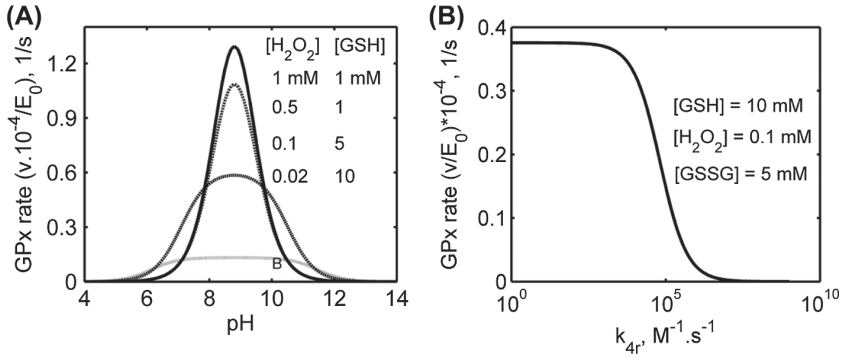
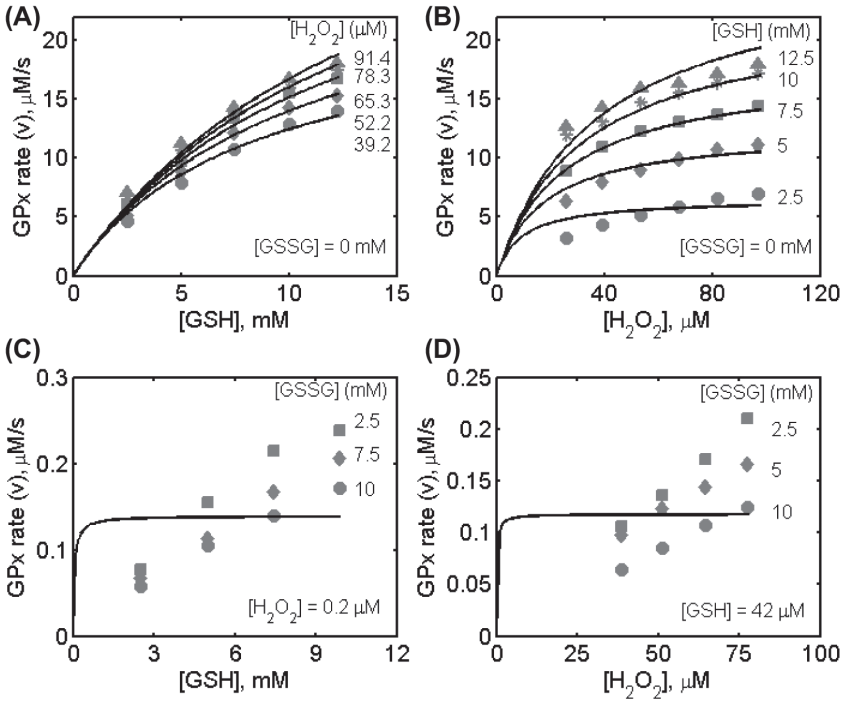
Supplementary material for Pannala VR, et al. A mechanistic mathematical model for the catalytic action of glutathione peroxidase. Free Radic Res 2014;48:487–502.



Supplementary Figure 1. Model simulations based on the values of the rate constants estimated for Flohé et al. [1] from Table II in the main text. (A) Simulation of the bi-modal behavior of the observed GPx activity with varying pH for different combinations of reaction substrates in the absence of the product GSSG. (B) Sensitivity analysis for the parameter k_{4r} for the interaction of reduced enzyme (E) with the product GSSG in the presence of 0.1 mM of H_2O_2 and 10 mM of GSH for a product [GSSG] of 5 mM at pH 7. A fixed value of 4×10^2 at which product inhibition was absent has been used in the model to describe the experimental data.



Supplementary Figure 2. Comparison of the initial-velocity data for Carsol et al. [2] using GPx-1 from bovine erythrocytes at a negligible fixed reverse rate constant value (k_{1r}). Here, the enzyme assays were carried out at 0.1 M ionic strength, pH 7.0, and 37ºC. (A) Comparison of the model predictions to the initial-velocity data with varying [GSH] for five different [H_2O_2] (39.2, 52.5, 65.3, 78.3, and 91.4 μM) in the absence of the product GSSG. (B) Comparison of the model predictions to the initial-velocity data with varying [H_2O_2] for five different [GSH] (2.5, 5, 7.5, 10 and 12.5 mM) in the absence of the product GSSG. (C) Comparison of the model predictions to the initial-velocity data with varying [GSH] for three different product [GSSG] (2.5, 7.5 and 10 mM) at a fixed estimated [H_2O_2] of 0.2 μM. (D) Comparison of the model predictions to the initial-velocity data with varying [H_2O_2] for three different product [GSSG] (2.5, 5 and 10 mM) at a fixed estimated [GSH] of 42 μM. Here, the plots clearly show that under conditions of fixed low value of the reverse rate constant (k_{1r}) for the reaction step of *F* to *E* in Figure 1B of the main text, the model was not able describe the experimental data for any values of the remaining parameters.

References

[1] Flohé L, Loschen G, Günzler WA, Eichele E. Glutathione peroxidase, V. The kinetic mechanism. Hoppe-Seyler's Zeitschrift fur Physiologische Chemie. 1972;353:987–99.

[2] Carsol MA, Pouliquen-Sonaglia I, Lesgards G, Marchis-Mouren G, Puigserver A, Santimone M. A new kinetic model for the mode of action of soluble and membrane- immobilized glutathione peroxidase from bovine erythrocytes: Effects of selenium. European Journal of Biochemistry. 1997;247:248–55.