

Figure S1. Workflow of the conducted study.

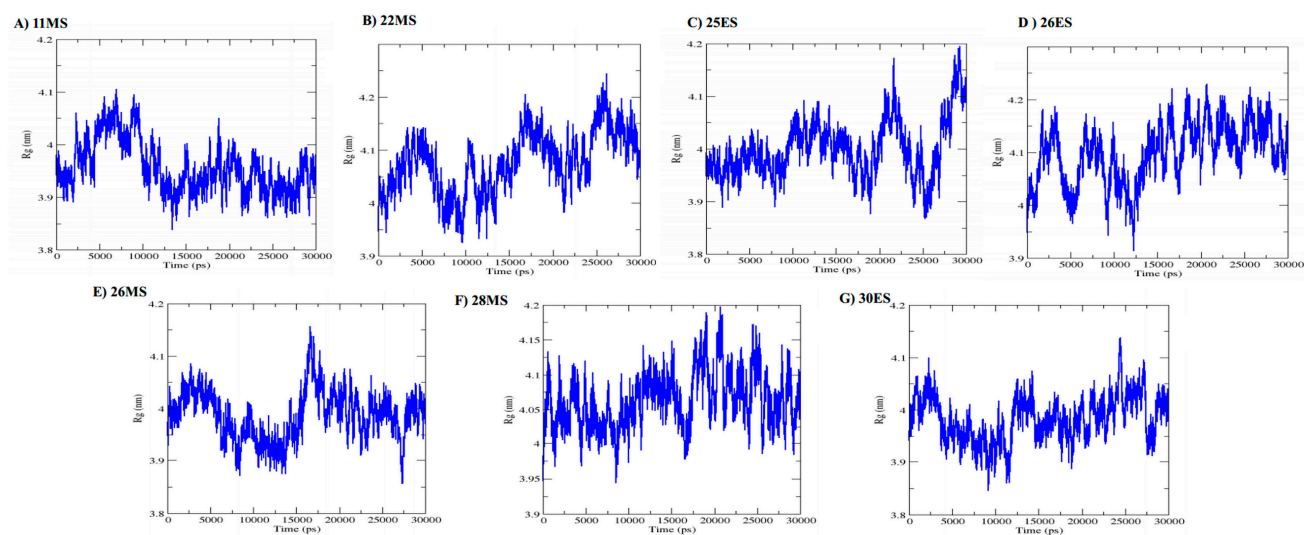


Figure S2. Radius of gyration (Rg) of target protein (HK2) for the entire simulation span whilst in the complex with (A) 11MS, (B) 22MS, (C) 25ES, (D) 26ES, (E) 26MS, (F) 28MS and (G) 30ES.

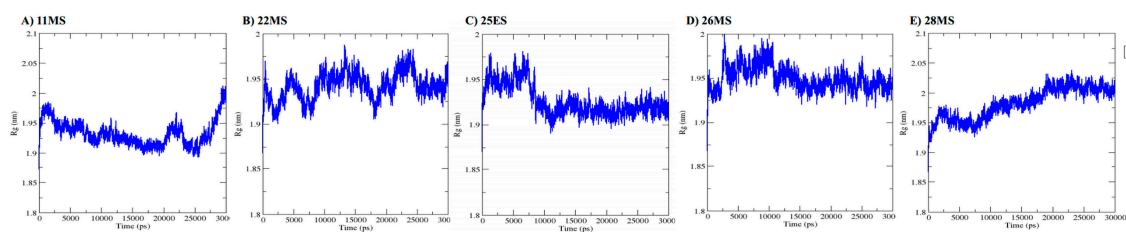


Figure S3. Radius of gyration (Rg) of target protein (GLS1) for the entire simulation span whilst in the complex with (A) 11MS, (B) 22MS, (C) 25ES, (D) 26MS and (E) 28MS