

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.17

Global applicability domain: Inside

Local applicability domain index: 5.60e-01

Confidence level: 7.14e-01

Nearest Neighbors from the Training Set

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Ametryn

Measured: 2.98

Predicted: 3.17

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Prometryn

Measured: 3.51

Predicted: 3.87

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Terbutryn

Measured: 3.74

Predicted: 3.88

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Desmetryn

Measured: 2.38

Predicted: 2.78

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Terbutylazine

Measured: 3.21

Predicted: 3.57