

Supporting Information for
BayBE: A Bayesian Back End for Experimental Planning in the Low-To-No-Data Regime

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1 Reaction Schema

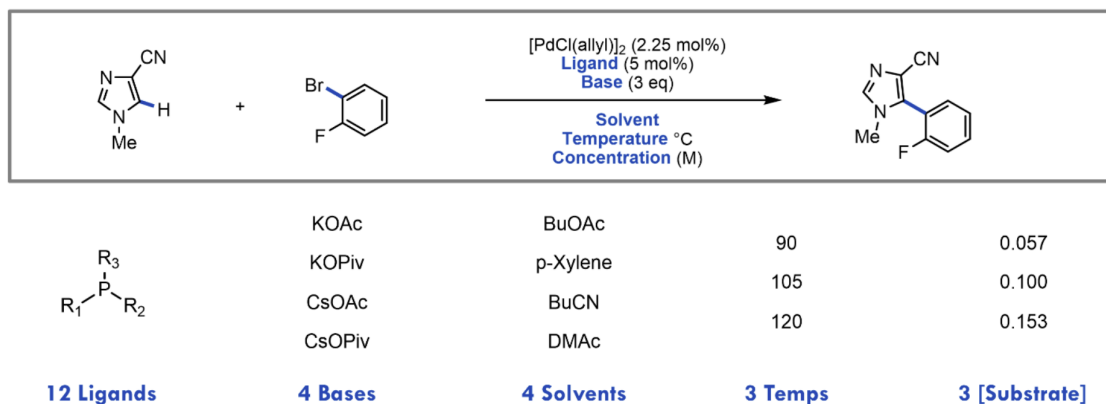


Figure S1 Reaction schema of the direct arylation investigated in this work, adapted from Shields et al¹.

2 Temperature Correlation

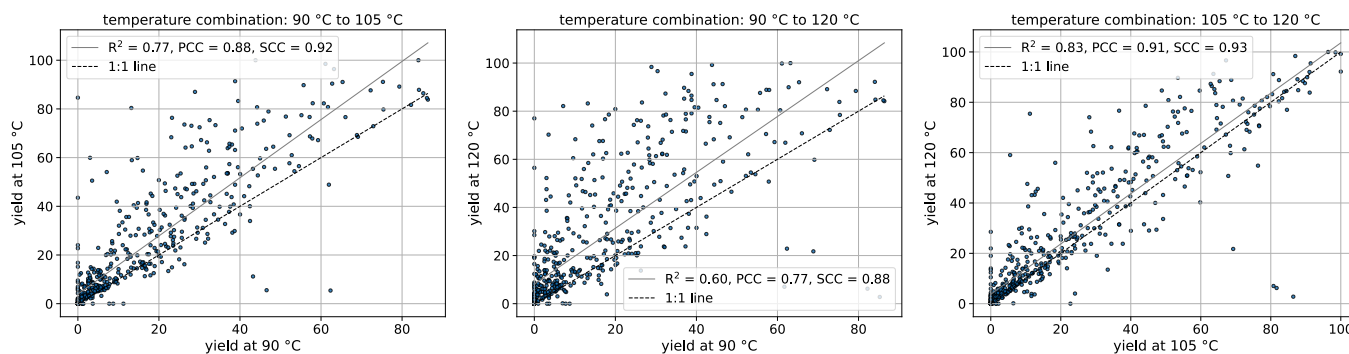


Figure S2 Correlation between data from the three different temperatures for the direct arylation data set¹.

3 Temperature Transfer Learning

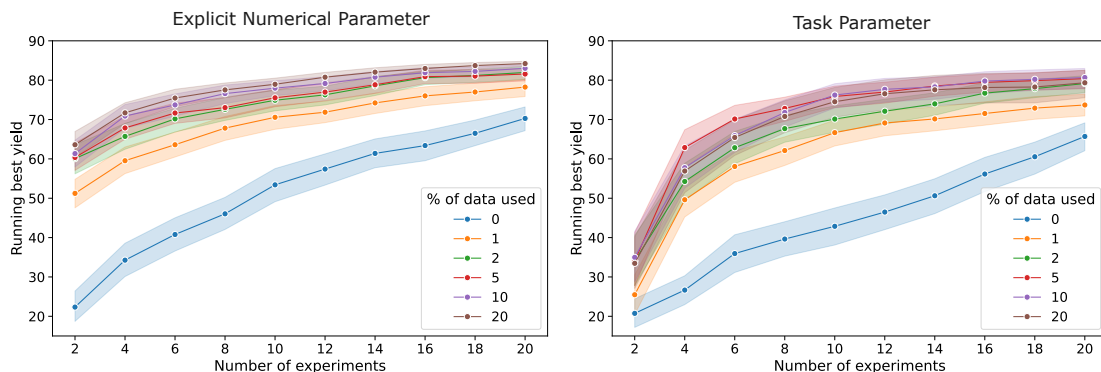


Figure S3 Transfer learning via explicit and implicit (task parameter) modeling for temperature 90°C, incorporating source data at 105°C and 120°C.

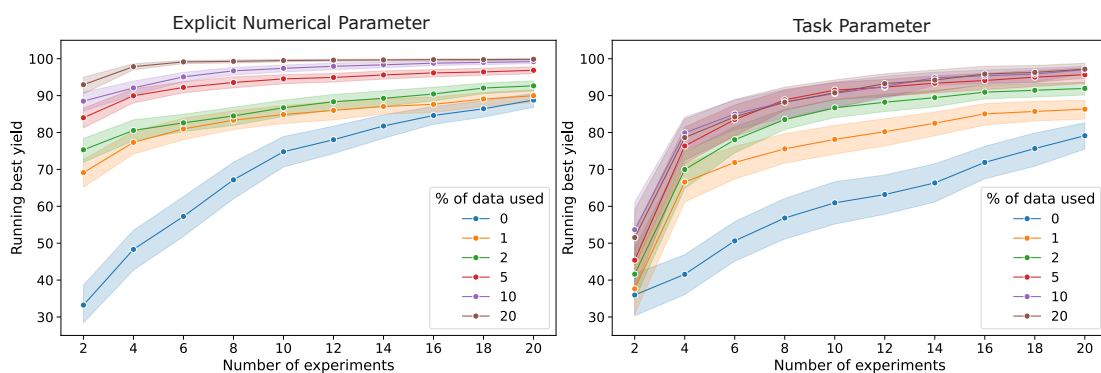


Figure S4 Transfer learning via explicit and implicit (task parameter) modeling for temperature 105°C, incorporating source data at 90°C and 120°C.

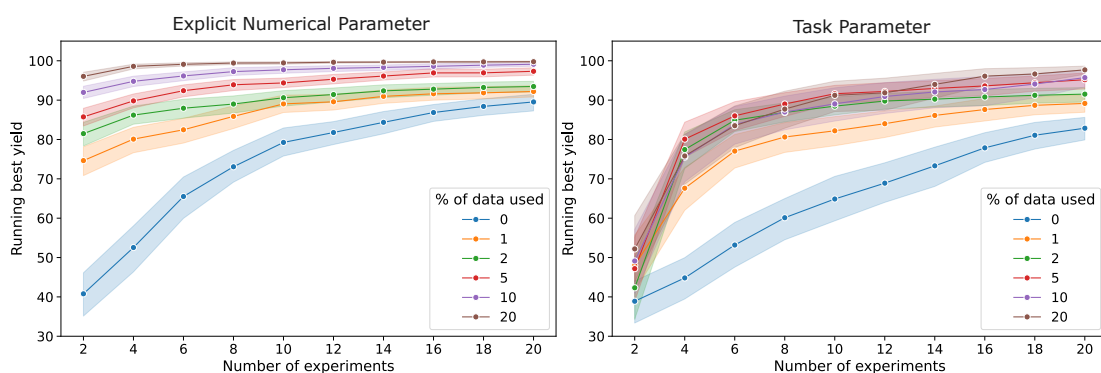


Figure S5 Transfer learning via explicit and implicit (task parameter) modeling for temperature 120°C, incorporating source data at 90°C and 105°C.

4 Concentration Correlation

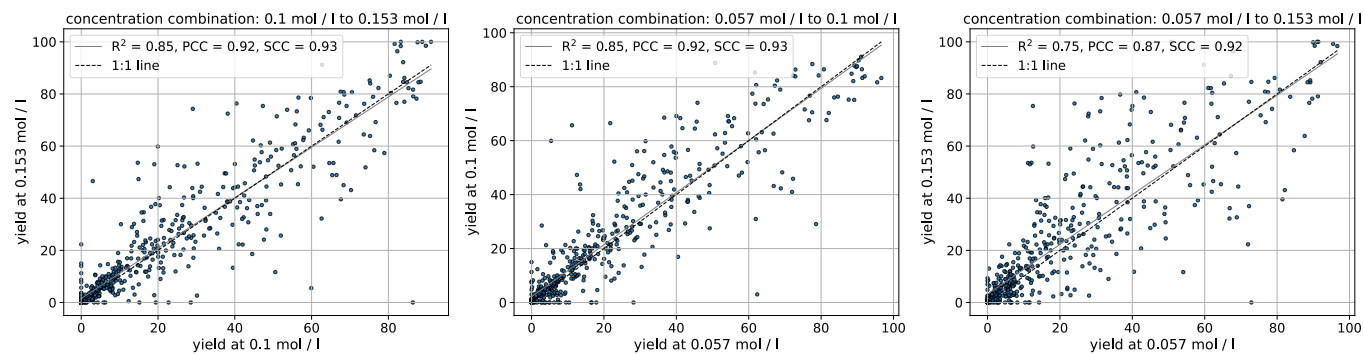


Figure S6 Correlation between data from the three different concentrations for the direct arylation data set¹.

5 Concentration Transfer Learning

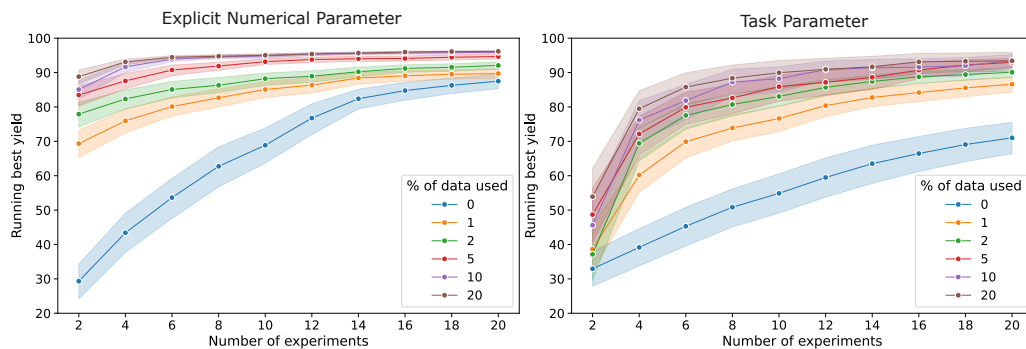


Figure S7 Transfer learning via explicit and implicit (task parameter) modeling for concentration 0.057 mol / l, incorporating source data at 0.1 mol / l and 0.153 mol / l.

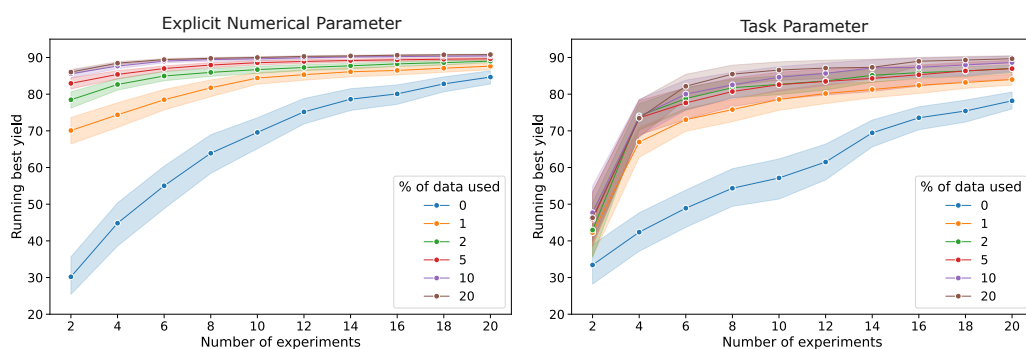


Figure S8 Transfer learning via explicit and implicit (task parameter) modeling for concentration 0.1 mol / l, incorporating source data at 0.057 mol / l and 0.153 mol / l.

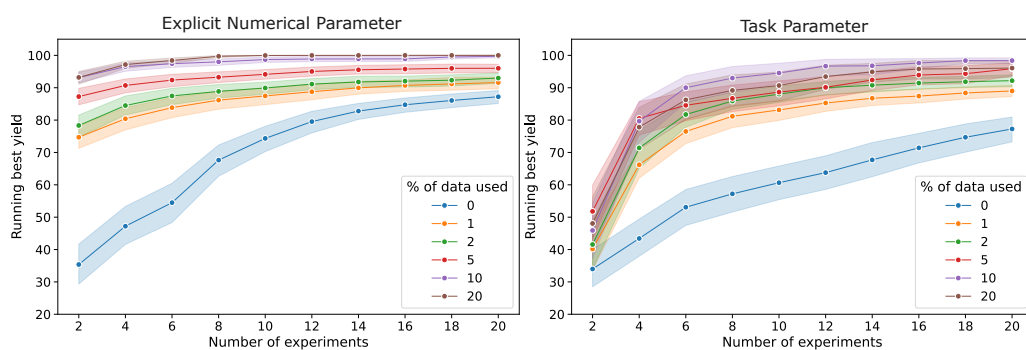


Figure S9 Transfer learning via explicit and implicit (task parameter) modeling for concentration 0.153 mol / l, incorporating source data at 0.057 mol / l and 0.153 mol / l.

Notes and References

- [1] B. J. Shields, J. Stevens, J. Li, M. Parasram, F. Damani, J. I. M. Alvarado, J. M. Janey, R. P. Adams and A. G. Doyle, *Nature*, 2021, **590**, 89–96.