

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.73e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.64e-01

Confidence level: 4.78e-01

Nearest Neighbors from the Training Set

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Malaoxon

Measured: 2.39e-02

Predicted: 6.73e-02

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Phosphamidon

Measured: 3.34

Predicted: 1.76

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Cyanthoate

Measured: 2.38e-01

Predicted: 3.86e-01

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Endothion

Measured: 5.35

Predicted: 2.95

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Dicrotophos

Measured: 4.22

Predicted: 2.95