

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: 2.36e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.13e-01

Confidence level: 5.42e-01

Nearest Neighbors from the Training Set

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1H-Pyridine-3-carbonitrile, 6-chloro-2-hydroxy-4-oxo-

Measured: 5.86e-02

Predicted: 7.62e-02

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(Carbamothioylsulfanyl)acetic acid

Measured: 1.79e-01

Predicted: 1.42e-01

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1-(Hydroxymethyl)-5,5-dimethylhydantoin

Measured: 6.32

Predicted: 2.12

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2-Amino-5,6-dihydro-4H-1,3-thiazine-4-carboxylic acid

Measured: 1.87e-01

Predicted: 1.97e-01

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L-Tryptophan

Measured: 6.56e-02

Predicted: 4.25e-02