Kinetic, molecular docking, and dynamics studies to determine the effect of inhibitors on the activity and structure of fused G6PD::6PGL protein from *Trichomonas vaginalis*

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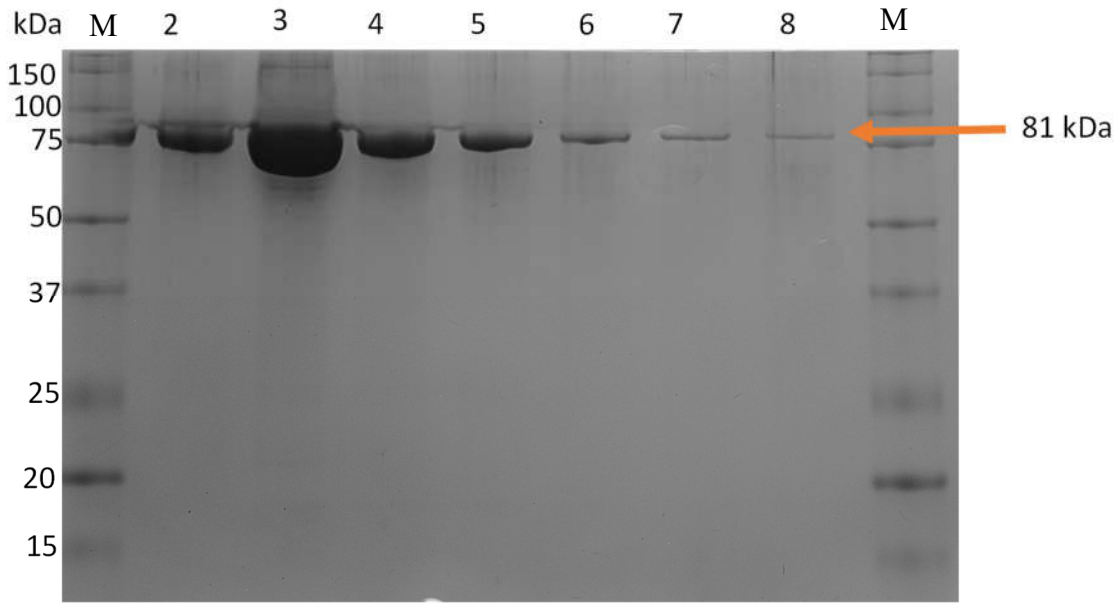

Figure S1. Purification of the recombinant TvG6PD::6PGL enzyme. M: molecular protein weight (MW) marker precision plus protein kaleidoscope standards from Bio-Rad. Lines 1 - 8: 10 µL of protein fractions showed G6PD activity. We stained the gel with a colloidal Coomassie solution. The SDS-PAGE gels are representative of three independent experiments.

Table S1. Data obtained by molecular docking assays with the SwissDock server for the most stable clusters.

Compound	Population	ΔG (Kcal/mol)	Full fitness (Kcal/mol)
JMM-3 Zone 1	16	-7.0833	-3770.4844
JMM-3 Zone 2	216	-8.6520	-3770.0078
MCC-7 Zone 1	64	-8.0406	-3867.0112
MCC-7 Zone 2	112	-7.3288	-3866.477

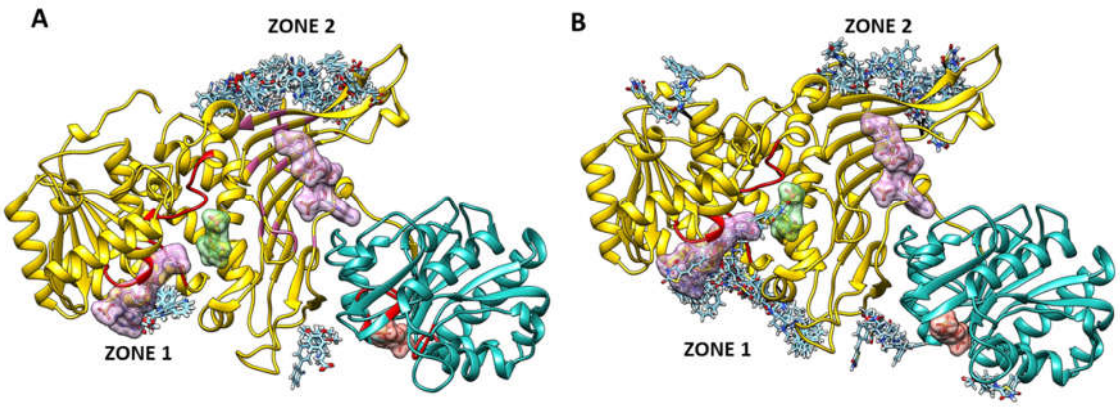

Figure S2. Molecular docking of the TvG6PD::6PGL model with compounds obtained with the SwissDock server. (**A**) General view of the binding affinities of all JMM-3 conformers with the TvG6PD::6PGL protein (**B**) General view of the binding affinities of all MCC-7 conformers with the TvG6PD::6PGL protein. The G6PD and 6PGL are shown in gold and light sea green color.