

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: -9.69 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.49e-02

Confidence level: 8.88e-01

Nearest Neighbors from the Training Set

[Image not found](#)

alpha-Humulene

Measured: -9.54

Predicted: N/A

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beta-Caryophyllene

Measured: -9.70

Predicted: N/A

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Myrcene

Measured: -9.67

Predicted: -9.69

[Image not found](#)

Ocimene (E)

Measured: -9.60

Predicted: -9.62

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beta-Ocimene

Measured: -9.60

Predicted: -9.62