Table S4. Optimized cellular parameters. Parameters were allowed to vary between "Min." and "Max." values obtained or approximated from literature. "Reaction #s" are the reactions associated with each rate parameter, with numbering corresponding to that in the model [1]. "Optimal" are optimized parameter values, and are only shown for parameters found to significantly affect the SSR between simulated and measured [NO•] and [O_2] curves for *E. coli* treated with 500 μM DPTA. "Prev. Opt." are the optimal values for significant parameters obtained in our previous study [1]. Dashed lines (--) in the "Optimal" and "Prev. Opt." columns indicate parameters found to have negligible effect on the SSR.

#	Parameter	Parameter description/reaction involved	Reaction #s	Min.	Max.	Optimal	Prev. Opt.	Units	Ref.
1	$k_{NO•-[Fe-S]}$	[Fe-S] nitrosylation by NO•	85,86	1.0×10^{4}	1.0×10^{8}	9.51×10^{7}	--	$M^{-2}s^{-1}$	[2]
2	$k_{DNIC-rem}$	DNIC removal from protein	87,89	1	100	62.7	--	$M^{-1}s^{-1}$	[3]
3	$k_{DNIC-bind}$	DNIC binding to apoprotein	88,90	1	100	--	--	$M^{-1}s^{-1}$	[3]
4	$k_{DNIC-deg}$	O_2-mediated DNIC degradation	91	0.1	100	--	--	$M^{-1}s^{-1}$	[4]
5	$k_{IscU-load-Fe}$	IscA-mediated Fe^{2+} transfer to IscU	92,93	2.5×10^{-3}	2.5	0.36	--	s^{-1}	[5]
6	$K_{IscU-load-S,Cys}$	IscS-mediated S transfer from Cys to IscU	151,152	1.0×10^{-6}	1.0×10^{-4}	--	--	M	[6]
7	$K_{IscU-load-S,IscU}$	IscS-mediated S transfer from Cys to IscU	151,152	1.0×10^{-6}	1.0×10^{-4}	1.55×10^{-5}	--	M	[6,7]
8	$k_{IscU-2Fe2S-insert,cat}$	IscU-mediated [2Fe-2S] insertion into apoprotein	153,154	1.0×10^{-4}	0.1	1.08×10^{-2}	--	s^{-1}	[8]
9	$K_{IscU-2Fe2S-insert,P2Fe2S(apo)}$	IscU-mediated [2Fe-2S] insertion into apoprotein	153,154	1.0×10^{-6}	1.0×10^{-4}	--	--	M	[8]
10	$k_{IscU-4Fe4S-insert}$	IscU-mediated [4Fe-4S] insertion into apoprotein	94	1	500	6.12	--	$M^{-1}s^{-1}$	[9]
11	$k_{dN-deam}$	N_2O_3-mediated DNA base deamination	95–97	1.0×10^{3}	1.0×10^{6}	--	--	$M^{-1}s^{-1}$	[10]
12	$K_{dX-excis,DNA(dX)}$	Excision of xanthine from DNA	155	1.0×10^{-8}	1.0×10^{-6}	--	--	M	[11]
13	$K_{dI-excis,DNA(dI)}$	Excision of hypoxanthine from DNA	156	1.0×10^{-8}	1.0×10^{-6}	--	--	M	[12]
14	$K_{dU-excis,DNA(dU)}$	Excision of uracil from DNA	157	1.0×10^{-8}	1.0×10^{-6}	--	--	M	[13]
15	$k_{Hmp,NO•-on}$	Hmp detoxification; NO• binding to Hmp-Fe^{2+}	110,113,118	4.0×10^{6}	2.6×10^{7}	8.19×10^{6}	4.13×10^{6}	$M^{-1}s^{-1}$	[14]
16	$k_{Hmp,NO•-ox}$	Hmp detoxification; NO• binding to Hmp-Fe^{2+}-O_2	103,108,125	9.6×10^{8}	2.4×10^{9}	--	--	$M^{-1}s^{-1}$	[14]
17	$k_{Hmp-exp,max}$	Hmp expression (maximum rate)	177	2.0×10^{-10}	2.0×10^{-8}	1.73×10^{-8}	1.93×10^{-8}	$M \cdot s^{-1}$	*a*
18	$K_{Hmp-exp,NO•}$	Hmp expression (regulatory NO• interaction)	177	1.0×10^{-8}	1.0×10^{-5}	1.72×10^{-6}	3.38×10^{-7}	M	*b*
19	$k_{NorV-exp,max}$	NorV expression (maximum rate)	178	2.0×10^{-10}	2.0×10^{-8}	--	--	$M \cdot s^{-1}$	*a*
20	$K_{NorV-exp,NO•}$	NorV expression (regulatory NO• interaction)	178	1.0×10^{-8}	1.0×10^{-5}	--	--	M	*b*
21	$k_{NorV-O2}$	O_2-mediated NorV inactivation	146,147	10	1000	849	549	$M^{-1}s^{-1}$	[15]
22	$k_{NrfA-exp,max}$	NrfA expression (maximum rate)	179	2.0×10^{-10}	2.0×10^{-8}	--	--	$M \cdot s^{-1}$	*a*
23	$K_{NrfA-exp,NO2-}$	NrfA expression (regulatory NO_2^- interaction)	179	1.0×10^{-6}	1.0×10^{-3}	--	--	M	*c*
24	$K_{NrfA-exp,O2}$	NrfA expression (regulatory O_2 interaction)	179	1.0×10^{-12}	1.0×10^{-10}	--	--	M	*c*
25	$[Cys]_0$	Initial concentration of cysteine	--	5.0×10^{-5}	2.0×10^{-4}	--	--	M	[16,17]
26	$[Trx_{red}]_0$	Initial concentration of reduced thioredoxin	--	5.0×10^{-6}	5.0×10^{-5}	--	--	M	[18,19]
27	$[IscU]_0$	Initial concentration of IscU	--	1.0×10^{-8}	1.0×10^{-5}	8.30×10^{-6}	--	M	[6,20]
28	$[IscS]_0$	Initial concentration of IscS	--	1.0×10^{-8}	1.0×10^{-5}	7.60×10^{-6}	--	M	[6,20]
29	$[P_{2Fe2S}(holo)]_0$	Initial concentration of *holo* [2Fe-2S] proteins	--	1.0×10^{-6}	1.0×10^{-4}	8.29×10^{-5}	--	M	[21,22]
30	$[P_{4Fe4S}(holo)]_0$	Initial concentration of *holo* [4Fe-4S] proteins	--	5.0×10^{-5}	5.0×10^{-4}	4.82×10^{-4}	--	M	[21,22]
31	$[LigA]_0$	Initial concentration of DNA ligase	--	1.0×10^{-8}	1.0×10^{-5}	--	--	M	[23]
32	$[PolI]_0$	Initial concentration of DNA polymerase	--	1.0×10^{-8}	1.0×10^{-5}	--	--	M	[23]
33	$[DNA(dN)]_0$	Initial concentration of DNA bases (dA,dC,dG)	--	0.001	0.1	--	--	M	[22]
34	$[Xth]_0$	Initial concentration of DNA exonuclease III	--	1.0×10^{-9}	1.0×10^{-6}	--	--	M	[24]
35	$[GS-FDH]_0$	Initial concentration of GSH-dependent FDH	--	1.0×10^{-8}	1.0×10^{-5}	--	--	M	[24]
36	$[AlkA]_0$	Initial concentration of DNA glycosylase (dX, dI)	--	1.0×10^{-9}	1.0×10^{-6}	--	--	M	[24]
37	$[Ung]_0$	Initial concentration of DNA glycosylase (dU)	--	1.0×10^{-9}	1.0×10^{-6}	--	--	M	[24]

a. The bounds of Hmp, NorV, and NrfA maximum expression rates were chosen based on those reported for various enzymes in [25]. Values were converted from $g_{protein}/g_{DW} \cdot s$ to $M \cdot s^{-1}$ assuming a cell density of 448 gDW/L [22], and ranged from 2×10^{-10} (Acs) to 2×10^{-8} $M \cdot s^{-1}$ (PfkA).

b. The NO• binding constant describing Hmp and NorV expression was varied in the nM to μM range based on reported physiological concentrations of NO• [26,27].
c. The NO_2^- binding constant describing NrfA expression was varied in the μM range, and the O_2 inhibition term was assumed to be much lower, as NrfA expression is primarily anaerobic [28,29].

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