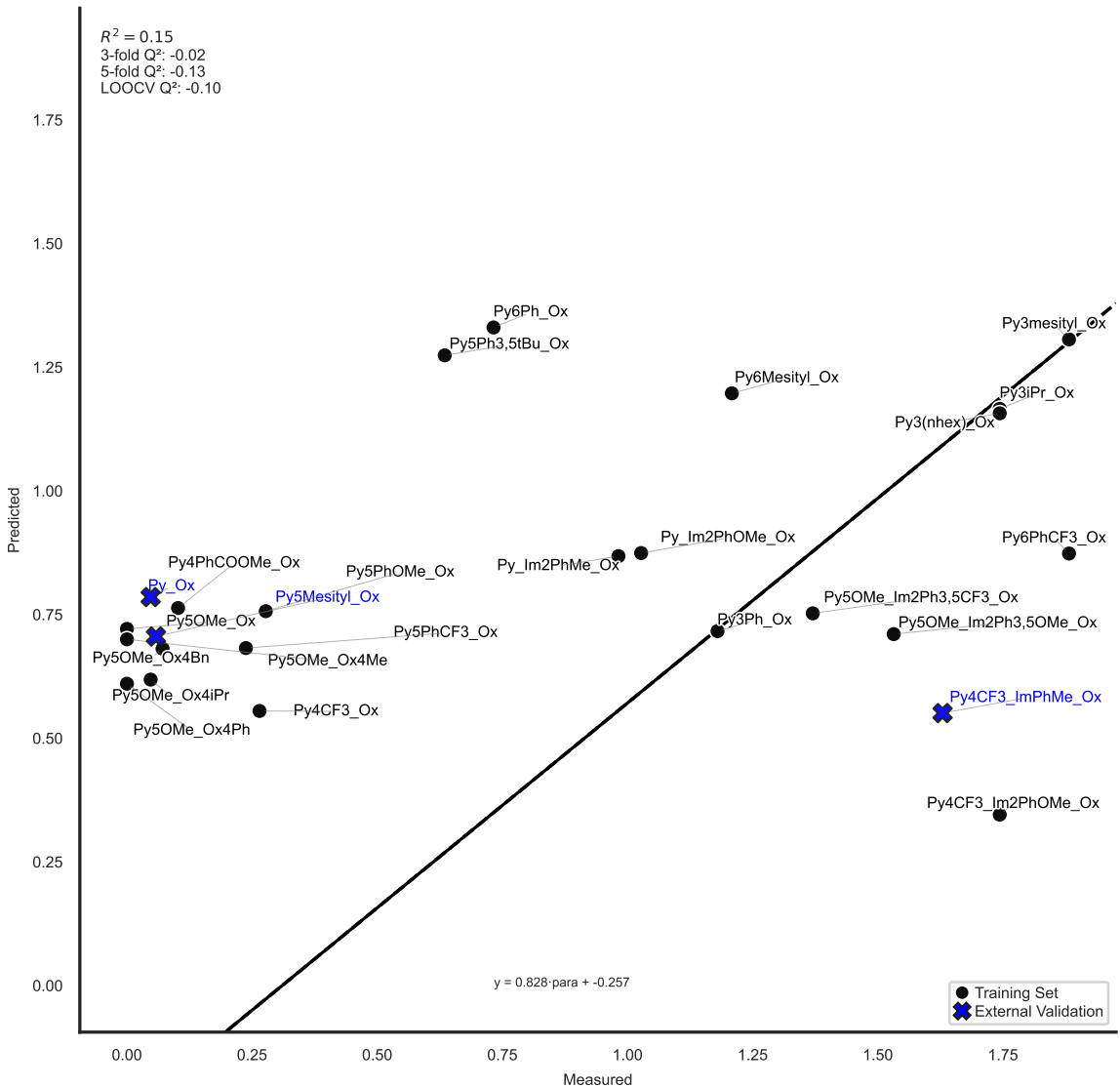


Predicted vs Measured



old CV Metrics

| Q2_3_MARMSD_3 |      |       |
|---------------|------|-------|
| -0.01         | 0.59 | 0.702 |

5-fold CV Metrics

| Q2_5_MARMSD_5 |      |       |
|---------------|------|-------|
| -0.11         | 0.64 | 0.739 |

LOOCV Metrics

| Q2_LOOCV_MARMSD_LO |      |       |
|--------------------|------|-------|
| -0.01              | 0.64 | 0.728 |

Variance Inflation Factors

(no data)

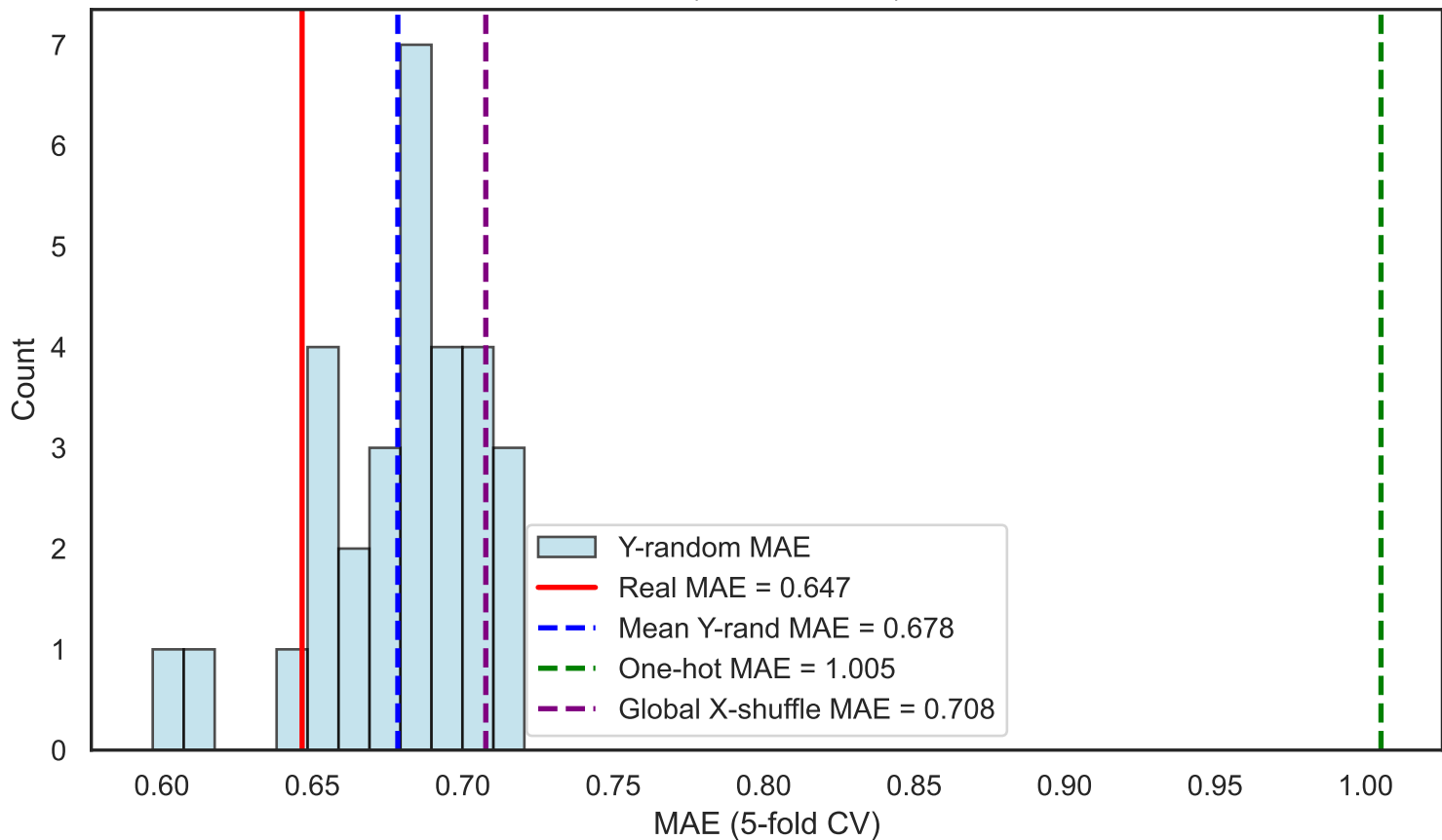
Coefficient Estimation

| Essential | Std. Error | Value |
|-----------|------------|-------|
| 0.8       | 0.15       | 5.7   |
| -0.1      | 0.1        | -1.4  |

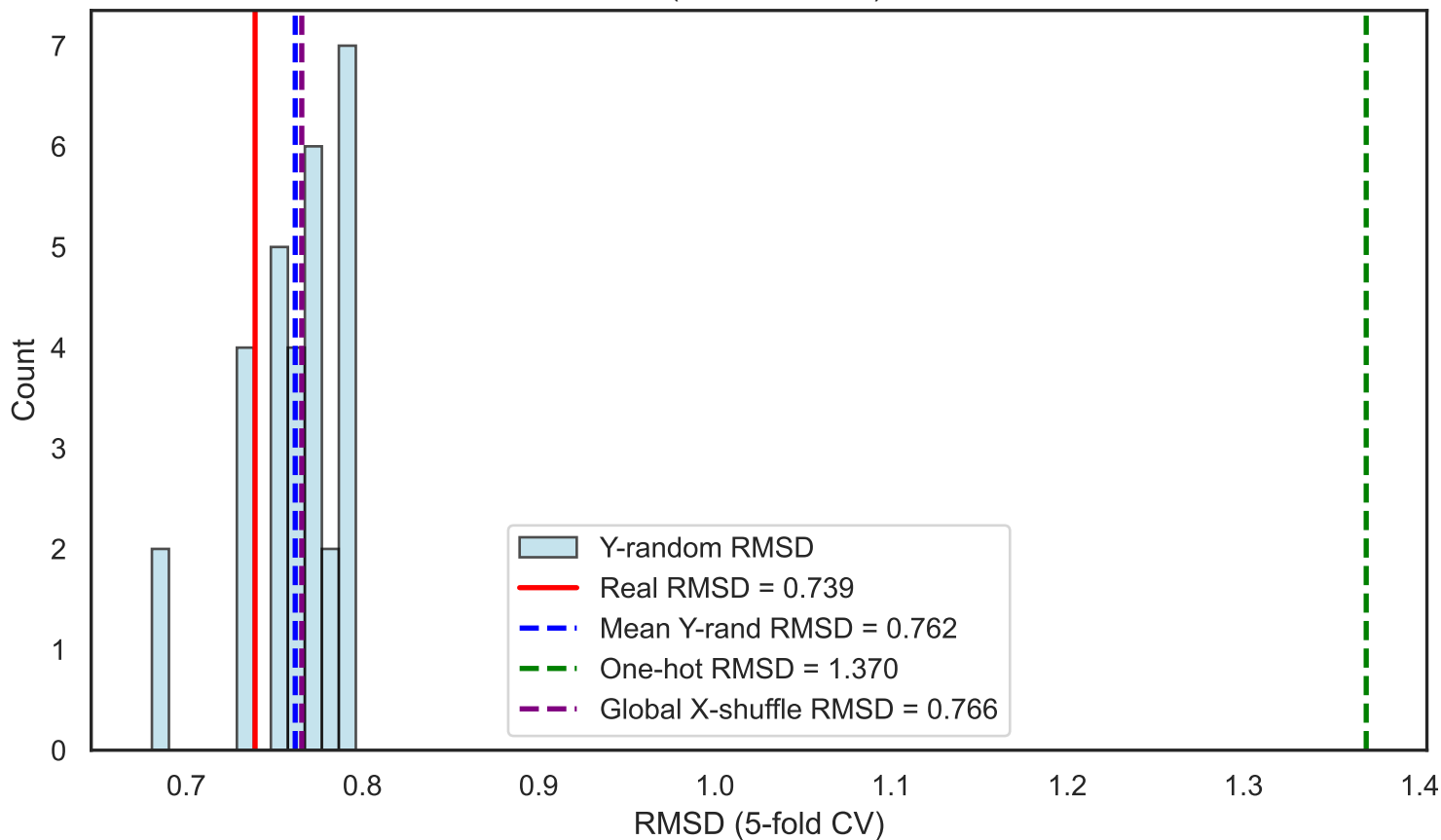
Left-out Predictions

| Molecule         | Actual | Predicted | Error in % |
|------------------|--------|-----------|------------|
| Py4CF3_ImPhMe_Ox | 1.629  | 0.551     | 66.191     |
| Py5Mesityl_Ox    | 0.058  | 0.706     | 1116.741   |
| Py_Ox            | 0.047  | 0.785     | 1557.015   |

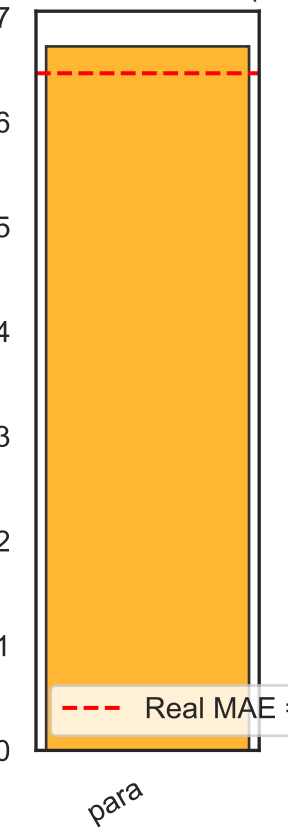
Validation (lower is better): MAE



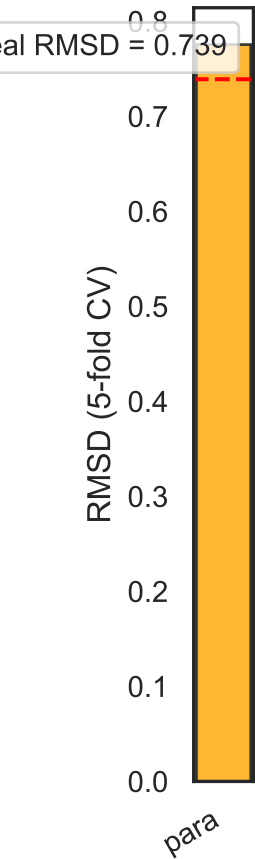
Validation (lower is better): RMSD



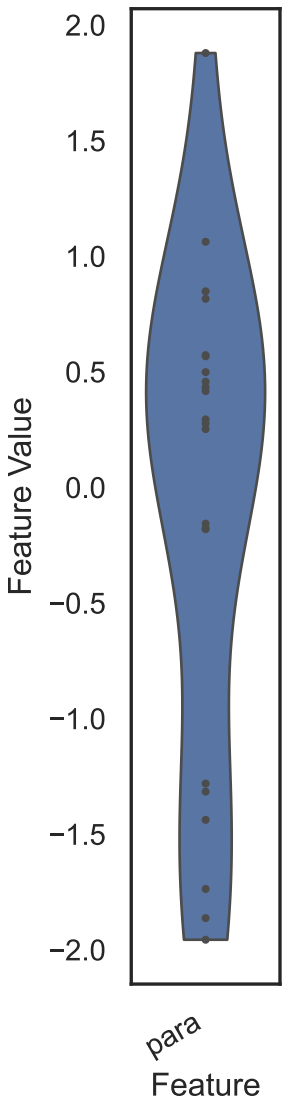
shuffle test: MAE (low



ture shuffle test: RMS



# Distribution of Selected



# Threshold analysis: para

