1 Branch point simulations with alpha = 0, beta = 0

Branch point model with artificial data (noise-free kinetic data, noise-free state data) - alpha = 0, beta = 0

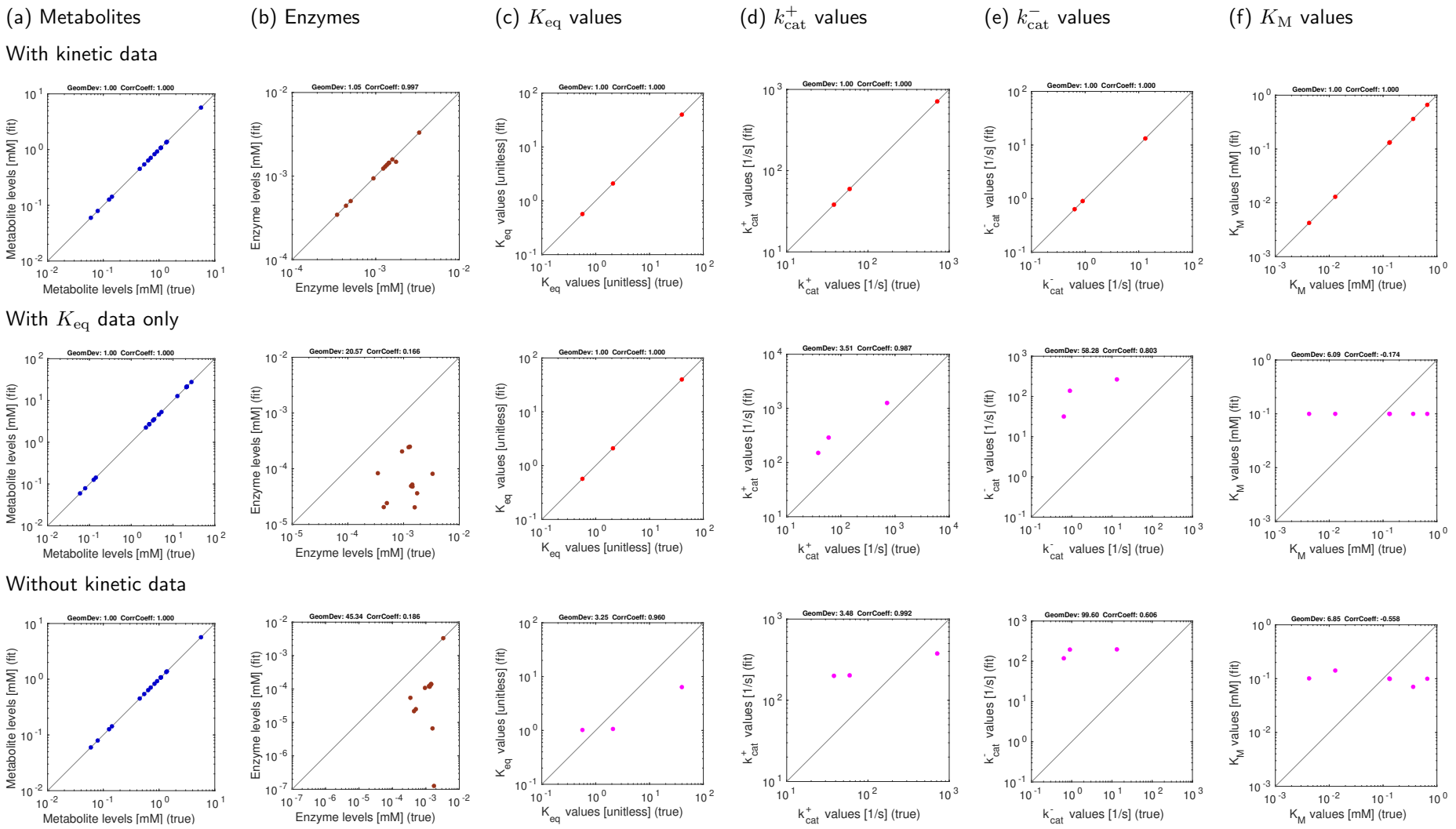


Figure 3: Model balancing results for Branch point model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation coefficients ("CorrCoeff"). (a) Metabolite levels. (b) Enzyme levels. (c)-(f) Different types of kinetic constants. Rows show different estimation scenarios (see Figure) Upper row: simple scenario S1 (noise-free artificial data, data for kinetic constants). Centre row: scenario S1K (noise-free artificial data, kinetic data given only for equilibrium constants). Lower row: scenario S2 (noise-free artificial data, no data for kinetic constants). Depending on the scenario, kinetic constants are either fitted (red dots) or predicted (magenta dots).

Branch point model with artificial data (noisy kinetic data, noise-free state data) - alpha = 0, beta = 0

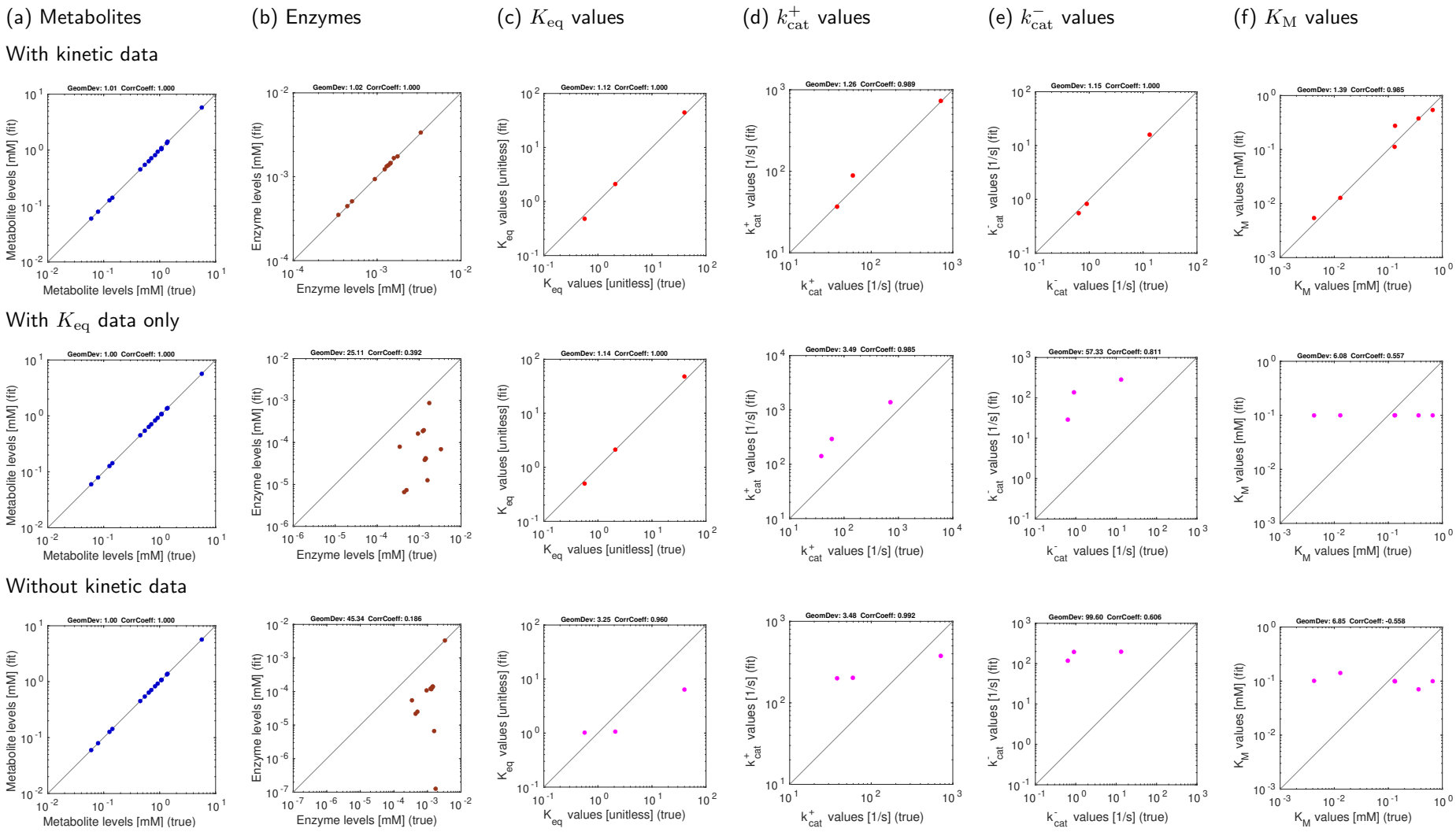
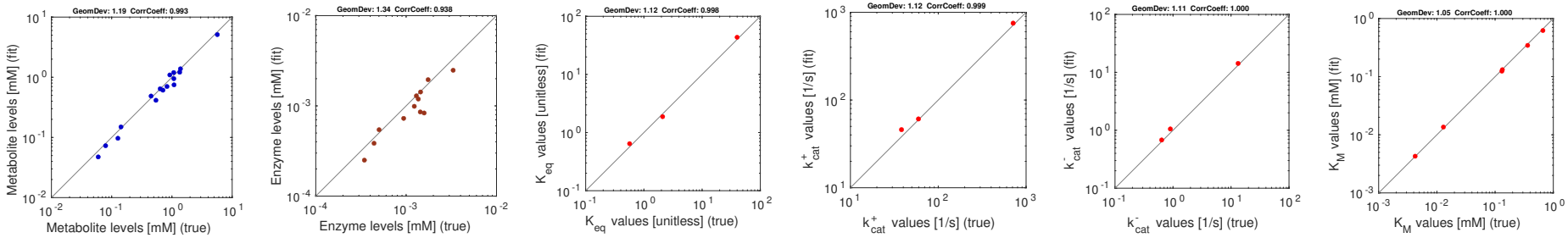


Figure 4: Same as Figure 8, with noisy kinetic data

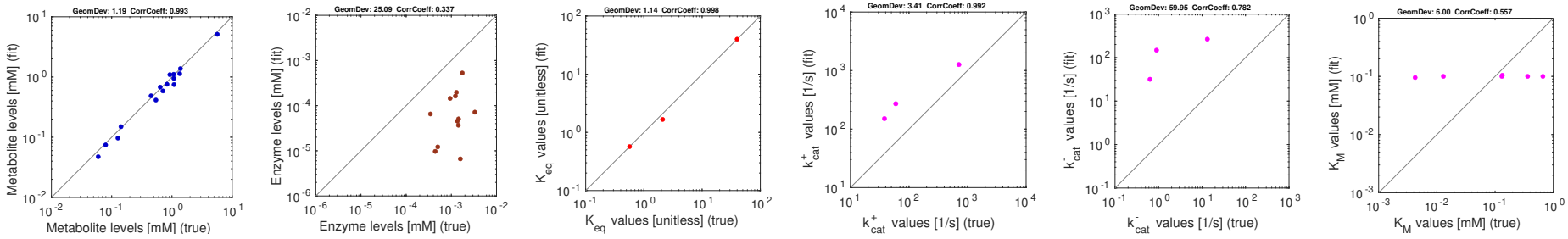
Branch point model with artificial data (noise-free kinetic data, noisy state data) - alpha = 0, beta = 0

(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

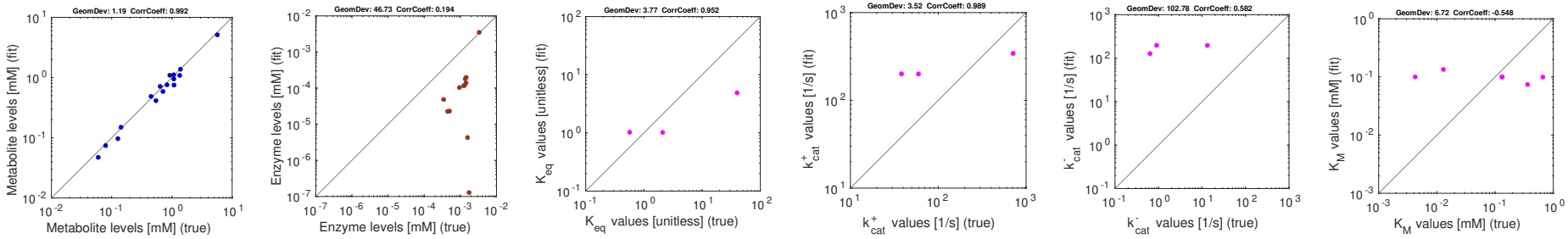
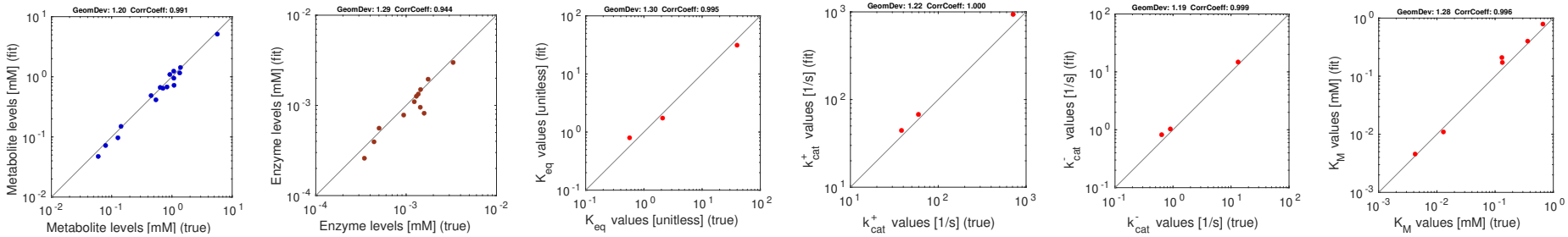


Figure 5: Results for Branch point with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial data, no data for kinetic constants).

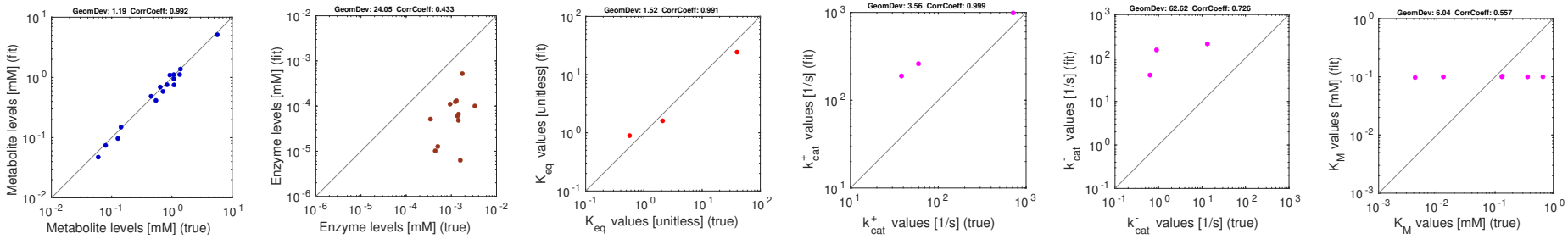
Branch point model with artificial data (noisy kinetic data, noisy state data) - alpha = 0, beta = 0

(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

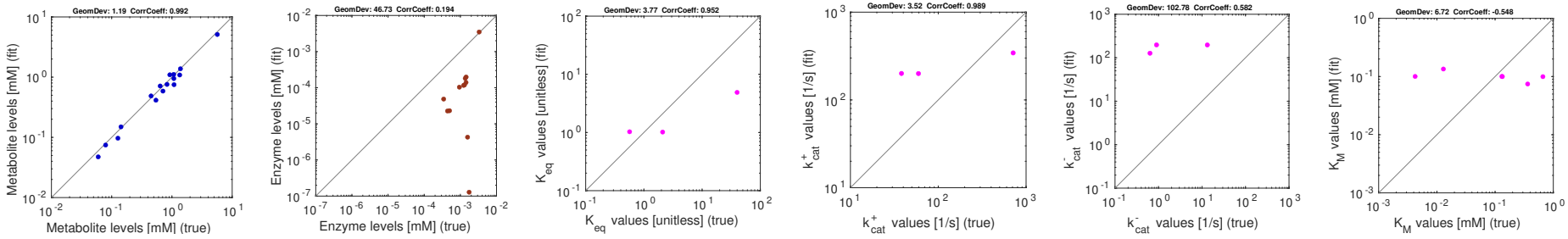


Figure 6: Same as Figure 10, with noisy kinetic data

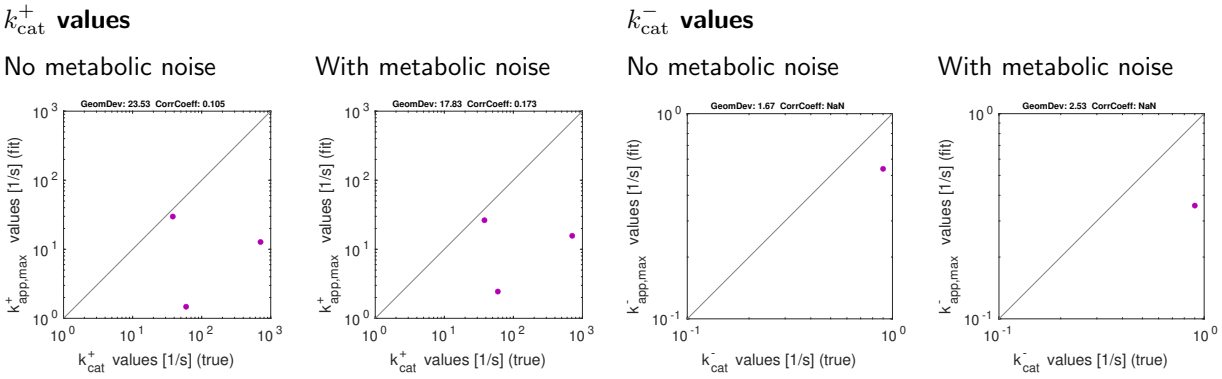


Figure 7: Catalytic constants in Branch point (artificial data), estimated by kinetic profiling. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).

2 Branch point simulations with alpha = 1, beta = 0

Branch point model with artificial data (noise-free kinetic data, noise-free state data) - alpha = 1, beta = 0

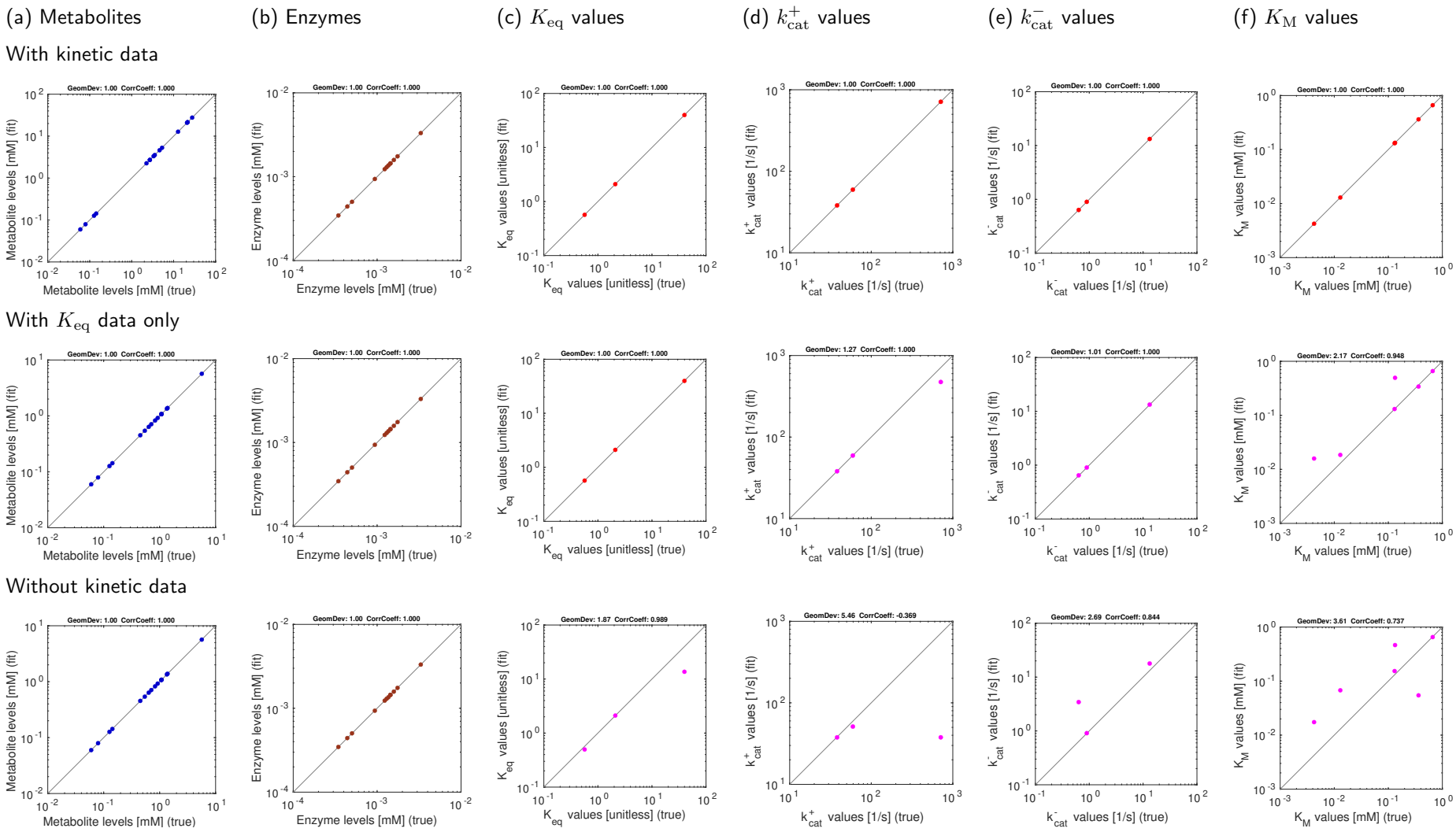


Figure 8: Model balancing results for Branch point model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation coefficients ("CorrCoeff"). (a) Metabolite levels. (b) Enzyme levels. (c)-(f) Different types of kinetic constants. Rows show different estimation scenarios (see Figure) Upper row: simple scenario S1 (noise-free artificial data, data for kinetic constants). Centre row: scenario S1K (noise-free artificial data, kinetic data given only for equilibrium constants). Lower row: scenario S2 (noise-free artificial data, no data for kinetic constants). Depending on the scenario, kinetic constants are either fitted (red dots) or predicted (magenta dots).

Branch point model with artificial data (noisy kinetic data, noise-free state data) - alpha = 1, beta = 0

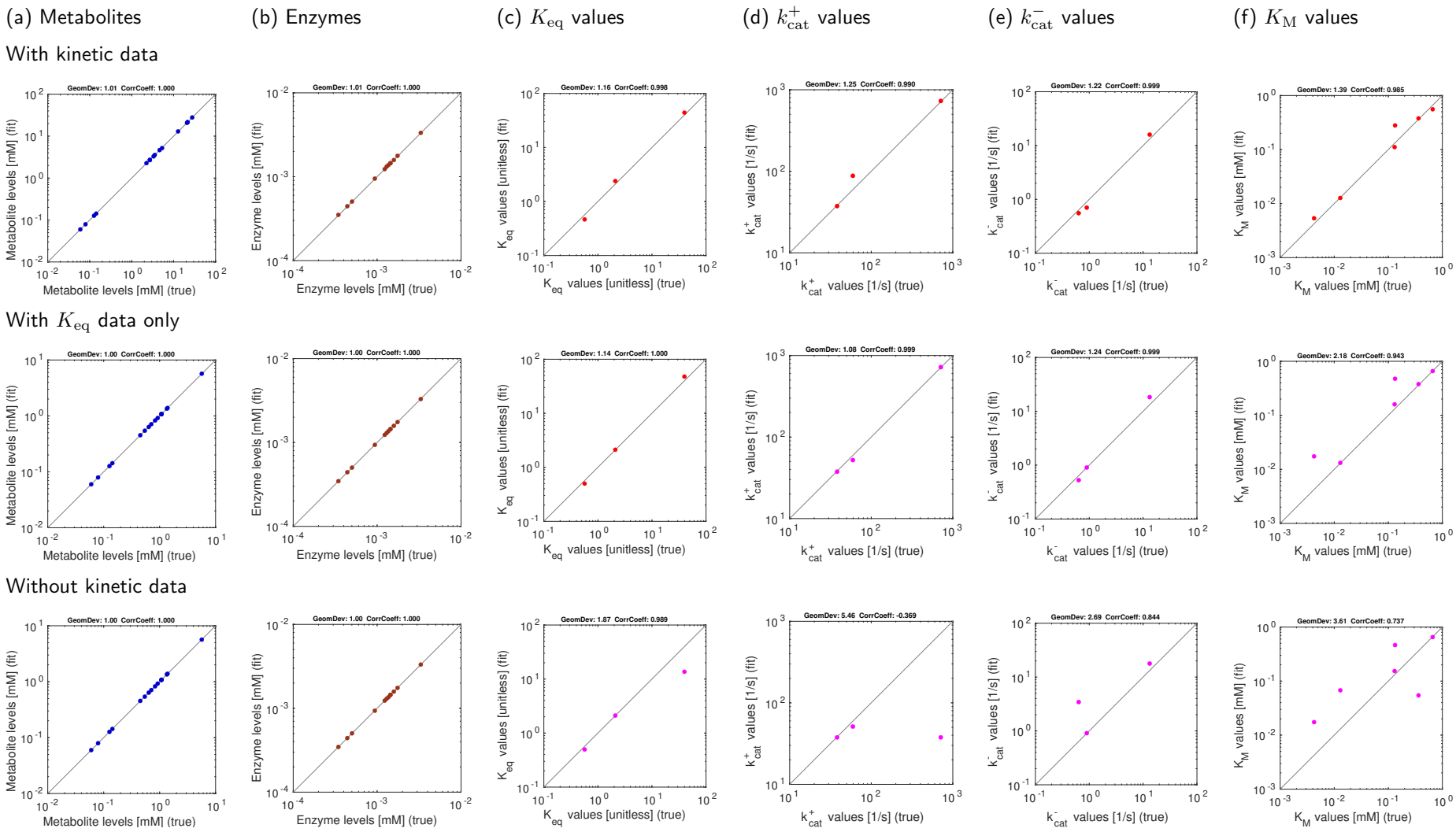


Figure 9: Same as Figure 8, with noisy kinetic data

Branch point model with artificial data (noise-free kinetic data, noisy state data) - alpha = 1, beta = 0

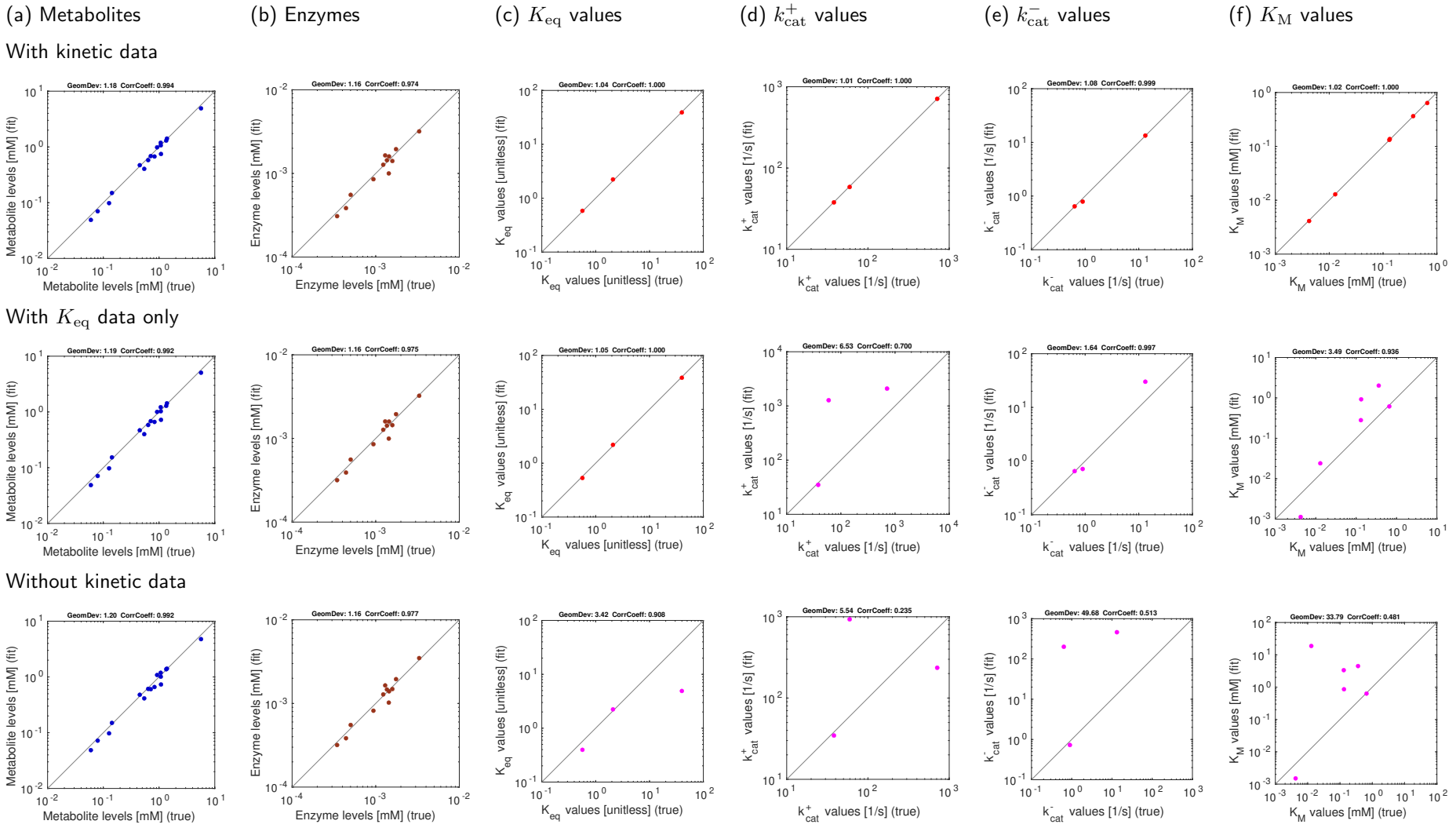


Figure 10: Results for Branch point with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial data, no data for kinetic constants).

Branch point model with artificial data (noisy kinetic data, noisy state data) - alpha = 1, beta = 0

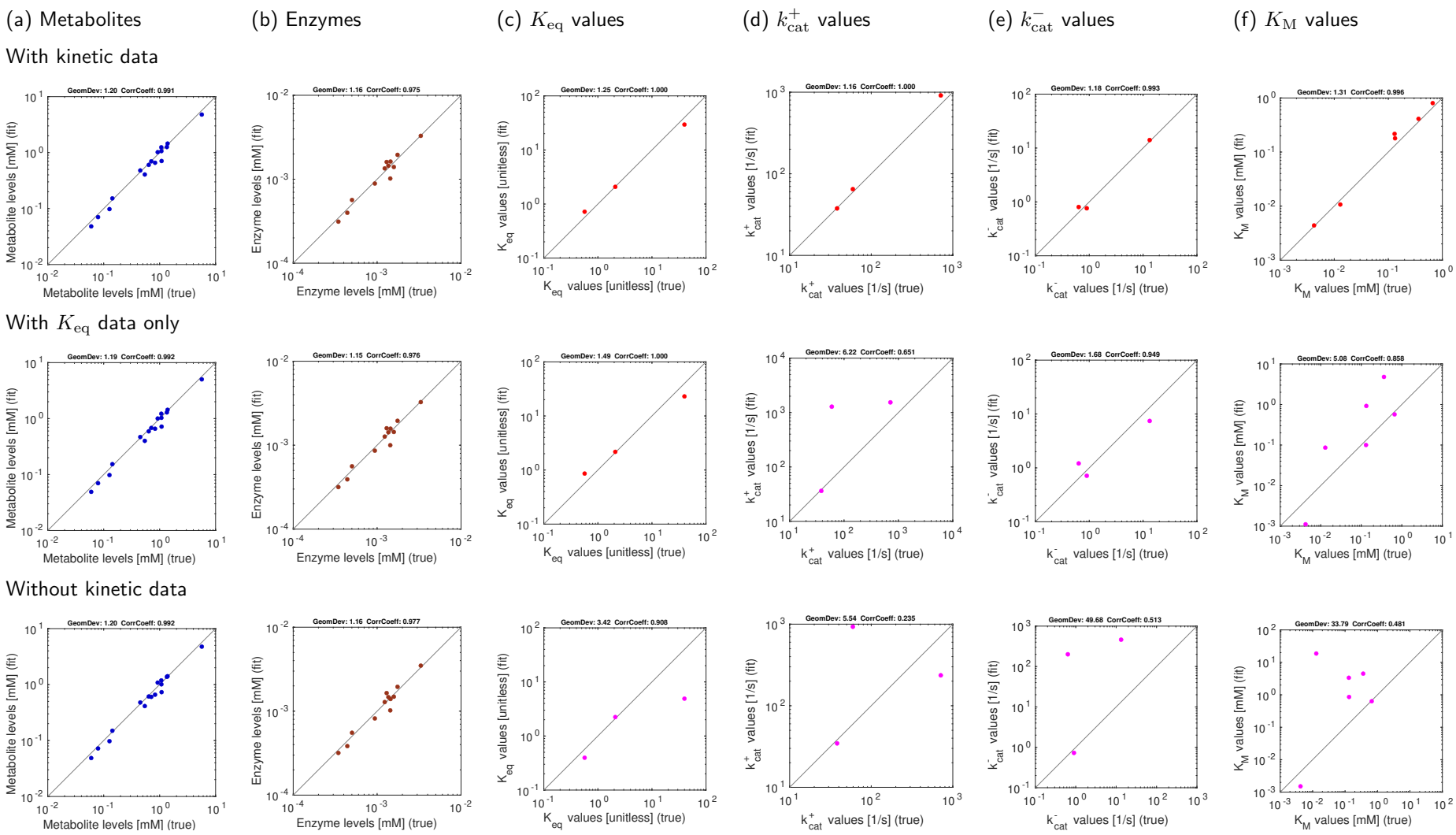


Figure 11: Same as Figure 10, with noisy kinetic data

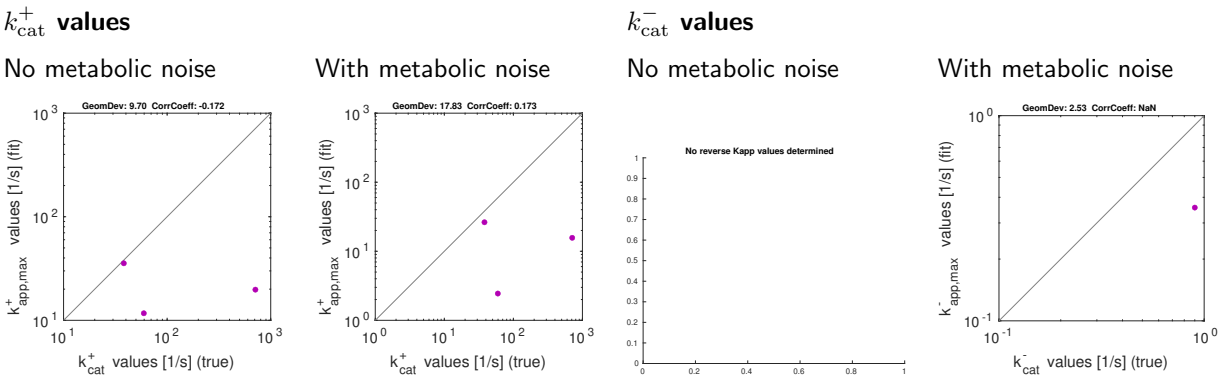


Figure 12: Catalytic constants in Branch point (artificial data), estimated by kinetic profiling. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).