Top 5 Models (ranked by R^2)

Overview

Rank	R^2 (train)	#Features	#Samples	Formula
1	0.632	2	15	Dist_1-2 + Dist_16-17
2	0.627	2	15	para + Dist_16-17
3	0.563	2	15	-17-18- + Dist_16-17
4	0.562	2	15	Dist_2-3 + Dist_16-17
5	0.552	2	15	-2-3- + Dist_16-17

Rank #1 | R^2=0.632 | Features=2 | Samples=15
Dist_1-2 + Dist_16-17

Coefficients

Estimate	Std. Error	t value	p value
0.7603	0.0345	22.03	4.488e-11
-0.07268	0.04484	-1.621	0.131
0.09985	0.04484	2.227	0.04586

VIF

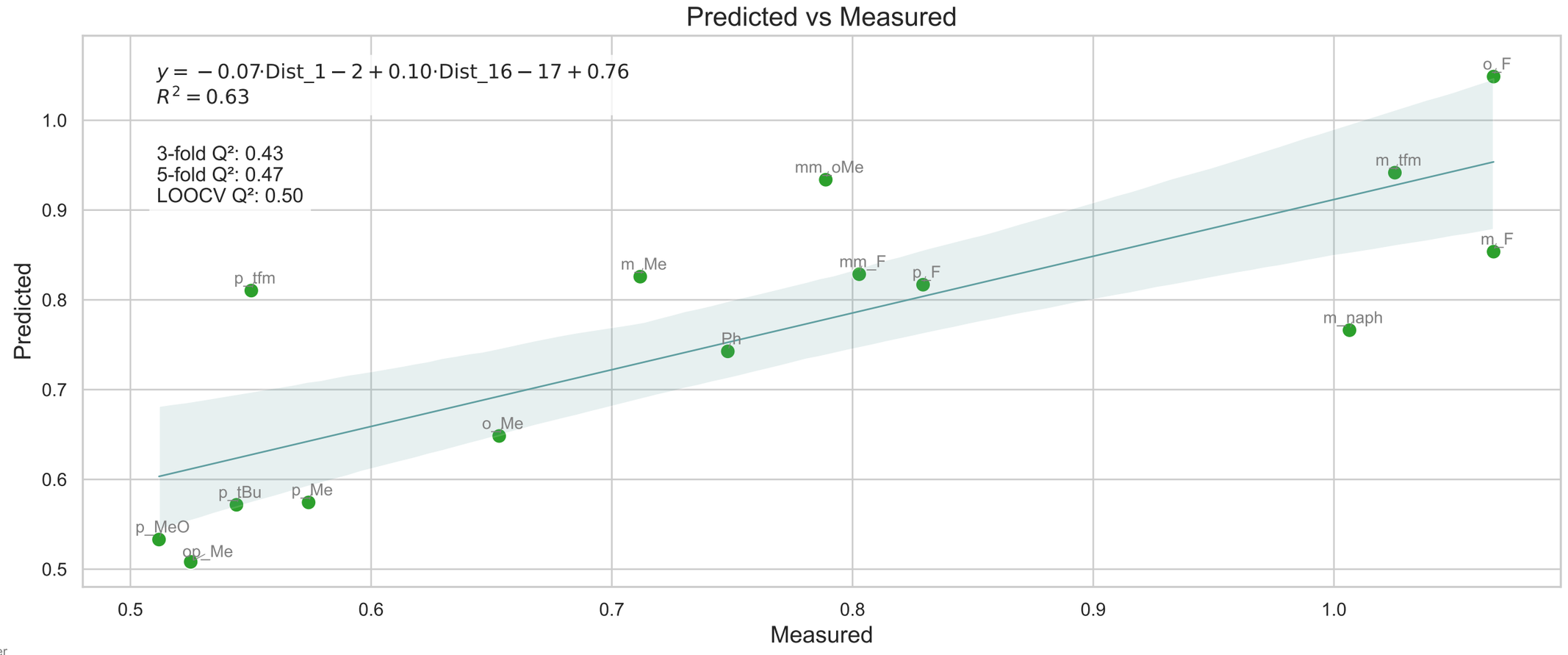
variable	VIF
Dist_1-2	1.689
Dist_16-17	1.689

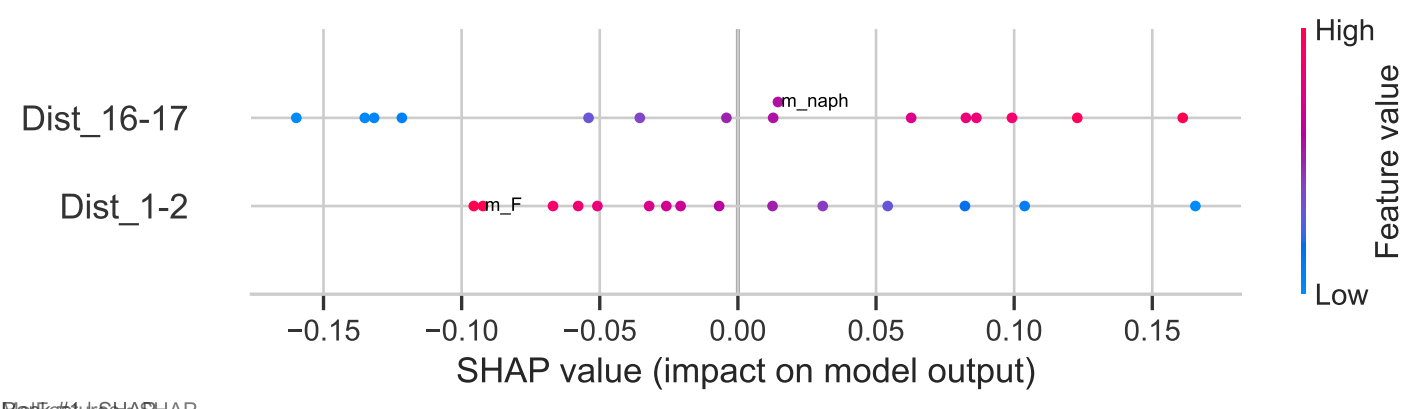
Cross-validation metrics

Q2_3_M	MAE	RMSD	Q2_5_M	MAE	RMSD	Q2_LOO	MAE	RMSD (LOO)
0.434	0.103	0.147	0.474	0.099	0.142	0.496	0.095	0.14

Model Summary

Formula: Dist_1-2 + Dist_16-17
Train R^2: 0.632
Q^2 (3/5/LOO): 0.434 / 0.474 / 0.496


Predicted vs Measured
$y = -0.07 \cdot \text{Dist_1-2} + 0.10 \cdot \text{Dist_16-17} + 0.76$
$R^2 = 0.63$
3-fold Q²: 0.43
5-fold Q²: 0.47
LOOCV Q²: 0.50
o_F
m_tfm
mm_oMe
m_F
m_Me
mm_F
p_F
p_tfm
m_naph
Ph
o_Me
p_tBu
p_Me
p_MeO
op_Me
Predicted
Measured
0.5
0.6
0.7
0.8
0.9
1.0


Dist_16-17
Dist_1-2
m_naph
m_F
High
Feature value
Low
−0.15
−0.10
−0.05
0.00
0.05
0.10
0.15
SHAP value (impact on model output)

Rank #1 | SHAP