DISSECTING THE CATALYTIC MECHANISM OF *TRYPANOSOMA BRUCEI* TRYPTANTHIONE SYNTHETASE BY KINETIC ANALYSIS AND COMPUTATIONAL MODELLING*

Overview of all data points with accompanying simulations
Fig 1: Comparison between the activities of TryS measured at fixed ATP and the model simulation.

The rates (open circles) measured by varying Spd or Gsp at 2.3 mM ATP and different fixed GSH concentrations are depicted together with the model simulations (dashed lines).
Fig 2: Comparison between the activities of TryS measured at fixed GSH and the model simulation.

The rates (open circles) measured by varying Spd or Gsp at 0.9 mM GSH and different fixed ATP concentrations are depicted together with the model simulations (dashed lines).
Fig 3: Comparison between the activities of TryS measured at fixed Spd or Gsp and the model simulations.

The rates (open circles) measured by varying ATP at 8 mM Spd or 0.5 mM Gsp and different fixed GSH concentrations are depicted together with the model simulations (dashed lines).
Fig 4: Comparison between the measured inhibitory effect of T(SH)$_2$ on TryS activity and the model simulations at variable GSH concentrations and fixed Spd.

The experimental values (open circles) measured at varying GSH and fixed concentrations of 8 mM Spd and 2.3 mM ATP are depicted together with the model simulation (dashed lines). The T(SH)$_2$ concentrations in the assays are shown inside each graph.
Fig 5: Comparison between the measured inhibitory effect of T(SH)$_2$ on TryS activity and the model simulations at variable GSH concentrations and fixed Gsp.

The experimental values (open circles) measured at varying GSH and fixed concentrations of 0.521 mM Gsp (A) or 0.608 mM Gsp (B) and 2.3 mM ATP are depicted together with the model simulations (dashed lines). The T(SH)$_2$ concentrations in the assays are shown inside each graph.
Fig 6: Comparison between the measured inhibitory effect of T(SH)$_2$ on TryS activity and the model simulations at variable Spd concentrations.

The experimental values (open circles) measured at varying Spd and fixed concentrations of 0.2 mM GSH and 2.3 mM ATP are depicted together with the model simulations (dashed lines). The T(SH)$_2$ concentrations in the assays are shown inside each graph.
Fig 7: Comparison between the measured inhibitory effect of T(SH)$_2$ on TryS activity and the model simulations at variable Gsp concentrations.

The experimental values (open circles) measured at varying Gsp and fixed concentrations of 0.2 mM GSH and 2.3 mM ATP are depicted together with the model simulations (dashed lines). The T(SH)$_2$ concentrations in the assays are shown inside each graph.