

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: 5.70e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.28e-01

Confidence level: 6.74e-01

Nearest Neighbors from the Training Set

[Image not found](#)

L-Alanine, N-
[(ethylthio)thioxomethyl]-

Measured: 7.98e-02

Predicted: 6.94e-02

[Image not found](#)

L-Alanine, N-
[(ethylthio)thioxomethyl]-

Measured: 7.98e-02

Predicted: 6.94e-02