MD SIMULATION ANALYSIS FOR COMPLEXES 2-6

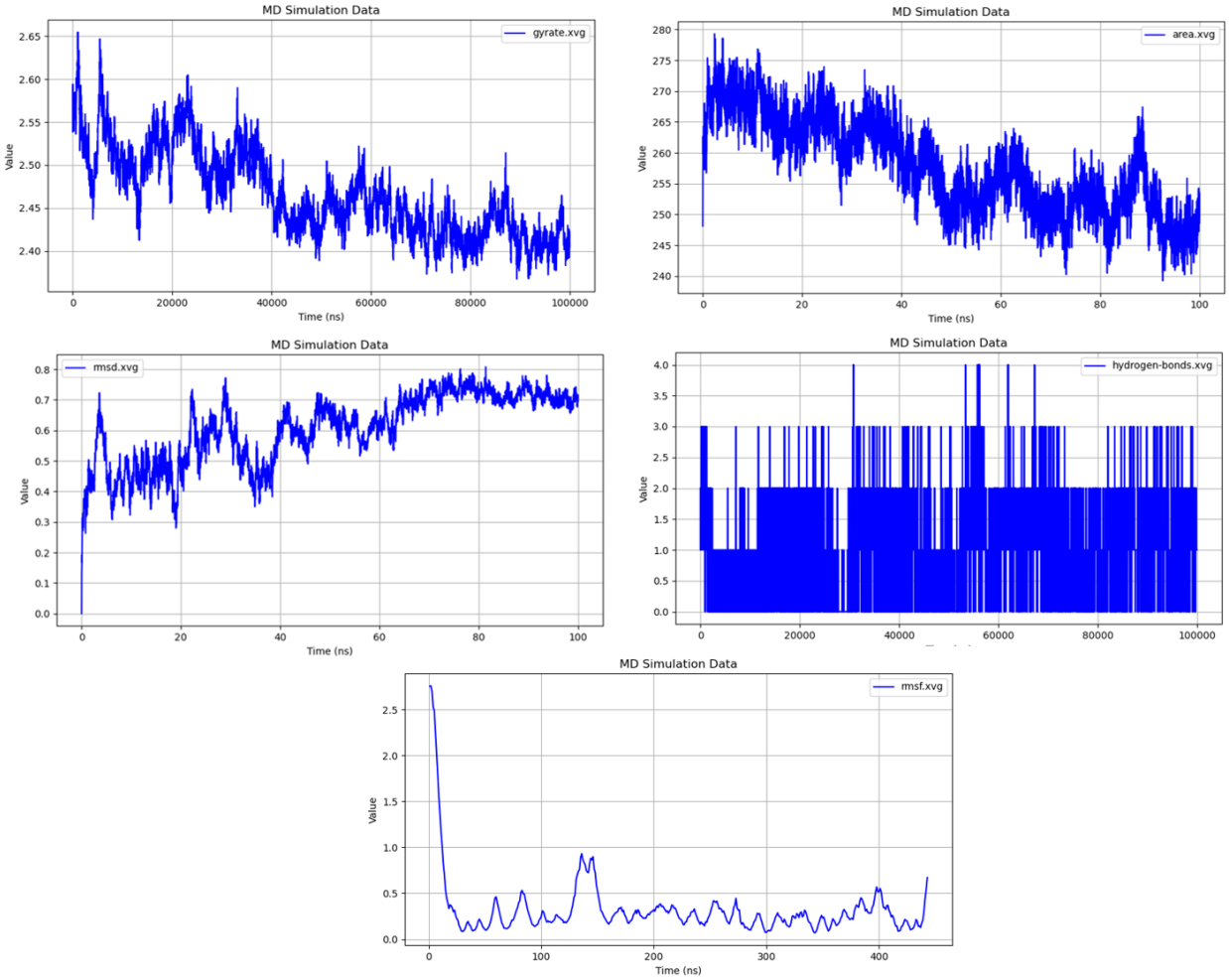

Figure 1 MD Simulation analysis of the 2nd top-ranked complex **perfluoro_curcumin (complex 2_)** with its receptor. The analysis indicates a stable, productive binding pose.

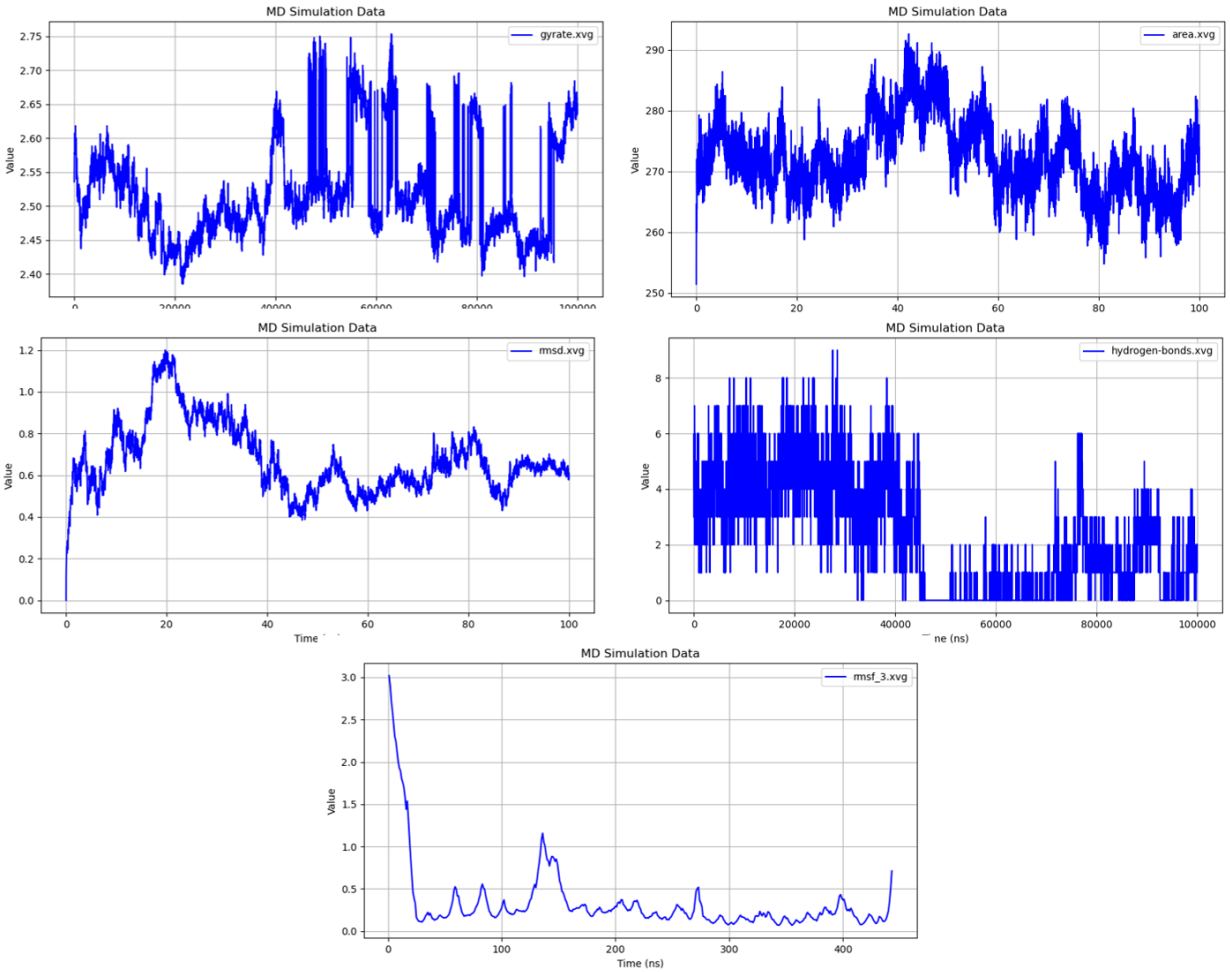

Figure 2 MD Simulation analysis of the 3rd top-ranked complex **curcumin_4'_O_beta_D_gentiobioside (complex 3_)** with its receptor.

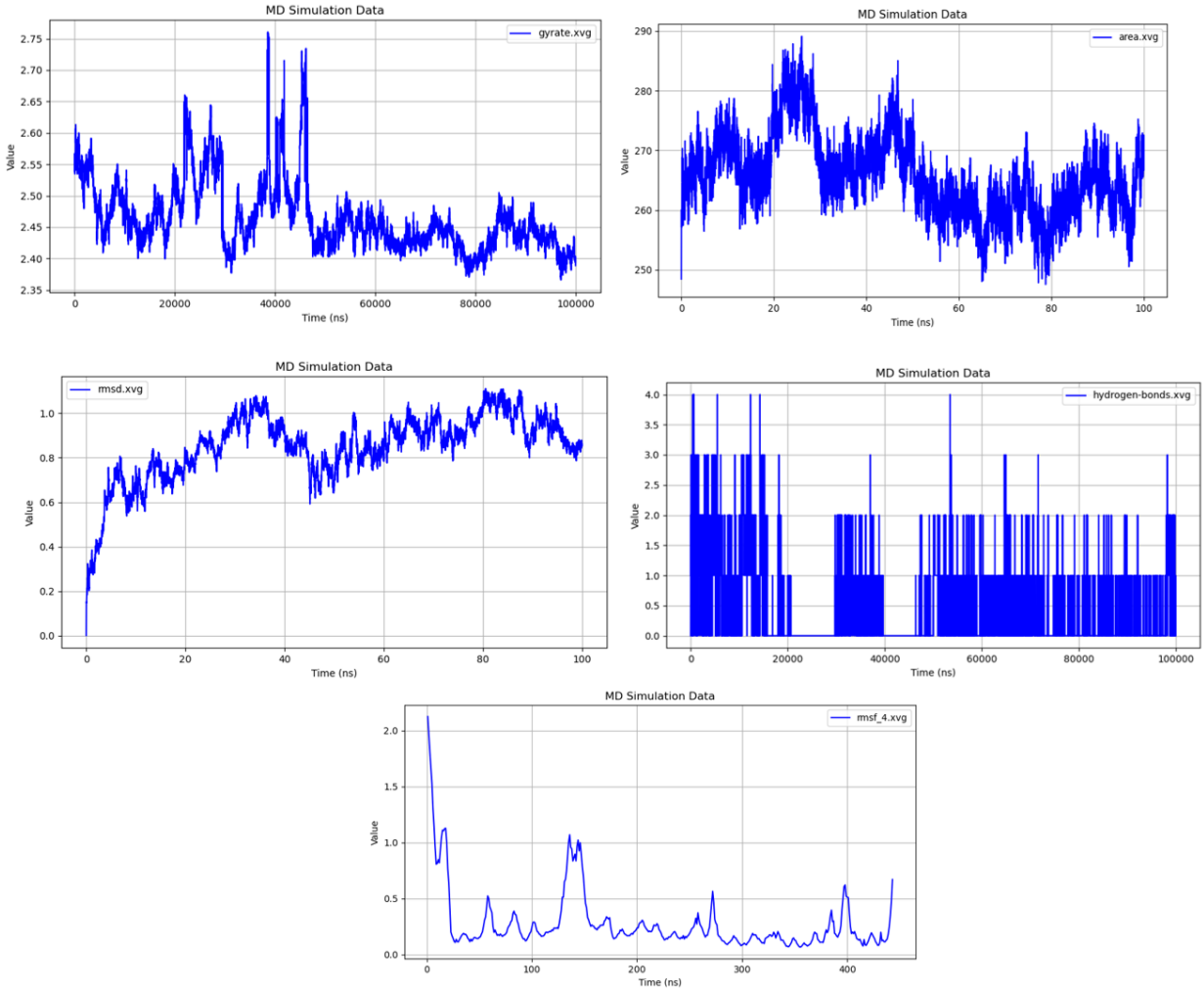

Figure 3 MD Simulation analysis of the 4th ranked complex **4-(4-Hydroxy-3-methoxybenzylidene)-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione (complex 4_)** with its receptor.

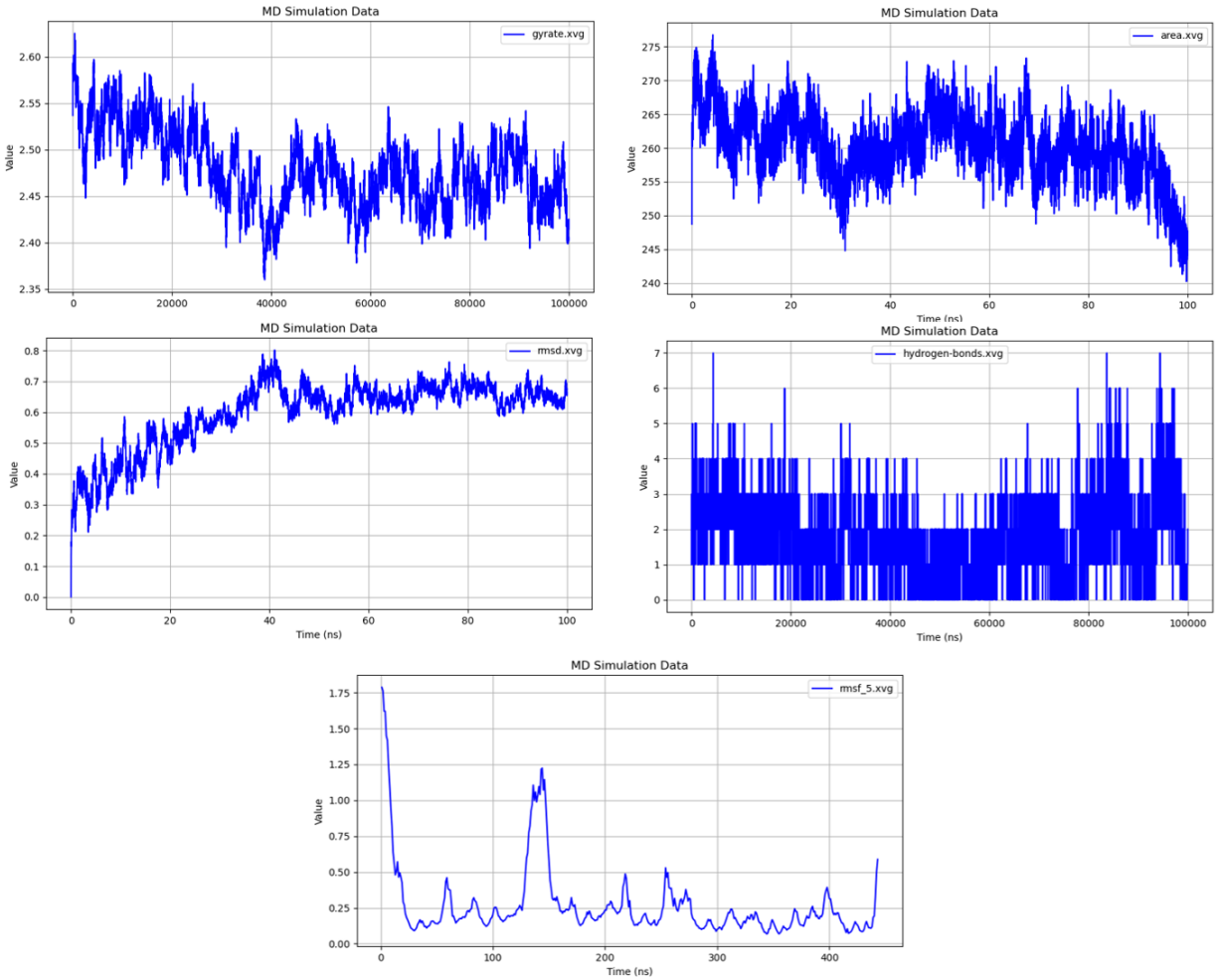

Figure 4 MD Simulation analysis of the 5th ranked complex **Curcumin_diglucoside (complex 5_)** with its receptor.

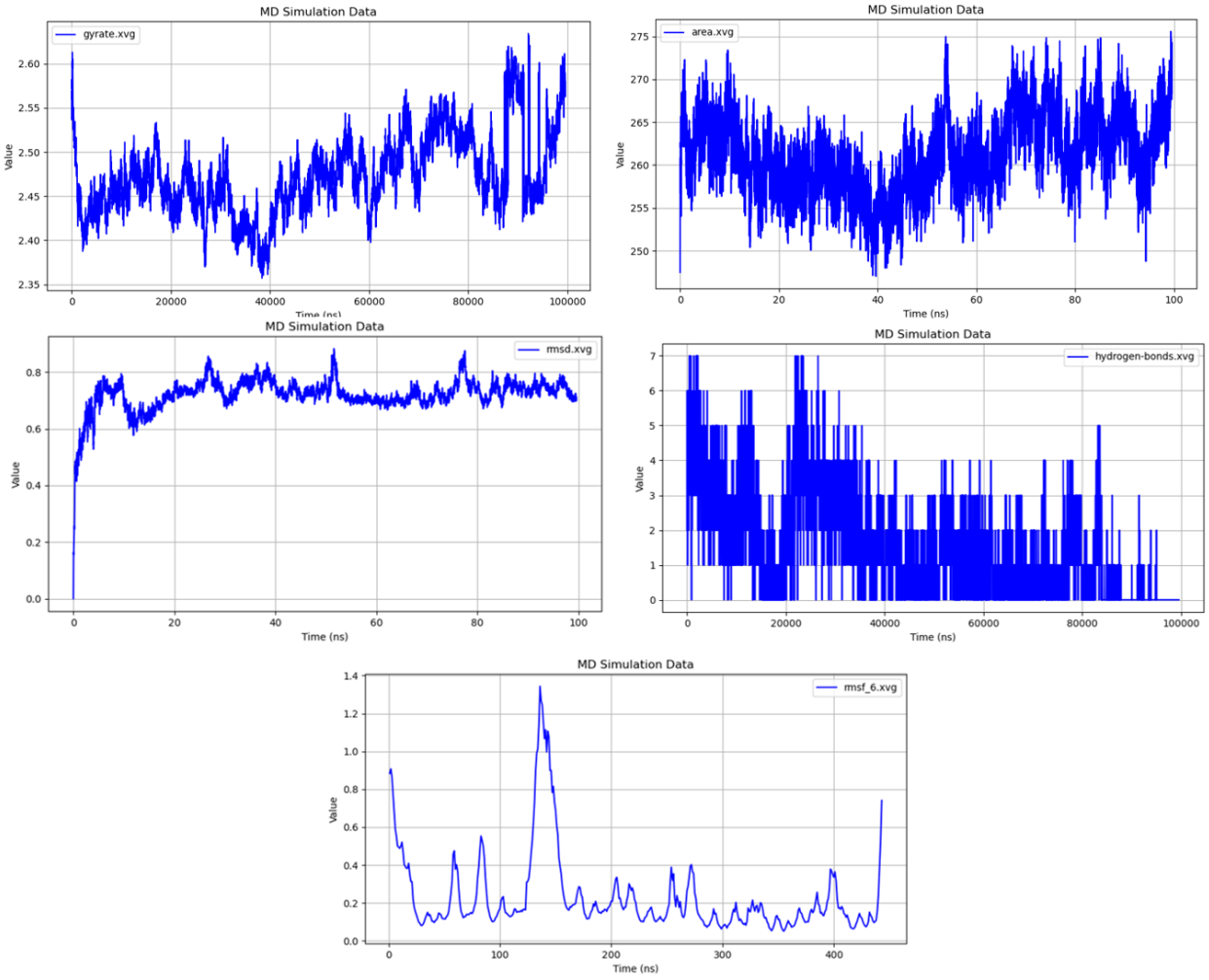

Figure 5 MD Simulation analysis of the 6th ranked complex **Curcumin_b_D_Glucuronide_Sodium_Salt (complex 6_)** with its receptor.