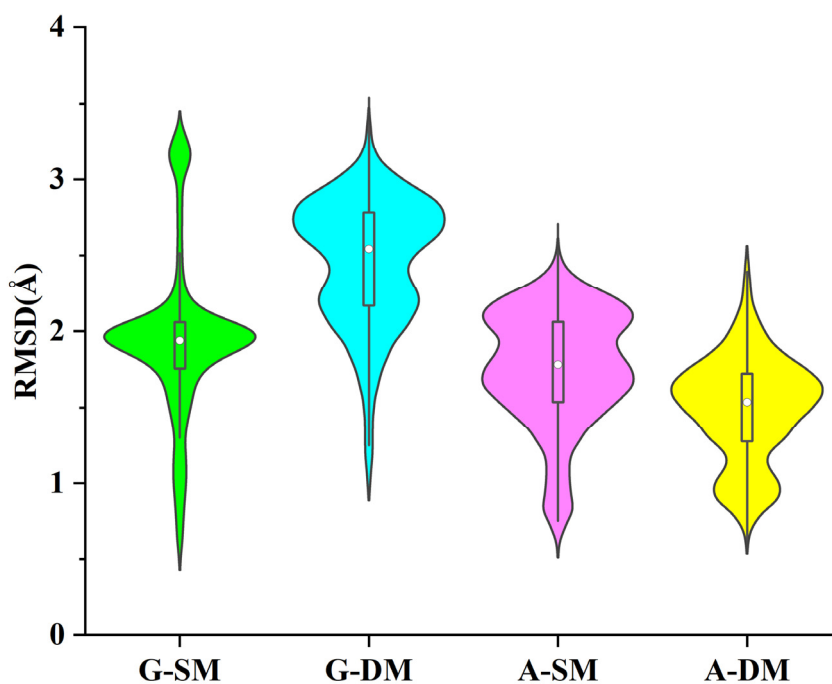


Figure S3. RMSD values for Gefitinib in the G-SM (green), and G-DM (cyan) system, Afatinib in the A-SM (pink), and A-DM (yellow) system.