

Microcystin LR

101043-37-2 | DTXSID3031654

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.18 days

Global applicability domain: Outside

Local applicability domain index: 1.57e-01

Confidence level: 9.16e-01

Nearest Neighbors from the Training Set

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1-Methyl-2-propylbenzene

Measured: 3.00

Predicted: 3.17

Image not found

3-Ethyltoluene

Measured: 3.00

Predicted: 3.26

Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: 4.00

Predicted: 3.89

Image not found

2-Ethyl-p-xylene

Measured: 3.00

Predicted: 3.70

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1H-Indene, 2-methyl-

Measured: 3.00

Predicted: 2.48