# Catalytic oxidant scavenging by selenium-containing compounds: reduction of selenoxides and *N*-chloramines by thiols and redox enzymes

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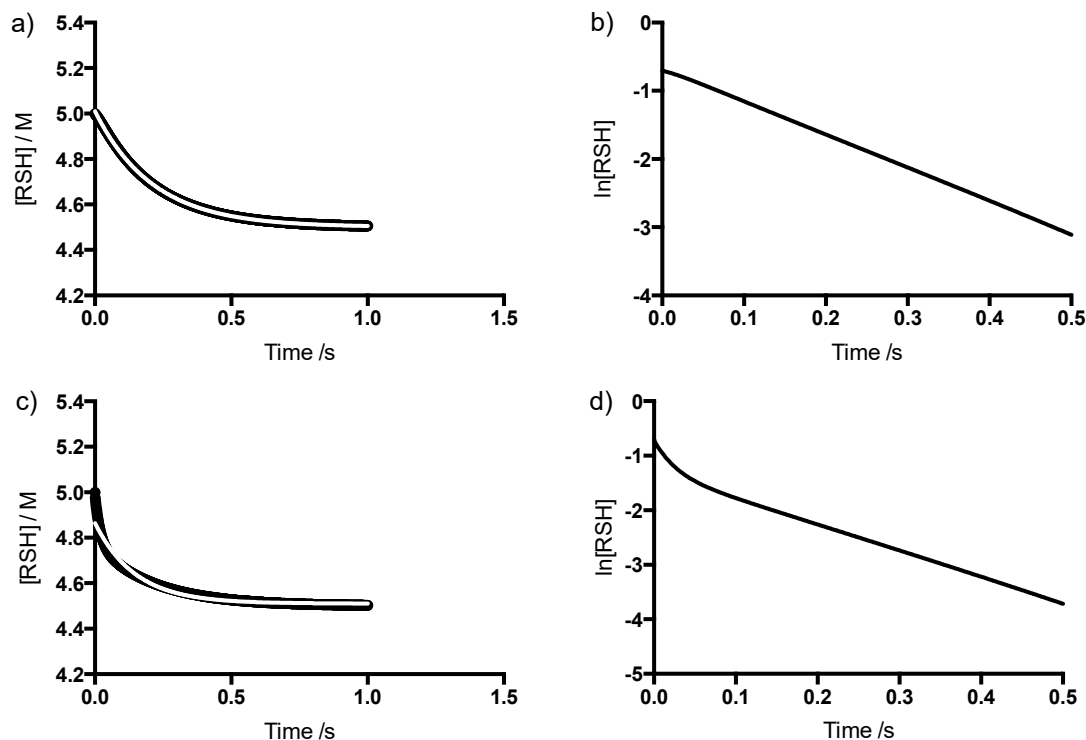
*Figure S.1 – Computational models showing reaction profile for the proposed two-step mechanism shown in Scheme 1*

Graph a) shows computational model (black line) of the reaction (A + RSH → C + RSH → D + E + F) where concentration of RSH is set to 5 M, representing a ten-fold excess of the concentration of A, set to 0.5 M. The rate constant for the $k_2$ was set to 10 and $k_1$ was set to 1. The simulation was run for 1000 points, with the theoretical concentrations of A and RSH calculated at 0.001 s intervals. An exponential decay function was fitted to the data obtained for concentrations of RSH (white line). Graph c) shows the same model (black line), with $k_2$ set to 1 and $k_1$ set to 10, with the exponential fit (white line). The concentration of RSH obtained in a) was plotted as ln[RSH] vs time in b). The concentration of RSH obtained in c) was plotted as ln[RSH] vs time in d). When $k_2 > k_1$ first-order conditions are observed, with concentration data fitting to single exponential curve, and ln[RSH] vs time plots linear. When $k_2 < k_1$, first-order mechanisms are not observed. Computational models were performed in Mechanism-Based Kinetics Simulator available at (http://www.stolaf.edu/depts/chemistry/courses/toolkits/126/js/kinetics/). Exponential fits were performed in Prism v6.
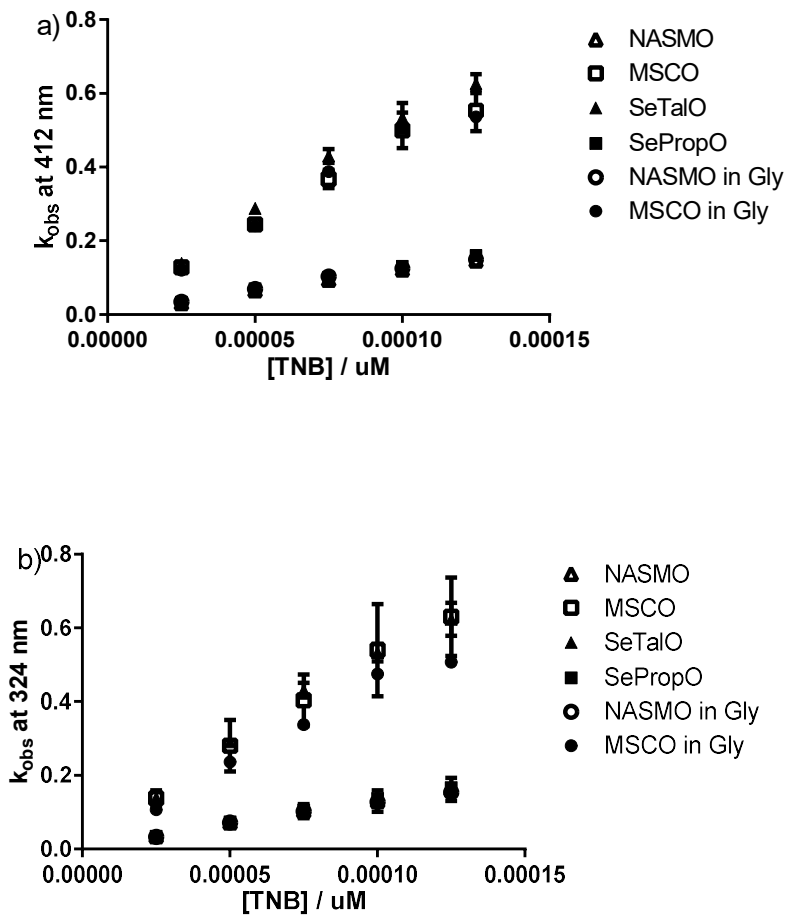
*Figure S.2 – Pseudo first-order plot for the reduction of selenoxides (5 µM) by increasing TNB (25 – 125 µM)*

The observed rate constant, $k_{obs}$, was determined at (a) 412 nm (consumption of TNB) or (b) 324 nm (formation of DTNB), from kinetic data obtained after mixing preformed selenoxides (5 µM) with TNB (25 – 125 µM) using single exponential fitting. $k_{obs}$ was plotted against initial TNB concentration and the second-order rate constants determined from the gradient of these plots and are reported in Table 1. Data represent mean ± SD of three independent experiments.
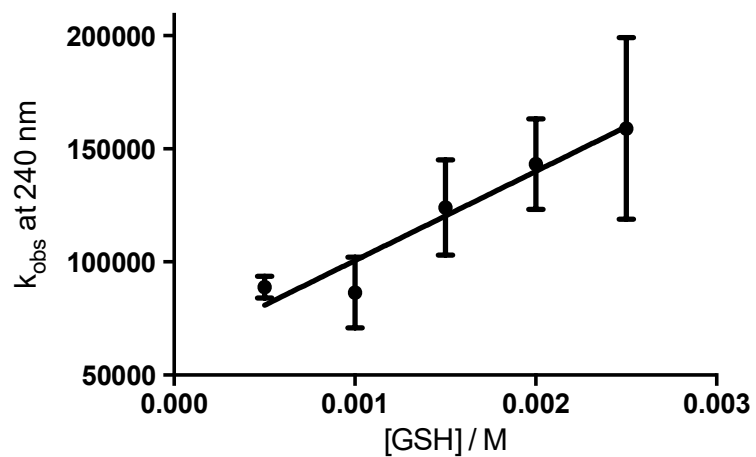
*Figure S.3 – Pseudo first-order plot for the initial phase measured during reduction of SeMetO with increasing [GSH]*

The observed rate constant, $k_{obs}$, was determined at 240 nm from kinetic data obtained after mixing SeMetO (125 μM) with GSH (0.5 – 2.5 mM) using single exponential fitting. $k_{obs}$ was plotted against the initial GSH concentration and the second-order rate constant determined from the gradient of this plot. Data represent mean ± SD of three independent experiments.
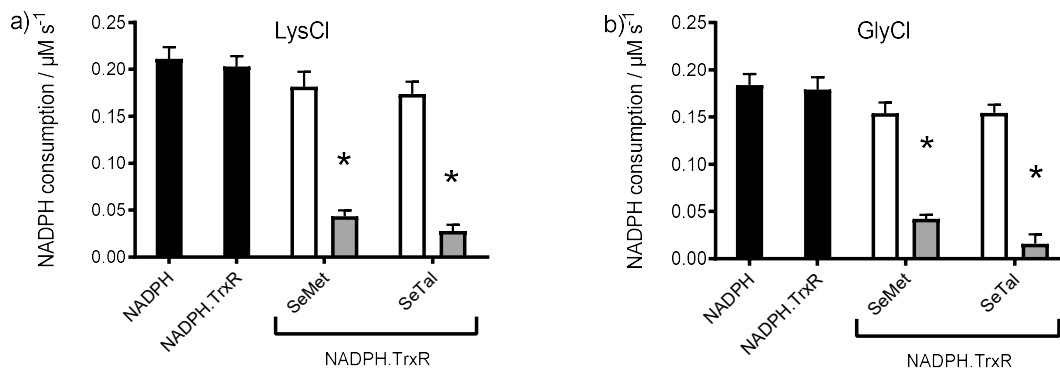
Figure S.4 – Rate of absorbance change at 340 nm after addition of LysCl and GlyCl to the TrxR system in the presence or absence of SeMet and SeTal

The initial rate of change in absorbance at 340 nm was determined over the first 15 min after (a) LysCl (200 µM) or (b) GlyCl (200 µM) was added to the TrxR (25 nM) and NADPH (700 µM) in the presence or absence of SeMet (20 µM – white bars; 200 µM grey bars) and SeTal (20 µM – white bars; 200 µM grey bars). Data represent mean ± SD of three independent experiments. * indicates significant difference (p < 0.05) from the control with no selenium compound by one-way ANOVA with Tukey's post-hoc test.
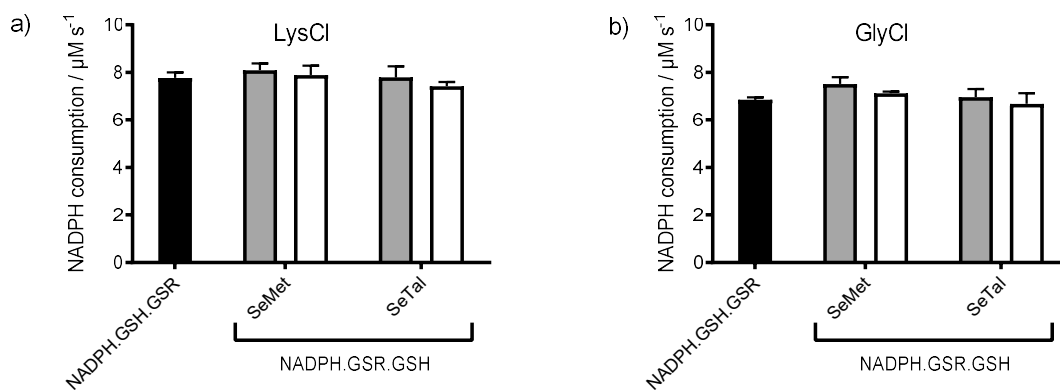


Figure S.5 – Rate of absorbance change at 340 nm after addition of LysCl and GlyCl to the GSR system in the presence or absence of SeMet and SeTal

The initial rate of change in absorbance at 340 nm was determined over the first 10 s after (a) LysCl (200 µM) or (b) GlyCl (200 µM) was added to the GSR (25 nM), GSH (400 µM) and NADPH (500 µM) in the presence or absence of SeMet (20 µM – white bars; 200 µM grey bars) and SeTal (20 µM – white bars; 200 µM grey bars). Data represent mean ± SD of three independent experiments.