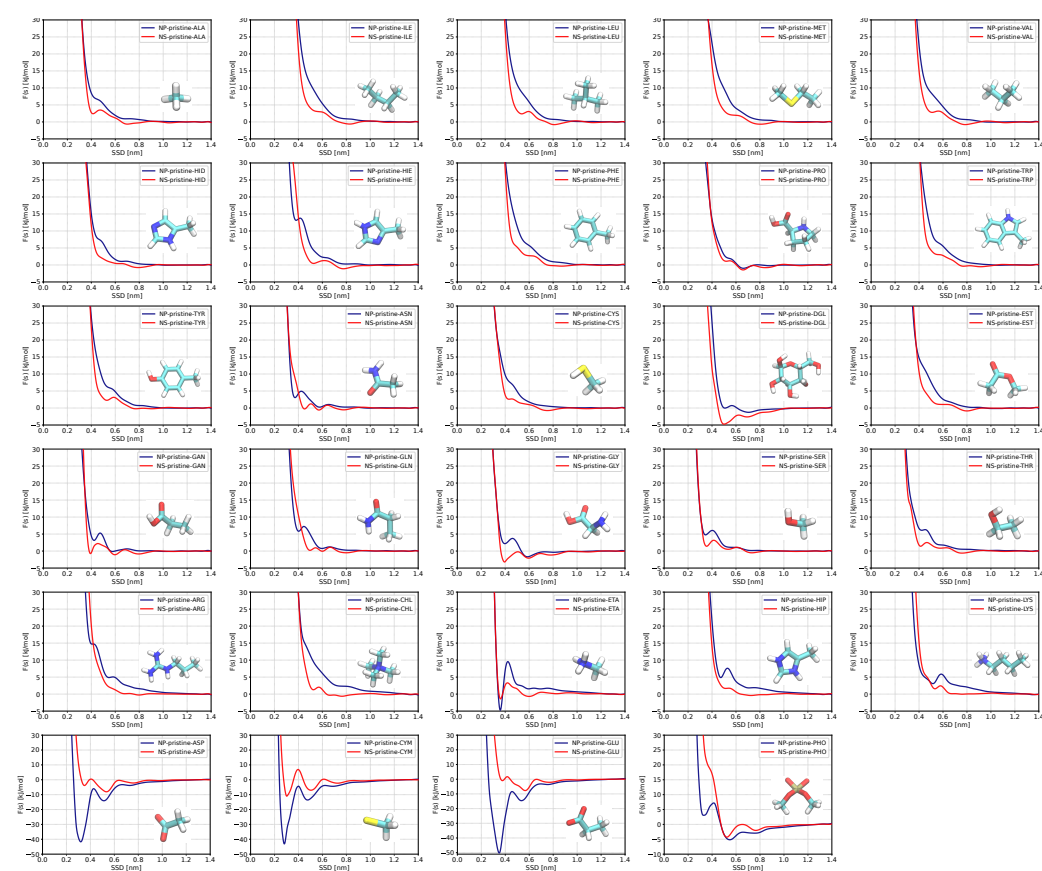
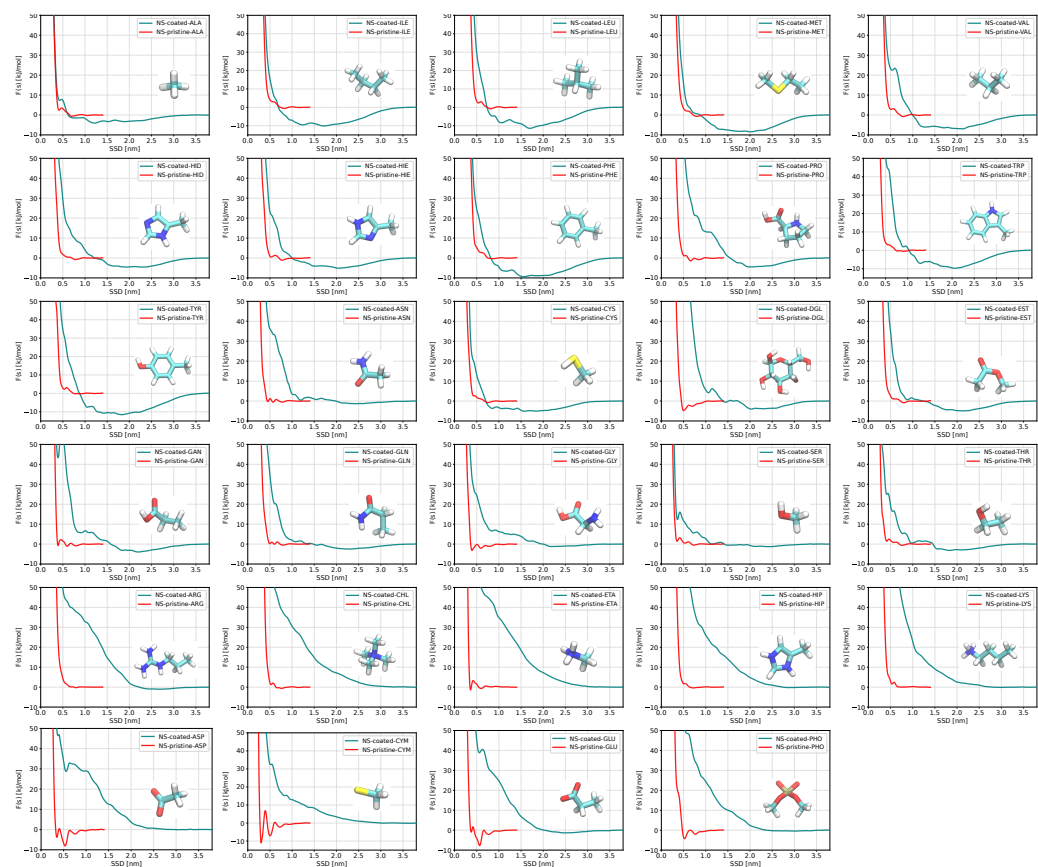


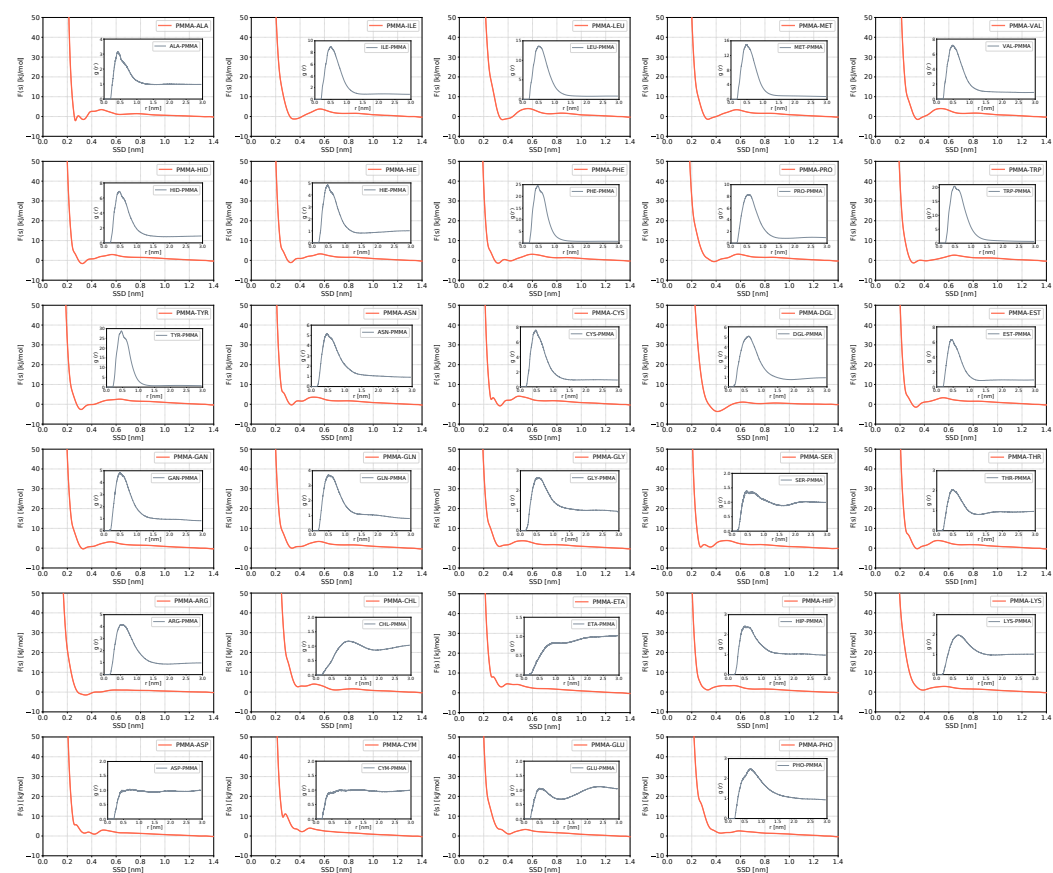
**Figure S1.** Root mean square deviation analysis for ZnS crystal structure.



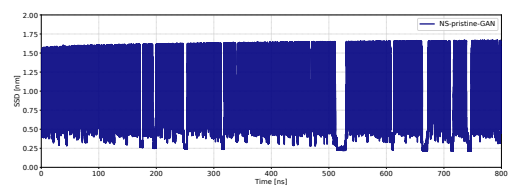
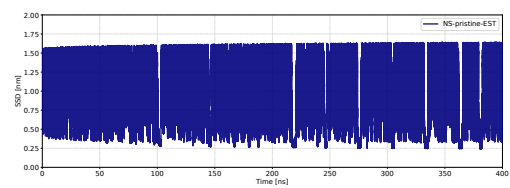
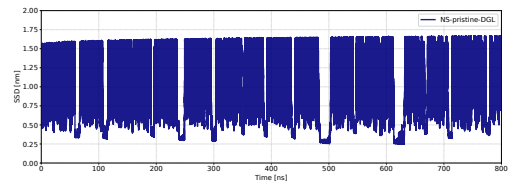
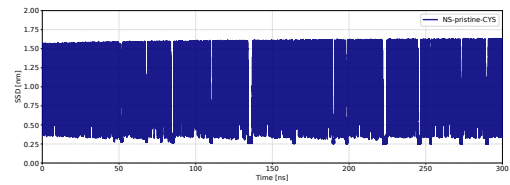
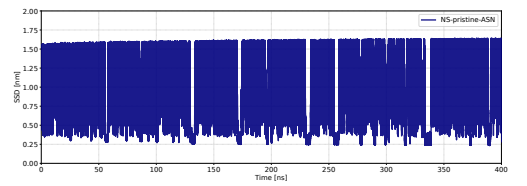
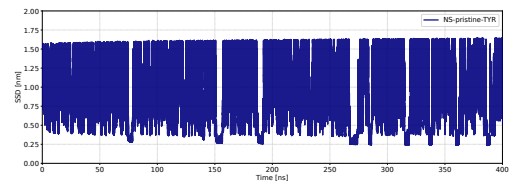
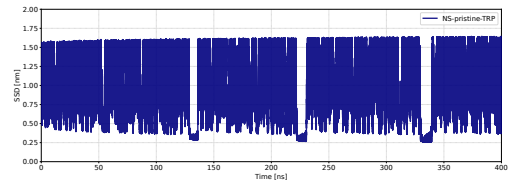
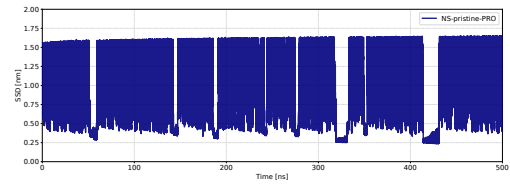
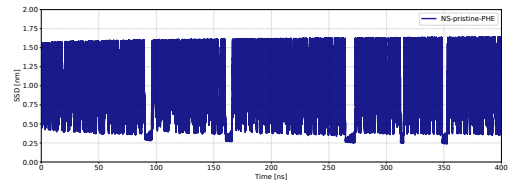
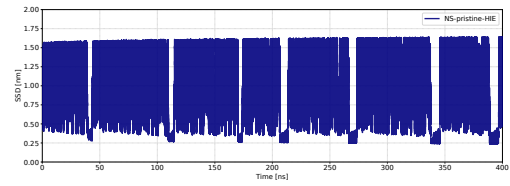
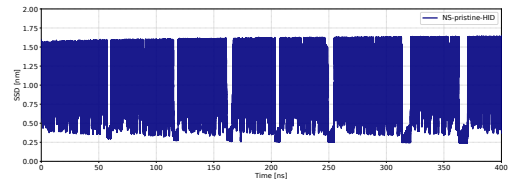
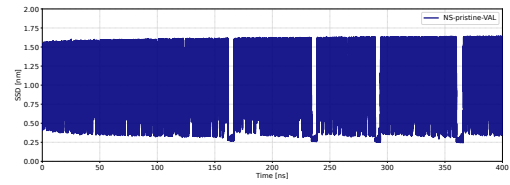
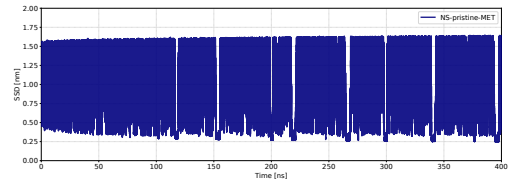
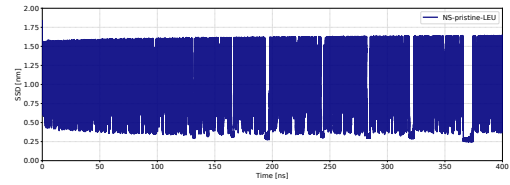
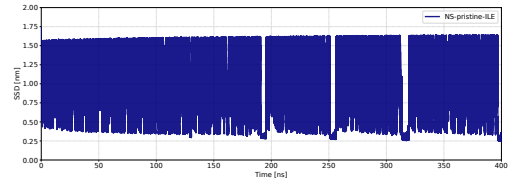
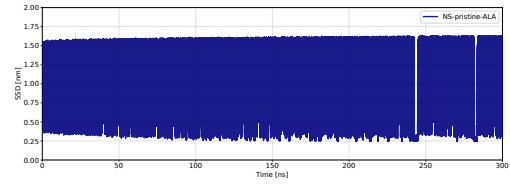
**Figure S2.** Adsorption free energy profiles as functions of the surface separation distance (SSD) for different biomolecules on ZnS (110) plane and ZnS nanoparticle in pristine (non-coated) form. The red curves correspond to ZnS (110) nanoslabs (NS), and the blue curves correspond to ZnS nanoparticle (NP). The chemical structure of biomolecules are shown in each corresponding plot.



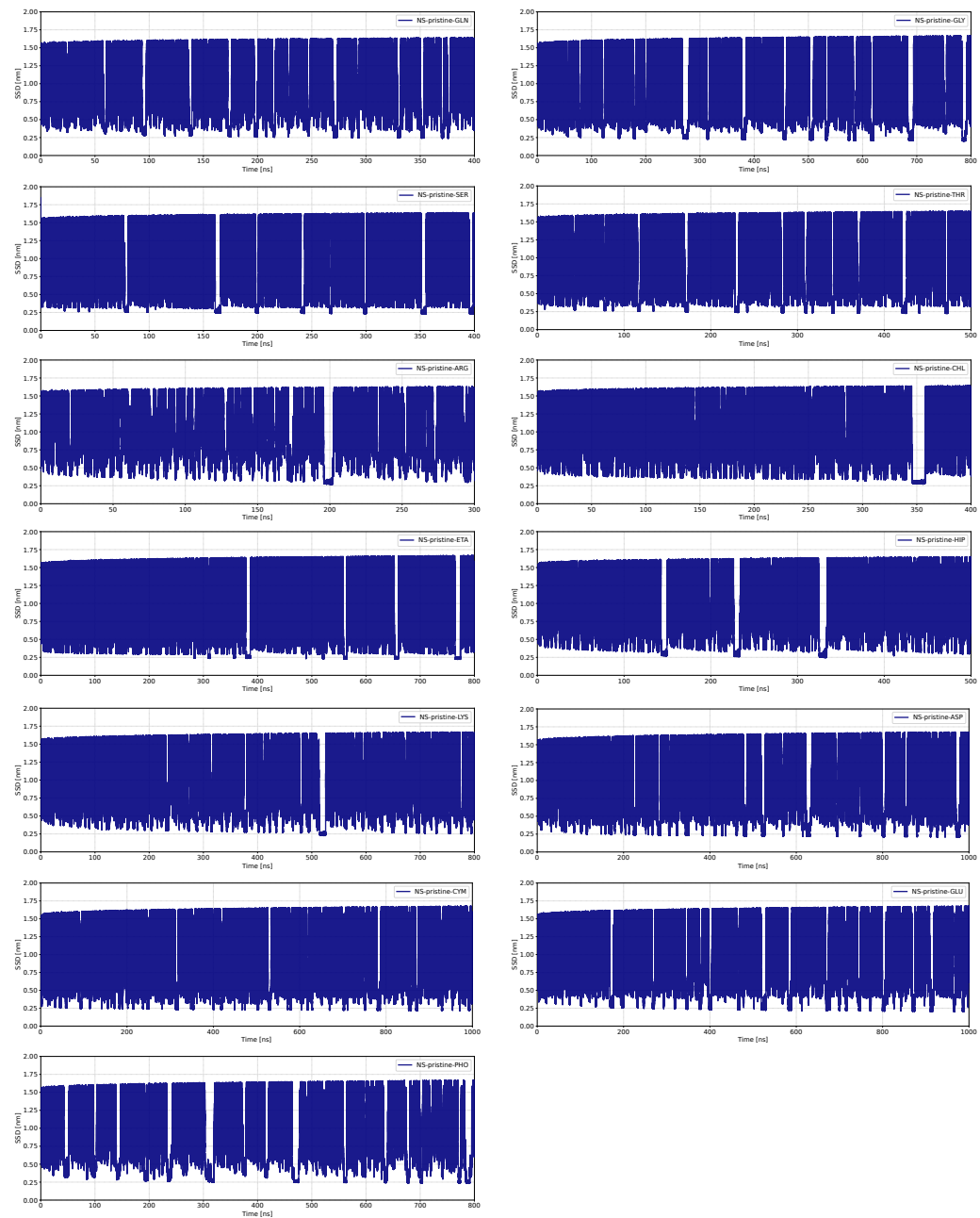
**Figure S3.** Adsorption free energy profiles as functions of the surface separation distance (SSD) for different biomolecules on ZnS (110) plane in pristine (non-coated) and coated (with PMMA) forms. The red and green curves correspond to the pristine and coated form of ZnS (110) respectively. The chemical structure of biomolecules are shown in each corresponding plot.



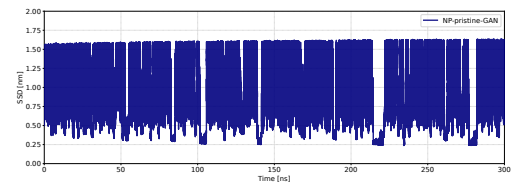
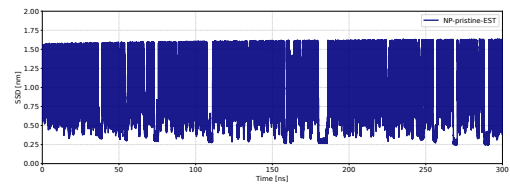
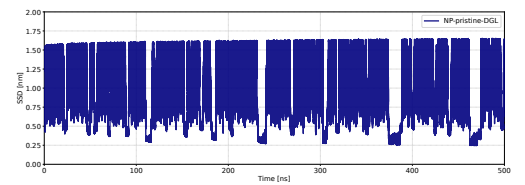
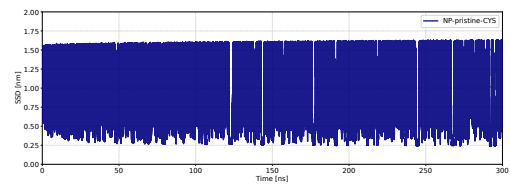
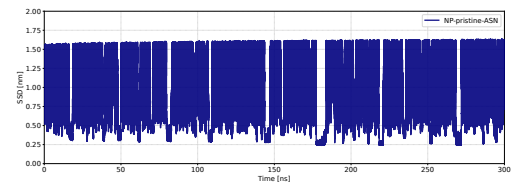
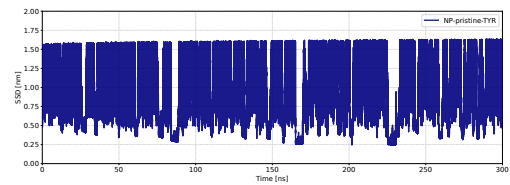
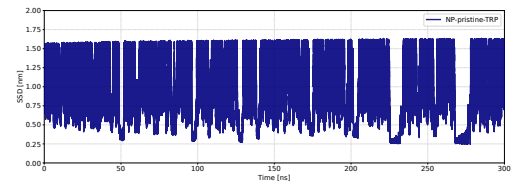
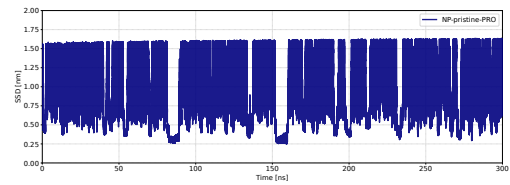
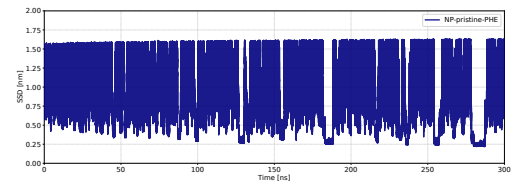
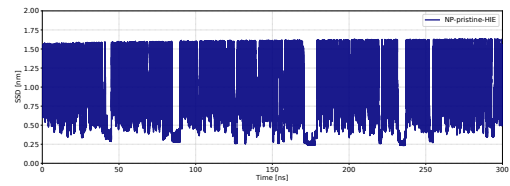
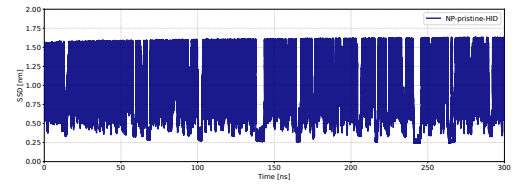
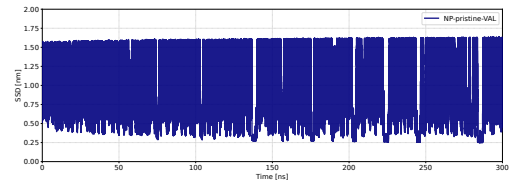
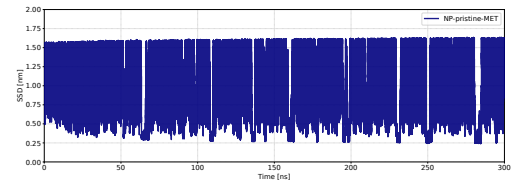
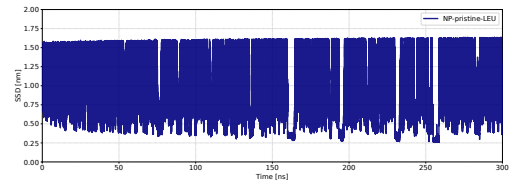
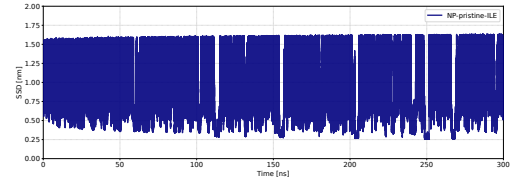
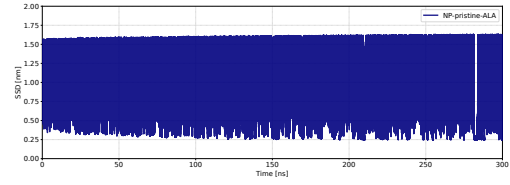
**Figure S4.** The outer plots represent adsorption free energy profiles as functions of the minimum distance between the center of mass of each biomolecules to the nearest atom of 3-MMA molecule. The RDF of each biomolecule to a 3-MMA molecule are shown in the inner plots.

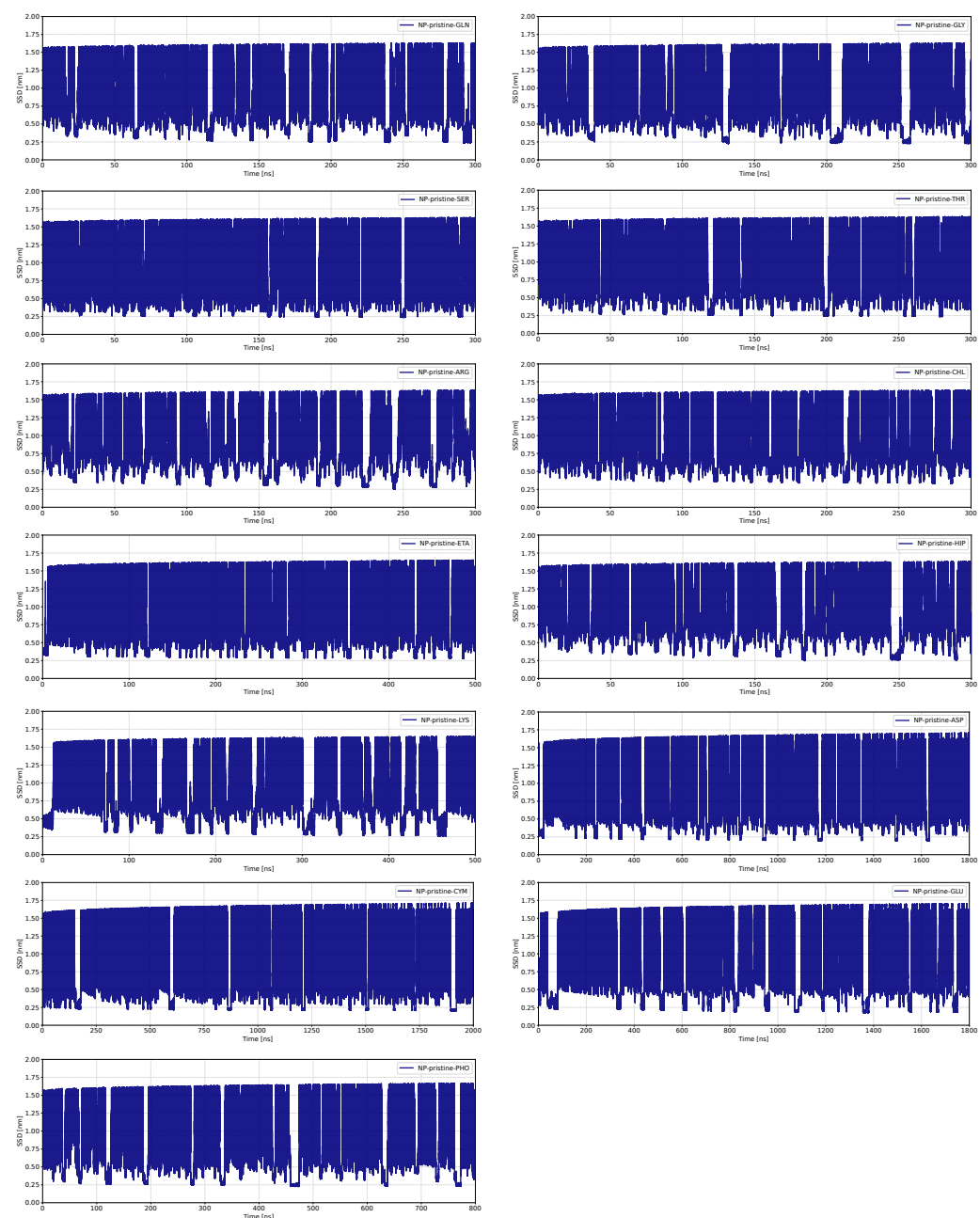




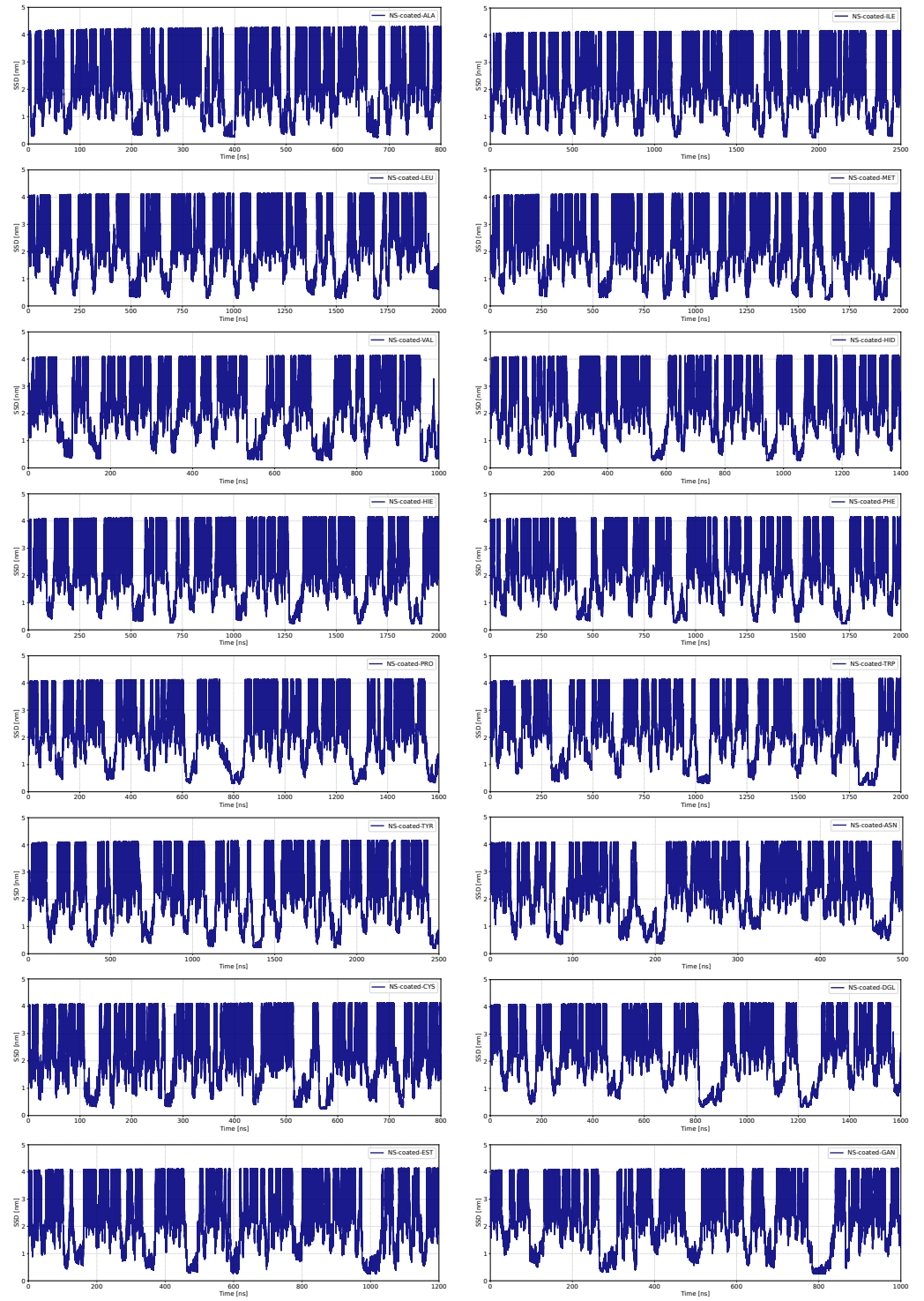


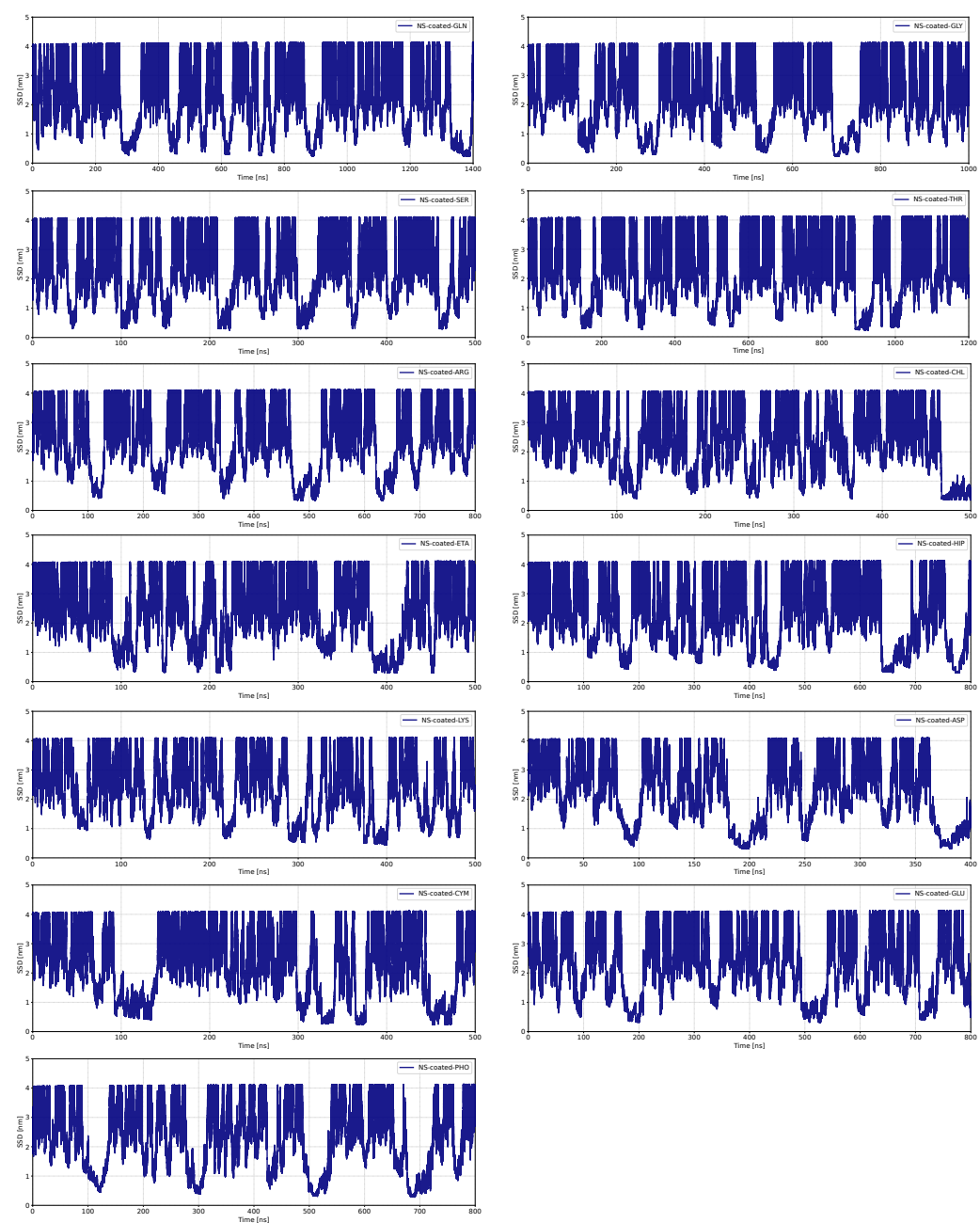
**Figure S5.** Surface separation distance (SSD) during metadynamics simulation of biomolecules on the pristine ZnS (110) slabs.



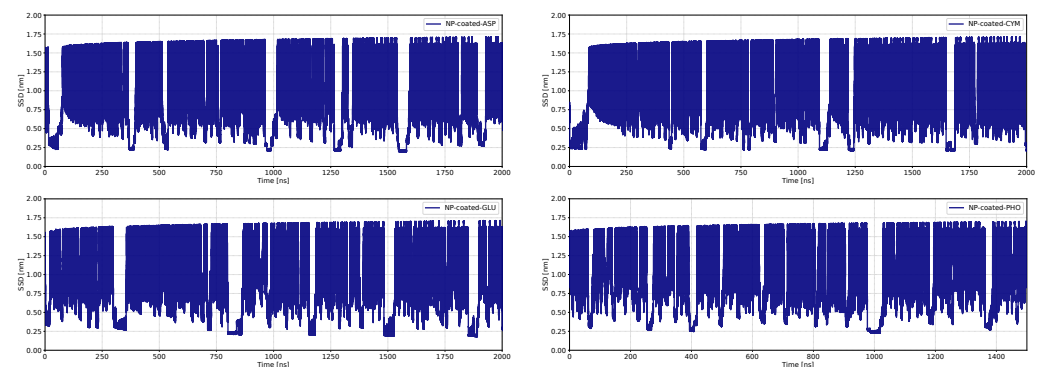


**Figure S6.** Surface separation distance (SSD) during metadynamics simulation of biomolecules on the pristine ZnS nanoparticle.

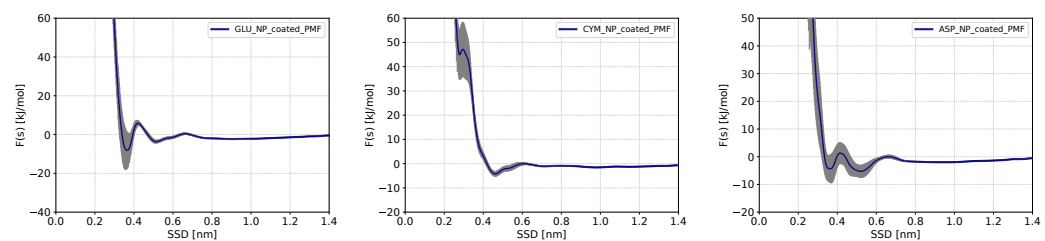




**Figure S7.** Surface separation distance (SSD) during metadynamics simulation of biomolecules on the coated ZnS (110) slabs.



**Figure S8.** Surface separation distance (SSD) during metadynamics simulation of biomolecules on the coated ZnS nanoparticles.



**Figure S9.** Adsorption profiles of biomolecules at ZnS nanoparticles. The gray curves show errors.