

Model Performance

Model	Data
-------	------

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: 282 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.28e-01

Confidence level: 8.42e-01

Nearest Neighbors from the Training Set

Image not found

Atraton

Measured: 437

Predicted: 282

Image not found

Propazine

Measured: 251

Predicted: 280

Image not found

Cyanazine

Measured: 191

Predicted: 253

Image not found

Terbutylazine

Measured: 209

Predicted: 255

Image not found

Prometon

Measured: 398

Predicted: 339