1 Three-chain simulations with alpha = 0.1, beta = 0

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

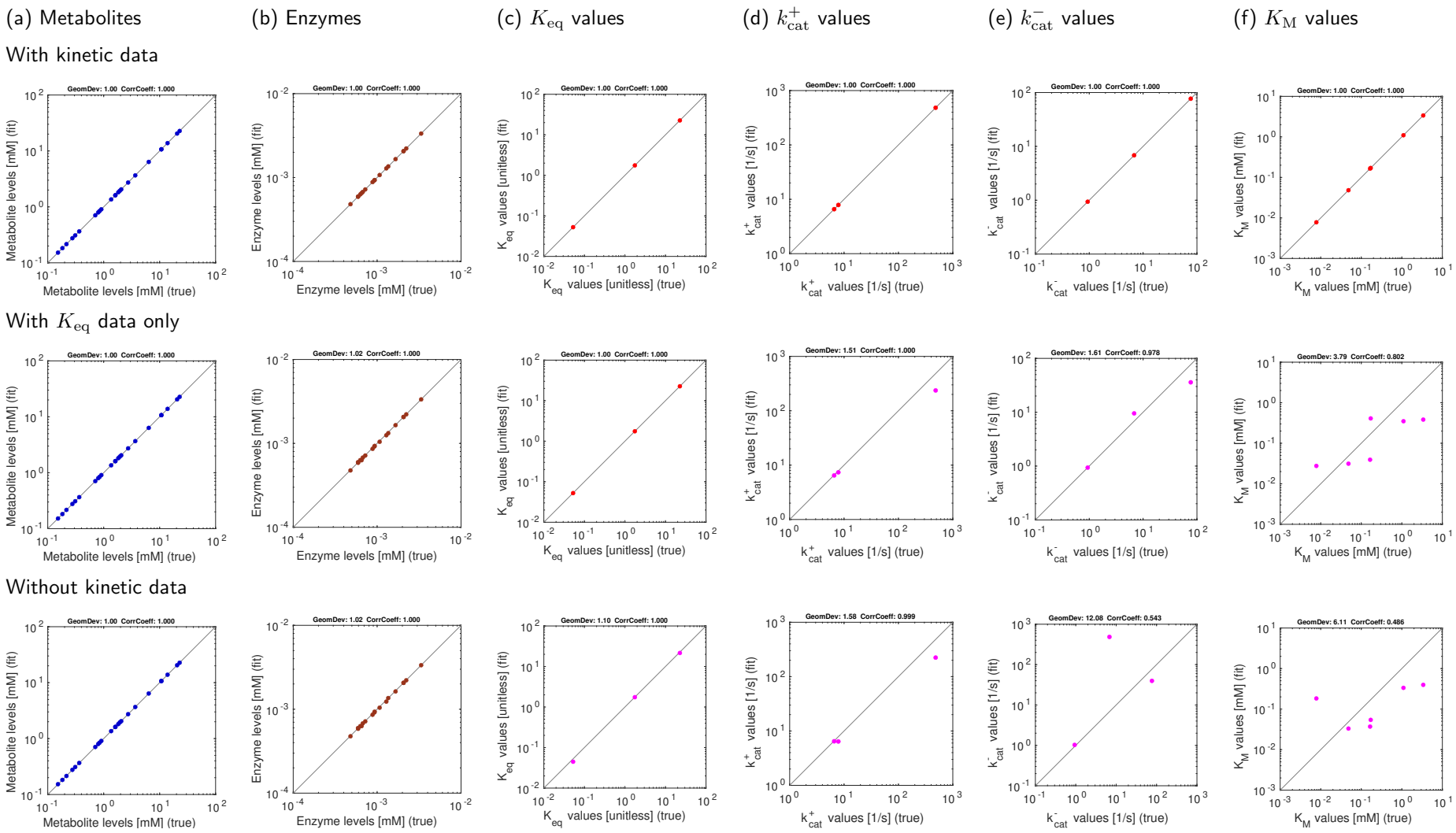

Figure 3: Model balancing results for Three-chain model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation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

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

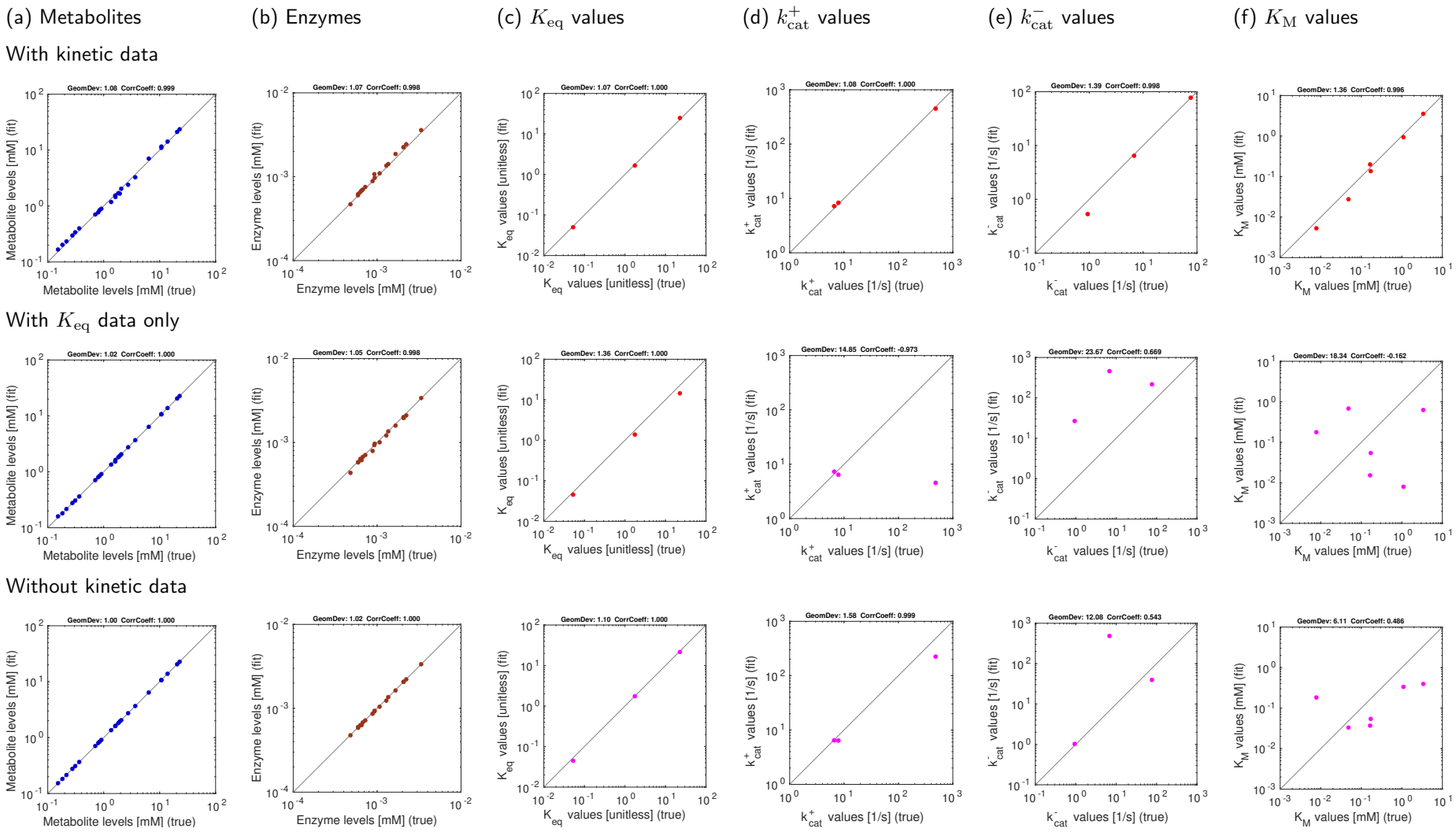

Figure 4: Same as Figure 8, with noisy kinetic data

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

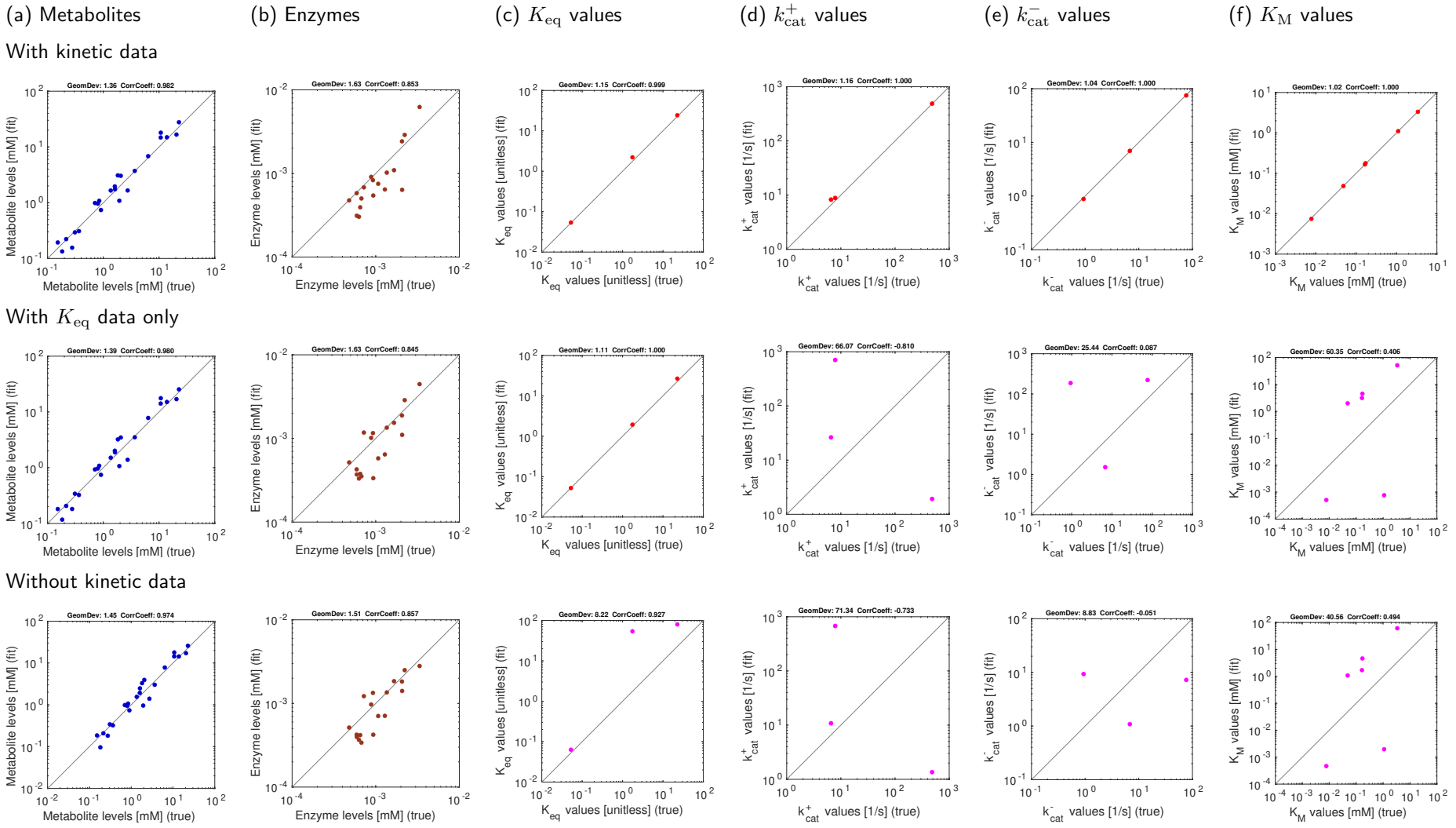

Figure 5: Results for Three-chain with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial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

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

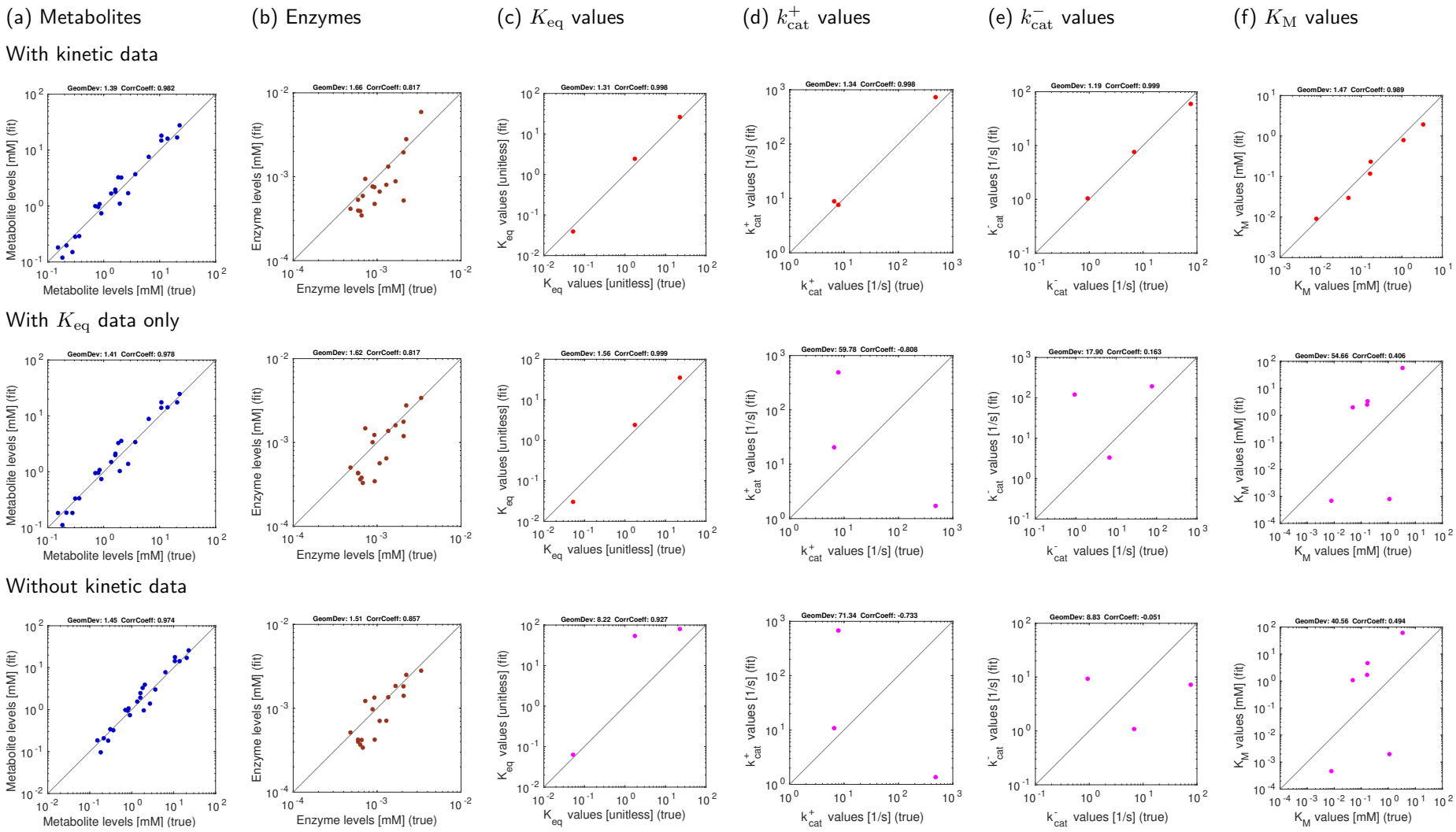

Figure 6: Same as Figure 10, with noisy kinetic data

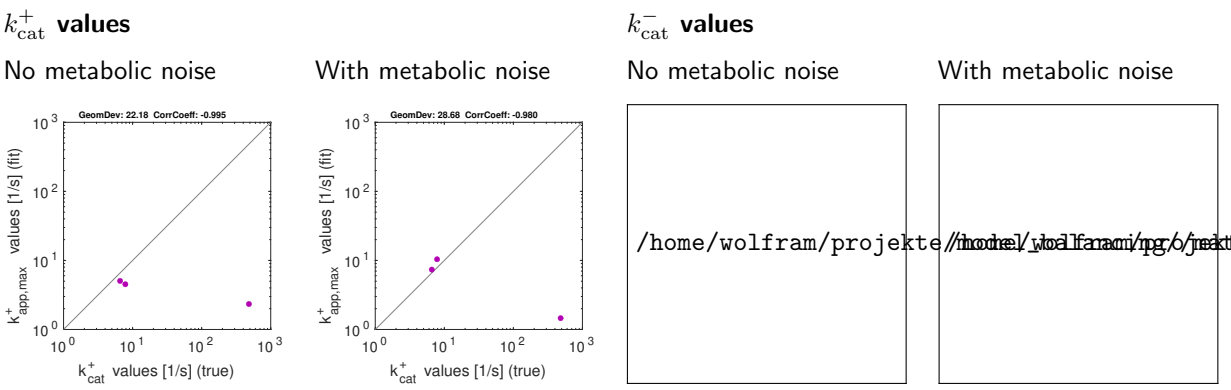

Figure 7: Catalytic constants in Three-chain (artificial data), estimated by kinetic profiling. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).

2 Three-chain simulations with alpha = 1, beta = 0

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

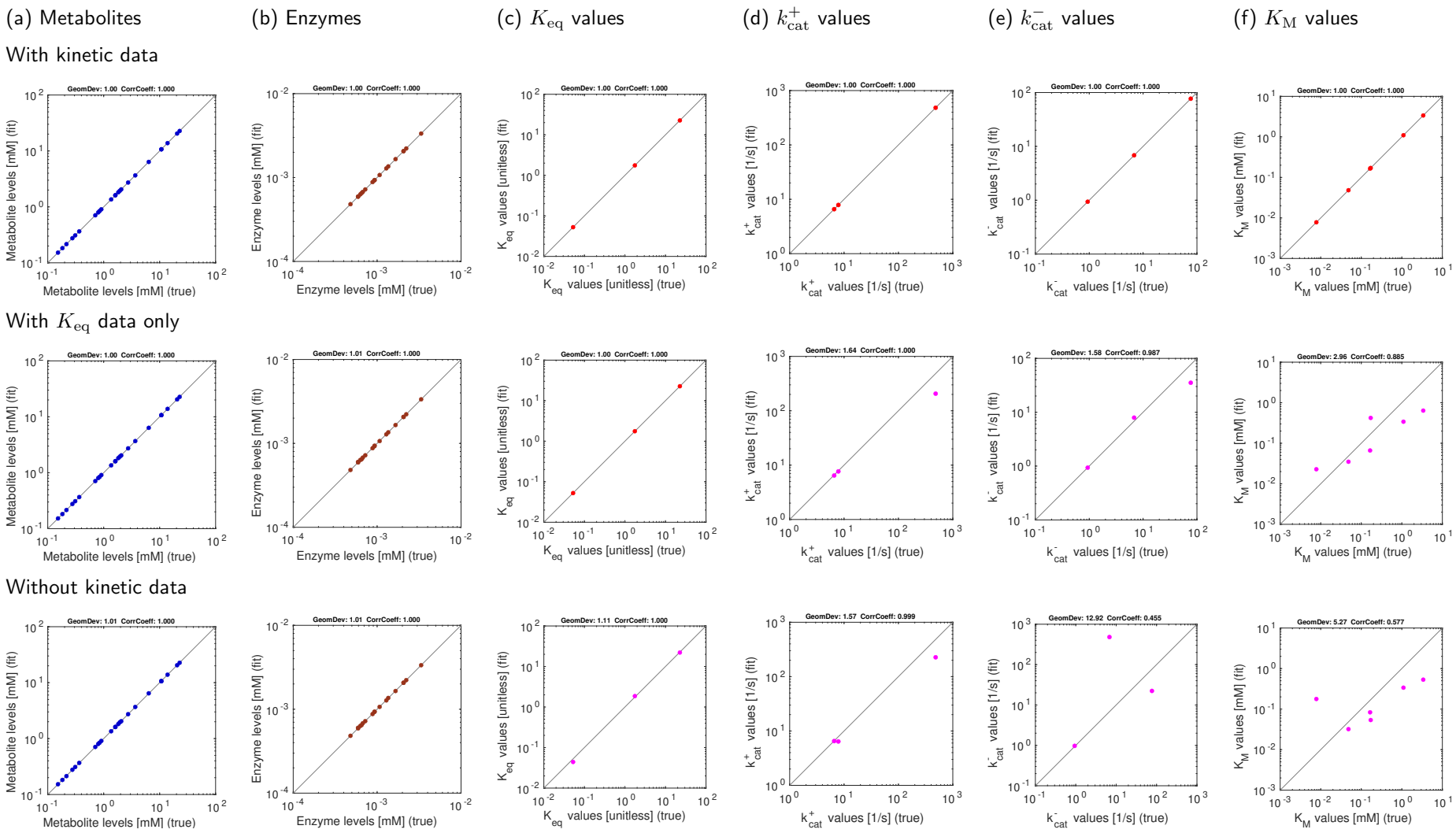

Figure 8: Model balancing results for Three-chain model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation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

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

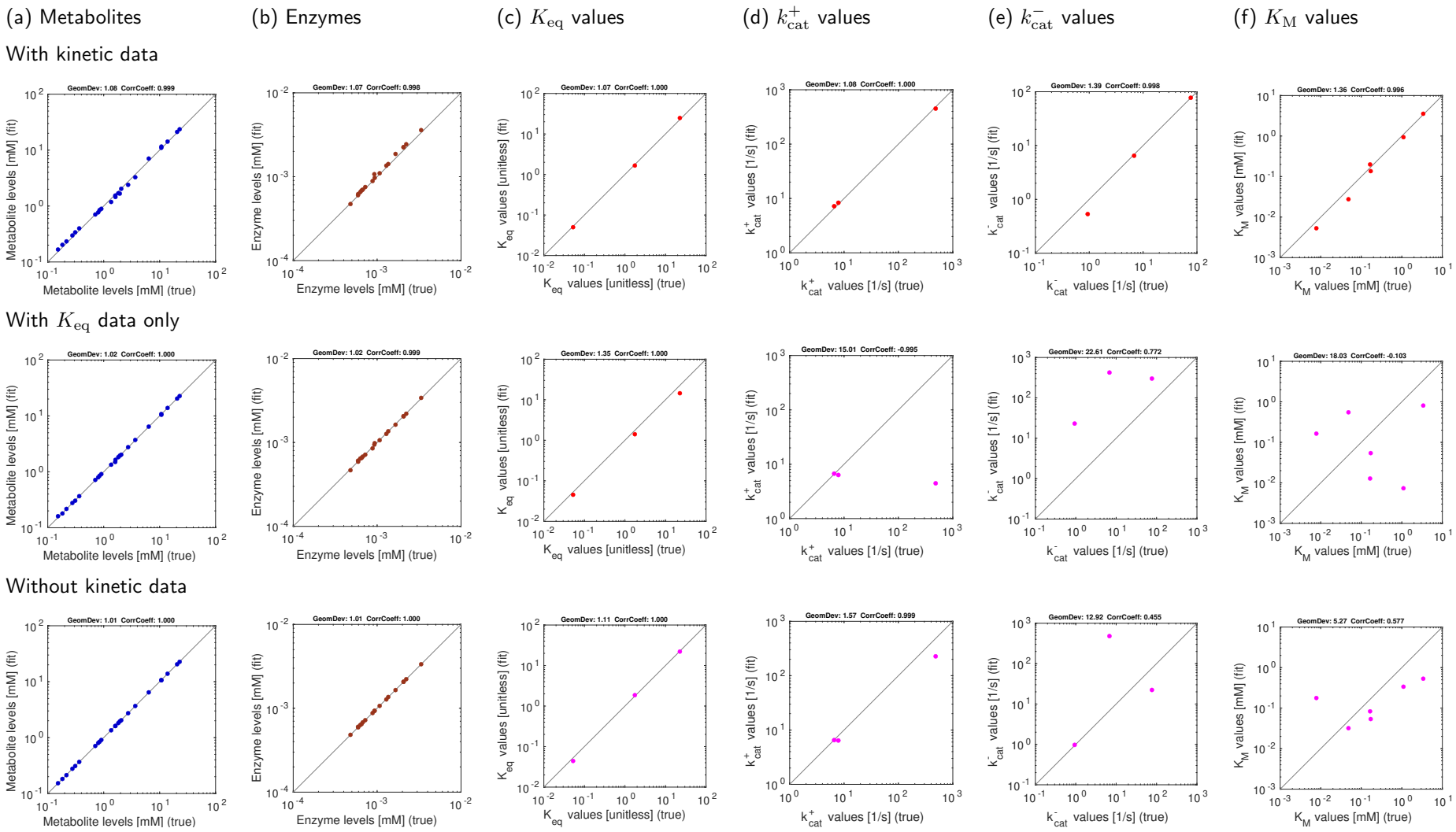

Figure 9: Same as Figure 8, with noisy kinetic data

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

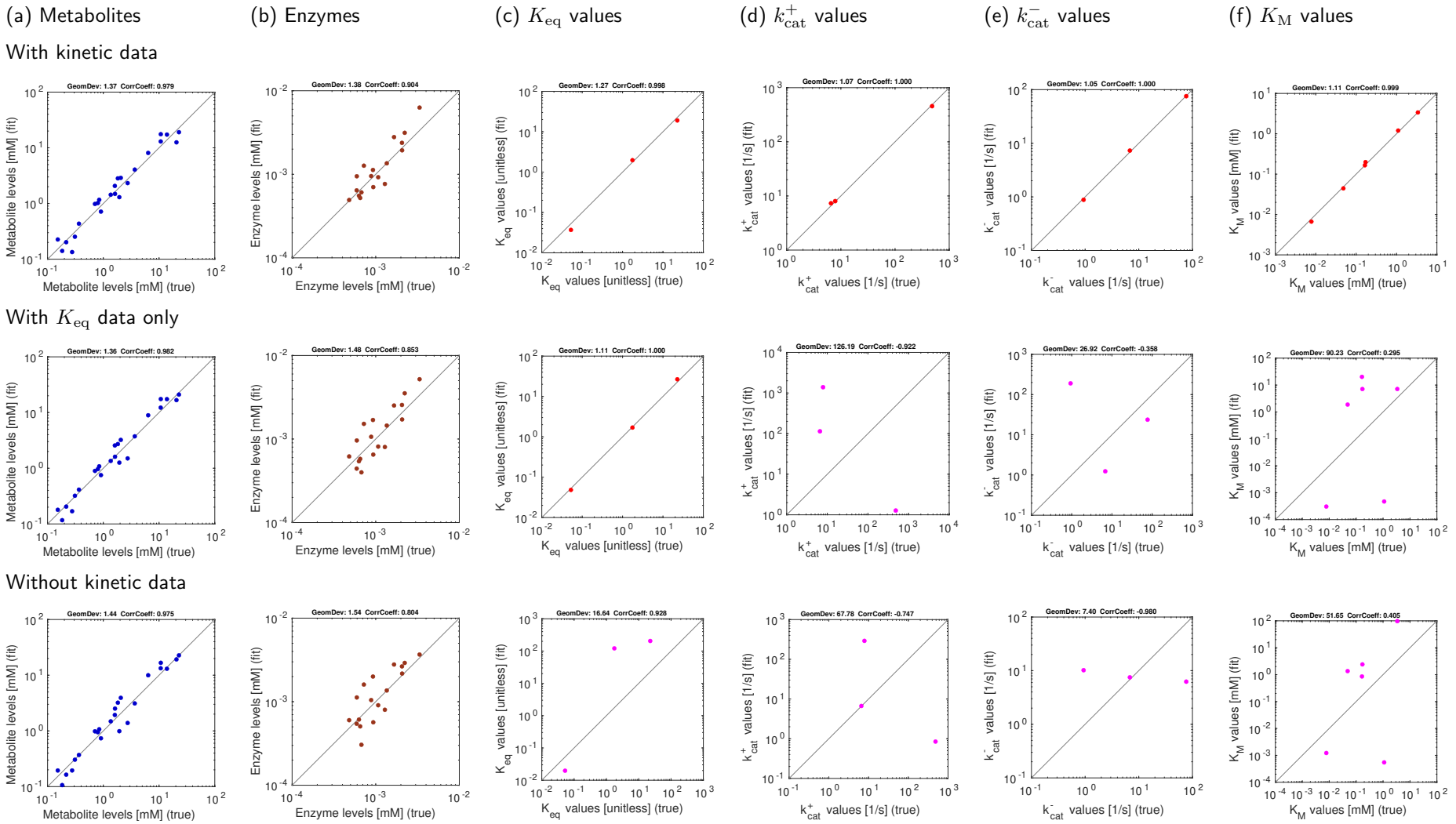

Figure 10: Results for Three-chain with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial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

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

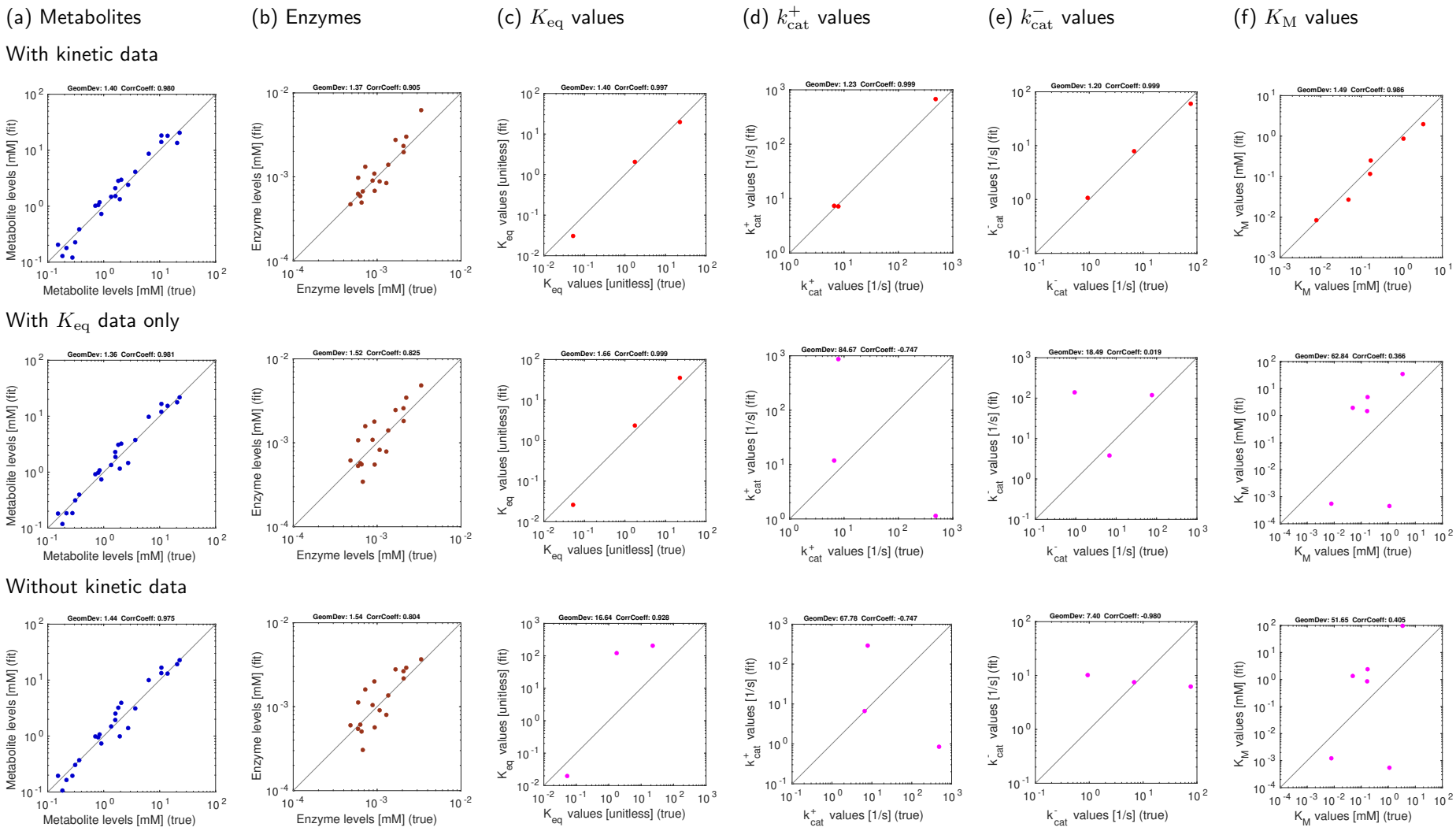

Figure 11: Same as Figure 10, with noisy kinetic data

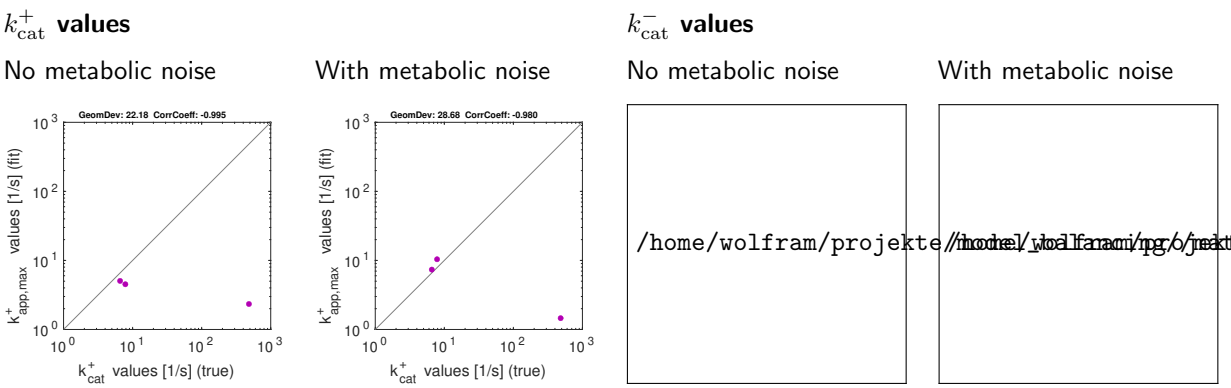

Figure 12: Catalytic constants in Three-chain (artificial data), estimated by kinetic profiling. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).