

Table S1. Respiration reactions, rate expressions, and associated kinetic parameters added to the model. Reaction numbers are continued from the existing set of 179 model reactions [1].

#	Reaction stoichiometry and rate equation	Parameters	References
180 ^a	$\text{O}_2 + 2 \text{Q}_8\text{H}_2 \xrightarrow{\text{Cyo}} 2 \text{H}_2\text{O} + 2 \text{Q}_8$ $r = \frac{k_{\text{cat}} [\text{Cyo}][\text{O}_2][\text{Q}_8\text{H}_2]^2}{K_{\text{iq1}}K_{\text{mq2}}[\text{O}_2] + K_{\text{Q}_8\text{H}_2}[\text{Q}_8\text{H}_2][\text{O}_2] + K_{\text{O}_2}[\text{Q}_8\text{H}_2]^2 + [\text{Q}_8\text{H}_2]^2[\text{O}_2]}$	$k_{\text{cat}} = 18.3 \text{ to } 150 \text{ s}^{-1}$ $K_{\text{iq1}}K_{\text{mq2}} = 2.13 \times 10^{-10} \text{ M}^2$ $K_{\text{Q}_8\text{H}_2} = 5.3 \times 10^{-5} \text{ M}$ $K_{\text{O}_2} = 6.05 \times 10^{-6} \text{ M}$	[2-4] [5] ^d [6] [2]
181	$\text{O}_2 + 2 \text{Q}_8\text{H}_2 \xrightarrow{\text{Cyd}} 2 \text{H}_2\text{O} + 2 \text{Q}_8$ $r = \frac{k_{\text{cat}} [\text{Cyd}][\text{O}_2][\text{Q}_8\text{H}_2]^2}{K_{\text{iq1}}K_{\text{mq2}}[\text{O}_2] + K_{\text{Q}_8\text{H}_2}[\text{Q}_8\text{H}_2][\text{O}_2] + K_{\text{O}_2}[\text{Q}_8\text{H}_2]^2 + [\text{Q}_8\text{H}_2]^2[\text{O}_2]}$	$k_{\text{cat}} = 12 \text{ to } 469 \text{ s}^{-1}$ $K_{\text{iq1}}K_{\text{mq2}} = 2.13 \times 10^{-10} \text{ M}^2$ $K_{\text{Q}_8\text{H}_2} = 4.2 \times 10^{-5} \text{ M}$ $K_{\text{O}_2} = 2.7 \times 10^{-7} \text{ M}$	[2,4,5] [5] [5] [2]
182 ^{b,c}	$\text{NADH} + \text{Q}_8 + \text{H}^+ \xrightarrow{\text{NDH-1}} \text{NAD}^+ + \text{Q}_8\text{H}_2$ $r = \left(\frac{P_{2\text{Fe}2\text{S}}(\text{holo}) + P_{4\text{Fe}4\text{S}}(\text{holo})}{P_{\text{FeS,TOT}}} \right) \left(\frac{k_{\text{cat}} [\text{NDH1}][\text{Q}_8][\text{NADH}]}{K_{\text{NADH}}K_{\text{d,Q}_8} + K_{\text{NADH}}[\text{Q}_8] + K_{\text{m,Q}_8}[\text{NADH}] + [\text{Q}_8][\text{NADH}]} \right)$ <p>where:</p> $P_{\text{FeS,TOT}} = P_{2\text{Fe}2\text{S}}(\text{holo}) + P_{4\text{Fe}4\text{S}}(\text{holo}) + P_{2\text{Fe}2\text{S}}(\text{DNIC})_2 + P_{4\text{Fe}4\text{S}}(\text{RRE})_2 + P_{2\text{Fe}2\text{S}}(\text{apo}) + P_{4\text{Fe}4\text{S}}(\text{apo})$	$k_{\text{cat}} = 50 \text{ to } 600 \text{ s}^{-1}$ $K_{\text{NADH}} = 7.2 \times 10^{-6} \text{ M}$ $K_{\text{d,Q}_8} = 3.0 \times 10^{-5} \text{ M}$ $K_{\text{m,Q}_8} = 3.0 \times 10^{-5} \text{ M}$	[7,8] [7] [9] ^e [9]
183 ^c	$\text{NADH} + \text{Q}_8 + \text{H}^+ \xrightarrow{\text{NDH-2}} \text{NAD}^+ + \text{Q}_8\text{H}_2$ $r = \left(\frac{k_{\text{cat}} [\text{NDH2}][\text{Q}_8][\text{NADH}]}{K_{\text{NADH}}K_{\text{d,Q}_8} + K_{\text{NADH}}[\text{Q}_8] + K_{\text{m,Q}_8}[\text{NADH}] + [\text{Q}_8][\text{NADH}]} \right)$	$k_{\text{cat}} = 17.1 \text{ to } 474 \text{ s}^{-1}$ $K_{\text{NADH}} = 5.7 \times 10^{-5} \text{ M}$ $K_{\text{d,Q}_8} = 5.9 \times 10^{-6} \text{ M}$ $K_{\text{m,Q}_8} = 5.9 \times 10^{-6} \text{ M}$	[10,11] ^f [10] [12] ^e [12]

a. Cytochrome *bo* quinol oxidation was assumed to proceed via a mechanism involving a ternary complex, as is reported for cytochrome *bd* [5].

b. The rate of NDH-1 was scaled by the ratio of undamaged [Fe-S] clusters to total [Fe-S] clusters to account for potential NO•-mediated inhibition of NDH-1 activity through nitrosylation of its [Fe-S] clusters.

c. The NDH-1 and NDH-2 rate equations are modeled following a sequential mechanism [13].

d. The $K_{\text{iq1}}K_{\text{mq2}}$ value for cytochrome *bo* was assumed to be equal to that of cytochrome *bd*.

e. The $K_{\text{d,Q}_8}$ values for NDH-1 and NDH-2 were assumed to be equal to that of their $K_{\text{m,Q}_8}$ values.

f. The literature NDH-2 k_{cat} values were reported in units of $\mu\text{mol NADH/mg protein/min}$ [10,11], and were converted to units of s^{-1} via multiplication by the molecular weight of NDH-2, reported as 47.359 kDa based on its nucleotide sequence [14].

References

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