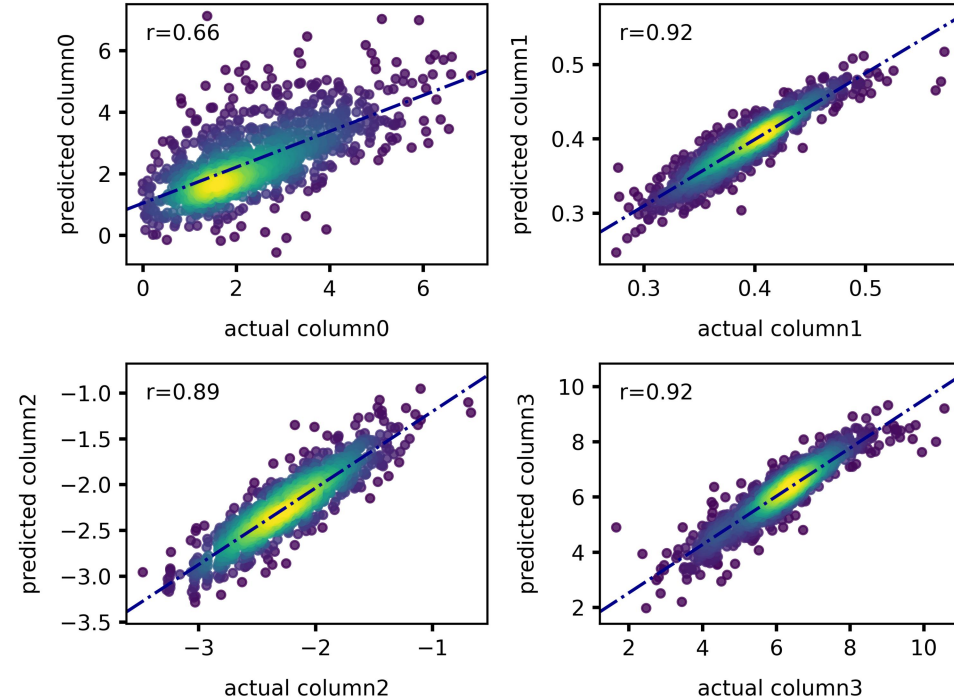
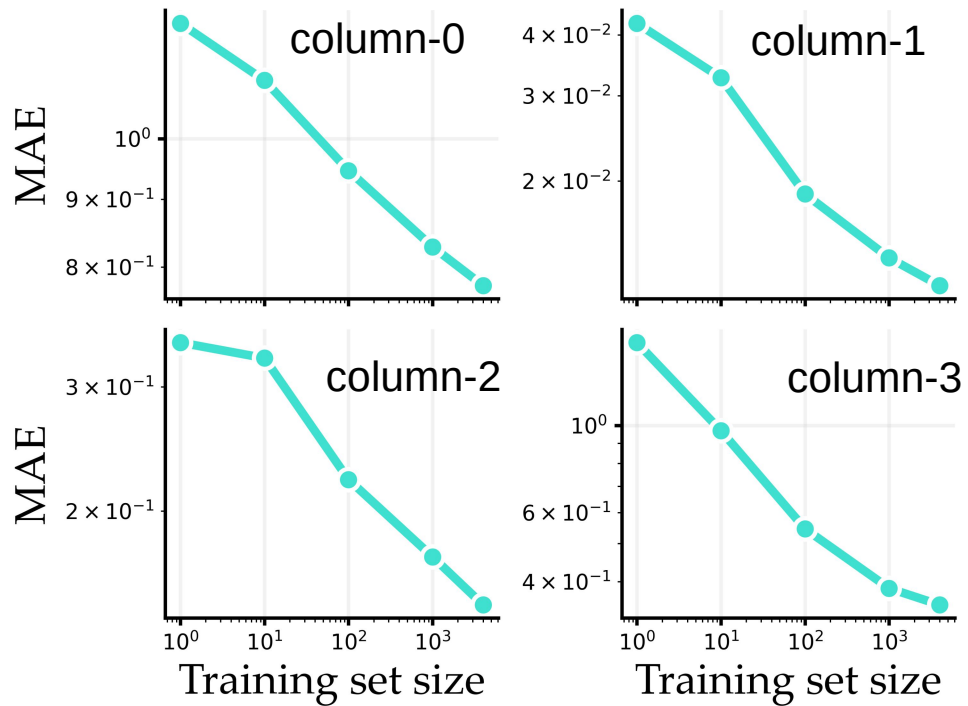




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Kernel Ridge Regression



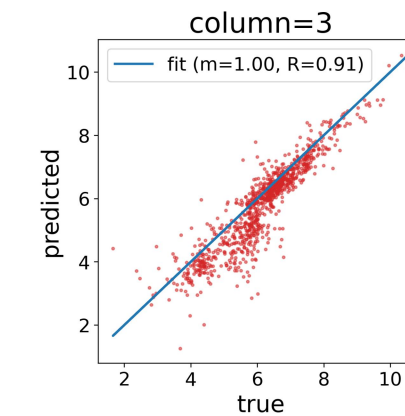
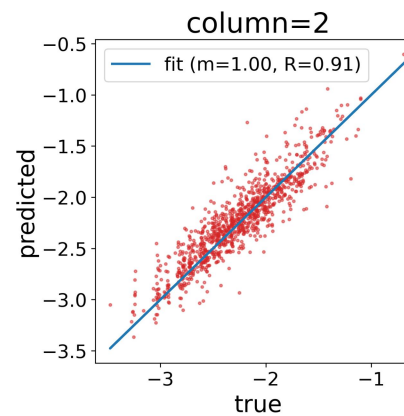
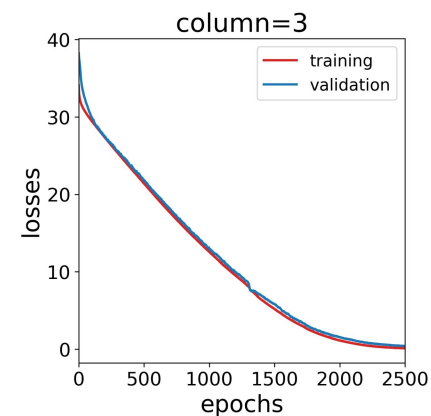
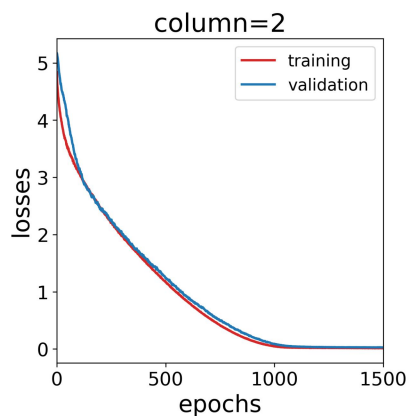
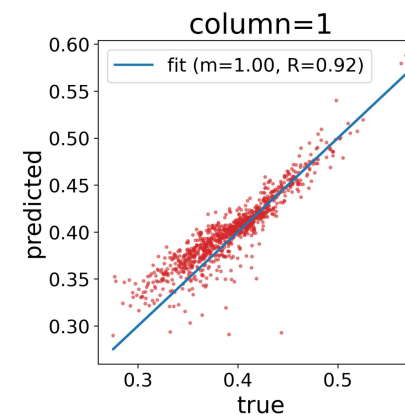
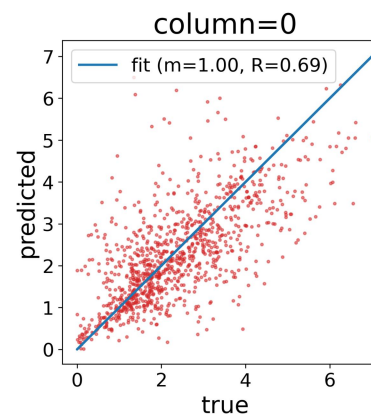
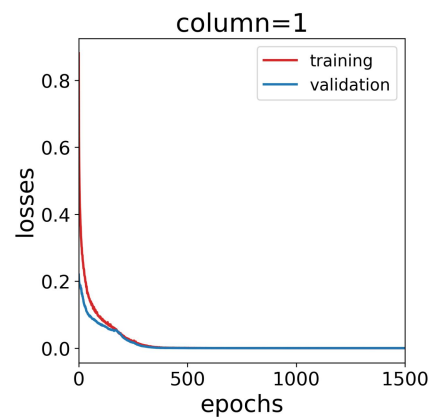
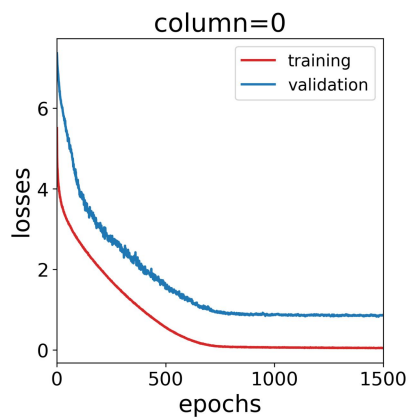
Single kernel recipe: No costly cross-validation required for hyper-parameters tuning



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Deep Neural Network



2048 long, default fingerprinting was too much of data for the small molecules. **Dropout layers** improved training.