

# Top 5 Models (ranked by R<sup>2</sup>)

## Overview

Rank	R <sup>2</sup> (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

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

Cross-validation metrics

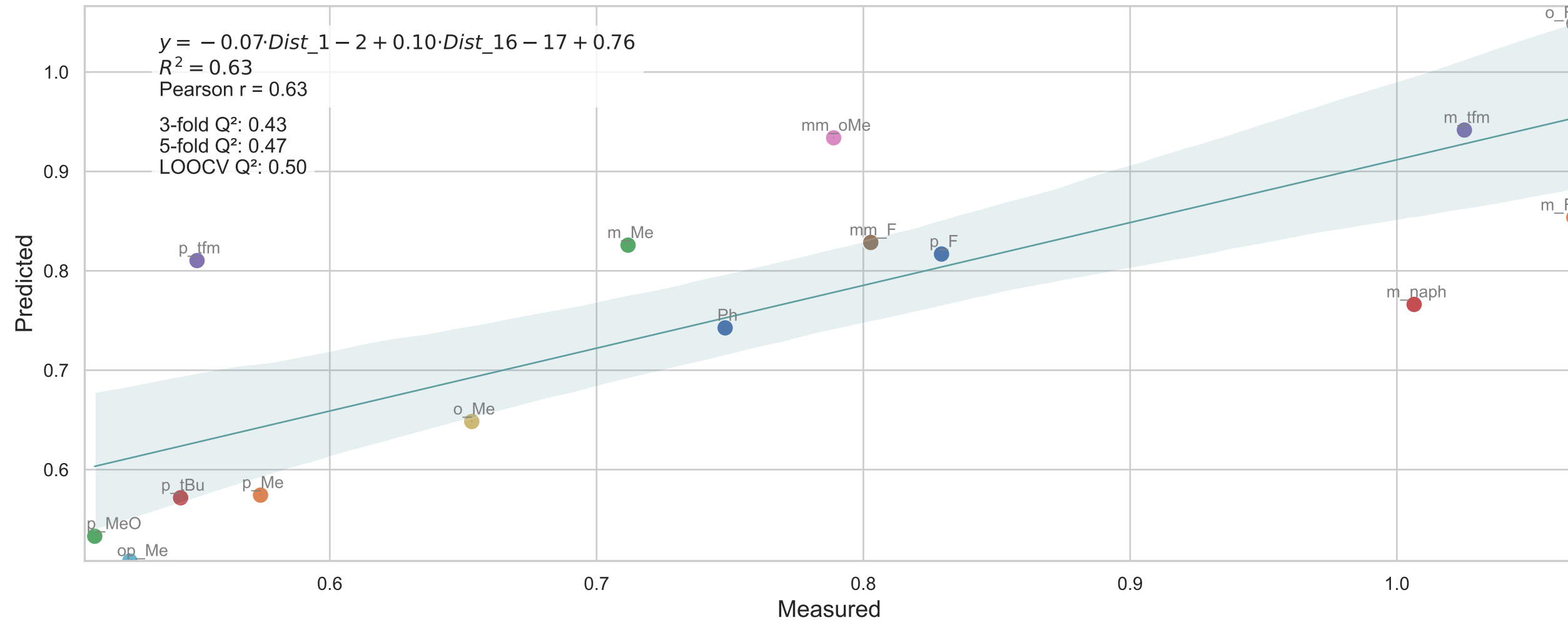
Model Summary

Formula: Dist\_1-2 + Dist\_16-17  
Train R²: 0.632  
Q² (3/5/LOO): 0.434 / 0.474 / 0.496

variable	VIF
Dist_1-2	1.689
Dist_16-17	1.689

Q²	3	MAE	MSD	5	MAE	MSD	LOO	MAE	MSD (LOO)
	0.434	0.103	0.147	0.474	0.099	0.142	0.496	0.095	0.14

# Predicted vs Measured



Dist\_16-17

Dist\_1-2

