

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -2.92

Global applicability domain: Inside

Local applicability domain index: 5.96e-01

Confidence level: 6.31e-01

Nearest Neighbors from the Training Set

Image not found

D-Glucose

Measured: -3.24

Predicted: -2.92

Image not found

D-Glucitol

Measured: -2.20

Predicted: -2.36

Image not found

D-Mannitol

Measured: -2.20

Predicted: -2.36

Image not found

D-Galactitol

Measured: -2.20

Predicted: -2.36

Image not found

D-Glucuronic acid

Measured: -2.57

Predicted: -2.55