

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: 190 °C

Global applicability domain: Inside

Local applicability domain index: 6.93e-01

Confidence level: 6.04e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Atrazine

Measured: 173

Predicted: 187

[Image not found](#)

Terbutylazine

Measured: 178

Predicted: 188

[Image not found](#)

Propazine

Measured: 213

Predicted: 197

[Image not found](#)

Simazine

Measured: 226

Predicted: 206

[Image not found](#)

Cyprazine

Measured: 167

Predicted: 179