**Supporting Material**

***In vitro* and *in silico* determination of the interaction of artemisinin with human serum albumin.**

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**Figure S1.** k-Nearest Neighbor distance plot of the center of mass coordinates from the results of multiple docking runs of ART.

**Figure S2**. k-Nearest Neighbor distance plot of the center of mass coordinates from the results of multiple docking runs of DEXA.

**Figure S3.** Distribution of HSA conformations over time.

**Figure S4.** Cluster analysis of the COM data from the docking results of ART with HSA using the DBSCAN algorithm. Roman numerals denote clusters, where the 1st cluster contains 58.2% of docking conformations.

**Figure S5.** Cluster analysis of the COM data from the docking results of DEXA with HSA using the DBSCAN algorithm. Roman numerals denote clusters, where the 1st cluster contains 68.8% of docking conformations.