

Description of Additional Supplementary Files

Supplementary Data 1: Analyses of hydrogen bonds in *Pf*GS and ΔI_2 *Pf*GS. Hydrogen bonds unique for *Pf*GS and ΔI_2 *Pf*GS are listed for all the four subunits used in MD simulations. Hydrogen bonds having $\geq 40\%$ occupancy are considered. Hydrogen bonds of the key residues associated with enzyme activity from the adjacent subunits (subunit A and B) are represented to highlight the variations between *Pf*GS and ΔI_2 *Pf*GS. Hydrogen bonds that were either absent or with significantly reduced occupancies ($< 40\%$) are highlighted in blue. The entire list of hydrogen bonds are also provided for *Pf*GS and ΔI_2 *Pf*GS.

Supplementary Data 2: Cumulative peptide intensities and normalized FC and Log₂FC values of downregulated and upregulated proteins in MSO-treated *Pf*3D7 parasites. The cumulative peptide intensities of the proteins that were commonly downregulated and upregulated in two independent sets of experiments are shown. For cumulative peptide intensities, peptides identified with $\geq 95\%$ confidence for the respective proteins were considered. Fold change (FC) values normalized with respect to parasite actin I are given along with Log₂FC values. For downregulated proteins, proteins identified in both the untreated controls of two independent experiments and either undetectable or significantly downregulated (≥ 1.5 fold) in MSO-treated *Pf*3D7 parasites are represented. For upregulated proteins, proteins significantly upregulated (≥ 1.5 fold) in both the MSO-treated parasites of two independent experiments and/or undetectable in the untreated controls but detectable in the MSO-treated parasites are represented. Asparagine-rich proteins are highlighted in bold. The entire peptide summary for the respective controls and MSO-treated samples are also provided.