1 Three-chain model Simulations with alpha = 0

Three-chain model with artificial data (noise-free kinetic data, noise-free state data)

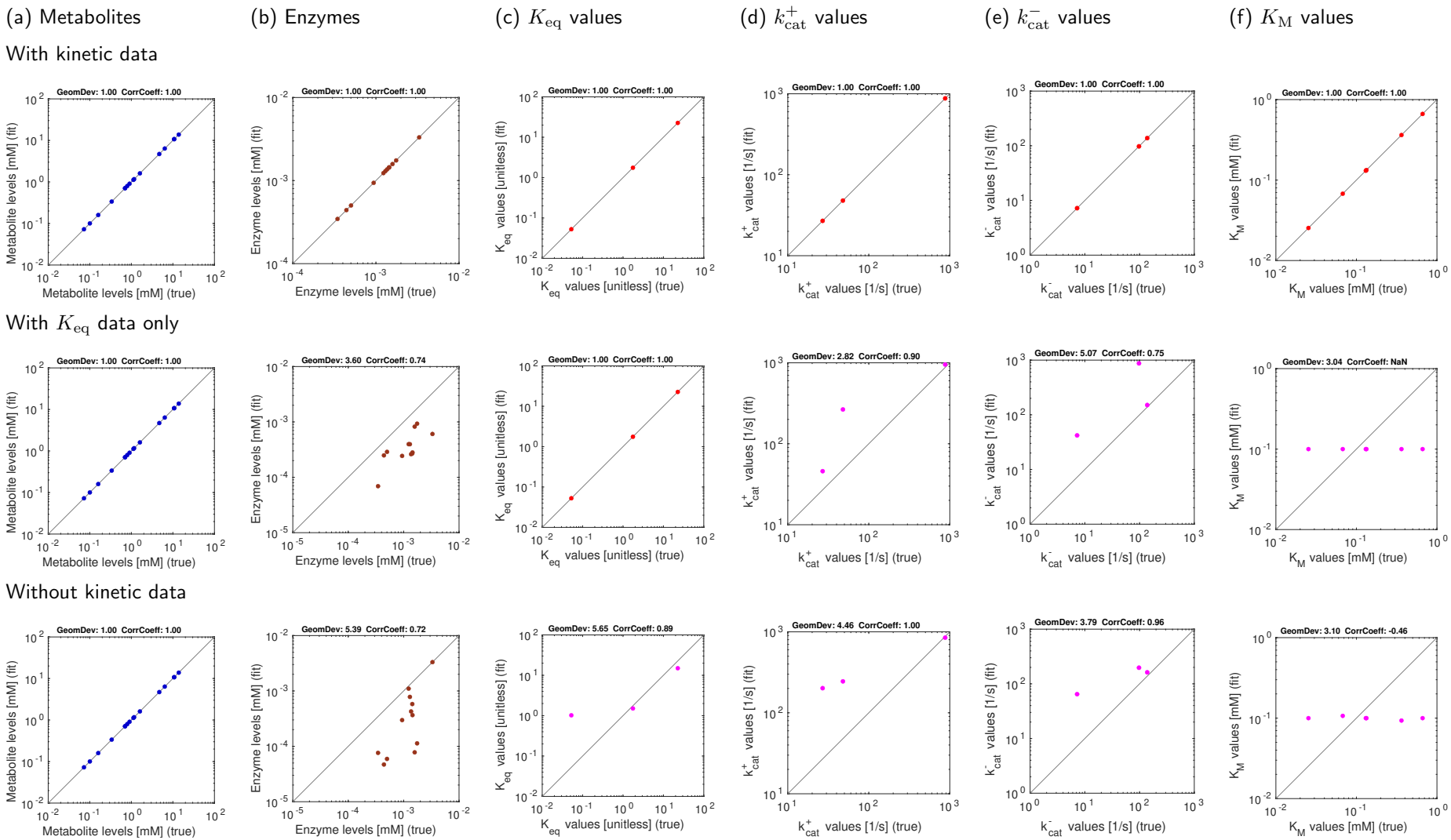


Figure 3: Model balancing results for Three-chain model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation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

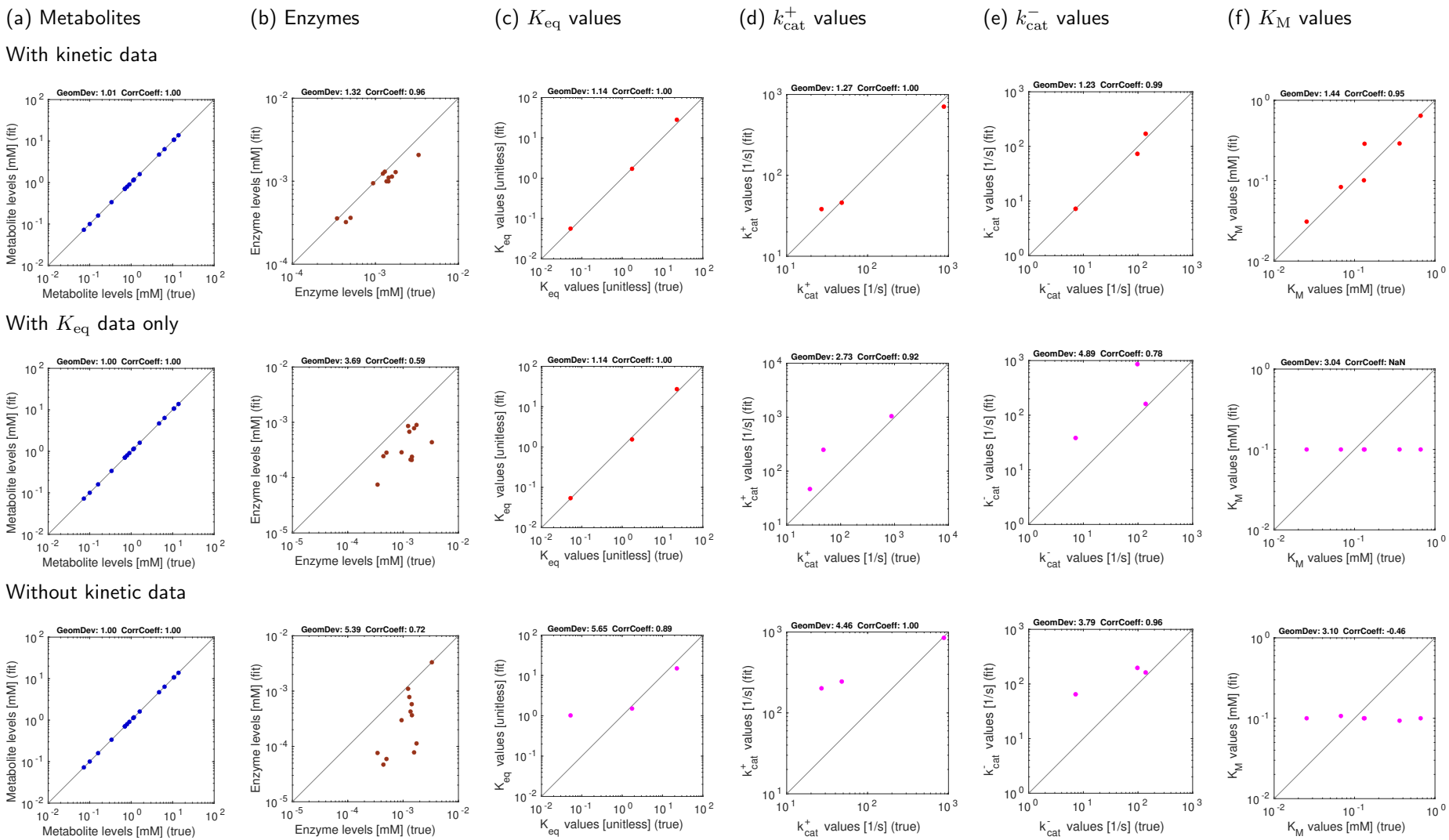


Figure 4: Same as Figure 28, with noisy kinetic data

Three-chain model with artificial data (noise-free kinetic data, noisy state data)

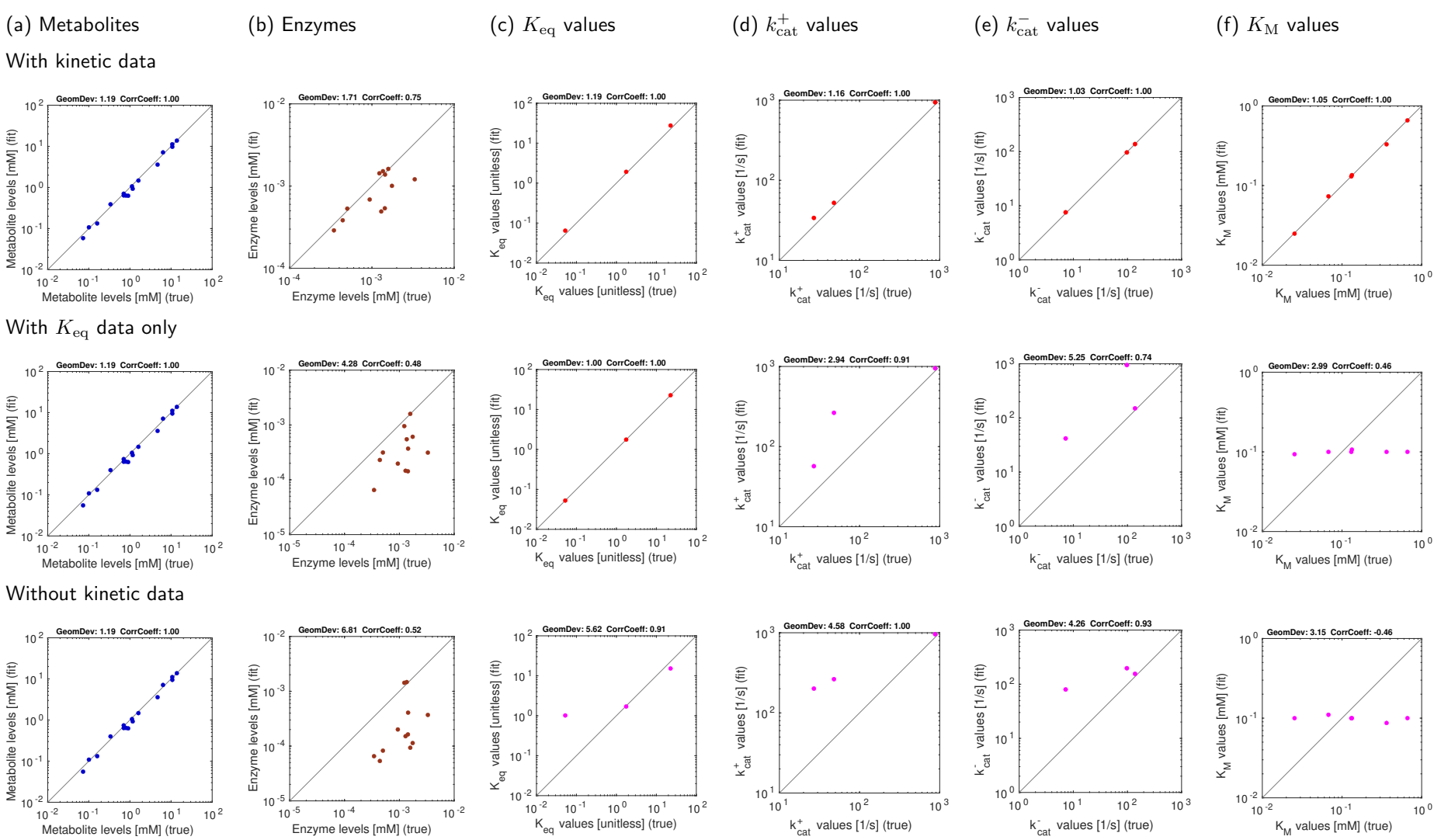


Figure 5: Results for Three-chain with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial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

Three-chain model with artificial data (noisy kinetic data, noisy state data)

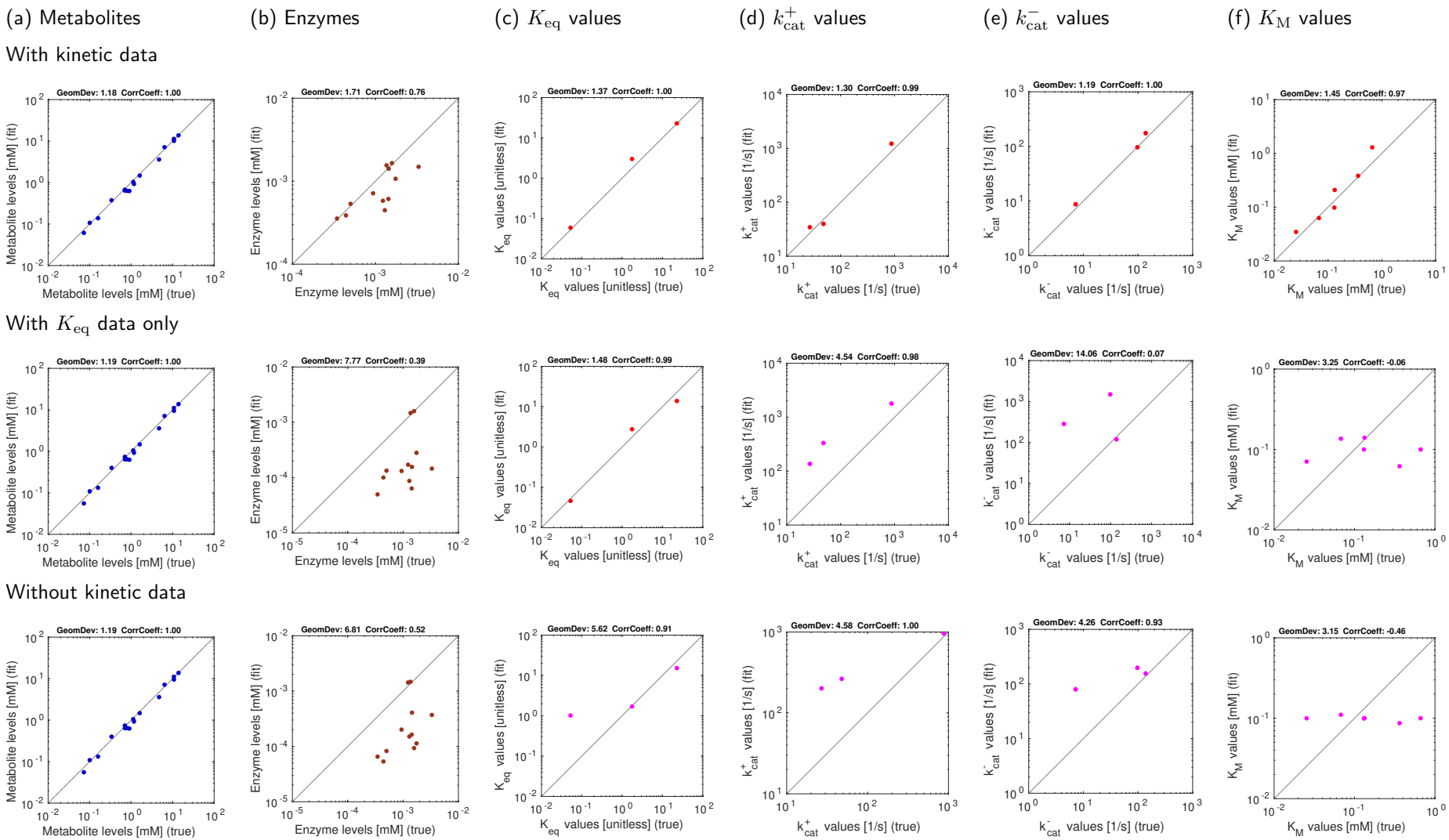


Figure 6: Same as Figure 30, with noisy kinetic data

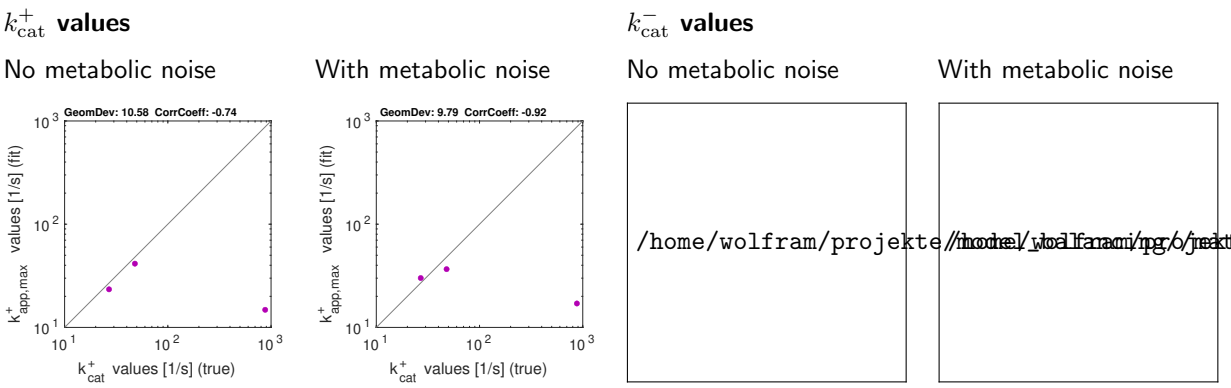


Figure 7: Catalytic constants in Three-chain (artificial data), estimated by kinetic profiling [**?**]. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).

2 Three-chain model Simulations with alpha = 0.001

Three-chain model with artificial data (noise-free kinetic data, noise-free state data)

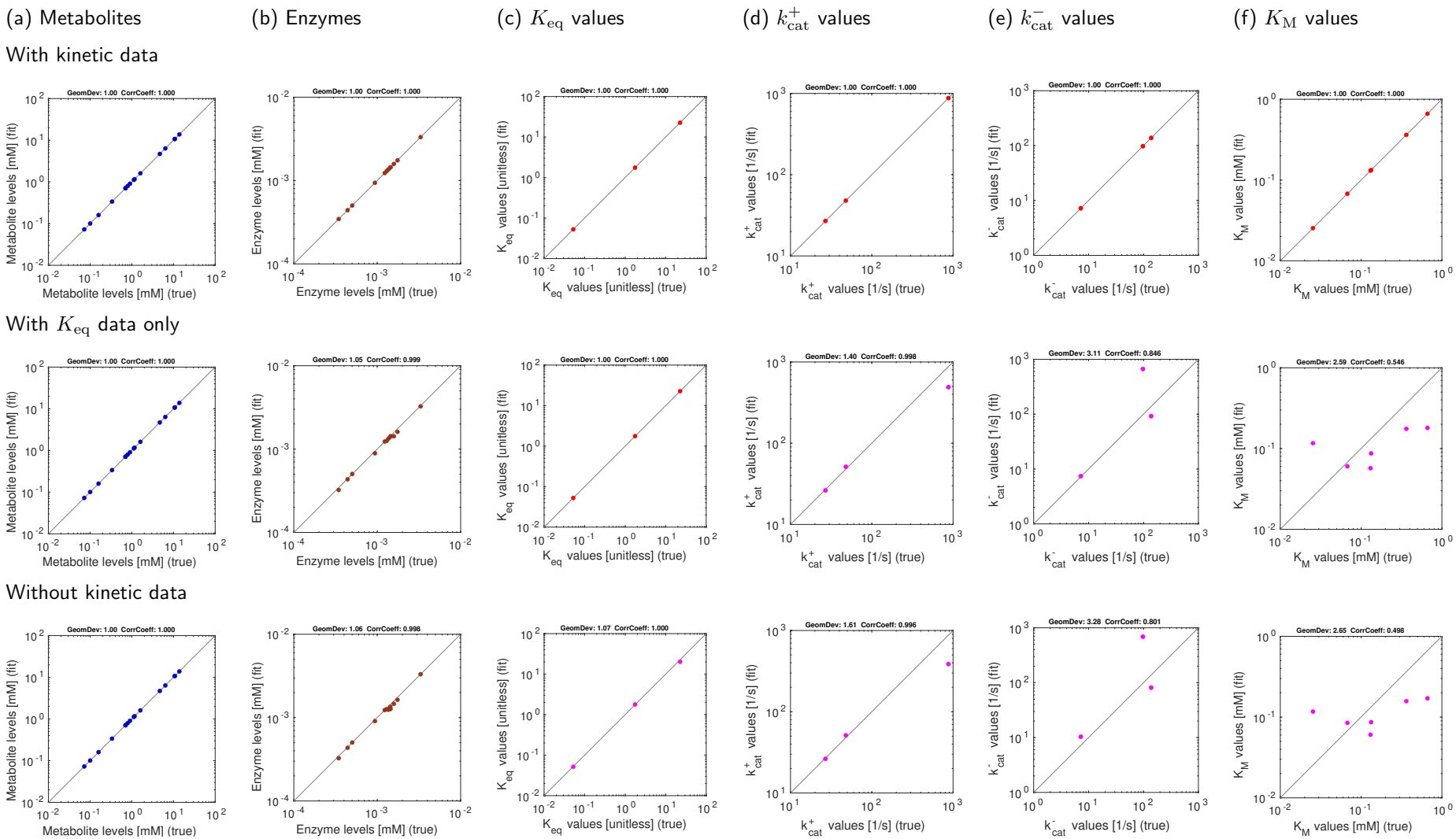


Figure 8: Model balancing results for Three-chain model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation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

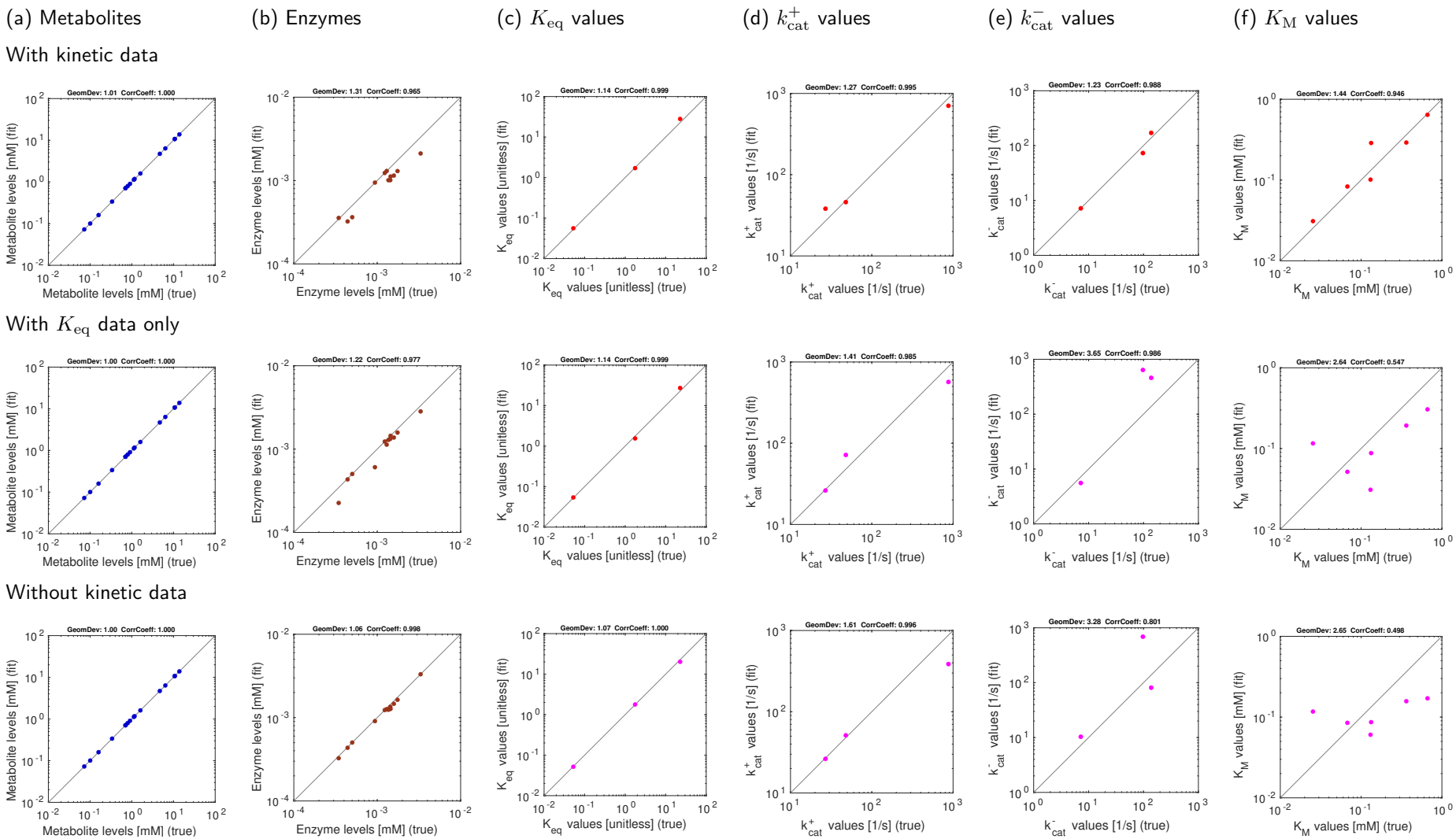


Figure 9: Same as Figure 28, with noisy kinetic data

Three-chain model with artificial data (noise-free kinetic data, noisy state data)

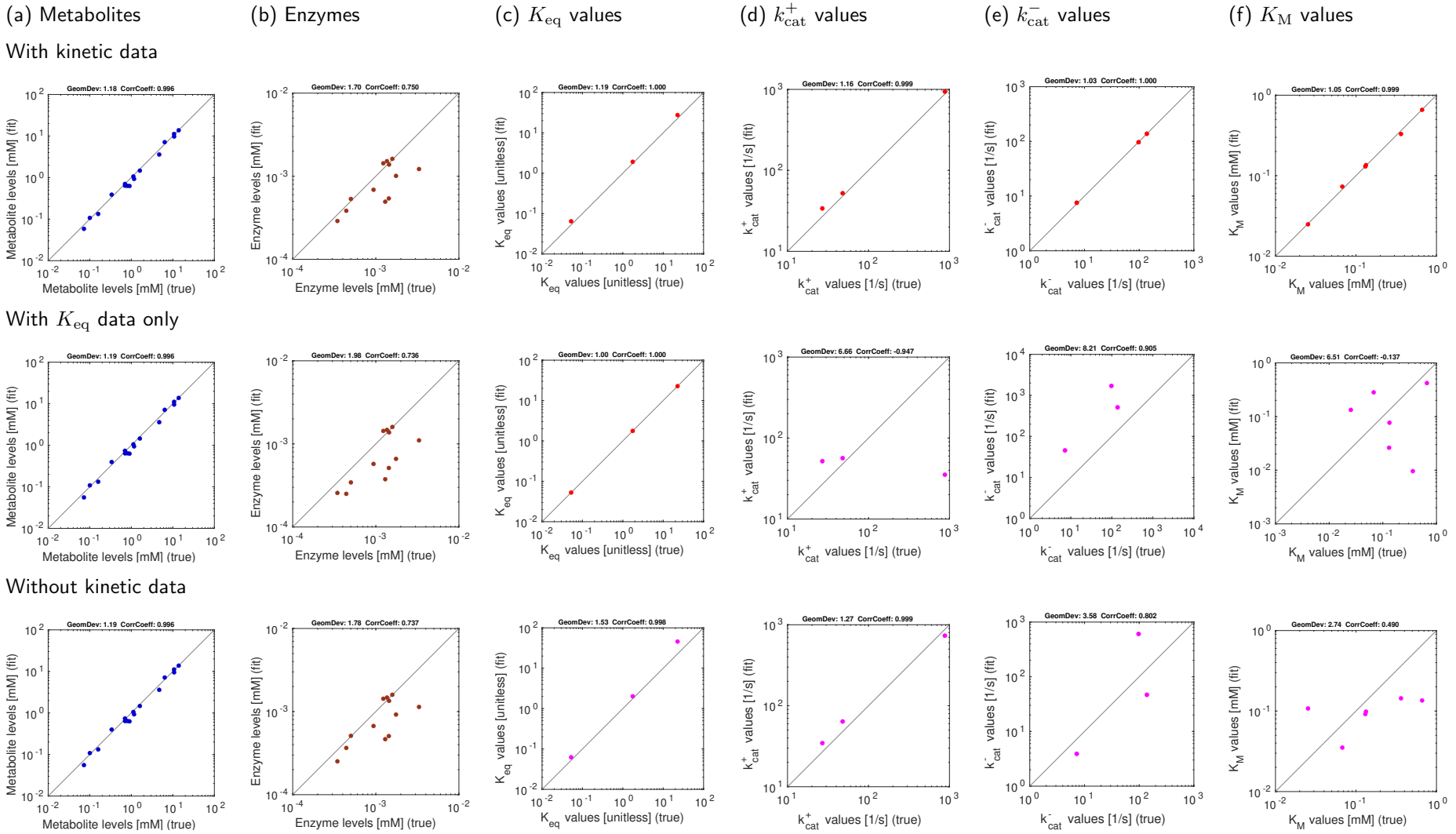


Figure 10: Results for Three-chain with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial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

Three-chain model with artificial data (noisy kinetic data, noisy state data)

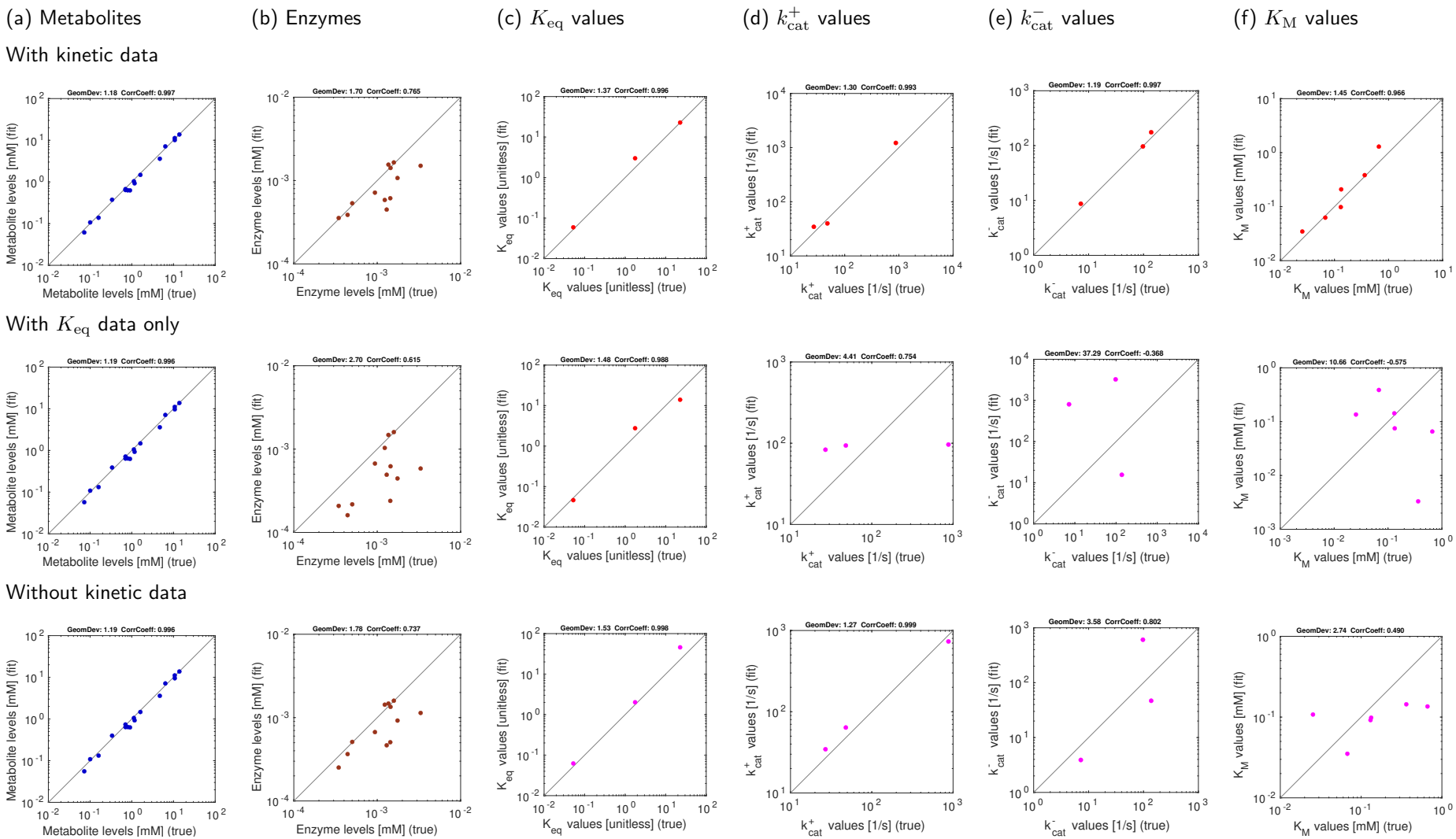


Figure 11: Same as Figure 30, with noisy kinetic data

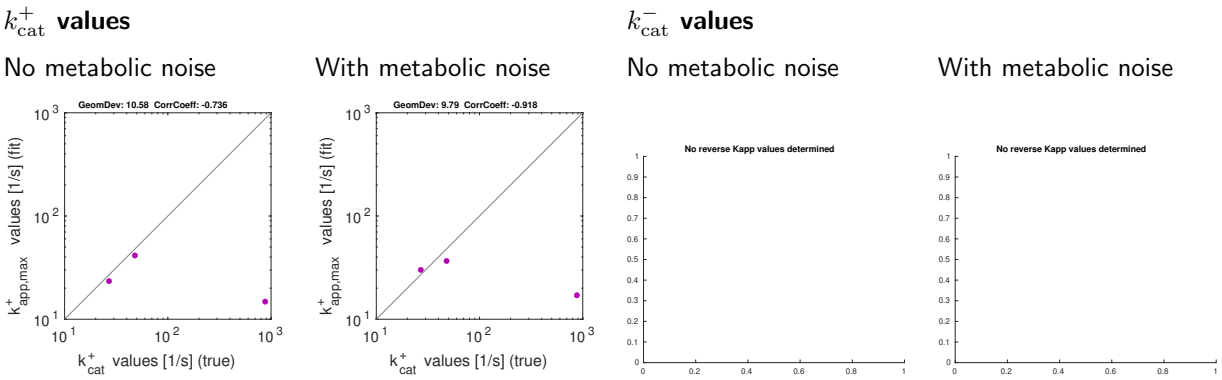


Figure 12: Catalytic constants in Three-chain (artificial data), estimated by kinetic profiling [**?**]. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).

3 Three-chain model Simulations with alpha = 0.01

Three-chain model with artificial data (noise-free kinetic data, noise-free state data)

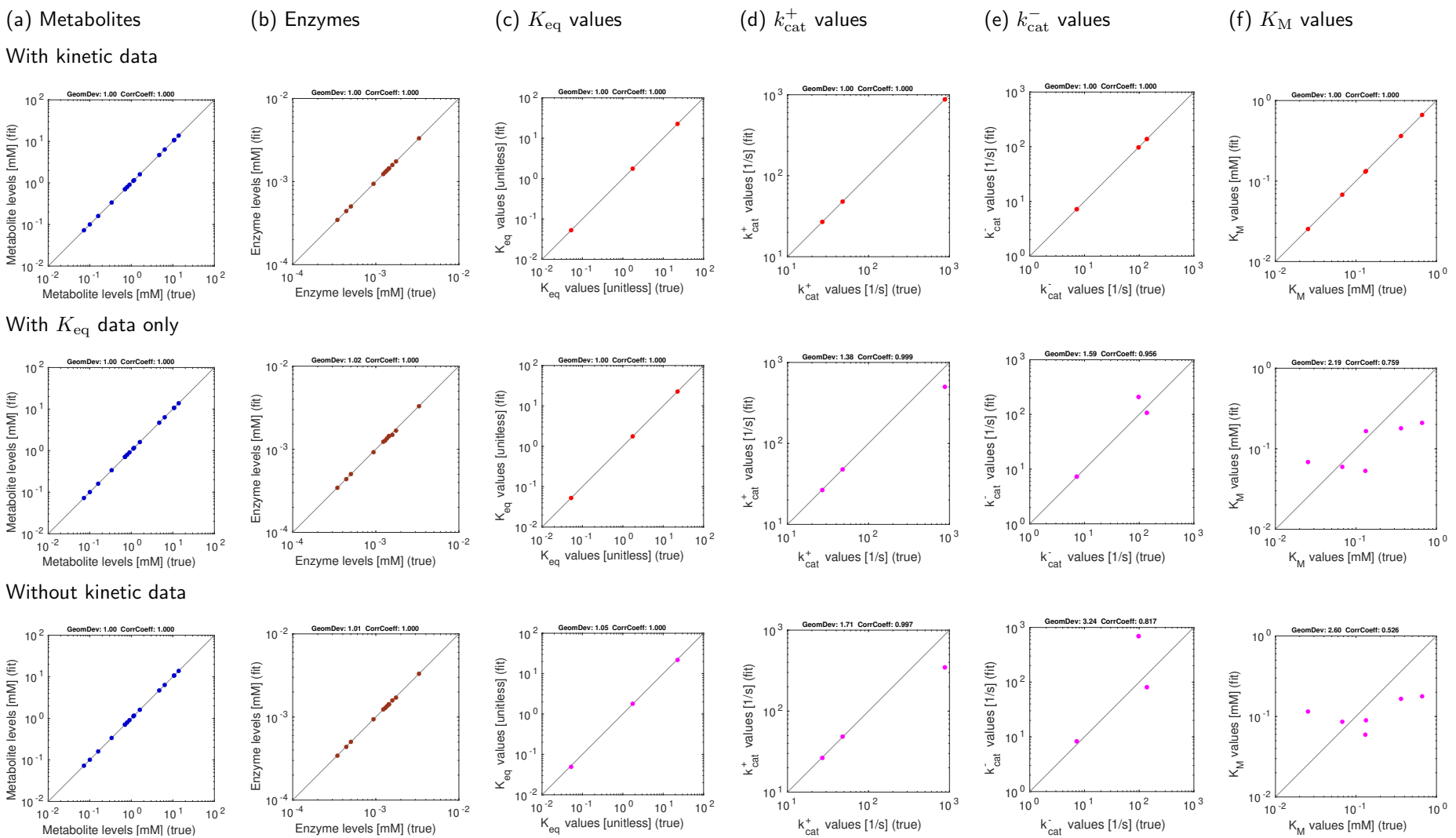


Figure 13: Model balancing results for Three-chain model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation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

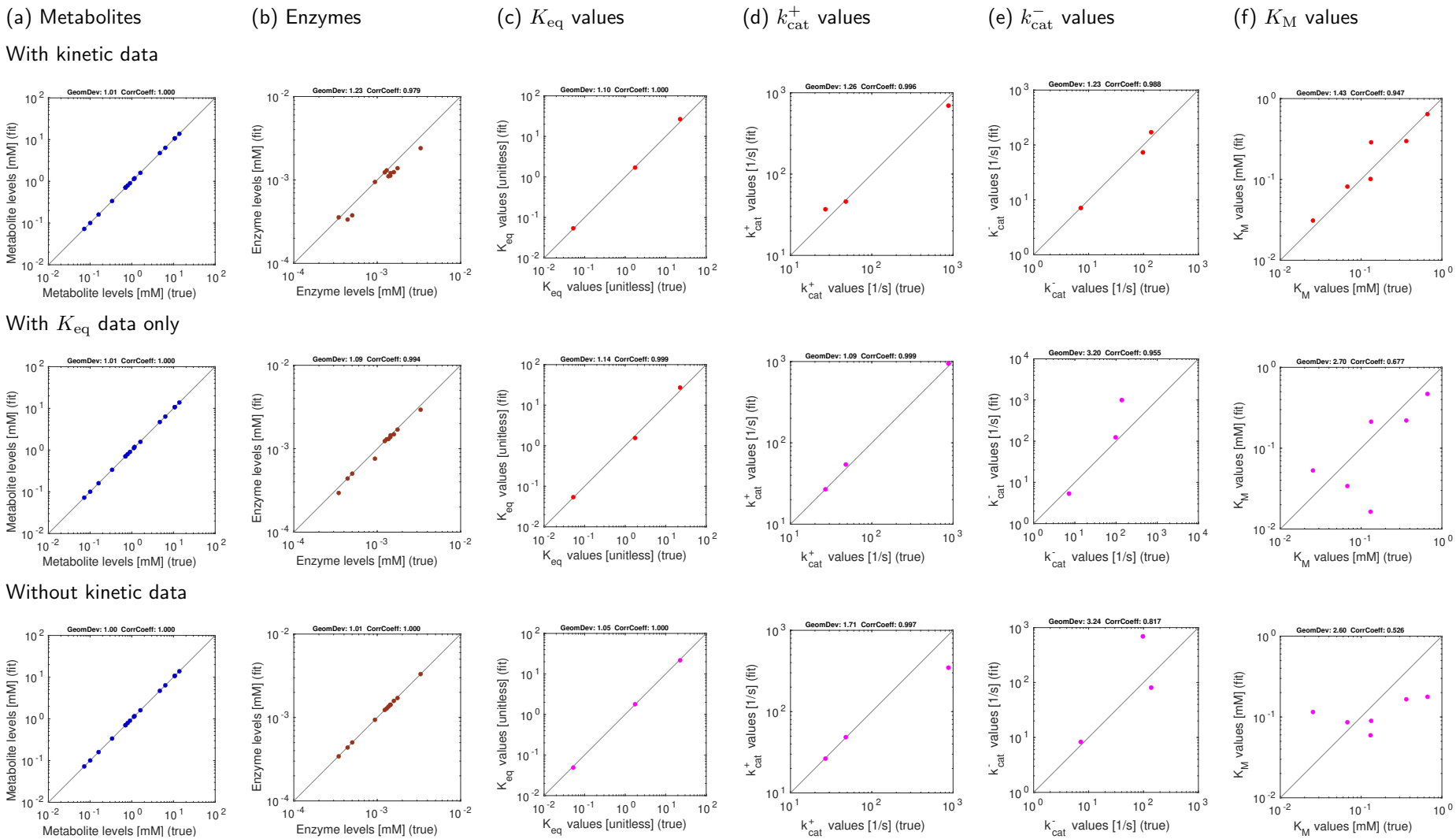


Figure 14: Same as Figure 28, with noisy kinetic data

Three-chain model with artificial data (noise-free kinetic data, noisy state data)

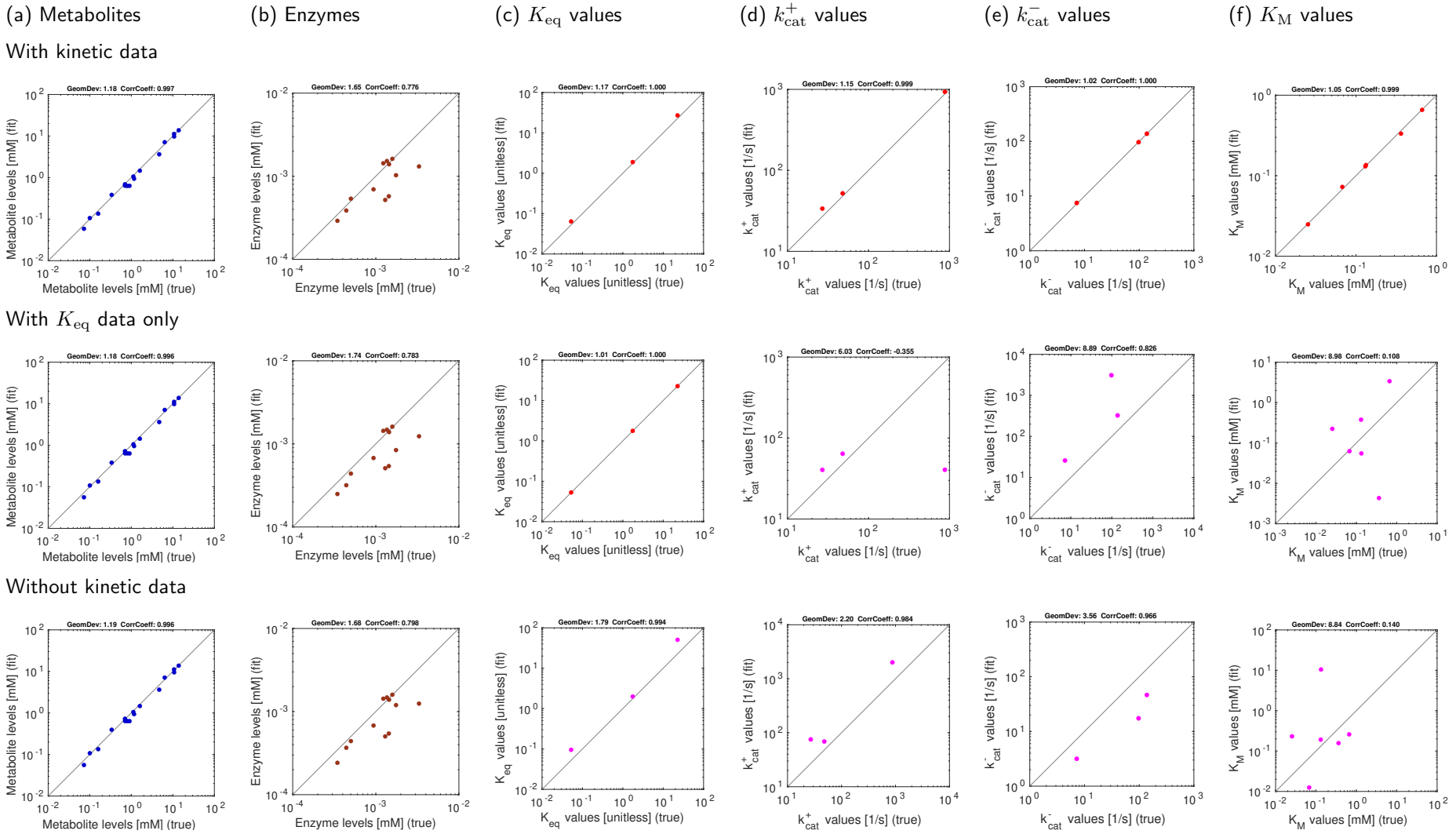


Figure 15: Results for Three-chain with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial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

Three-chain model with artificial data (noisy kinetic data, noisy state data)

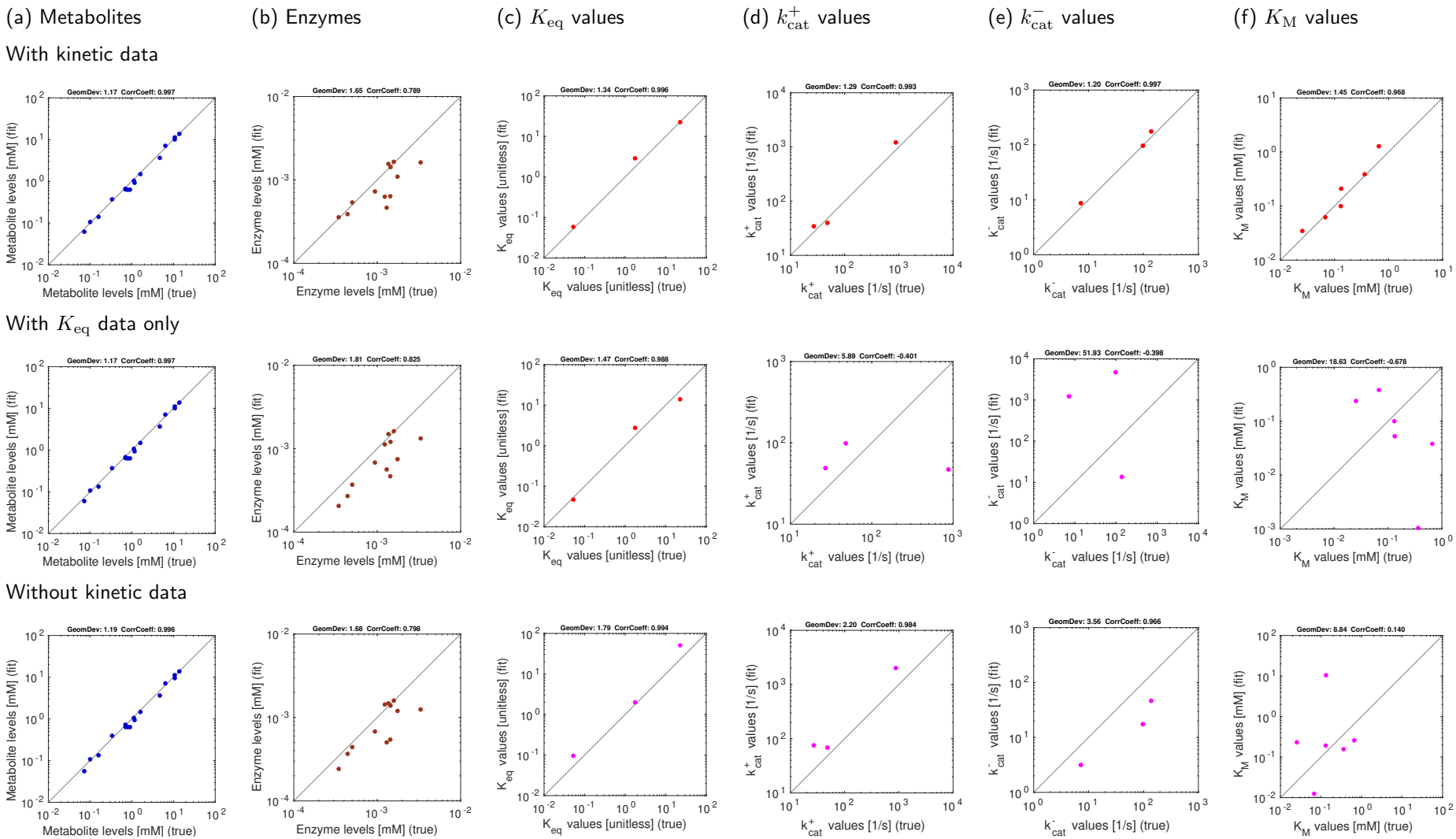


Figure 16: Same as Figure 30, with noisy kinetic data

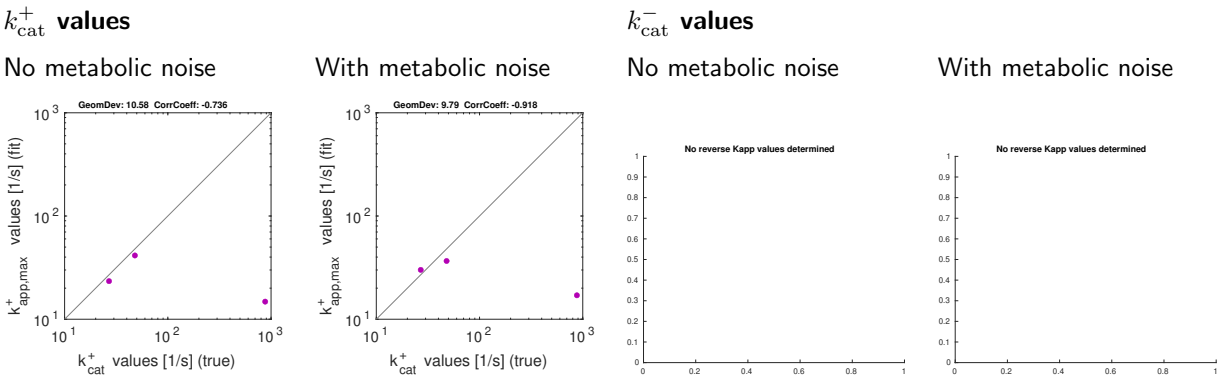


Figure 17: Catalytic constants in Three-chain (artificial data), estimated by kinetic profiling [**?**]. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).

4 Three-chain model Simulations with alpha = 0.1

Three-chain model with artificial data (noise-free kinetic data, noise-free state data)

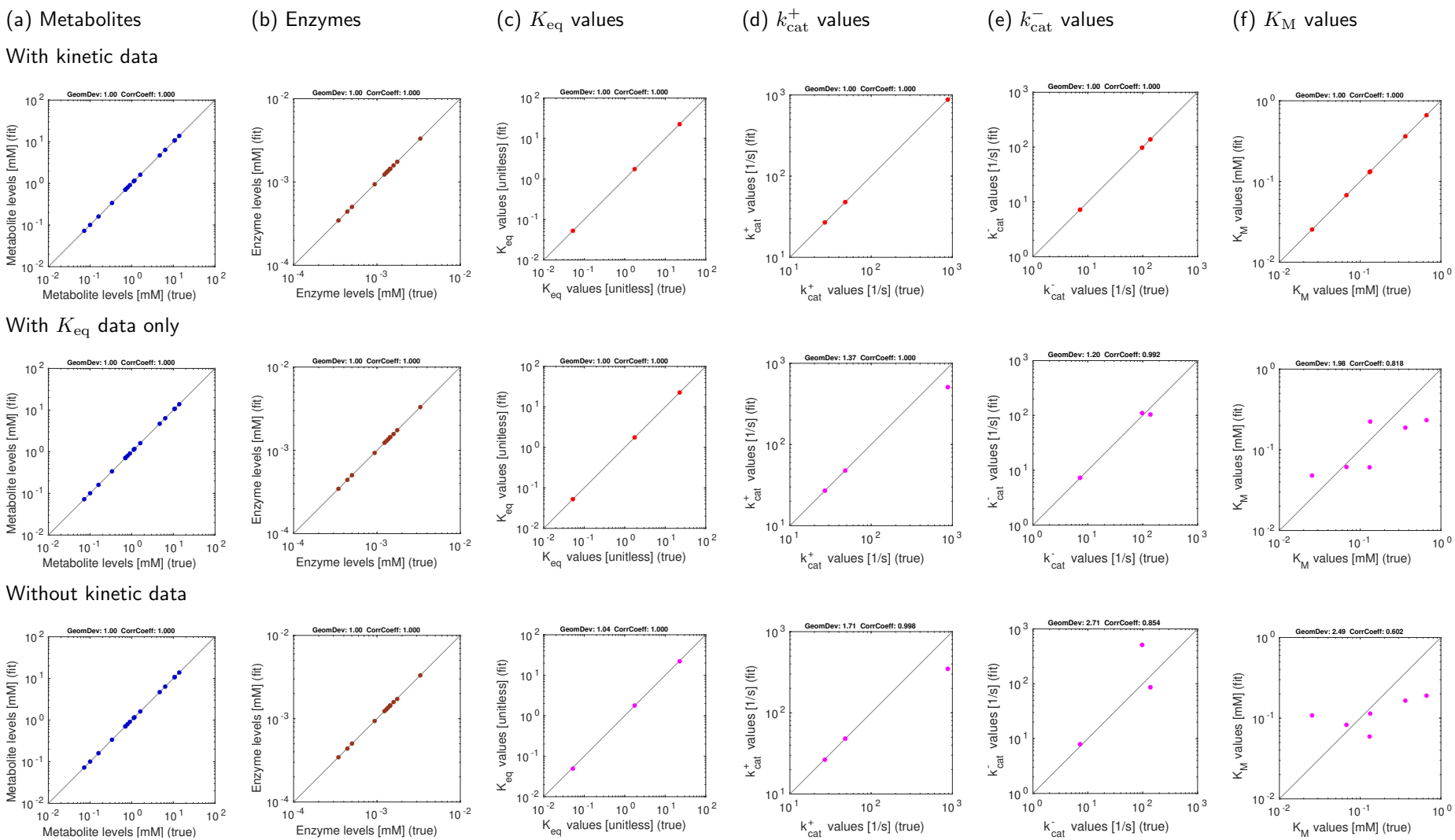


Figure 18: Model balancing results for Three-chain model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation 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)

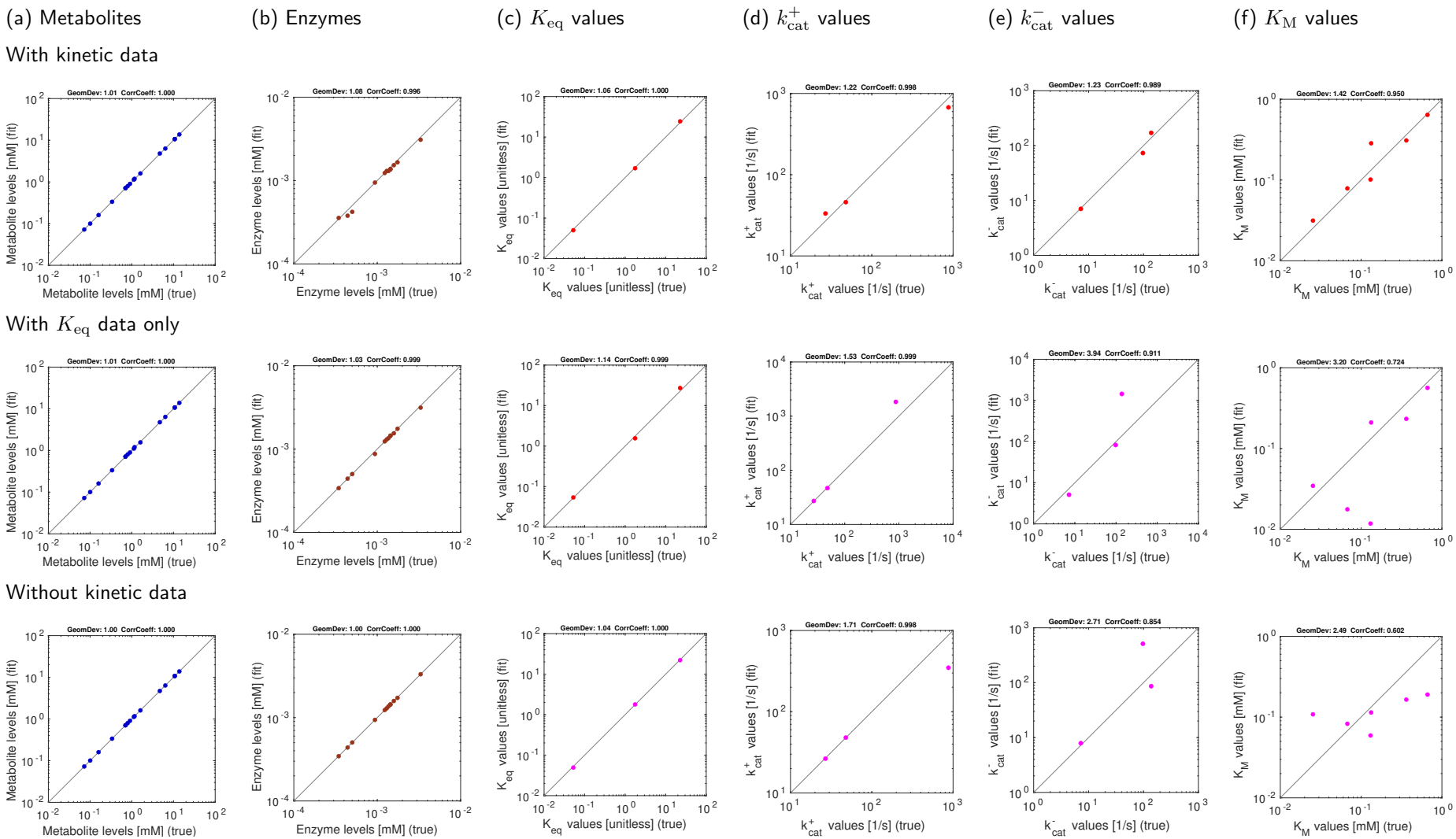


Figure 19: Same as Figure 28, with noisy kinetic data

Three-chain model with artificial data (noise-free kinetic data, noisy state data)

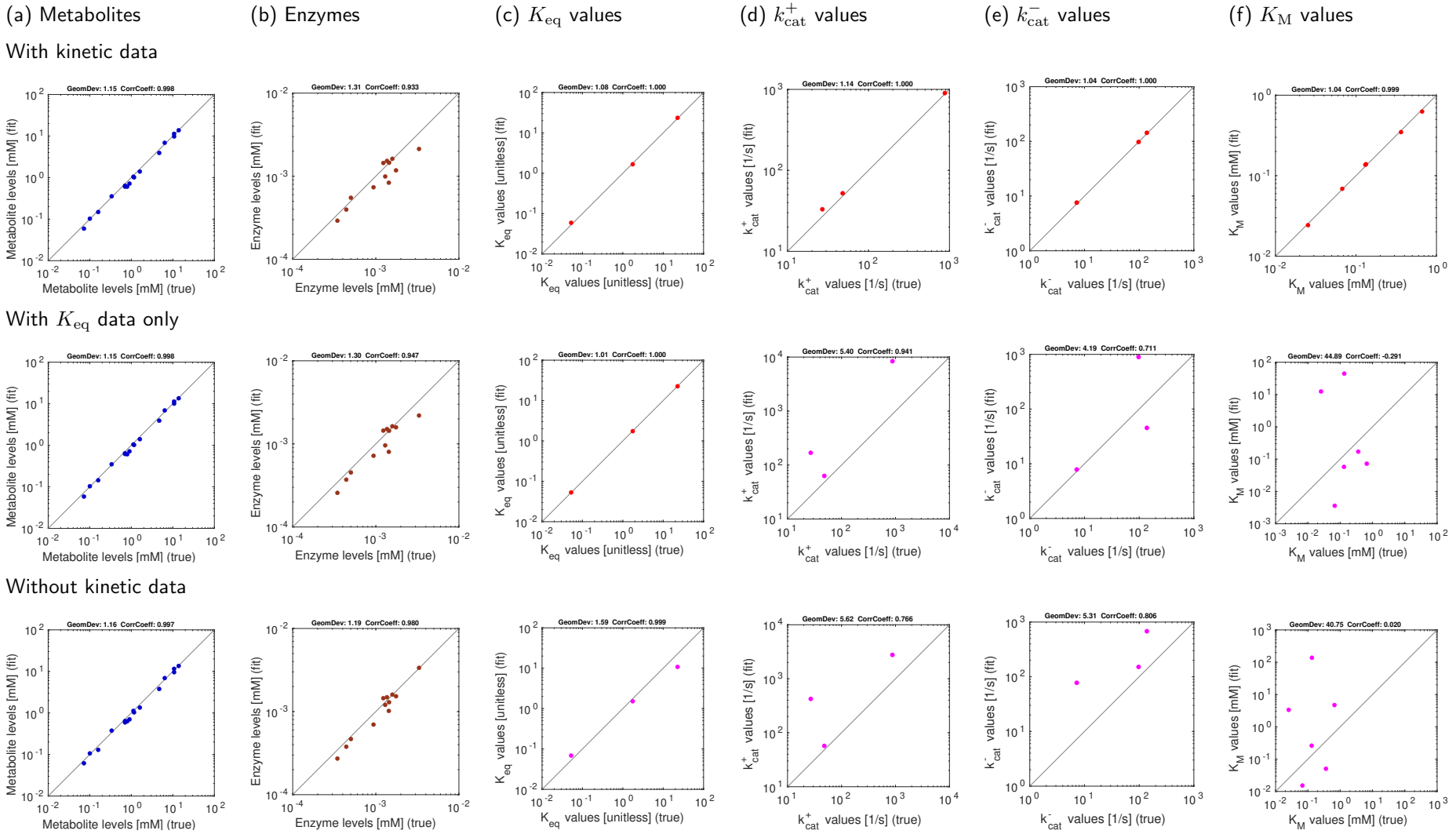


Figure 20: Results for Three-chain with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial data, no data for kinetic constants).

Three-chain model with artificial data (noisy kinetic data, noisy state data)

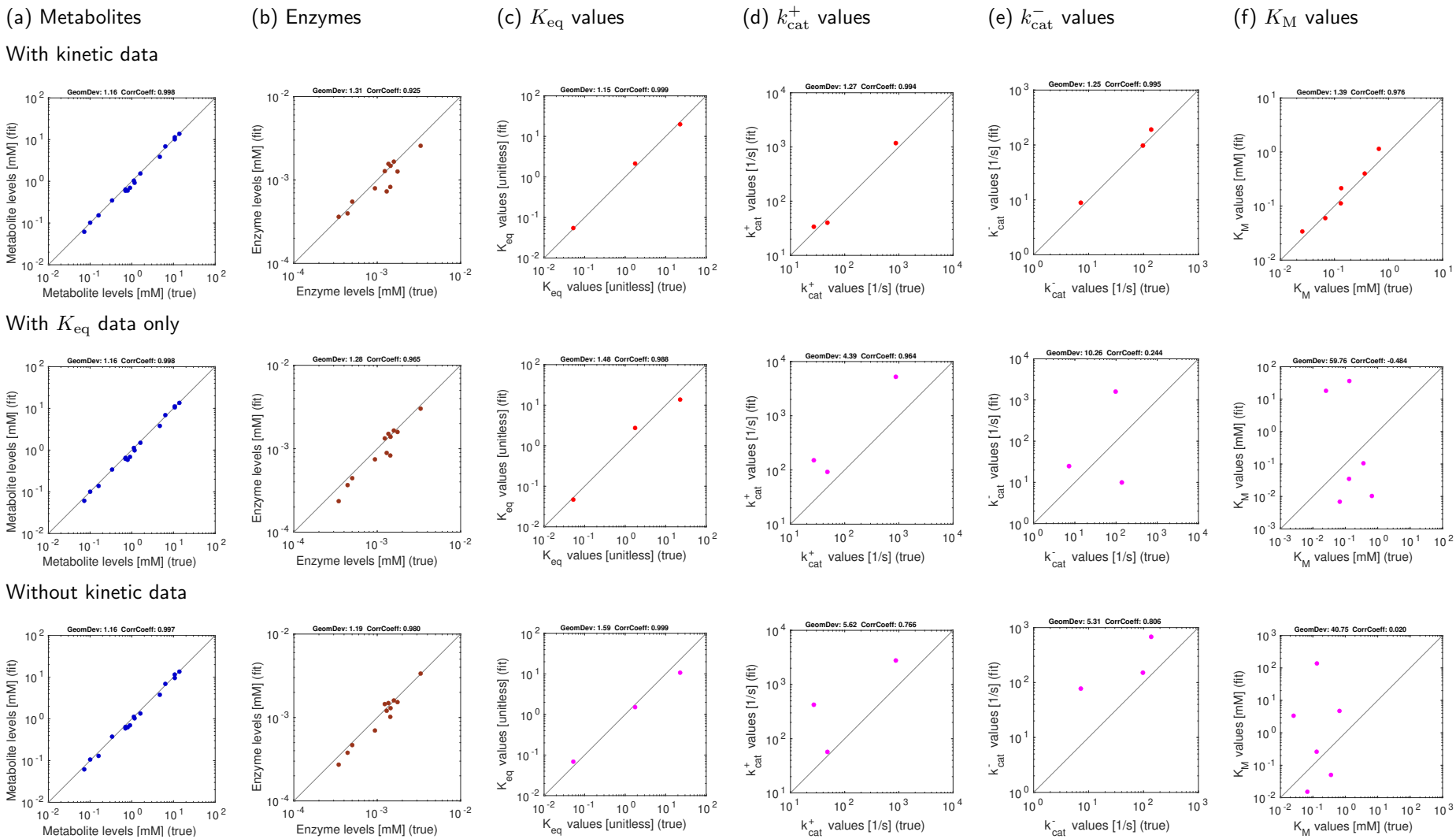


Figure 21: Same as Figure 30, with noisy kinetic data

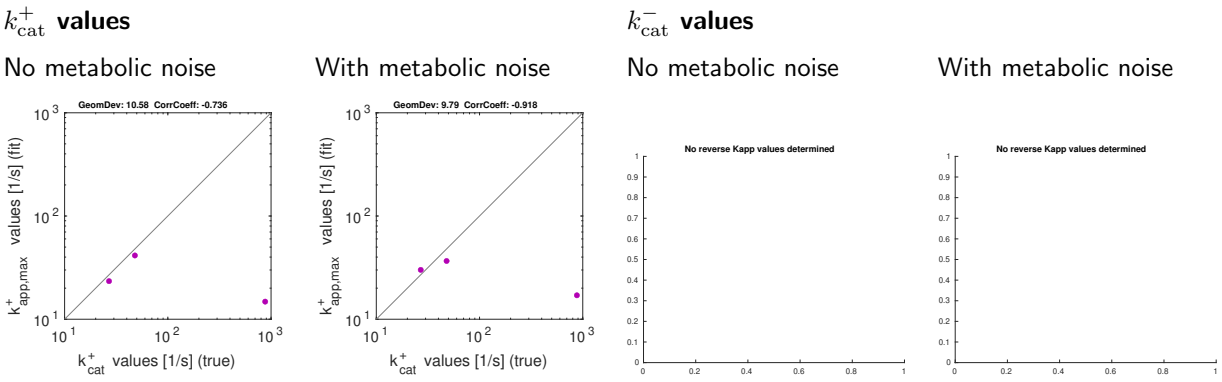


Figure 22: Catalytic constants in Three-chain (artificial data), estimated by kinetic profiling [**?**]. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).

5 Three-chain model Simulations with alpha = 0.5

Three-chain model with artificial data (noise-free kinetic data, noise-free state data)

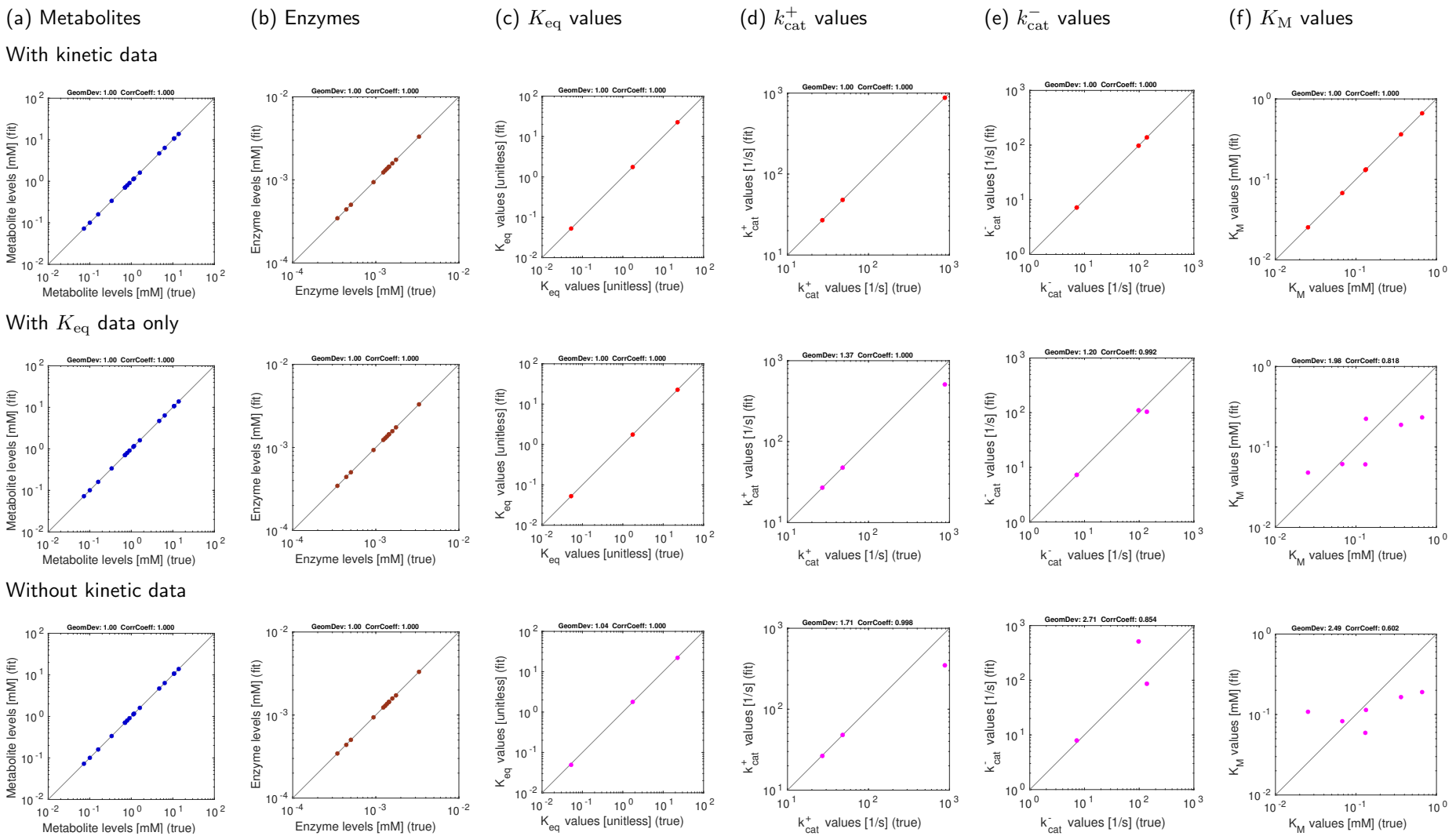


Figure 23: Model balancing results for Three-chain model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation 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)

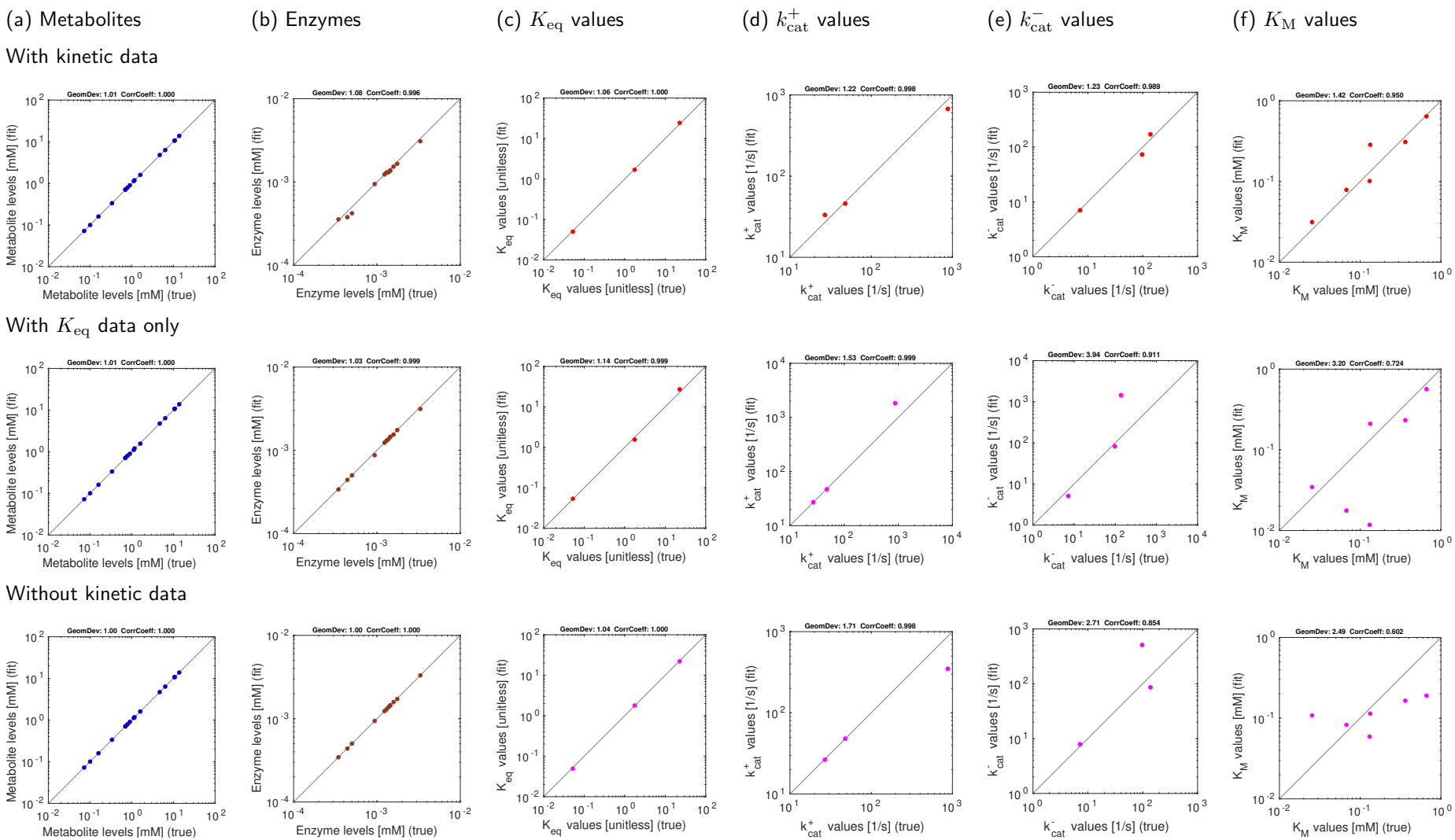


Figure 24: Same as Figure 28, with noisy kinetic data

Three-chain model with artificial data (noise-free kinetic data, noisy state data)

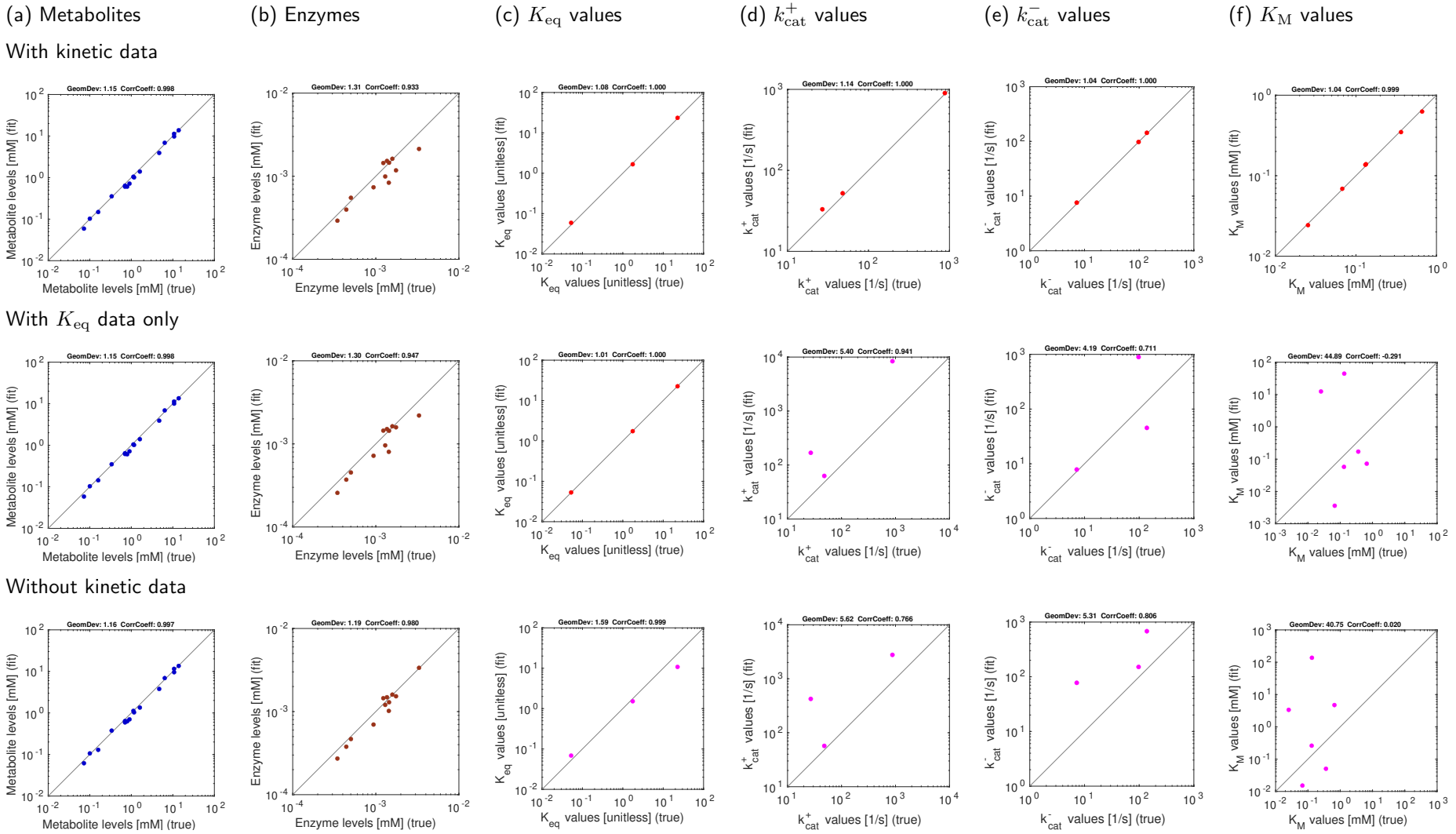


Figure 25: Results for Three-chain with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial data, no data for kinetic constants).

Three-chain model with artificial data (noisy kinetic data, noisy state data)

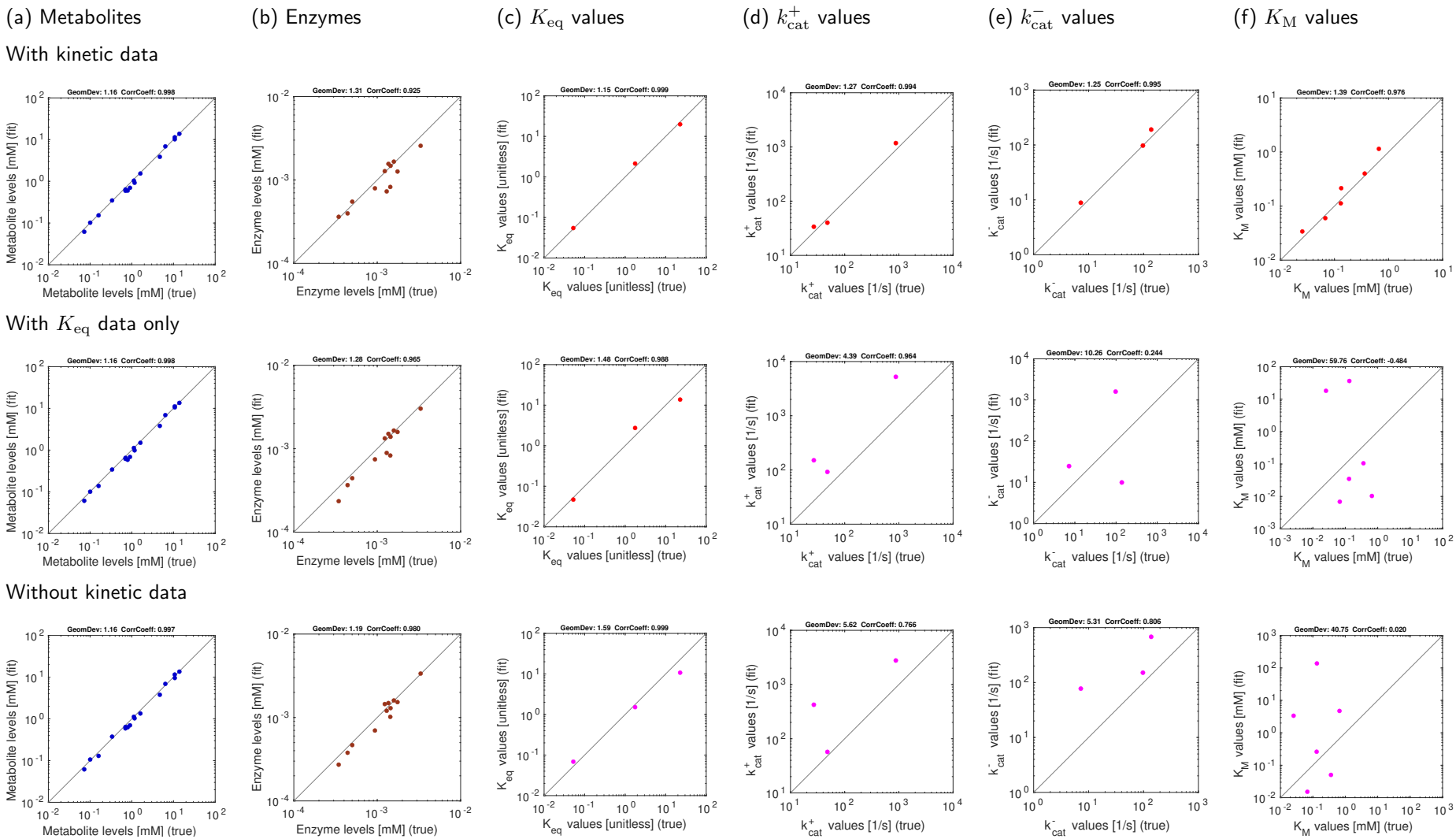


Figure 26: Same as Figure 30, with noisy kinetic data

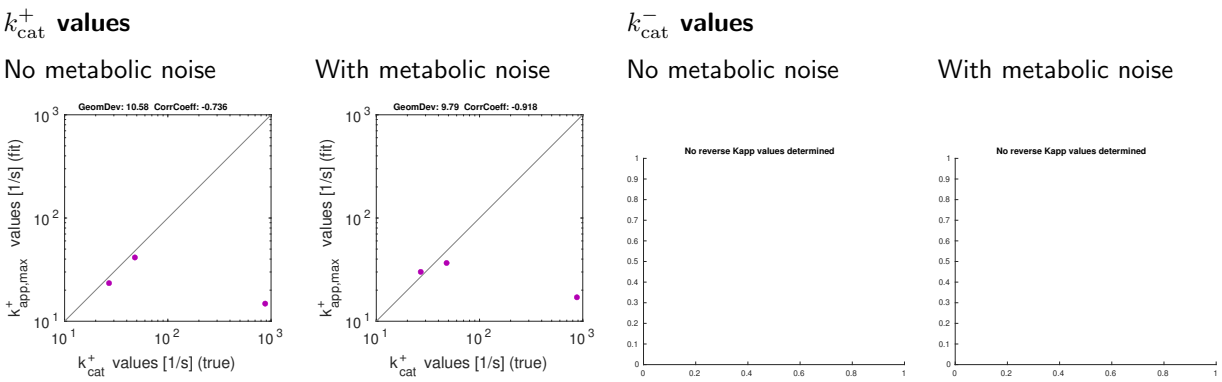


Figure 27: Catalytic constants in Three-chain (artificial data), estimated by kinetic profiling [**?**]. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).

6 Three-chain model Simulations with alpha = 1

Three-chain model with artificial data (noise-free kinetic data, noise-free state data)

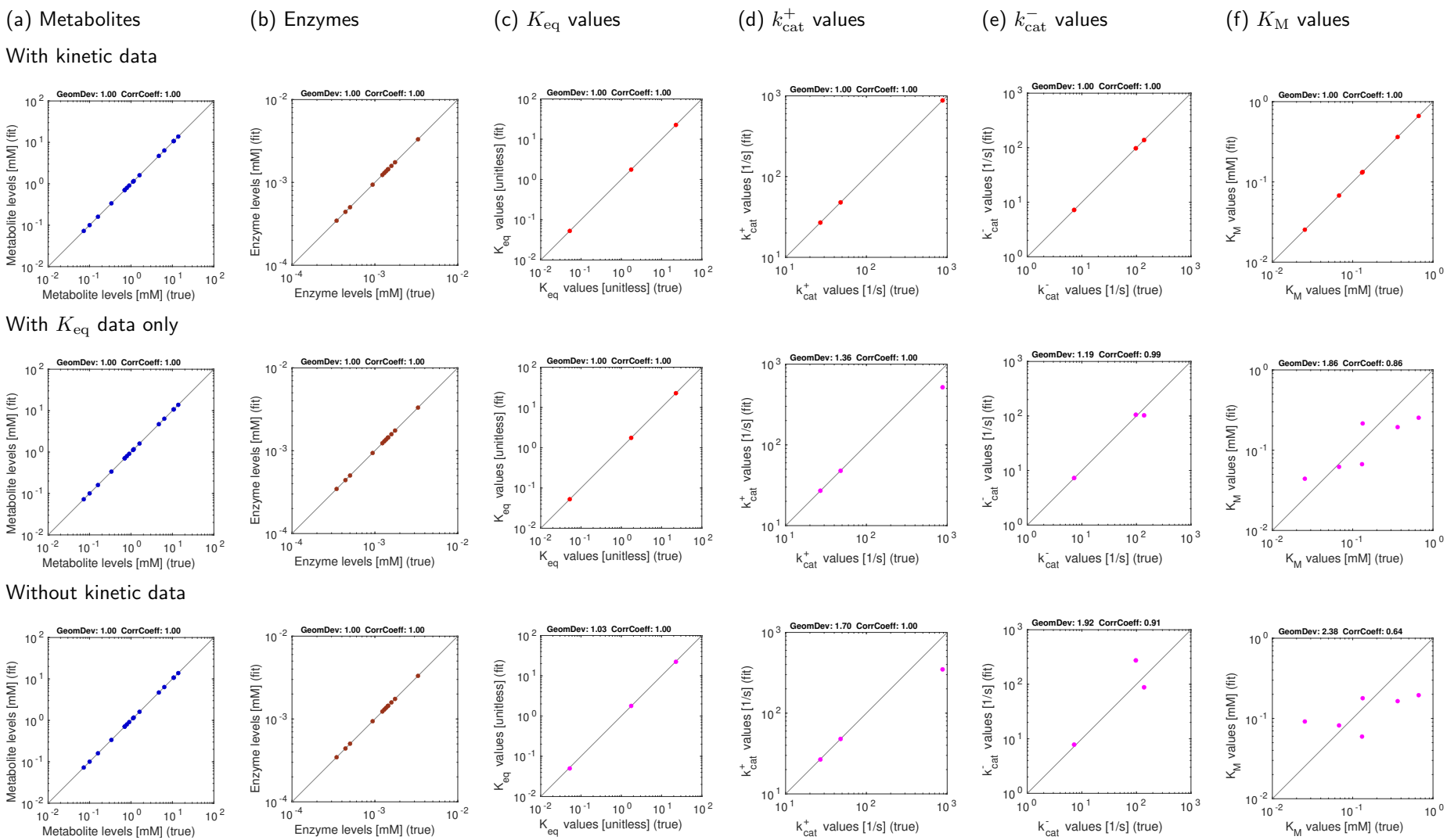
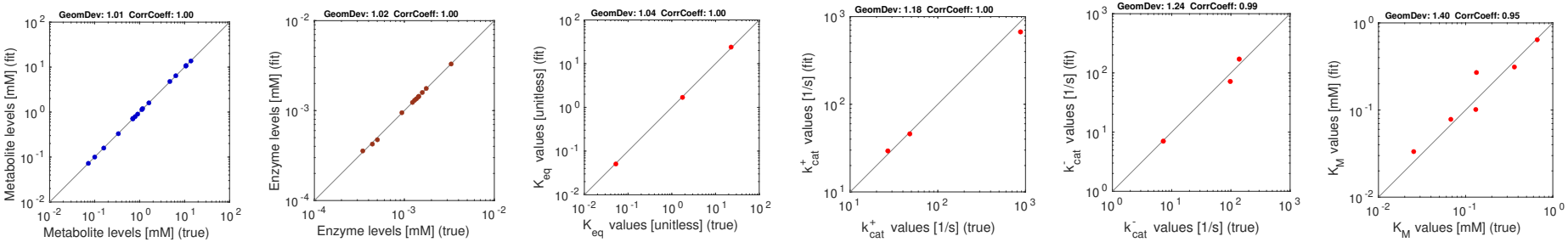


Figure 28: Model balancing results for Three-chain model with artificial data. The model structure is shown in Figure **??**. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation 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).

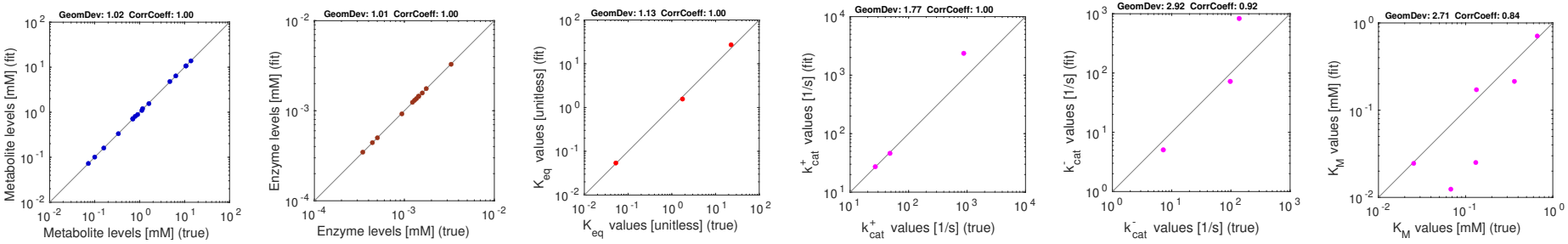
Three-chain model with artificial data (noisy kinetic data, noise-free state data)

(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

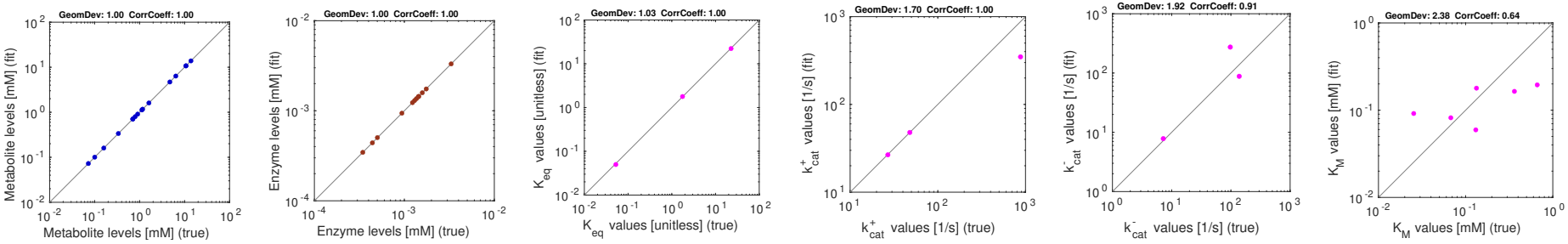


Figure 29: Same as Figure 28, with noisy kinetic data

Three-chain model with artificial data (noise-free kinetic data, noisy state data)

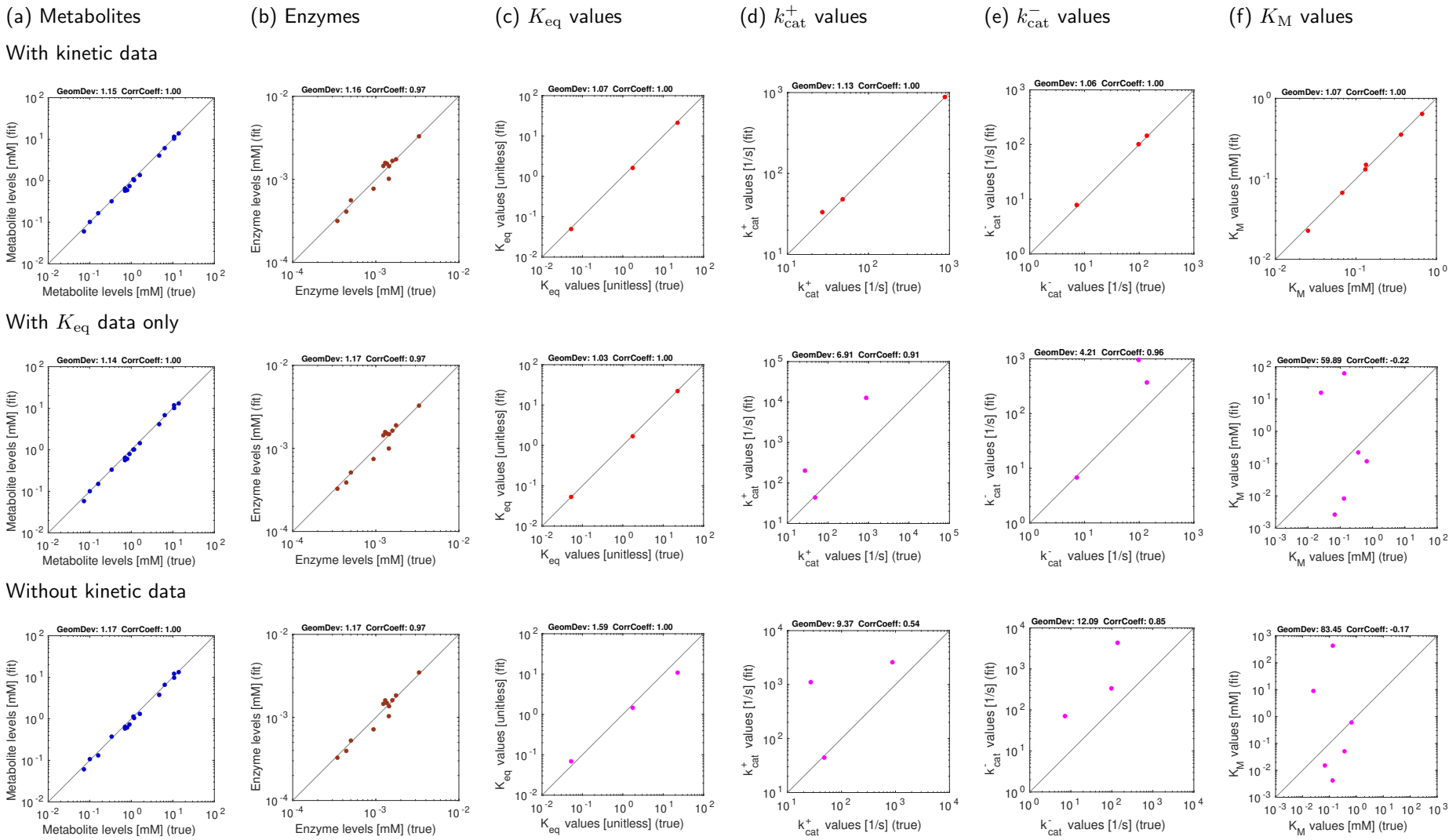


Figure 30: Results for Three-chain with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial data, no data for kinetic constants).

Three-chain model with artificial data (noisy kinetic data, noisy state data)

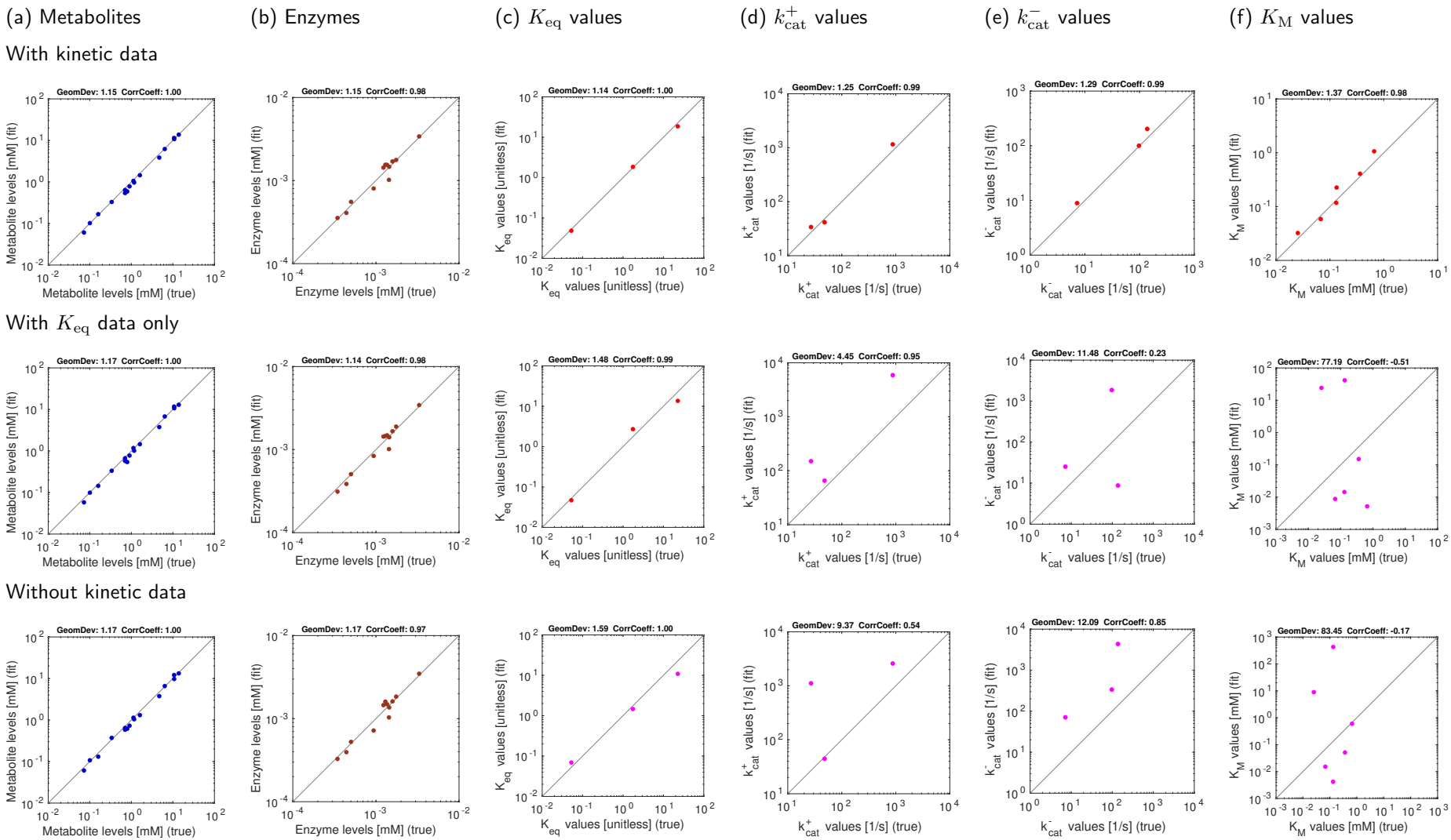


Figure 31: Same as Figure 30, with noisy kinetic data

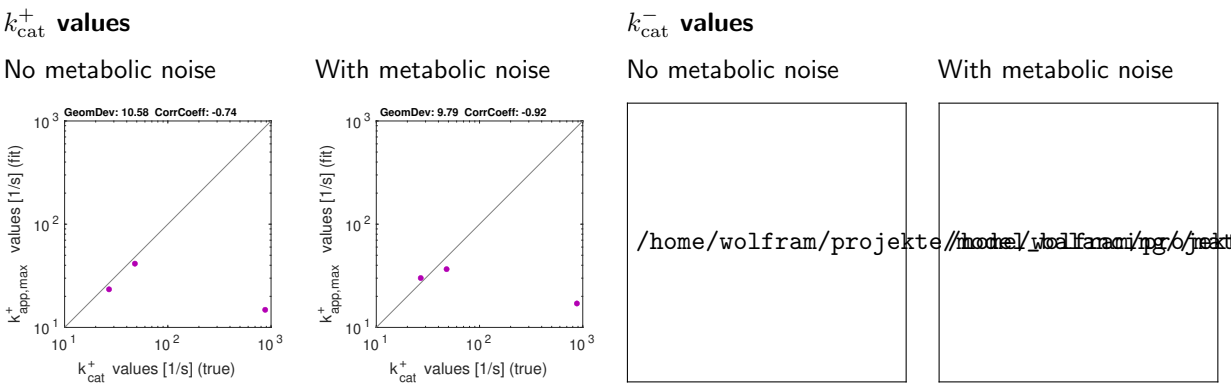


Figure 32: Catalytic constants in Three-chain (artificial data), estimated by kinetic profiling [**?**]. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k^+_{cat} for reactions with forward fluxe).