

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: 2.87

Global applicability domain: Inside

Local applicability domain index: 5.28e-01

Confidence level: 8.65e-01

Nearest Neighbors from the Training Set

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Bromacil

Measured: 3.24

Predicted: 2.87

Image not found

Dimethoate

Measured: 1.58

Predicted: 1.88

Image not found

2-Isopropyl-6-methyl-4-pyrimidone

Measured: 1.82

Predicted: 2.23

Image not found

Carbendazim

Measured: 2.51

Predicted: 2.38

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Paraldehyde

Measured: 3.02

Predicted: 2.77