

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: 6.37e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.72e-01

Confidence level: 4.07e-01

Nearest Neighbors from the Training Set

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Methabenzthiazuron

Measured: 2.67e-04

Predicted: 1.49e-03

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Guanidine, (2-benzothiazolyl)-

Measured: 3.62e-03

Predicted: 2.64e-03

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Benzthiazuron

Measured: 5.79e-05

Predicted: 1.30e-03

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S-[2-Oxo-2-(phenylamino)ethyl]
thiocarbamate

Measured: 4.76e-02

Predicted: 6.62e-02

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Lenacil

Measured: 2.56e-05

Predicted: 1.78e-04