

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.29

Global applicability domain: Inside

Local applicability domain index: 5.42e-01

Confidence level: 4.30e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Indole-3-butyric acid

Measured: 2.30

Predicted: 3.40e-01

[Image not found](#)

Tacrine

Measured: 2.71

Predicted: 2.60

[Image not found](#)

Quinmerac

Measured: 0.78

Predicted: 2.50