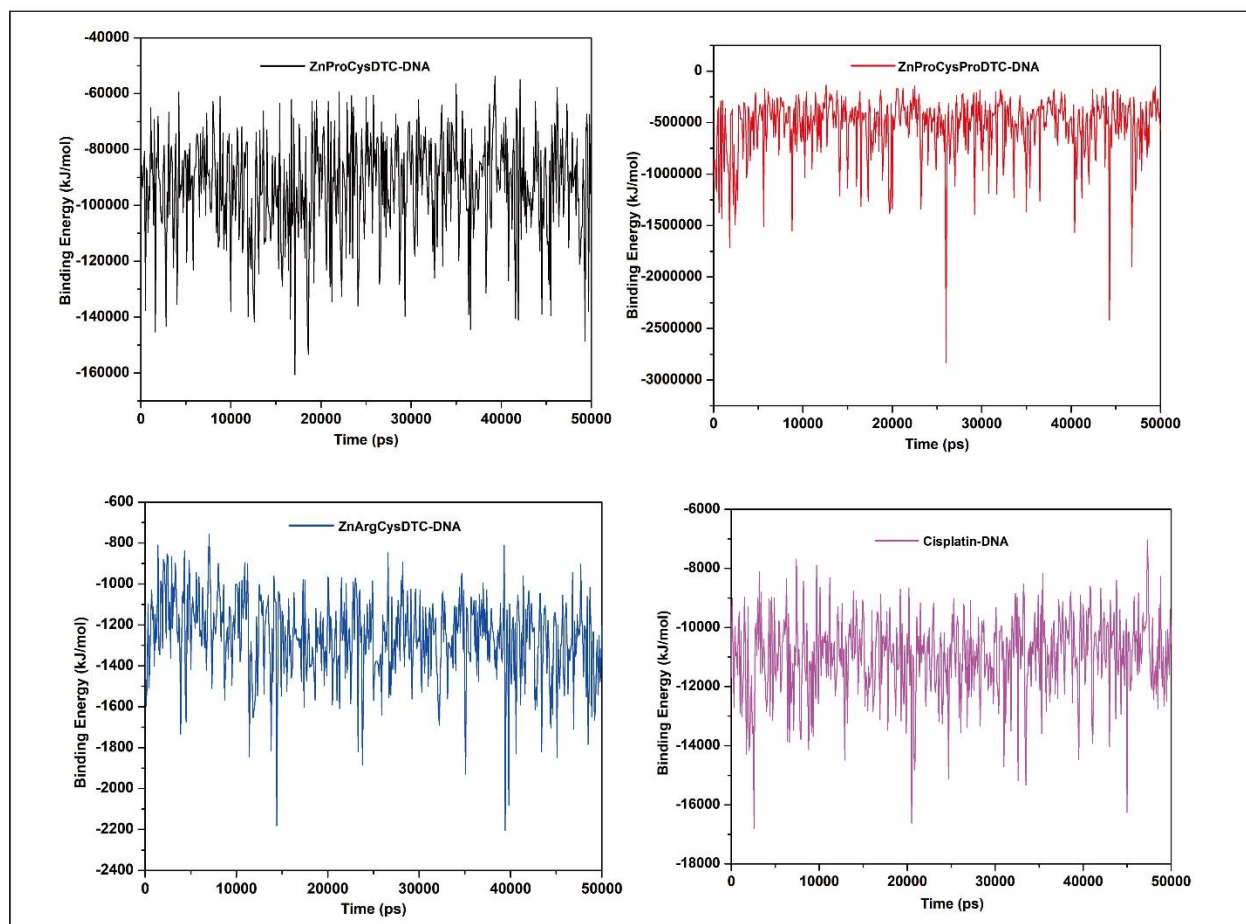
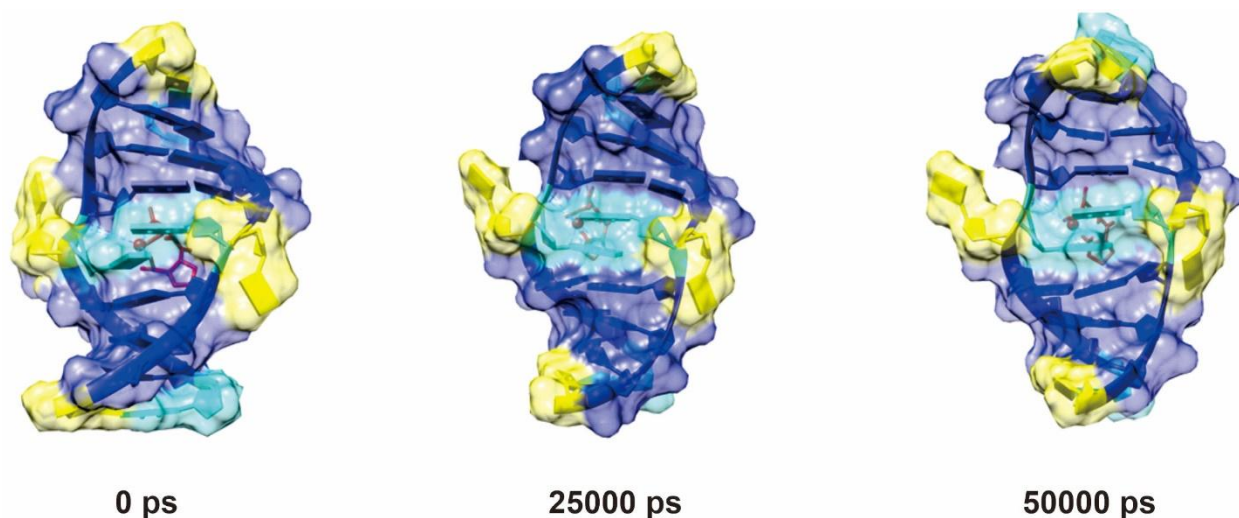
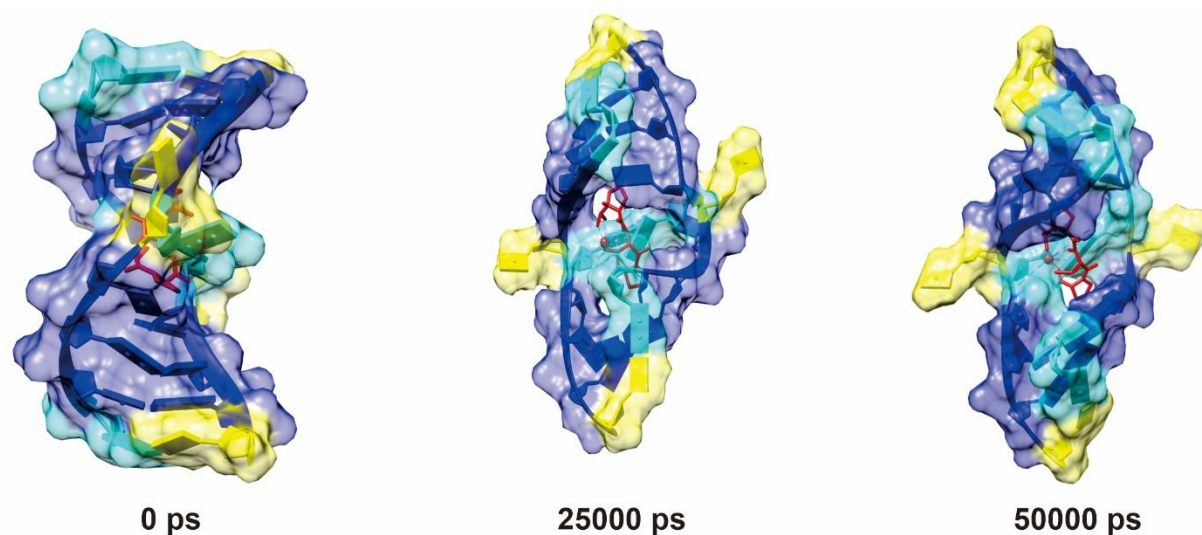




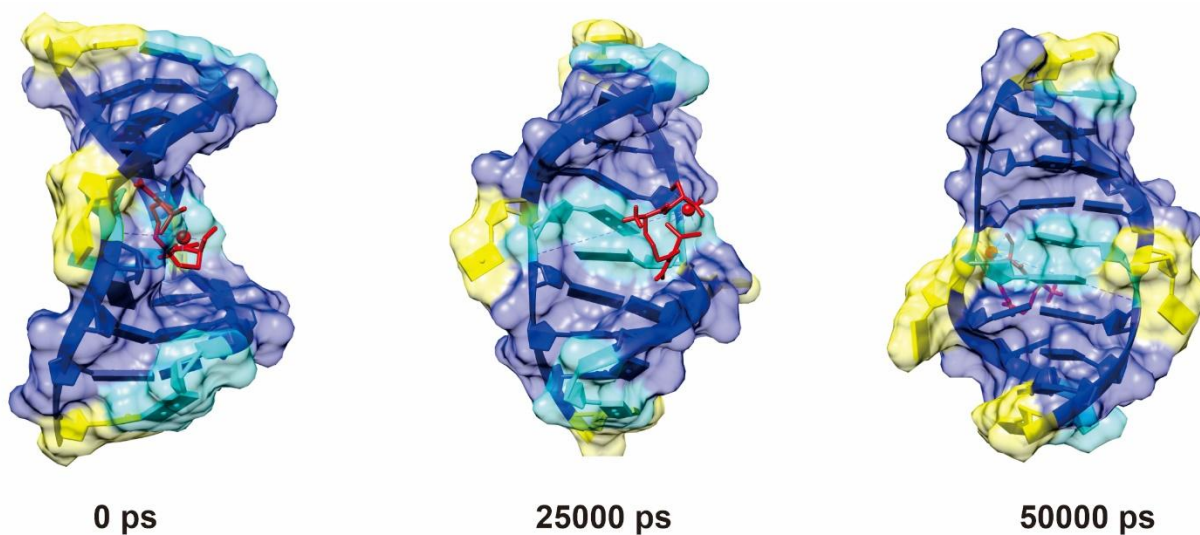
Supplementary Figure 1. Binding Energy of ZnProCysDTC-DNA, ZnProCysProDTC-DNA, ZnArgCysDTC-DNA, and Cisplatin-DNA



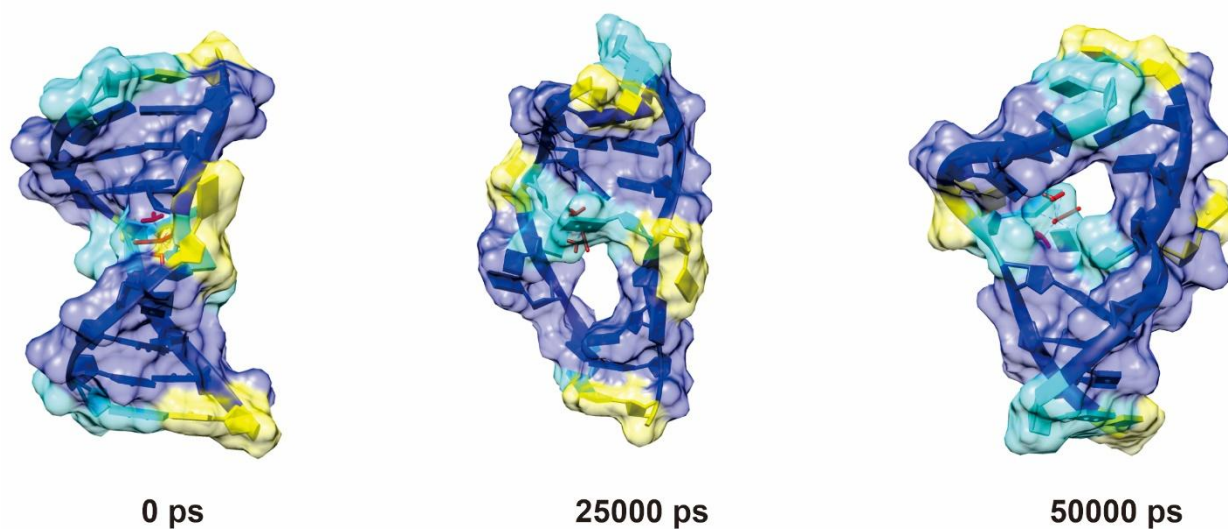
Supplementary Figure 2. Molecular interactions between ZnProCysDTC at the DNA binding site in different time intervals. The DC base pairing region is illustrated in the yellow cavity, the DG base pairing region is in the light blue cavity and the complex compound ZnProCysDTC has been shown in red color.



Supplementary Figure 3. Molecular interactions between ZnProCysProDTC at the DNA binding site in different time intervals. The DC base pairing region is illustrated in the yellow cavity, the DG base pairing region is in the light blue cavity and the complex compound ZnProCysProDTC has been shown in red color.



Supplementary Figure 4. Molecular interactions between ZnArgCysDTC at the DNA binding site in different time intervals. The DC base pairing region is illustrated in the yellow cavity, the DG base pairing region is in the light blue cavity and the complex compound ZnArgCysDTC has been shown in red color.



Supplementary Figure 5. Molecular interactions between Cisplatin at the DNA binding site in different time intervals. The DC base pairing region is illustrated in the yellow cavity, the DG base pairing region is in the light blue cavity and the complex compound Cisplatin has been shown in red color.