## Supplementary file 1 A: Model equations

| Reaction nr | reaction | Function | Present in model(s) |
|---|---|---|---|
| 1 PTS_Glc Glucose proton symporter | GLC_Ext + PEP -> G6P + PYR; FBP Pi_Int | $\frac{\mathrm{PTS\_Glc}\cdot\frac{\mathrm{Pi\_Int}}{\mathrm{Pi\_Int}+\mathrm{kaPi\_Int\_PTS\_Glc}}\cdot\frac{\mathrm{kiFBP\_PTS\_Glc}}{\mathrm{FBP}+\mathrm{kiFBP\_PTS\_Glc}}\cdot\mathrm{kcat\_PTS\_Glc}\cdot\frac{\mathrm{GLC\_Ext}}{\mathrm{kmGLC\_PTS\_Glc}}\cdot\frac{\mathrm{PEP}}{\mathrm{kmPEP\_PTS\_Glc}}}{\left(1+\frac{\mathrm{GLC\_Ext}}{\mathrm{kmGLC\_PTS\_Glc}}\right)\cdot\left(1+\frac{\mathrm{PEP}}{\mathrm{kmPEP\_PTS\_Glc}}\right)+\left(1+\frac{\mathrm{G6P}}{\mathrm{kmG6P\_PTS\_Glc}}\right)\cdot\left(1+\frac{\mathrm{PYR}}{\mathrm{kmPYR\_PTS\_Glc}}\right)-1}$ | 1,2,3,4,5,6 |
| 2 PGI Glucose-6-phosphate isomerase | G6P = F6P | $\frac{\mathrm{PGI}\cdot\left(\mathrm{kcat\_PGI}\cdot\frac{\mathrm{G6P}}{\mathrm{kmG6P\_PGI}}-\frac{\mathrm{kcat\_PGI}}{\mathrm{Keq\_PGI}}\cdot\frac{\mathrm{F6P}}{\mathrm{kmG6P\_PGI}}\right)}{1+\frac{\mathrm{G6P}}{\mathrm{kmG6P\_PGI}}+\frac{\mathrm{F6P}}{\mathrm{kmF6P\_PGI}}}$ | 1,2,3,4,5,6 |
| 3 PFK Phosphofructokinase | F6P + ATP -> FBP + ADP | $\frac{\mathrm{PFK}\cdot\mathrm{kcat\_PFK}\cdot\frac{\mathrm{ATP}}{\mathrm{kmF6P\_PFK}}\cdot\frac{\mathrm{F6P}}{\mathrm{kmATP\_PFK}}}{\left(1+\frac{\mathrm{ATP}}{\mathrm{kmF6P\_PFK}}\right)\cdot\left(1+\frac{\mathrm{F6P}}{\mathrm{kmATP\_PFK}}\right)+\left(1+\frac{\mathrm{ADP}}{\mathrm{kmFBP\_PFK}}\right)\cdot\left(1+\frac{\mathrm{FBP}}{\mathrm{kmADP\_PFK}}\right)-1}$ | 1,2,3,4,5,6 |
| 4 FBA Fructose-bisphosphate aldolase | GAP + Pi_Int + NAD = DGP + NADH | $\frac{\mathrm{FBA}\cdot\left(\mathrm{kcat\_FBA}\cdot\frac{\mathrm{FBP}}{\mathrm{kmFBP\_FBA}}-\frac{\mathrm{kcat\_FBA}}{\mathrm{Keq\_FBA}}\cdot\frac{\mathrm{GAP}^2}{\mathrm{kmFBP\_FBA}}\right)}{1+\frac{\mathrm{FBP}}{\mathrm{kmFBP\_FBA}}+\frac{\mathrm{GAP}}{\mathrm{kmGAP\_FBA}}+\left(\frac{\mathrm{GAP}}{\mathrm{kmGAP\_FBA}}\right)^2}$ | 1,2,3,4,5,6 |
| 5 GAPDH Glyceraldehyde-3-phosphate dehydrogenase | DGP + ADP = PEP + ATP | $\frac{\mathrm{GAPDH}\cdot\left(\mathrm{kcat\_GAPDH}\cdot\frac{\mathrm{GAP}}{\mathrm{kmGAP\_GAPDH}}\cdot\frac{\mathrm{NAD}}{\mathrm{kmNAD\_GAPDH}}\cdot\frac{\mathrm{Pi\_Int}}{\mathrm{kmPi\_Int\_GAPDH}}-\frac{\mathrm{kcat\_GAPDH}}{\mathrm{Keq\_GAPDH}}\cdot\frac{\mathrm{DGP}}{\mathrm{kmGAP\_GAPDH}}\cdot\frac{\mathrm{NADH}}{\mathrm{kmNAD\_GAPDH}}\right.}{\left(1+\frac{\mathrm{GAP}}{\mathrm{kmGAP\_GAPDH}}\right)\cdot\left(1+\frac{\mathrm{Pi\_Int}}{\mathrm{kmPi\_Int\_GAPDH}}\right)\cdot\left(1+\frac{\mathrm{NAD}}{\mathrm{kmNAD\_GAPDH}}\right)+\left(1+\frac{\mathrm{DGP}}{\mathrm{kmDGP\_GAPDH}}\right)\cdot\left(1+\frac{\mathrm{NADH}}{\mathrm{kmNADH\_GAP}}\right.}$ | 1,2,3,4,5,6 |

| | | | |
|---|---|---|---|
| 6 ENO<br>Enolase | PEP + ADP -> PYR + ATP;  FBP Pi_Int | $\frac{\mathrm{ENO}\cdot\left(\mathrm{kcat\_ENO}\cdot\frac{\mathrm{DGP}}{\mathrm{kmDGP\_ENO}}\cdot\frac{\mathrm{ADP}}{\mathrm{kmADP\_ENO}}-\frac{\mathrm{kcat\_ENO}}{\mathrm{Keq\_ENO}}\cdot\frac{\mathrm{PEP}}{\mathrm{kmDGP\_ENO}}\cdot\frac{\mathrm{ATP}}{\mathrm{kmADP\_ENO}}\right)}{\left(1+\frac{\mathrm{DGP}}{\mathrm{kmDGP\_ENO}}\right)\cdot\left(1+\frac{\mathrm{ADP}}{\mathrm{kmADP\_ENO}}\right)+\left(1+\frac{\mathrm{PEP}}{\mathrm{kmPEP\_ENO}}\right)\cdot\left(1+\frac{\mathrm{ATP}}{\mathrm{kmATP\_ENO}}\right)-1}$ | 1,2,3,4,5,6 |
| 7 PYK<br>Pyruvate kinase | PYR + CoA + NAD = AcCoA + NADH; GAP | $\frac{\frac{\mathrm{PYK}\cdot\mathrm{FBP}}{\mathrm{FBP}+\mathrm{kaFBP\_PYK}}\cdot\frac{\mathrm{kiPi\_Int\_PYK}^{\mathrm{nPYK}}}{\mathrm{Pi\_Int}^{\mathrm{nPYK}}+\mathrm{kiPi\_Int\_PYK}^{\mathrm{nPYK}}}\cdot\mathrm{kcat\_PYK}\cdot\frac{\mathrm{ADP}}{\mathrm{kmADP\_PYK}}\cdot\frac{\mathrm{PEP}}{\mathrm{kmPEP\_PYK}}}{\left(1+\frac{\mathrm{ADP}}{\mathrm{kmADP\_PYK}}\right)\cdot\left(1+\frac{\mathrm{PEP}}{\mathrm{kmPEP\_PYK}}\right)+\left(1+\frac{\mathrm{ATP}}{\mathrm{kmATP\_PYK}}\right)\cdot\left(1+\frac{\mathrm{PYR}}{\mathrm{kmPYR\_PYK}}\right)-1}$ | 1,2,3,4,5,6 |
| 8 LDH<br>Lactate dehydrogenase | PYR + NADH -> LAC + NAD;  FBP Pi_Int* O2 | $\frac{\frac{\mathrm{LDH}\cdot\mathrm{FBP}}{\mathrm{FBP}+\mathrm{kaFBP\_LDH}}\cdot\frac{\mathrm{kiPi\_Int\_LDH}}{\mathrm{Pi\_Int}+\mathrm{kiPi\_Int\_LDH}}\cdot\frac{\mathrm{kiO2\_LDH}}{\mathrm{O2}+\mathrm{kiO2\_LDH}}\cdot\mathrm{kcat\_LDH}\cdot\frac{\mathrm{NADH}}{\mathrm{kmPYR\_LDH}}\cdot\frac{\mathrm{PYR}}{\mathrm{kmNADH\_LDH}}}{\left(1+\frac{\mathrm{NADH}}{\mathrm{kmPYR\_LDH}}\right)\cdot\left(1+\frac{\mathrm{PYR}}{\mathrm{kmNADH\_LDH}}\right)+\left(1+\frac{\mathrm{LAC}}{\mathrm{kmLAC\_LDH}}\right)\cdot\left(1+\frac{\mathrm{NAD}}{\mathrm{kmNAD\_LDH}}\right)-1}$ | 1*,2*,3*,4*,5, 6 |
| 9 PDH<br>Pyruvate dehydrogenase | PYR + CoA + NAD = AcCoA + NADH; GAP | $\frac{\mathrm{PDH}\cdot\frac{\mathrm{kiGAP\_PDH}}{\mathrm{GAP}+\mathrm{kiGAP\_PDH}}\cdot\left(\mathrm{kcat\_PDH}\cdot\frac{\mathrm{NAD}}{\mathrm{kmPYR\_PDH}}\cdot\frac{\mathrm{PYR}}{\mathrm{kmCoA\_PDH}}\cdot\frac{\mathrm{CoA}}{\mathrm{kmNAD\_PDH}}-\frac{\mathrm{kcat\_PDH}}{\mathrm{Keq\_PDH}}\cdot\frac{\mathrm{AcCoA}}{\mathrm{kmPYR\_PDH}}\cdot\frac{\mathrm{NADH}}{\mathrm{kmCoA\_PDH}}\right)}{\left(1+\frac{\mathrm{NAD}}{\mathrm{kmPYR\_PDH}}\right)\cdot\left(1+\frac{\mathrm{PYR}}{\mathrm{kmCoA\_PDH}}\right)\cdot\left(1+\frac{\mathrm{CoA}}{\mathrm{kmNAD\_PDH}}\right)+\left(1+\frac{\mathrm{AcCoA}}{\mathrm{kmAcCoA\_PDH}}\right)\cdot\left(1+\frac{\mathrm{NADH}}{\mathrm{kmNADH\_PDH}}\right)-1}$ | 1,2,3,4,5,6 |
| 10 PTA_ACK<br>Phosphotransacetylase | AcCoA + ADP -> ACE + ATP + CoA | $\frac{\mathrm{PTA\_ACK}\cdot\mathrm{kcat\_PTA\_ACK}\cdot\frac{\mathrm{AcCoA}}{\mathrm{kmAcCoA\_PTA\_ACK}}\cdot\frac{\mathrm{ADP}}{\mathrm{kmADP\_PTA\_ACK}}}{\left(1+\frac{\mathrm{AcCoA}}{\mathrm{kmAcCoA\_PTA\_ACK}}\right)\cdot\left(1+\frac{\mathrm{ADP}}{\mathrm{kmADP\_PTA\_ACK}}\right)+\left(1+\frac{\mathrm{ACE}}{\mathrm{kmACE\_PTA\_ACK}}\right)\cdot\left(1+\frac{\mathrm{ATP}}{\mathrm{kmATP\_PTA\_ACK}}\right)\cdot\left(1+\frac{\mathrm{CoA}}{\mathrm{kmCoA\_PTA\_ACK}}\right.}$ | 1,2,3,4,5,6 |
| 11 ATPase | ATP -> ADP + Pi_Int | $\mathrm{ATPase}\cdot\mathrm{kcat\_ATPase}\cdot\frac{\left(\frac{\mathrm{ATP}}{\mathrm{kmATP\_ATPase}}\right)^{\mathrm{nATPase}}}{\left(\frac{\mathrm{ATP}}{\mathrm{kmATP\_ATPase}}\right)^{\mathrm{nATPase}}+1}$ | 2,4,6 |
| 12 NOXE<br>NADH oxidase | O2 + 2 * NADH -> 2 * NAD | $\frac{\mathrm{NOXE}\cdot\mathrm{kcat\_NOXE}\cdot\left(\frac{\mathrm{O2}}{\mathrm{kmNADH\_NOXE}}\right)^{2}\cdot\frac{\mathrm{NADH}}{\mathrm{kmO2\_NOXE}}}{\left(1+\frac{\mathrm{O2}}{\mathrm{kmNADH\_NOXE}}\right)^{2}\cdot\left(1+\frac{\mathrm{NADH}}{\mathrm{kmO2\_NOXE}}\right)+1+\frac{\mathrm{NAD}}{\mathrm{kmNAD\_NOXE}}-1}$ | 3,4,6 |

*Models marked with an asterisk contain the function for Lactate Dehydrogenase without the oxygen inhibition term $\frac{kiO2\_LHD}{O2+kiO2\_LDH}$

# Supplementary file 1 B comparison of model additions

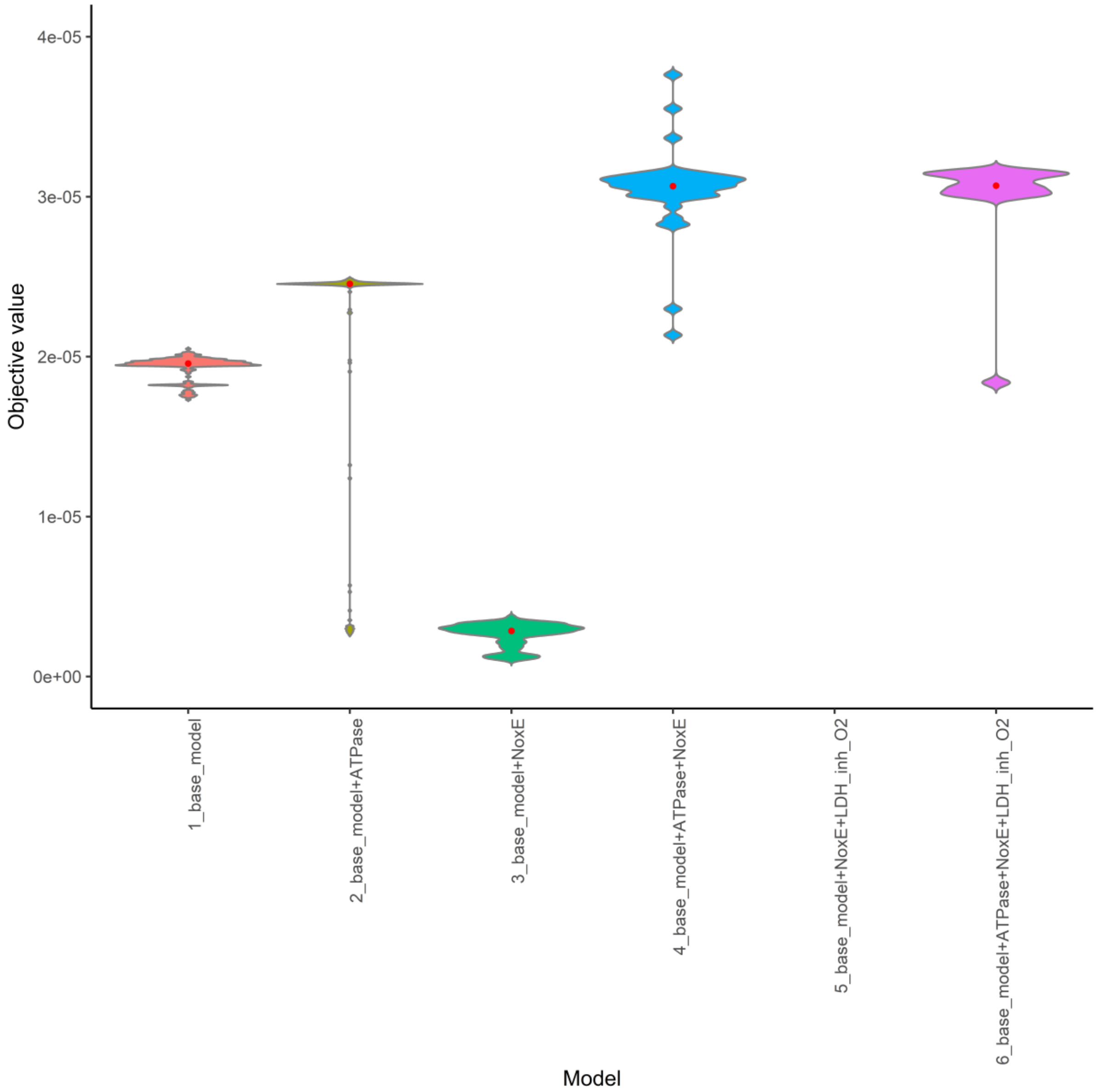



*Figure 1 Zoomed in version of comparison of 100 parameter sets for the model with and without additions. Outliers on the top were removed to better show overall performance of the models.*

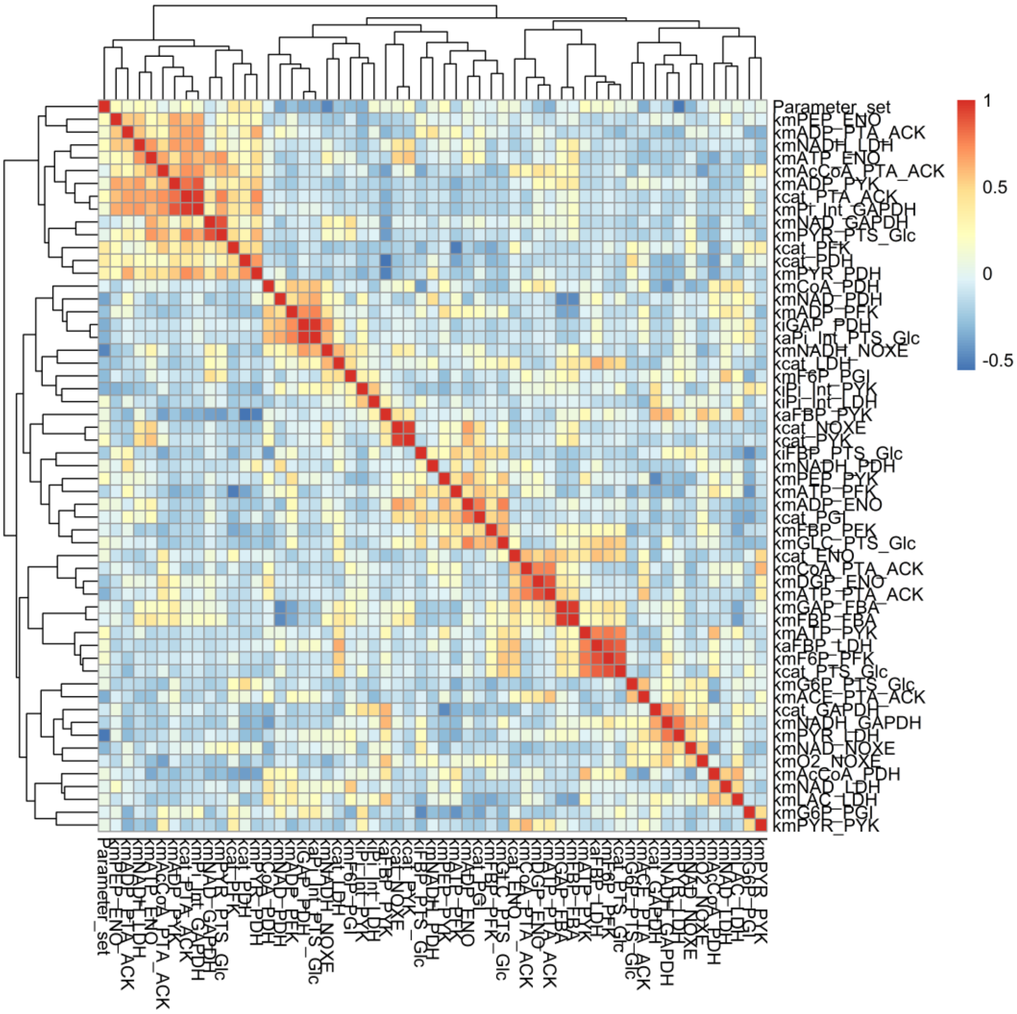
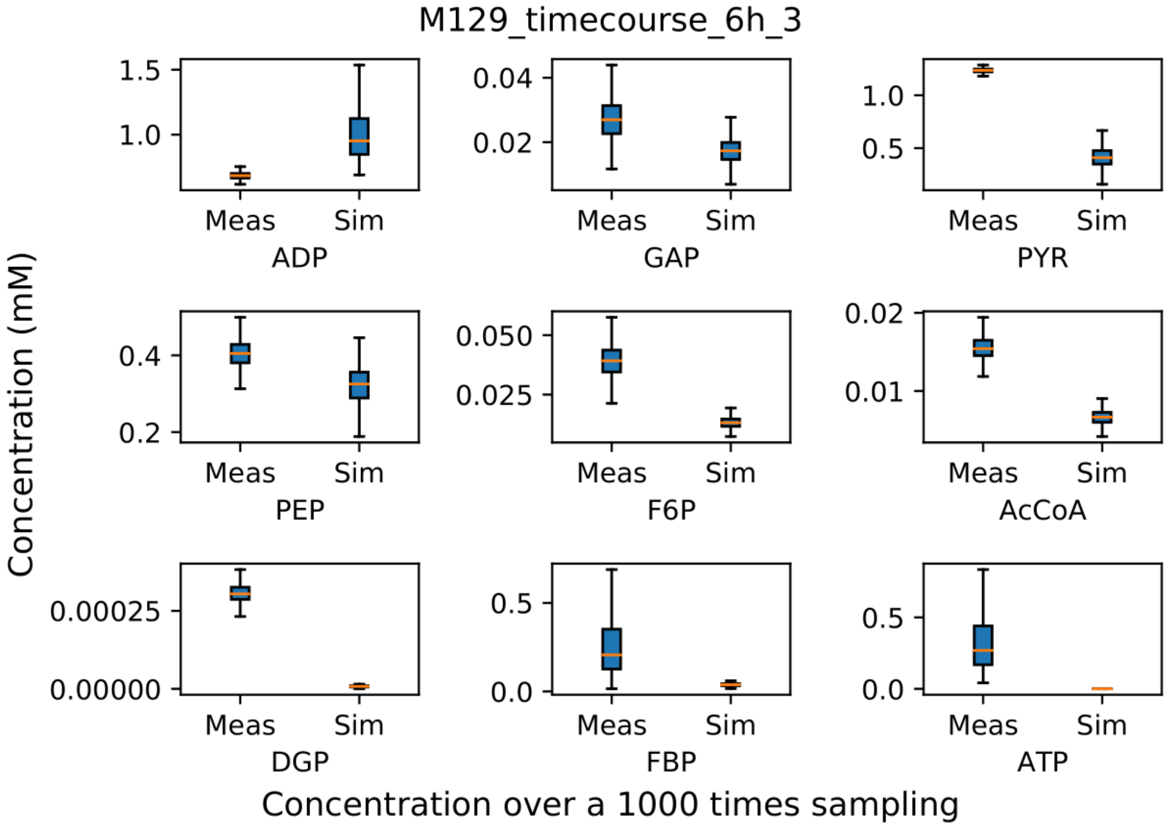


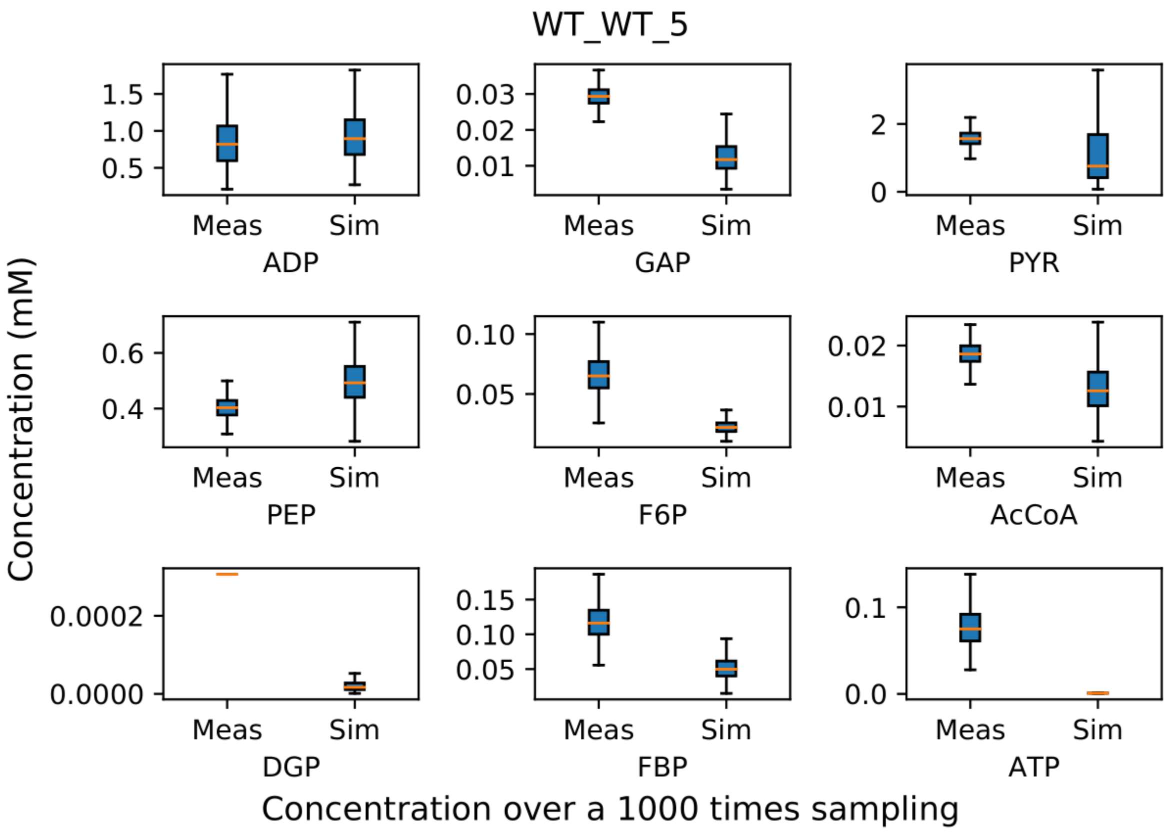
*Figure 2 Correlation of the parameter sets for model 3 that includes NoxE for the best 10 performing parameter sets.*

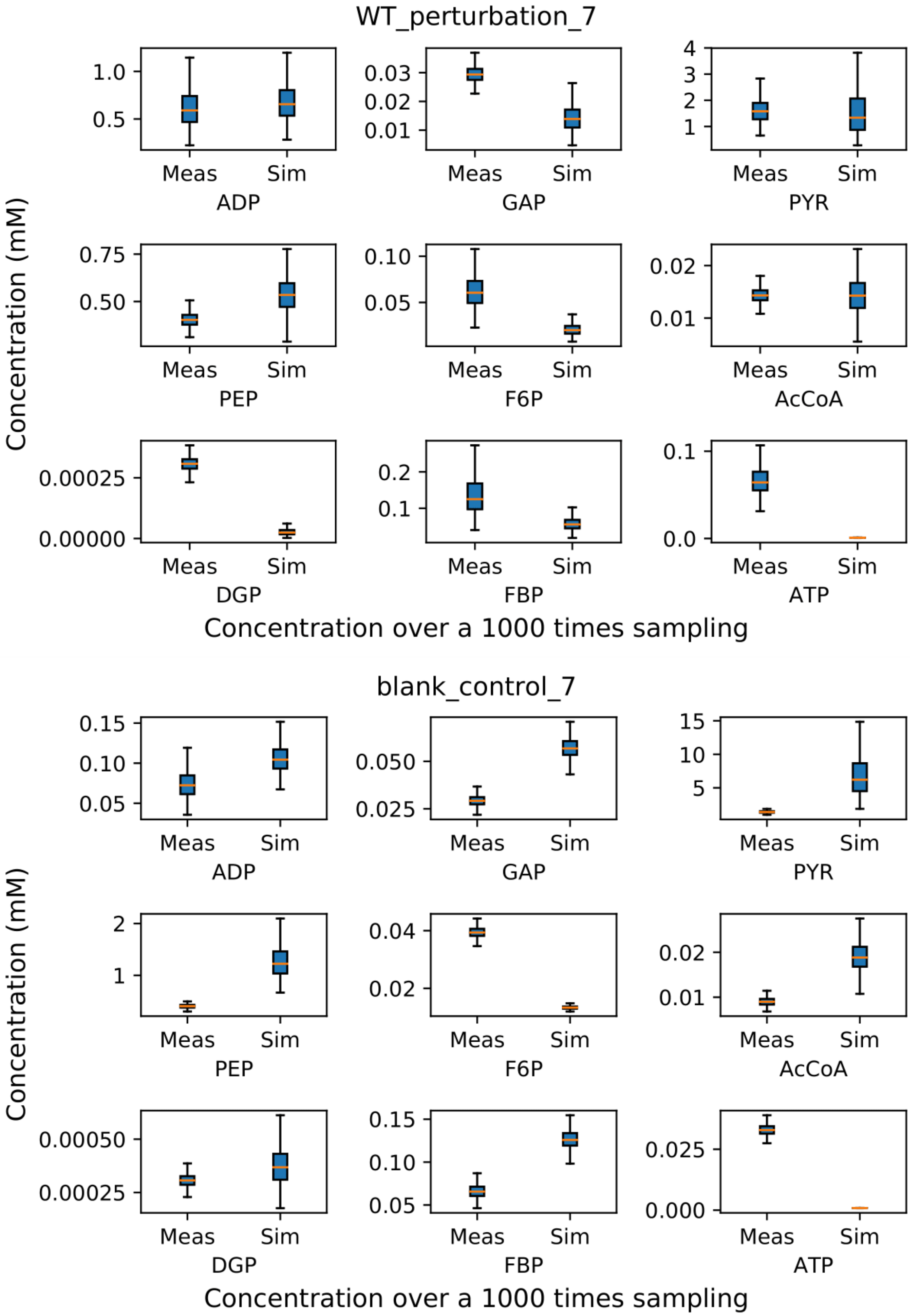
Parameter distributions for each of the 6 models over 100 parameter sets as well as heatmaps showing the correlation between parameters over all 100 fittings for each of the six model configurations are available upon request.

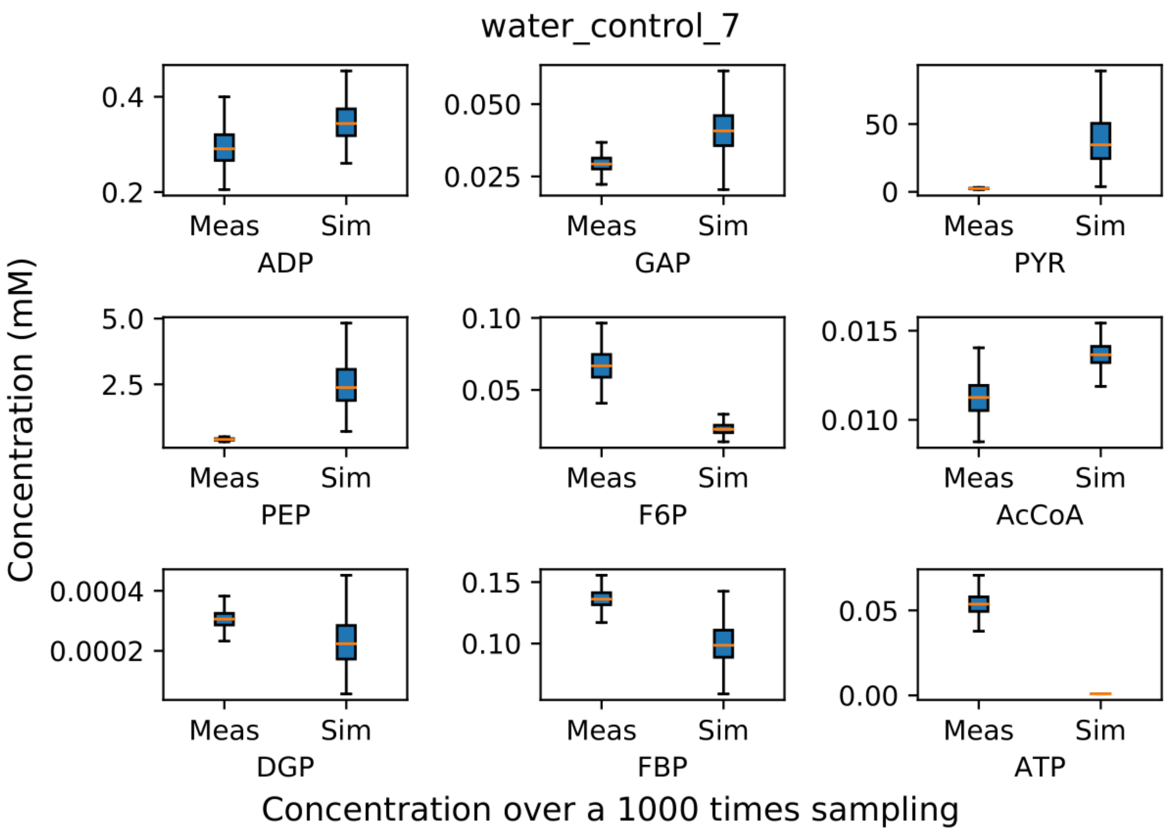
## Supplementary file 1 C Simulating 40 independent samples.

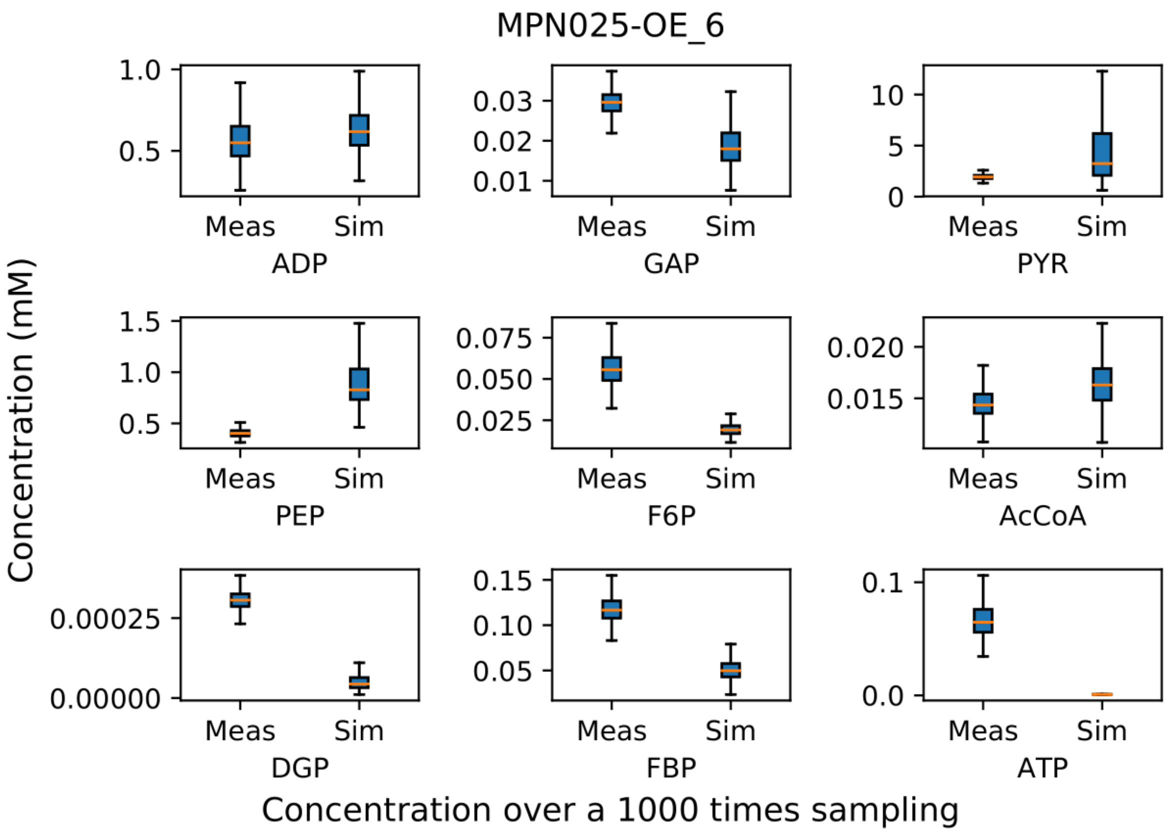
Metabolite concentrations measured and predicted using a 1000x sampling.

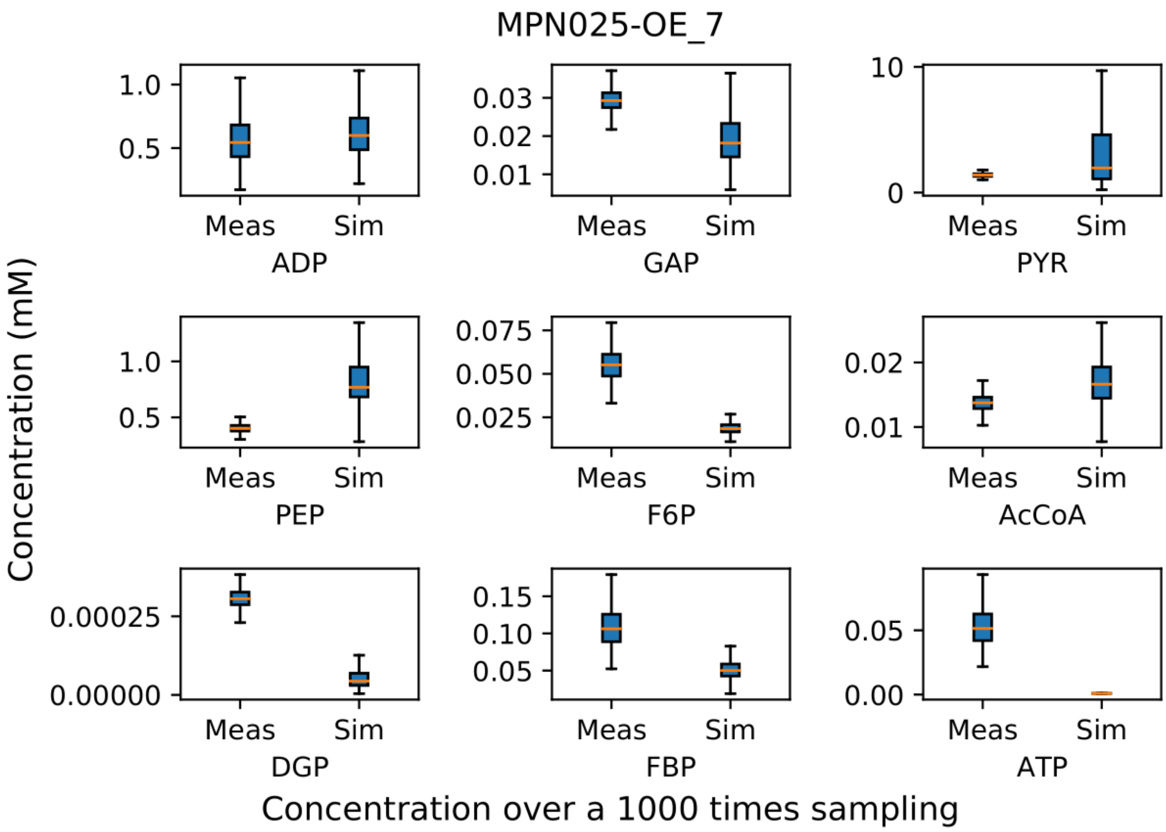


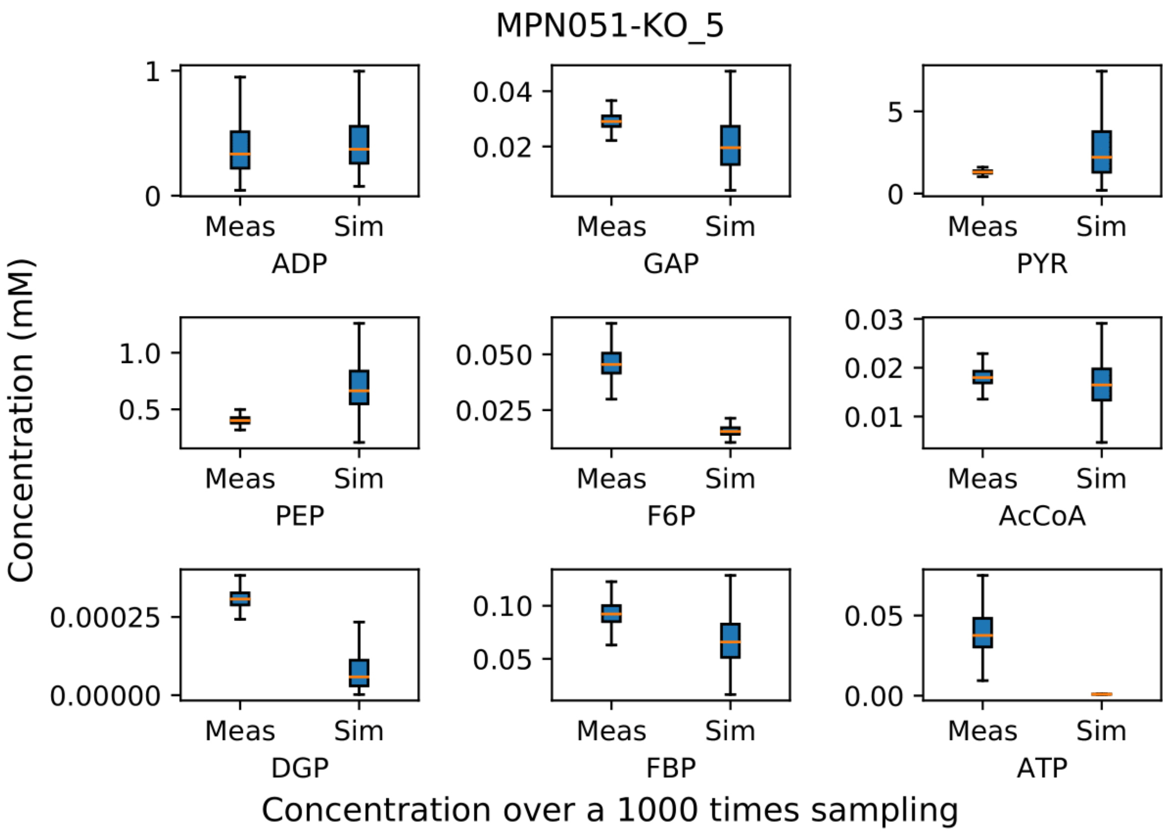



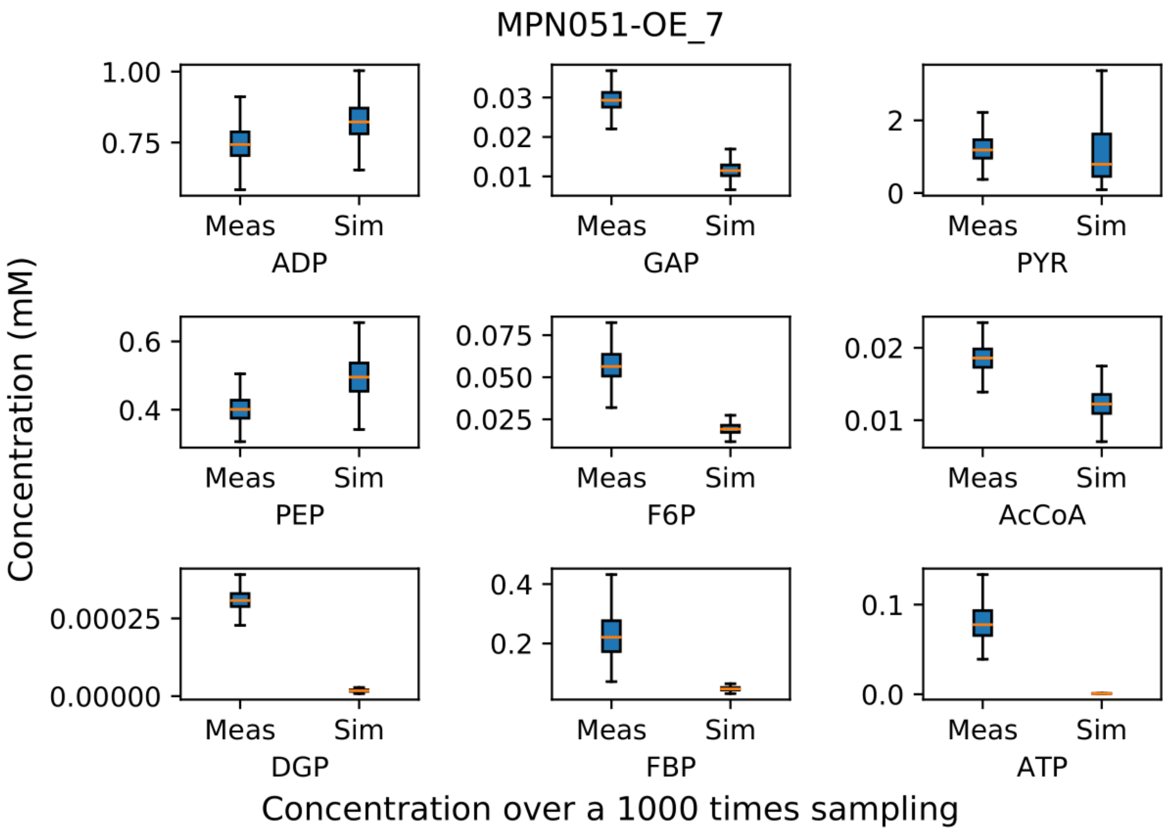

WT_perturbation_7
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling
blank_control_7
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

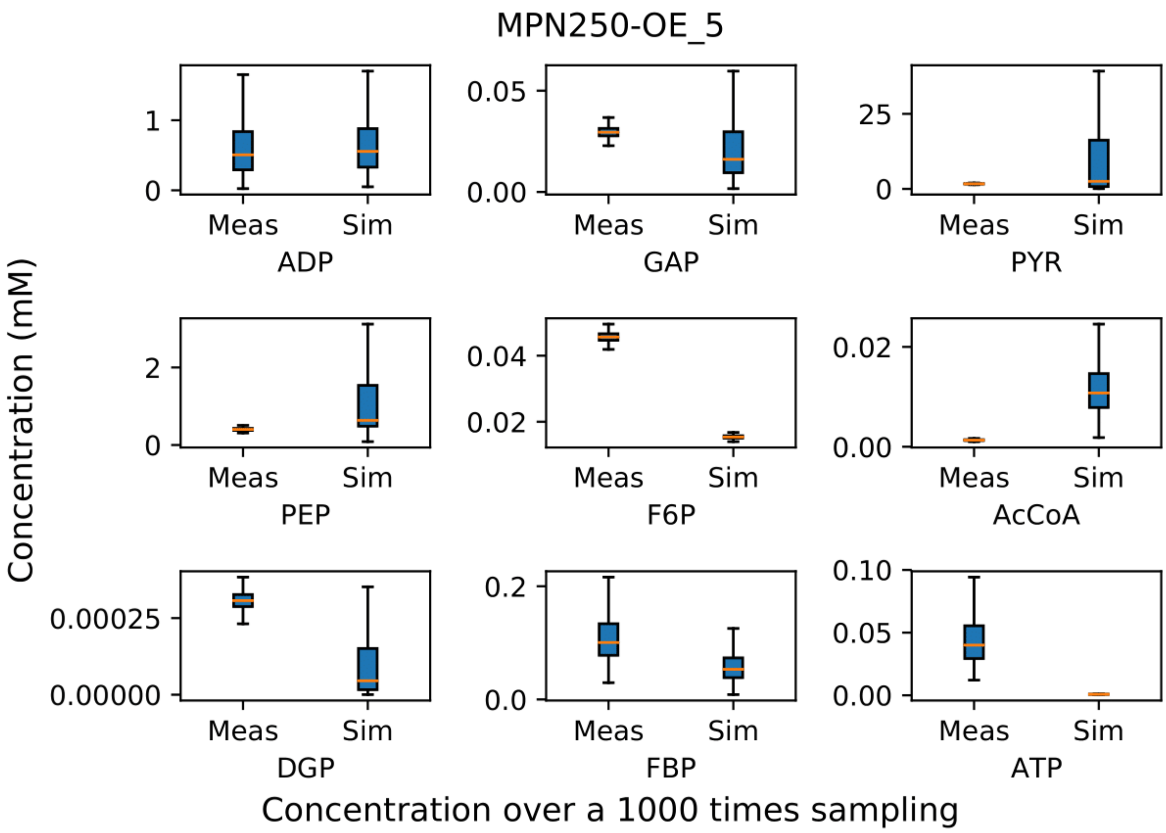

water_control_7
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

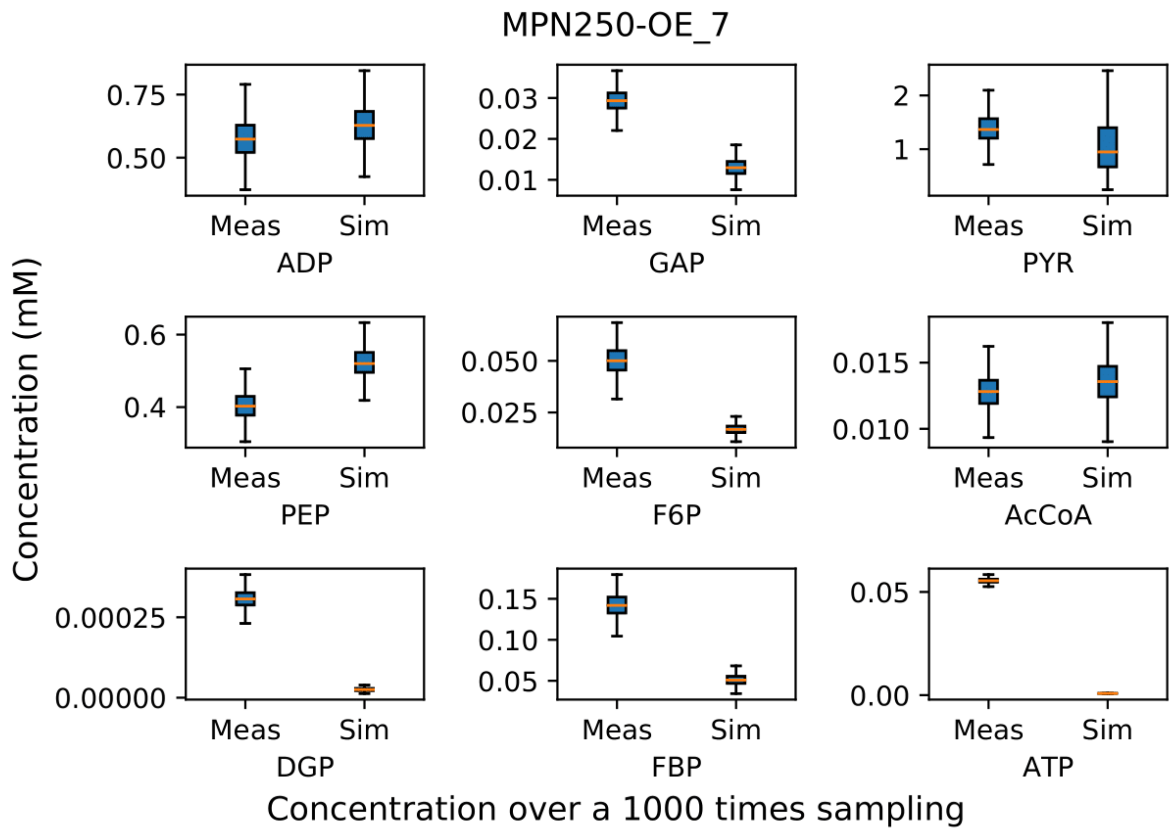

MPN025-OE_6
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

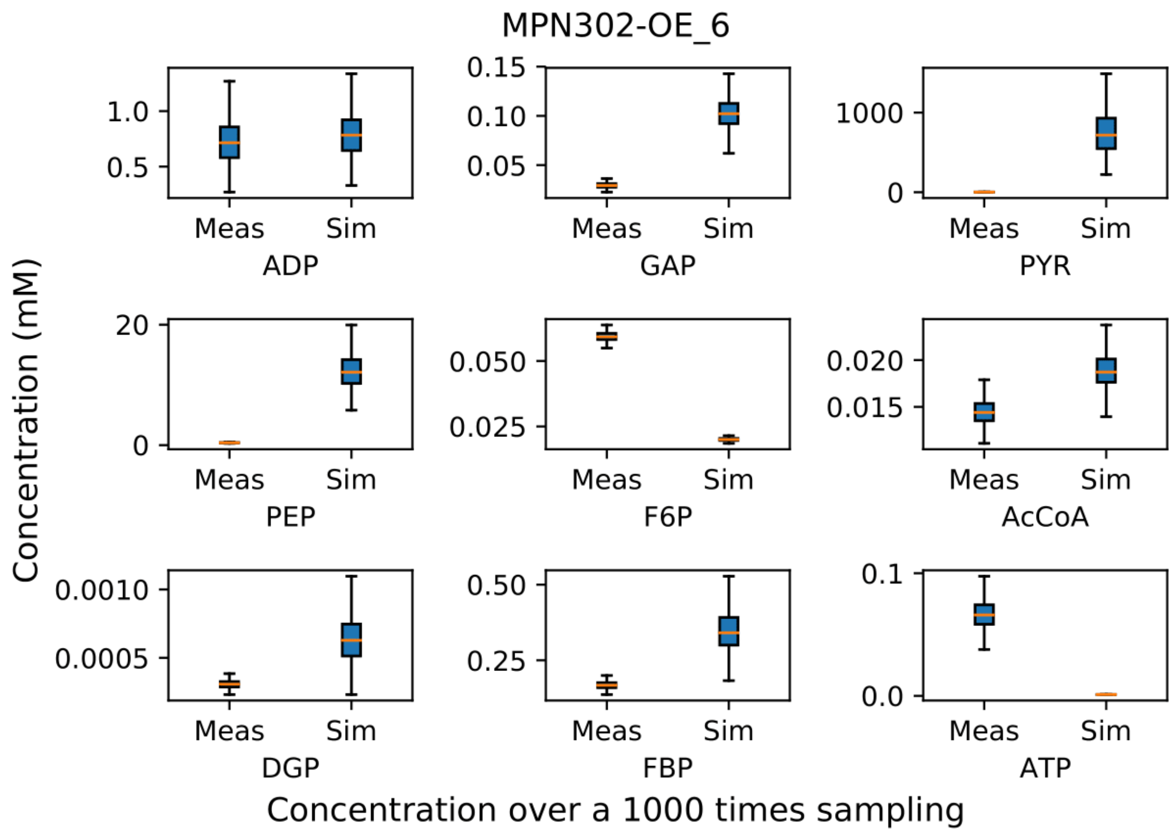

MPN025-OE_7
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

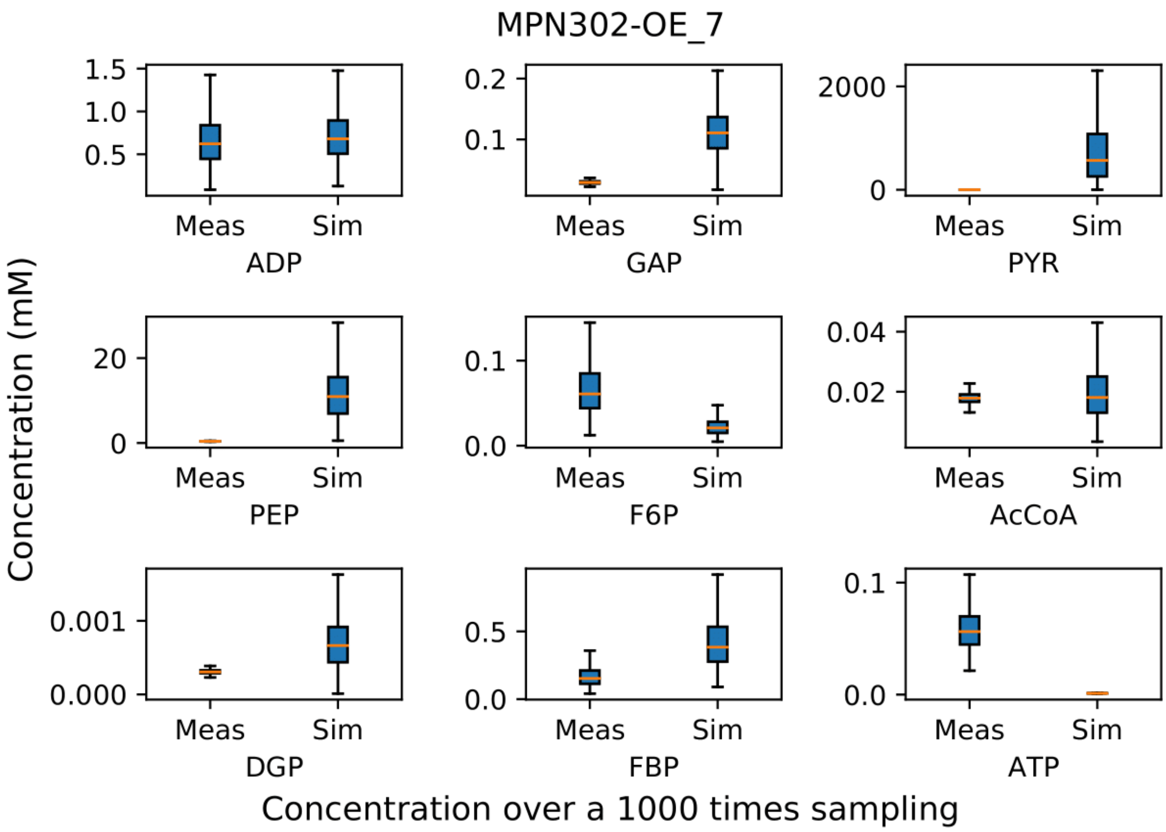

MPN051-KO_5
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

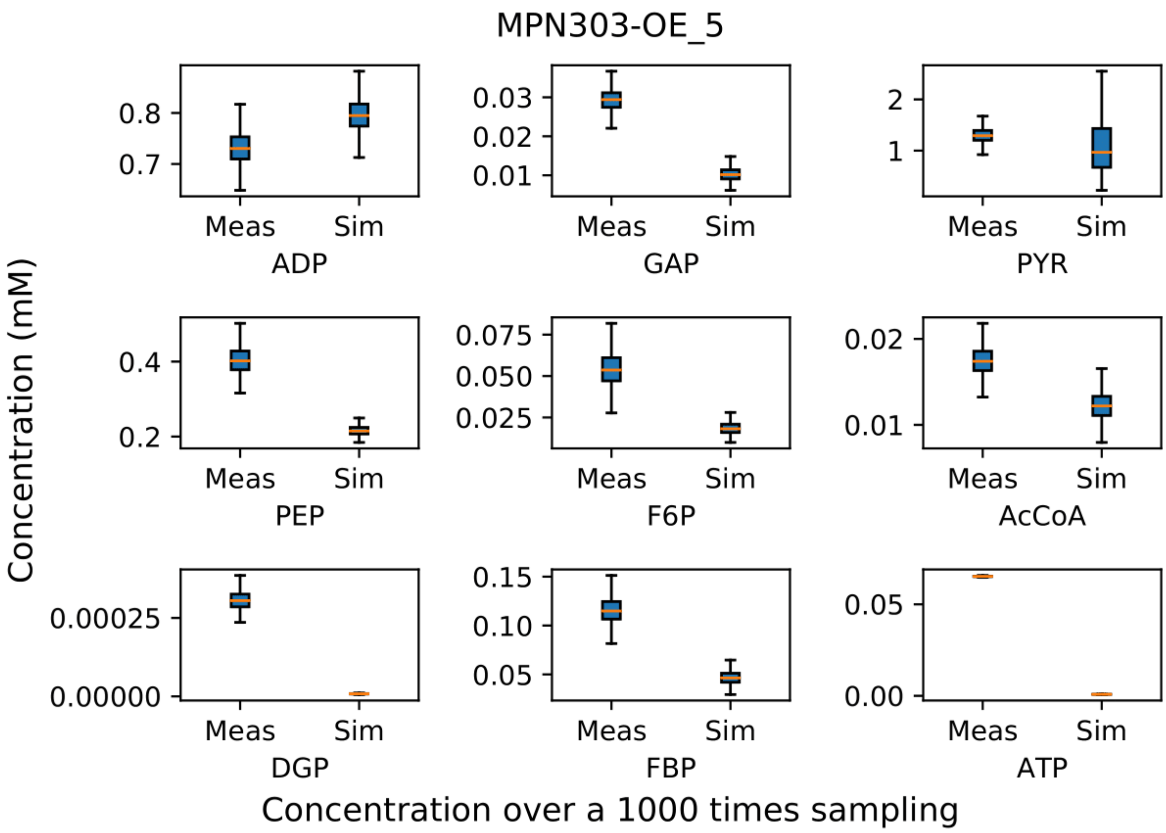

MPN051-OE_7
Concentration (mM)
1.00
0.75
Meas
Sim
ADP
0.03
0.02
0.01
Meas
Sim
GAP
2
0
Meas
Sim
PYR
0.6
0.4
Meas
Sim
PEP
0.075
0.050
0.025
Meas
Sim
F6P
0.02
0.01
Meas
Sim
AcCoA
0.00025
0.00000
Meas
Sim
DGP
0.4
0.2
Meas
Sim
FBP
0.1
0.0
Meas
Sim
ATP
Concentration over a 1000 times sampling

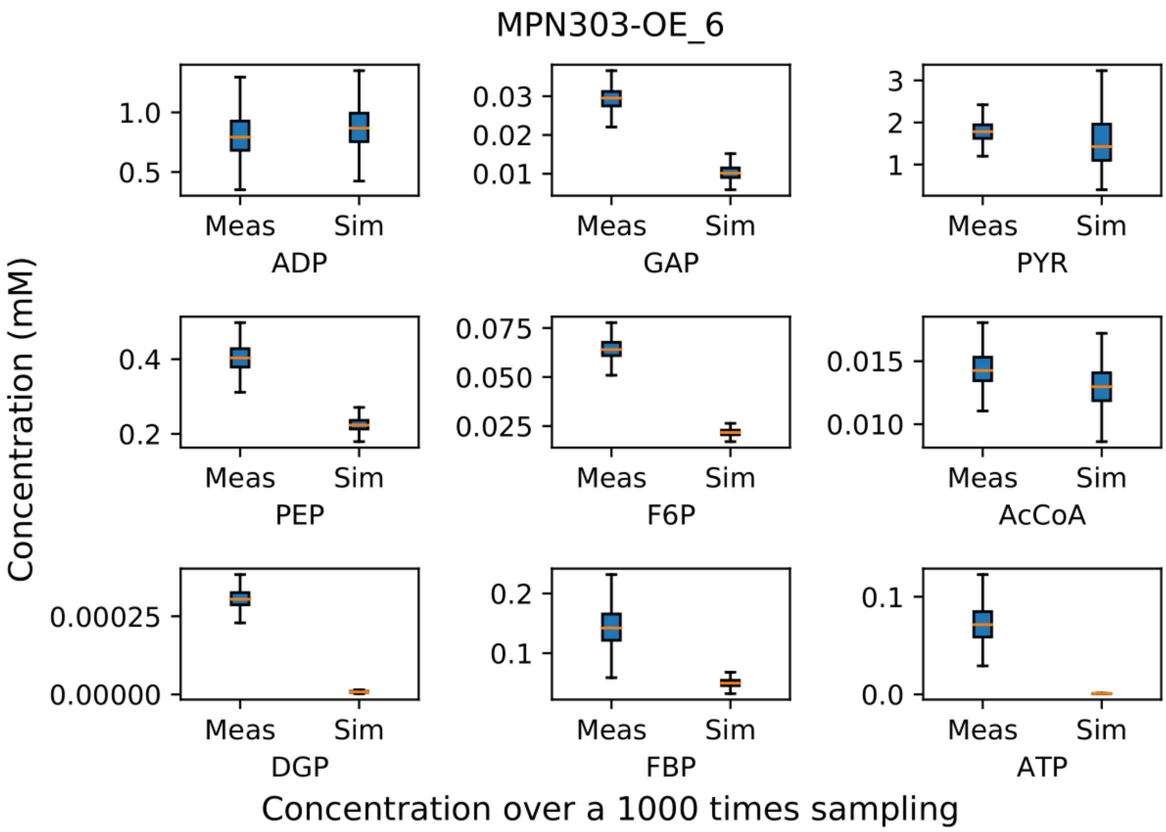

MPN250-OE_5
Concentration (mM)
1
0
Meas
Sim
ADP
0.05
0.00
Meas
Sim
GAP
25
0
Meas
Sim
PYR
2
0
Meas
Sim
PEP
0.04
0.02
Meas
Sim
F6P
0.02
0.00
Meas
Sim
AcCoA
0.00025
0.00000
Meas
Sim
DGP
0.2
0.0
Meas
Sim
FBP
0.10
0.05
0.00
Meas
Sim
ATP
Concentration over a 1000 times sampling

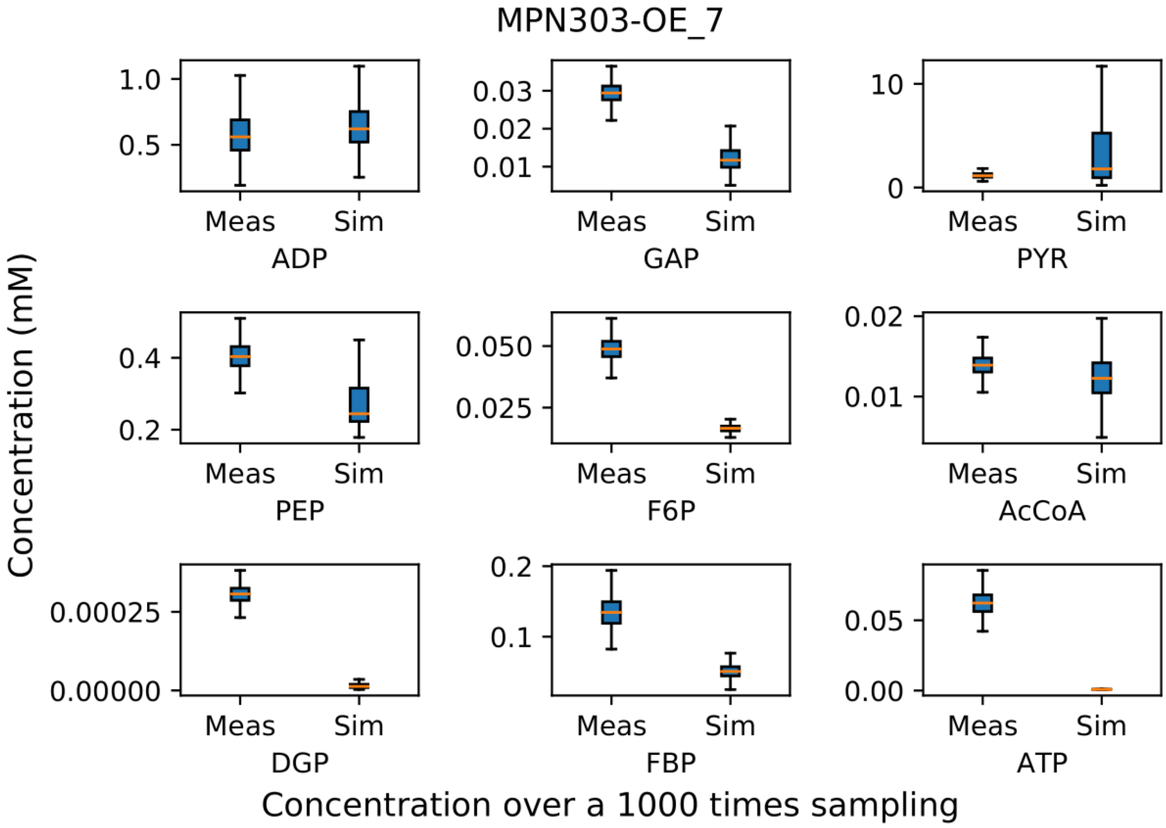

MPN250-OE_7
Concentration (mM)
0.75
0.50
Meas
Sim
ADP
0.03
0.02
0.01
Meas
Sim
GAP
2
1
Meas
Sim
PYR
0.6
0.4
Meas
Sim
PEP
0.050
0.025
Meas
Sim
F6P
0.015
0.010
Meas
Sim
AcCoA
0.00025
0.00000
Meas
Sim
DGP
0.15
0.10
0.05
Meas
Sim
FBP
0.05
0.00
Meas
Sim
ATP
Concentration over a 1000 times sampling

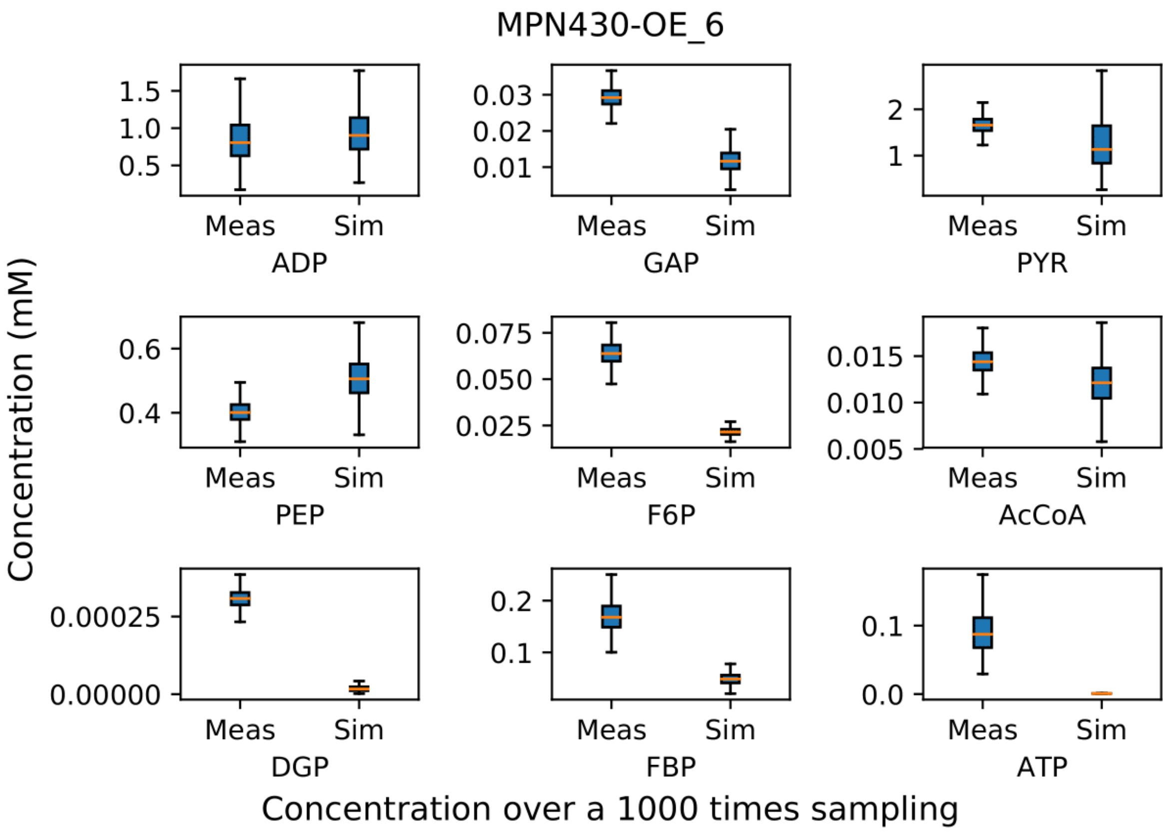

MPN302-OE_6
Concentration (mM)
1.0
0.5
Meas
Sim
ADP
0.15
0.10
0.05
Meas
Sim
GAP
1000
0
Meas
Sim
PYR
20
0
Meas
Sim
PEP
0.050
0.025
Meas
Sim
F6P
0.020
0.015
Meas
Sim
AcCoA
0.0010
0.0005
Meas
Sim
DGP
0.50
0.25
Meas
Sim
FBP
0.1
0.0
Meas
Sim
ATP
Concentration over a 1000 times sampling

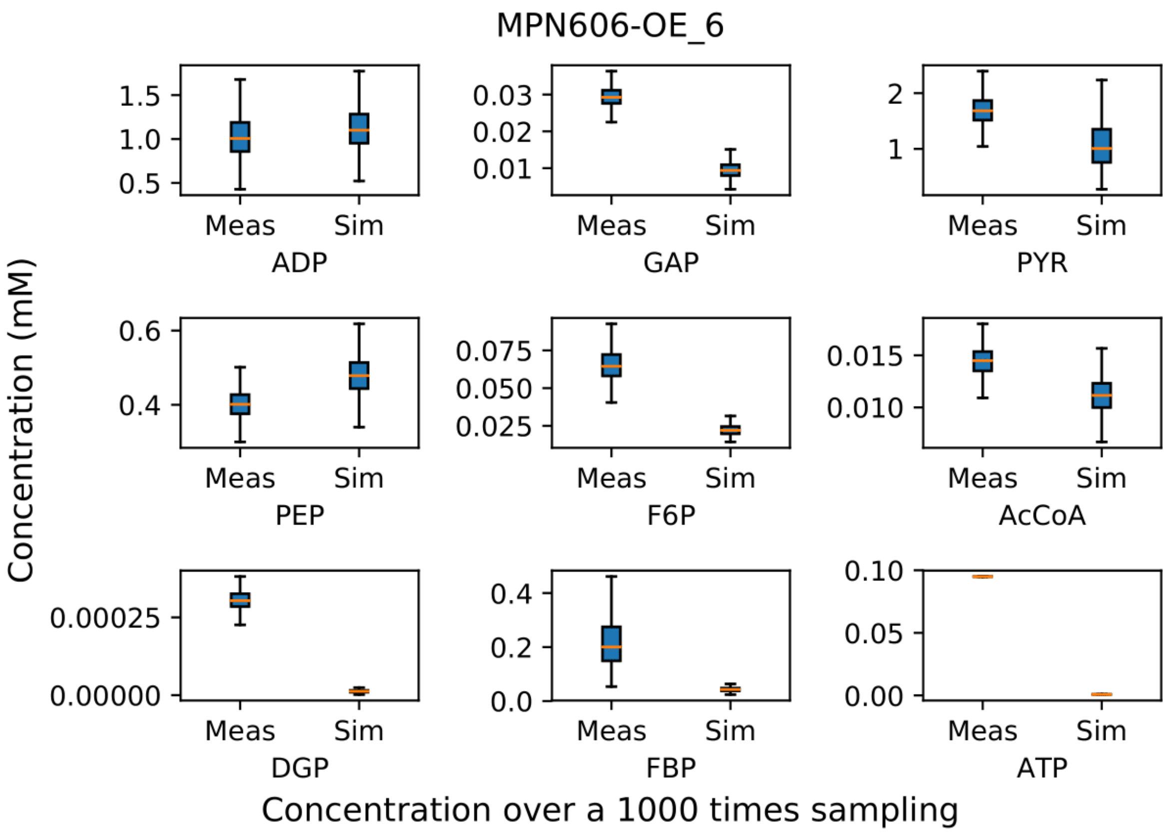

MPN302-OE_7
Concentration (mM)
Meas
Sim
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
1.5
1.0
0.5
0.2
0.1
2000
0
20
0.0
0.04
0.02
0.001
0.000
Concentration over a 1000 times sampling

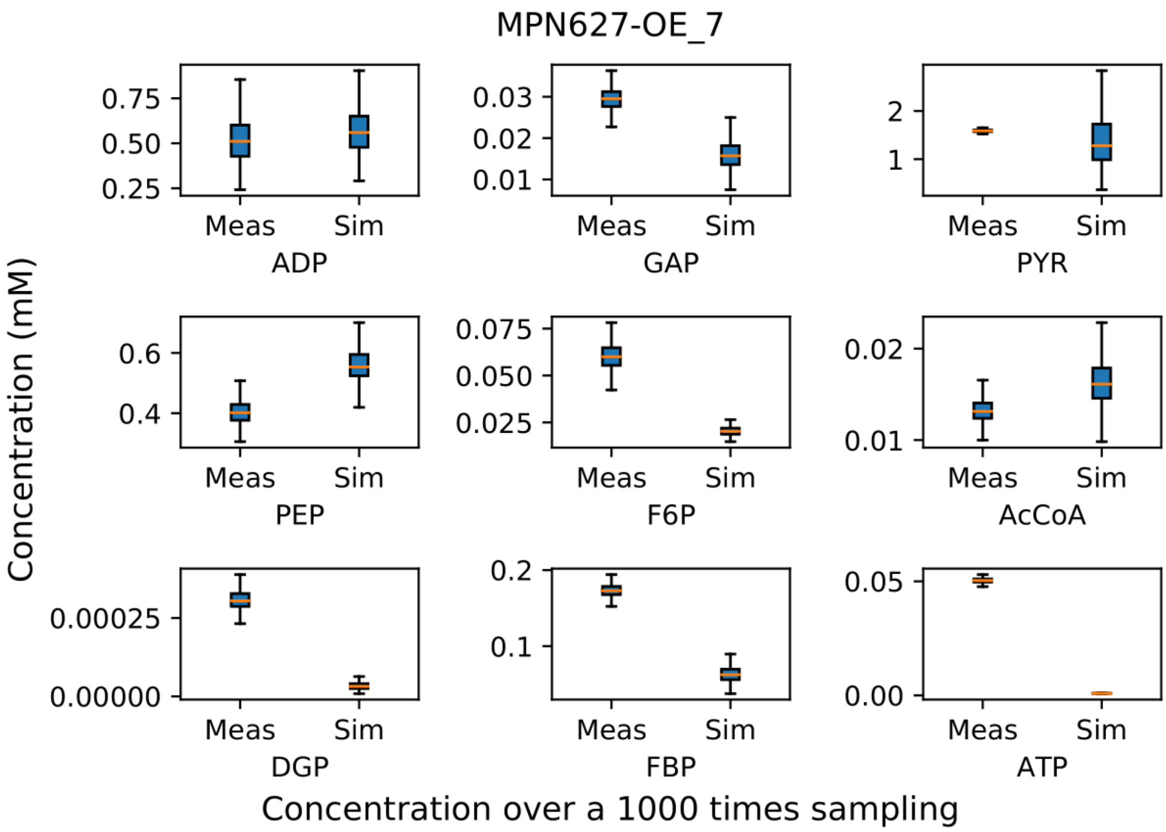

MPN303-OE_5
Concentration (mM)
Meas
Sim
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
0.8
0.7
0.03
0.02
0.01
2
1
0.4
0.2
0.075
0.050
0.025
0.00025
0.00000
0.15
0.10
0.05
0.00
Concentration over a 1000 times sampling

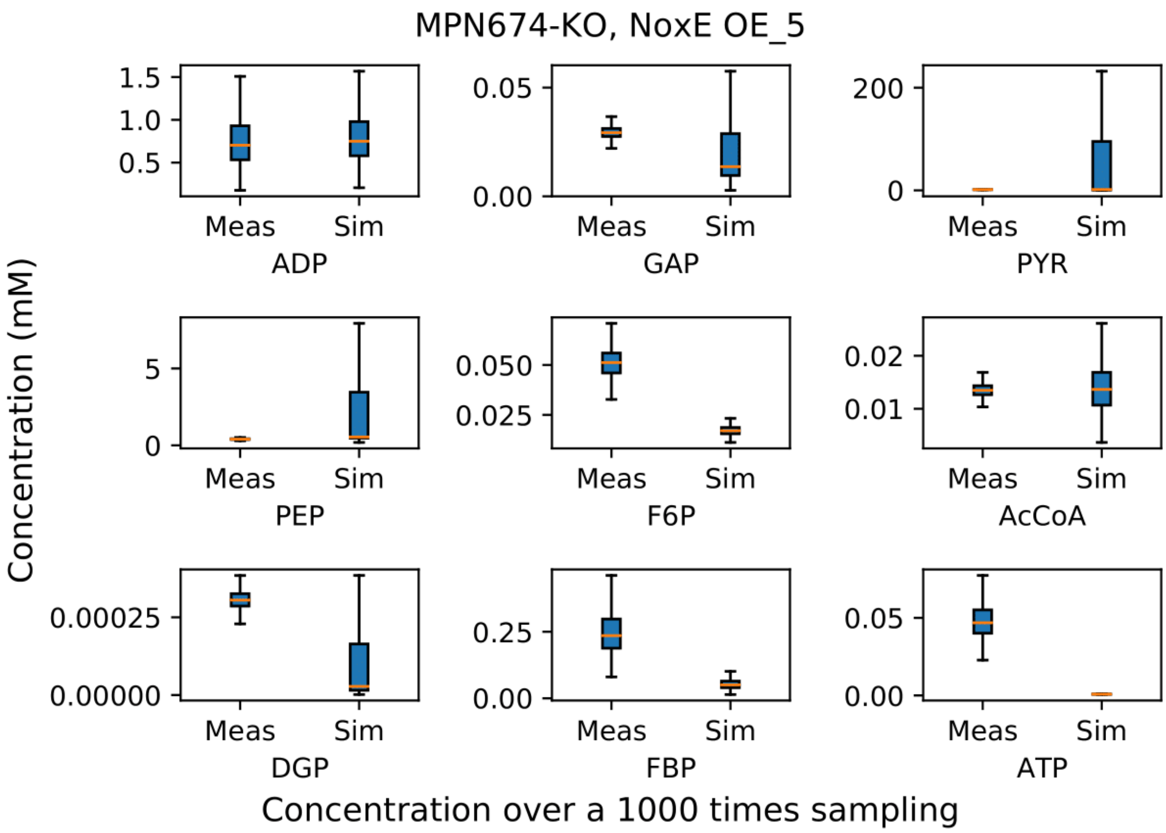

MPN303-OE_6
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

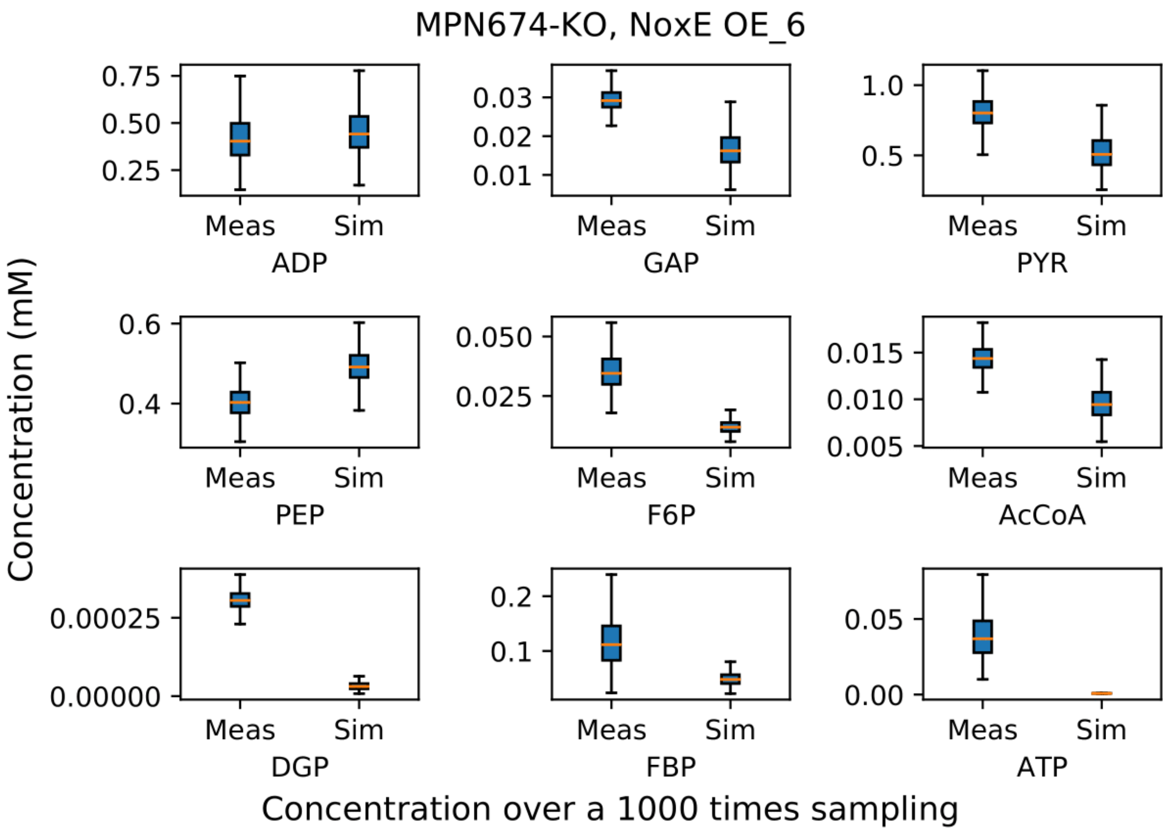

MPN303-OE_7
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

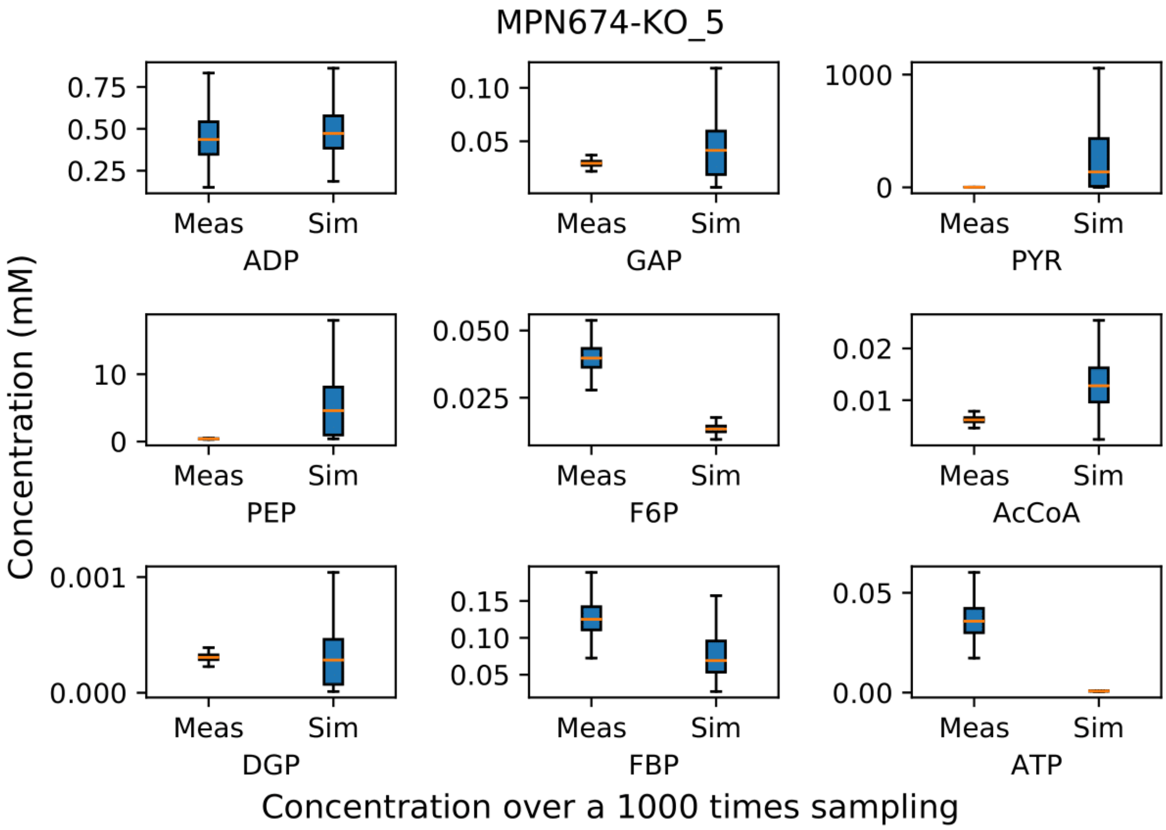

MPN430-OE_6
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

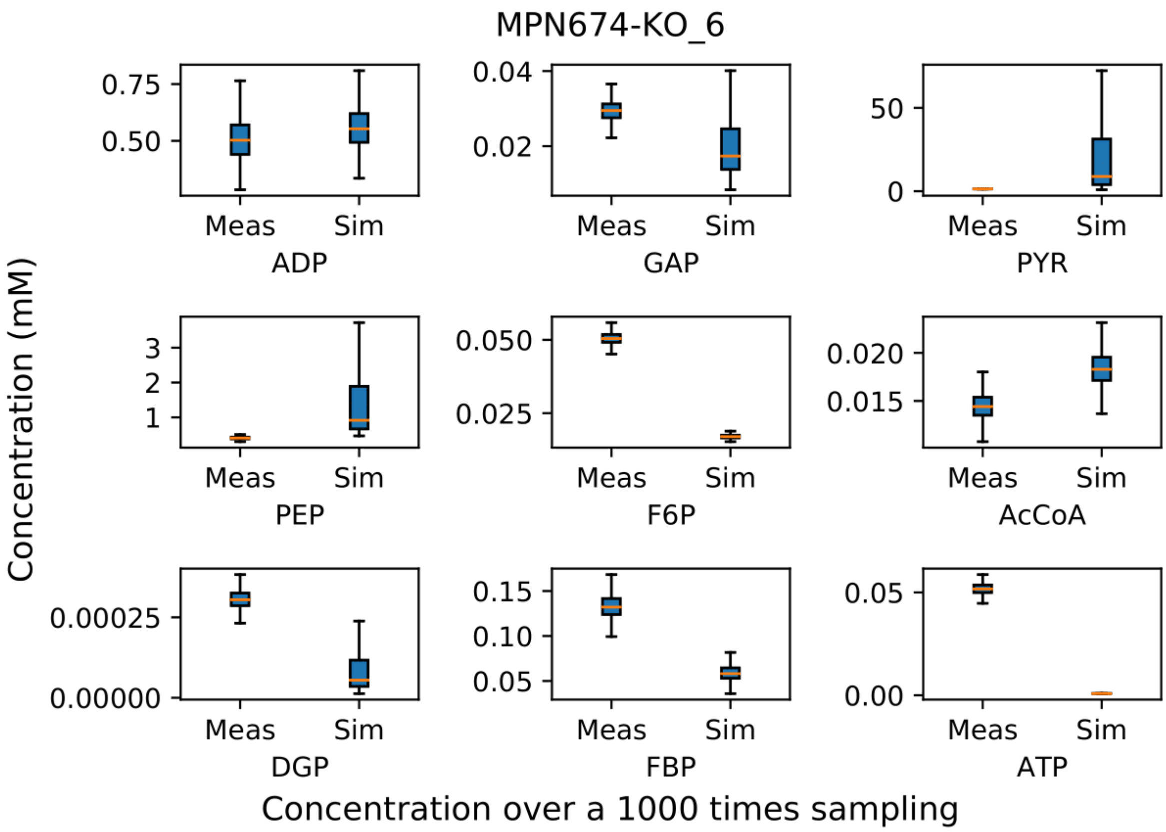

MPN606-OE_6
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

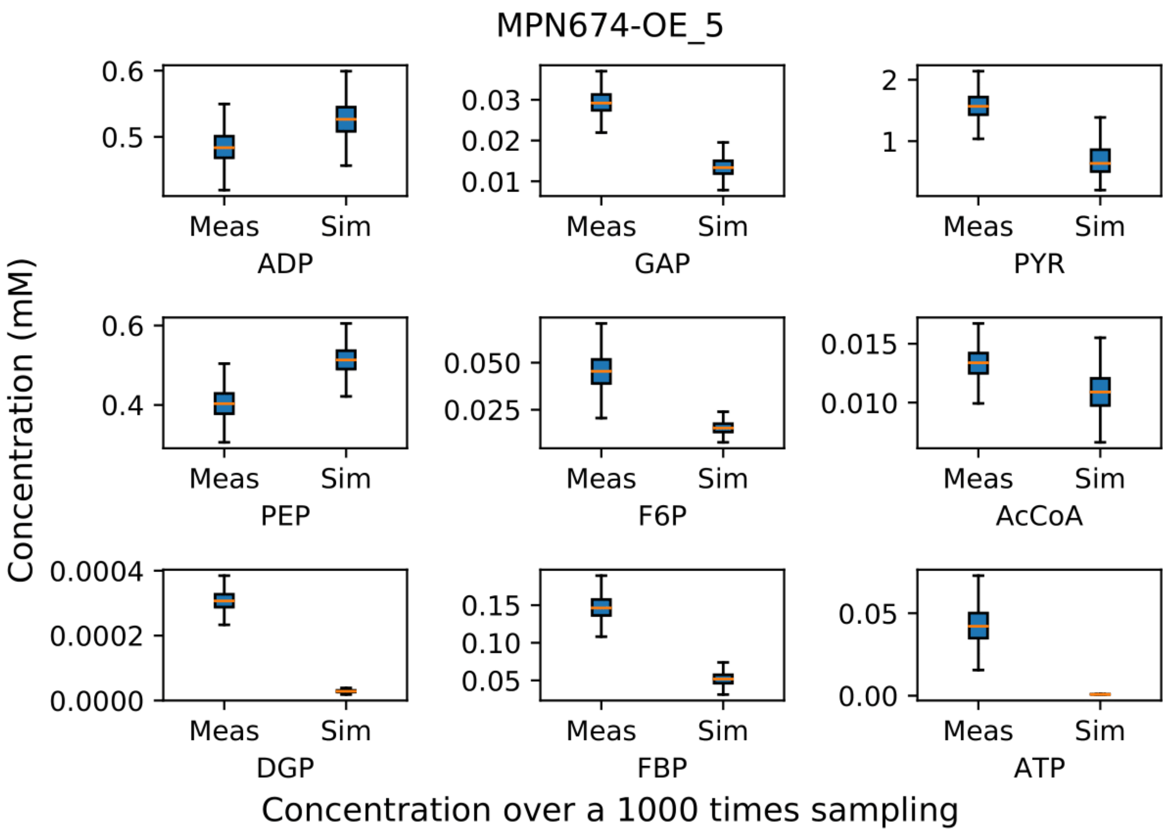

MPN627-OE_7
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

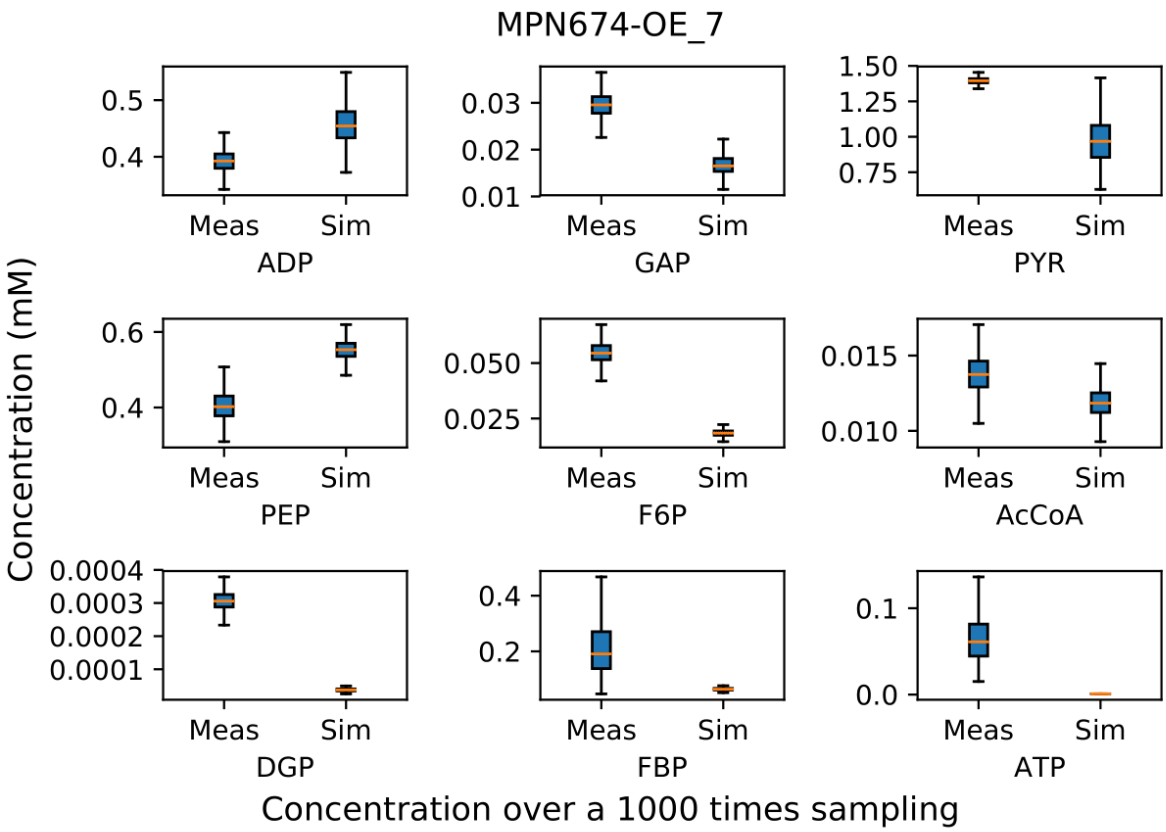

MPN674-KO, NoxE OE_5
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

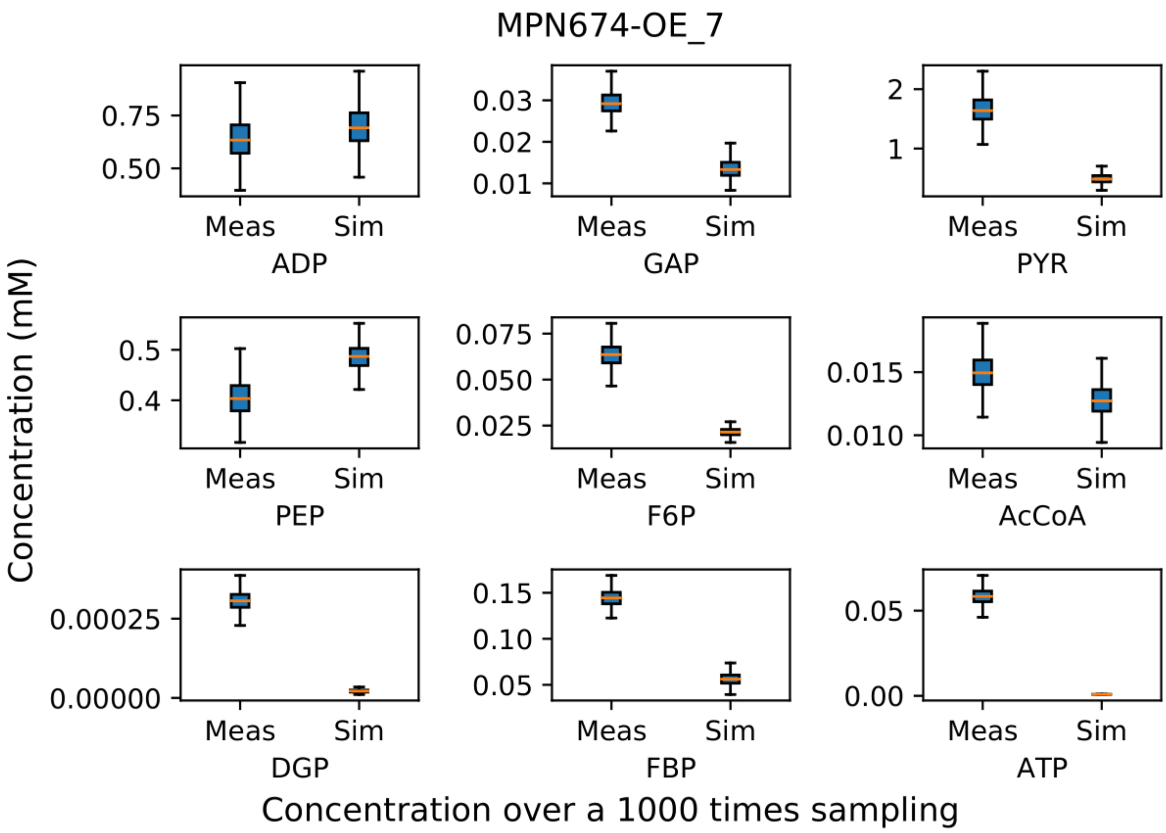

MPN674-KO, NoxE OE_6
Concentration (mM)
Meas
Sim
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Concentration over a 1000 times sampling

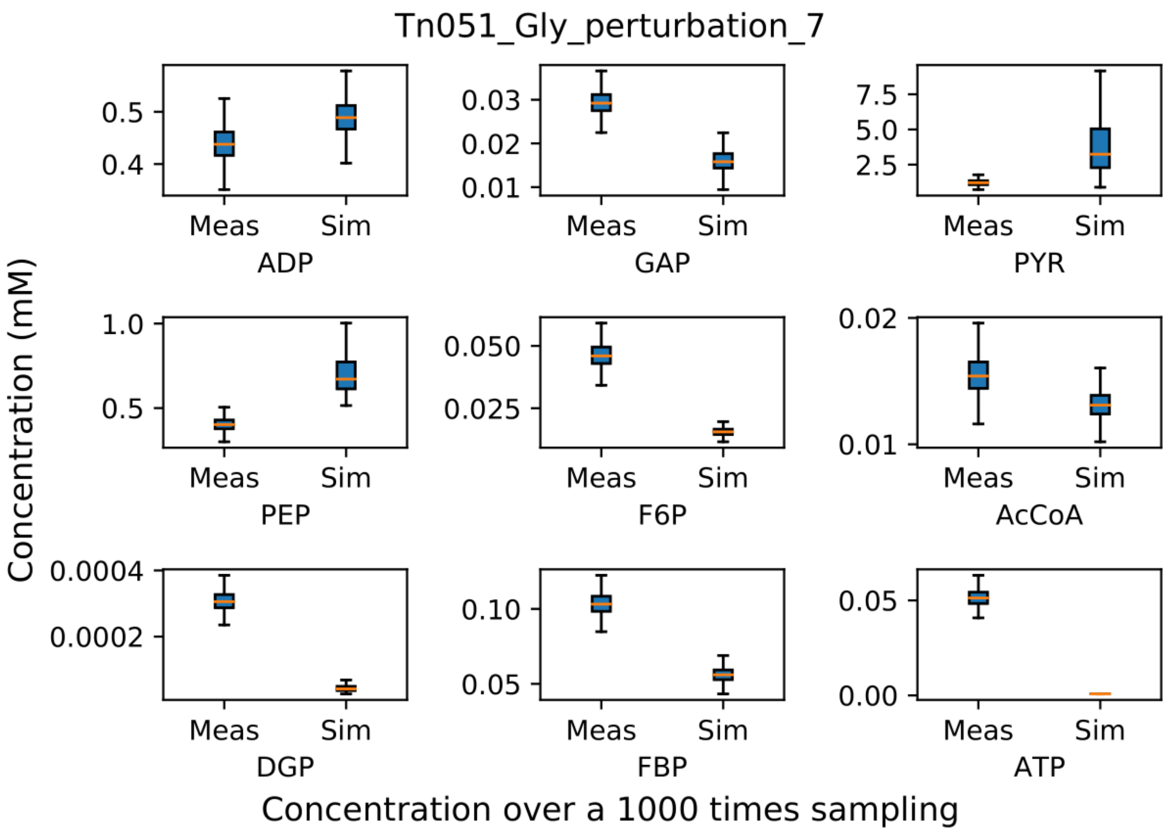

MPN674-KO_5
Concentration (mM)
Meas
Sim
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Concentration over a 1000 times sampling

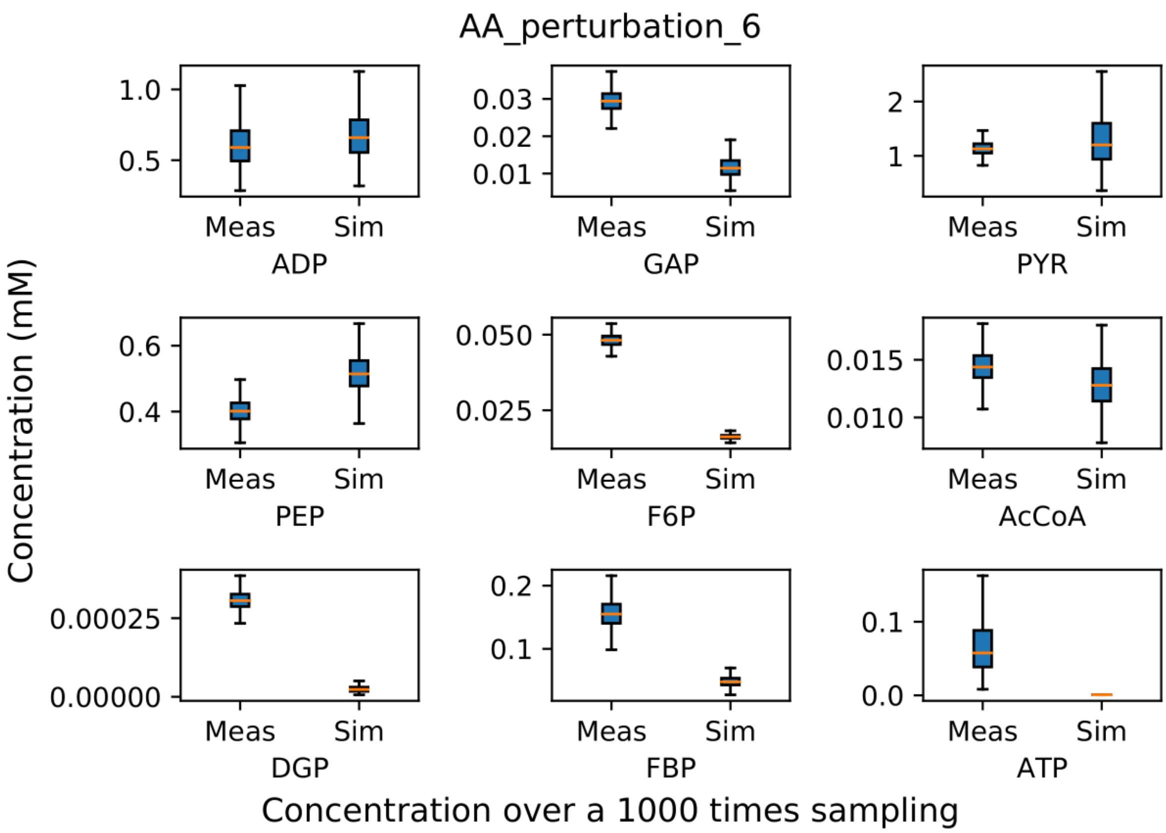

MPN674-KO_6
Concentration (mM)
0.75
0.50
Meas
Sim
ADP
0.04
0.02
GAP
50
0
PYR
3
2
1
PEP
0.050
0.025
F6P
0.020
0.015
AcCoA
0.00025
0.00000
DGP
0.15
0.10
0.05
FBP
0.05
0.00
ATP
Concentration over a 1000 times sampling

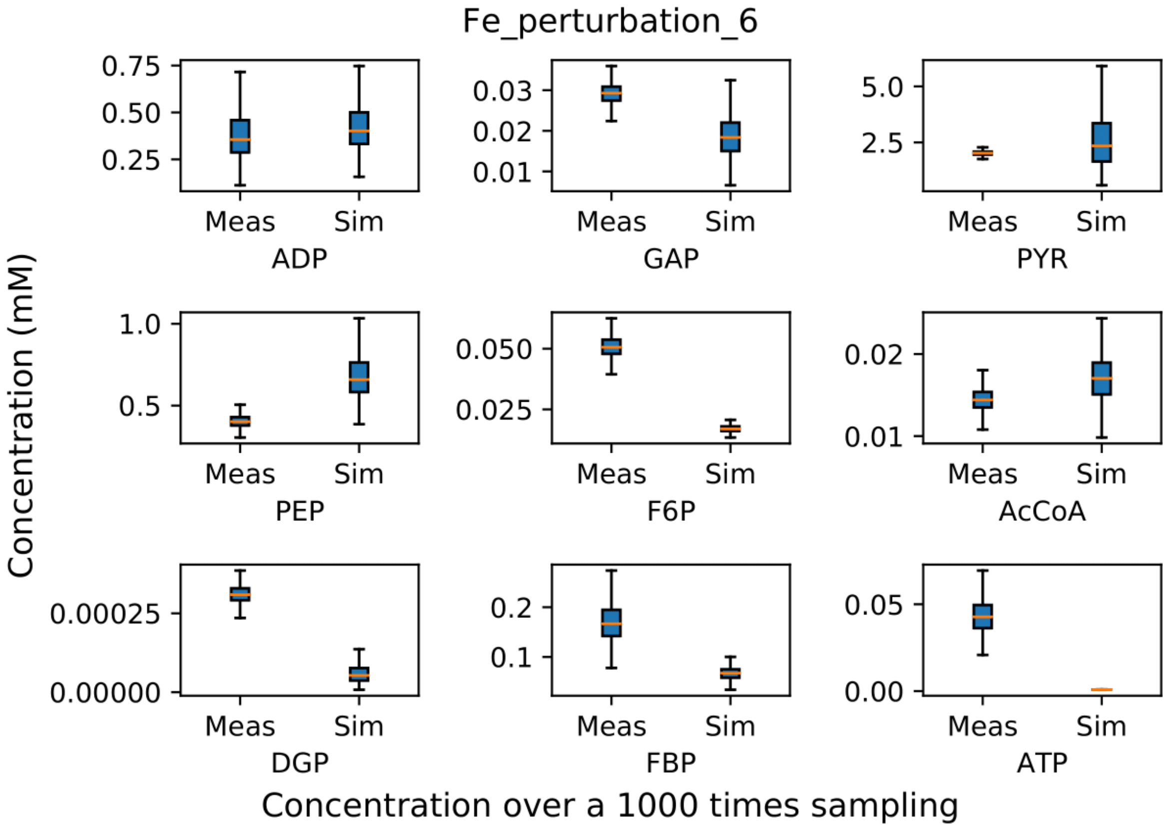

MPN674-OE_5
Concentration (mM)
0.6
0.5
Meas
Sim
ADP
0.03
0.02
0.01
GAP
2
1
PYR
0.6
0.4
PEP
0.050
0.025
F6P
0.015
0.010
AcCoA
0.0004
0.0002
0.0000
DGP
0.15
0.10
0.05
FBP
0.05
0.00
ATP
Concentration over a 1000 times sampling

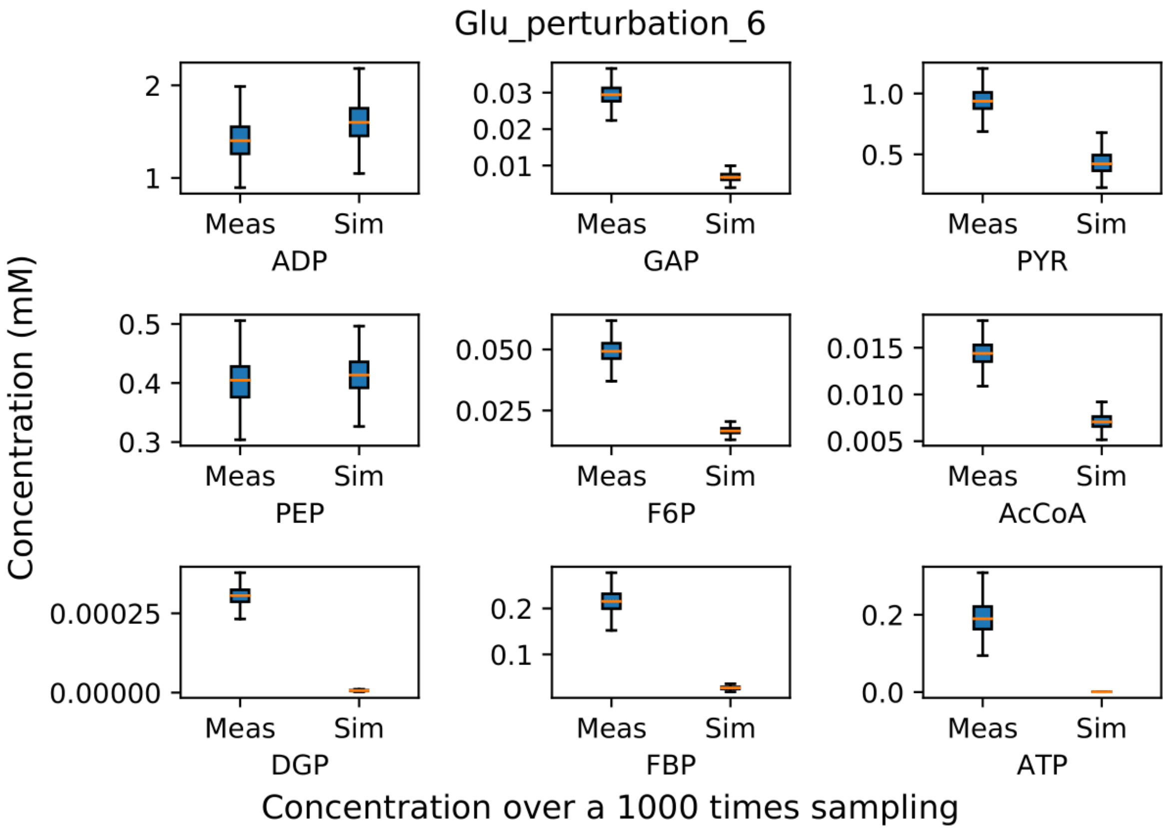

MPN674-OE_7
Concentration (mM)
0.5
0.4
Meas
Sim
ADP
0.03
0.02
0.01
GAP
1.50
1.25
1.00
0.75
PYR
0.6
0.4
PEP
0.050
0.025
F6P
0.015
0.010
AcCoA
0.0004
0.0003
0.0002
0.0001
DGP
0.4
0.2
FBP
0.1
0.0
ATP
Concentration over a 1000 times sampling

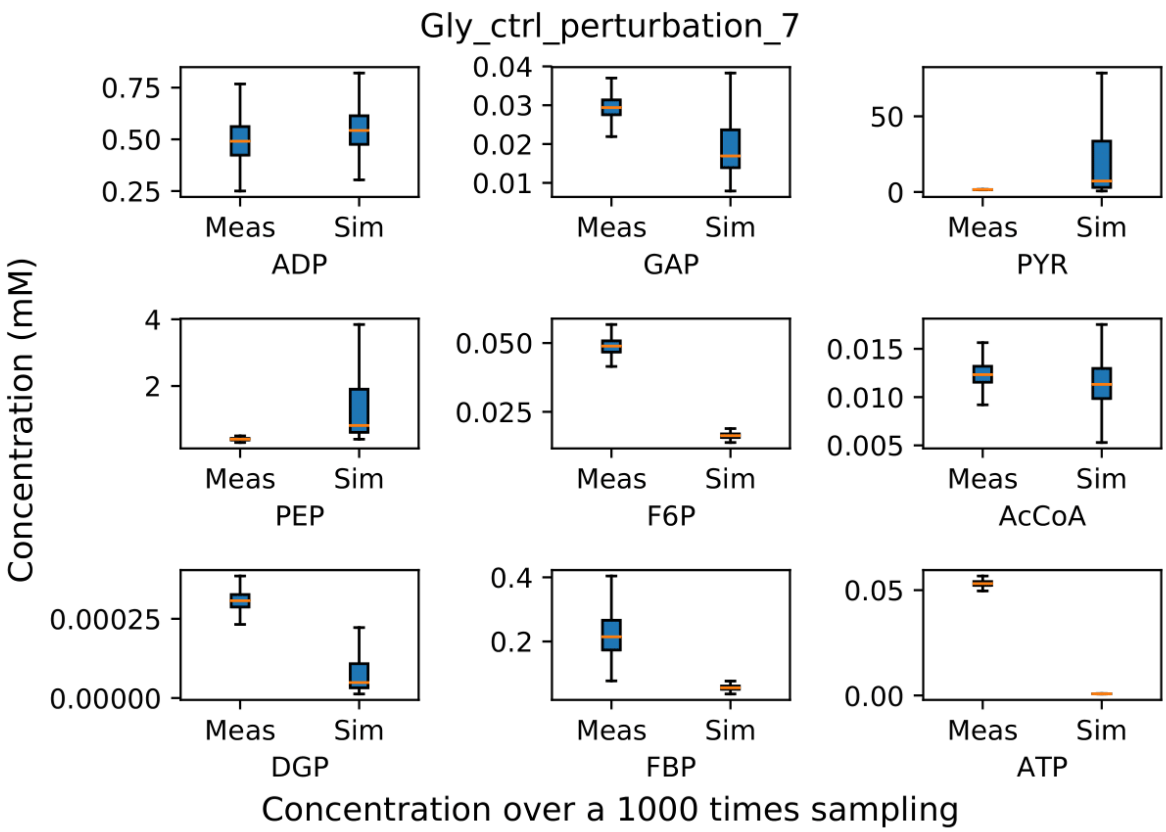

MPN674-OE_7
Concentration (mM)
0.75
0.50
Meas
Sim
ADP
0.03
0.02
0.01
GAP
2
1
PYR
0.5
0.4
PEP
0.075
0.050
0.025
F6P
0.015
0.010
AcCoA
0.00025
0.00000
DGP
0.15
0.10
0.05
FBP
0.05
0.00
ATP
Concentration over a 1000 times sampling

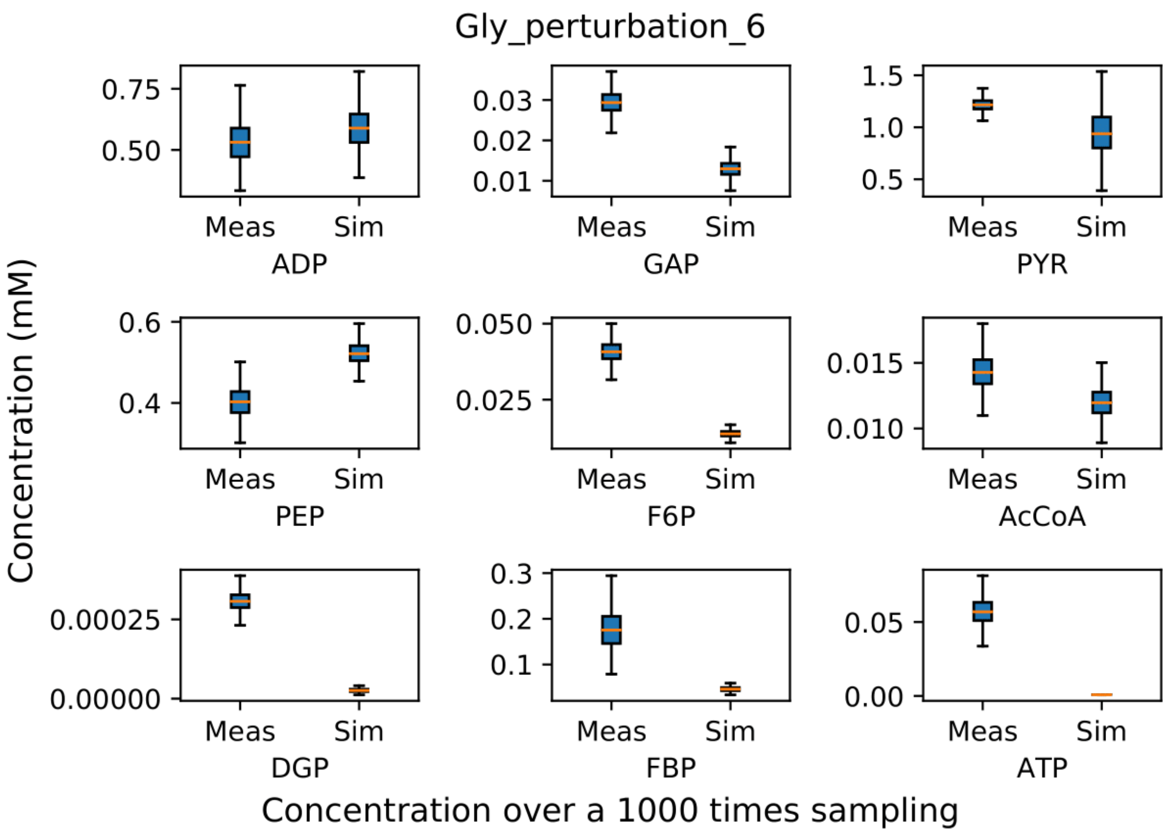

Tn051_Gly_perturbation_7
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

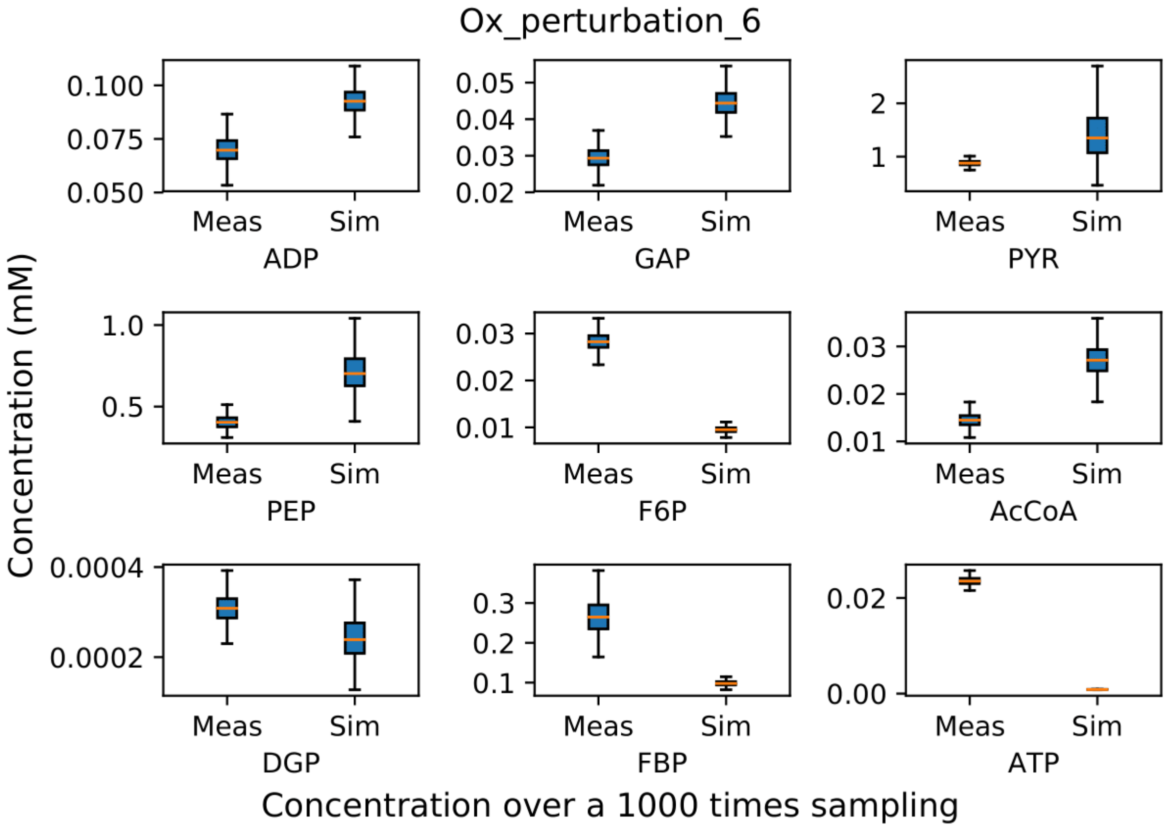

AA_perturbation_6
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

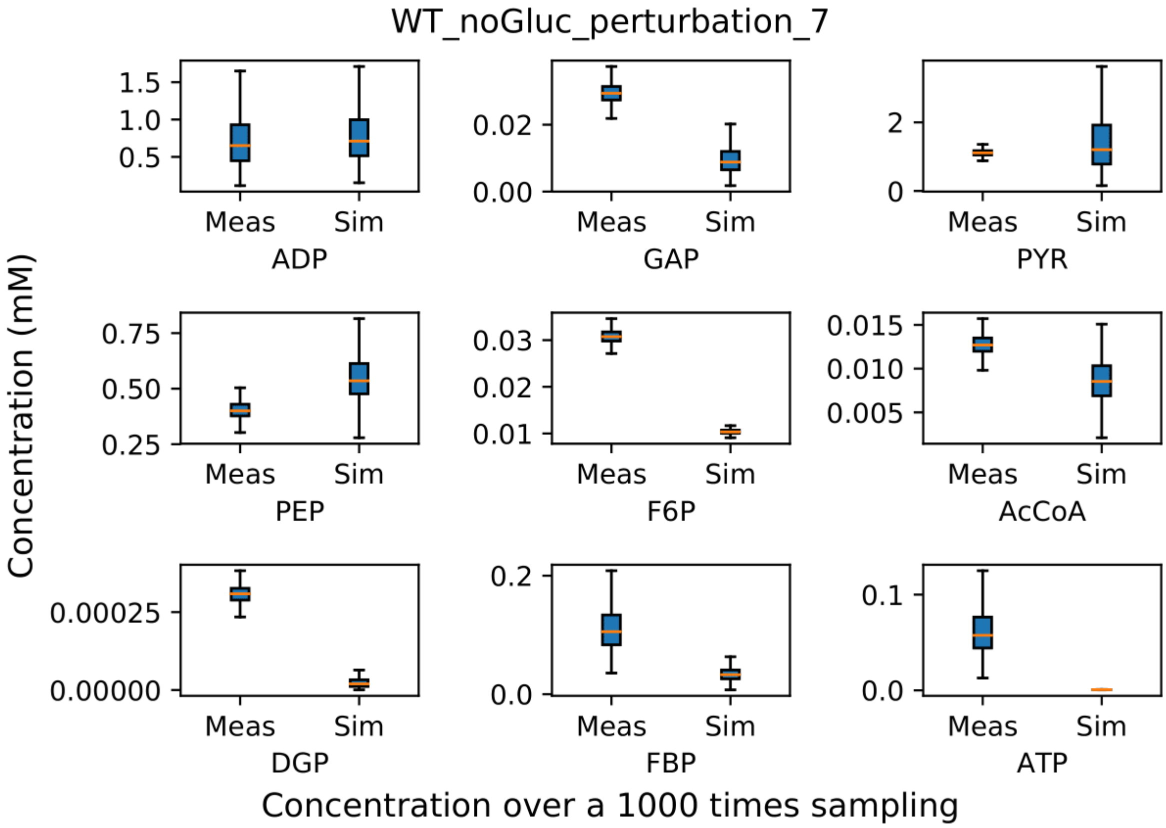

Fe_perturbation_6
Concentration (mM)
0.75
0.50
0.25
Meas
Sim
ADP
0.03
0.02
0.01
GAP
5.0
2.5
PYR
1.0
0.5
PEP
0.050
0.025
F6P
0.02
0.01
AcCoA
0.00025
0.00000
DGP
0.2
0.1
FBP
0.05
0.00
ATP
Concentration over a 1000 times sampling

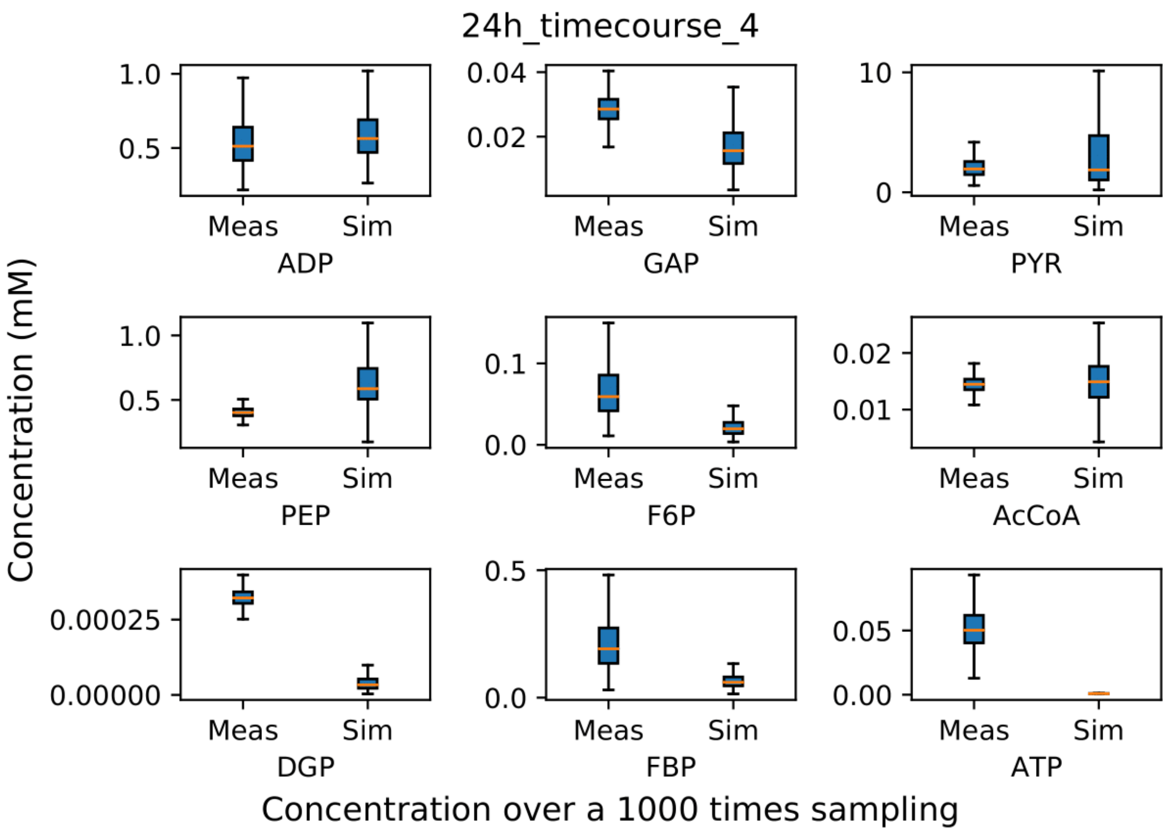

Glu_perturbation_6
Concentration (mM)
2
1
Meas
Sim
ADP
0.03
0.02
0.01
GAP
1.0
0.5
PYR
0.5
0.4
0.3
PEP
0.050
0.025
F6P
0.015
0.010
0.005
AcCoA
0.00025
0.00000
DGP
0.2
0.1
FBP
0.2
0.0
ATP
Concentration over a 1000 times sampling


Gly_ctrl_perturbation_7
Concentration (mM)
Meas
Sim
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
0.75
0.50
0.25
0.04
0.03
0.02
0.01
50
0
4
2
0.050
0.025
0.015
0.010
0.005
0.00025
0.00000
0.4
0.2
0.05
0.00
Concentration over a 1000 times sampling

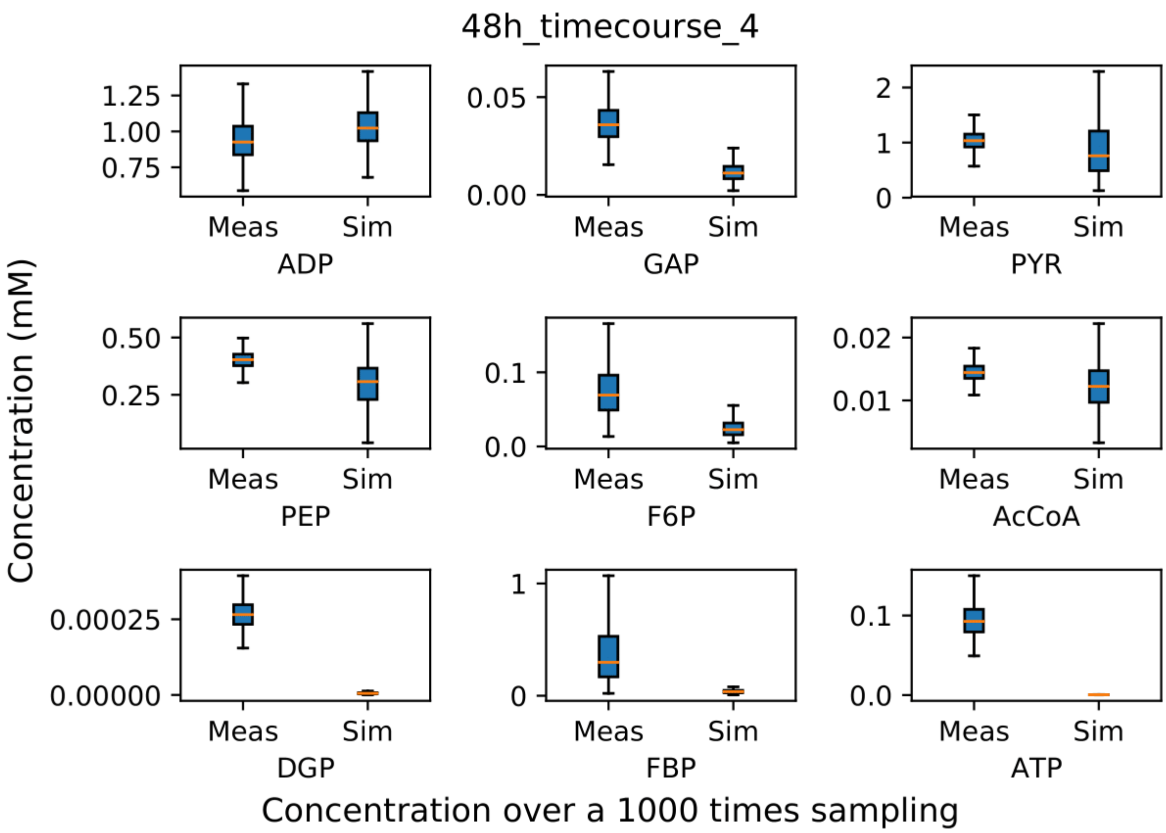

Gly_perturbation_6
Concentration (mM)
Meas
Sim
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
0.75
0.50
0.03
0.02
0.01
1.5
1.0
0.5
0.6
0.4
0.050
0.025
0.015
0.010
0.00025
0.00000
0.3
0.2
0.1
0.05
0.00
Concentration over a 1000 times sampling


Ox_perturbation_6
Concentration (mM)
Meas
Sim
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Concentration over a 1000 times sampling

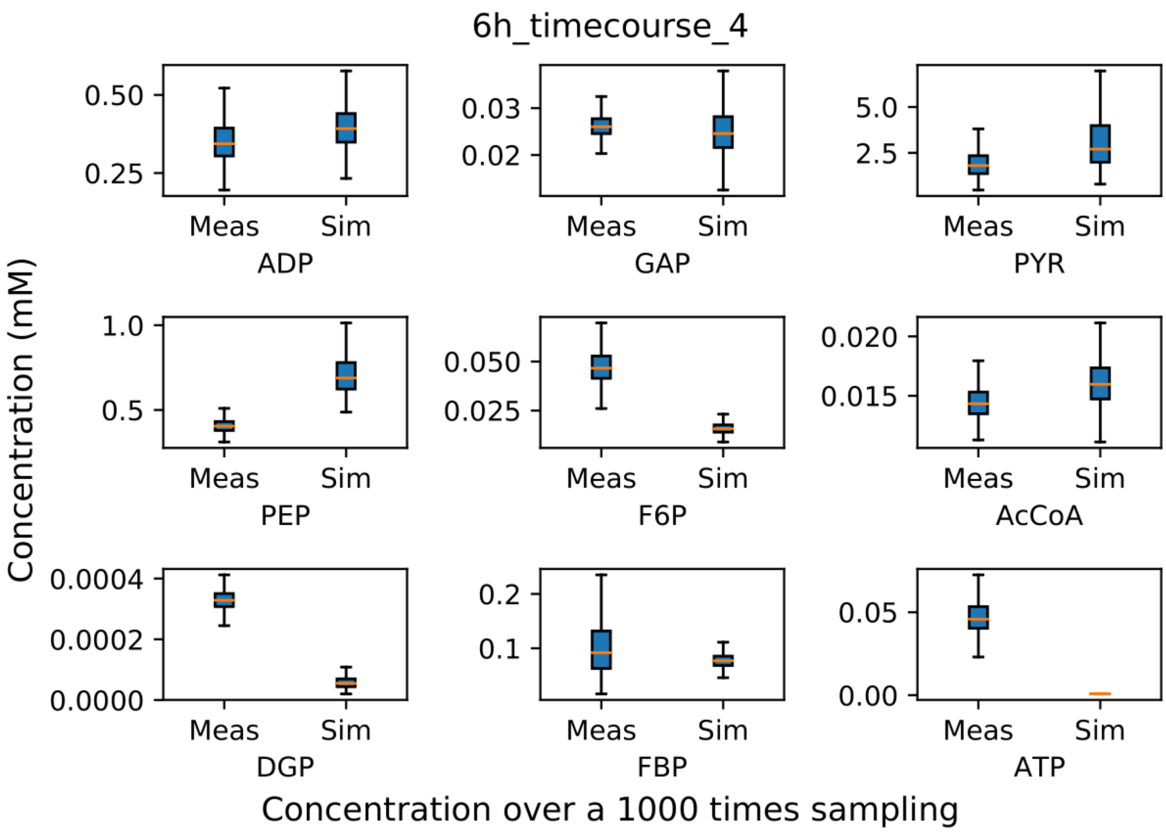

WT_noGluc_perturbation_7
Concentration (mM)
Meas
Sim
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Concentration over a 1000 times sampling

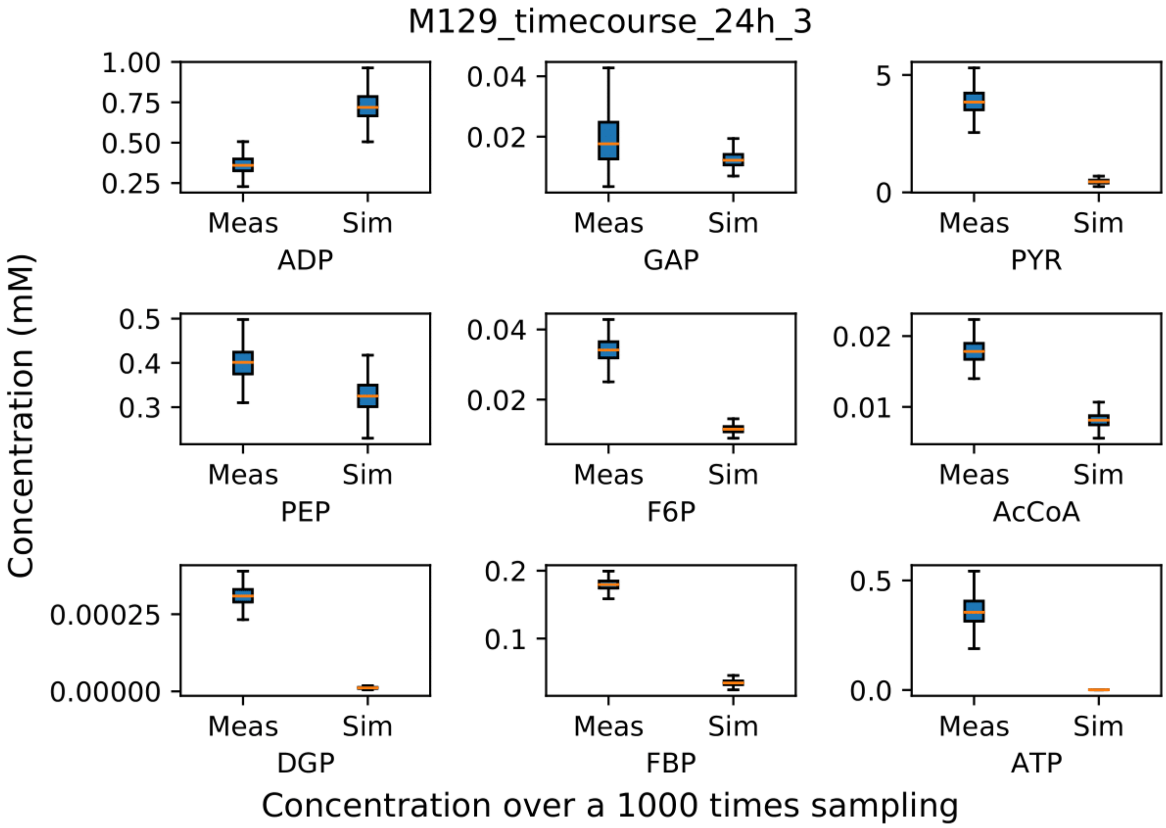


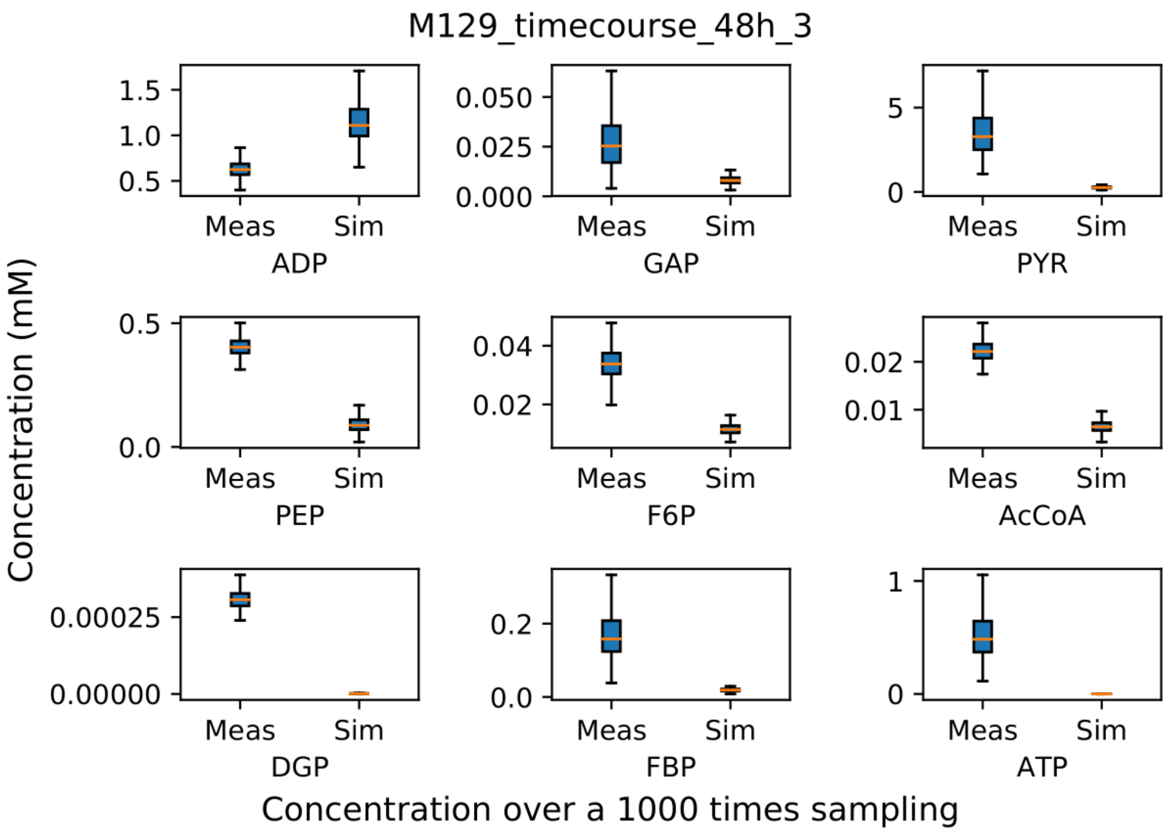
24h_timecourse_4
Concentration (mM)
1.0
0.5
Meas
Sim
ADP
0.04
0.02
GAP
10
0
PYR
PEP
0.1
0.0
F6P
0.02
0.01
AcCoA
0.00025
0.00000
DGP
FBP
0.05
0.00
ATP
Concentration over a 1000 times sampling

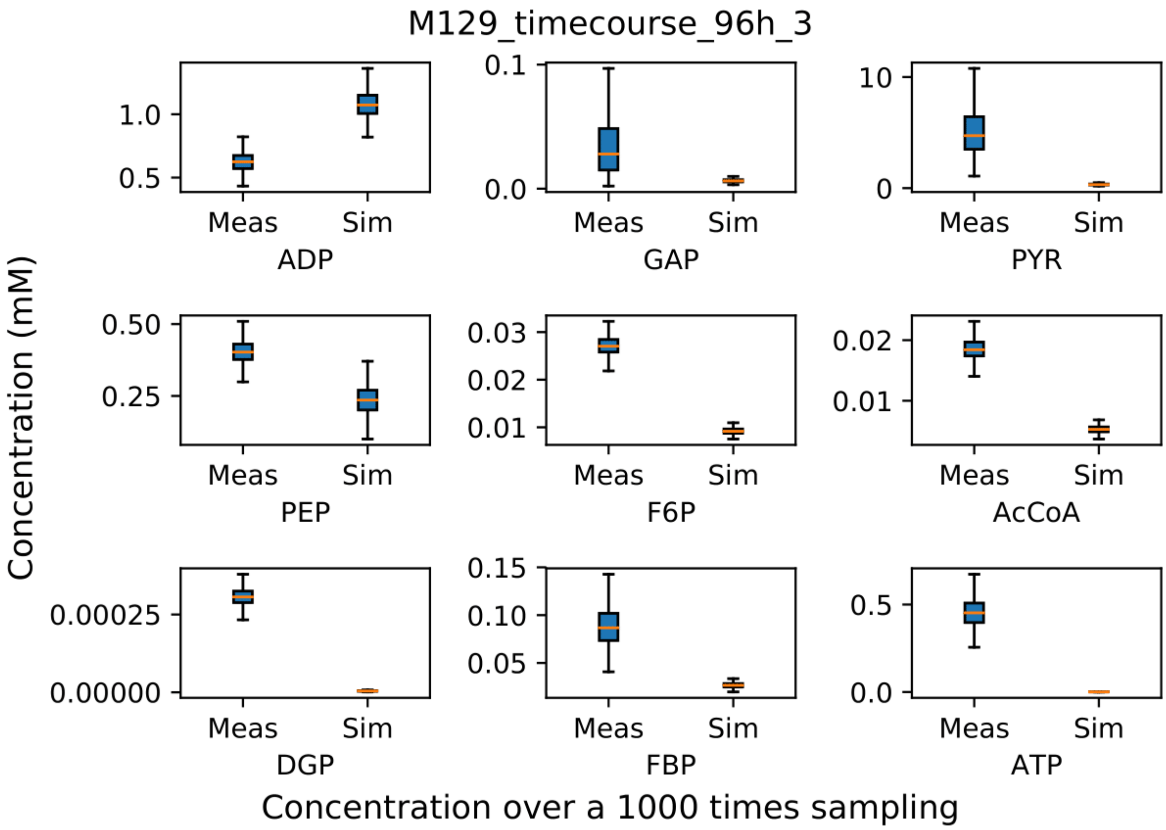



48h_timecourse_4
Concentration (mM)
1.25
1.00
0.75
Meas
Sim
ADP
0.05
0.00
GAP
2
1
0
PYR
0.50
0.25
PEP
0.1
0.0
F6P
0.02
0.01
AcCoA
0.00025
0.00000
DGP
1
0
FBP
0.1
0.0
ATP
Concentration over a 1000 times sampling


6h_timecourse_4
Concentration (mM)
0.50
0.25
Meas
Sim
ADP
0.03
0.02
GAP
5.0
2.5
PYR
1.0
0.5
PEP
0.050
0.025
F6P
0.020
0.015
AcCoA
0.0004
0.0002
0.0000
DGP
0.2
0.1
FBP
0.05
0.00
ATP
Concentration over a 1000 times sampling


M129_timecourse_24h_3
Concentration (mM)
1.00
0.75
0.50
0.25
Meas
Sim
ADP
0.04
0.02
GAP
5
0
PYR
0.5
0.4
0.3
PEP
0.04
0.02
F6P
0.02
0.01
AcCoA
0.00025
0.00000
DGP
0.2
0.1
FBP
0.5
0.0
ATP
Concentration over a 1000 times sampling


M129_timecourse_48h_3
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling


M129_timecourse_96h_3
Concentration (mM)
ADP
GAP
PYR
PEP
F6P
AcCoA
DGP
FBP
ATP
Meas
Sim
Concentration over a 1000 times sampling

# Supplementary file 1 D Metabolomics analysis.

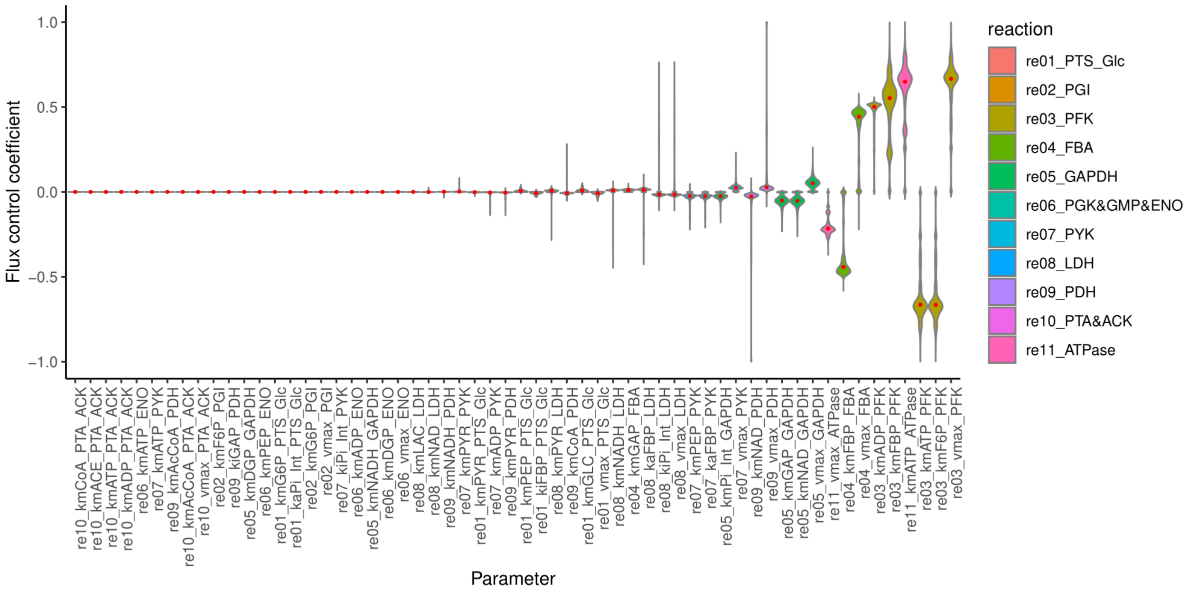



*Figure 3 Local sensitivity analysis using 1000x sampling from the measurement distribution.*

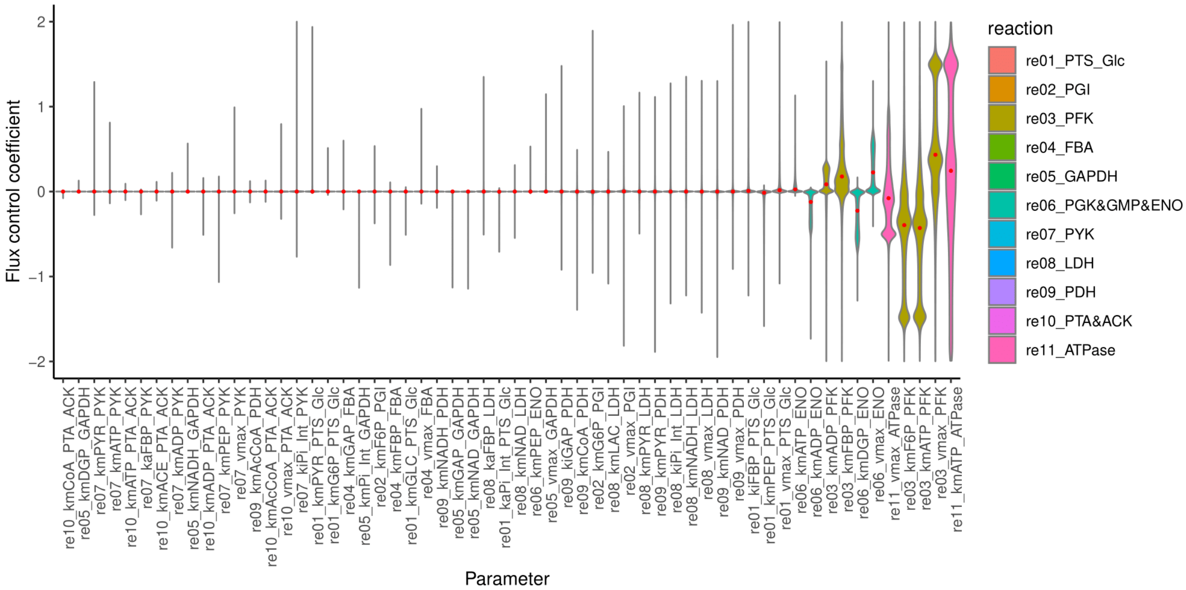



*Figure 4 Global sensitivity analysis using a 100,000 Latin Hypercube sampling withing the parameter search range.*

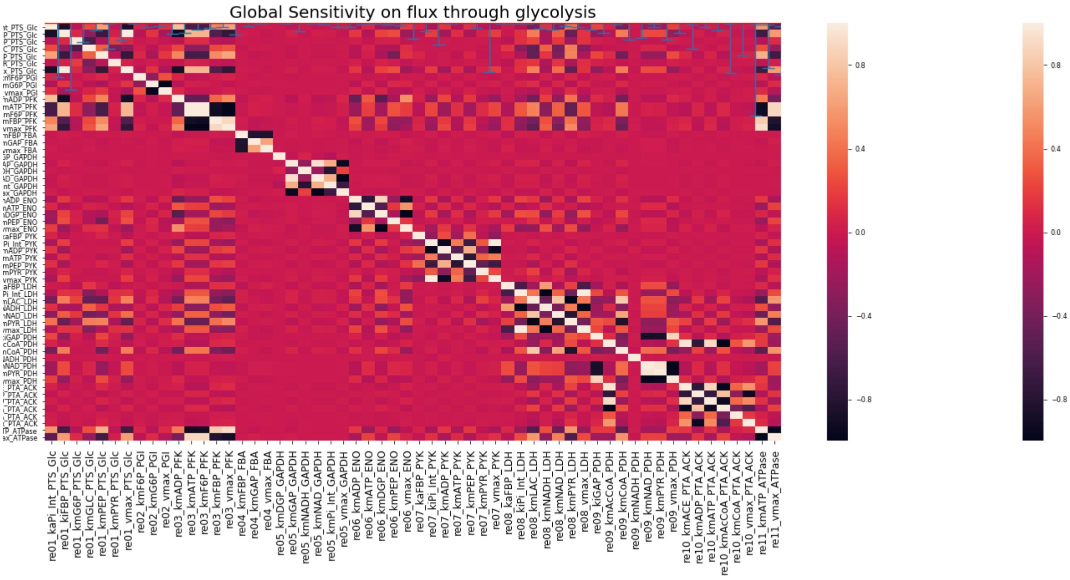



*Figure 5 Correlation analysis of control coefficients control over flux through glycolysis using a 100,000 Latin Hypercube sampling.*