

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 4.49

Global applicability domain: Outside

Local applicability domain index: 4.73e-02

Confidence level: 5.98e-01

Nearest Neighbors from the Training Set

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Fluvalinate

Measured: 5.71

Predicted: 5.47

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tau-Fluvalinate

Measured: 5.71

Predicted: 5.47

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Triflusulfuron-methyl

Measured: 1.84

Predicted: 1.70

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Hydramethylnon

Measured: 5.86

Predicted: 5.63

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Nonylphenyl diphenyl
phosphate, mixed isomers

Measured: 4.06

Predicted: 4.74

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Flucythrinate

Measured: 5.00

Predicted: 5.19