Top 5 Models (ranked by R²)

Overview

Rank	R² (train)	#Features	#Samples	Formula
1	0.695	3	18	cross_6_0 + para_14_0 + total_dipole_6-11-4
2	0.687	3	18	para_14_0 + loc_B5_11-27 + aniso
3	0.63	3	18	para_14_0 + Amplitude_Stretch_12_13 + total_dipole_6-11-4
4	0.627	3	18	para_14_0 + Amplitude_Stretch_24_25 + Frequency_Stretch_12_13
5	0.627	3	18	Frequency_Stretch_12_13 + Amplitude_Stretch_12_13 + dipole_z_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

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

Cross-validation metrics

Q2_3_FARM	RMSD	Q2_5_FARM	RMSD	Q2_LOO	RMSD	MAE	RMSD	RMSD (LOO)
-0.072	0.313	0.405	0.260	0.286	0.349	0.3	0.28	0.341

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

Predicted vs Measured

$R^2 = 0.70$
3-fold Q²: -0.07
5-fold Q²: 0.27
LOOCV Q²: 0.30

Labels on plot: tB14, 1-Ad, CH□CF□, Cy, 4-tBu-Ph, CH□tBu, Et, Ph, CH□iPr, 4-Et-Ph, 4-MeO-Ph, CHEt□

● Training set

$y = +0.18 \cdot cross\_6\_0 - 0.24 \cdot para\_14\_0 - 0.23 \cdot total\_dipole\_6 - 11 - 4 + 0.77$