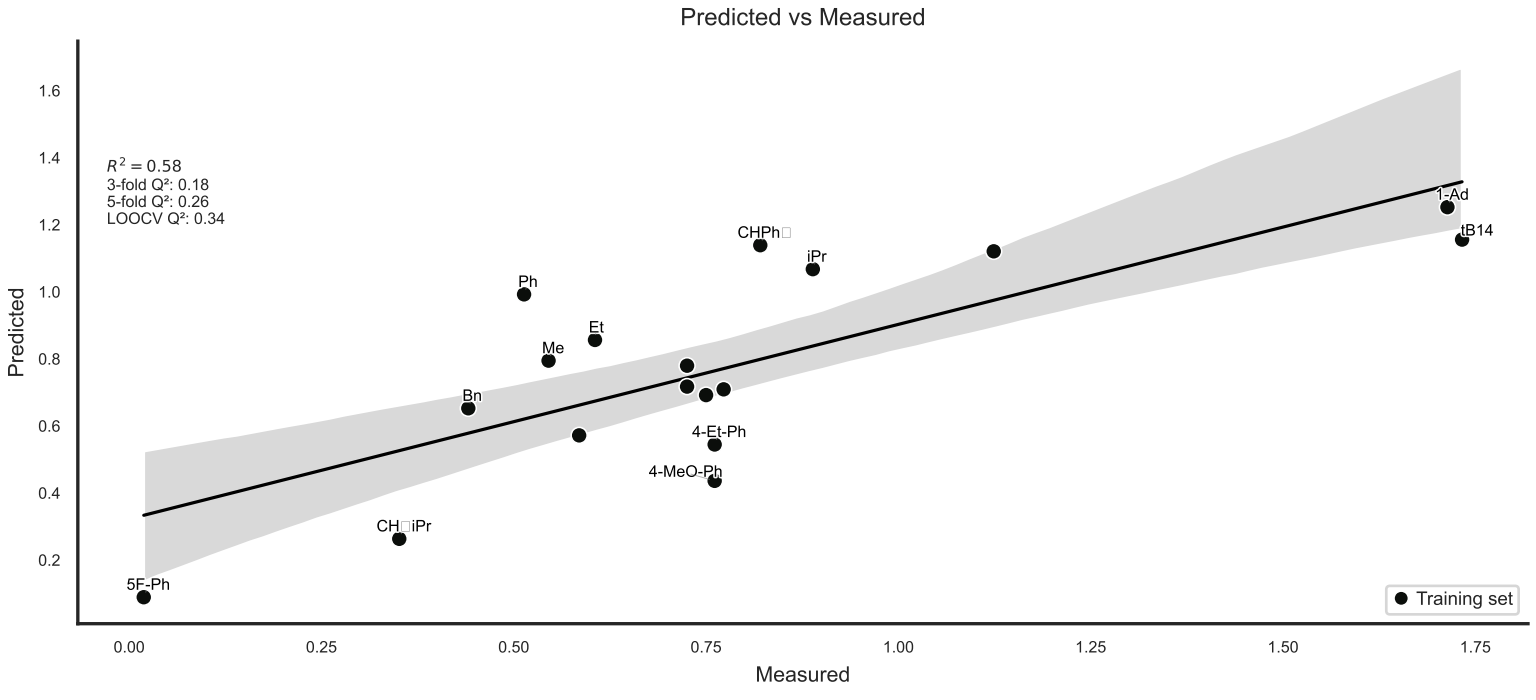

Predicted vs Measured
$R^2 = 0.58$
3-fold Q²: 0.18
5-fold Q²: 0.26
LOOCV Q²: 0.34
Predicted
Measured
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
1-Ad
tB14
CHPh□
iPr
Ph
Et
Me
Bn
4-Et-Ph
4-MeO-Ph
CH□iPr
5F-Ph
Training set
$y = +10.42 \cdot \text{Amplitude\_Stretch\_12\_13} + 0.20 \cdot \text{dipole\_z\_6-11-4} - 0.18 \cdot \text{total\_dipole\_6-11-4} - 9.37$

old CV Metrics

Q2_3_	MAE_	RMSD_3
0.18	0.29	0.367

5-fold CV Metrics

Q2_5_	MAE_	RMSD_5
0.25	0.27	0.351

LOOCV Metri

Q2_	MAE_	RMSD_LO
0.34	0.25	0.33

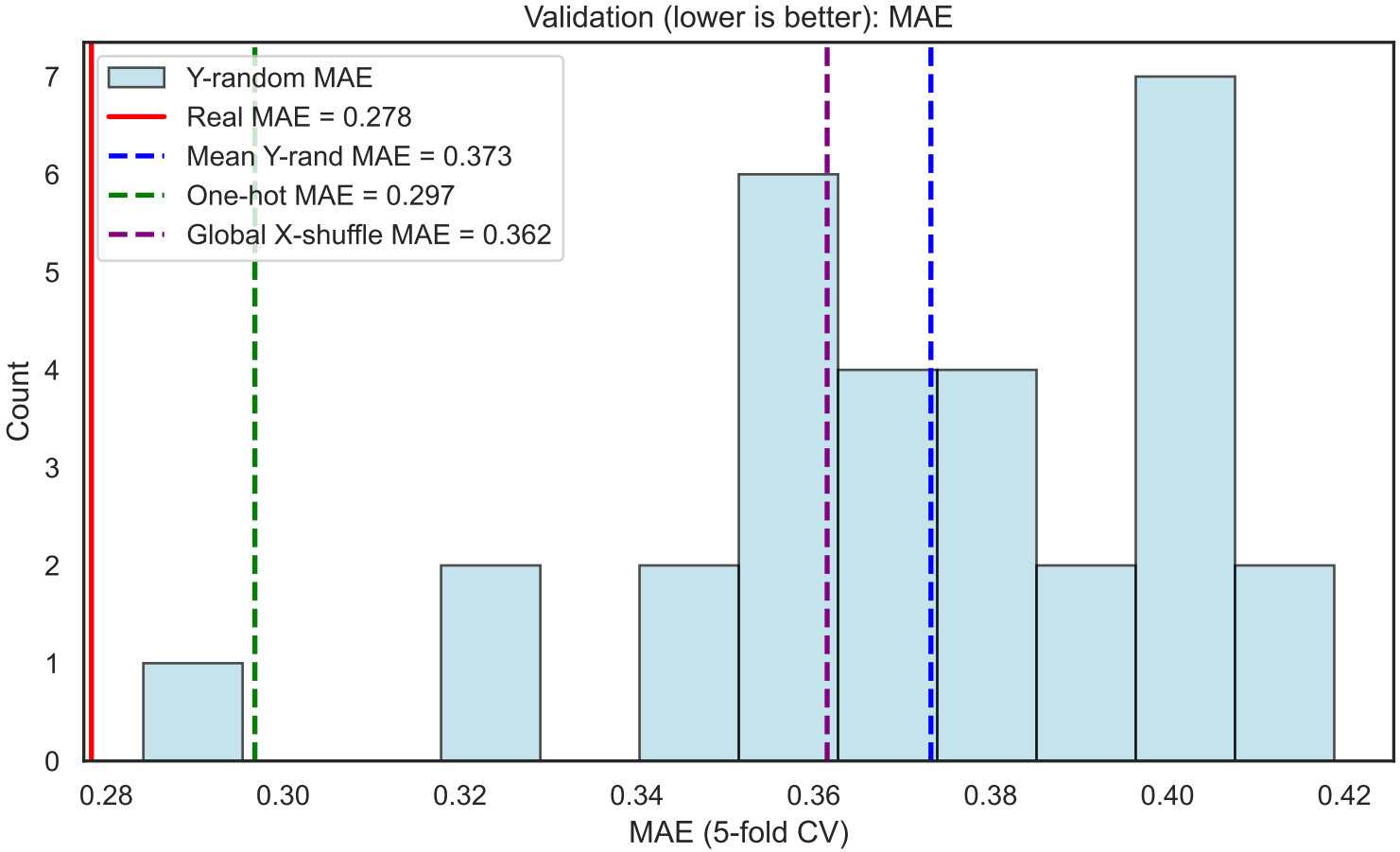
Variance Inflation Factors

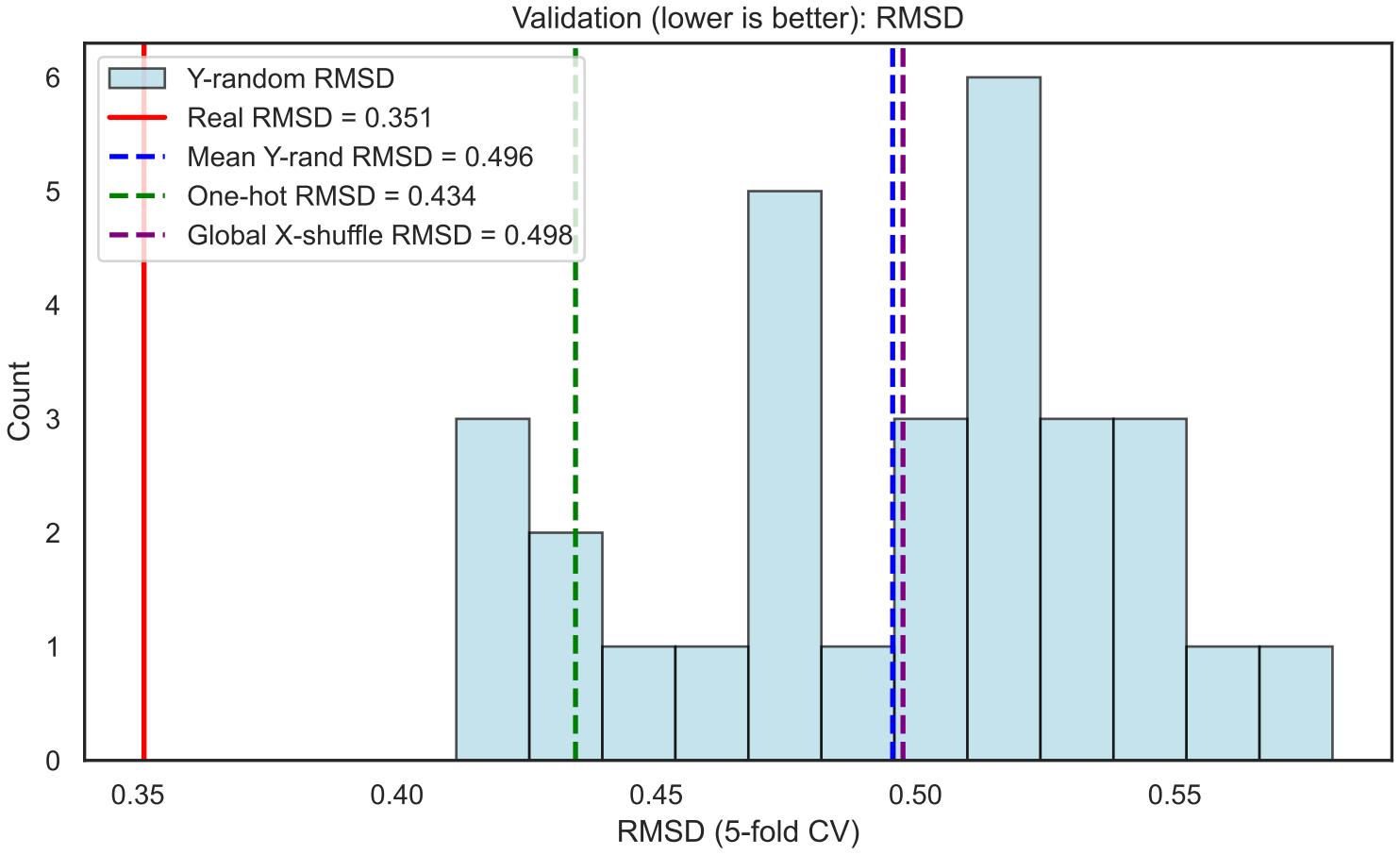
variable	VIF
total_dipole_6-11-4	1.38
dipole_z_6-11-4	1.33
Amplitude_Stretch_12_13	1.19

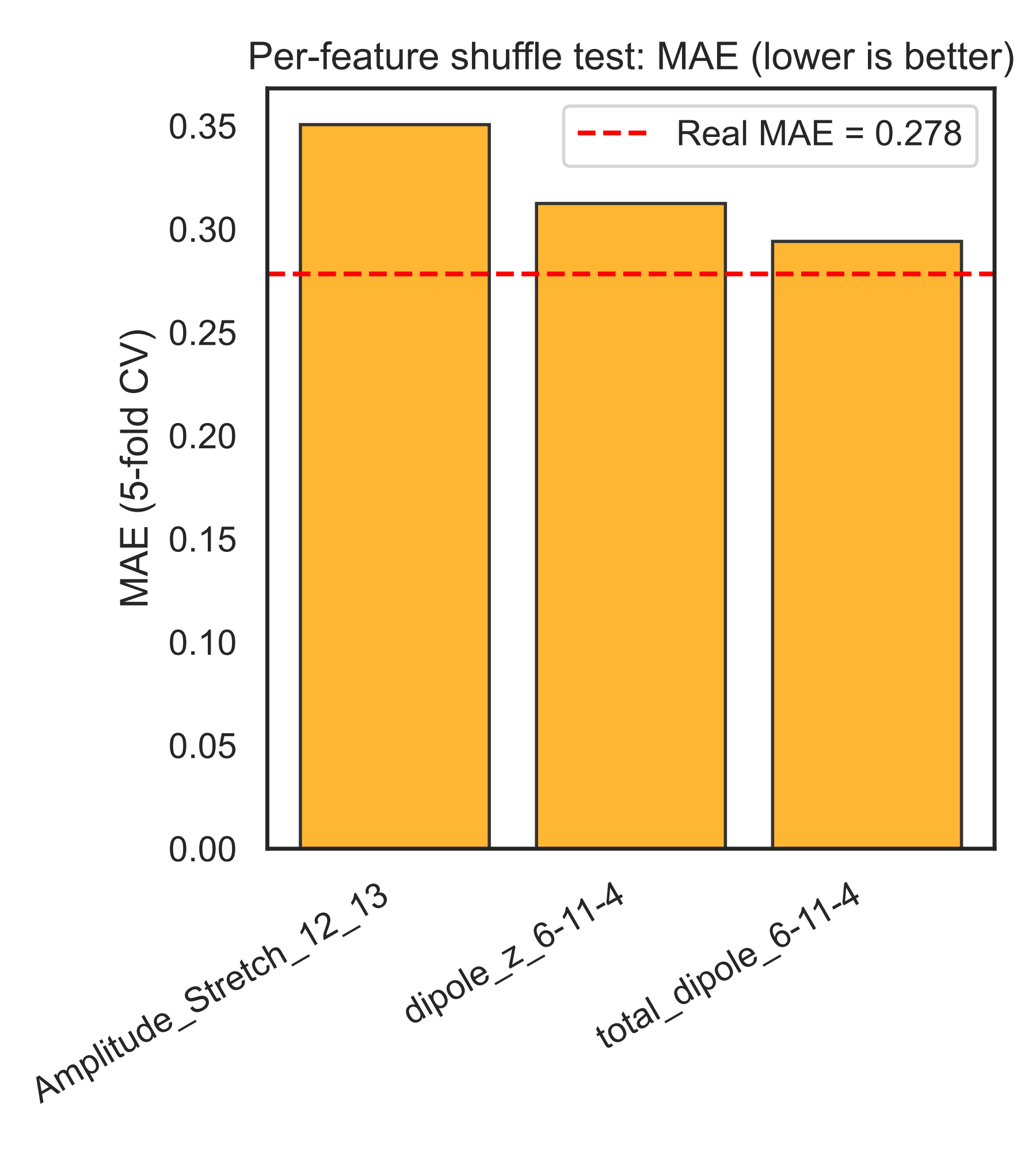
Coefficient Estim

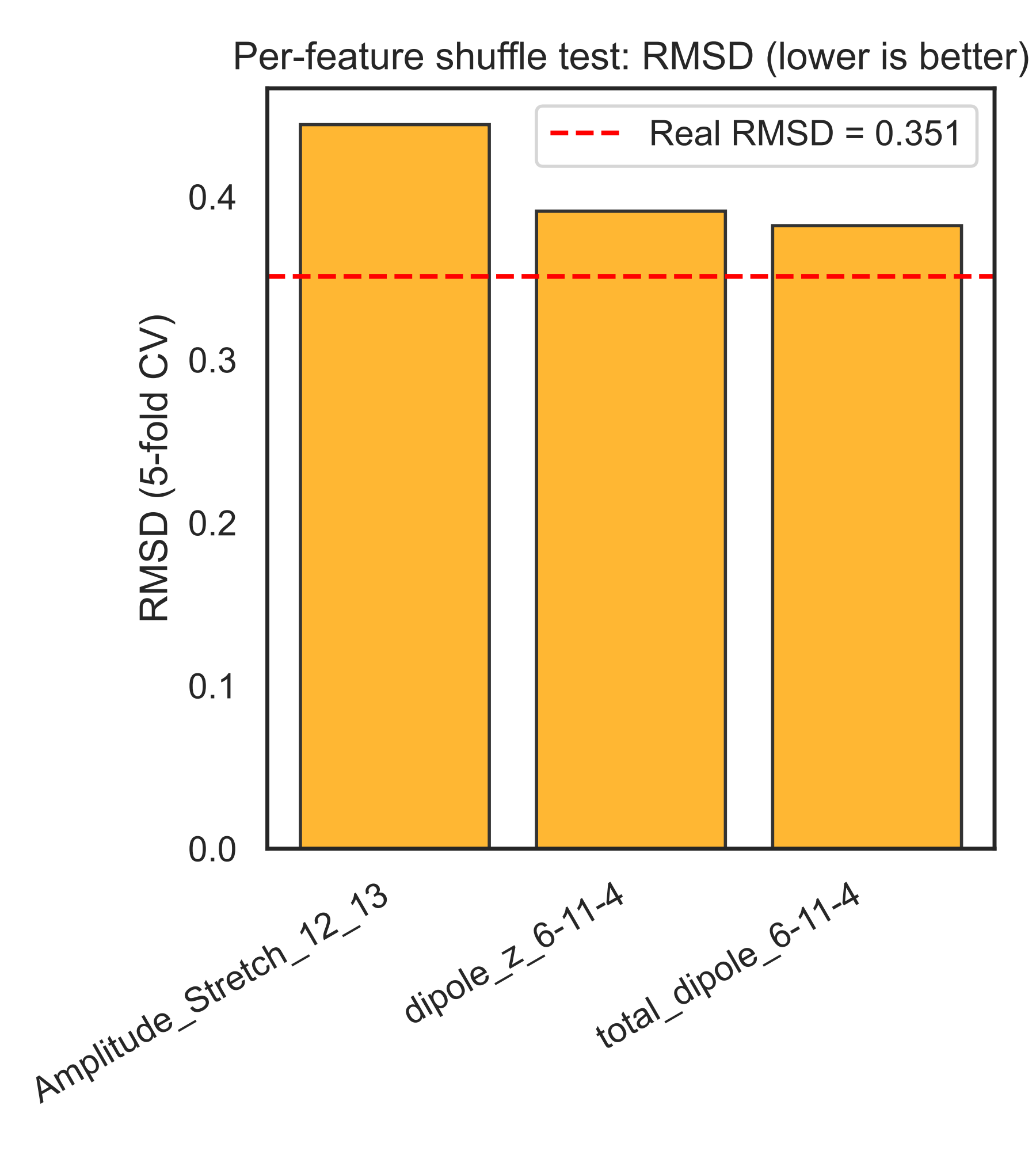
Estim	Std. E	t val	p.valu
-9.3	3.1	-2.9	0.01
10.	3.1	3.2	0.00
0.1	0.0	2.2	0.03
-0.1	0.0	-2.0	0.05

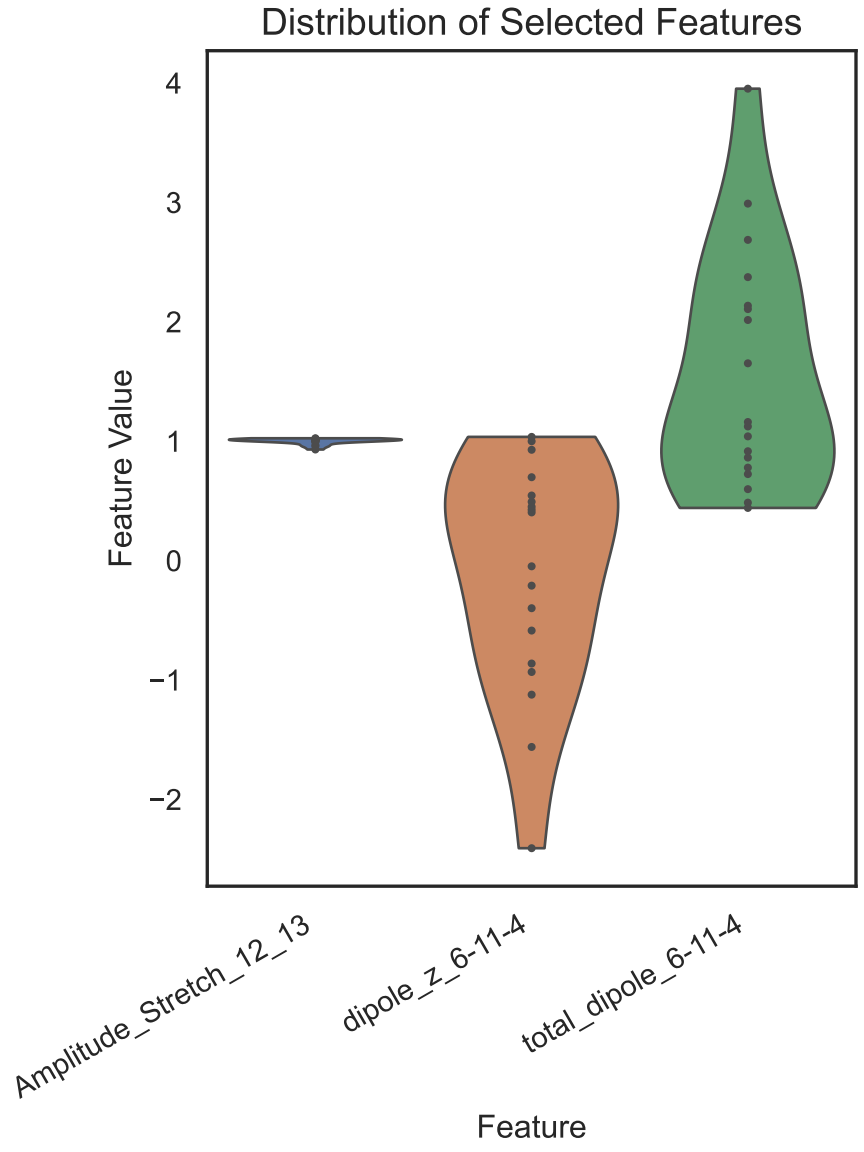
Left-out Predictions (none)

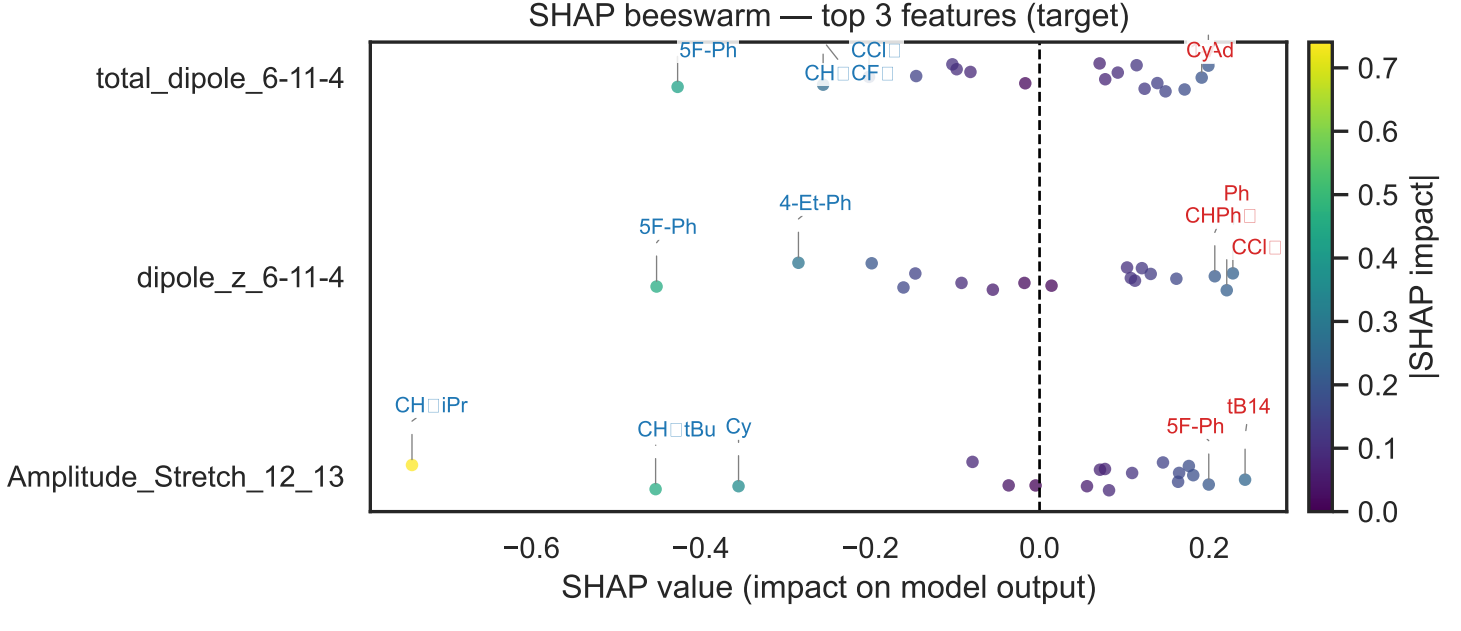

Validation (lower is better): MAE
Y-random MAE
Real MAE = 0.278
Mean Y-rand MAE = 0.373
One-hot MAE = 0.297
Global X-shuffle MAE = 0.362
Count
0
1
2
3
4
5
6
7
0.28
0.30
0.32
0.34
0.36
0.38
0.40
0.42
MAE (5-fold CV)

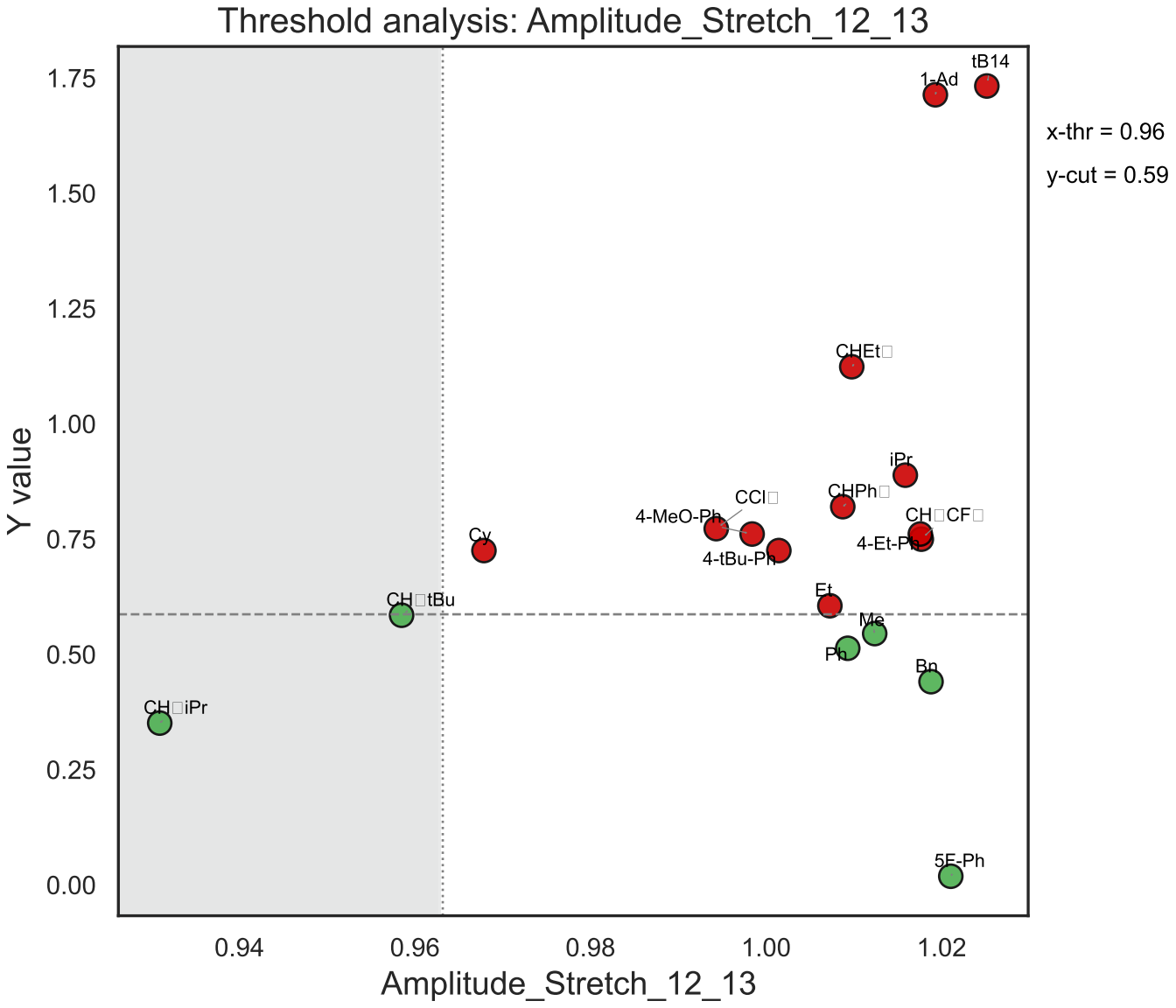

Validation (lower is better): RMSD
Y-random RMSD
Real RMSD = 0.351
Mean Y-rand RMSD = 0.496
One-hot RMSD = 0.434
Global X-shuffle RMSD = 0.498
Count
RMSD (5-fold CV)
0
1
2
3
4
5
6
0.35
0.40
0.45
0.50
0.55

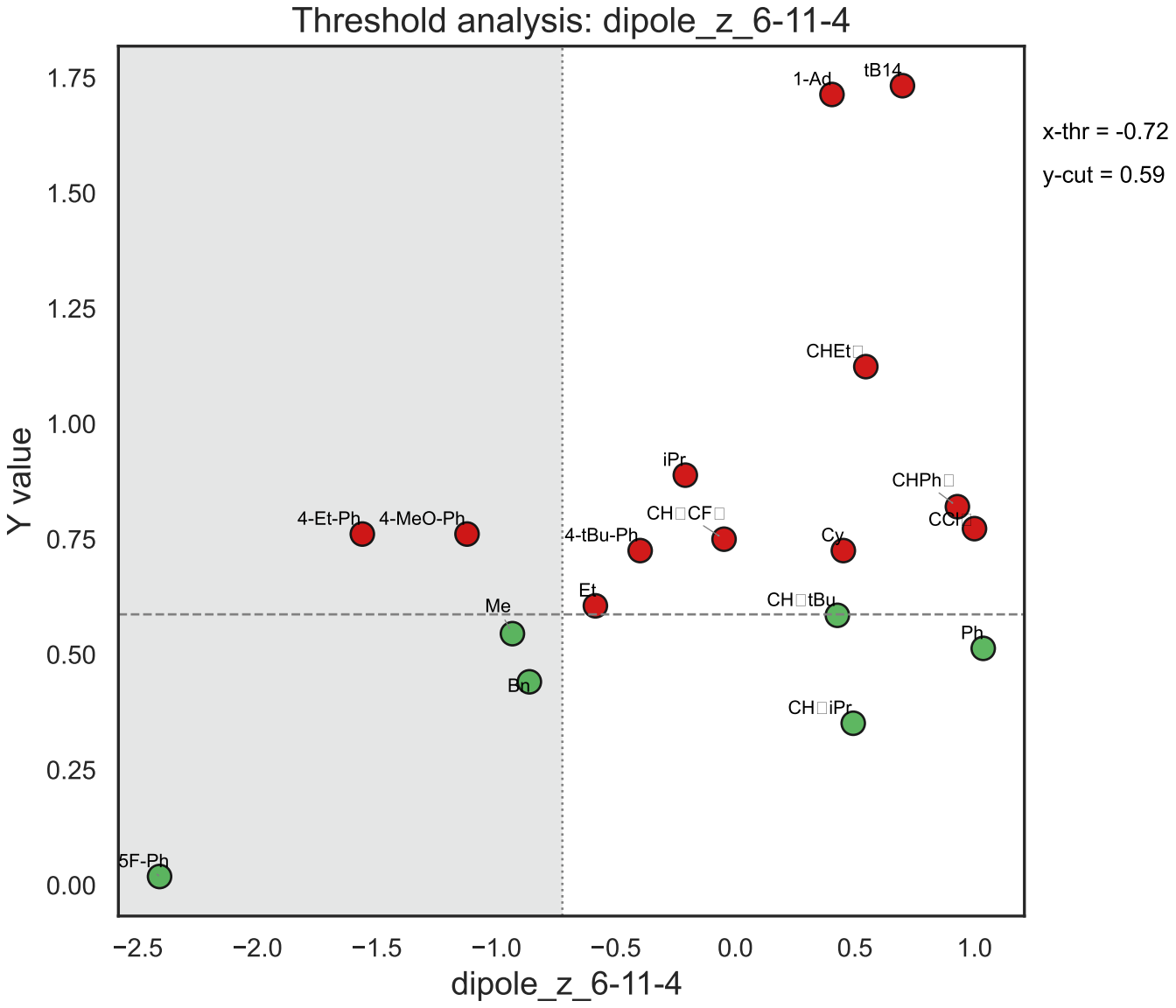

Per-feature shuffle test: MAE (lower is better)
Real MAE = 0.278
MAE (5-fold CV)
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Amplitude_Stretch_12_13
dipole_z_6-11-4
total_dipole_6-11-4

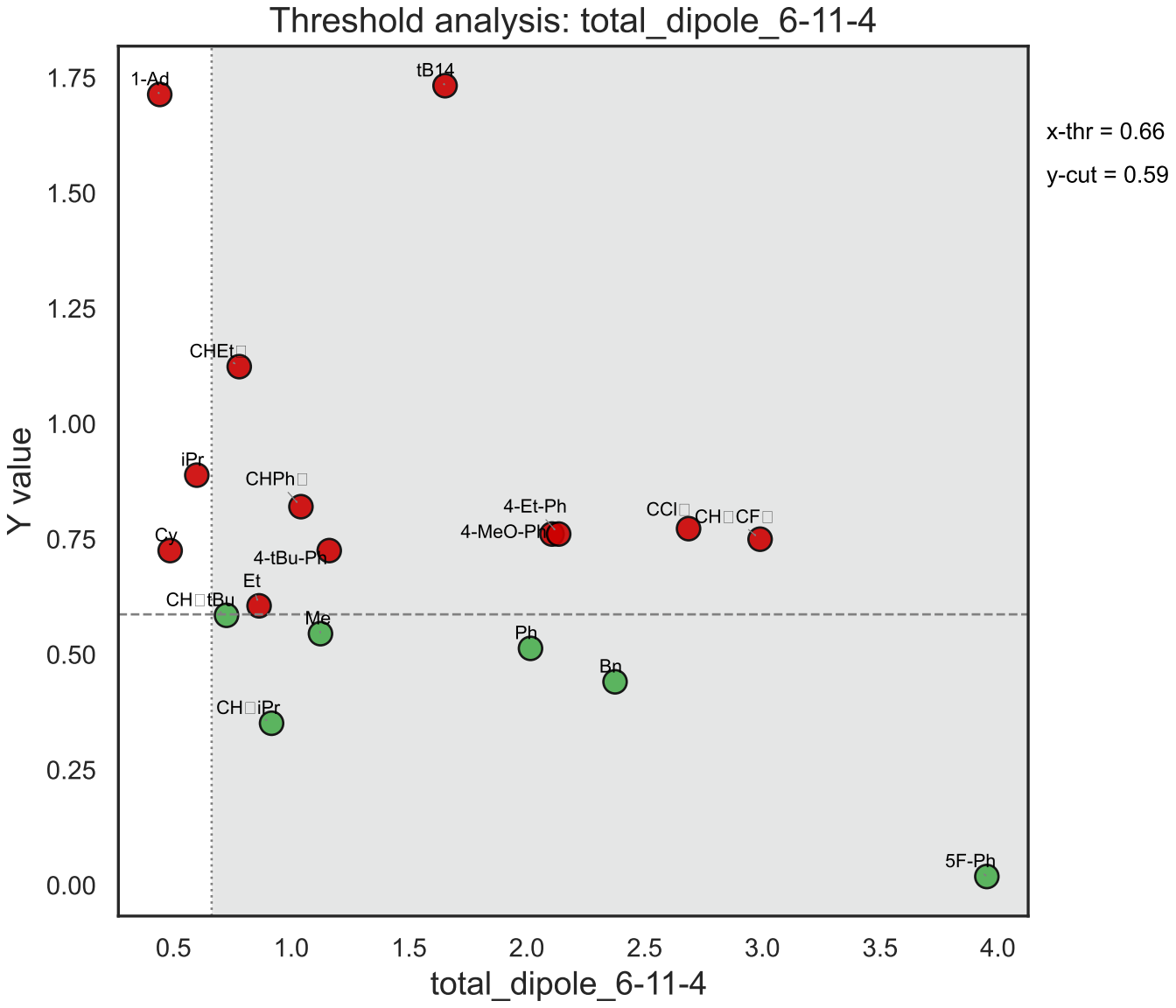

Per-feature shuffle test: RMSD (lower is better)
Real RMSD = 0.351
RMSD (5-fold CV)
0.0
0.1
0.2
0.3
0.4
Amplitude_Stretch_12_13
dipole_z_6-11-4
total_dipole_6-11-4


Distribution of Selected Features
Feature Value
4
3
2
1
0
−1
−2
Amplitude_Stretch_12_13
dipole_z_6-11-4
total_dipole_6-11-4
Feature


SHAP beeswarm — top 3 features (target)
total_dipole_6-11-4
dipole_z_6-11-4
Amplitude_Stretch_12_13
5F-Ph
CCl□
CH□CF□
Cy4d
4-Et-Ph
5F-Ph
Ph
CHPh□
CCl□
CH□iPr
CH□tBu
Cy
5F-Ph
tB14
−0.6
−0.4
−0.2
0.0
0.2
SHAP value (impact on model output)
|SHAP impact|
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7


Threshold analysis: Amplitude_Stretch_12_13
x-thr = 0.96
y-cut = 0.59
Y value
Amplitude_Stretch_12_13
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.94
0.96
0.98
1.00
1.02
tB14
1-Ad
CHEt□
iPr
CHPh□
CCl□
4-MeO-Ph
CH□CF□
Cy
4-Et-Ph
4-tBu-Ph
Et
CH□tBu
Me
Ph
Bn
CH□iPr
5F-Ph


Threshold analysis: dipole_z_6-11-4
x-thr = -0.72
y-cut = 0.59
Y value
dipole_z_6-11-4
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
−2.5
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1-Ad
tB14
CHEt□
iPr
CHPh□
CH□CF□
CCl
4-Et-Ph
4-MeO-Ph
4-tBu-Ph
Cy
Et
Me
CH□tBu
Ph
Bn
CH□iPr
5F-Ph


Threshold analysis: total_dipole_6-11-4
x-thr = 0.66
y-cut = 0.59
Y value
total_dipole_6-11-4
1-Ad
tB14
CHEt
iPr
CHPh
4-Et-Ph
4-MeO-Ph
CCl
CH
CF
Cy
4-tBu-Ph
Et
CH
tBu
Me
Ph
Bn
CH
iPr
5F-Ph
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0