

Table S3. Ordinary Differential Equations for each of the kinetic reaction used in four models.

$$\begin{aligned}
 \frac{d([Met] \cdot V_{cell})}{d t} &= -V_{cell} \cdot \left(\frac{V_{(SAMsyn)} \cdot [Met]^{h_{(SAMsyn)}}}{Shalve_{(SAMsyn)}^{h_{(SAMsyn)}} + [Met]^{h_{(SAMsyn)}}} \right) \\
 \frac{d([SAM] \cdot V_{cell})}{d t} &= +V_{cell} \cdot \left(\frac{V_{(SAMsyn)} \cdot [Met]^{h_{(SAMsyn)}}}{Shalve_{(SAMsyn)}^{h_{(SAMsyn)}} + [Met]^{h_{(SAMsyn)}}} \right) \\
 &\quad - V_{cell} \cdot \left(\frac{V_{(SAMdc)} \cdot [SAM]}{Km_{(SAMdc)} + [SAM]} \right) \\
 \frac{d([dcSAM] \cdot V_{cell})}{d t} &= +V_{cell} \cdot \left(\frac{V_{(SAMdc)} \cdot [SAM]}{Km_{(SAMdc)} + [SAM]} \right) \\
 &\quad - V_{cell} \cdot \left(\frac{VmPut_{(SpdS)} \cdot [Put] \cdot [dcSAM]}{KmdcSAM_{(SpdS)} \cdot [Put] + KmPut_{(SpdS)} \cdot [dcSAM] + [Put] \cdot [dcSAM] + KddcSAM_{(SpdS)} \cdot KmPut_{(SpdS)}} \right) \\
 \frac{d([Arg] \cdot V_{cell})}{d t} &= -V_{cell} \cdot \left(\frac{V_{(Arginase)} \cdot [Arg]}{Km_{(Arginase)} + [Arg]} \right) \\
 \frac{d([Orn] \cdot V_{cell})}{d t} &= +V_{cell} \cdot \left(\frac{V_{(Arginase)} \cdot [Arg]}{Km_{(Arginase)} + [Arg]} \right) \\
 &\quad - V_{cell} \cdot \left(\frac{V_{(ODC)} \cdot [Orn]}{Km_{(ODC)} + [Orn]} \right) \\
 \frac{d([Put] \cdot V_{cell})}{d t} &= +V_{cell} \cdot \left(\frac{V_{(ODC)} \cdot [Orn]}{Km_{(ODC)} + [Orn]} \right) \\
 &\quad - V_{cell} \cdot \left(\frac{VmPut_{(SpdS)} \cdot [Put] \cdot [dcSAM]}{KmdcSAM_{(SpdS)} \cdot [Put] + KmPut_{(SpdS)} \cdot [dcSAM] + [Put] \cdot [dcSAM] + KddcSAM_{(SpdS)} \cdot KmPut_{(SpdS)}} \right) \\
 \frac{d([Spd] \cdot V_{cell})}{d t} &= +V_{cell} \cdot \left(\frac{VmPut_{(SpdS)} \cdot [Put] \cdot [dcSAM]}{KmdcSAM_{(SpdS)} \cdot [Put] + KmPut_{(SpdS)} \cdot [dcSAM] + [Put] \cdot [dcSAM] + KddcSAM_{(SpdS)} \cdot KmPut_{(SpdS)}} \right) \\
 &\quad - V_{cell} \cdot \left(\frac{vmax_{(TryS1)} \cdot [Spd] \cdot [GSH]}{Kma_{(TryS1)} \cdot Kmb_{(TryS1)} + [Spd] \cdot Kmb_{(TryS1)} + [GSH] \cdot Kma_{(TryS1)} + [Spd] \cdot [GSH]} \right) \\
 \frac{d([Cys] \cdot V_{cell})}{d t} &= -V_{cell} \cdot \left(\frac{Vm_{(yECS)} \cdot [Cys] \cdot [Glu]}{Km2_{(yECS)} \cdot [Cys] + Km1_{(yECS)} \cdot [Glu] + [Cys] \cdot [Glu] + kd1_{(yECS)} \cdot Km2_{(yECS)}} \right) \\
 \frac{d([Glu] \cdot V_{cell})}{d t} &= -V_{cell} \cdot \left(\frac{Vm_{(yECS)} \cdot [Cys] \cdot [Glu]}{Km2_{(yECS)} \cdot [Cys] + Km1_{(yECS)} \cdot [Glu] + [Cys] \cdot [Glu] + kd1_{(yECS)} \cdot Km2_{(yECS)}} \right) \\
 \frac{d([GluCys] \cdot V_{cell})}{d t} &= +V_{cell} \cdot \left(\frac{Vm_{(yECS)} \cdot [Cys] \cdot [Glu]}{Km2_{(yECS)} \cdot [Cys] + Km1_{(yECS)} \cdot [Glu] + [Cys] \cdot [Glu] + kd1_{(yECS)} \cdot Km2_{(yECS)}} \right) \\
 &\quad - V_{cell} \cdot \left(\frac{Vm_{(GS)} \cdot [Gly] \cdot [GluCys]}{Km2_{(GS)} \cdot [Gly] + Km1_{(GS)} \cdot [GluCys] + [Gly] \cdot [GluCys] + kd1_{(GS)} \cdot Km2_{(GS)}} \right)
 \end{aligned}$$

$$\begin{aligned}
& \frac{d([\text{GSH}] \cdot V_{\text{cell}})}{d t} \\
& \frac{d([\text{Gly}] \cdot V_{\text{cell}})}{d t} \\
& \frac{d([\text{Gspd}] \cdot V_{\text{cell}})}{d t} \\
& \frac{d([\text{TS2}] \cdot V_{\text{cell}})}{d t} \\
& \frac{d([\text{T[SH]2}] \cdot V_{\text{cell}})}{d t} \\
& \frac{d([\text{CO2}] \cdot V_{\text{cell}})}{d t}
\end{aligned}
=
\begin{aligned}
& -V_{\text{cell}} \cdot \left(\frac{V_{m_{(\text{GS})}} \cdot [\text{Gly}] \cdot [\text{GluCys}]}{K_{m2_{(\text{GS})}} \cdot [\text{Gly}] + K_{m1_{(\text{GS})}} \cdot [\text{GluCys}] + [\text{Gly}] \cdot [\text{GluCys}] + k_{d1_{(\text{GS})}} \cdot K_{m2_{(\text{GS})}}} \right) \\
& +V_{\text{cell}} \cdot \left(\frac{V_{m_{(\text{GS})}} \cdot [\text{Gly}] \cdot [\text{GluCys}]}{K_{m2_{(\text{GS})}} \cdot [\text{Gly}] + K_{m1_{(\text{GS})}} \cdot [\text{GluCys}] + [\text{Gly}] \cdot [\text{GluCys}] + k_{d1_{(\text{GS})}} \cdot K_{m2_{(\text{GS})}}} \right) \\
& -V_{\text{cell}} \cdot \left(\frac{v_{\text{max}_{(\text{TryS1})}} \cdot [\text{Spd}] \cdot [\text{GSH}]}{K_{\text{ma}_{(\text{TryS1})}} \cdot K_{\text{mb}_{(\text{TryS1})}} + [\text{Spd}] \cdot K_{\text{mb}_{(\text{TryS1})}} + [\text{GSH}] \cdot K_{\text{ma}_{(\text{TryS1})}} + [\text{Spd}] \cdot [\text{GSH}]} \right) \\
& -V_{\text{cell}} \cdot \left(\frac{v_{\text{max}_{(\text{TryS2})}} \cdot [\text{Gspd}] \cdot [\text{GSH}]}{K_{\text{ma}_{(\text{TryS2})}} \cdot K_{\text{mb}_{(\text{TryS2})}} + [\text{Gspd}] \cdot K_{\text{mb}_{(\text{TryS2})}} + [\text{GSH}] \cdot K_{\text{ma}_{(\text{TryS2})}} + [\text{Gspd}] \cdot [\text{GSH}]} \right) \\
& = -V_{\text{cell}} \cdot \left(\frac{V_{m_{(\text{GS})}} \cdot [\text{Gly}] \cdot [\text{GluCys}]}{K_{m2_{(\text{GS})}} \cdot [\text{Gly}] + K_{m1_{(\text{GS})}} \cdot [\text{GluCys}] + [\text{Gly}] \cdot [\text{GluCys}] + k_{d1_{(\text{GS})}} \cdot K_{m2_{(\text{GS})}}} \right) \\
& +V_{\text{cell}} \cdot \left(\frac{v_{\text{max}_{(\text{TryS1})}} \cdot [\text{Spd}] \cdot [\text{GSH}]}{K_{\text{ma}_{(\text{TryS1})}} \cdot K_{\text{mb}_{(\text{TryS1})}} + [\text{Spd}] \cdot K_{\text{mb}_{(\text{TryS1})}} + [\text{GSH}] \cdot K_{\text{ma}_{(\text{TryS1})}} + [\text{Spd}] \cdot [\text{GSH}]} \right) \\
& -V_{\text{cell}} \cdot \left(\frac{v_{\text{max}_{(\text{TryS2})}} \cdot [\text{Gspd}] \cdot [\text{GSH}]}{K_{\text{ma}_{(\text{TryS2})}} \cdot K_{\text{mb}_{(\text{TryS2})}} + [\text{Gspd}] \cdot K_{\text{mb}_{(\text{TryS2})}} + [\text{GSH}] \cdot K_{\text{ma}_{(\text{TryS2})}} + [\text{Gspd}] \cdot [\text{GSH}]} \right) \\
& = +V_{\text{cell}} \cdot (k1_{(\text{"TXNo Reduction"})} \cdot [\text{T[SH]2}] \cdot [\text{TXNo}]) \\
& +V_{\text{cell}} \cdot (k1_{(\text{"Grx1 reduction"})} \cdot [\text{Grx1}] \cdot [\text{T[SH]2}]) \\
& +V_{\text{cell}} \cdot (k1_{(\text{"Grx2 reduction"})} \cdot [\text{Grx2}] \cdot [\text{T[SH]2}]) \\
& -V_{\text{cell}} \cdot \left(\frac{V_{(\text{TR})} \cdot [\text{TS2}] \cdot [\text{NADPH}]}{K_{\text{mA}_{(\text{TR})}} \cdot K_{\text{mB}_{(\text{TR})}} + K_{\text{mB}_{(\text{TR})}} \cdot [\text{TS2}] + K_{\text{mA}_{(\text{TR})}} \cdot [\text{NADPH}]} \right) \\
& = -V_{\text{cell}} \cdot (k1_{(\text{"TXNo Reduction"})} \cdot [\text{T[SH]2}] \cdot [\text{TXNo}]) \\
& -V_{\text{cell}} \cdot (k1_{(\text{"Grx1 reduction"})} \cdot [\text{Grx1}] \cdot [\text{T[SH]2}]) \\
& -V_{\text{cell}} \cdot (k1_{(\text{"Grx2 reduction"})} \cdot [\text{Grx2}] \cdot [\text{T[SH]2}]) \\
& +V_{\text{cell}} \cdot \left(\frac{v_{\text{max}_{(\text{TryS2})}} \cdot [\text{Gspd}] \cdot [\text{GSH}]}{K_{\text{ma}_{(\text{TryS2})}} \cdot K_{\text{mb}_{(\text{TryS2})}} + [\text{Gspd}] \cdot K_{\text{mb}_{(\text{TryS2})}} + [\text{GSH}] \cdot K_{\text{ma}_{(\text{TryS2})}} + [\text{Gspd}] \cdot [\text{GSH}]} \right) \\
& +V_{\text{cell}} \cdot \left(\frac{V_{(\text{TR})} \cdot [\text{TS2}] \cdot [\text{NADPH}]}{K_{\text{mA}_{(\text{TR})}} \cdot K_{\text{mB}_{(\text{TR})}} + K_{\text{mB}_{(\text{TR})}} \cdot [\text{TS2}] + K_{\text{mA}_{(\text{TR})}} \cdot [\text{NADPH}]} \right) \\
& = +V_{\text{cell}} \cdot \left(\frac{V_{(\text{ODC})} \cdot [\text{Orn}]}{K_{\text{m}_{(\text{ODC})}} + [\text{Orn}]} \right)
\end{aligned}$$

$$\frac{d([\text{TXNo}] \cdot V_{\text{cell}})}{d t}$$

$$= -V_{\text{cell}} \cdot (k1_{(\text{"TXNo Reduction"})} \cdot [\text{T[SH]2}] \cdot [\text{TXNo}])$$

$$+ V_{\text{cell}} \cdot \left(\frac{Kcat_{(\text{TDPx})} \cdot [\text{TDPx}] \cdot [\text{H2O2}] \cdot [\text{TXNr}]}{Kb_{(\text{TDPx})} \cdot [\text{H2O2}] + Ka_{(\text{TDPx})} \cdot [\text{TXNr}] + [\text{H2O2}] \cdot [\text{TXNr}]} \right)$$

$$+ V_{\text{cell}} \cdot \left(\frac{Kcat_{(\text{TryP})} \cdot [\text{TryP}] \cdot [\text{H2O2}] \cdot [\text{TXNr}]}{Kb_{(\text{TryP})} \cdot [\text{H2O2}] + Ka_{(\text{TryP})} \cdot [\text{TXNr}] + [\text{H2O2}] \cdot [\text{TXNr}]} \right)$$

$$\frac{d([\text{TXNr}] \cdot V_{\text{cell}})}{d t}$$

$$= +V_{\text{cell}} \cdot (k1_{(\text{"TXNo Reduction"})} \cdot [\text{T[SH]2}] \cdot [\text{TXNo}])$$

$$- V_{\text{cell}} \cdot \left(\frac{Kcat_{(\text{TDPx})} \cdot [\text{TDPx}] \cdot [\text{H2O2}] \cdot [\text{TXNr}]}{Kb_{(\text{TDPx})} \cdot [\text{H2O2}] + Ka_{(\text{TDPx})} \cdot [\text{TXNr}] + [\text{H2O2}] \cdot [\text{TXNr}]} \right)$$

$$- V_{\text{cell}} \cdot \left(\frac{Kcat_{(\text{TryP})} \cdot [\text{TryP}] \cdot [\text{H2O2}] \cdot [\text{TXNr}]}{Kb_{(\text{TryP})} \cdot [\text{H2O2}] + Ka_{(\text{TryP})} \cdot [\text{TXNr}] + [\text{H2O2}] \cdot [\text{TXNr}]} \right)$$

$$\frac{d([\text{H2O}] \cdot V_{\text{cell}})}{d t}$$

$$= +V_{\text{cell}} \cdot \left(\frac{Kcat_{(\text{TDPx})} \cdot [\text{TDPx}] \cdot [\text{H2O2}] \cdot [\text{TXNr}]}{Kb_{(\text{TDPx})} \cdot [\text{H2O2}] + Ka_{(\text{TDPx})} \cdot [\text{TXNr}] + [\text{H2O2}] \cdot [\text{TXNr}]} \right)$$

$$+ V_{\text{cell}} \cdot \left(\frac{Kcat_{(\text{TryP})} \cdot [\text{TryP}] \cdot [\text{H2O2}] \cdot [\text{TXNr}]}{Kb_{(\text{TryP})} \cdot [\text{H2O2}] + Ka_{(\text{TryP})} \cdot [\text{TXNr}] + [\text{H2O2}] \cdot [\text{TXNr}]} \right)$$

$$\frac{d([\text{H2O2}] \cdot V_{\text{cell}})}{d t}$$

$$= -V_{\text{cell}} \cdot \left(\frac{Kcat_{(\text{TDPx})} \cdot [\text{TDPx}] \cdot [\text{H2O2}] \cdot [\text{TXNr}]}{Kb_{(\text{TDPx})} \cdot [\text{H2O2}] + Ka_{(\text{TDPx})} \cdot [\text{TXNr}] + [\text{H2O2}] \cdot [\text{TXNr}]} \right)$$

$$- V_{\text{cell}} \cdot \left(\frac{Kcat_{(\text{TryP})} \cdot [\text{TryP}] \cdot [\text{H2O2}] \cdot [\text{TXNr}]}{Kb_{(\text{TryP})} \cdot [\text{H2O2}] + Ka_{(\text{TryP})} \cdot [\text{TXNr}] + [\text{H2O2}] \cdot [\text{TXNr}]} \right)$$

$$+ V_{\text{cell}} \cdot (k1_{(\text{"Aconitase_O2.-"})} \cdot [\text{"O2.-"}] \cdot [\text{"aconitase[4Fe-4S]"}])$$

$$+ V_{\text{cell}} \cdot (k1_{(\text{"Fumarase_O2.-"})} \cdot [\text{"O2.-"}] \cdot [\text{"fumarase[4Fe-4S]"}])$$

$$- V_{\text{cell}} \cdot (k1_{(\text{"Fenton reaction"})} \cdot [\text{H2O2}] \cdot [\text{"Fe+3"}])$$

$$\begin{aligned}
\frac{d([\text{aconitase}] \cdot V_{\text{cell}})}{d t} &= -V_{\text{cell}} \cdot \left(\frac{V_{(\text{Aco_activation_grx1})} \cdot [\text{aconitase}] \cdot [{}^{\text{''ISC-Grx1r[4Fe-4S]''}}]}{K_{\text{mA}}_{(\text{Aco_activation_grx1})} \cdot K_{\text{mB}}_{(\text{Aco_activation_grx1})} + K_{\text{mB}}_{(\text{Aco_activation_grx1})} \cdot [\text{aconitase}] + K_{\text{mA}}_{(\text{Aco_activation_grx1})} \cdot [{}^{\text{''ISC-Grx1r[4Fe-4S]''}}}]} \right) \\
&\quad - V_{\text{cell}} \cdot \left(\frac{V_{(\text{Aco_activation_grx2})} \cdot [\text{aconitase}] \cdot [{}^{\text{''ISC-Grx2r[4Fe-4S]''}}]}{K_{\text{mA}}_{(\text{Aco_activation_grx2})} \cdot K_{\text{mB}}_{(\text{Aco_activation_grx2})} + K_{\text{mB}}_{(\text{Aco_activation_grx2})} \cdot [\text{aconitase}] + K_{\text{mA}}_{(\text{Aco_activation_grx2})} \cdot [{}^{\text{''ISC-Grx2r[4Fe-4S]''}}}]} \right) \\
\frac{d([{}^{\text{''fumarase[4Fe-4S]''}}] \cdot V_{\text{cell}})}{d t} &= +V_{\text{cell}} \cdot \left(\frac{V_{(\text{Fum_activation_grx1})} \cdot [{}^{\text{''Fumarase''}}] \cdot [{}^{\text{''ISC-Grx1r[4Fe-4S]''}}]}{K_{\text{mA}}_{(\text{Fum_activation_grx1})} \cdot K_{\text{mB}}_{(\text{Fum_activation_grx1})} + K_{\text{mB}}_{(\text{Fum_activation_grx1})} \cdot [{}^{\text{''Fumarase''}}] + K_{\text{mA}}_{(\text{Fum_activation_grx1})} \cdot [{}^{\text{''ISC-Grx1r[4Fe-4S]''}}}]} \right) \\
&\quad + V_{\text{cell}} \cdot \left(\frac{V_{(\text{Fum_activation_grx2})} \cdot [{}^{\text{''Fumarase''}}] \cdot [{}^{\text{''ISC-Grx2r[4Fe-4S]''}}]}{K_{\text{mA}}_{(\text{Fum_activation_grx2})} \cdot K_{\text{mB}}_{(\text{Fum_activation_grx2})} + K_{\text{mB}}_{(\text{Fum_activation_grx2})} \cdot [{}^{\text{''Fumarase''}}] + K_{\text{mA}}_{(\text{Fum_activation_grx2})} \cdot [{}^{\text{''ISC-Grx2r[4Fe-4S]''}}}]} \right) \\
&\quad - V_{\text{cell}} \cdot (k1_{(\text{''Fumarase O2-''}}) \cdot [{}^{\text{''O2-''}}] \cdot [{}^{\text{''fumarase[4Fe-4S]''}}]) \\
&\quad + V_{\text{cell}} \cdot (k1_{(\text{''Fum_activation_Fe+2''}}) \cdot [{}^{\text{''fumarase[3Fe-4S]''}}] \cdot [{}^{\text{''Fe+2''}}]) \\
&\quad - V_{\text{cell}} \cdot (k1_{(\text{''Fum_ONOO-''}}) \cdot [{}^{\text{''fumarase[4Fe-4S]''}}] \cdot [{}^{\text{''ONOO-''}}]) \\
\frac{d([{}^{\text{''Fumarase''}}] \cdot V_{\text{cell}})}{d t} &= -V_{\text{cell}} \cdot \left(\frac{V_{(\text{Fum_activation_grx1})} \cdot [{}^{\text{''Fumarase''}}] \cdot [{}^{\text{''ISC-Grx1r[4Fe-4S]''}}]}{K_{\text{mA}}_{(\text{Fum_activation_grx1})} \cdot K_{\text{mB}}_{(\text{Fum_activation_grx1})} + K_{\text{mB}}_{(\text{Fum_activation_grx1})} \cdot [{}^{\text{''Fumarase''}}] + K_{\text{mA}}_{(\text{Fum_activation_grx1})} \cdot [{}^{\text{''ISC-Grx1r[4Fe-4S]''}}}]} \right) \\
&\quad - V_{\text{cell}} \cdot \left(\frac{V_{(\text{Fum_activation_grx2})} \cdot [{}^{\text{''Fumarase''}}] \cdot [{}^{\text{''ISC-Grx2r[4Fe-4S]''}}]}{K_{\text{mA}}_{(\text{Fum_activation_grx2})} \cdot K_{\text{mB}}_{(\text{Fum_activation_grx2})} + K_{\text{mB}}_{(\text{Fum_activation_grx2})} \cdot [{}^{\text{''Fumarase''}}] + K_{\text{mA}}_{(\text{Fum_activation_grx2})} \cdot [{}^{\text{''ISC-Grx2r[4Fe-4S]''}}}]} \right) \\
\frac{d([\text{Grx1}] \cdot V_{\text{cell}})}{d t} &= -V_{\text{cell}} \cdot (k1_{(\text{''Grx1 reduction''}}) \cdot [\text{Grx1}] \cdot [{}^{\text{''T[SH]2''}}]) \\
\frac{d([\text{Grx1r}] \cdot V_{\text{cell}})}{d t} &= +V_{\text{cell}} \cdot (k1_{(\text{''Grx1 reduction''}}) \cdot [\text{Grx1}] \cdot [{}^{\text{''T[SH]2''}}]) \\
&\quad - V_{\text{cell}} \cdot (k1_{(\text{''ISCU-grx1 complex''}}) \cdot [{}^{\text{''ISCU[2Fe-2S]''}}] \cdot [\text{Grx1r}]) \\
\frac{d([\text{Grx2}] \cdot V_{\text{cell}})}{d t} &= -V_{\text{cell}} \cdot (k1_{(\text{''Grx2 reduction''}}) \cdot [\text{Grx2}] \cdot [{}^{\text{''T[SH]2''}}])
\end{aligned}$$

$$\frac{d([\text{Grx2}] \cdot V_{\text{cell}})}{d t} = -V_{\text{cell}} \cdot (k1_{(\text{"Grx2 reduction"})} \cdot [\text{Grx2}] \cdot [\text{T[SH]2}])$$

$$\frac{d([\text{Grx2r}] \cdot V_{\text{cell}})}{d t} = +V_{\text{cell}} \cdot (k1_{(\text{"Grx2 reduction"})} \cdot [\text{Grx2}] \cdot [\text{T[SH]2}])$$

$$-V_{\text{cell}} \cdot (k1_{(\text{"ISCU-grx2 complex"})} \cdot [\text{"ISCU[2Fe-2S]"}] \cdot [\text{Grx2r}])$$

$$\frac{d([\text{"aconitase[4Fe-4S]"}] \cdot V_{\text{cell}})}{d t} = +V_{\text{cell}} \cdot \left(\frac{V_{(\text{Aco_activation_grx1})} \cdot [\text{"aconitase"}] \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]}{KmA_{(\text{Aco_activation_grx1})} \cdot KmB_{(\text{Aco_activation_grx1})} + KmB_{(\text{Aco_activation_grx1})} \cdot [\text{"aconitase"}] + KmA_{(\text{Aco_activation_grx1})} \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]} \right)$$

$$+V_{\text{cell}} \cdot \left(\frac{V_{(\text{Aco_activation_grx2})} \cdot [\text{"aconitase"}] \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]}{KmA_{(\text{Aco_activation_grx2})} \cdot KmB_{(\text{Aco_activation_grx2})} + KmB_{(\text{Aco_activation_grx2})} \cdot [\text{"aconitase"}] + KmA_{(\text{Aco_activation_grx2})} \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]} \right)$$

$$-V_{\text{cell}} \cdot (k1_{(\text{"Aconitase_O2-"})} \cdot [\text{"O2-"}] \cdot [\text{"aconitase[4Fe-4S]"}])$$

$$+V_{\text{cell}} \cdot (k1_{(\text{"Aco_activation_Fe+2"})} \cdot [\text{"aconitase[3Fe-4S]+"}] \cdot [\text{"Fe+2"}])$$

$$-V_{\text{cell}} \cdot (k1_{(\text{"Aco_ONOO-"})} \cdot [\text{"aconitase[4Fe-4S]"}] \cdot [\text{"ONOO-"}])$$

$$\frac{d([\text{ISCU}] \cdot V_{\text{cell}})}{d t} = +V_{\text{cell}} \cdot \left(\frac{V_{(\text{Aco_activation_grx1})} \cdot [\text{"aconitase"}] \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]}{KmA_{(\text{Aco_activation_grx1})} \cdot KmB_{(\text{Aco_activation_grx1})} + KmB_{(\text{Aco_activation_grx1})} \cdot [\text{"aconitase"}] + KmA_{(\text{Aco_activation_grx1})} \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]} \right)$$

$$+V_{\text{cell}} \cdot \left(\frac{V_{(\text{Fum_activation_grx1})} \cdot [\text{Fumarase}] \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]}{KmA_{(\text{Fum_activation_grx1})} \cdot KmB_{(\text{Fum_activation_grx1})} + KmB_{(\text{Fum_activation_grx1})} \cdot [\text{Fumarase}] + KmA_{(\text{Fum_activation_grx1})} \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]} \right)$$

$$+V_{\text{cell}} \cdot \left(\frac{V_{(\text{Aco_activation_grx2})} \cdot [\text{"aconitase"}] \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]}{KmA_{(\text{Aco_activation_grx2})} \cdot KmB_{(\text{Aco_activation_grx2})} + KmB_{(\text{Aco_activation_grx2})} \cdot [\text{"aconitase"}] + KmA_{(\text{Aco_activation_grx2})} \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]} \right)$$

$$+V_{\text{cell}} \cdot \left(\frac{V_{(\text{Fum_activation_grx2})} \cdot [\text{Fumarase}] \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]}{KmA_{(\text{Fum_activation_grx2})} \cdot KmB_{(\text{Fum_activation_grx2})} + KmB_{(\text{Fum_activation_grx2})} \cdot [\text{Fumarase}] + KmA_{(\text{Fum_activation_grx2})} \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]} \right)$$

$$\begin{aligned}
\frac{d([\text{"ISCU[2Fe-2S]"}] \cdot V_{\text{cell}})}{d t} &= +V_{\text{cell}} \cdot \left(\frac{V_{(\text{"ISCU activation"})} \cdot [\text{"Fe+2"}] \cdot [\text{"Fe+2"}]}{\text{KmA}_{(\text{"ISCU activation"})} \cdot \text{KmB}_{(\text{"ISCU activation"})} + \text{KmB}_{(\text{"ISCU activation"})} \cdot [\text{"Fe+2"}] + \text{KmA}_{(\text{"ISCU activation"})} \cdot [\text{"Fe+2"}]} \right) \\
&\quad - V_{\text{cell}} \cdot (k1_{(\text{"ISCU-grx1 complex"})} \cdot [\text{"ISCU[2Fe-2S]"}] \cdot [\text{Grx1r}]) \\
&\quad - V_{\text{cell}} \cdot (k1_{(\text{"ISCU-grx2 complex"})} \cdot [\text{"ISCU[2Fe-2S]"}] \cdot [\text{Grx2r}]) \\
\frac{d([\text{ISCU[2S]}] \cdot V_{\text{cell}})}{d t} &= -V_{\text{cell}} \cdot \left(\frac{V_{(\text{"ISCU activation"})} \cdot [\text{"Fe+2"}] \cdot [\text{"Fe+2"}]}{\text{KmA}_{(\text{"ISCU activation"})} \cdot \text{KmB}_{(\text{"ISCU activation"})} + \text{KmB}_{(\text{"ISCU activation"})} \cdot [\text{"Fe+2"}] + \text{KmA}_{(\text{"ISCU activation"})} \cdot [\text{"Fe+2"}]} \right) \\
\frac{d([\text{"ISC-Grx1r[4Fe-4S]"}] \cdot V_{\text{cell}})}{d t} &= -V_{\text{cell}} \cdot \left(\frac{V_{(\text{Aco_activation_grx1})} \cdot [\text{aconitase}] \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]}{\text{KmA}_{(\text{Aco_activation_grx1})} \cdot \text{KmB}_{(\text{Aco_activation_grx1})} + \text{KmB}_{(\text{Aco_activation_grx1})} \cdot [\text{aconitase}] + \text{KmA}_{(\text{Aco_activation_grx1})} \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]} \right) \\
&\quad - V_{\text{cell}} \cdot \left(\frac{V_{(\text{Fum_activation_grx1})} \cdot [\text{Fumarase}] \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]}{\text{KmA}_{(\text{Fum_activation_grx1})} \cdot \text{KmB}_{(\text{Fum_activation_grx1})} + \text{KmB}_{(\text{Fum_activation_grx1})} \cdot [\text{Fumarase}] + \text{KmA}_{(\text{Fum_activation_grx1})} \cdot [\text{"ISC-Grx1r[4Fe-4S]"}]} \right) \\
&\quad + V_{\text{cell}} \cdot (k1_{(\text{"ISCU-grx1 complex"})} \cdot [\text{"ISCU[2Fe-2S]"}] \cdot [\text{Grx1r}]) \\
\frac{d([\text{"ISC-Grx2r[4Fe-4S]"}] \cdot V_{\text{cell}})}{d t} &= +V_{\text{cell}} \cdot (k1_{(\text{"ISCU-grx2 complex"})} \cdot [\text{"ISCU[2Fe-2S]"}] \cdot [\text{Grx2r}]) \\
&\quad - V_{\text{cell}} \cdot \left(\frac{V_{(\text{Aco_activation_grx2})} \cdot [\text{aconitase}] \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]}{\text{KmA}_{(\text{Aco_activation_grx2})} \cdot \text{KmB}_{(\text{Aco_activation_grx2})} + \text{KmB}_{(\text{Aco_activation_grx2})} \cdot [\text{aconitase}] + \text{KmA}_{(\text{Aco_activation_grx2})} \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]} \right) \\
&\quad - V_{\text{cell}} \cdot \left(\frac{V_{(\text{Fum_activation_grx2})} \cdot [\text{Fumarase}] \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]}{\text{KmA}_{(\text{Fum_activation_grx2})} \cdot \text{KmB}_{(\text{Fum_activation_grx2})} + \text{KmB}_{(\text{Fum_activation_grx2})} \cdot [\text{Fumarase}] + \text{KmA}_{(\text{Fum_activation_grx2})} \cdot [\text{"ISC-Grx2r[4Fe-4S]"}]} \right) \\
\frac{d([\text{"O2.-"}] \cdot V_{\text{cell}})}{d t} &= -V_{\text{cell}} \cdot (k1_{(\text{"Aconitase O2.-"})} \cdot [\text{"O2.-"}] \cdot [\text{"aconitase[4Fe-4S]"}]) \\
&\quad - V_{\text{cell}} \cdot (k1_{(\text{"Fumarase O2.-"})} \cdot [\text{"O2.-"}] \cdot [\text{"fumarase[4Fe-4S]"}])
\end{aligned}$$

$$\frac{d([\text{OH}^-] \cdot V_{\text{cell}})}{d t} = + V_{\text{cell}} \cdot (k1_{(\text{"Fenton reaction"})} \cdot [\text{H2O2}] \cdot [\text{"Fe+3"}])$$

$$\begin{aligned} \frac{d([\text{"Fe+3"}] \cdot V_{\text{cell}})}{d t} &= + V_{\text{cell}} \cdot (k1_{(\text{"Aconitase_O2.-"})} \cdot [\text{"O2.-"}] \cdot [\text{"aconitase[4Fe-4S]"}]) \\ &+ V_{\text{cell}} \cdot (k1_{(\text{"Fumarase O2.-"})} \cdot [\text{"O2.-"}] \cdot [\text{"fumarase[4Fe-4S]"}]) \\ &- V_{\text{cell}} \cdot (k1_{(\text{"Fenton reaction"})} \cdot [\text{H2O2}] \cdot [\text{"Fe+3"}]) \\ &+ V_{\text{cell}} \cdot (k1_{(\text{"Aco_ONOO-"})} \cdot [\text{"aconitase[4Fe-4S]"}] \cdot [\text{"ONOO-"}]) \\ &+ V_{\text{cell}} \cdot (k1_{(\text{"Fum_ONOO-"})} \cdot [\text{"fumarase[4Fe-4S]"}] \cdot [\text{"ONOO-"}]) \end{aligned}$$

$$\frac{d([\text{"OH-"}] \cdot V_{\text{cell}})}{d t} = + V_{\text{cell}} \cdot (k1_{(\text{"Fenton reaction"})} \cdot [\text{H2O2}] \cdot [\text{"Fe+3"}])$$

$$\begin{aligned} \frac{d([\text{"aconitase[3Fe-4S]+"}] \cdot V_{\text{cell}})}{d t} &= + V_{\text{cell}} \cdot (k1_{(\text{"Aconitase_O2.-"})} \cdot [\text{"O2.-"}] \cdot [\text{"aconitase[4Fe-4S]"}]) \\ &- V_{\text{cell}} \cdot (k1_{(\text{"Aco_activation_Fe+2"})} \cdot [\text{"aconitase[3Fe-4S]+"}] \cdot [\text{"Fe+2"}]) \\ &+ V_{\text{cell}} \cdot (k1_{(\text{"Aco_ONOO-"})} \cdot [\text{"aconitase[4Fe-4S]"}] \cdot [\text{"ONOO-"}]) \end{aligned}$$

$$\begin{aligned} \frac{d([\text{"fumarase[3Fe-4S]+"}] \cdot V_{\text{cell}})}{d t} &= + V_{\text{cell}} \cdot (k1_{(\text{"Fumarase O2.-"})} \cdot [\text{"O2.-"}] \cdot [\text{"fumarase[4Fe-4S]"}]) \\ &- V_{\text{cell}} \cdot (k1_{(\text{"Fum_activation_Fe+2"})} \cdot [\text{"fumarase[3Fe-4S]+"}] \cdot [\text{"Fe+2"}]) \\ &+ V_{\text{cell}} \cdot (k1_{(\text{"Fum_ONOO-"})} \cdot [\text{"fumarase[4Fe-4S]"}] \cdot [\text{"ONOO-"}]) \end{aligned}$$

$$\begin{aligned} \frac{d([\text{"ONOO-"}] \cdot V_{\text{cell}})}{d t} &= - V_{\text{cell}} \cdot (k1_{(\text{"Aco_ONOO-"})} \cdot [\text{"aconitase[4Fe-4S]"}] \cdot [\text{"ONOO-"}]) \\ &- V_{\text{cell}} \cdot (k1_{(\text{"Fum_ONOO-"})} \cdot [\text{"fumarase[4Fe-4S]"}] \cdot [\text{"ONOO-"}]) \end{aligned}$$

$$\frac{d([\text{NADP}] \cdot V_{\text{cell}})}{d t} = + V_{\text{cell}} \cdot \left(\frac{V_{(\text{TR})} \cdot [\text{TS2}] \cdot [\text{NADPH}]}{KmA_{(\text{TR})} \cdot KmB_{(\text{TR})} + KmB_{(\text{TR})} \cdot [\text{TS2}] + KmA_{(\text{TR})} \cdot [\text{NADPH}]} \right)$$

$$\frac{d([\text{NADPH}] \cdot V_{\text{cell}})}{d t} = - V_{\text{cell}} \cdot \left(\frac{V_{(\text{TR})} \cdot [\text{TS2}] \cdot [\text{NADPH}]}{KmA_{(\text{TR})} \cdot KmB_{(\text{TR})} + KmB_{(\text{TR})} \cdot [\text{TS2}] + KmA_{(\text{TR})} \cdot [\text{NADPH}]} \right)$$