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

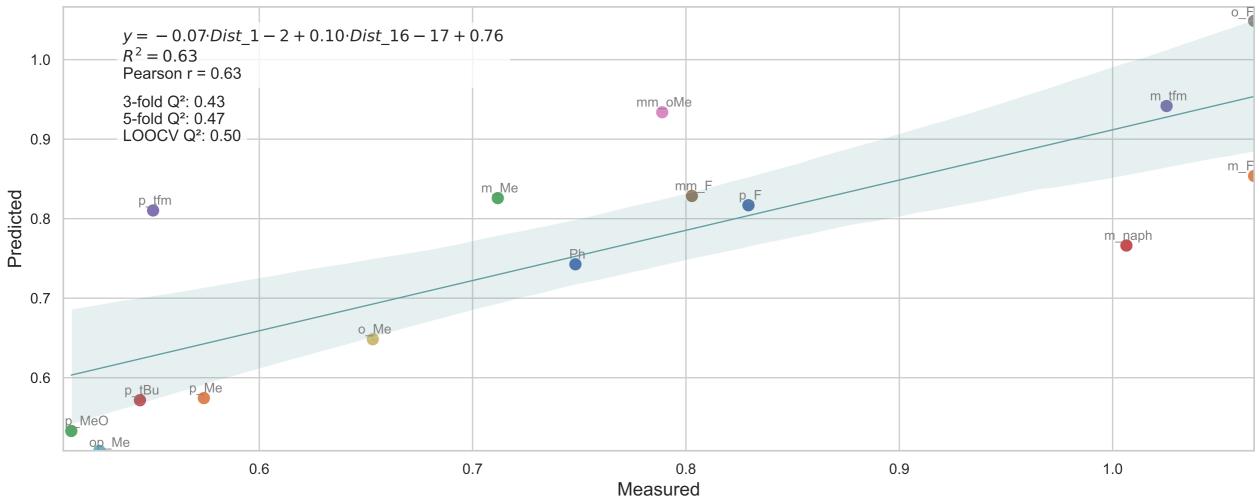
Q2 (3/5/LOO): 0.434 / 0.474 / 0.496

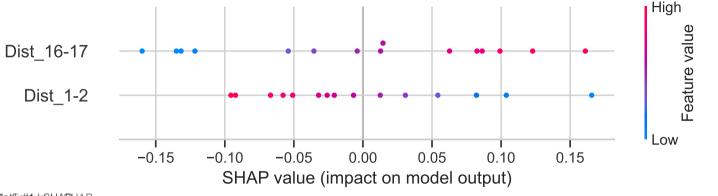
variable	VIF
Dist_1-2	1.689
Dist_16-17	1.689

 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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Rank #2 | R²=0.627 | Features=2 | Samples=15 para + Dist_16-17

Coefficients

Estimate	Std. Error	t value	p value
0.7603	0.03474	21.89	4.859e-11
0.0552	0.03541	1.559	0.145
0.157	0.03541	4.433	0.0008168

VIF

Cross-validation metrics

Model Summary

Formula: para + Dist_16-17 Train R²: 0.627

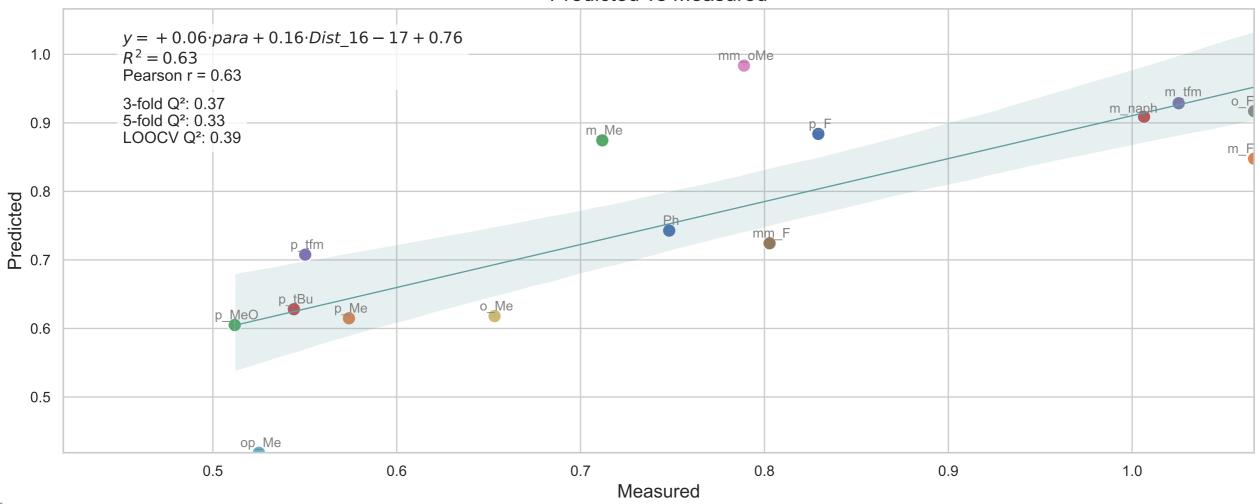
Q² (3/5/LOO): 0.374 / 0.326 / 0.391

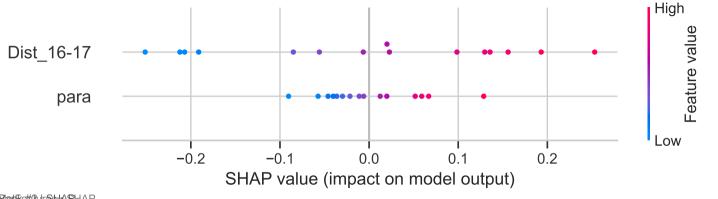
variable	VIF
para	1.039
Dist_16-17	1.039

 Q_2^2 MAR(MSQ_2^2 5 MAR(MSQ_2^2 LONGE RIMSD (LOO)

p. 5 MolFeatures • Summary







Rlantke#2ulr&HABHAP

Rank #3 | R²=0.563 | Features=2 | Samples=15 -17-18- + Dist_16-17

Coefficients

Estimate	Std. Error	t value	p value
0.7603	0.03761	20.21	1.232e-10
0.02102	0.03779	0.5562	0.5883
0.1442	0.03779	3.817	0.002452

VIF

Cross-validation metrics

Model Summary

Formula: -17-18- + Dist_16-17

Train R²: 0.563

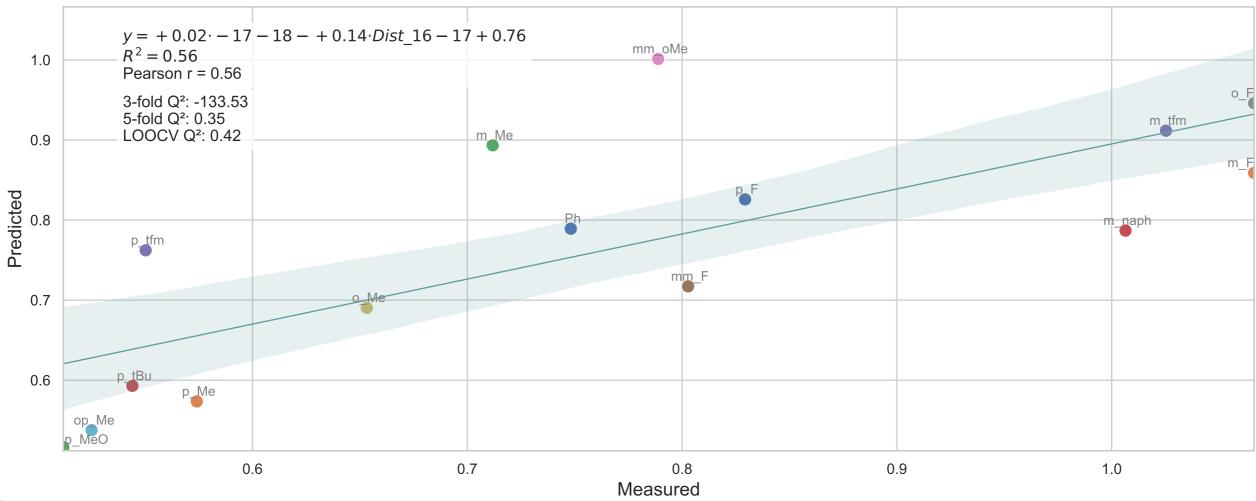
Q² (3/5/LOO): -133.530 / 0.345 / 0.417

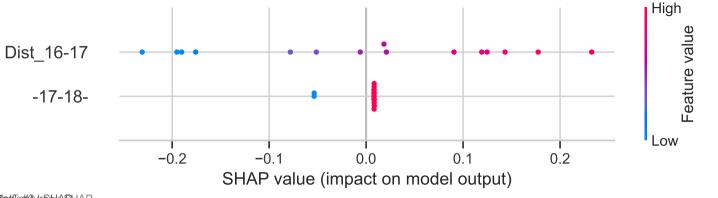
variable	VIF
-17-18-	1.009
Dist_16-17	1.009

Q2_3_MAR(//SQ2_5_MAR(//SQ2_LOMAE RMSD (LOO) -133.50 496 .148 0.3450 1250 .1590 .417 0.116 0.15

MolFeatures • Summary p. 8







Rlantke#3ulr&HABHAP p. 10

Rank #4 | R²=0.562 | Features=2 | Samples=15 Dist_2-3 + Dist_16-17

Coefficients

Estimate	Std. Error	t value	p value
0.7603	0.03765	20.19	1.248e-10
0.022	0.04134	0.5321	0.6044
0.1372	0.04134	3.319	0.006124

VIF

Cross-validation metrics

Model Summary

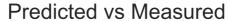
Formula: Dist_2-3 + Dist_16-17 Train R²: 0.562

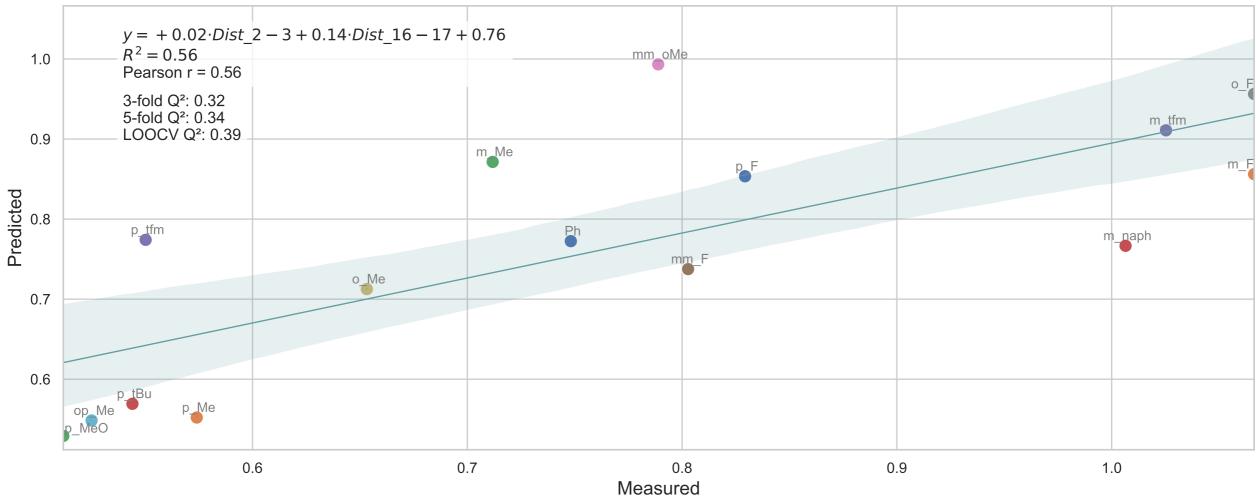
Q² (3/5/LOO): 0.315 / 0.341 / 0.391

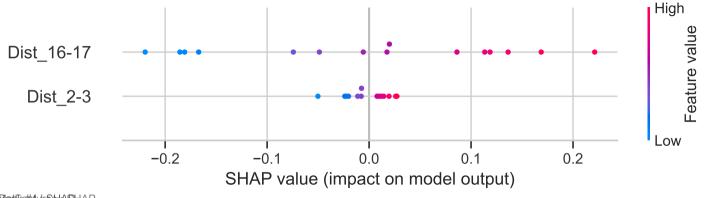
variable	VIF
Dist_2-3	1.205
Dist_16-17	1.205

 Q_2^2 MAR(MSQ_2^2 5 MAR(MSQ_2^2 LONGE RIMSD (LOO)

MolFeatures • Summary p. 11







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Rank #5 | R²=0.552 | Features=2 | Samples=15 -2-3- + Dist_16-17

Coefficients

Estimate	Std. Error	t value	p value
0.7603	0.03806	19.98	1.414e-10
0.005931	0.03979	0.1491	0.884
0.148	0.03979	3.72	0.002929

VIF

Cross-validation metrics

Model Summary

Formula: -2-3- + Dist_16-17 Train R²: 0.552

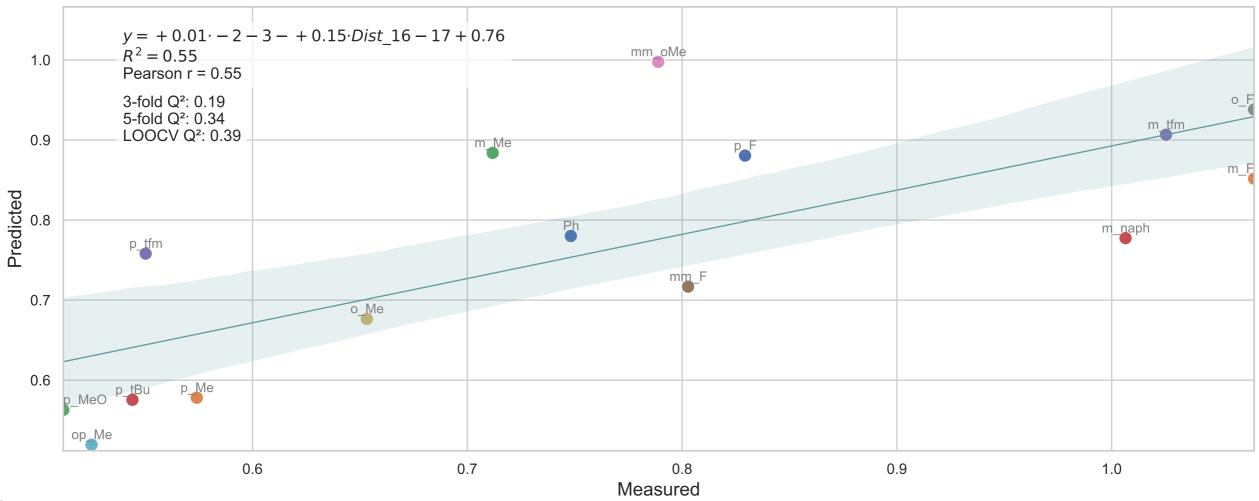
Q2 (3/5/LOO): 0.190 / 0.340 / 0.393

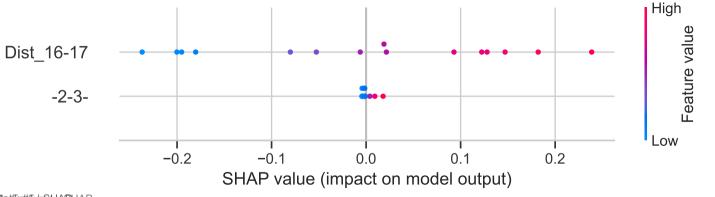
variable	VIF
-2-3-	1.093
Dist_16-17	1.093

 Q_2^2 MAR(MSQ_2^2 5 MAR(MSQ_2^2 LONGE RIMSD (LOO) 0.190 1420.175 0.340 127 0.160 393 0.123 0.153

MolFeatures • Summary p. 14







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