1 Double branch simulations with alpha = 0, beta = 0

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

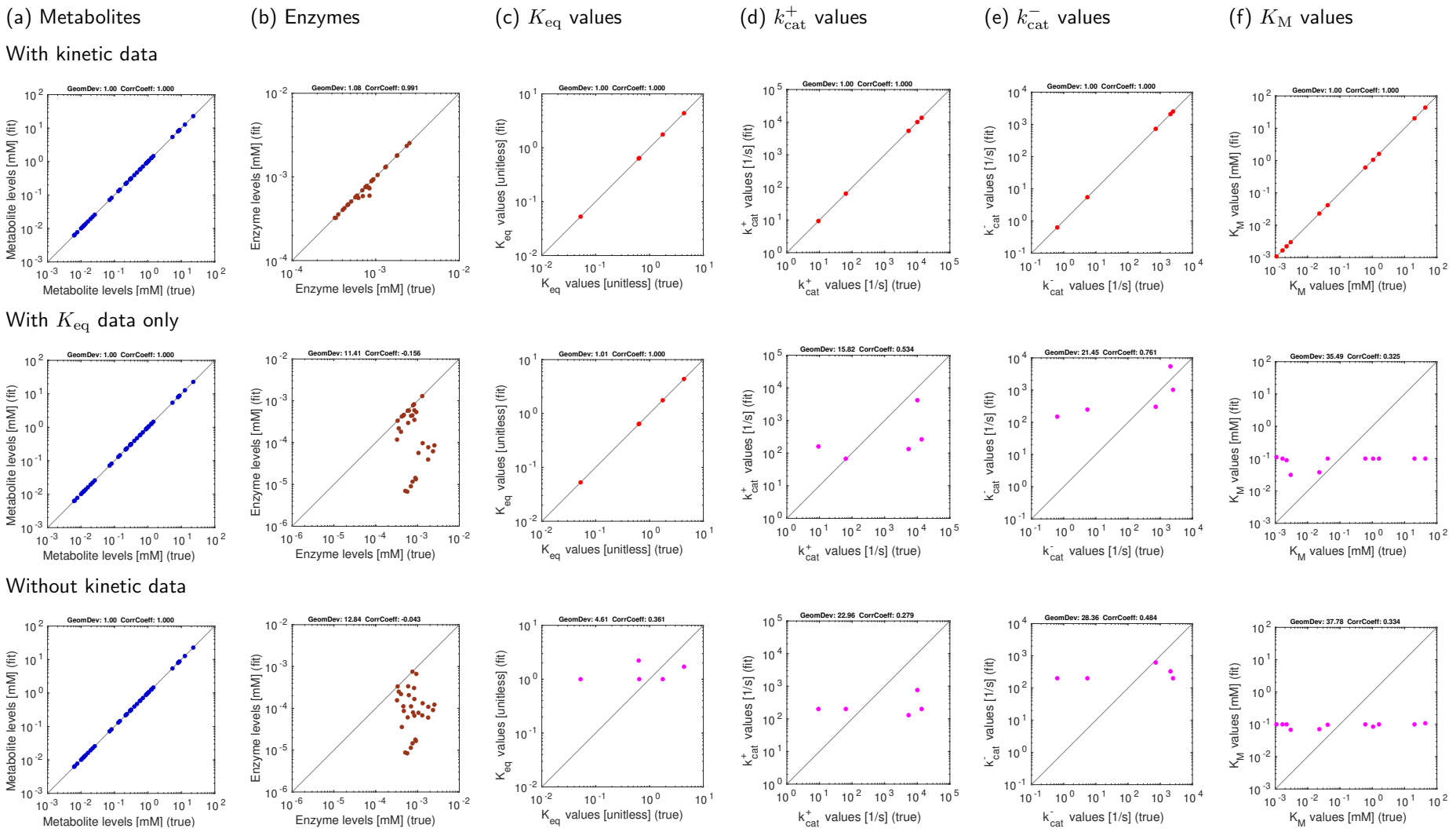

Figure 3: Model balancing results for Double branch model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quantified by geometric standard deviations ("GeomDev") and Pearson correlation 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).

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

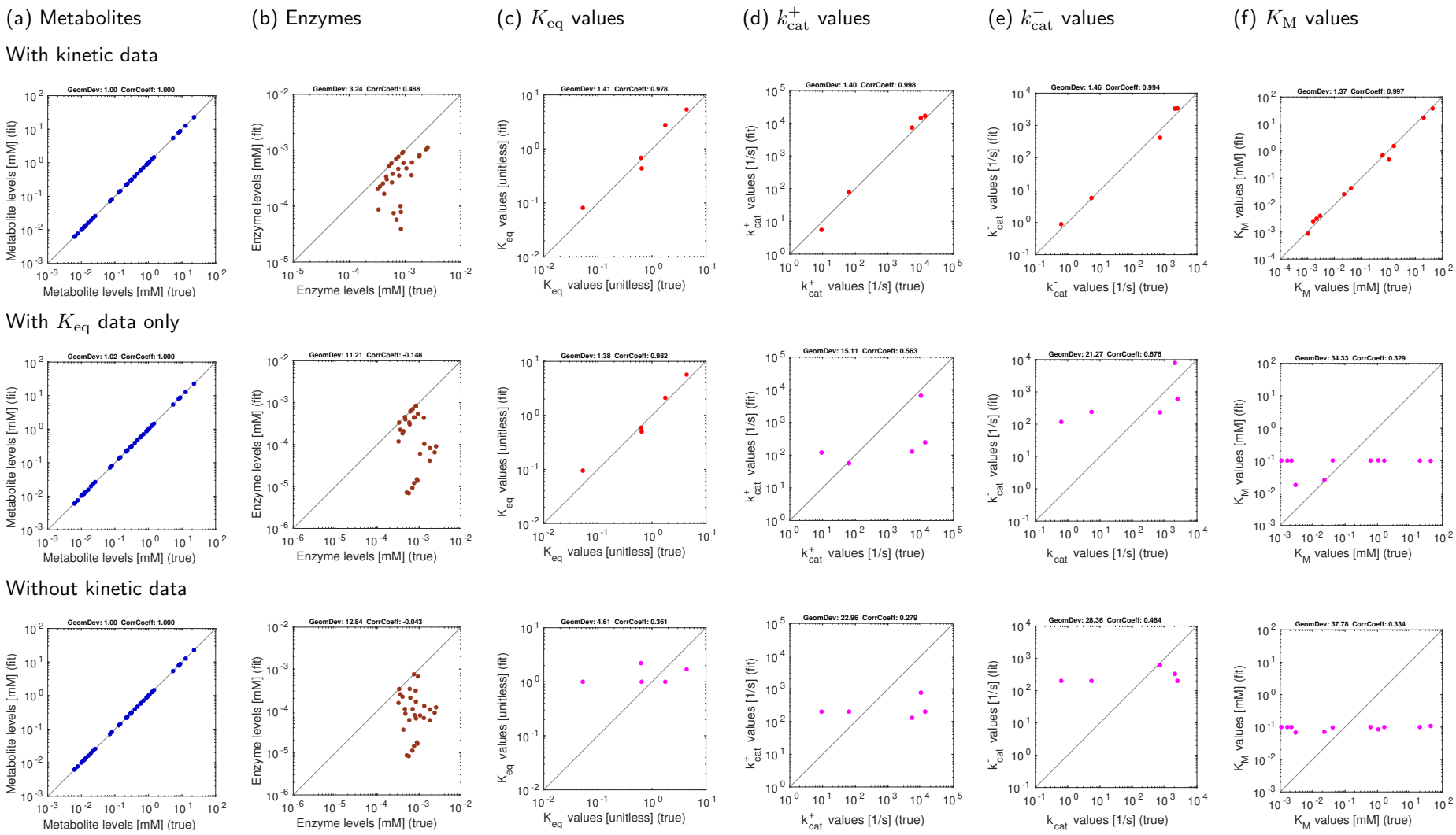

Figure 4: Same as Figure 13, with noisy kinetic data

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

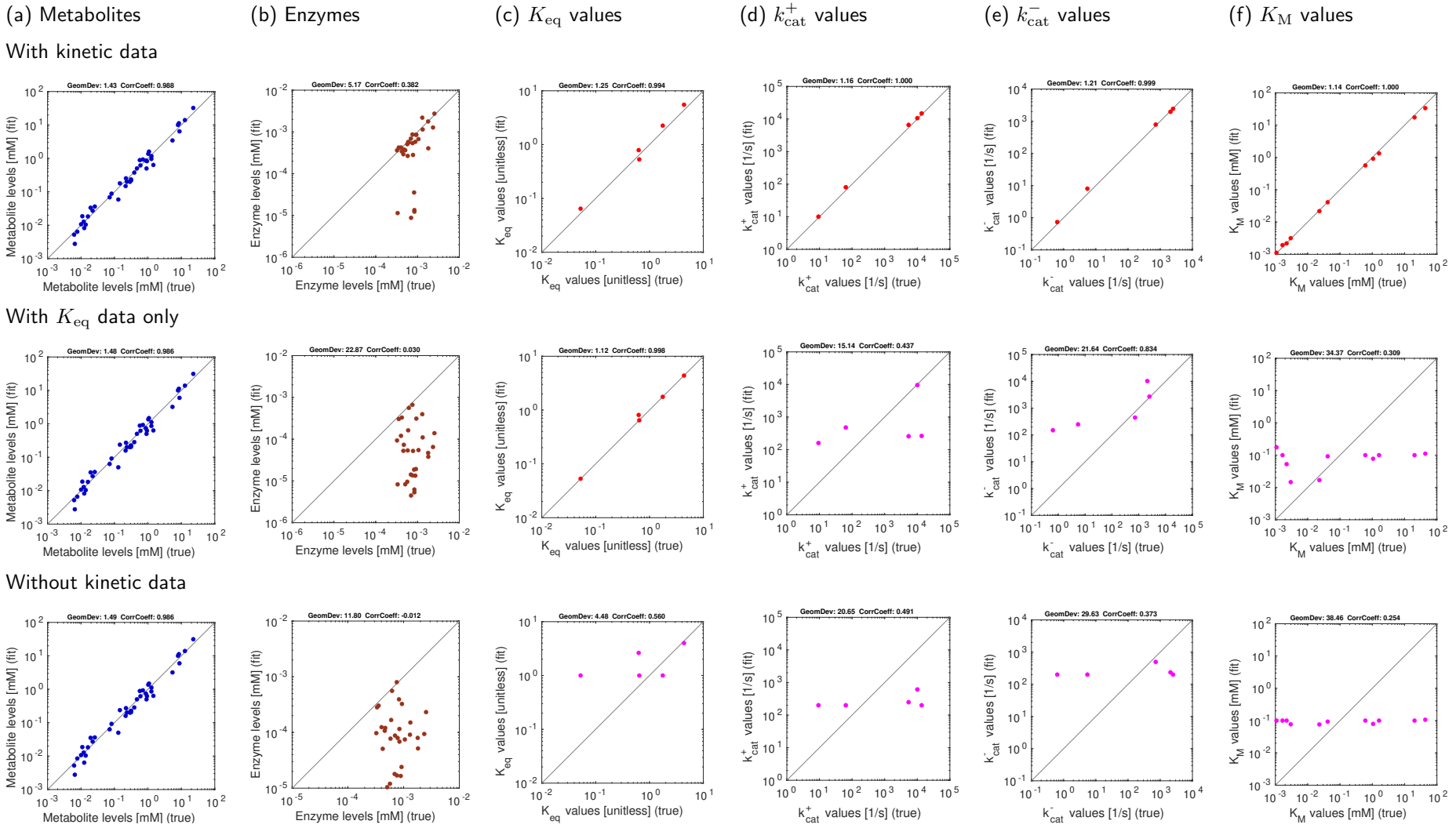

Figure 5: Results for Double branch with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial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

Double branch model with artificial data (noisy kinetic data, noisy state data) - alpha = 0, beta = 0

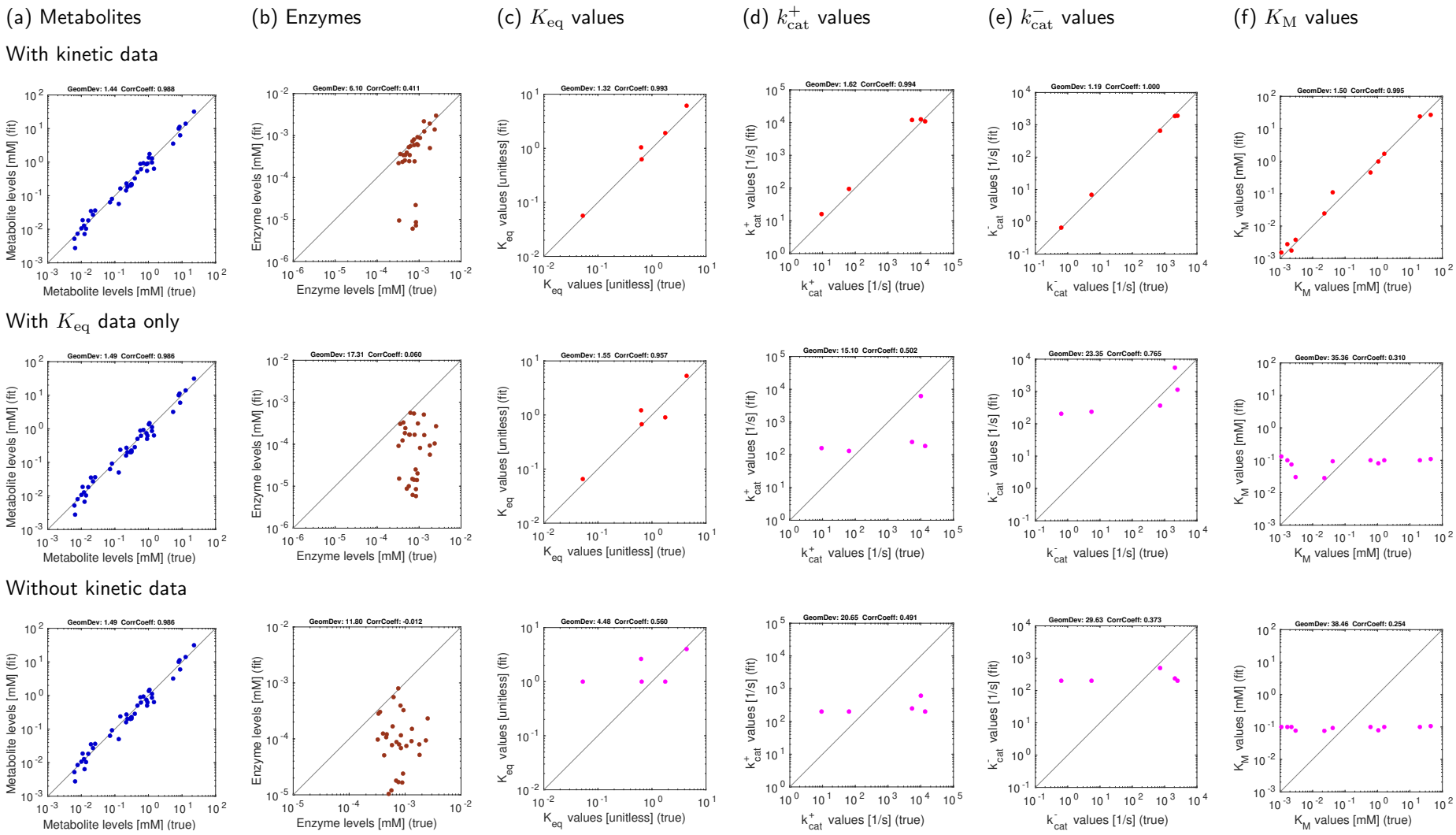

Figure 6: Same as Figure 15, with noisy kinetic data

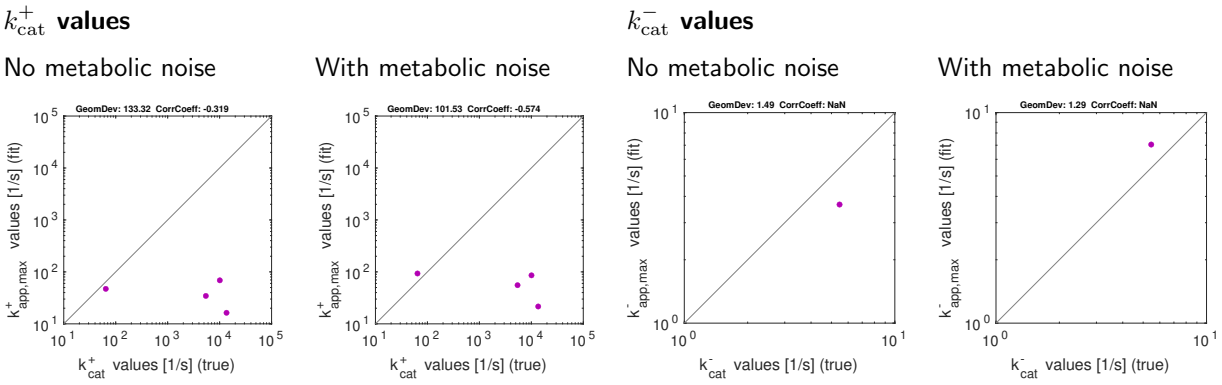

Figure 7: Catalytic constants in Double branch (artificial data), estimated by kinetic profiling. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).

2 Double branch model Simulations with alpha = 0.1

3 Double branch simulations with alpha = 0.1, beta = 0

Double branch model with artificial data (noise-free kinetic data, noise-free state data) - alpha = 0.1, beta = 0

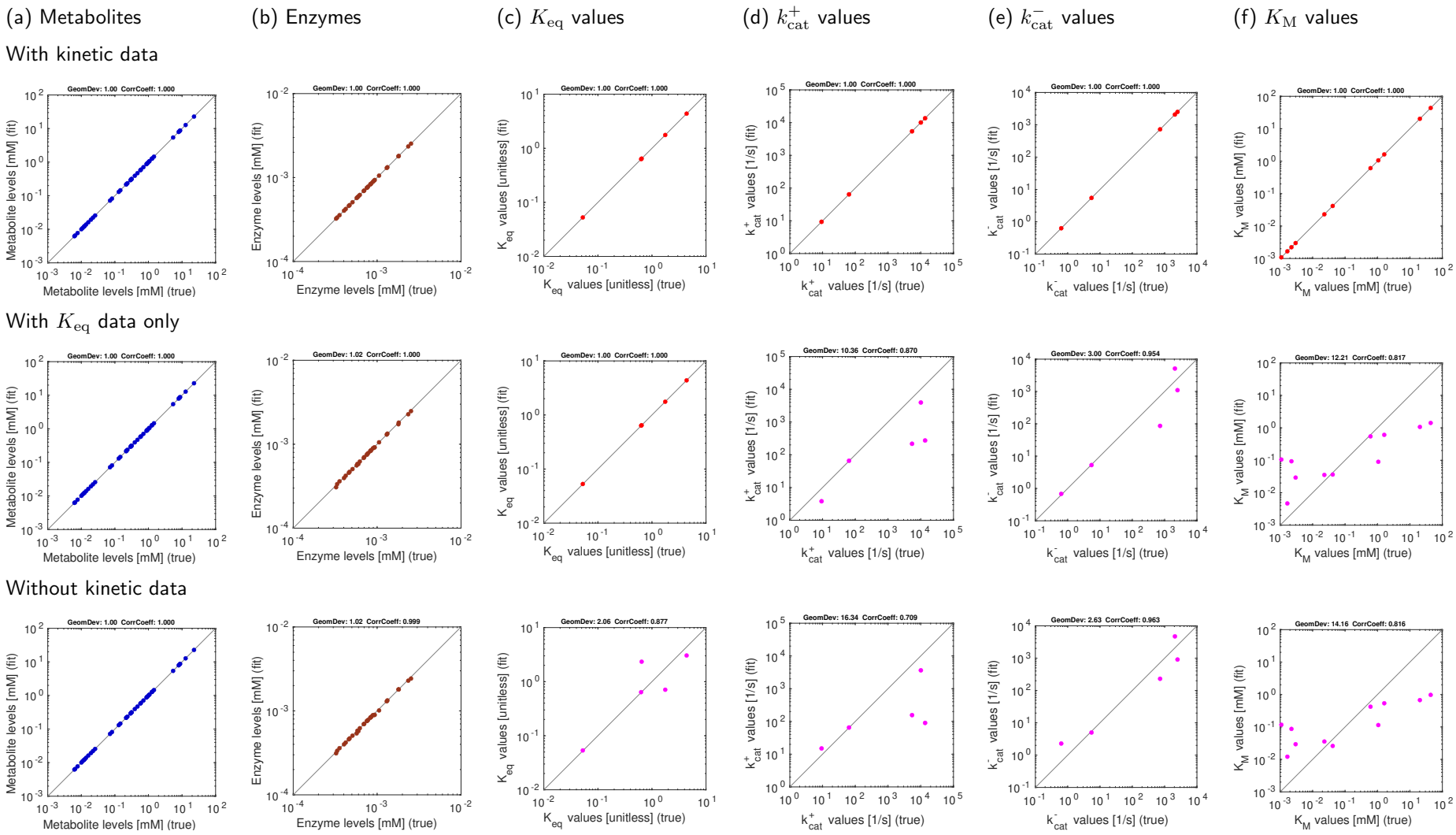

Figure 8: Model balancing results for Double branch model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quantified by geometric standard deviations ("GeomDev") and Pearson correlation 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).

Double branch model with artificial data (noisy kinetic data, noise-free state data) - alpha = 0.1, beta = 0

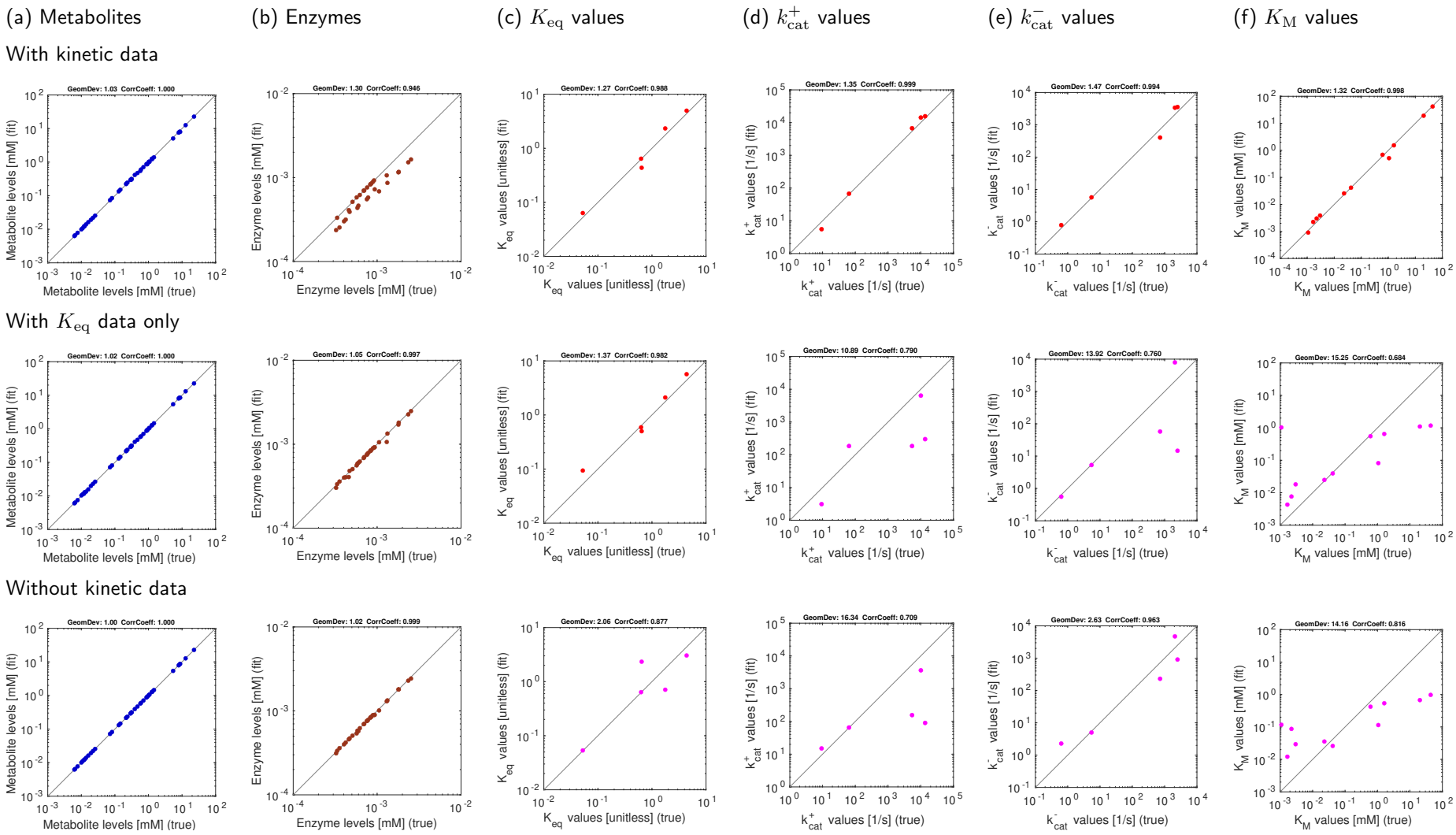

Figure 9: Same as Figure 13, with noisy kinetic data

Double branch model with artificial data (noise-free kinetic data, noisy state data) - alpha = 0.1, beta = 0

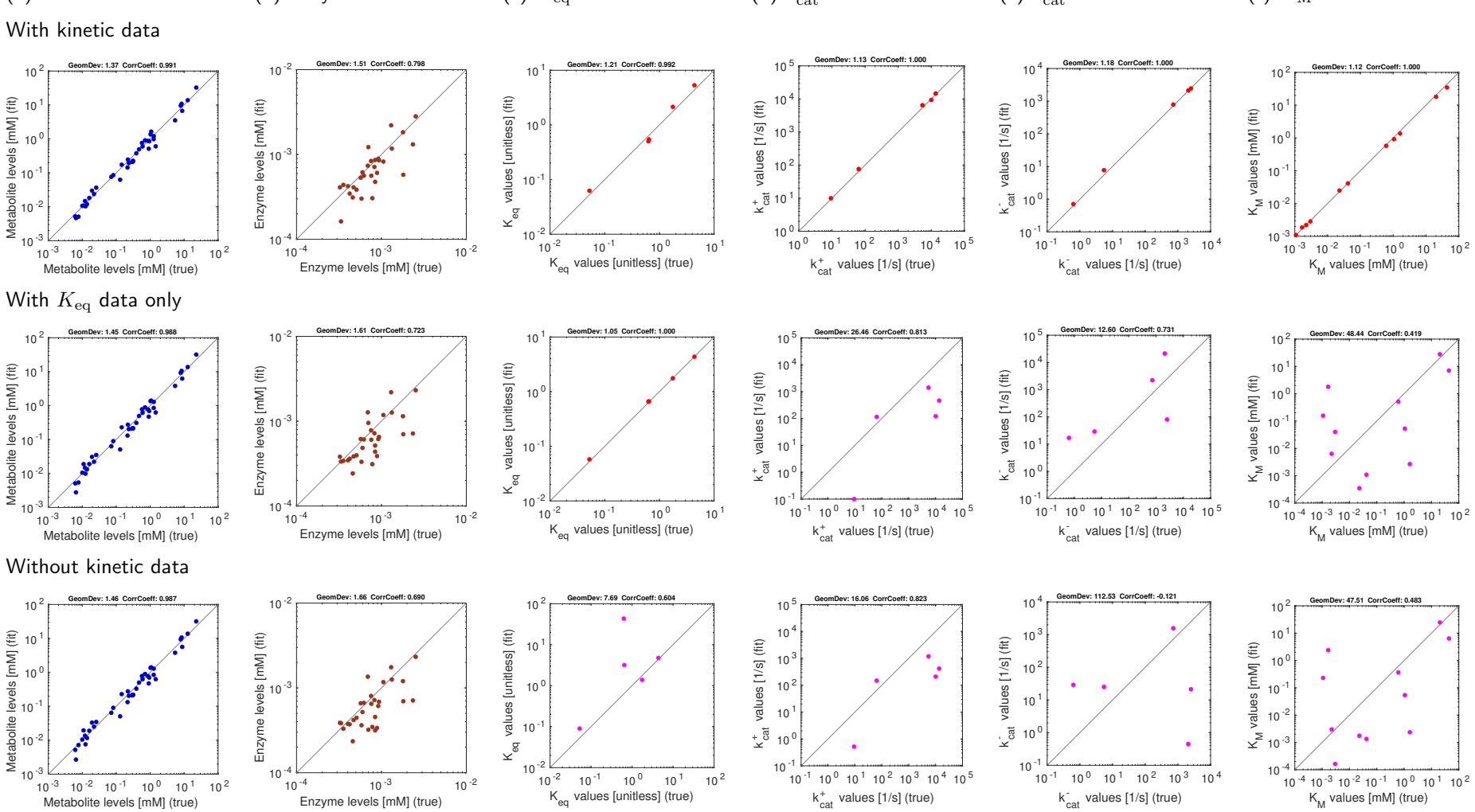

Figure 10: Results for Double branch with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial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

Double branch model with artificial data (noisy kinetic data, noisy state data) - alpha = 0.1, beta = 0

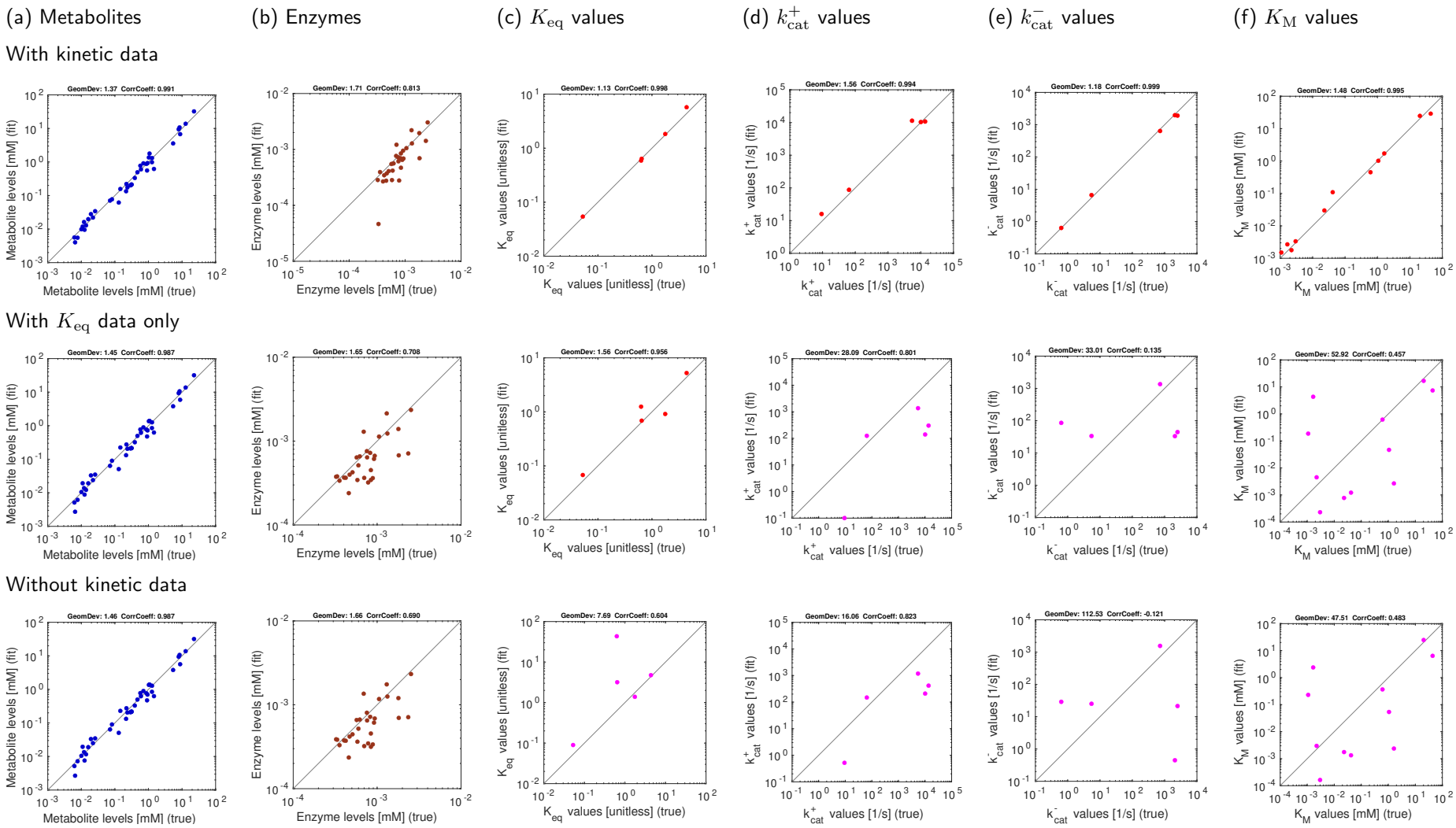

Figure 11: Same as Figure 15, with noisy kinetic data

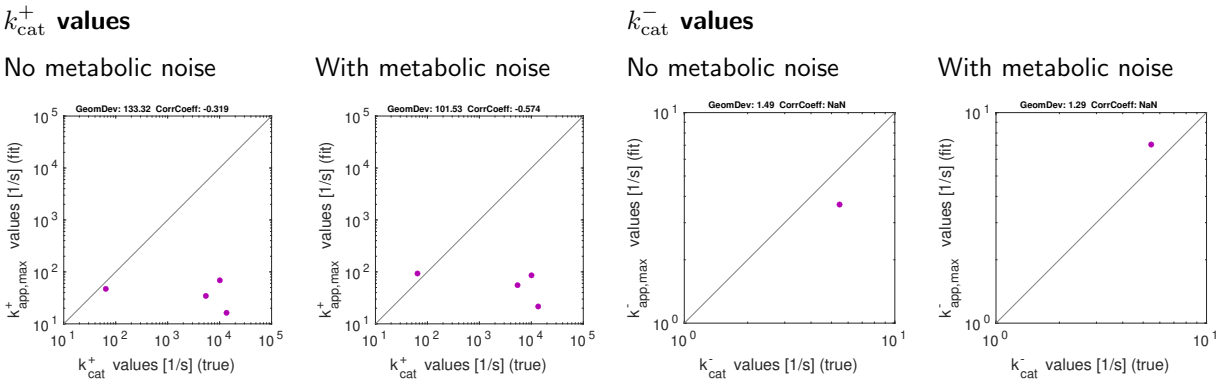

Figure 12: Catalytic constants in Double branch (artificial data), estimated by kinetic profiling. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).

4 Double branch model Simulations with alpha = 1

5 Double branch simulations with alpha = 1, beta = 0

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

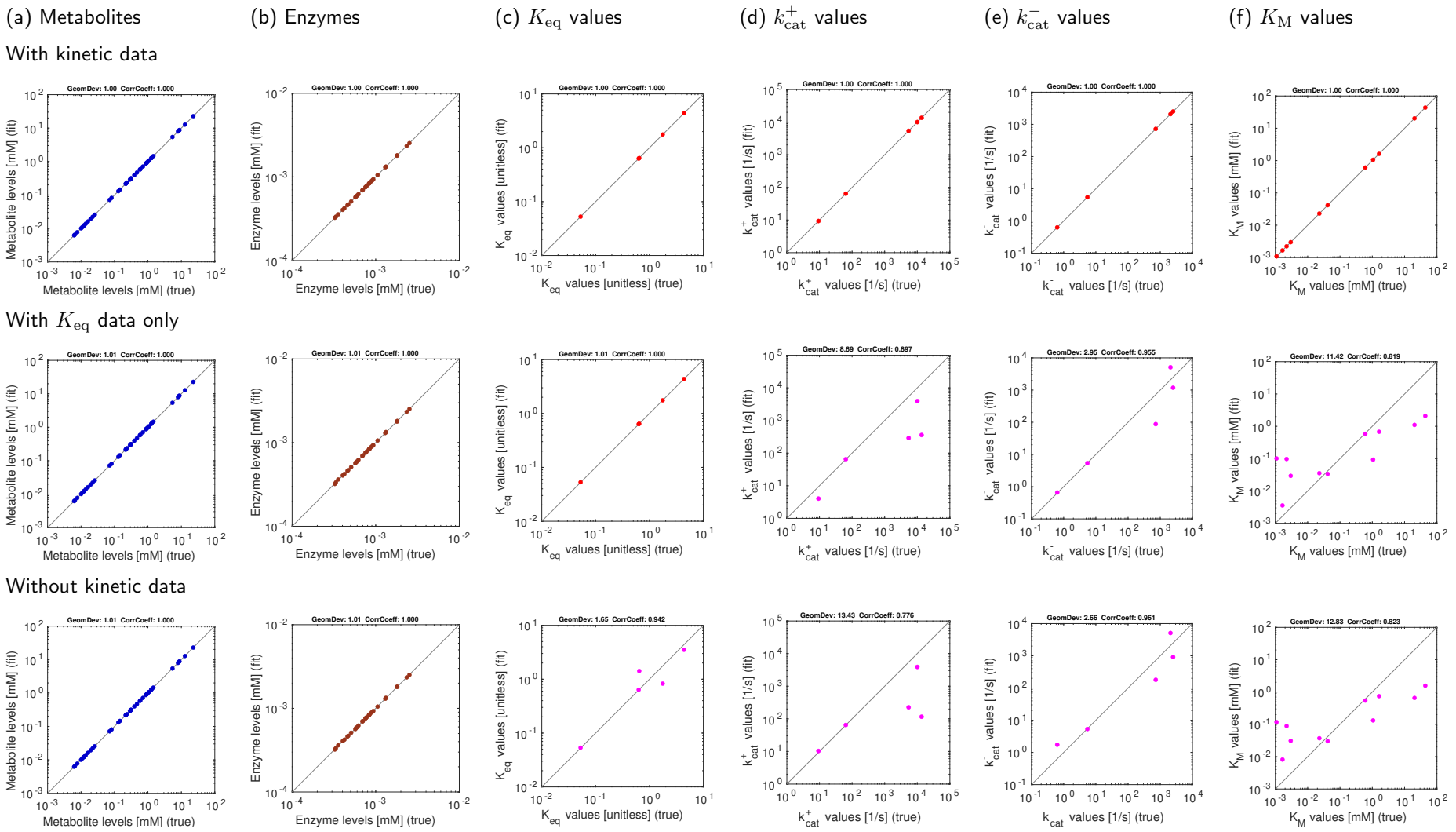

Figure 13: Model balancing results for Double branch model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quantified by geometric standard deviations ("GeomDev") and Pearson correlation 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).

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

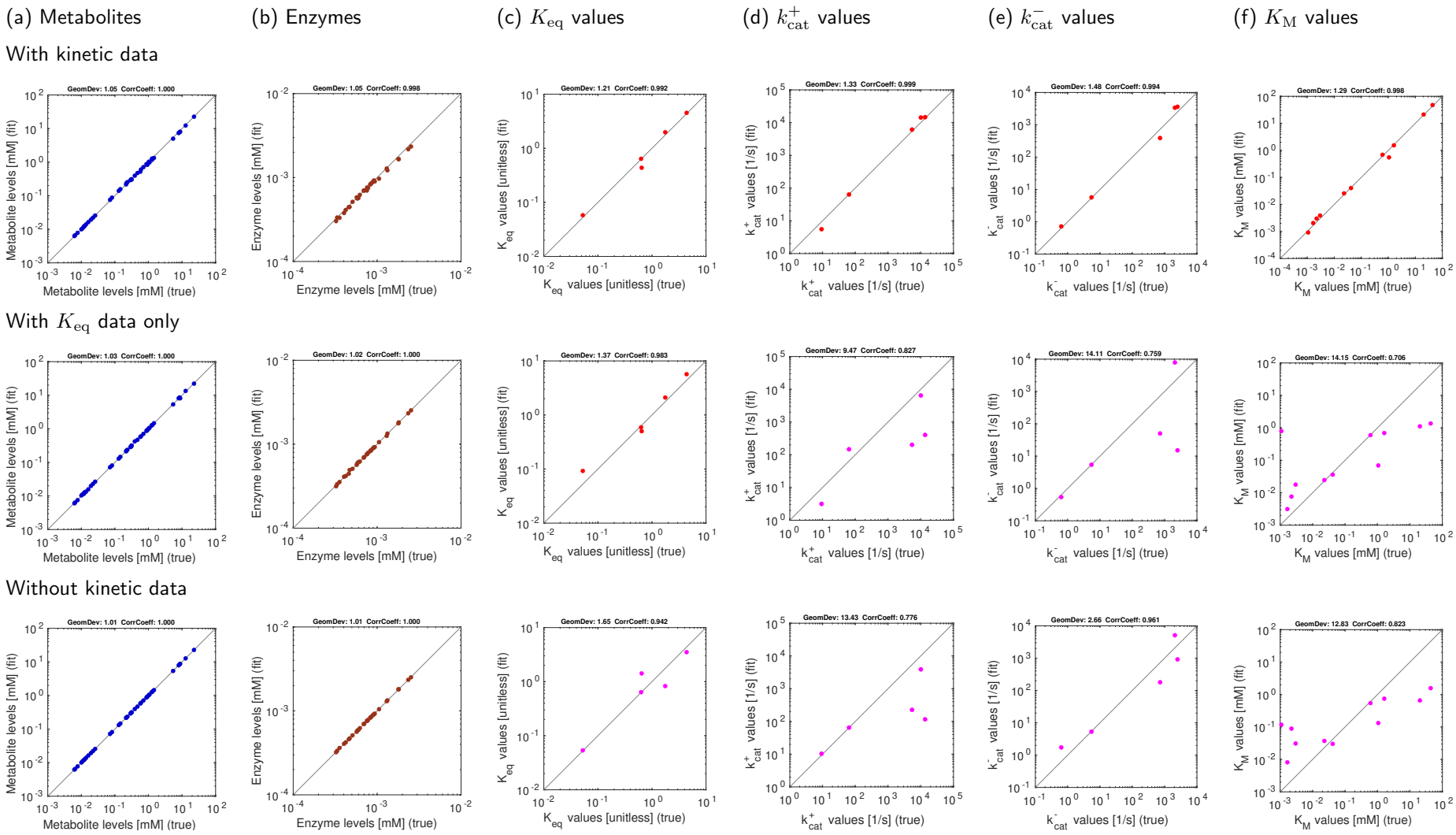

Figure 14: Same as Figure 13, with noisy kinetic data

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

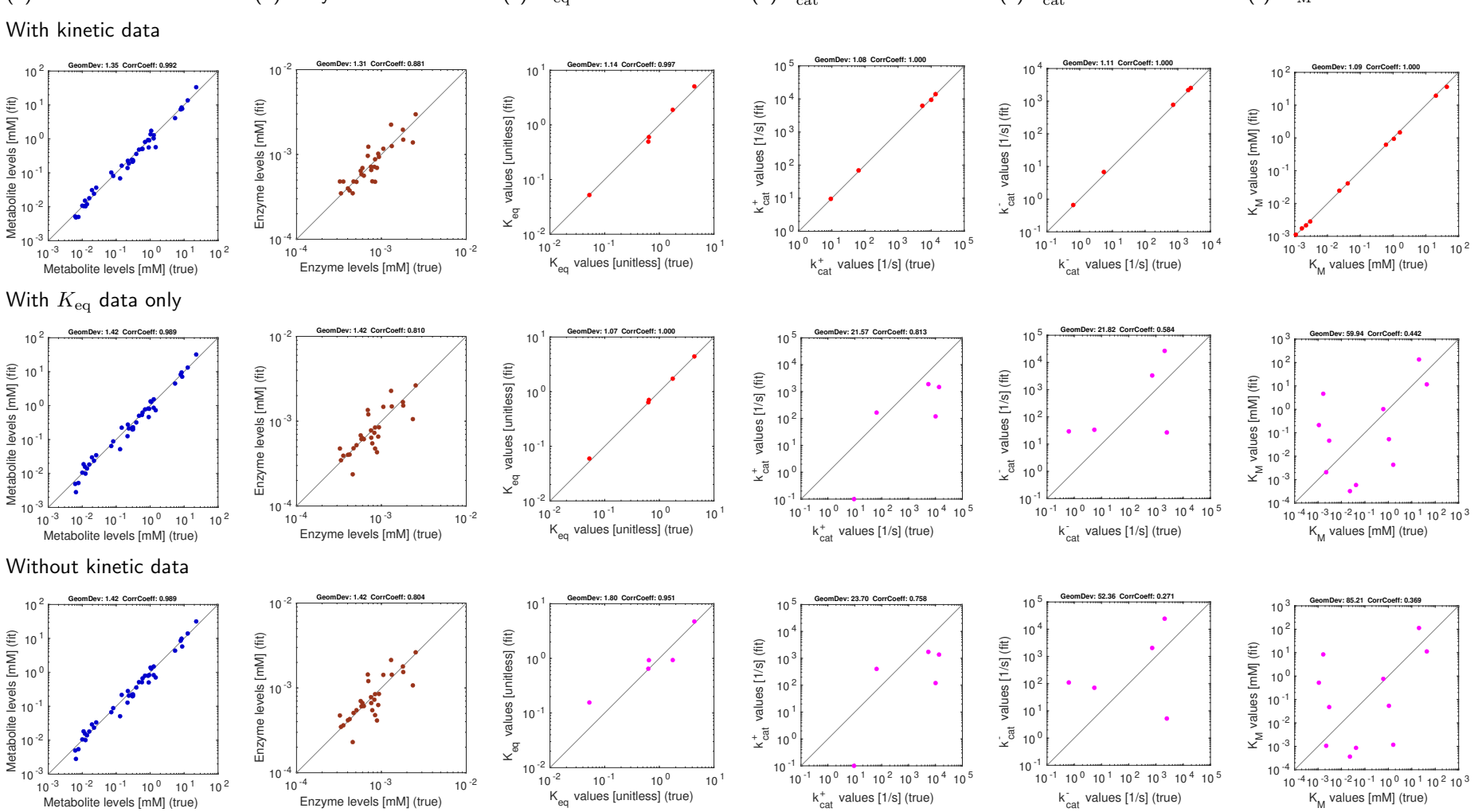

Figure 15: Results for Double branch with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial data, no data for kinetic constants).

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

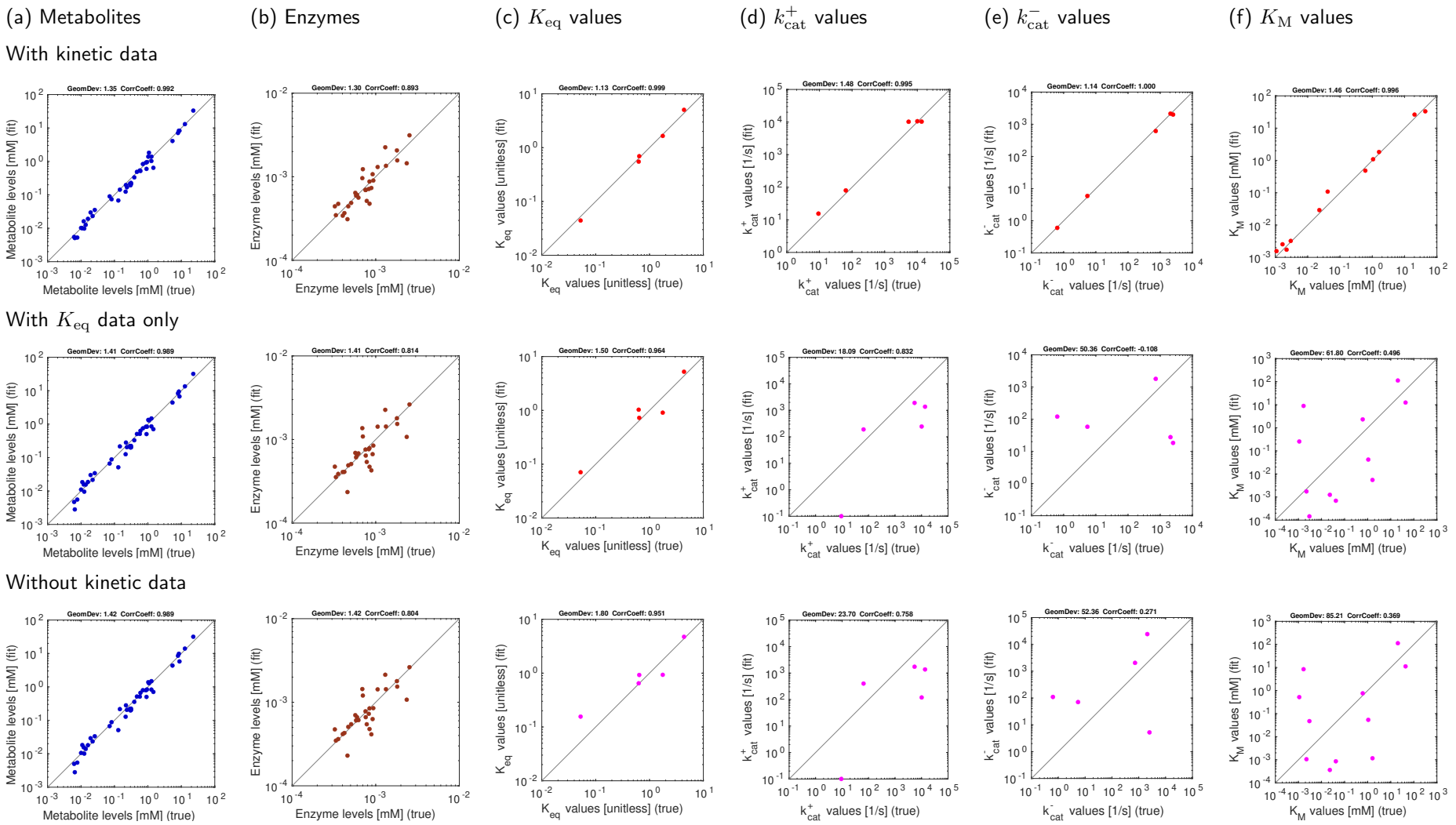

Figure 16: Same as Figure 15, with noisy kinetic data

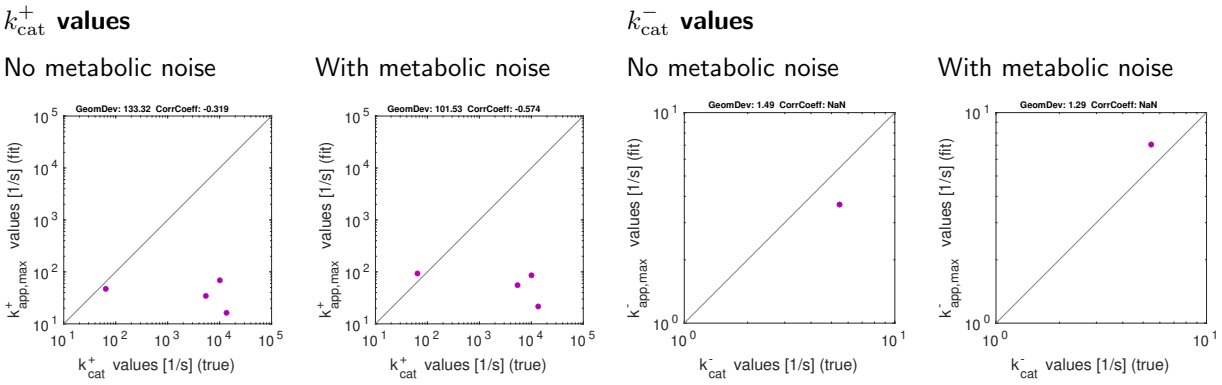

Figure 17: Catalytic constants in Double branch (artificial data), estimated by kinetic profiling. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).