1 E. coli Glucose simulations with alpha = 0.1, beta = 0

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

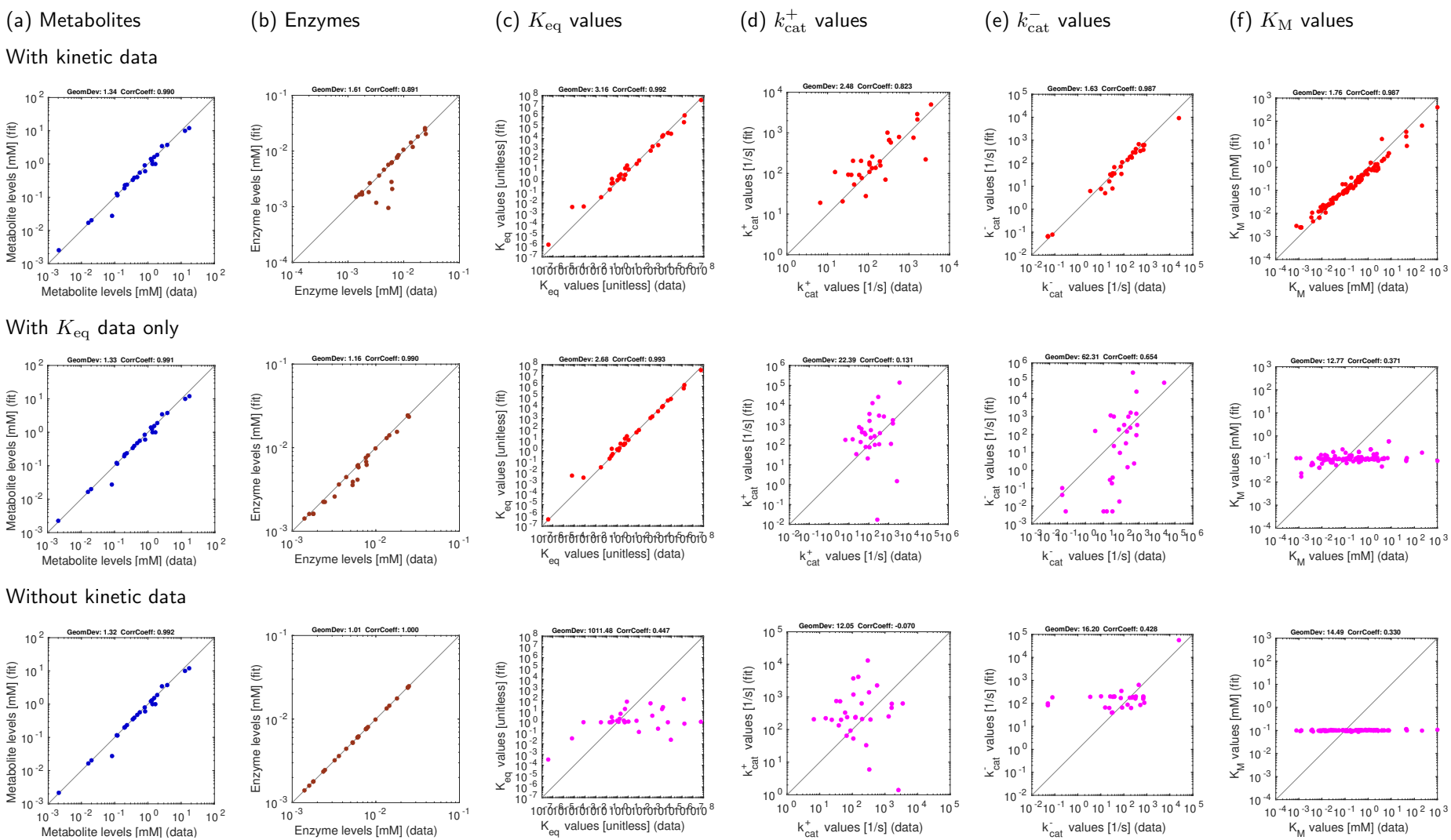


Figure 3: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). The kinetic data stem from previous parameter balancing based on *in-vitro* data. Top: estimation using kinetic data. Centre: estimation using equilibrium constants as the only kinetic data. Centre: 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

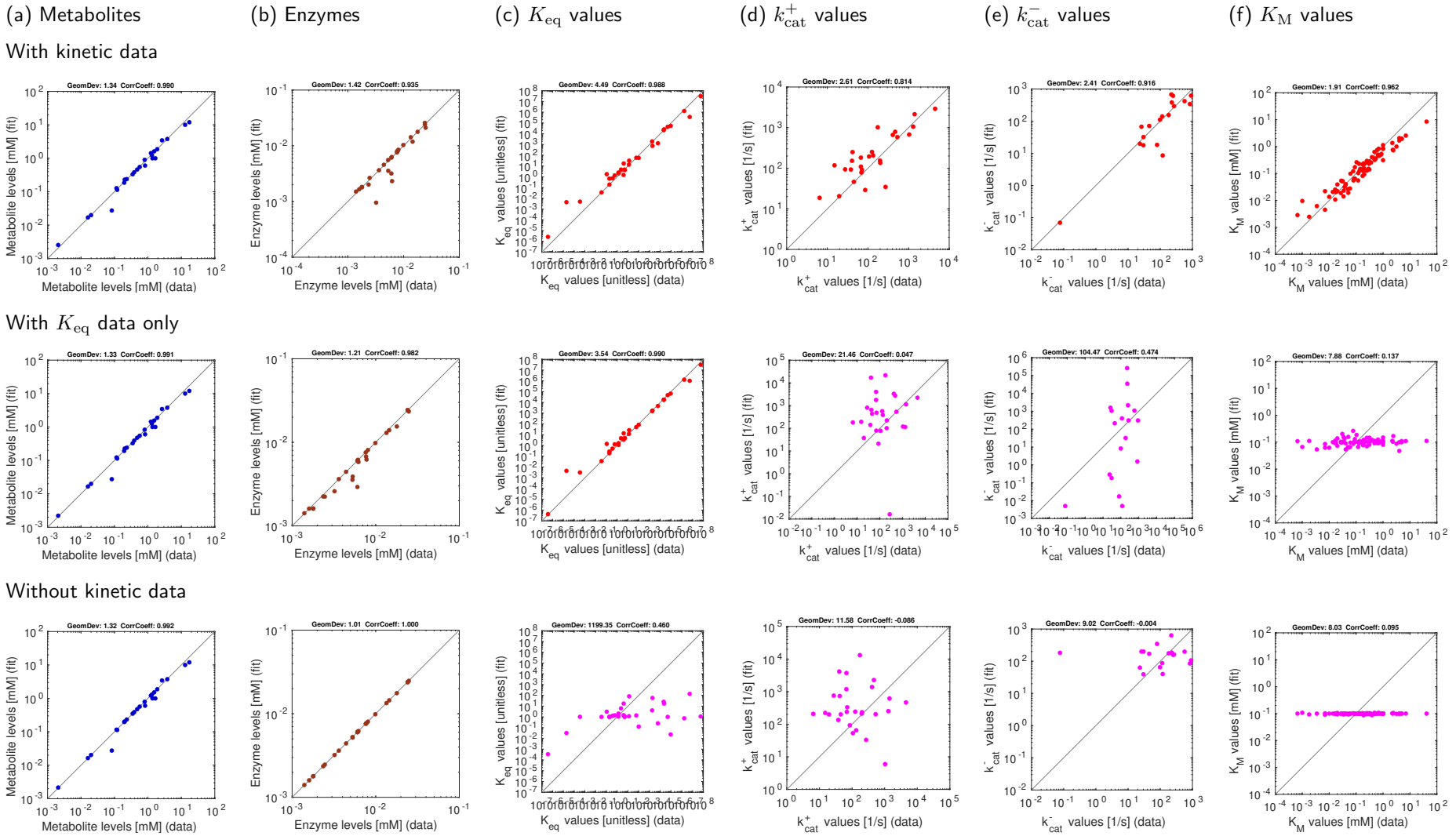


Figure 4: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). Same as Figure 3, but based on original kinetic *in-vitro* data instead of balanced kinetic data.

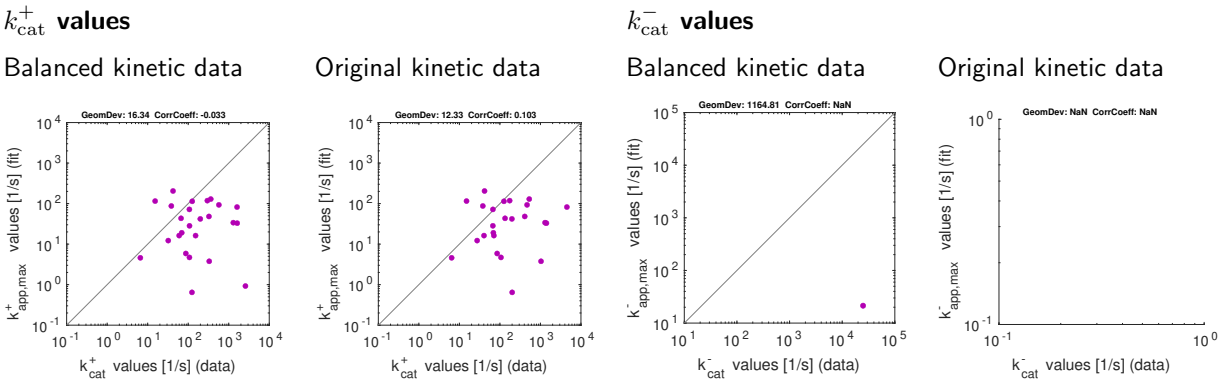


Figure 5: Catalytic constants in *E. coli* central metabolism model (aerobic growth on glucose), estimated by kinetic profiling.

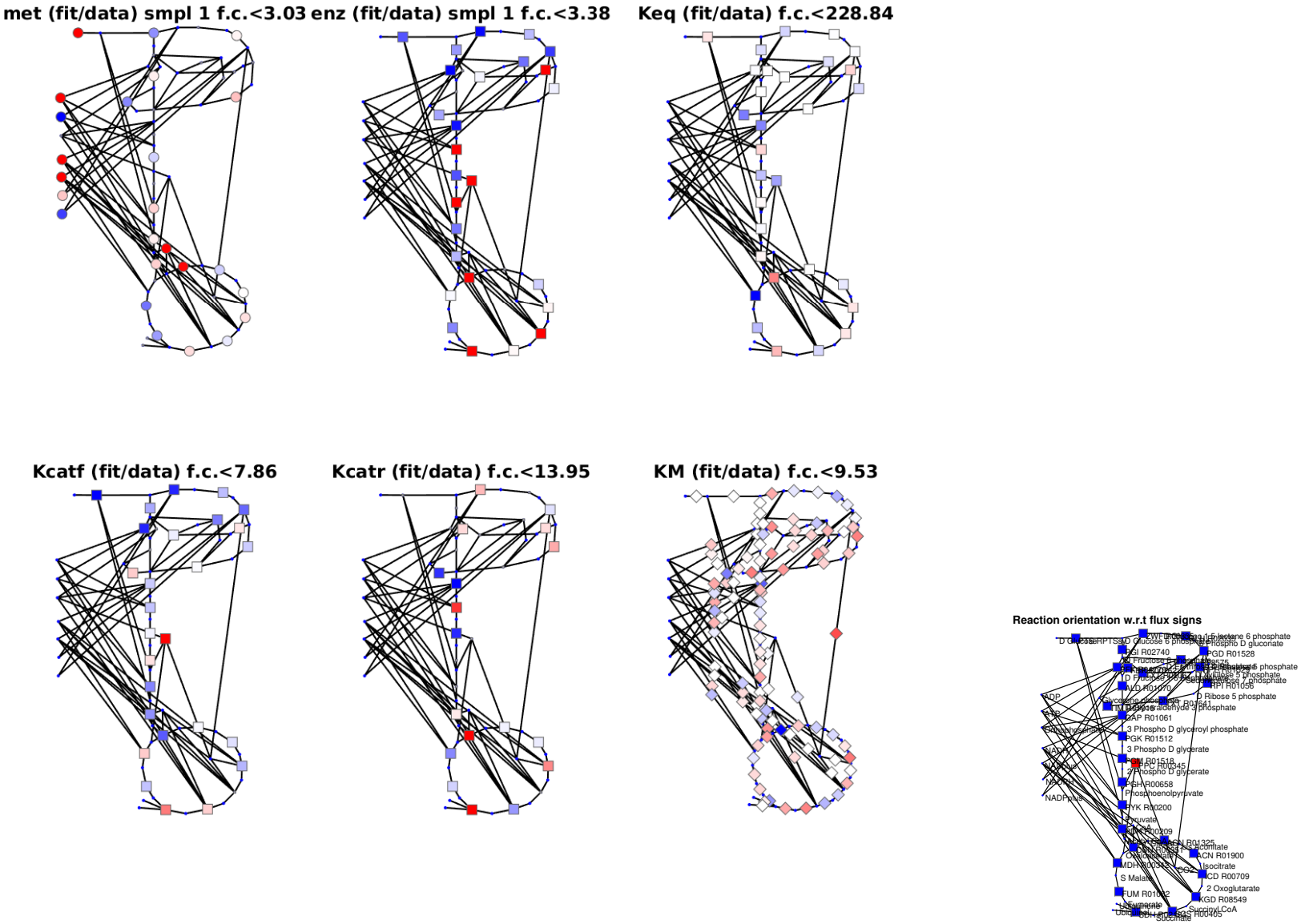


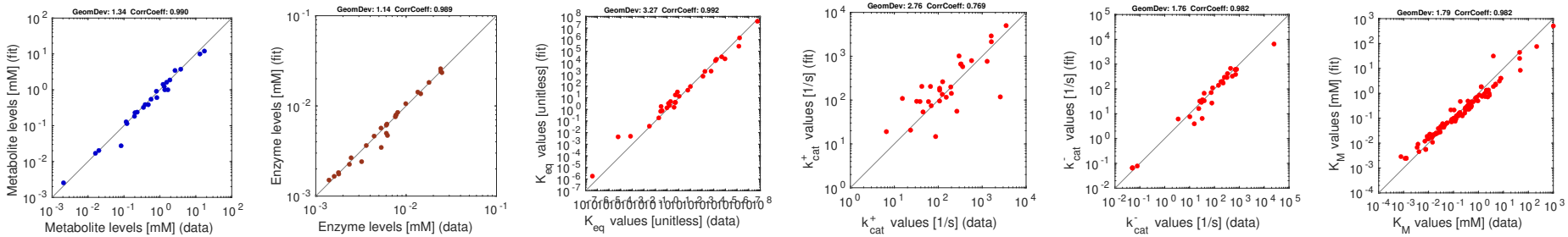
Figure 6: Diagnostic plots for fit with original kinetic data. Left: Relative fitting errors. Blue: fitted value too high. Red: fitted value too low. Maximal fold changes (whether up or down) are given by numbers. Right: Reaction orientatation (defining "forward" and "reverse"). Blue: in flux direction;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

2 E. coli Glucose simulations with alpha = 0.5, beta = 0

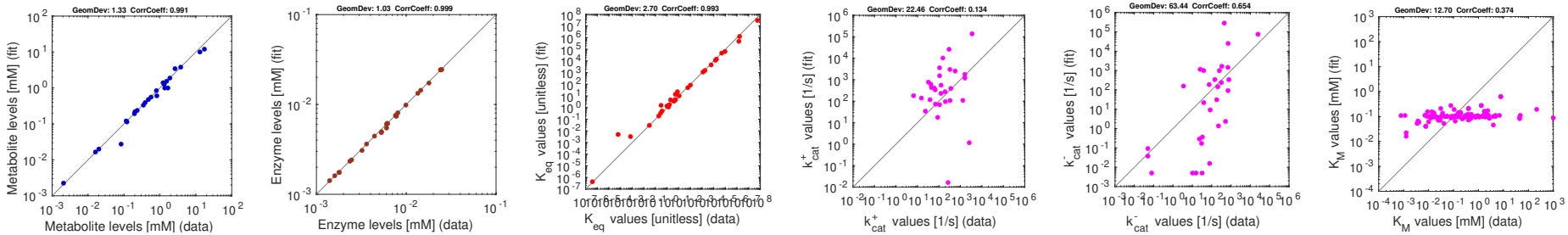
E. coli model (aerobic growth on glucose), balanced kinetic data

(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

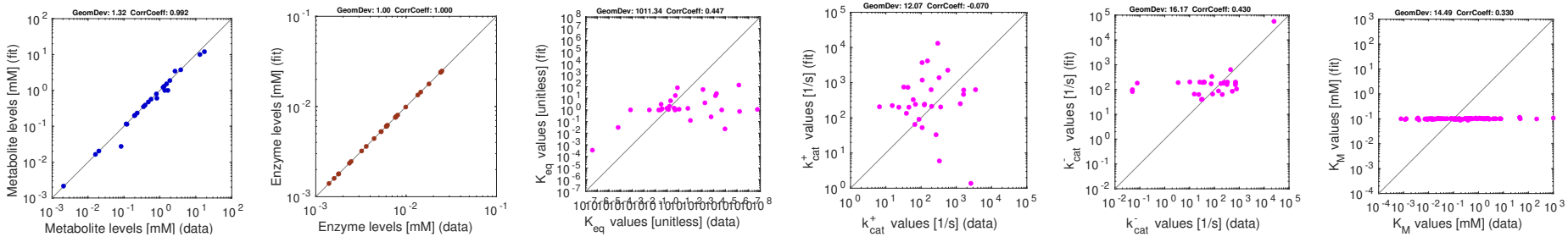


Figure 7: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). The kinetic data stem from previous parameter balancing based on *in-vitro* data. Top: estimation using kinetic data. Centre: estimation using equilibrium constants as the only kinetic data. Centre: 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

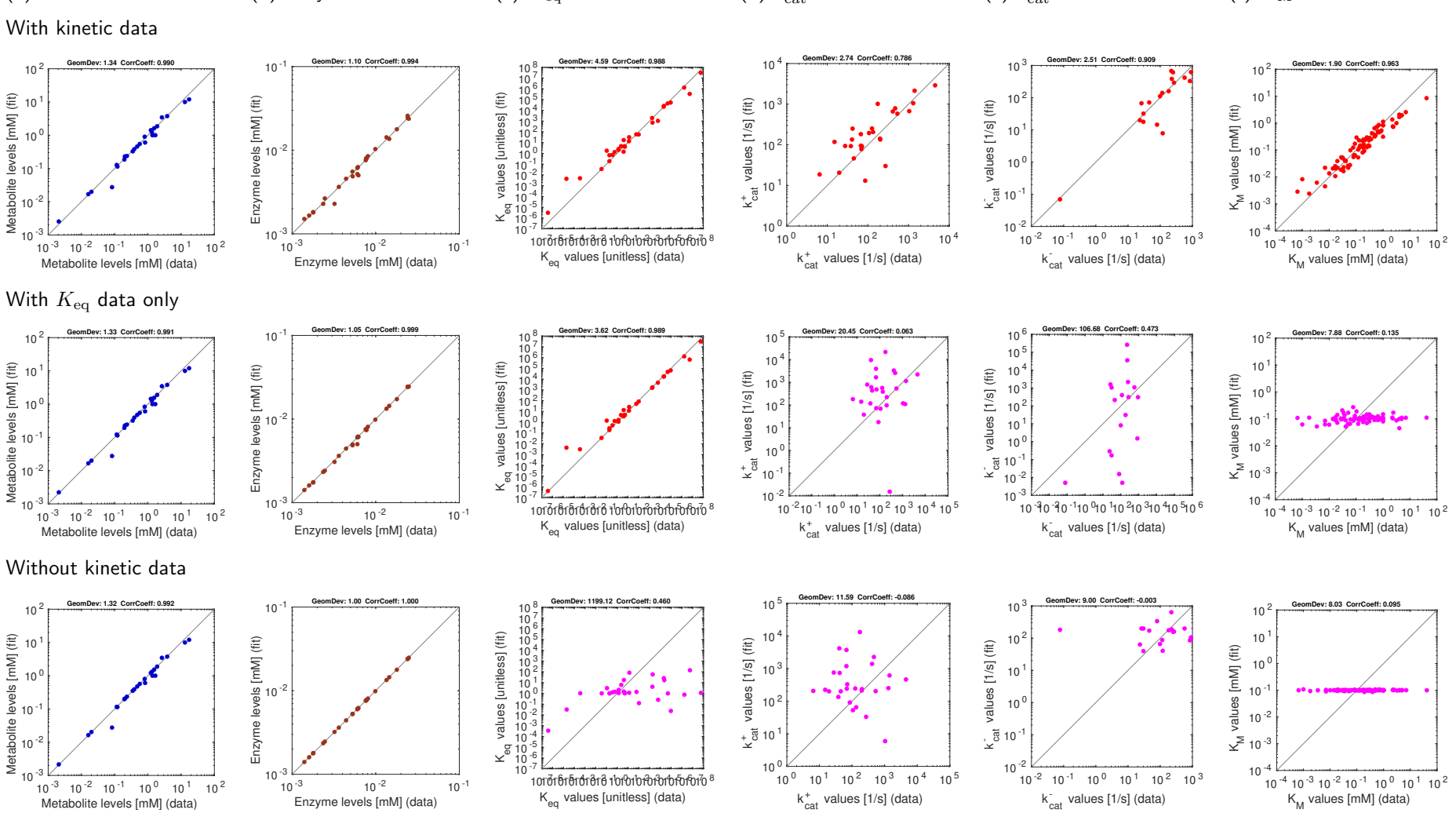


Figure 8: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). Same as Figure 3, but based on original kinetic *in-vitro* data instead of balanced kinetic data.

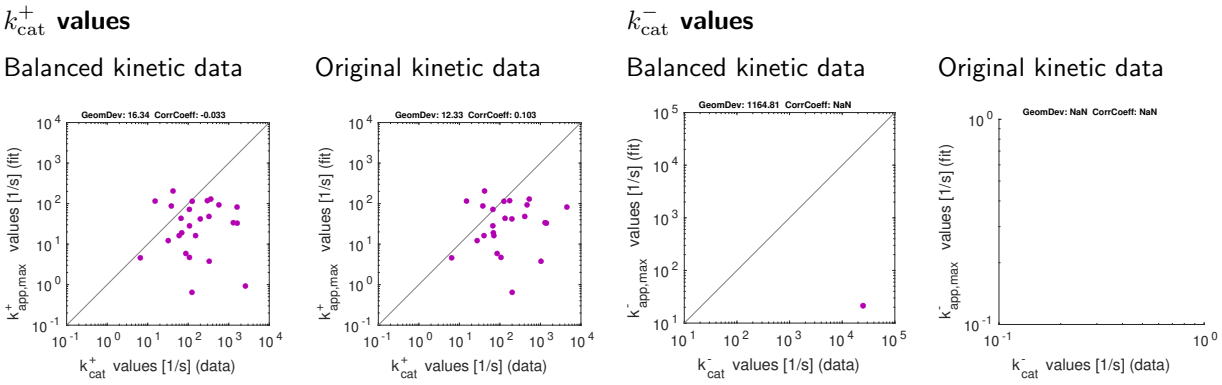


Figure 9: Catalytic constants in *E. coli* central metabolism model (aerobic growth on glucose), estimated by kinetic profiling.

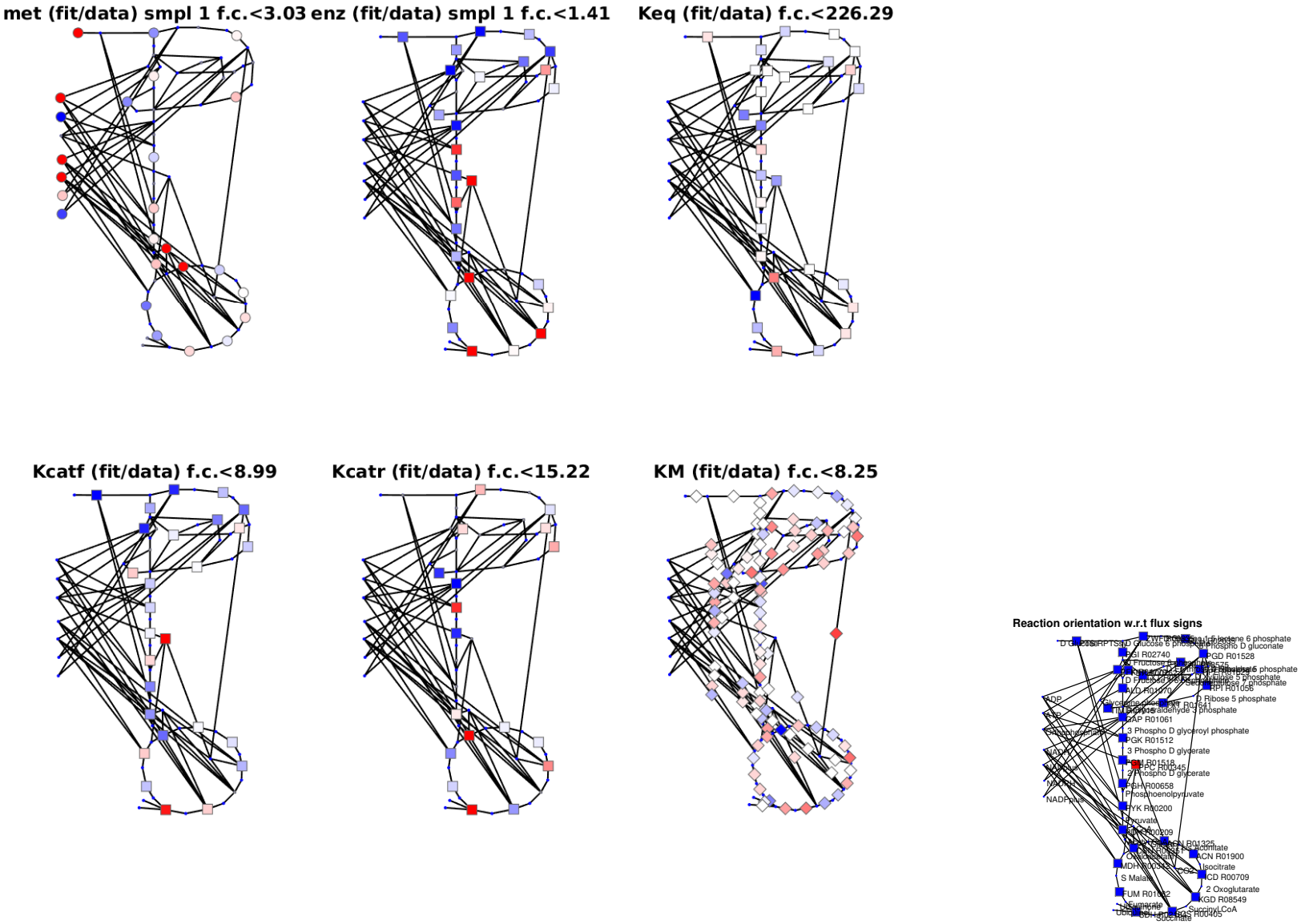


Figure 10: Diagnostic plots for fit with original kinetic data. Left: Relative fitting errors. Blue: fitted value too high. Red: fitted value too low. Maximal fold changes (whether up or down) are given by numbers. Right: Reaction orientatation (defining "forward" and "reverse"). Blue: in flux direction;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

3 E. coli Glucose simulations with alpha = 1, beta = 0

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

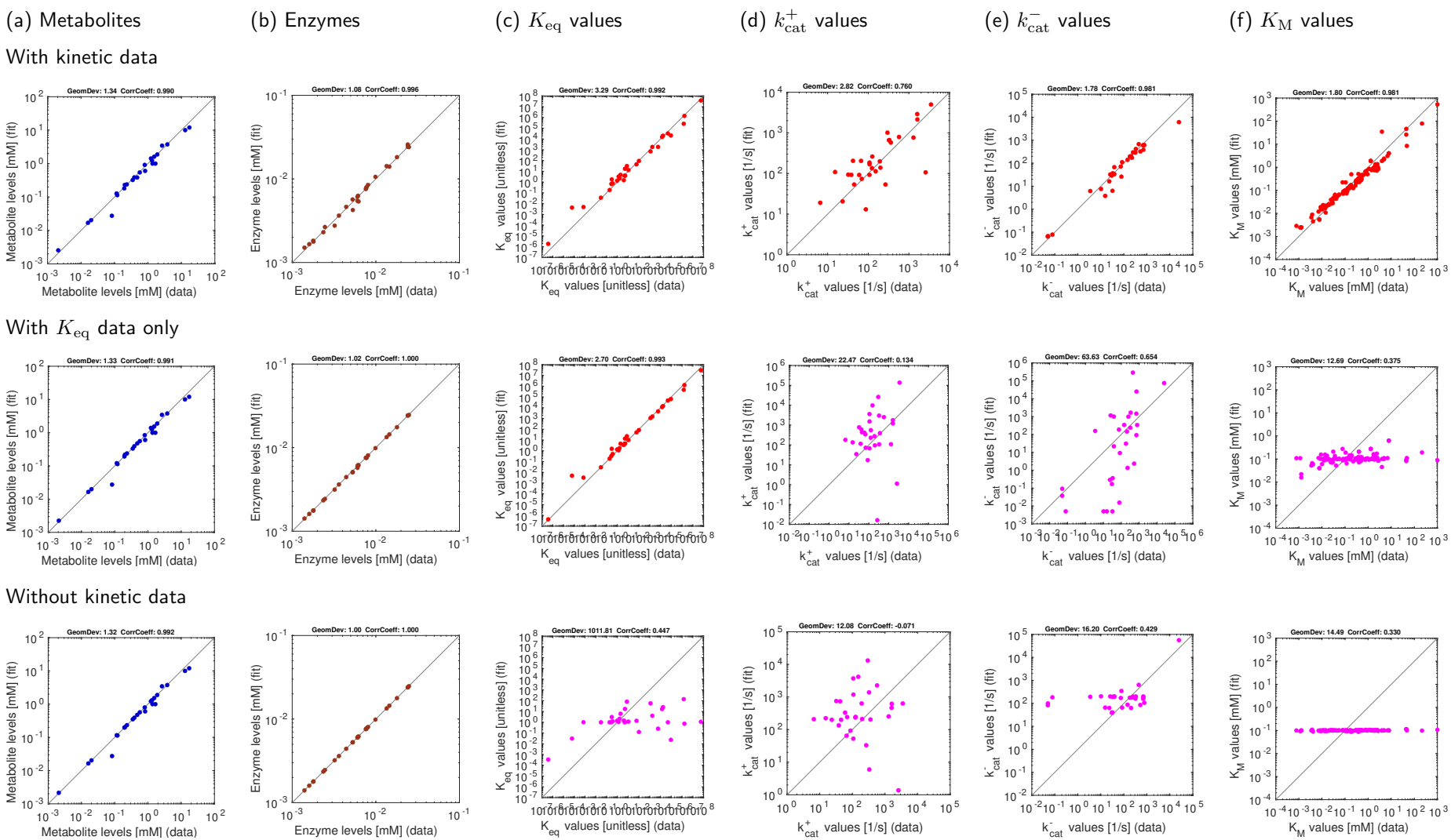


Figure 11: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). The kinetic data stem from previous parameter balancing based on *in-vitro* data. Top: estimation using kinetic data. Centre: estimation using equilibrium constants as the only kinetic data. Centre: 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

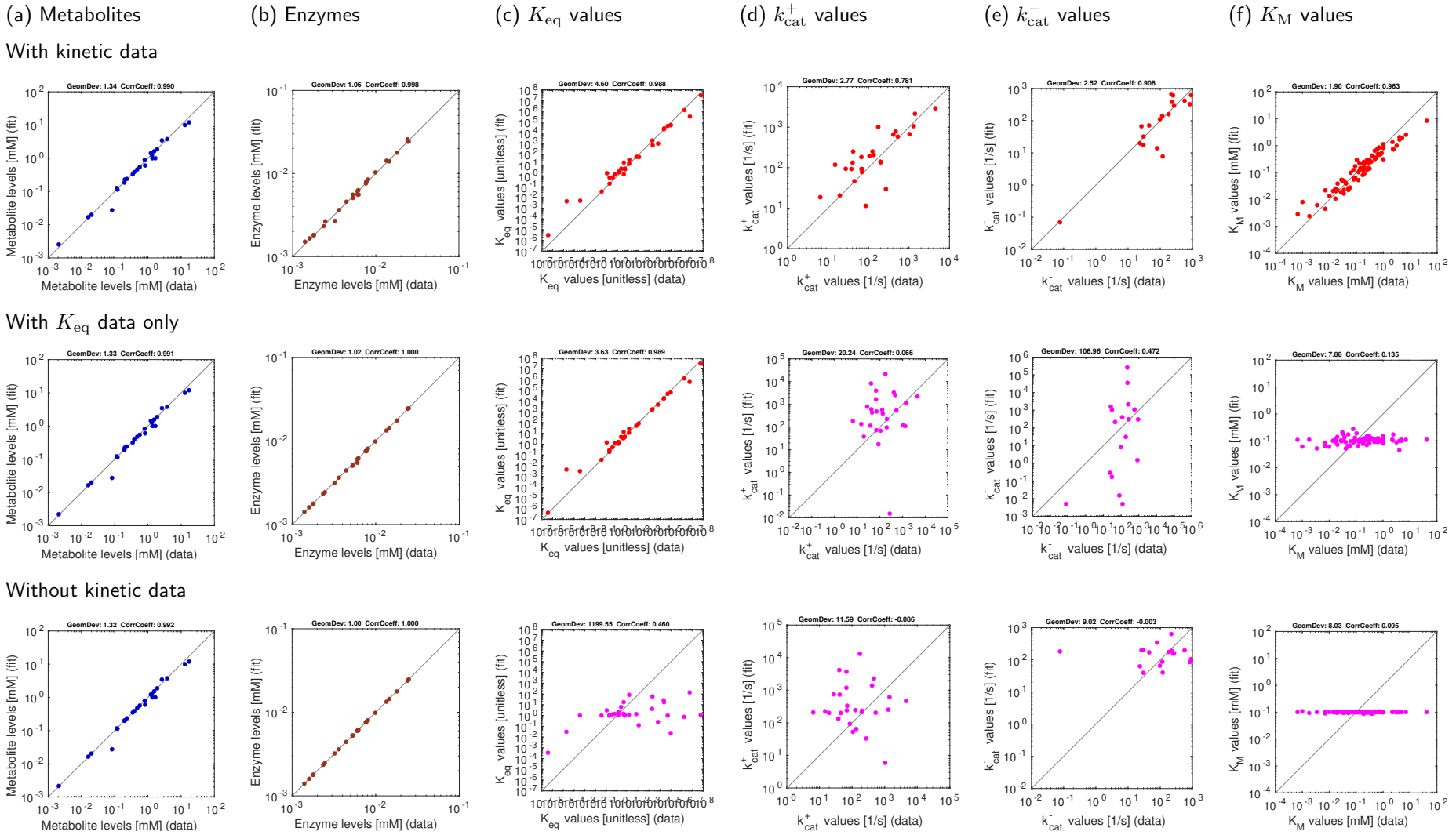


Figure 12: Results for *E. coli* central metabolism with experimental data (aerobic growth on glucose). Same as Figure 3, but based on original kinetic *in-vitro* data instead of balanced kinetic data.

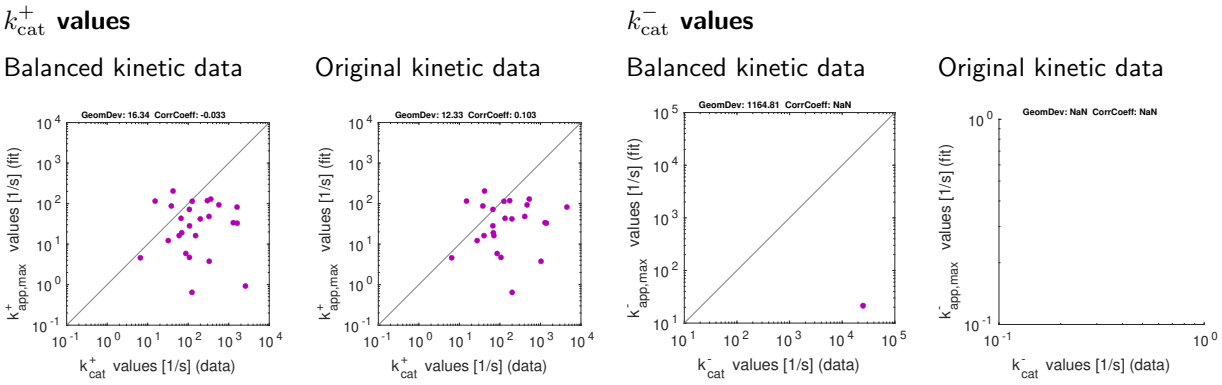


Figure 13: Catalytic constants in *E. coli* central metabolism model (aerobic growth on glucose), estimated by kinetic profiling.

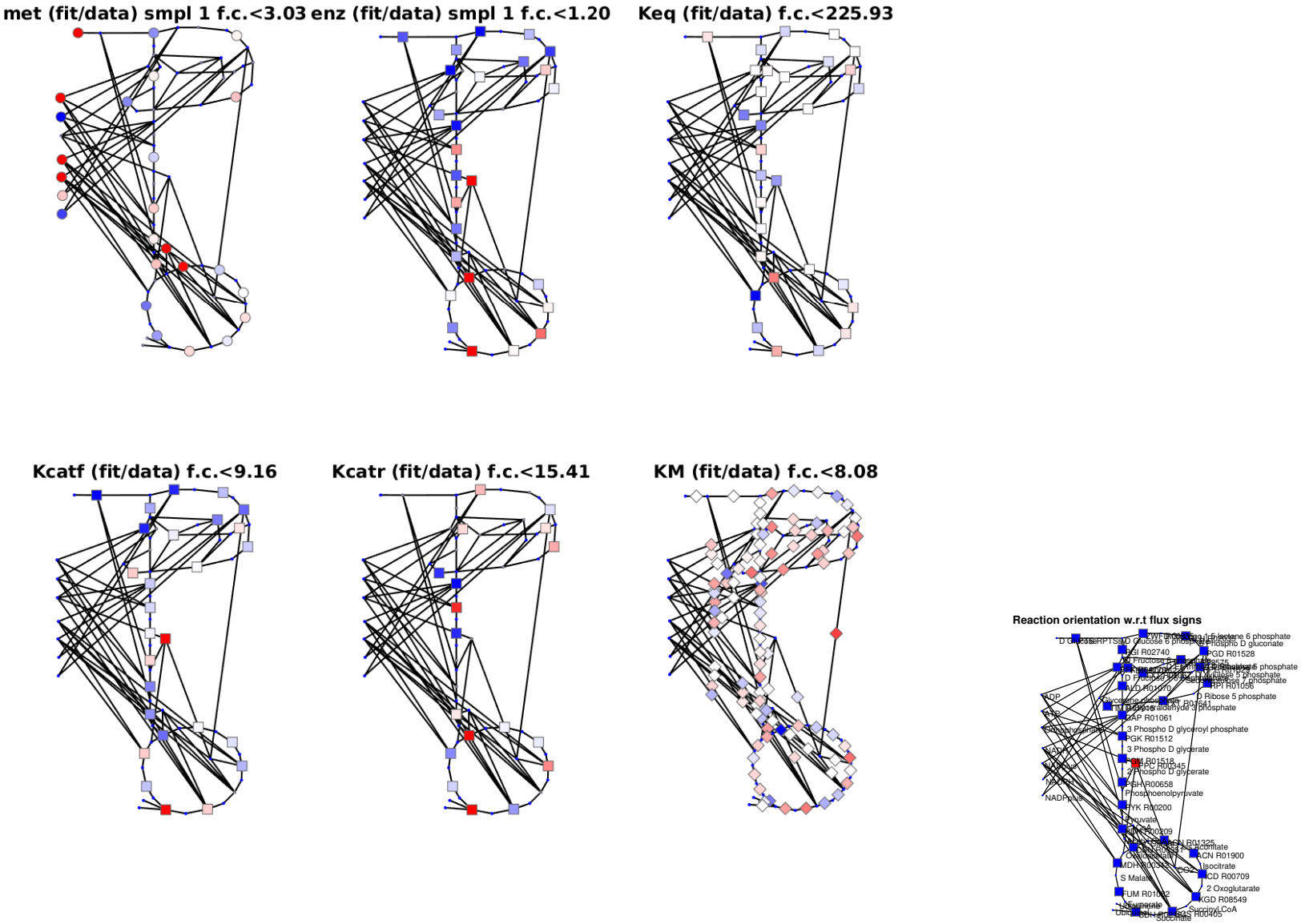


Figure 14: Diagnostic plots for fit with original kinetic data. Left: Relative fitting errors. Blue: fitted value too high. Red: fitted value too low. Maximal fold changes (whether up or down) are given by numbers. Right: Reaction orientatation (defining "forward" and "reverse"). Blue: in flux direction;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