

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 177 °C

Global applicability domain: Inside

Local applicability domain index: 4.01e-01

Confidence level: 9.08e-01

Nearest Neighbors from the Training Set

Image not found

Imazethapyr

Measured: 171

Predicted: 177

Image not found

Imazapyr

Measured: 171

Predicted: 189

Image not found

Imazamox

Measured: 166

Predicted: 177

Image not found

Nalidixic acid

Measured: 230

Predicted: 191

Image not found

Metoclopramide

Measured: 147

Predicted: 147