

# Use %Mass-Change as target

|           | RMSE(train)        | PCC(train)         | RMSE(valid)       | PCC(valid)        |
|-----------|--------------------|--------------------|-------------------|-------------------|
| NN        | 0.037 $\pm$ 0.012  | 0.988 $\pm$ 0.008  | 0.103 $\pm$ 0.031 | 0.947 $\pm$ 0.039 |
| SVR       | 0.072 $\pm$ 0.004  | 0.972 $\pm$ 0.008  | 0.095 $\pm$ 0.03  | 0.941 $\pm$ 0.102 |
| LinearReg | 0.060 $\pm$ 0.009  | 0.973 $\pm$ 0.008  | 0.094 $\pm$ 0.03  | 0.970 $\pm$ 0.025 |
| KRR       | 0.0098 $\pm$ 0.002 | 0.999 $\pm$ 0.0003 | 0.04 $\pm$ 0.017  | 0.992 $\pm$ 0.011 |

\*all features and target property are normalized to [0,1] range

# Comparison

