

1 E. coli Three states data with $\alpha = 0.01$

E. coli model (aerobic growth on glucose), balanced kinetic data

(a) Metabolites

(b) Enzymes

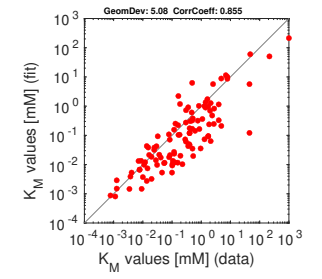
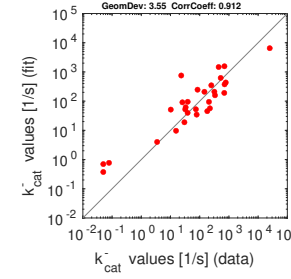
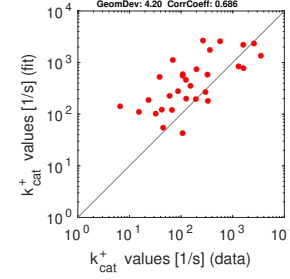
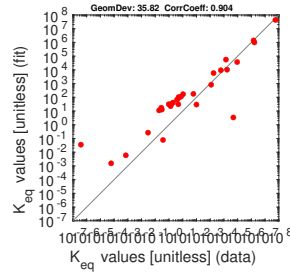
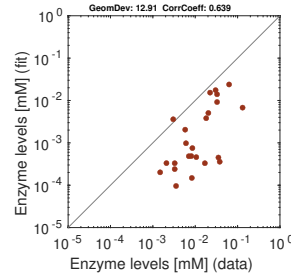
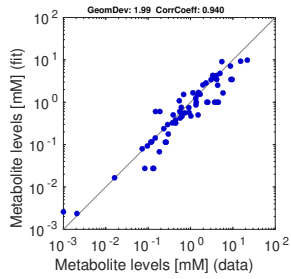
(c) K_{eq} values

(d) k_{cat}^+ values

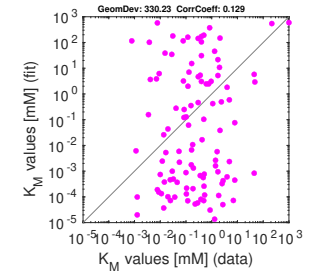
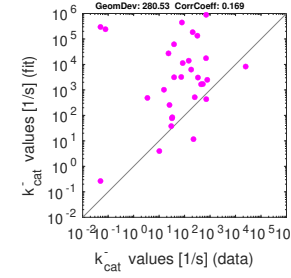
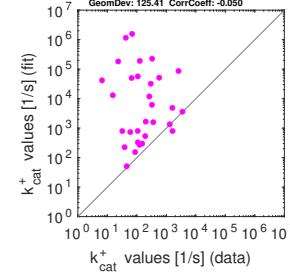
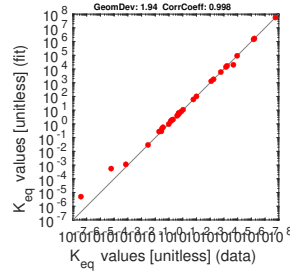
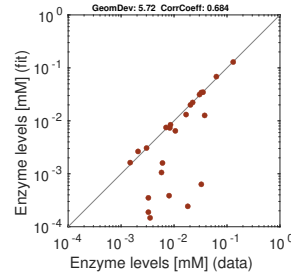
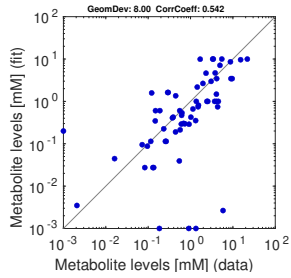
(e) k_{cat}^- values

(f) K_M values

With kinetic data



With K_{eq} data only



Without kinetic data

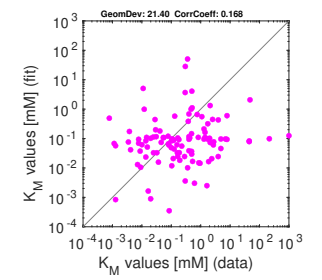
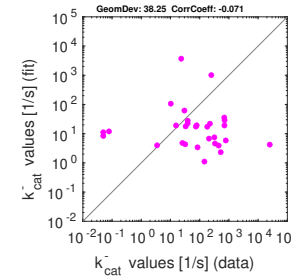
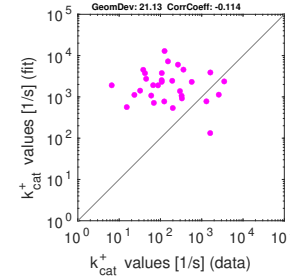
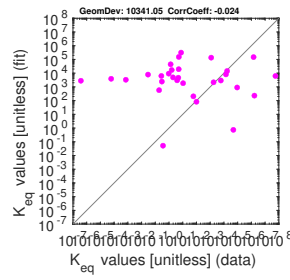
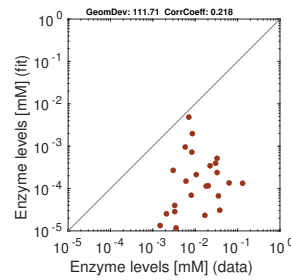
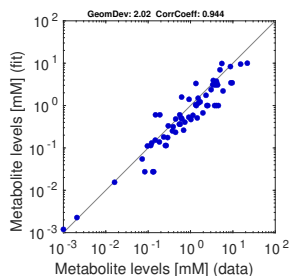


Figure 3: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). The kinetic data stem from previous parameter balancing based on *in-vitro* data. Top: estimation using kinetic data. Centre: estimation using equilibrium constants as the only kinetic data. Bottom: estimation without usage of kinetic data. The same metabolite, enzyme, and kinetic data were used in [?].

E. coli central metabolism model (aerobic growth on glucose), in-vitro kinetic data

(a) Metabolites

(b) Enzymes

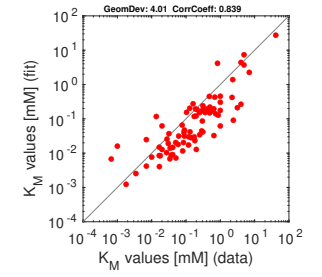
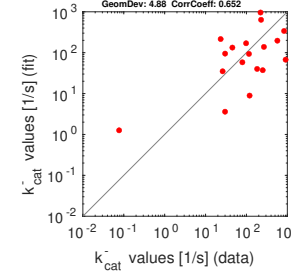
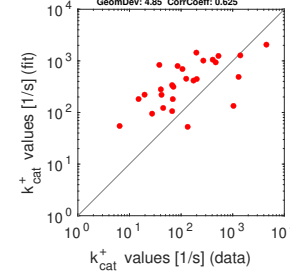
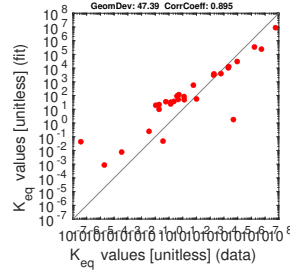
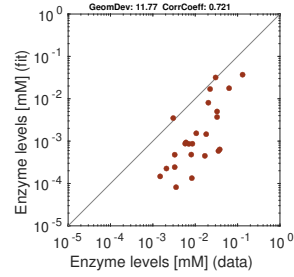
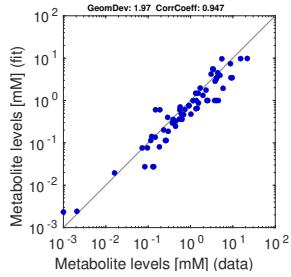
(c) K_{eq} values

(d) k_{cat}^+ values

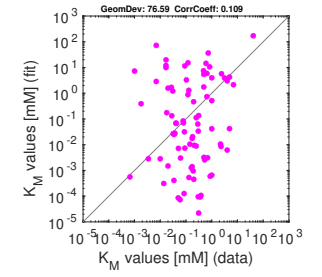
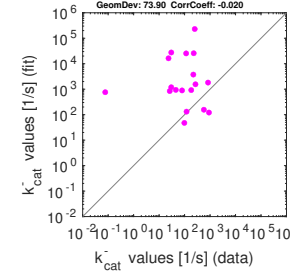
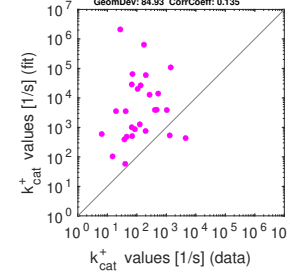
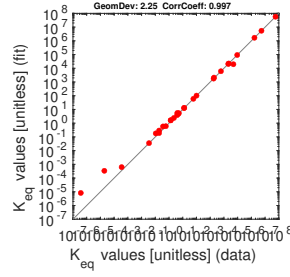
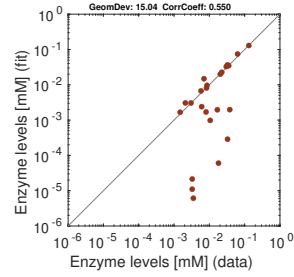
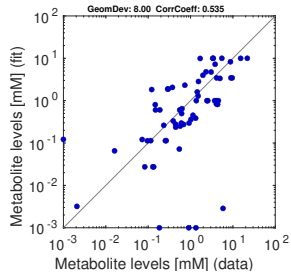
(e) k_{cat}^- values

(f) K_M values

With kinetic data



With K_{eq} data only



Without kinetic data

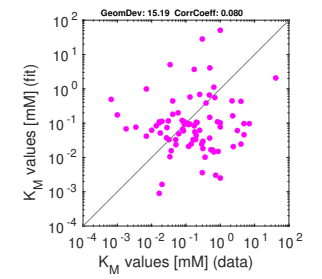
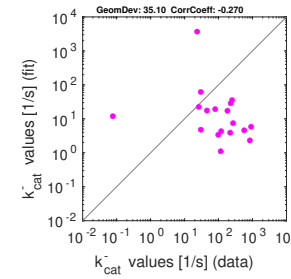
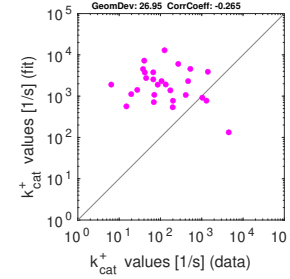
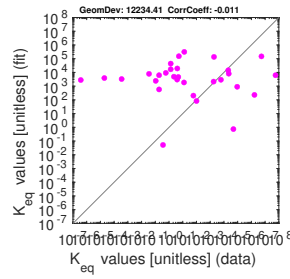
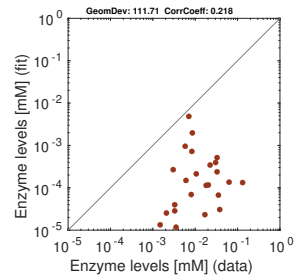
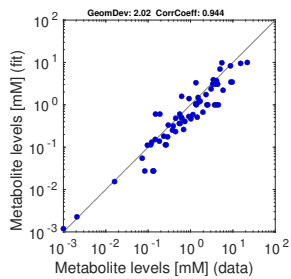


Figure 4: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). Same as Figure 15, but based on original kinetic *in-vitro* data instead of balanced kinetic data.

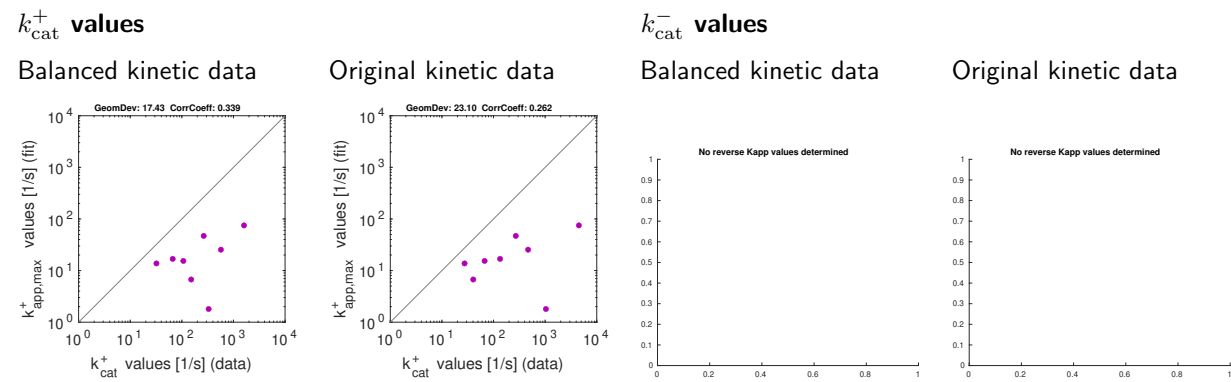
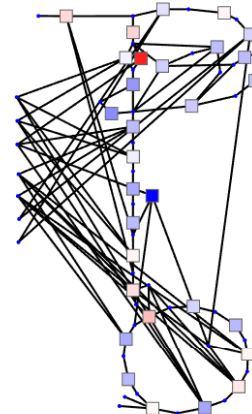
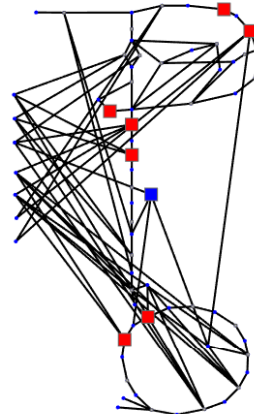
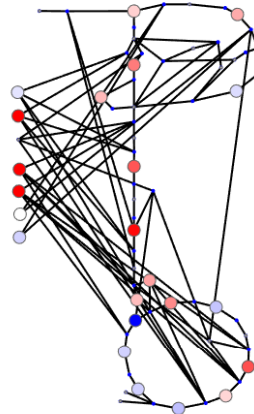
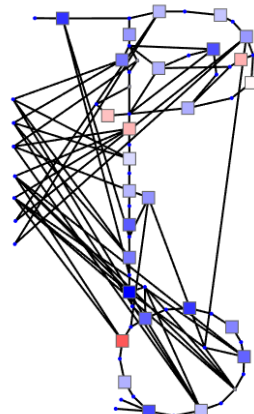


Figure 5: Catalytic constants in *E. coli* central metabolism model (aerobic growth on glucose), estimated by kinetic profiling [?].

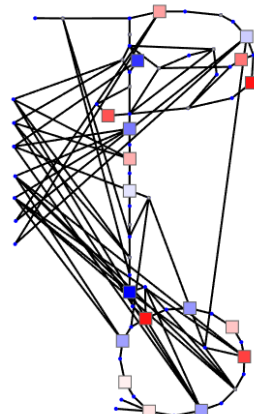
met (fit/data) smpl 1 f.c.<3.03enz (fit/data) smpl 1 f.c.<62.21Keq (fit/data) f.c.<116957.24



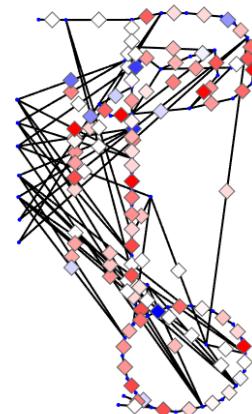
Kcatf (fit/data) f.c.<22.05



Kcatr (fit/data) f.c.<16.39



KM (fit/data) f.c.<26.55



Reaction orientation w.r.t flux signs

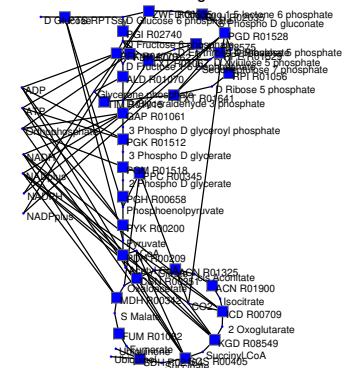


Figure 6: Diagnostic plots for fit with original kinetic data. Left: Relative fitting errors. Blue: fitted value too high. Red: fitted value too low. Maximal fold changes (whether up or down) are given by numbers. Right: Reaction orientatation (defining “forward” and “reverse”). Blue: in flux direction; Red: against flux direction.

2 E. coli Three states data with $\alpha = 0.1$

E. coli model (aerobic growth on glucose), balanced kinetic data

(a) Metabolites

(b) Enzymes

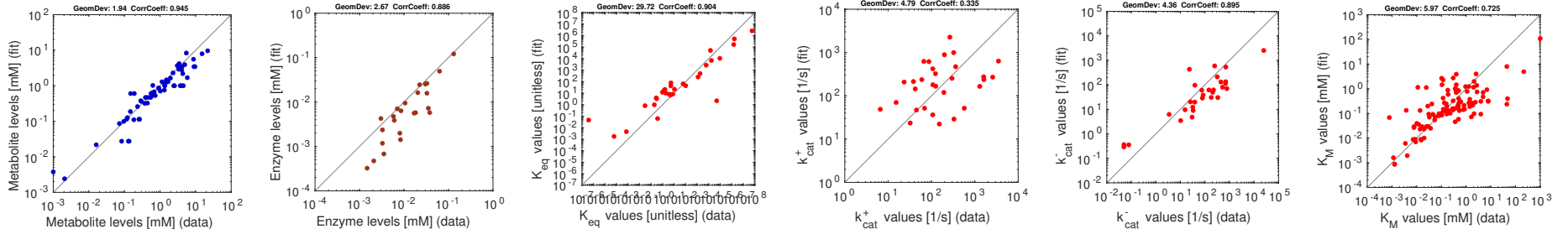
(c) K_{eq} values

(d) k_{cat}^+ values

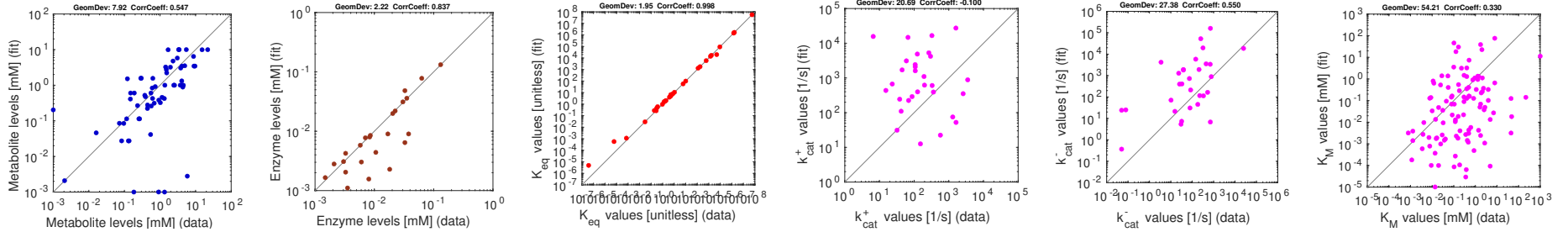
(e) k_{cat}^- values

(f) K_M values

With kinetic data



With K_{eq} data only



Without kinetic data

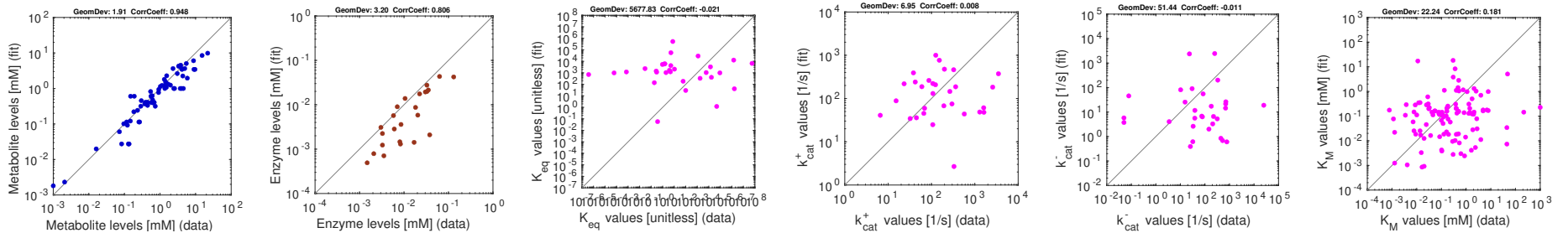


Figure 7: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). The kinetic data stem from previous parameter balancing based on *in-vitro* data. Top: estimation using kinetic data. Centre: estimation using equilibrium constants as the only kinetic data. Bottom: estimation without usage of kinetic data. The same metabolite, enzyme, and kinetic data were used in [?].

E. coli central metabolism model (aerobic growth on glucose), in-vitro kinetic data

(a) Metabolites

(b) Enzymes

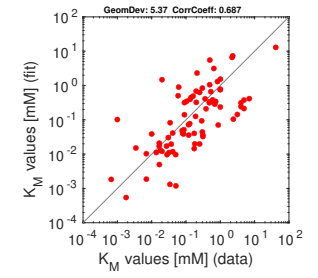
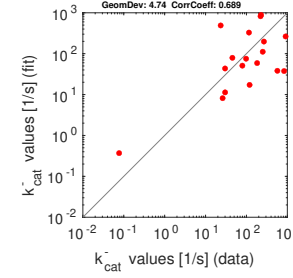
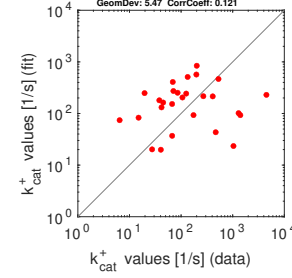
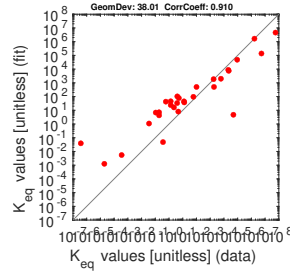
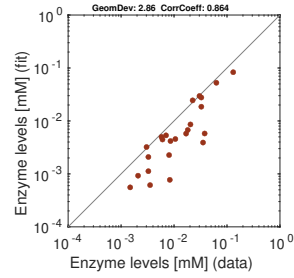
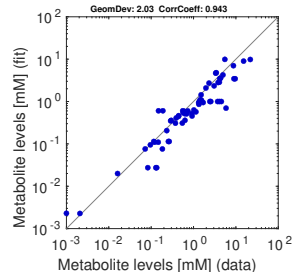
(c) K_{eq} values

(d) k_{cat}^+ values

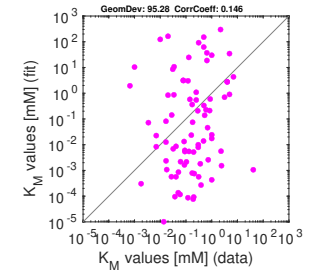
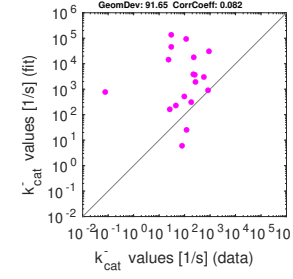
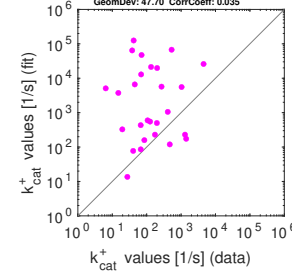
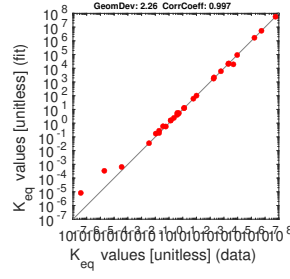
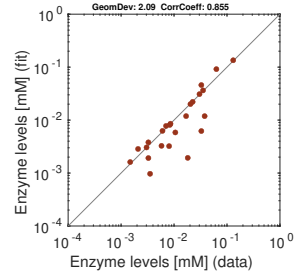
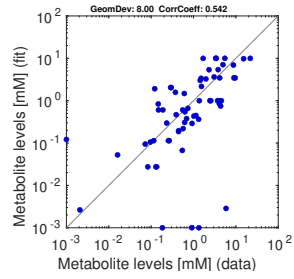
(e) k_{cat}^- values

(f) K_M values

With kinetic data



With K_{eq} data only



Without kinetic data

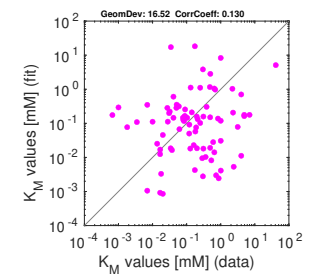
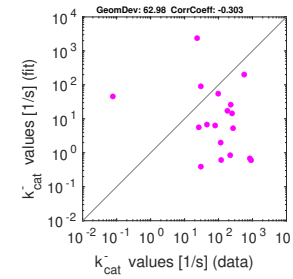
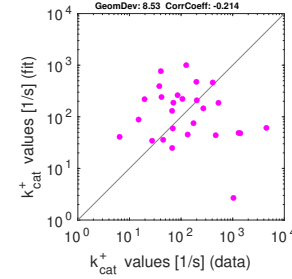
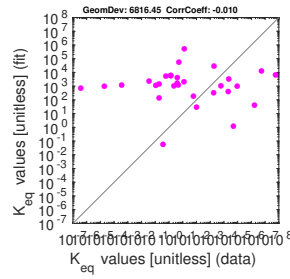
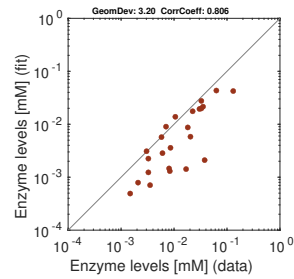
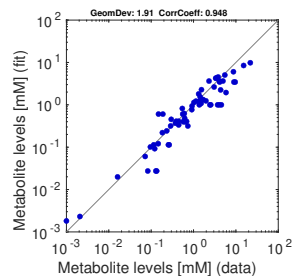


Figure 8: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). Same as Figure 15, but based on original kinetic *in-vitro* data instead of balanced kinetic data.

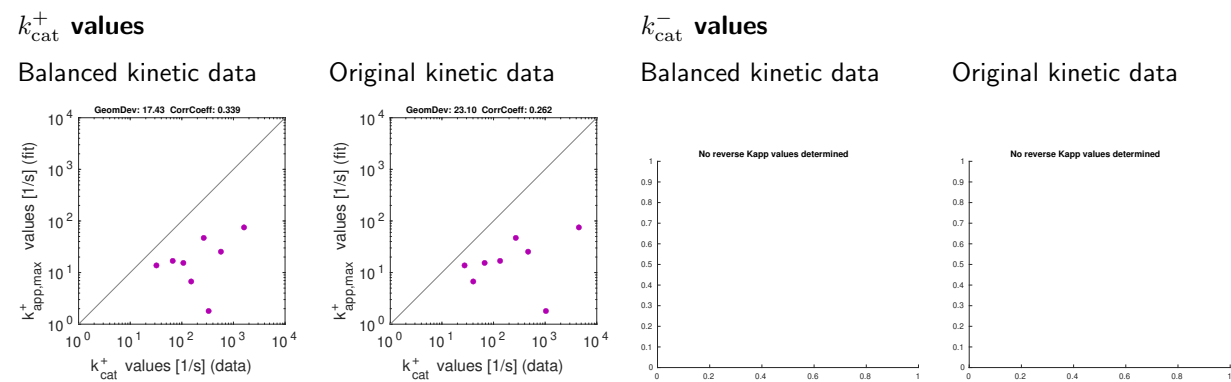
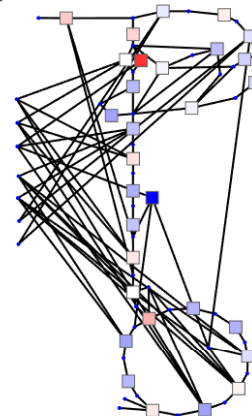
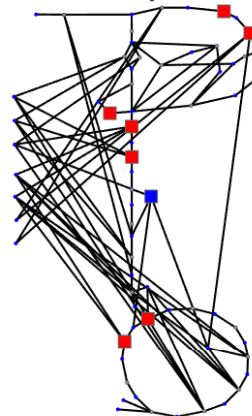
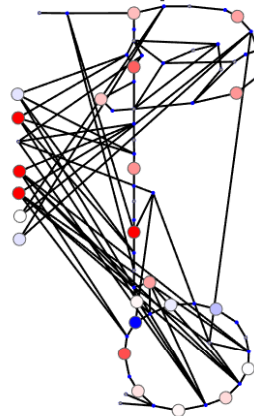
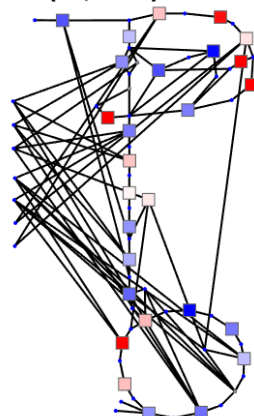


Figure 9: Catalytic constants in *E. coli* central metabolism model (aerobic growth on glucose), estimated by kinetic profiling [?].

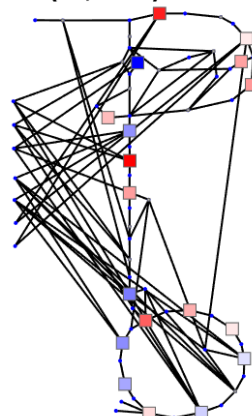
met (fit/data) smpl 1 f.c.<3.03 enz (fit/data) smpl 1 f.c.<10.77 Keq (fit/data) f.c.<105266.83



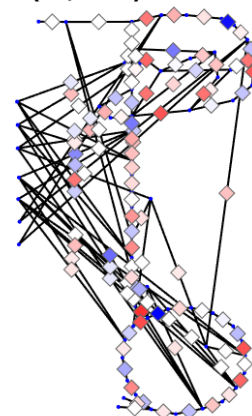
Kcatf (fit/data) f.c.<44.19



Kcatr (fit/data) f.c.<22.17



KM (fit/data) f.c.<101.74



Reaction orientation w.r.t flux signs

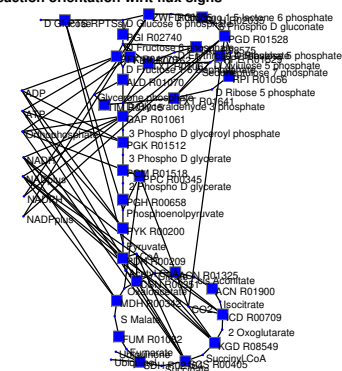


Figure 10: Diagnostic plots for fit with original kinetic data. Left: Relative fitting errors. Blue: fitted value too high. Red: fitted value too low. Maximal fold changes (whether up or down) are given by numbers. Right: Reaction orientatation (defining “forward” and “reverse”). Blue: in flux direction; Red: against flux direction.

3 E. coli Three states data with $\alpha = 0.5$

E. coli model (aerobic growth on glucose), balanced kinetic data

(a) Metabolites

(b) Enzymes

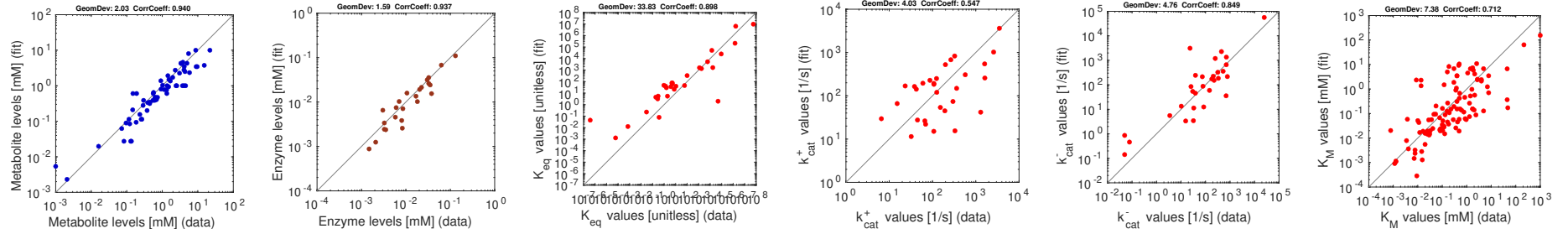
(c) K_{eq} values

(d) k_{cat}^+ values

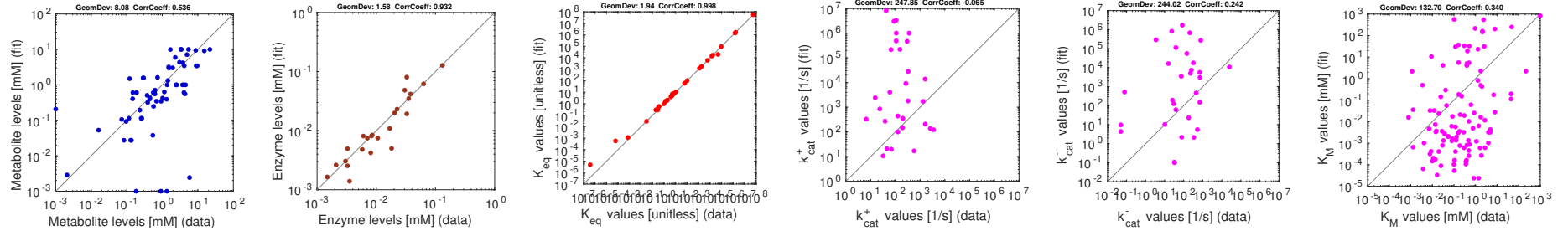
(e) k_{cat}^- values

(f) K_M values

With kinetic data



With K_{eq} data only



Without kinetic data

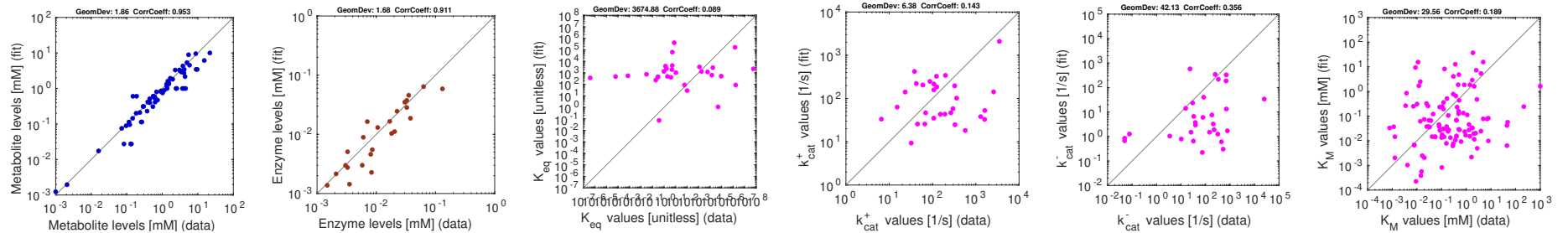


Figure 11: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). The kinetic data stem from previous parameter balancing based on *in-vitro* data. Top: estimation using kinetic data. Centre: estimation using equilibrium constants as the only kinetic data. Bottom: estimation without usage of kinetic data. The same metabolite, enzyme, and kinetic data were used in [?].

E. coli central metabolism model (aerobic growth on glucose), in-vitro kinetic data

(a) Metabolites

(b) Enzymes

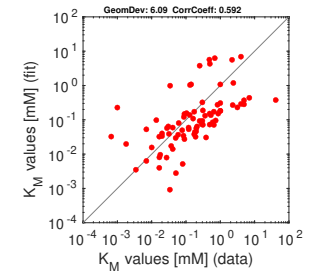
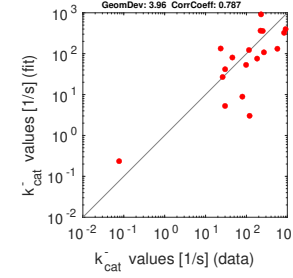
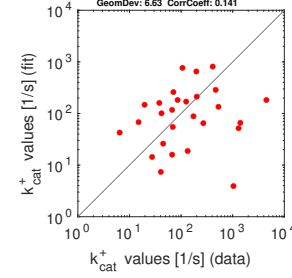
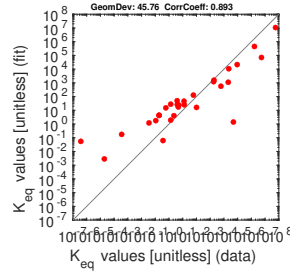
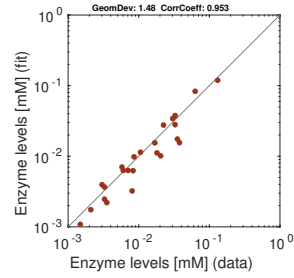
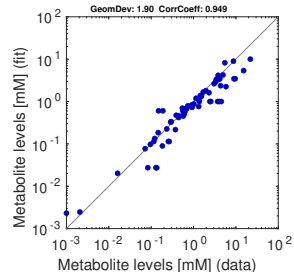
(c) K_{eq} values

(d) k_{cat}^+ values

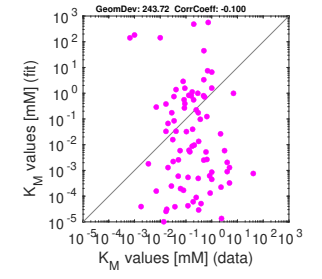
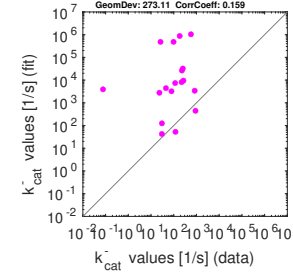
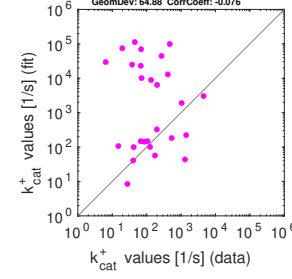
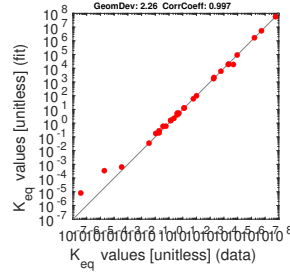
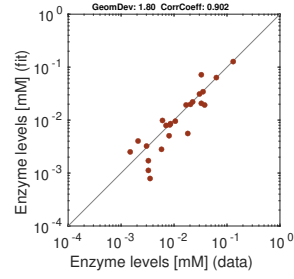
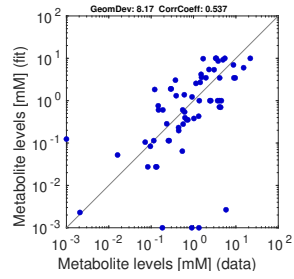
(e) k_{cat}^- values

(f) K_M values

With kinetic data



With K_{eq} data only



Without kinetic data

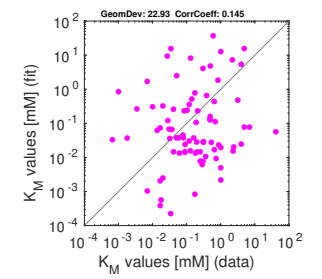
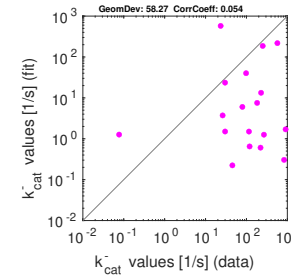
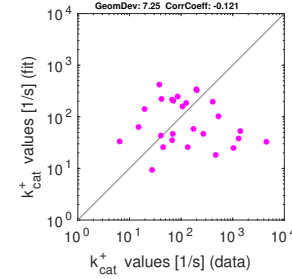
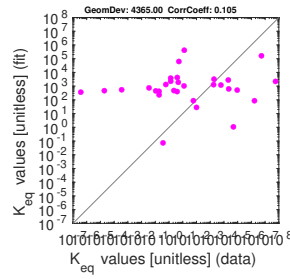
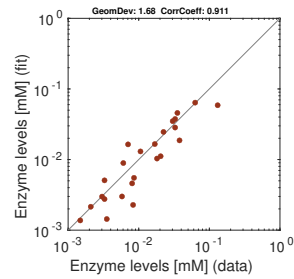
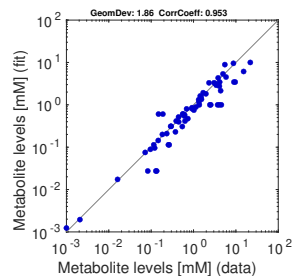


Figure 12: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). Same as Figure 15, but based on original kinetic *in-vitro* data instead of balanced kinetic data.

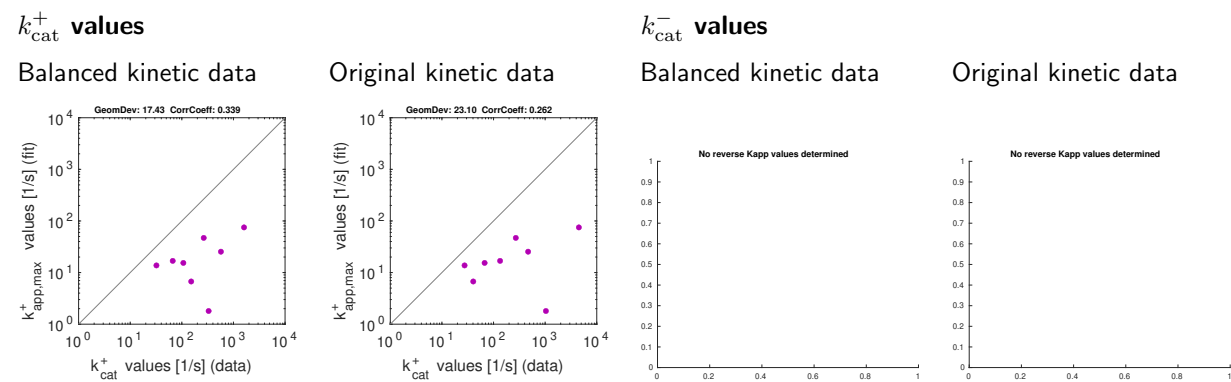
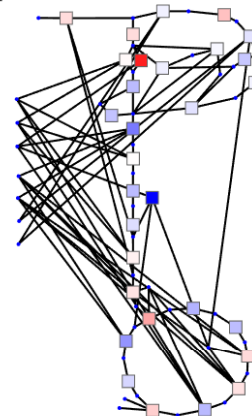
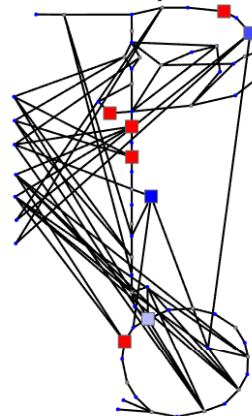
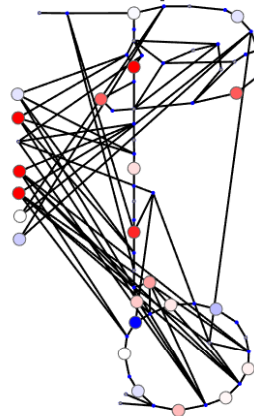
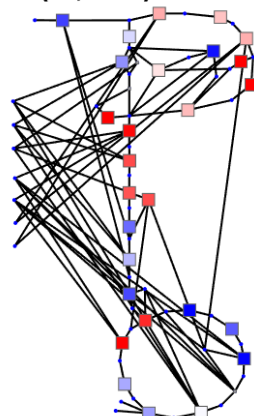


Figure 13: Catalytic constants in *E. coli* central metabolism model (aerobic growth on glucose), estimated by kinetic profiling [?].

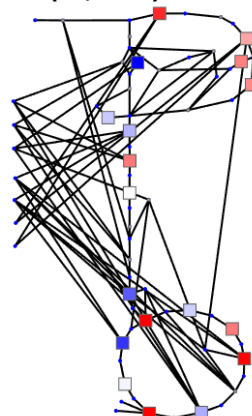
met (fit/data) smpl 1 f.c.<3.03 enz (fit/data) smpl 1 f.c.<2.02 Keq (fit/data) f.c.<146086.66



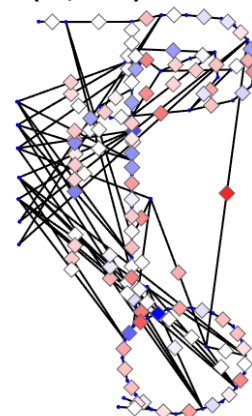
Kcatf (fit/data) f.c.<264.15



Kcatr (fit/data) f.c.<39.41



KM (fit/data) f.c.<227.21



Reaction orientation w.r.t flux signs

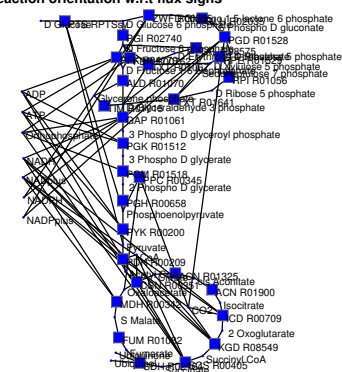


Figure 14: Diagnostic plots for fit with original kinetic data. Left: Relative fitting errors. Blue: fitted value too high. Red: fitted value too low. Maximal fold changes (whether up or down) are given by numbers. Right: Reaction orientatation (defining “forward” and “reverse”). Blue: in flux direction; Red: against flux direction.

4 E. coli Three states data with $\alpha = 1$

E. coli model (aerobic growth on glucose), balanced kinetic data

(a) Metabolites

(b) Enzymes

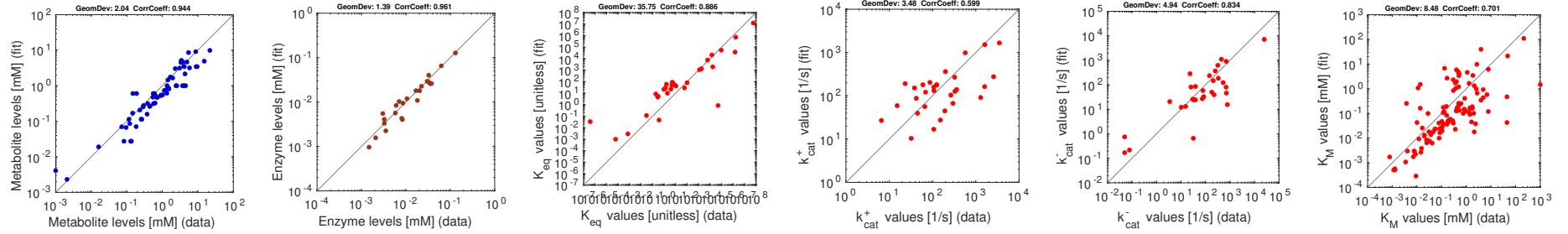
(c) K_{eq} values

(d) k_{cat}^+ values

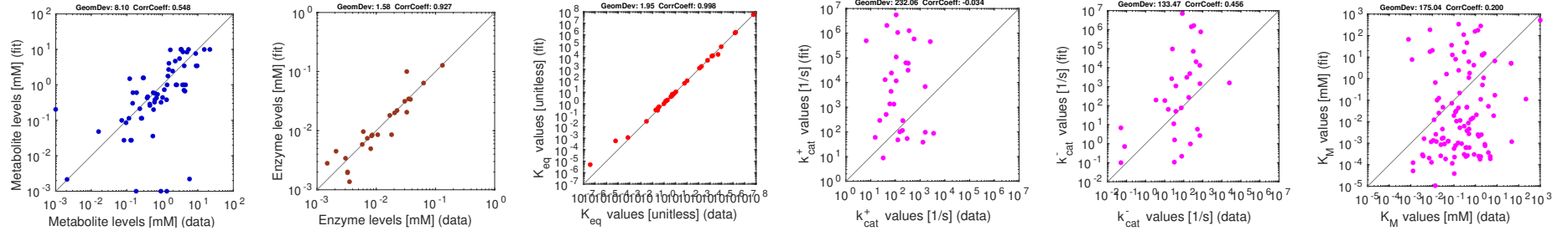
(e) k_{cat}^- values

(f) K_M values

With kinetic data



With K_{eq} data only



Without kinetic data

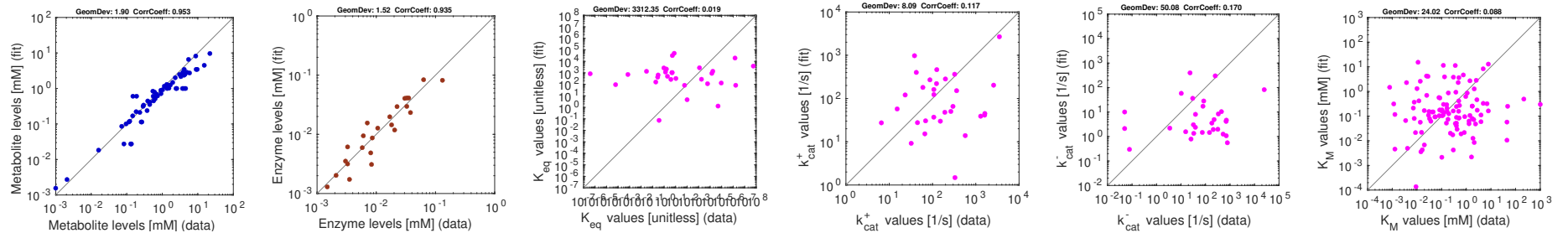


Figure 15: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). The kinetic data stem from previous parameter balancing based on *in-vitro* data. Top: estimation using kinetic data. Centre: estimation using equilibrium constants as the only kinetic data. Bottom: estimation without usage of kinetic data. The same metabolite, enzyme, and kinetic data were used in [?].

E. coli central metabolism model (aerobic growth on glucose), in-vitro kinetic data

(a) Metabolites

(b) Enzymes

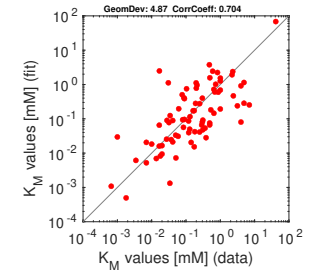
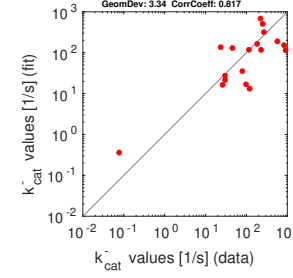
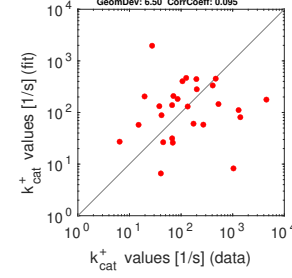
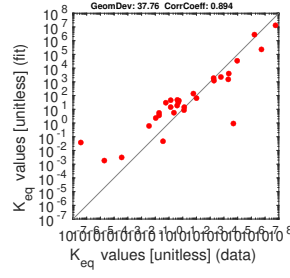
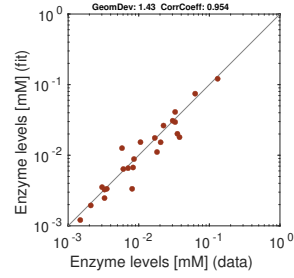
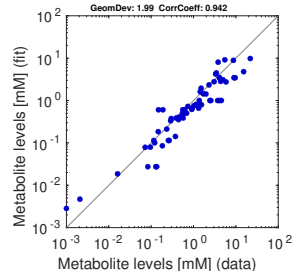
(c) K_{eq} values

(d) k_{cat}^+ values

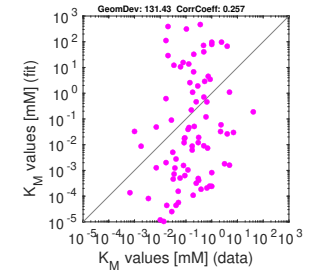
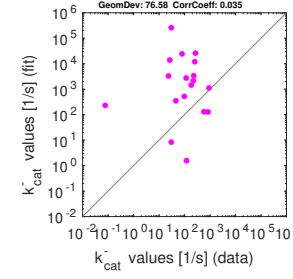
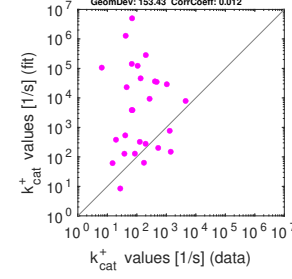
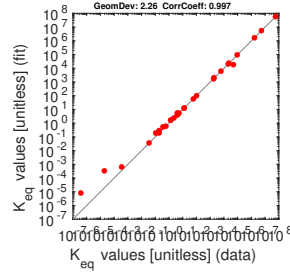
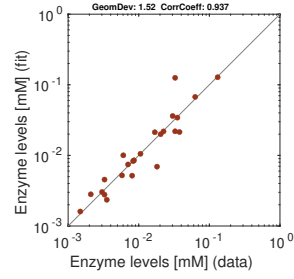
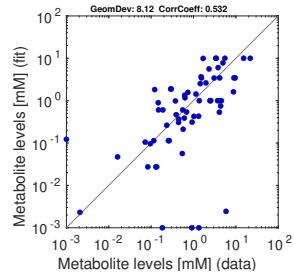
(e) k_{cat}^- values

(f) K_M values

With kinetic data



With K_{eq} data only



Without kinetic data

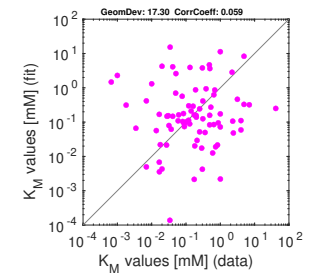
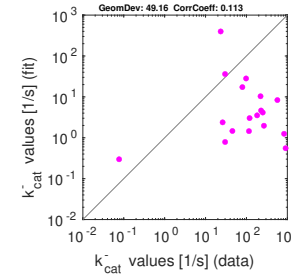
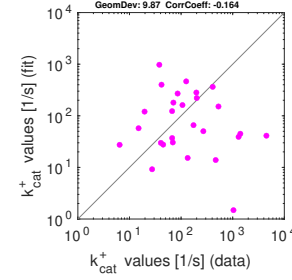
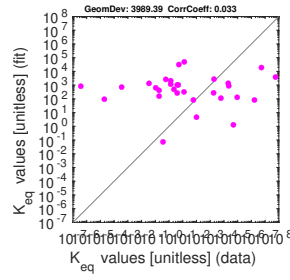
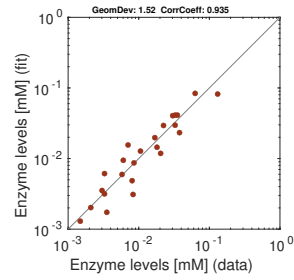
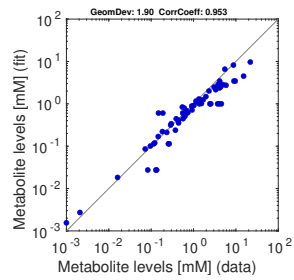


Figure 16: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). Same as Figure 15, but based on original kinetic *in-vitro* data instead of balanced kinetic data.

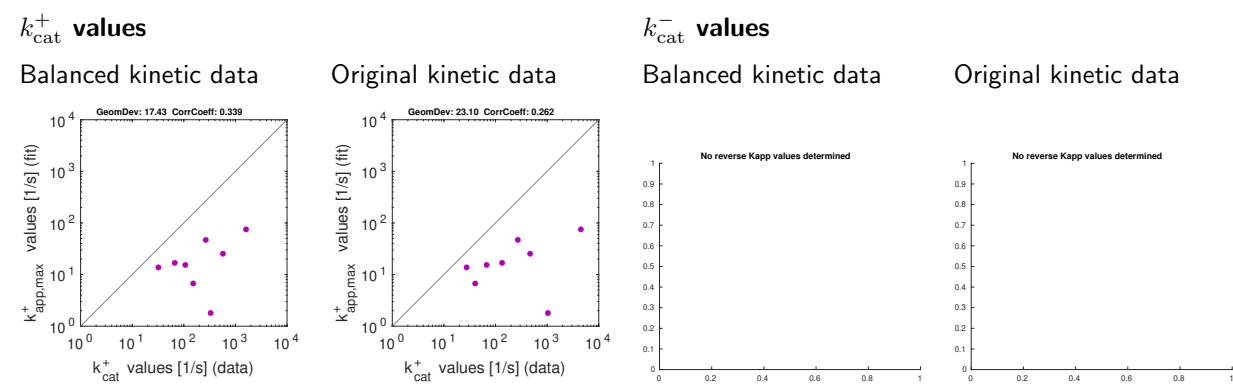
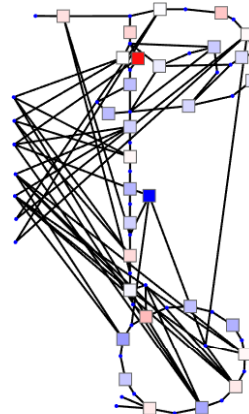
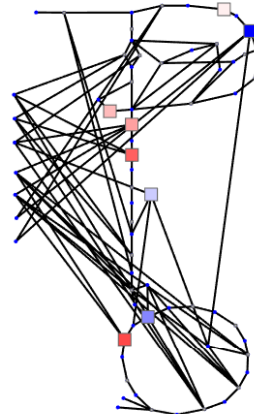
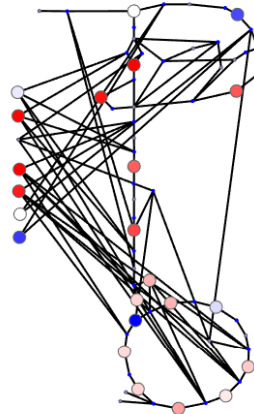
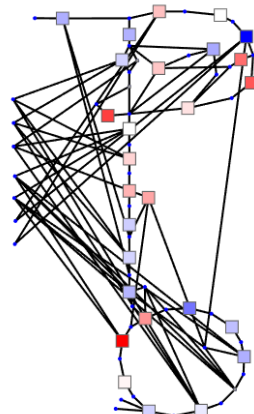


Figure 17: Catalytic constants in *E. coli* central metabolism model (aerobic growth on glucose), estimated by kinetic profiling [?].

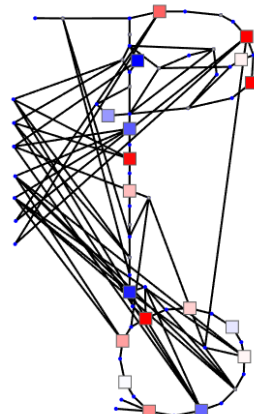
met (fit/data) smpl 1 f.c.<3.16 enz (fit/data) smpl 1 f.c.<2.18 Keq (fit/data) f.c.<102208.59



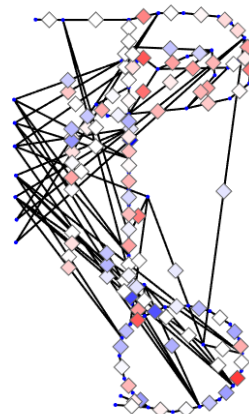
Kcatf (fit/data) f.c.<125.47



Kcatr (fit/data) f.c.<9.06



KM (fit/data) f.c.<148.07



Reaction orientation w.r.t flux signs

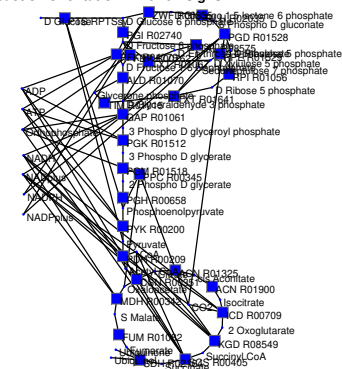


Figure 18: Diagnostic plots for fit with original kinetic data. Left: Relative fitting errors. Blue: fitted value too high. Red: fitted value too low. Maximal fold changes (whether up or down) are given by numbers. Right: Reaction orientation (defining “forward” and “reverse”). Blue: in flux direction; Red: against flux direction.