Supporting Information for "When Machine Learning Models Learn Chemistry II: Applying WISP to Real-World Examples"

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December 11, 2025

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1 LCAP yield

Figure SI-1 shows the WISP output plots for the LCAP yield, highlighting regions where the model fails to capture the underlying chemistry (b). For this case, no distinction between training and test data was made, as a pre-trained model was used.
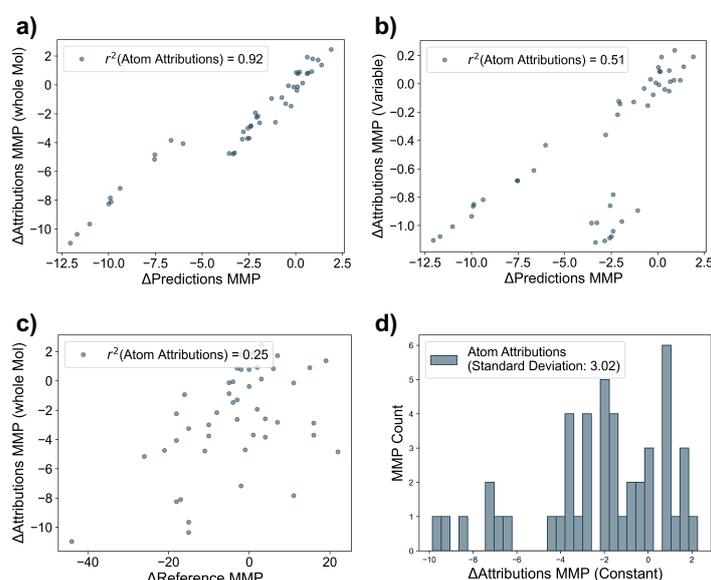

Figure SI-1: Shown are the atom attributions for the entire molecule (a) and for the variable part (b) with respect to the predicted LCAP yield. Additionally, the correlation between the attributed contributions and the experimental LCAP is presented (c), along with a histogram of the variance in the contributions of the constant part of the molecules (d). All values are derived from the entire data set.

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2 AMES

In Figures SI-2 and SI-3, the WISP output plots for the AMES dataset are shown: the training set results for the atom attributor (Fig. SI-2) and the RDKit attributor (Fig. SI-3). The plots differ in appearance from the plots on the other datasets due to the classification nature of the underlying model.
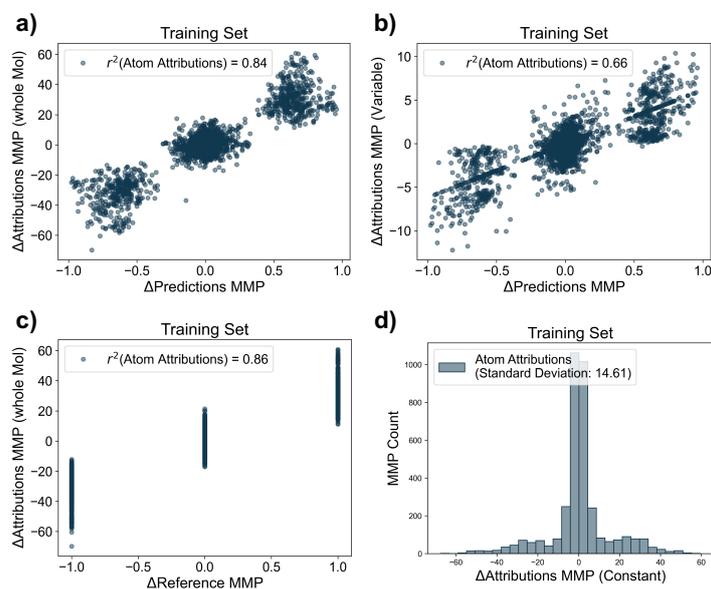

Figure SI-2: Shown are the atom attributions for the entire molecule (a) and the variable part (b) with respect to the predicted Ames mutagenicity. Additionally, the correlation between the attributed contributions and the experimental log P is presented (c), along with a histogram of the variance in contributions from the constant part of the molecules (d). All values are derived from the model's training set.
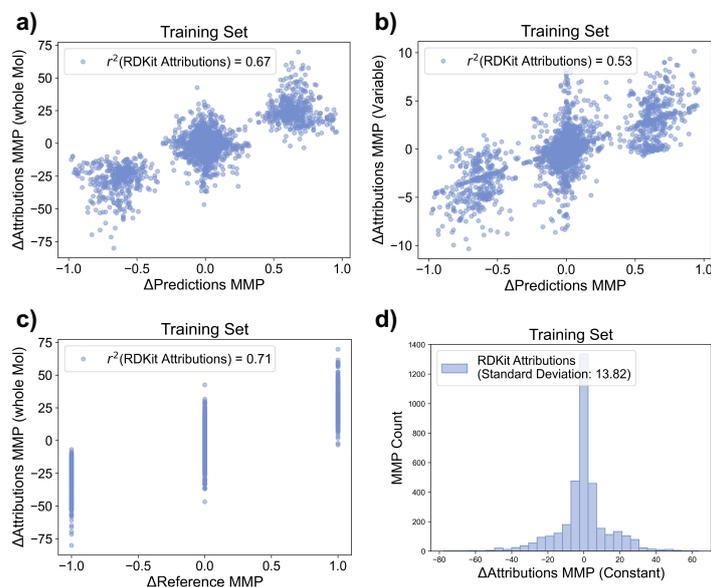

Figure SI-3: Shown are the rdkit attributions for the entire molecule (a) and the variable part (b) with respect to the predicted Ames mutagenicity. Additionally, the correlation between the attributed contributions and the experimental log P is presented (c), along with a histogram of the variance in contributions from the constant part of the molecules (d). All values are derived from the model's training set.

3 General Trends

Figure SI-4 illustrates the calculation of the correlation reported in Table 5 of the main paper, exemplified by the relationship between the standard deviation of the constant part and the r^2 of the whole-molecule predictions on the test set. This yields a correlation of 0.79, as displayed in Table 5 in the main paper.
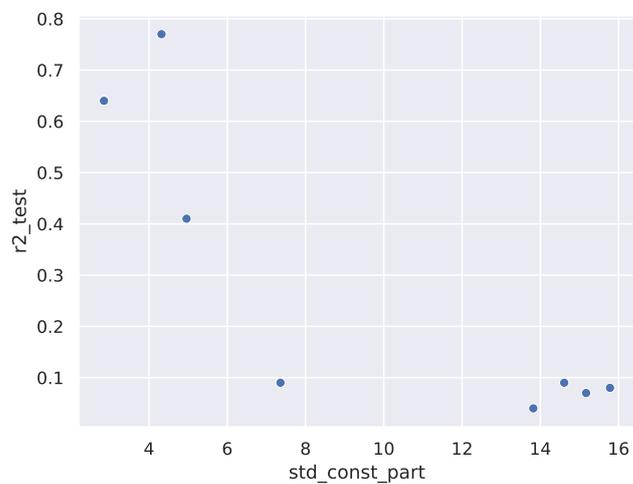

Figure SI-4: Example correlation plot between the standard deviation of the constant part and the r^2 of the whole-molecule on the property of interest on the test set.