

Microcystin LR

101043-37-2 | DTXSID3031654

Model Performance

Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
|------|------|------|------|------|------|
| 0.84 | 0.55 | 0.85 | 0.53 | 0.83 | 0.64 |

Model Results

Predicted value: 6.41e-01

Global applicability domain: Outside

Local applicability domain index: 7.12e-02

Confidence level: 6.60e-01

Nearest Neighbors from the Training Set

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Docusate sodium

Measured: 0.97

Predicted: 9.52e-01

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N,N,N',N',N'',N''-

Hexakis(methoxymethyl)-
1,3,5-triazine-2,4,6-triamine

Measured: 0.54

Predicted: 6.53e-01

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Tris(2-butoxyethyl)
phosphate

Measured: 0.76

Predicted: 8.01e-01

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7,7'-(Carbonyldiimino)bis[4-
hydroxy-2-
naphthalenesulfonic acid]

Measured: 0.26

Predicted: 4.30e-01

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Bis(2-ethylhexyl) phosphate

Measured: 0.64

Predicted: 7.46e-01