

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: 2.82

Global applicability domain: Inside

Local applicability domain index: 3.89e-01

Confidence level: 8.60e-01

Nearest Neighbors from the Training Set

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Carbendazim

Measured: 2.51

Predicted: 2.38

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Bromacil

Measured: 3.24

Predicted: 2.87

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Cycloheximide

Measured: 2.82

Predicted: 2.70

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Dimethoate

Measured: 1.58

Predicted: 1.88

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Methidathion

Measured: 5.50

Predicted: 4.97