

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.49

Global applicability domain: Inside

Local applicability domain index: 2.84e-01

Confidence level: 5.63e-01

Nearest Neighbors from the Training Set

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Malaoxon

Measured: 1.12

Predicted: 1.49

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Malathion

Measured: 33.1

Predicted: 21.9

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Pyridaphenthion

Measured: 4.68

Predicted: 10.1

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Methodathion

Measured: 5.50

Predicted: 4.97

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Cycloheximide

Measured: 2.82

Predicted: 2.70