

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: 1.14e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.67e-01

Confidence level: 5.08e-01

Nearest Neighbors from the Training Set

[Image not found](#)

alpha-Santonin

Measured: 8.12e-04

Predicted: 5.45e-04

[Image not found](#)

Oxabentrinil

Measured: 8.61e-05

Predicted: 1.53e-03

[Image not found](#)

.alpha.-

[(Cyanomethoxy)imino]benzeneacetonitrile

Measured: 5.13e-04

Predicted: 5.60e-02

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Sparteine

Measured: 1.30e-02

Predicted: 8.29e-03