

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.39e-04 mmHg

Global applicability domain: Outside

Local applicability domain index: 7.60e-01

Confidence level: 5.65e-01

Nearest Neighbors from the Training Set

Image not found

Oxazole

Measured: 9.75e-05

Predicted: 99.5

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Hymexazol

Measured: 3.20e-04

Predicted: 1.02e-02

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cis-Mevinphos

Measured: 6.38e-04

Predicted: 1.88e-04

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Tricosane

Measured: 1.70e-05

Predicted: 1.26e-05

Image not found

Terbutryn

Measured: 3.00e-04

Predicted: 1.66e-06