Top 5 Models (ranked by R²)

Overview

R² (train)	#Features	#Samples	Formula
0.695	3	18	total dinale 6-11-1
0.687	3	18	para_14_0 + loc_B5_11-27 + aniso_
0.63	3	18	total dimoles foodstade Stretch 24 25
0.627	3	18	reguency Stretch 12 13 +
0.627	3	18	Amplitude_Stretch_12_13 +
	0.695 0.687 0.63 0.627	0.695 3 0.687 3 0.63 3 0.627 3	0.695 3 18 0.687 3 18 0.63 3 18 0.627 3 18

dipole_z_6-11-4

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Rank #1 | R²=0.695 | Features=3 | Samples=18 cross_6_0 + para_14_0 + total_dipole_6-11-4

Coefficients

Estimate	Std. Error	t value	p value
0.7686	0.06014	12.78	4.152e-09
0.1797	0.06143	2.925	0.01108
-0.2431	0.0606	-4.011	0.001288
-0.2331	0.06189	-3.766	0.002086

VIF

Cross-validation metrics

Model Summary

Formula: cross_6_0 + para_14_0 + total_dipole_6-11-4

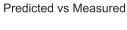
Train R²: 0.695

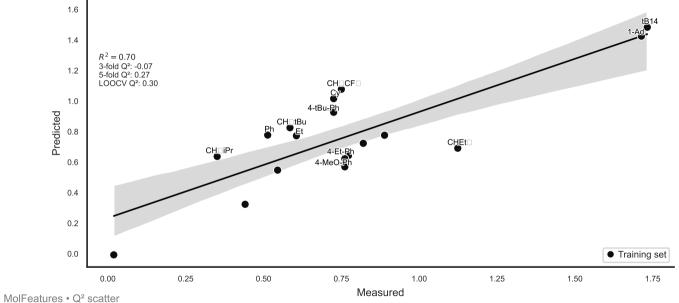
Q2 (3/5/LOO): -0.073 / 0.267 / 0.300

variable	VIF
cross_6_0	1.043
para_14_0	1.015
total_dipole_6-11-4	1.059

Q2 3 MARWSQ2 5 MARWSQ2 LV04 FRMSD (LOO) -0.070.3130.4050.260.2860.349 0.3 0.28 0.341

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 $y = +0.18 \cdot \text{cross} = 6.0 - 0.24 \cdot \text{para} = 14.0 - 0.23 \cdot \text{total_dipole} = 6 - 11 - 4 + 0.77$