

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 86.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.49e-01

Confidence level: 5.98e-01

Nearest Neighbors from the Training Set

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Imazapyr

Measured: 100

Predicted: 65.8

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Imazethapyr

Measured: 7.08

Predicted: 77.7

[Image not found](#)

Ethyl phthalyl ethyl glycolate

Measured: 347

Predicted: 319

[Image not found](#)

Phenazopyridine

Measured: 209

Predicted: 268

[Image not found](#)

Ancymidol

Measured: 120

Predicted: 112