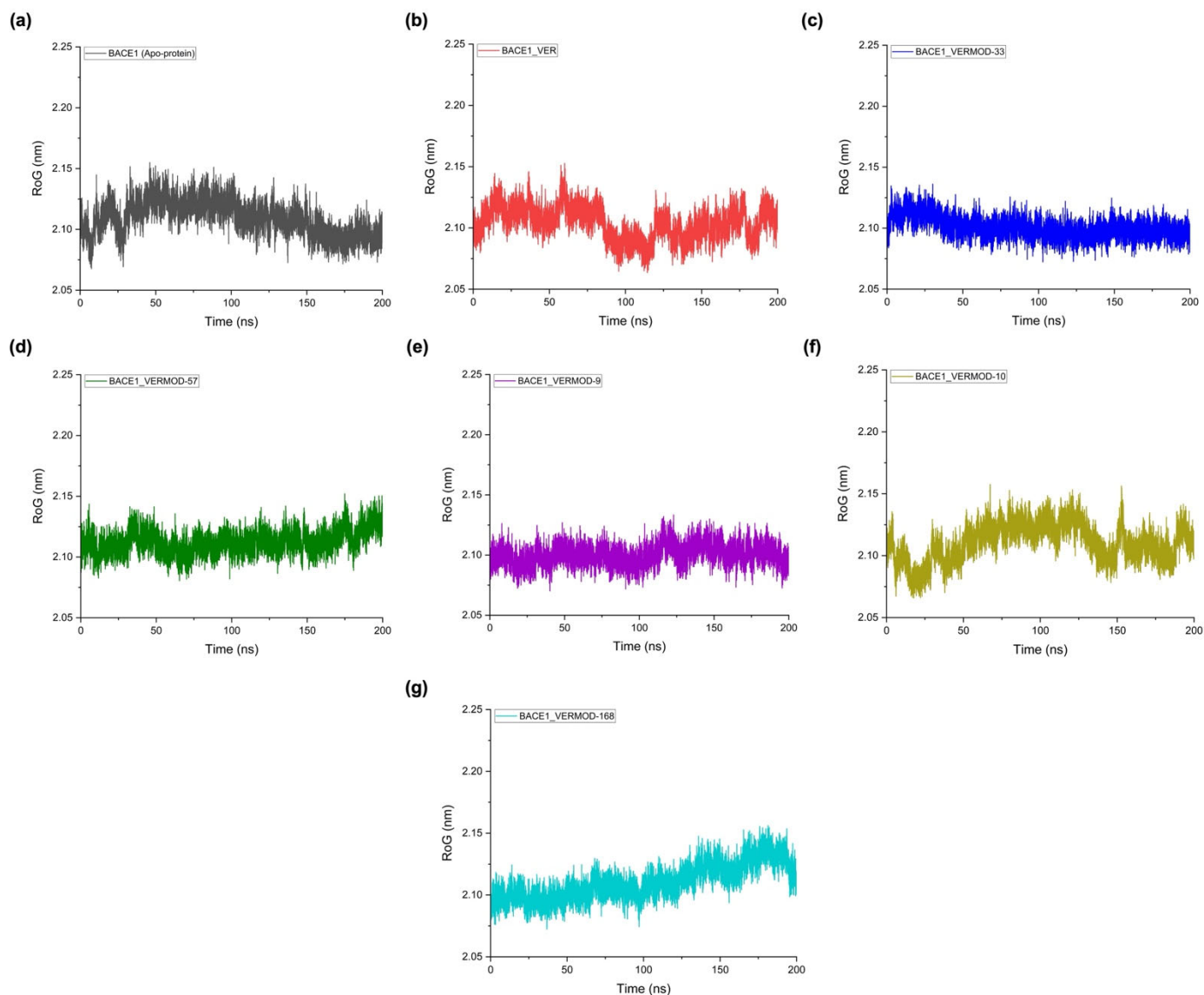
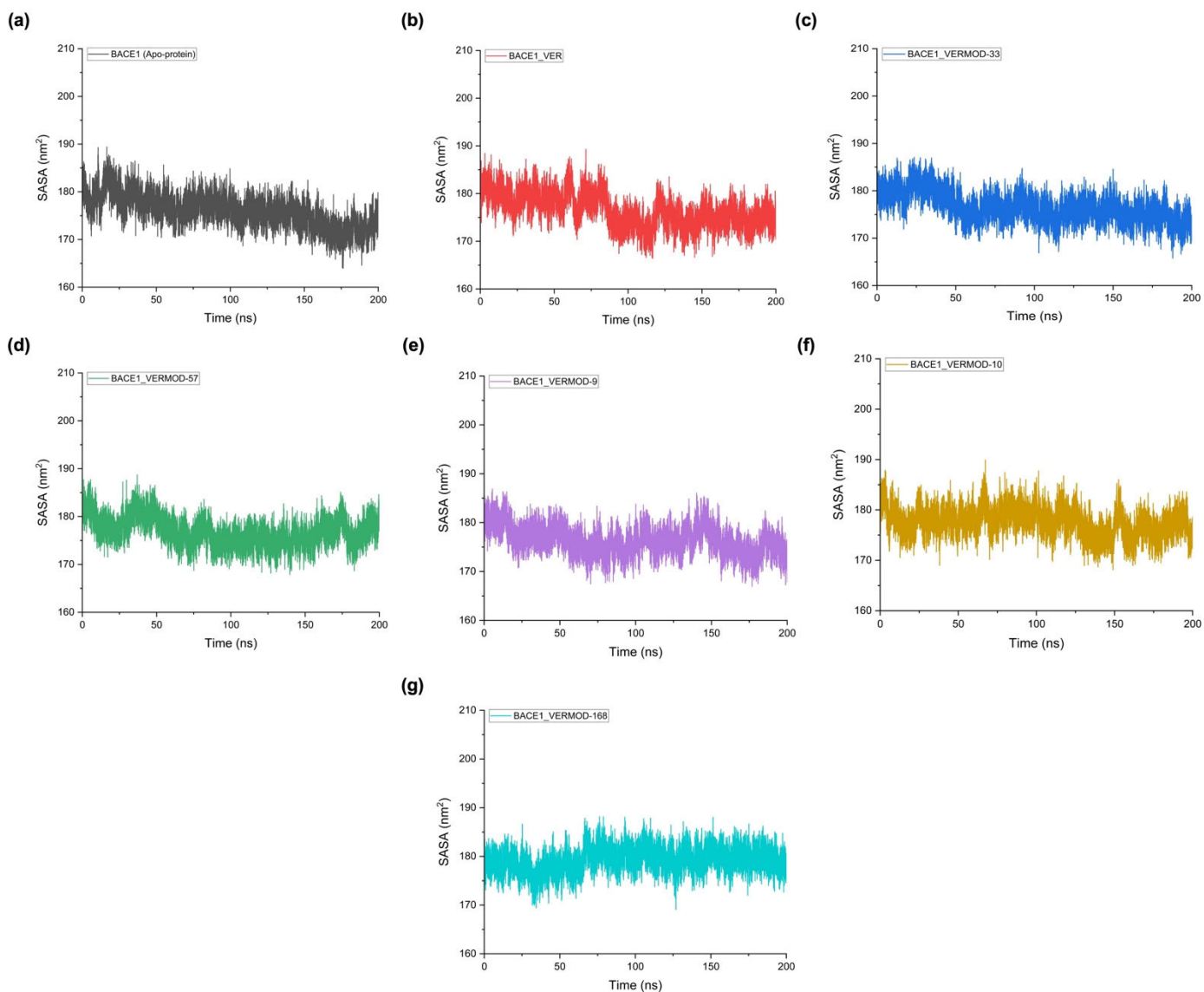


Supplementary Data S4

Detailed RoG and SASA profiles for each simulated complex, including single-complex plots and stability analyses.



Supplementary Figure 1. Radius of gyration (RoG) plots. (a) BACE1 (Apo-protein). (b) BACE1_VER complex. (c) BACE1_VERMOD-33 complex. (d) BACE1_VERMOD-57 complex. (e) BACE1_VERMOD-9 complex. (f) BACE1_VERMOD-10 complex. (g) BACE1_VERMOD-168 complex.



Supplementary Figure 2. Solvent-Accessible Surface Area (SASA) plots. (a) BACE1 (Apo-protein). (b) BACE1_VER complex. (c) BACE1_VERMOD-33 complex. (d) BACE1_VERMOD-57 complex. (e) BACE1_VERMOD-9 complex. (f) BACE1_VERMOD-10 complex. (g) BACE1_VERMOD-168 complex.