

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: 3180 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.41e-01

Confidence level: 4.52e-01

Nearest Neighbors from the Training Set

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Bifenox

Measured: 10000

Predicted: 3180

[Image not found](#)

Niclosamide

Measured: 2240

Predicted: 4670

[Image not found](#)

Acifluorfen-sodium

Measured: 112

Predicted: 1480

[Image not found](#)

Clofentezine

Measured: 45700

Predicted: 6520

[Image not found](#)

Naptalam-sodium

Measured: 2190

Predicted: 1690