

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: 2.55e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.62e-01

Confidence level: 5.13e-01

Nearest Neighbors from the Training Set

[Image not found](#)

alpha-Santonin

Measured: 8.12e-04

Predicted: 5.45e-04

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N-(1-Naphthyl)ethylenediamine

Measured: 1.07e-02

Predicted: 9.11e-02

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Oxabentrinil

Measured: 8.61e-05

Predicted: 1.53e-03

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1,10-Phenanthroline

Measured: 1.49e-02

Predicted: 5.60e-03

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1-Naphthylamine

Measured: 1.19e-02

Predicted: 3.04e-02