Table S3. Model reactions with complex rate expressions. Reactions are listed with their associated rate expression and rate constants. Reaction numbering is continued from Table S2. Asterisks (*) denote uncertain parameter values that were varied during parametric analysis and optimization.

#	Reaction and kinetic expression	Parameters	References
151	$\mathrm{IscU} + 2\,\mathrm{Cys} \xrightarrow{IscS} \mathrm{IscU(2S)}^{2-} + 2\,\mathrm{Ala} + 2\,\mathrm{H}^{+}$ $r = \frac{k_{\mathrm{cat}}[\mathrm{IscS}][\mathrm{IscU}][\mathrm{Cys}]}{[\mathrm{IscU}][\mathrm{Cys}] + K_{\mathrm{Cys}}[\mathrm{IscU}] + K_{\mathrm{IscU}}[\mathrm{Cys}]}$	$k_{\mathrm{cat}} = 0.07\ \mathrm{s}^{-1}$ $K_{\mathrm{Cys}} = 2.7\times10^{-6}$ M * $K_{\mathrm{IscU}} = 2.6\times10^{-6}$ M *	[1][a] [1] [1,2]
152	$\mathrm{IscU([2Fe\text{-}2S])}^{2-} + 2\,\mathrm{Cys} \xrightarrow{IscS} \mathrm{IscU([2Fe\text{-}2S]\text{-}2S)}^{4-} + \mathrm{Ala} + 2\,\mathrm{H}^{+}$ $r = \frac{k_{\mathrm{cat}}[\mathrm{IscS}][\mathrm{IscU(2Fe2S)}][\mathrm{Cys}]}{[\mathrm{IscU(2Fe2S)}][\mathrm{Cys}] + K_{\mathrm{Cys}}[\mathrm{IscU(2Fe2S)}] + K_{\mathrm{IscU(2Fe2S)}}[\mathrm{Cys}]}$	$k_{\mathrm{cat}} = 0.07\ \mathrm{s}^{-1}$ $K_{\mathrm{Cys}} = 2.7\times10^{-6}$ M * $K_{\mathrm{IscU}} = 2.6\times10^{-6}$ M *	[1][a] [1] [1,2]
153	$P_{\mathrm{2Fe2S}}(apo) + \mathrm{IscU([2Fe\text{-}2S])}^{2-} + \mathrm{ATP} + \mathrm{H_2O} \xrightarrow{HscAB} \mathrm{IscU} + P_{\mathrm{2Fe2S}}(holo) + \mathrm{ADP} + \mathrm{P_i} + \mathrm{H}^{+}$ $r = \frac{k_{\mathrm{cat}}[\mathrm{IscU(2Fe2S)}][P_{\mathrm{2Fe2S}}(apo)]}{K_{P_{\mathrm{2Fe2S}}(apo)} + [P_{\mathrm{2Fe2S}}(apo)]}$	$k_{\mathrm{cat}} = 3.5\times10^{-3}\ \mathrm{s}^{-1}$ * $K_{P\mathrm{2Fe2S}(apo)} = 2.7\times10^{-5}$ M *	[3][b] [3]
154	$P_{\mathrm{2Fe2S}}(apo) + \mathrm{IscU([2Fe\text{-}2S]_2)}^{4-} + \mathrm{ATP} + \mathrm{H_2O} \xrightarrow{HscAB} \mathrm{IscU([2Fe\text{-}2S])} + P_{\mathrm{2Fe2S}}(holo) + \mathrm{ADP} + \mathrm{P_i} + \mathrm{H}^{+}$ $r = \frac{k_{\mathrm{cat}}[\mathrm{IscU(2Fe2S)_2}][P_{\mathrm{2Fe2S}}(apo)]}{K_{P_{\mathrm{2Fe2S}}(apo)} + [P_{\mathrm{2Fe2S}}(apo)]}$	$k_{\mathrm{cat}} = 3.5\times10^{-3}\ \mathrm{s}^{-1}$ * $K_{P\mathrm{2Fe2S}(apo)} = 2.7\times10^{-5}$ M *	[3][b,c] [3]
155	$\mathrm{DNA(dX)} + \mathrm{H_2O} \xrightarrow{AlkA} \mathrm{DNA(AP_G)} + \mathrm{X}$ $r = \frac{k_{\mathrm{cat}}[\mathrm{AlkA}][\mathrm{DNA(dX)}]}{K_{\mathrm{DNA(dX)}} + [\mathrm{DNA(dX)}]}$	$k_{\mathrm{cat}} = 4.0\times10^{-4}\ \mathrm{s}^{-1}$ $K_{\mathrm{DNA(dX)}} = 5.3\times10^{-8}$ M *	[4][d] [4]
156	$\mathrm{DNA(dI)} + \mathrm{H_2O} \xrightarrow{AlkA} \mathrm{DNA(AP_A)} + \mathrm{hX}$ $r = \frac{k_{\mathrm{cat}}[\mathrm{AlkA}][\mathrm{DNA(dI)}]}{K_{\mathrm{DNA(dI)}} + [\mathrm{DNA(dI)}]}$	$k_{\mathrm{cat}} = 1.3\times10^{-3}\ \mathrm{s}^{-1}$ $K_{\mathrm{DNA(dI)}} = 4.2\times10^{-8}$ M *	[5] [5]

157	$DNA(dU) + H_2O \xrightarrow{Ung} DNA(AP_C) + U$ $$r = \frac{k_{cat}[Ung][DNA(dU)]}{K_{DNA(dU)} + [DNA(dU)]}$$	$k_{cat} = 0.5\ s^{-1}$ $K_{DNA(dU)} = 2.78 \times 10^{-7}$ M *	[6] [6,7][e]
158	$DNA(AP_G) + 2\ H_2O \xrightarrow{Xth} DNA(dG)_{gap} + 2\ H^+ + dR5P$ $$r = \frac{k_{cat}[Xth][DNA(AP_G)]}{K_{DNA(AP_G)} + [DNA(AP_G)]}$$	$k_{cat} = 0.23\ s^{-1}$ $K_{DNA(APG)} = 1.6 \times 10^{-8}$ M	[8][f] [8]
159	$DNA(AP_A) + 2\ H_2O \xrightarrow{Xth} DNA(dA)_{gap} + 2\ H^+ + dR5P$ $$r = \frac{k_{cat}[Xth][DNA(AP_A)]}{K_{DNA(AP_A)} + [DNA(AP_A)]}$$	$k_{cat} = 0.23\ s^{-1}$ $K_{DNA(APA)} = 1.6 \times 10^{-8}$ M	[8][f] [8]
160	$DNA(AP_C) + 2\ H_2O \xrightarrow{Xth} DNA(dC)_{gap} + 2\ H^+ + dR5P$ $$r = \frac{k_{cat}[Xth][DNA(AP_C)]}{K_{DNA(AP_C)} + [DNA(AP_C)]}$$	$k_{cat} = 0.23\ s^{-1}$ $K_{DNA(APC)} = 1.6 \times 10^{-8}$ M	[8][f] [8]
161	$DNA(dG)_{gap} + dGTP \xrightarrow{PolI} DNA(dG)_{nick} + PP_i$ $$r = \frac{k_{cat}[PolI][dGTP][DNA(dG)_{gap}]}{K_{i,DNA(dG)_{gap}} K_{dGTP} + K_{DNA(dG)_{gap}}[dGTP] + K_{dGTP}[DNA(dG)_{gap}]\left(1 + \frac{K_{i,DNA(dG)_{gap}}}{K_{i,DNA(dG)_{nick}}}\right) + [DNA(dG)_{gap}][dGTP]\left(1 + \frac{K_{DNA(dG)_{gap}}}{K_{i,DNA(dG)_{nick}}}\right)}$$	$k_{cat} = 14\ s^{-1}$ $K_{DNA(dG)gap} = 5.4 \times 10^{-9}$ M $K_{i,DNA(dG)gap} = 8.1 \times 10^{-9}$ M $K_{i,DNA(dG)nick} = 2.2 \times 10^{-8}$ M $K_{dGTP} = 1.3 \times 10^{-6}$ M	[9][g] [9] [9] [9] [10][h]
162	$DNA(dA)_{gap} + dATP \xrightarrow{PolI} DNA(dA)_{nick} + PP_i$ $$r = \frac{k_{cat}[PolI][dATP][DNA(dA)_{gap}]}{K_{i,DNA(dA)_{gap}} K_{dATP} + K_{DNA(dA)_{gap}}[dATP] + K_{dATP}[DNA(dA)_{gap}]\left(1 + \frac{K_{i,DNA(dA)_{gap}}}{K_{i,DNA(dA)_{nick}}}\right) + [DNA(dA)_{gap}][dATP]\left(1 + \frac{K_{DNA(dA)_{gap}}}{K_{i,DNA(dA)_{nick}}}\right)}$$	$k_{cat} = 14\ s^{-1}$ $K_{DNA(dA)gap} = 5.4 \times 10^{-9}$ M $K_{i,DNA(dA)gap} = 8.1 \times 10^{-9}$ M $K_{i,DNA(dA)nick} = 2.2 \times 10^{-8}$ M $K_{dATP} = 3.7 \times 10^{-6}$ M	[9][g] [9] [9] [9] [10][h]

163	$DNA(dC)_{gap} + dCTP \xrightarrow{PolI} DNA(dC)_{nick} + PP_i$ $$r = \frac{k_{cat}[PolI][dCTP][DNA(dC)_{gap}]}{K_{i,DNA(dC)_{gap}} K_{dCTP} + K_{DNA(dC)_{gap}}[dCTP] + K_{dCTP}[DNA(dC)_{gap}]\left(1+\frac{K_{i,DNA(dC)_{gap}}}{K_{i,DNA(dC)_{nick}}}\right) + [DNA(dC)_{gap}][dCTP]\left(1+\frac{K_{DNA(dC)_{gap}}}{K_{i,DNA(dC)_{nick}}}\right)}$$	$k_{cat} = 14\ s^{-1}$ $K_{DNA(dC)gap} = 5.4\times10^{-9}$ M $K_{i,DNA(dC)gap} = 8.1\times10^{-9}$ M $K_{i,DNA(dC)nick} = 2.2\times10^{-8}$ M $K_{dCTP} = 2.1\times10^{-6}$ M	[9] [g] [9] [9] [9] [10] [h]
164	$DNA(dG)_{nick} + NAD^+ \xrightarrow{LigA} DNA(dG) + AMP + NMN + H^+$ $$r = \frac{k_{cat}[LigA][DNA(dG)_{nick}][NAD^+]}{[DNA(dG)_{nick}][NAD^+] + K_{NAD^+}[DNA(dG)_{nick}] + K_{DNA(dG)_{nick}}[NAD^+]}$$	$k_{cat} = 0.023\ s^{-1}$ $K_{NAD+} = 7.0\times10^{-6}$ M $K_{DNA(dG)nick} = 5.0\times10^{-8}$ M	[11] [i] [11] [11]
165	$DNA(dA)_{nick} + NAD^+ \xrightarrow{LigA} DNA(dA) + AMP + NMN + H^+$ $$r = \frac{k_{cat}[LigA][DNA(dA)_{nick}][NAD^+]}{[DNA(dA)_{nick}][NAD^+] + K_{NAD^+}[DNA(dA)_{nick}] + K_{DNA(dA)_{nick}}[NAD^+]}$$	$k_{cat} = 0.023\ s^{-1}$ $K_{NAD+} = 7.0\times10^{-6}$ M $K_{DNA(dA)nick} = 5.0\times10^{-8}$ M	[11] [i] [11] [11]
166	$DNA(dC)_{nick} + NAD^+ \xrightarrow{LigA} DNA(dC) + AMP + NMN + H^+$ $$r = \frac{k_{cat}[LigA][DNA(dC)_{nick}][NAD^+]}{[DNA(dC)_{nick}][NAD^+] + K_{NAD^+}[DNA(dC)_{nick}] + K_{DNA(dC)_{nick}}[NAD^+]}$$	$k_{cat} = 0.023\ s^{-1}$ $K_{NAD+} = 7.0\times10^{-6}$ M $K_{DNA(dC)nick} = 5.0\times10^{-8}$ M	[11] [i] [11] [11]
167	$GSNO + 2\ NADH + 2\ H^+ + GSH \xrightarrow{GSFDH} GSSG + NH_3 + H_2O + 2\ NAD^+$ $$r = \frac{k_{cat}[GSFDH][GSNO]}{K_{GSNO} + [GSNO]}$$	$k_{cat} = 3.1\ s^{-1}$ $K_{GSNO} = 7.4\times10^{-4}$ M	[12] [j] [12]
168	$GSSG + H^+ + NADPH \xrightarrow{Gor} 2\ GSH + NADP^+$ $$r = \frac{k_1[Gor][GSSG][NADPH] + k_2[Gor][GSSG]^2[NADPH]}{K_{NADPH}[GSSG] + K_{GSSG}[NADPH] + [GSSG][NADPH] + K_1[GSSG]^2 + K_2[GSSG]^2[NADPH]}$$	$k_1 = 267\ s^{-1}$ $k_2 = 6.55\times10^5\ M^{-1}s^{-1}$ $K_{NADPH} = 2.2\times10^{-5}$ M $K_{GSSG} = 9.7\times10^{-5}$ M $K_1 = 0.022$ $K_2 = 3.9\times10^3\ M^{-1}$	[13] [k] [14] [13] [13] [14] [14]

169	$Trx_{ox} + NADPH + H^+ \xrightarrow{TrxR} Trx_{red} + NADP^+$ $$r = \frac{k_{cat}[TrxR][Trx_{ox}][NADPH]}{[Trx_{ox}][NADPH] + K_{NADPH}[Trx_{ox}] + K_{Trx_{ox}}[NADPH]}$$	$k_{cat} = 41.25\ s^{-1}$ $K_{NADPH} = 4.6\times10^{-6}$ M $K_{Trxox} = 1.7\times10^{-6}$ M	[15][l] [15] [15]
170	$Trx_{red} + GSNO \rightarrow Trx_{ox} + HNO + GSH$ $$r = \frac{k_{cat}[Trx_{red}][GSNO]}{K_{GSNO} + [GSNO]}$$	$k_{cat} = 0.02\ s^{-1}$ $K_{GSNO} = 1.0\times10^{-5}$ M	[16] [16]
171	Cyo + NO• ⇌ Cyo(NO) $$r = \frac{k_{on,NO\bullet}[NO^\bullet][Cyo]}{1 + \frac{[O_2]}{K_{O_2}}} - k_{off,NO\bullet}[Cyo(NO)]$$	$k_{on,NO\bullet} = 6.8\times10^{6}\ M^{-1}s^{-1}$ $k_{off,NO\bullet} = 0.03\ s^{-1}$ $K_{\bullet} = 6.05\times10^{-6}$ M $K_{d,NO\bullet} = 4.4\times10^{-9}$ M	[17] [m] [17] [17] [17]
172	Cyd + NO• ⇌ Cyd(NO) $$r = \frac{k_{on,NO\bullet}[NO^\bullet][Cyd]}{1 + \frac{[O_2]}{K_{O_2}}} - k_{off,NO\bullet}[Cyd(NO)]$$	$k_{on,NO\bullet} = 3.8\times10^{8}\ M^{-1}s^{-1}$ $k_{off,NO\bullet} = 0.163\ s^{-1}$ $K_{O2} = 2.7\times10^{-7}$ M $K_{d,NO\bullet} = 5.5\times10^{-10}$ M	[17] [m] [17] [17] [17]
173	$NorV_{ox} + NADH \rightarrow NorV_{red} + NAD^+ + H^+$ $$r = \frac{k_{cat}[NorV_{ox}][NADH]}{1 + \frac{[NO^\bullet]}{K_{i,NO\bullet}}}$$	$k_{cat} = 5.5\times10^{6}\ M^{-1}s^{-1}$ $K_{i,NO\bullet} = 1.35\times10^{-5}$ M	[18][n] [19][o]
174	$NorV_{red} + 2\ NO\bullet + 2\ H^+ \rightarrow NorV_{ox} + N_2O + H_2O$ $$r = \frac{k_{cat}[NorV_{red}][NO^\bullet]}{K_{NO\bullet} + [NO^\bullet]}$$	$k_{cat} = 7.45\ s^{-1}$ $K_{NO\bullet} = 1.2\times10^{-6}$ M	[20][p] [21]

175	$NO\bullet + 6\ H^+ + 2.5\ NADH \rightarrow NH_4^+ + H_2O + 2.5\ NAD^+ + 2.5\ H^+$ $$r = \frac{k_{cat}[\mathrm{NrfA}][\mathrm{NO}^\bullet]}{K_{\mathrm{NO}\bullet} + [\mathrm{NO}^\bullet]}$$	$k_{cat} = 390\ s^{-1}$ $K_{NO\bullet} = 3.0 \times 10^{-4}$ M	[22][q] [23][r]
176	$O_{2,air} \rightleftharpoons O_{2,culture}$ $$r = k_L a_{O_2}\left([\mathrm{O_2}]_{sat} - [\mathrm{O_2}]\right)$$	$k_L a_{O2} = 1.36 \times 10^3\ s^{-1}$	*s*
177	$\rightarrow Hmp_{FAD,Fe3}$ $$r = \frac{k_{\mathrm{Hmp\text{-}exp,max}}[\mathrm{NO}^\bullet]}{[\mathrm{NO}^\bullet] + K_{\mathrm{Hmp\text{-}exp,NO}\bullet}}$$	$k_{Hmp\text{-}exp,max}$ $= 1.93 \times 10^{-8}\ M{\cdot}s^{-1}$ * $K_{Hmp\text{-}exp,NO\bullet}$ $= 3.38 \times 10^{-7}$M *	*t*
178	$\rightarrow NorV_{ox}$ $$r = \frac{k_{\mathrm{NorV\text{-}exp,max}}[\mathrm{NO}^\bullet]}{[\mathrm{NO}^\bullet] + K_{\mathrm{NorV\text{-}exp,NO}\bullet}}$$	$k_{NorV\text{-}exp,max}$ $= 6.81 \times 10^{-9}\ M{\cdot}s^{-1}$ * $K_{NorV\text{-}exp,NO\bullet}$ $= 9.41 \times 10^{-6}$ M *	*t*
179	$\rightarrow$ NrfA $$r = \frac{k_{\mathrm{NrfA\text{-}exp,max}}[\mathrm{NO_2^-}]}{[\mathrm{NO_2^-}] + K_{\mathrm{NrfA\text{-}exp,NO_2^-}}\left(1 + \frac{[\mathrm{O_2}]}{K_{\mathrm{NrfA\text{-}exp,O_2}}}\right)}$$	$k_{NrfA\text{-}exp,max}$ $= 7.72 \times 10^{-9}\ M{\cdot}s^{-1}$ * $K_{NrfA\text{-}exp,NO2-}$ $= 9.32 \times 10^{-4}$ M * $K_{NrfA\text{-}exp,O2}$ $= 3.45 \times 10^{-11}$ M *	*t*

a. Literature k_{cat} is per mol cysteine; value shown has been halved according to the stoichiometry used.

b. Rate constants shown are for the reaction in the absence of the HscAB chaperone system. When present, the chaperone system has been shown to increase the [Fe-S] cluster transfer rate by approximately 10-fold [24].

c. [2Fe-2S] cluster transfer to an apoprotein was assumed to occur with both [2Fe-2S] and 2×[2Fe-2S]-loaded forms of IscU, and at similar rates.

d. The k_{cat} was calculated from the reported V_{max} by dividing by the concentration of AlkA enzyme used in the assay (300 fmol per 10 µl, or 30 nM).

e. The Michaelis constant for the deaminated base ($K_{DNA(dU)}$) was calculated from the constants associated with binding and unbinding (k_1 and k_{-1}, respectively) of the enzyme to the DNA strand [7], and the reported k_{cat} value [6], assuming intermediate enzyme complexes are in rapid equilibrium: $K_{DNA(dU)} = (k_{cat} + k_{-1})/k_1$.

f. Kinetics constants are for the rate of excision of deoxyribose (regular AP site) in oligonucleotides by Xth. For the reaction, we assumed the AP site and adjacent phosphate were removed in a single step to release 5dRP. The rate was also assumed to be independent of the base removed to form the AP site.

g. The rate expression was obtained from [9]. $K_{DNA(dN)gap}$ is the constant associated with the damaged DNA binding as a substrate, $K_{i,DNA(dN)gap}$ is the substrate inhibition constant for the damaged DNA, and $K_{i,DNA(dN)nick}$ is the constant describing product inhibition by the repaired DNA (where N = A, C, or G).

h. K_{dNTP} is the average of the two values reported for base re-insertion into two different types of template DNA strands.

i. Based on the reported reaction mechanism [11], we assumed ping-pong kinetics, and therefore used the corresponding form of the rate equation. The rate constants were also assumed to be independent of the nucleotides adjacent to the backbone nick. A proton (H^+) was added to the products of the reported reaction to balance stoichiometry.

j. The rate constants were approximated from Figure 1b in [12].

k. The rate expression was obtained from literature [14]. Values for rate constants k_2, K_1, and K_2 are for glutathione reductase in rat liver [14], while k_1, K_{NADPH}, and K_{GSSG} were measured for the *E. coli* enzyme [13].

l. Ping-pong kinetics were assumed based on the report of ping-pong behavior for human placenta thioredoxin reductase [25].

m. Reversible binding of NO• to Cyo and Cyd was modeled as following Michaelis-Menten behavior. Due to normal respiration activity (consumption of O_2), the effective enzyme concentration will be reduced. This was taken into account by adding a competitive inhibition term to the denominator, as O_2 and NO• are competing for the same active site.

n. Reported rate constant was measured at 5°C.

o. NorV is inhibited upon binding of NO• to its oxidized form. The inhibition rate constant shown is for the NO• reductase of *Paracoccus denitrificans*.

p. Literature k_{cat} is per mol NO•; value shown has been halved according to the stoichiometry used.

q. k_{cat} is reported to range from 30 to 1000 s^{-1} [22].

r. $K_{NO•}$ value was measured at 4°C.

s. The oxygen mass transfer coefficient ($k_L a_{O2}$) was measured in our experimental system (see Figure S12 and Text S1).

t. Parameters governing enzyme expression were determined via parameter optimization with experimentally measured [NO•] curves for aerobic, wild-type *E. coli* cultures dosed with 0.5 mM DPTA (see Table S4 and Text S1).

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