molecular informatics

Supporting Information

Prediction of the Chemical Context for Buchwald-Hartwig Coupling Reactions

Samuel Genheden,* Agnes Mårdh, Gustav Lahti, Ola Engkvist, Simon Olsson,* and Thierry Kogej

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Prediction of the chemical context for Buchwald-Hartwig coupling reactions

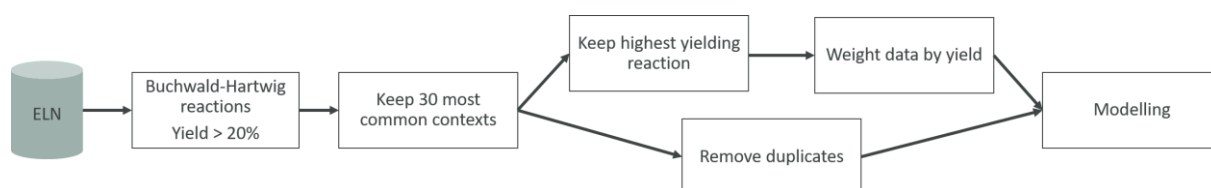Samuel Genheden, Agnes Mårdh, Gustav Lahti, Ola Engkvist, Simon Olsson, Thierry Kogej

Figure S1 – Overview of the data-processing pipeline to arrive at modelling-ready data.
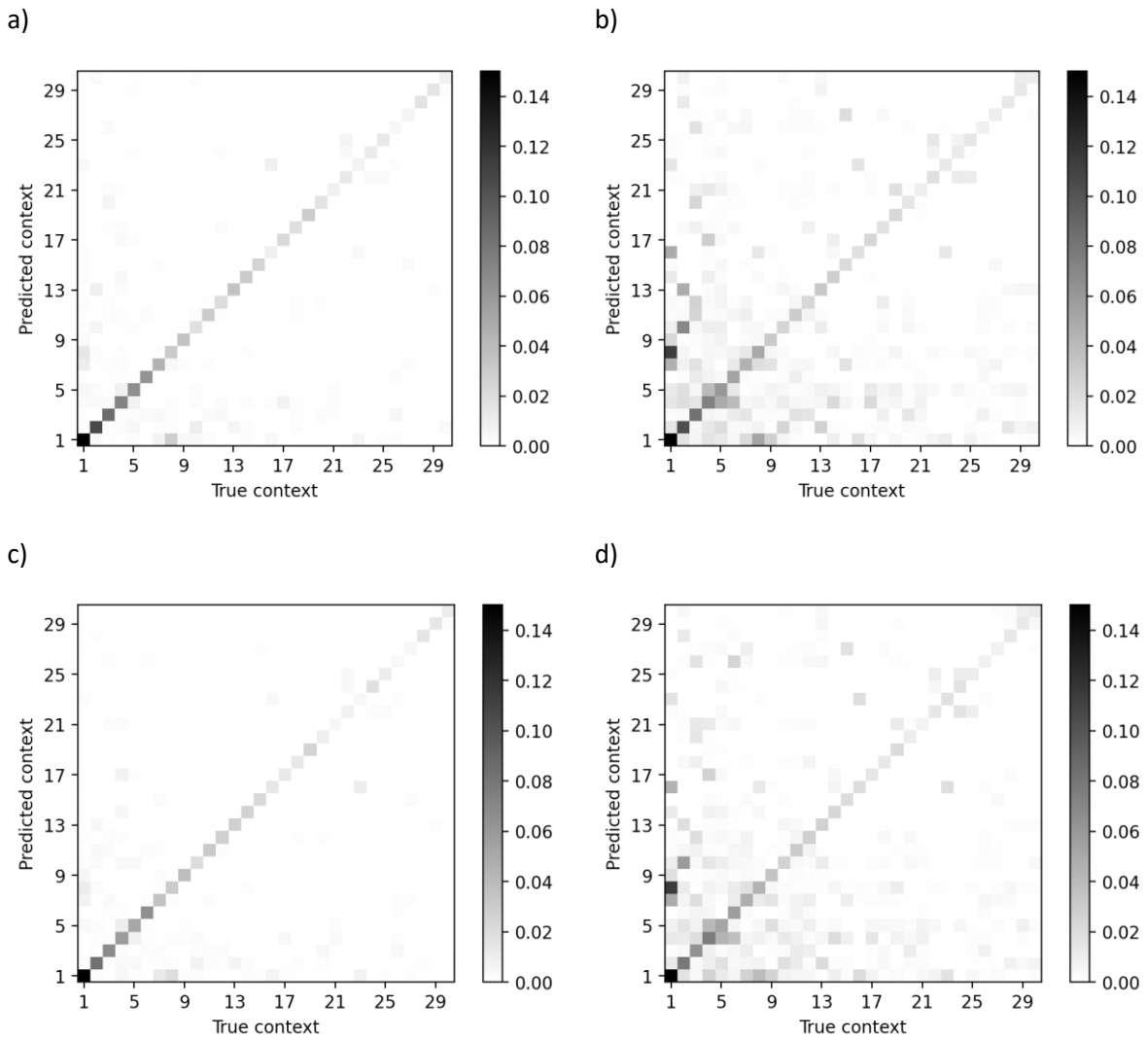
Figure S2 – Likelihood of predicting a context *x* when the ground-truth context is *y*. a) Single-label predictions in top-1, b) Single-label predictions in top-3, c) Multi-label predictions in top-1, d) Multi-label predictions in top-3. The likelihood is normalized based on the total number of data points and is computed over all three trained models. The contexts are sorted based on popularity in the full dataset, where 1 is the most common context.