

Model Performance

Model	Data
-------	------

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: 89.4 °C

Global applicability domain: Inside

Local applicability domain index: 6.47e-01

Confidence level: 6.89e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Desmetryn

Measured: 85.0

Predicted: 89.4

[Image not found](#)

Ametryn

Measured: 88.0

Predicted: 92.2

[Image not found](#)

Terbutryn

Measured: 104

Predicted: 96.7

[Image not found](#)

Prometryn

Measured: 119

Predicted: 102

[Image not found](#)

Dimethametryn

Measured: 65.0

Predicted: 89.9