

Top 5 Models (ranked by R²)

Overview

Rank	R² (train)	#Features	#Samples	Formula
1	0.627	3	18	Frequency Stretch 12 13 + Amplitude Stretch 12 13 +
2	0.61	3	18	Amplitude Stretch 24 25 + Amplitude Stretch 12 13 +
3	0.594	3	18	Amplitude Stretch 12 13 + Amplitude z 6-11-4 + nb6 - nbm 14
4	0.58	3	18	dipole z 6-11-4 + Amplitude Stretch 12 13 +
5	0.555	3	18	dipole_z_6-11-4 + iso

Coefficients

Estimate	Std. Error	t value	p value
-503.4	193.2	-2.605	0.02076
0.1275	0.04971	2.564	0.02248
10.21	2.946	3.467	0.003778
0.2303	0.07632	3.017	0.009232

VIF

Cross-validation metrics

Model Summary

Formula: Frequency_Stretch_12_13 + Amplitude_Stretch_12_13 + dipole_z_6-11-4
Train R²: 0.627
Q² (3/5/LOO): 0.198 / 0.246 / 0.304

variable	VIF
Frequency_Stretch_12_13	1.121
Amplitude_Stretch_12_13	1.16
dipole_z_6-11-4	1.164

Q2	3_F	5_F	10_F	15_F	20_F	25_F	30_F	35_F	40_F	45_F	50_F	55_F	60_F	65_F	70_F	75_F	80_F	85_F	90_F	95_F	100_F	LOO	
0.198	0.287	0.362	0.424	0.473	0.512	0.542	0.564	0.579	0.588	0.592	0.594	0.595	0.596	0.597	0.598	0.599	0.6	0.601	0.602	0.603	0.604	0.605	0.34

Predicted vs Measured

