

Quinic acid
86-68-0 | DTXSID70323339

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: 6.04e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.72e-01

Confidence level: 6.75e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Phenylalanine

Measured: 1.34e-01

Predicted: 3.30e-01

[Image not found](#)

Phenylalanine

Measured: 1.34e-01

Predicted: 3.30e-01

[Image not found](#)

D-Phenylalanine

Measured: 1.34e-01

Predicted: 3.30e-01

[Image not found](#)

I-Tryptophan

Measured: 6.56e-02

Predicted: 4.25e-02