

Model Performance

Model	Data
-------	------

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: 1.66e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.73e-01

Confidence level: 7.13e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Methacrifos

Measured: 1.67e-03

Predicted: 2.32e-03

[Image not found](#)

Phosphonothioic dihydrazide, P-phenyl-

Measured: 3.76e-02

Predicted: 1.83e-02

[Image not found](#)

Thionazin

Measured: 4.59e-03

Predicted: 1.69e-03

[Image not found](#)

Cyanophos

Measured: 1.89e-04

Predicted: 1.66e-03

[Image not found](#)

Sulfotepp

Measured: 9.31e-05

Predicted: 8.30e-05