Top 5 Models (ranked by R²)

Overview

Rank	R² (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 | R²=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

Cross-validation metrics

Model Summary

Formula: Dist_1-2 + Dist_16-17 Train R²: 0.632

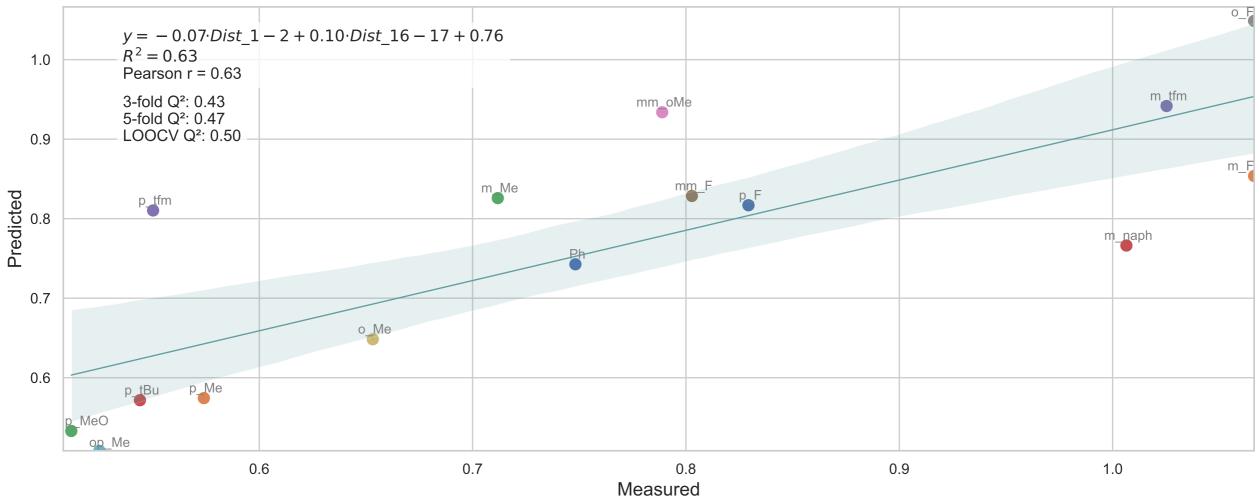
Q2 (3/5/LOO): 0.434 / 0.474 / 0.496

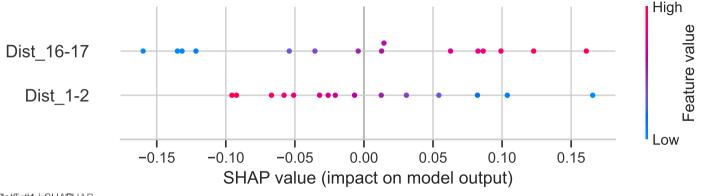
variable	VIF
Dist_1-2	1.689
Dist_16-17	1.689

 Q_2^2 MAR(MSQ_2^2 5 MAR(MSQ_2^2 LONGE RIMSD (LOO) 0.4340 1030 147 0.4740 0990 1420 496 0.095 0.14

p. 2 MolFeatures • Summary







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