Data Loading

```
!pip install 'pycaret[full]'
```

```
from google.colab import drive
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error, mean_absolute_error,accuracy_score, r2_score
from pycaret.regression import*
from google.colab import files

drive.mount('/content/drive')

dfVanco = pd.read_excel('/content/drive/MyDrive/data/original_dataset.xlsx')
```

```
Mounted at /content/drive
```

```
!pip install shap
```

```
import warnings
import numba

warnings.filterwarnings("ignore", category=numba.NumbaDeprecationWarning)

import pandas as pd
import numpy as np
import shap
import math
from pycaret.regression import*
from math import isnan
from IPython.display import display

pd.set_option('display.max_columns', None)
pd.set_option('display.max_rows', None)
```

```
print(dfVanco)
```

19	0	0	116.239316	5.027179	42.00	0.100879	6.869641
20	0	0	71.759259	3.142361	35.00	0.100879	6.869641
21	0	0	78.282828	3.414394	35.00	0.063960	10.834865
22	0	1	55.645161	2.482403	37.80	0.050585	13.699582
23	0	0	52.888889	2.358467	35.70	0.048298	14.348486
24	0	0	60.763889	2.743854	49.00	0.054834	12.638138
25	0	0	96.848291	4.185574	34.30	0.084784	8.173704
26	0	0	36.612166	1.676727	35.00	0.034788	19.920606
27	0	0	84.785354	3.685549	35.00	0.074772	9.268195
28	0	0	93.423423	4.039757	33.60	0.081941	8.457259
29	0	0	56.496063	2.544886	44.10	0.081941	8.457259
30	0	0	133.807588	5.729776	35.00	0.115460	6.002063
31	0	0	72.629630	3.187656	37.10	0.064683	10.713856
32	0	0	36.213992	1.675123	38.50	0.034458	20.111666
33	0	0	69.917081	3.101542	43.40	0.062431	11.100223
34	0	0	74.275114	3.249372	35.49	0.066048	10.492314
35	0	0	55.851064	2.508989	42.00	0.050756	13.653455
36	0	0	66.872428	2.968580	42.00	0.050756	13.653455
37	0	0	94.387755	4.070969	31.50	0.082742	8.375449
38	0	1	70.386905	3.064134	30.10	0.062821	11.031320
39	0	1	67.777778	3.006333	42.00	0.060656	11.425169
40	0	0	94.256757	4.116507	43.40	0.082633	8.386469
41	0	0	83.040936	3.654807	44.80	0.073324	9.451206
42	0	0	69.439891	3.051643	36.40	0.062035	11.171093
43	0	0	92.953216	4.074149	46.20	0.081551	8.497732

Pre-processing

```
# This code is rounding certain columns to a specified decimal place using the round() function in pan

dfVanco['BMI'] = round(dfVanco['BMI'], 1)
dfVanco['WBC'] = round(dfVanco['WBC'], 1)
dfVanco['Crcl'] = round(dfVanco['Crcl'], 1)
dfVanco['Clvanco'] = round(dfVanco['Clvanco'], 1)
dfVanco['Half_life'] = round(dfVanco['Half_life'], 1)
dfVanco['Ke'] = round(dfVanco['Ke'], 3)
```

```
dfVanco[:3]
```

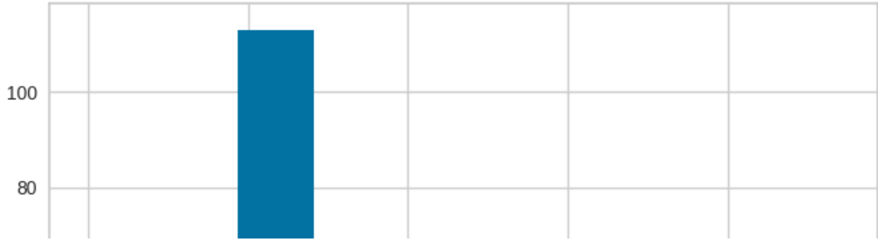
	Case_no	Gender	Age	Weight	Height	BMI	Initial VCM_daily_dose	ICU	WBC	Hb	PLT	CRP	eGFR	BUN	SCr	Albumin	TP	UA	NSAIDs
0	43	0	79	69.0	158.0	27.6	1000	0	5.9	7.3	134	43.23	90	35.6	0.45	2.5	5.6	4.5	0
1	89	0	74	72.0	163.0	27.1	1000	0	9.5	11.4	286	72.22	58	11.4	0.95	3.5	6.4	3.5	0

```
dfVanco=dfVanco.drop(columns='Case_no')
dfVanco[:3]
```

	Gender	Age	Weight	Height	BMI	Initial VCM_daily_dose	ICU	WBC	Hb	PLT	CRP	eGFR	BUN	SCr	Albumin	TP	UA	NSAIDs	ARB	ACE
0	0	79	69.0	158.0	27.6	1000	0	5.9	7.3	134	43.23	90	35.6	0.45	2.5	5.6	4.5	0	0	
1	0	74	72.0	163.0	27.1	1000	0	9.5	11.4	286	72.22	58	11.4	0.95	3.5	6.4	3.5	0	0	

```
dfVanco['Initial VCM_daily_dose'].plot.hist()
dfVanco['Initial VCM_daily_dose'].describe()
```

```
count     166.000000
mean     1963.765060
std       500.652737
min      1000.000000
25%      1940.000000
50%      2000.000000
75%      2000.000000
max      5700.000000
Name: Initial VCM_daily_dose, dtype: float64
```



Outlier Removal

```
# To remove outliers, remove the top and bottom 5% of the dataset

q1 = dfVanco['Initial VCM_daily_dose'].quantile(0.05)
q2 = dfVanco['Initial VCM_daily_dose'].quantile(0.5)
q3 = dfVanco['Initial VCM_daily_dose'].quantile(0.95)
iqr = q3 - q1

print(f'iqr: {iqr}')
print(f'low threshold : {q1-1.5*iqr}')
print(f'high theshold : {q3+1.5*iqr}')
```

```
iqr: 1300.0
low threshold : -750.0
high theshold : 4450.0
```

```
outlier1 = dfVanco['Initial VCM_daily_dose']>(q3+1.5*iqr)
outlier2 = dfVanco['Initial VCM_daily_dose']<(q1-1.5*iqr)
```

```
a = list(dfVanco[outlier2].index)
b = list(dfVanco[outlier1].index)
a.extend(b)
df1 = dfVanco.drop(a)

# df1 is the dataset after removing the top and bottom 5% of the dataset to remove outliers
print(f'# data: {len(df1)}')
df1['Initial VCM_daily_dose'].plot.hist(bins=10)
```

```
# data: 164
<Axes: ylabel='Frequency'>
```

```
1 df1.describe()
```

	Gender	Age	Weight	Height	BMI	Initial VCM_daily_dose	ICU	WBC	Hb	PLT	
count	164.000000	164.000000	164.000000	164.000000	164.000000	164.000000	164.000000	164.000000	164.000000	164.000000	164.00
mean	0.573171	69.701220	60.856707	161.765854	23.247561	1925.152439	0.158537	10.019512	10.276220	246.323171	79.42
std	0.496132	13.215152	11.752599	9.032419	4.047698	353.886148	0.366362	8.898955	1.895615	118.723163	75.80
min	0.000000	22.000000	33.000000	135.000000	14.300000	1000.000000	0.000000	0.100000	5.500000	14.000000	1.00
25%	0.000000	63.000000	53.000000	155.000000	20.600000	1890.000000	0.000000	6.325000	9.000000	167.000000	14.92
50%	1.000000	73.000000	60.000000	163.000000	23.300000	2000.000000	0.000000	8.900000	10.100000	238.000000	54.79
75%	1.000000	79.000000	69.000000	169.250000	25.700000	2000.000000	0.000000	11.350000	11.525000	320.500000	130.00
max	1.000000	91.000000	100.000000	180.000000	33.300000	3000.000000	1.000000	97.100000	14.700000	646.000000	300.00

1000 1250 1500 1750 2000 2250 2500 2750 3000

Modeling training using pycaret, an auto machine library

```
1 reg1 = setup(data=df1, target='Initial VCM_daily_dose',
2              train_size = 0.8,
3              fold = 5, fold_shuffle = True,
4              use_gpu=True,
5              session_id = 42
6             )
```

	Description	Value
0	Session id	42
1	Target	Initial VCM_daily_dose
2	Target type	Regression
3	Original data shape	(164, 33)
4	Transformed data shape	(164, 33)
5	Transformed train set shape	(131, 33)
6	Transformed test set shape	(33, 33)
7	Numeric features	32
8	Preprocess	True
9	Imputation type	simple
10	Numeric imputation	mean
11	Categorical imputation	mode
12	Fold Generator	KFold
13	Fold Number	5
14	CPU Jobs	-1
15	Use GPU	True
16	Log Experiment	False
17	Experiment Name	reg-default-name
18	USI	0ec9

Evaluation

```
1 best = compare_models(sort='mse')
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MA
et	Extra Trees Regressor	213.1982	107018.1676	324.7718	0.1405	0.1880	0.1
lightgbm	Light Gradient Boosting Machine	241.5854	112739.0369	332.2827	0.0909	0.1914	0.1
rf	Random Forest Regressor	223.7567	113796.5242	334.8708	0.0850	0.1950	0.1
catboost	CatBoost Regressor	230.4799	113844.6089	334.3818	0.0889	0.1954	0.1
ada	AdaBoost Regressor	229.7622	114563.9985	335.1575	0.0863	0.1936	0.1
br	Bayesian Ridge	234.2260	115319.1758	337.3491	0.0674	0.1980	0.1
huber	Huber Regressor	220.7969	125404.9419	352.7258	-0.0170	0.2087	0.1
omp	Orthogonal Matching Pursuit	241.0297	125413.9385	352.9780	-0.0328	0.2063	0.1
dummy	Dummy Regressor	235.6235	125955.9228	353.1710	-0.0168	0.2089	0.1
en	Elastic Net	253.7400	129943.5931	357.2337	-0.0450	0.2070	0.1
knn	K Neighbors Regressor	248.6442	130333.1501	359.8911	-0.0662	0.2095	0.1

```
1 best_tune = tune_model(best)
```

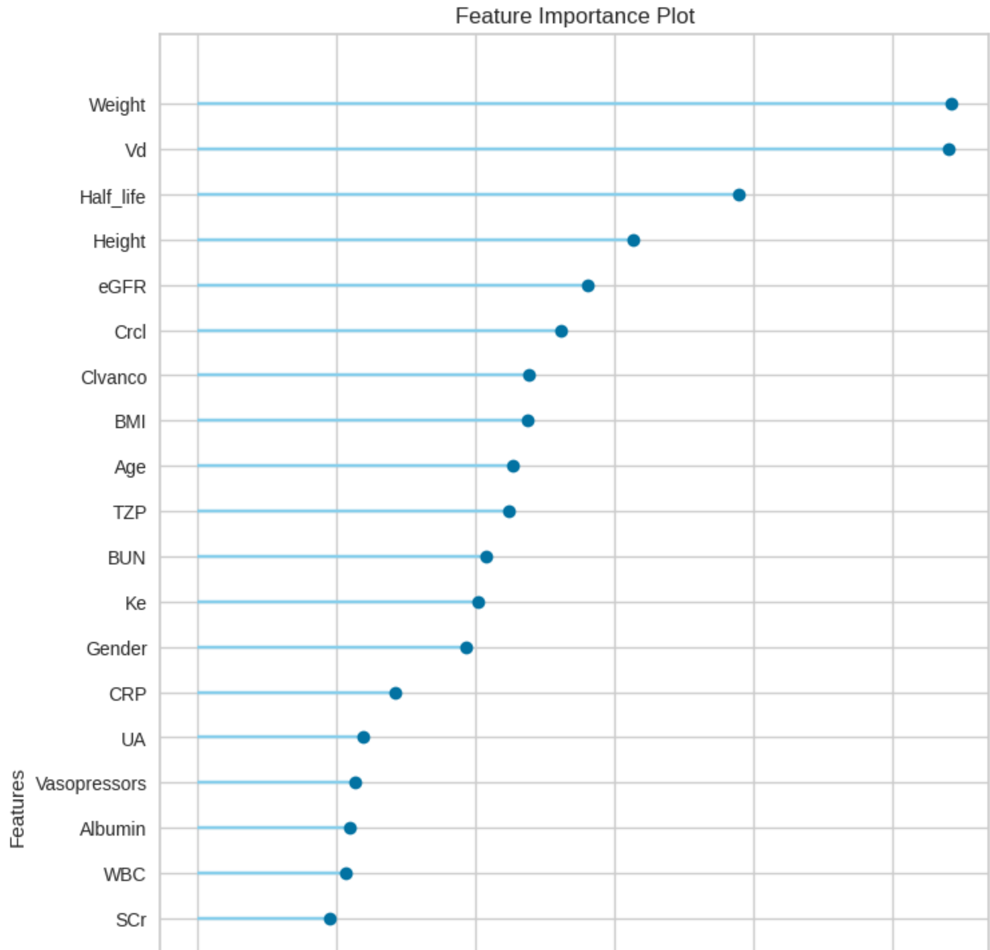
Fold	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	172.0221	89976.3895	299.9606	0.2912	0.1843	0.1139
1	183.6236	69715.2506	264.0365	0.2208	0.1524	0.1087
2	270.5127	142981.3852	378.1288	0.0380	0.2094	0.1472
3	221.9522	128962.3257	359.1132	0.1109	0.2063	0.1413
4	181.3184	83082.0580	288.2396	0.2298	0.1798	0.1156
Mean	205.8858	102943.4818	317.8957	0.1781	0.1864	0.1254
Std	36.5532	28095.3766	43.4255	0.0910	0.0207	0.0157

```
Fitting 5 folds for each of 10 candidates, totalling 50 fits
```

```
1 evaluate_model(best_tune)
```

Plot Type:

Pipeline Plot | Hyperparameters | Residuals | Prediction Error | Cooks Distance | Feature Selection
Learning Curve | Manifold Learning | Validation Curve | Feature Importance | Feature Importance… | Decision Tree
Interactive Residuals




```
predictions = predict_model(best_tune)
predictions[:5]
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	Extra Trees Regressor	241.1974	105707.4193	325.1268	0.1315	0.1771	0.1380

	Gender	Age	Weight	Height	BMI	ICU	WBC	Hb	PLT	CRP	...	TZP	FLC	FQ	Crcl	Clvanco	Vd	Ke
135	1	84	85.0	170.0	29.400000	0	10.4	10.3	192	129.479996	...	0	0	0	83.699997	3.7	59.500000	0.074
115	1	84	68.0	170.0	23.500000	0	6.7	12.5	259	47.610001	...	0	0	0	67.800003	3.0	47.599998	0.061
131	1	76	68.0	175.0	22.200001	0	9.2	11.5	230	39.410000	...	0	0	0	94.400002	4.1	47.599998	0.083
55	0	58	60.0	160.0	23.400000	1	19.9	11.0	393	90.570000	...	0	0	0	98.400002	4.3	42.000000	0.086
95	1	40	69.0	166.0	25.000000	0	18.1	13.0	280	163.240005	...	0	0	0	121.300003	5.3	48.299999	0.105

```
df_result = pd.DataFrame()
df_result['true'] = predictions['Initial VCM_daily_dose']
df_result['prediction'] = predictions['prediction_label']

# Since vancomycin is prescribed in units of 100 anyway, the numerical value is rounded up to 100.
def round_to_nearest_fifty(number):
    return round(number / 50.0) * 50

rounded_values = [round_to_nearest_fifty(num) for num in predictions['prediction_label']]
predictions["prediction_label"]= rounded_values
predictions
```

	Gender	Age	Weight	Height	BMI	ICU	WBC	Hb	PLT	CRP	...	TZP	FLC	FQ	Crcl	Clvanco	Vd	
135	1	84	85.0	170.0	29.400000	0	10.4	10.3	192	129.479996	...	0	0	0	83.699997	3.7	59.500000	0.0
115	1	84	68.0	170.0	23.500000	0	6.7	12.5	259	47.610001	...	0	0	0	67.800003	3.0	47.599998	0.0
131	1	76	68.0	175.0	22.200001	0	9.2	11.5	230	39.410000	...	0	0	0	94.400002	4.1	47.599998	0.0
55	0	58	60.0	160.0	23.400000	1	19.9	11.0	393	90.570000	...	0	0	0	98.400002	4.3	42.000000	0.0
95	1	40	69.0	166.0	25.000000	0	18.1	13.0	280	163.240005	...	0	0	0	121.300003	5.3	48.299999	0.1
29	1	58	63.0	168.0	22.299999	0	7.3	11.1	223	24.450001	...	0	0	0	56.500000	2.5	44.099998	0.0
157	1	71	70.0	170.0	24.200001	0	9.4	10.6	177	179.339996	...	1	0	0	82.800003	3.7	49.000000	0.0
51	0	75	55.0	154.0	23.200001	0	10.9	10.1	383	5.340000	...	0	0	0	69.199997	3.1	38.500000	0.0
101	1	65	67.0	167.0	24.000000	0	8.0	13.5	285	7.550000	...	0	0	0	90.599998	4.0	46.900002	0.0
145	1	48	80.0	171.0	27.400000	0	8.7	10.1	396	113.989998	...	0	0	0	152.600006	6.6	56.000000	0.1
19	0	76	60.0	153.0	25.600000	1	6.4	10.9	279	24.340000	...	0	0	0	116.199997	5.0	42.000000	0.1
85	0	76	43.0	159.0	17.000000	0	7.7	9.7	295	99.320000	...	0	0	0	58.000000	2.5	30.100000	0.0
15	1	59	68.0	165.0	25.000000	0	5.1	10.8	198	7.600000	...	0	0	0	70.800003	3.2	47.599998	0.0
66	0	76	60.0	145.0	28.500000	0	6.6	10.8	227	161.970001	...	0	0	0	65.699997	2.9	42.000000	0.0
24	1	85	70.0	165.0	25.700001	0	12.2	8.3	221	185.979996	...	0	0	0	60.799999	2.7	49.000000	0.0
30	1	61	50.0	160.0	19.500000	1	13.0	8.3	176	78.860001	...	0	0	0	133.800003	5.7	35.000000	0.1
132	1	71	50.0	172.0	16.900000	0	3.4	8.2	90	3.930000	...	1	0	0	90.400002	3.9	35.000000	0.0
105	1	78	64.0	180.0	19.799999	0	18.6	9.2	217	157.429993	...	0	0	0	122.500000	5.3	44.799999	0.1
152	1	37	58.0	173.0	19.400000	0	10.0	5.5	202	142.759995	...	0	0	0	150.899994	6.5	40.599998	0.1
16	1	81	43.0	150.0	19.100000	0	2.5	8.8	300	131.580002	...	0	0	0	34.900002	1.6	30.100000	0.0
75	0	69	54.0	159.0	21.400000	1	0.8	9.4	155	300.000000	...	0	0	0	54.500000	2.4	37.799999	0.0
18	0	82	51.0	135.0	28.000000	0	6.9	14.2	186	1.000000	...	0	0	0	57.200001	2.5	35.700001	0.0
12	0	81	75.0	150.0	33.299999	0	10.5	10.1	352	103.440002	...	0	0	0	66.099998	3.0	52.500000	0.0
9	0	71	70.0	168.0	24.799999	1	13.1	7.5	202	252.940002	...	0	0	0	54.299999	2.5	49.000000	0.0
31	1	66	53.0	156.0	21.799999	0	9.2	8.2	301	133.399994	...	0	0	0	72.599998	3.2	37.099998	0.0
155	1	67	65.0	163.0	24.500000	0	9.3	9.7	607	41.669998	...	1	0	0	92.800003	4.1	45.500000	0.0
98	1	83	60.0	165.0	22.000000	0	7.3	13.6	187	3.860000	...	0	0	0	64.199997	2.9	42.000000	0.0
56	0	72	44.0	155.0	18.299999	0	10.0	10.9	444	79.419998	...	1	0	0	70.599998	3.1	30.799999	0.0
134	1	65	58.0	160.0	22.700001	0	5.1	9.9	191	1.000000	...	0	0	0	80.599998	3.5	40.599998	0.0
160	1	59	53.0	165.0	19.500000	0	10.8	10.7	271	94.449997	...	0	0	0	91.699997	4.0	37.099998	0.0
139	1	79	68.0	165.0	25.000000	0	7.1	14.5	245	128.649994	...	0	0	0	50.099998	2.3	47.599998	0.0
78	0	81	60.0	152.0	26.000000	0	7.8	11.9	186	5.470000	...	0	0	0	68.500000	3.0	42.000000	0.0
60	0	73	50.0	151.0	21.900000	0	5.6	8.8	142	63.880001	...	0	0	0	92.000000	4.0	35.000000	0.0

```
1 df_result['prediction']
```

```
135    2007.555487
115    2023.853162
131    2071.346032
55     1998.173686
95     2036.220125
29     1975.344562
157    2051.056657
51     1976.986221
101    2039.870315
145    2024.522200
19     1980.268815
85     1638.200696
15     2019.613864
66     1960.596171
24     2000.841945
30     1831.280865
132    1883.687596
105    2096.465141
152    2031.064895
16     1535.573482
75     1864.311616
18     1821.083830
12     1918.628636
9      1836.806006
31     1964.324092
```

```
155    2012.708891
98     1999.624005
56     1821.995045
134    1986.274837
160    1972.078726
139    1881.710616
78     1963.245349
60     1883.324713
Name: prediction, dtype: float64
```

```
1 df_result['prediction']=predictions["prediction_label"]
2 df_result['prediction']
```

```
135    2000
115    2000
131    2050
55     2000
95     2050
29     2000
157    2050
51     2000
101    2050
145    2000
19     2000
85     1650
15     2000
66     1950
24     2000
30     1850
132    1900
105    2100
152    2050
16     1550
75     1850
18     1800
12     1900
9      1850
31     1950
155    2000
98     2000
56     1800
134    2000
160    1950
139    1900
78     1950
60     1900
Name: prediction, dtype: int64
```

Results

```
1 df_result
```

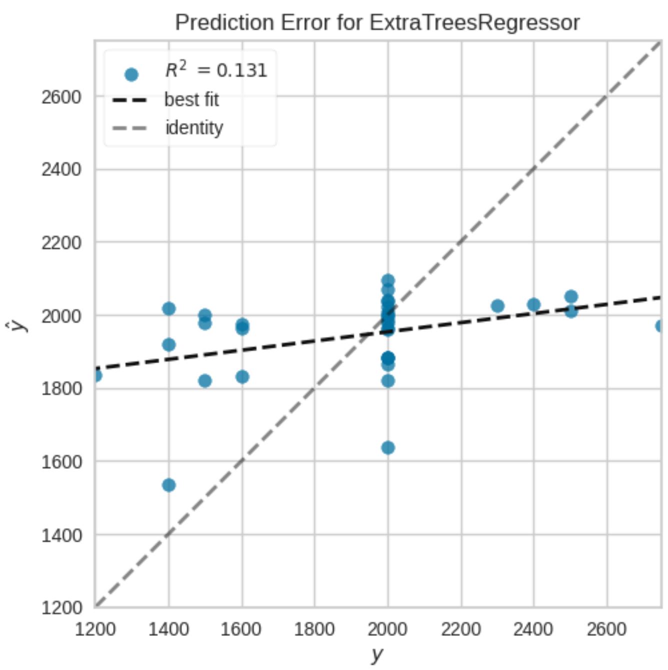
	true	prediction
135	2000	2000
115	2000	2000
131	2000	2050
55	2000	2000
95	2000	2050
29	1600	2000
157	2500	2050
51	2000	2000
101	2000	2050
145	2300	2000
19	1500	2000
85	2000	1650
15	1400	2000
66	2000	1950
24	1500	2000
30	1600	1850

```
1 df_result['accuracy'] = np.where(abs(df_result['true'] - df_result['prediction']) <=50, 1, 0)
2 accuracy = round((len(df_result.loc[df_result['accuracy'] == 1])/ len(df_result)) * 100, 1)
3 print('Accuracy: ', accuracy, '%')
4
```

```
Accuracy:  33.3 %
```

75 2000 1850

```
1 plot_model(best_tune, plot = 'error')
```



Log Transformation of 'Initial VCM_daily_dose'

```
1 # Applying a log transformation to the 'Initial VCM_daily_dose' column in the df_D2 dataframe.
2 # This process is often used in data science to manage skewed data or to linearize relationships that
```

```
1 df1['Initial VCM_daily_dose_log'] = df1['Initial VCM_daily_dose'].apply(lambda x: math.log(x))
```

```
1 df2=df1.drop(columns='Initial VCM_daily_dose')
```

```
df2
```

	Gender	Age	Weight	Height	BMI	ICU	WBC	Hb	PLT	CRP	...	AG	TZP	FLC	FQ	Crcl	Clvanco	Vd	Ke	Half_life	VCM
0	0	79	69.0	158.0	27.6	0	5.9	7.3	134	43.23	...	0	1	0	0	110.4	4.8	48.3	0.096	7.2	
1	0	74	72.0	163.0	27.1	0	9.5	11.4	286	72.22	...	0	1	0	0	59.1	2.7	50.4	0.053	13.0	
2	0	74	52.0	146.0	24.4	0	97.1	7.2	14	55.73	...	0	0	0	0	51.3	2.3	36.4	0.047	14.8	
3	0	83	48.0	153.0	20.5	0	6.1	8.4	285	39.53	...	0	0	0	0	32.0	1.5	33.6	0.031	22.4	
4	0	88	40.0	148.0	18.3	0	7.4	9.4	221	56.37	...	1	0	0	0	35.6	1.6	28.0	0.034	20.4	
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	
159	0	73	54.0	150.0	24.0	0	12.1	5.5	41	144.89	...	0	0	0	0	59.3	2.6	37.8	0.054	12.9	
160	1	59	53.0	165.0	19.5	0	10.8	10.7	271	94.45	...	0	0	0	0	91.7	4.0	37.1	0.081	8.6	
161	1	63	74.0	168.0	26.2	0	11.2	9.5	130	52.92	...	0	1	0	0	88.9	3.9	51.8	0.078	8.9	
162	0	64	63.0	155.0	26.2	0	6.9	7.5	179	260.20	...	0	0	0	0	113.0	4.9	44.1	0.098	7.1	
163	1	74	77.0	176.0	24.9	0	11.2	12.3	358	26.25	...	0	0	0	0	72.8	3.3	53.9	0.065	10.7	

```
reg1 = setup(data=df2, target='Initial VCM_daily_dose_log',
             train_size = 0.8,
             fold = 5, fold_shuffle = True,
             use_gpu=True,
             session_id = 42
            )
```

	Description	Value
0	Session id	42
1	Target	Initial VCM_daily_dose_log
2	Target type	Regression
3	Original data shape	(164, 33)
4	Transformed data shape	(164, 33)
5	Transformed train set shape	(131, 33)
6	Transformed test set shape	(33, 33)
7	Numeric features	32
8	Preprocess	True
9	Imputation type	simple
10	Numeric imputation	mean
11	Categorical imputation	mode
12	Fold Generator	KFold
13	Fold Number	5
14	CPU Jobs	-1
15	Use GPU	True
16	Log Experiment	False
17	Experiment Name	reg-default-name
18	USI	c7da

```
best = compare_models(sort='mse')
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE
et	Extra Trees Regressor	0.1214	0.0359	0.1880	0.1741	0.0224	0.0164
xgboost	Extreme Gradient Boosting	0.1307	0.0371	0.1915	0.1390	0.0228	0.0175
lightgbm	Light Gradient Boosting Machine	0.1349	0.0376	0.1924	0.1135	0.0229	0.0181
ada	AdaBoost Regressor	0.1371	0.0389	0.1959	0.0978	0.0233	0.0185
catboost	CatBoost Regressor	0.1279	0.0391	0.1962	0.0966	0.0234	0.0172
rf	Random Forest Regressor	0.1264	0.0394	0.1973	0.0882	0.0235	0.0170
br	Bayesian Ridge	0.1357	0.0394	0.1975	0.0790	0.0235	0.0183

```
1 best_tune = tune_model(best)
```

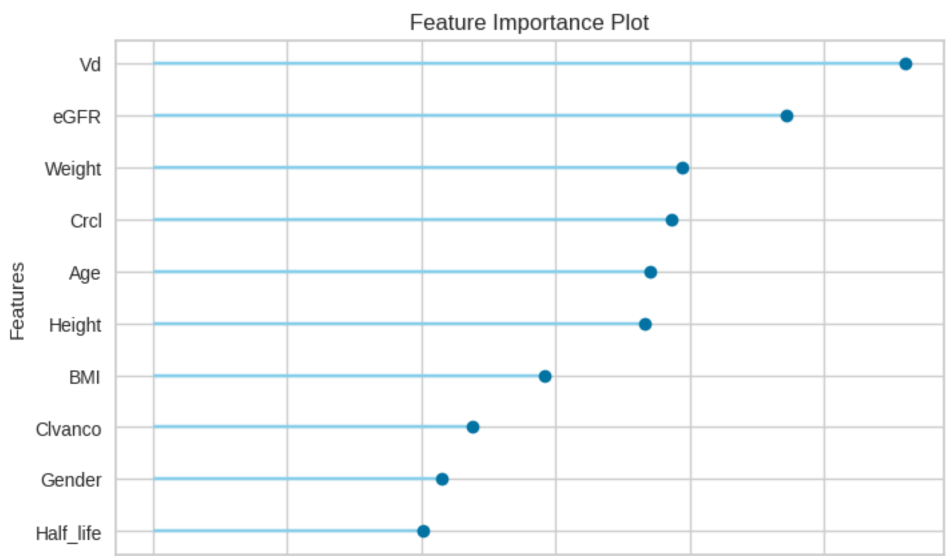
Fold	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	0.1069	0.0341	0.1846	0.2784	0.0222	0.0146
1	0.1020	0.0215	0.1466	0.2744	0.0174	0.0137
2	0.1515	0.0474	0.2176	0.0766	0.0259	0.0203
3	0.1302	0.0418	0.2045	0.1002	0.0243	0.0177
4	0.1143	0.0340	0.1844	0.1657	0.0221	0.0155
Mean	0.1210	0.0357	0.1875	0.1790	0.0224	0.0164
Std	0.0180	0.0087	0.0240	0.0847	0.0029	0.0024

```
Fitting 5 folds for each of 10 candidates, totalling 50 fits
```

```
1 evaluate_model(best_tune)
```

Plot Type:

Pipeline Plot	Hyperparameters	Residuals	Prediction Error	Cooks Distance	Feature Selection
Learning Curve	Manifold Learning	Validation Curve	Feature Importance	Feature Importance…	Decision Tree
Interactive Residuals					




```
1 predictions = predict_model(best_tune)
```

```
1 predictions
```

	Gender	Age	Weight	Height	BMI	ICU	WBC	Hb	PLT	CRP	...	TZP	FLC	FQ	Crcl	Clvanco	Vd	
135	1	84	85.0	170.0	29.400000	0	10.4	10.3	192	129.479996	...	0	0	0	83.699997	3.7	59.500000	0.0
115	1	84	68.0	170.0	23.500000	0	6.7	12.5	259	47.610001	...	0	0	0	67.800003	3.0	47.599998	0.0
131	1	76	68.0	175.0	22.200001	0	9.2	11.5	230	39.410000	...	0	0	0	94.400002	4.1	47.599998	0.0
55	0	58	60.0	160.0	23.400000	1	19.9	11.0	393	90.570000	...	0	0	0	98.400002	4.3	42.000000	0.0
95	1	40	69.0	166.0	25.000000	0	18.1	13.0	280	163.240005	...	0	0	0	121.300003	5.3	48.299999	0.1
29	1	58	63.0	168.0	22.299999	0	7.3	11.1	223	24.450001	...	0	0	0	56.500000	2.5	44.099998	0.0
157	1	71	70.0	170.0	24.200001	0	9.4	10.6	177	179.339996	...	1	0	0	82.800003	3.7	49.000000	0.0
51	0	75	55.0	154.0	23.200001	0	10.9	10.1	383	5.340000	...	0	0	0	69.199997	3.1	38.500000	0.0
101	1	65	67.0	167.0	24.000000	0	8.0	13.5	285	7.550000	...	0	0	0	90.599998	4.0	46.900002	0.0
145	1	48	80.0	171.0	27.400000	0	8.7	10.1	396	113.989998	...	0	0	0	152.600006	6.6	56.000000	0.1
19	0	76	60.0	153.0	25.600000	1	6.4	10.9	279	24.340000	...	0	0	0	116.199997	5.0	42.000000	0.1
85	0	76	43.0	159.0	17.000000	0	7.7	9.7	295	99.320000	...	0	0	0	58.000000	2.5	30.100000	0.0
15	1	59	68.0	165.0	25.000000	0	5.1	10.8	198	7.600000	...	0	0	0	70.800003	3.2	47.599998	0.0
66	0	76	60.0	145.0	28.500000	0	6.6	10.8	227	161.970001	...	0	0	0	65.699997	2.9	42.000000	0.0
24	1	85	70.0	165.0	25.700001	0	12.2	8.3	221	185.979996	...	0	0	0	60.799999	2.7	49.000000	0.0
30	1	61	50.0	160.0	19.500000	1	13.0	8.3	176	78.860001	...	0	0	0	133.800003	5.7	35.000000	0.1
132	1	71	50.0	172.0	16.900000	0	3.4	8.2	90	3.930000	...	1	0	0	90.400002	3.9	35.000000	0.0
105	1	78	64.0	180.0	19.799999	0	18.6	9.2	217	157.429993	...	0	0	0	122.500000	5.3	44.799999	0.1
152	1	37	58.0	173.0	19.400000	0	10.0	5.5	202	142.759995	...	0	0	0	150.899994	6.5	40.599998	0.1
16	1	81	43.0	150.0	19.100000	0	2.5	8.8	300	131.580002	...	0	0	0	34.900002	1.6	30.100000	0.0
75	0	69	54.0	159.0	21.400000	1	0.8	9.4	155	300.000000	...	0	0	0	54.500000	2.4	37.799999	0.0
18	0	82	51.0	135.0	28.000000	0	6.9	14.2	186	1.000000	...	0	0	0	57.200001	2.5	35.700001	0.0
12	0	81	75.0	150.0	33.299999	0	10.5	10.1	352	103.440002	...	0	0	0	66.099998	3.0	52.500000	0.0
9	0	71	70.0	168.0	24.799999	1	13.1	7.5	202	252.940002	...	0	0	0	54.299999	2.5	49.000000	0.0
31	1	66	53.0	156.0	21.799999	0	9.2	8.2	301	133.399994	...	0	0	0	72.599998	3.2	37.099998	0.0
155	1	67	65.0	163.0	24.500000	0	9.3	9.7	607	41.669998	...	1	0	0	92.800003	4.1	45.500000	0.0
98	1	83	60.0	165.0	22.000000	0	7.3	13.6	187	3.860000	...	0	0	0	64.199997	2.9	42.000000	0.0
56	0	72	44.0	155.0	18.299999	0	10.0	10.9	444	79.419998	...	1	0	0	70.599998	3.1	30.799999	0.0
134	1	65	58.0	160.0	22.700001	0	5.1	9.9	191	1.000000	...	0	0	0	80.599998	3.5	40.599998	0.0
160	1	59	53.0	165.0	19.500000	0	10.8	10.7	271	94.449997	...	0	0	0	91.699997	4.0	37.099998	0.0
139	1	79	68.0	165.0	25.000000	0	7.1	14.5	245	128.649994	...	0	0	0	50.099998	2.3	47.599998	0.0
78	0	81	60.0	152.0	26.000000	0	7.8	11.9	186	5.470000	...	0	0	0	68.500000	3.0	42.000000	0.0
60	0	73	50.0	151.0	21.900000	0	5.6	8.8	142	63.880001	...	0	0	0	92.000000	4.0	35.000000	0.0

```
1 df_result = pd.DataFrame()
2 df_result['Initial VCM_daily_dose_log'] = predictions['Initial VCM_daily_dose_log']
3 df_result['prediction_label_log']=predictions['prediction_label']
4 df_result
```

	Initial VCM_daily_dose_log	prediction_label_log
135	7.600903	7.591751
115	7.600903	7.599697
131	7.600903	7.609170
55	7.600903	7.561296
95	7.600903	7.613971
29	7.377759	7.547644
157	7.824046	7.600560
51	7.600903	7.556880
101	7.600903	7.606026
145	7.740664	7.593808
19	7.313221	7.572926
85	7.600903	7.443332
15	7.244227	7.590630
66	7.600903	7.558088
24	7.313221	7.592218
30	7.377759	7.529913
132	7.600903	7.556802
105	7.600903	7.597727
152	7.783224	7.581211
16	7.244227	7.375715
75	7.600903	7.469156
18	7.313221	7.499468
12	7.244227	7.564832
9	7.090077	7.462667
31	7.377759	7.556428

```
index_list = [135, 115, 131, 55, 95, 29, 157, 51, 101, 145, 19, 85, 15, 66, 24, 30, 132, 105, 152, 16,
index_series = pd.Series(index_list)  # Convert the list to a pandas Series

# List comprehension to store values
value_list = [df1.loc[index, 'Initial VCM_daily_dose'] for index in index_series]

print(value_list)

```

```
[2000, 2000, 2000, 2000, 2000, 1600, 2500, 2000, 2000, 2300, 1500, 2000, 1400, 2000, 1500, 1600, 2000, 2000, 2400, 1400, 2000, 1500, 1400, 1200,
```

```
df_result['Initial VCM_daily_dose']=value_list
df_result
```

	Initial VCM_daily_dose_log	prediction_label_log	Initial VCM_daily_dose
135	7.600903	7.591751	2000
115	7.600903	7.599697	2000
131	7.600903	7.609170	2000
55	7.600903	7.561296	2000
95	7.600903	7.613971	2000
29	7.377759	7.547644	1600
157	7.824046	7.600560	2500
51	7.600903	7.556880	2000
101	7.600903	7.606026	2000
145	7.740664	7.593808	2300
19	7.313221	7.572926	1500
85	7.600903	7.443332	2000
15	7.244227	7.590630	1400
66	7.600903	7.558088	2000
24	7.313221	7.592218	1500
30	7.377759	7.529913	1600
132	7.600903	7.556802	2000
105	7.600903	7.597727	2000
152	7.783224	7.581211	2400
16	7.244227	7.375715	1400
75	7.600903	7.469156	2000
18	7.313221	7.499468	1500

```
1 df_result['prediction'] = np.exp(df_result['prediction_label_log'])
```

```
1 df_result
```

	Initial VCM_daily_dose_log	prediction_label_log	Initial VCM_daily_dose	prediction
135	7.600903	7.591751	2000	1981.780232
115	7.600903	7.599697	2000	1997.589857
131	7.600903	7.609170	2000	2016.602619
55	7.600903	7.561296	2000	1922.335154
95	7.600903	7.613971	2000	2026.309476
29	7.377759	7.547644	1600	1896.270271
157	7.824046	7.600560	2500	1999.315232
51	7.600903	7.556880	2000	1913.865346
101	7.600903	7.606026	2000	2010.273127
145	7.740664	7.593808	2300	1985.861322

```
# round off the prediction values to the nearest fifty
rounded_values = [round_to_nearest_fifty(num) for num in df_result['prediction']]
df_result['prediction']= rounded_values

```

```
df_result
```

	Initial VCM_daily_dose_log	prediction_label_log	Initial VCM_daily_dose	prediction
51	7.600903	7.556880	2000	1900

```
df_result['accuracy'] = np.where(abs(df_result['Initial VCM_daily_dose'] - df_result['prediction']) <=
accuracy = round((len(df_result.loc[df_result['accuracy'] == 1])/ len(df_result)) * 100, 1)
print('Accuracy: ', accuracy, '%')
```

```
Accuracy:  24.2 %
```

Dataset augmentation

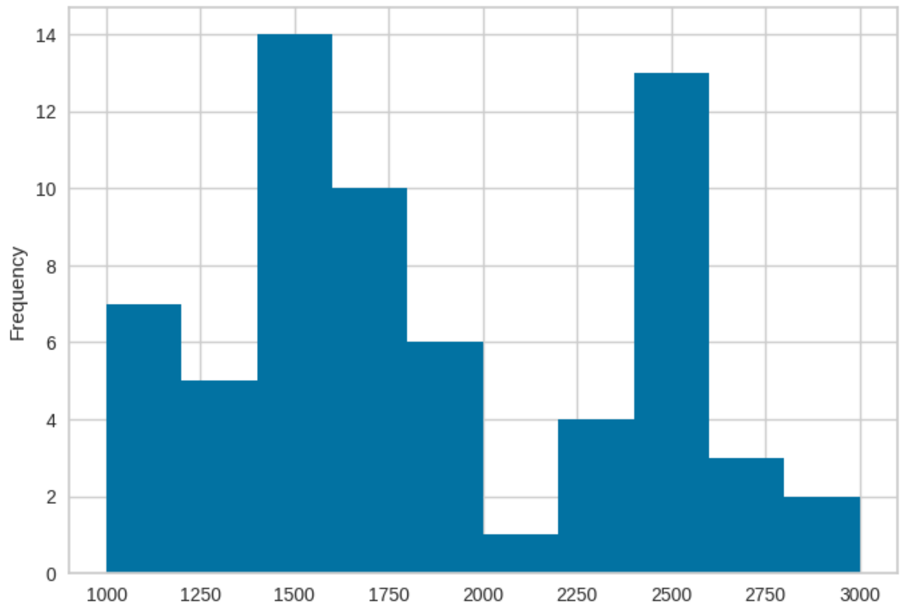
```
df1 = df1.drop(columns=['Initial VCM_daily_dose_log'])
```

```
# Dataset imbalance check

percentage = (df1['Initial VCM_daily_dose'].value_counts(normalize=True).loc[2000] * 100)
print(f"The percentage of data with 'Initial VCM_daily_dose' = 2000 is {percentage.round(1)} %")
```

```
The percentage of data with 'Initial VCM_daily_dose' = 2000 is 60.4 %
```

```
# Check the dataset except for the value of ['Initial VCM_daily_dose']  = 2000
df_temp = df1[df1['Initial VCM_daily_dose'] != 2000]


# the number of remaining data after erasing
print(f'# data: {len(df_temp)}')

# check with histogram
df_temp['Initial VCM_daily_dose'].plot.hist(bins=10)
```

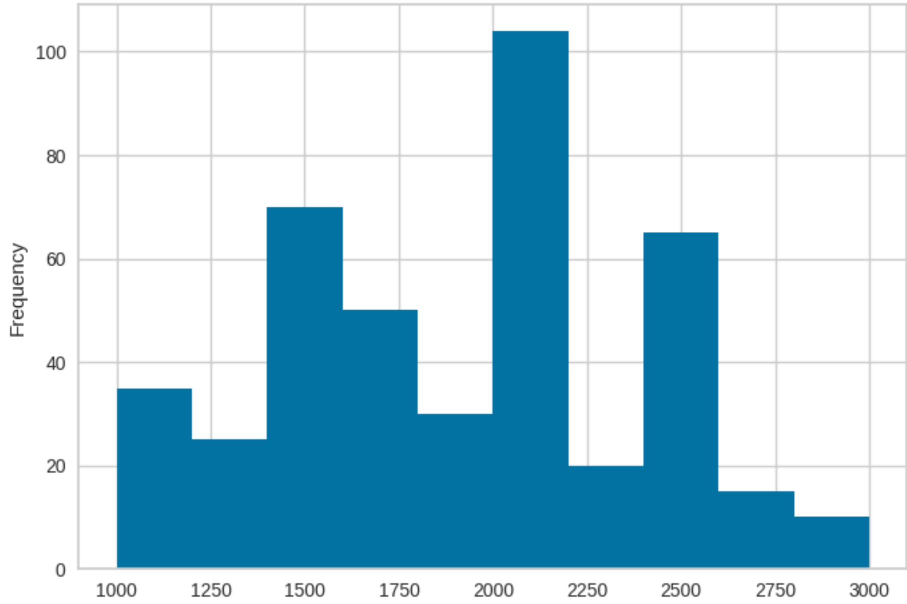
```
# data: 65
<Axes: ylabel='Frequency'>
```




```
# Amplify other datasets to match data imbalance
# n times data amplification: Amplify the original data using the data 'without' the initial dose valu
# After many attempts, it is reasonable to amplify it by about 4 times.

n = 4
df_list = [df_temp] * n
df_iter = pd.concat(df_list)
df_D = pd.concat([df1, df_iter])


```

```
# the number of data after amplification
print(f'# data: {len(df_D)}')

# check with histogram
df_D['Initial VCM_daily_dose'].plot.hist(bins=10)
```

```
# data: 424
<Axes: ylabel='Frequency'>
```




```
df_D
```

	Gender	Age	Weight	Height	BMI	Initial VCM_daily_dose	ICU	WBC	Hb	PLT	...	LAB	AG	TZP	FLC	FQ	Crcl	Clvanco	Vd	Ke
0	0	79	69.0	158.0	27.6	1000	0	5.9	7.3	134	...	0	0	1	0	0	110.4	4.8	48.3	0.096
1	0	74	72.0	163.0	27.1	1000	0	9.5	11.4	286	...	0	0	1	0	0	59.1	2.7	50.4	0.053
2	0	74	52.0	146.0	24.4	1000	0	97.1	7.2	14	...	0	0	0	0	0	51.3	2.3	36.4	0.047
3	0	83	48.0	153.0	20.5	1000	0	6.1	8.4	285	...	0	0	0	0	0	32.0	1.5	33.6	0.031
4	0	88	40.0	148.0	18.3	1000	0	7.4	9.4	221	...	0	1	0	0	0	35.6	1.6	28.0	0.034
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
159	0	73	54.0	150.0	24.0	2600	0	12.1	5.5	41	...	0	0	0	0	0	59.3	2.6	37.8	0.054
160	1	59	53.0	165.0	19.5	2750	0	10.8	10.7	271	...	0	0	0	0	0	91.7	4.0	37.1	0.081
161	1	63	74.0	168.0	26.2	2760	0	11.2	9.5	130	...	0	0	1	0	0	88.9	3.9	51.8	0.078
162	0	64	63.0	155.0	26.2	2840	0	6.9	7.5	179	...	0	0	0	0	0	113.0	4.9	44.1	0.098
163	1	74	77.0	176.0	24.9	3000	0	11.2	12.3	358	...	0	0	0	0	0	72.8	3.3	53.9	0.065

```
augmented_dataset = pd.ExcelWriter('augmented_dataset.xlsx')
```

```
df_D.to_excel(augmented_dataset, index=False)
```

```
augmented_dataset.save()
```

```
files.download('augmented_dataset.xlsx')
```

Model training with amplified data

```
# The amplified data is randomly corrupted and stored
df_D = df_D.sample(frac=1).reset_index(drop=True)
```

```

reg2 = setup(data=df_D,
             target='Initial VCM_daily_dose',
             train_size=0.8,
             fold=5,
             fold_shuffle=True,
             use_gpu=True,
             session_id=42
            )

```

	Description	Value
0	Session id	42
1	Target	Initial VCM_daily_dose
2	Target type	Regression
3	Original data shape	(424, 33)
4	Transformed data shape	(424, 33)
5	Transformed train set shape	(339, 33)
6	Transformed test set shape	(85, 33)
7	Numeric features	32
8	Preprocess	True
9	Imputation type	simple
10	Numeric imputation	mean
11	Categorical imputation	mode
12	Fold Generator	KFold
13	Fold Number	5
14	CPU Jobs	-1
15	Use GPU	True
16	Log Experiment	False
17	Experiment Name	reg-default-name
18	USI	de06

Evaluation

```
# find and tune the best model
best = compare_models(sort='mse')
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MA
et	Extra Trees Regressor	29.0796	6898.4477	81.6594	0.9697	0.0433	0.(
catboost	CatBoost Regressor	62.7350	11455.7905	106.0780	0.9492	0.0575	0.(
xgboost	Extreme Gradient	43.8438	16759.8443	127.3179	0.9266	0.0734	0.(

```
1 best_tune = tune_model(best)
```

Fold	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	162.4343	40883.6865	202.1971	0.8099	0.1147	0.0931
1	189.7252	63270.3435	251.5360	0.7449	0.1409	0.1108
2	159.4690	39133.5211	197.8219	0.8177	0.1256	0.1000
3	167.5104	44081.7959	209.9567	0.7878	0.1223	0.0966
4	146.8399	33261.2860	182.3768	0.8639	0.0959	0.0789
Mean	165.1958	44126.1266	208.7777	0.8048	0.1199	0.0959
Std	14.0315	10197.9144	23.1948	0.0389	0.0147	0.0104

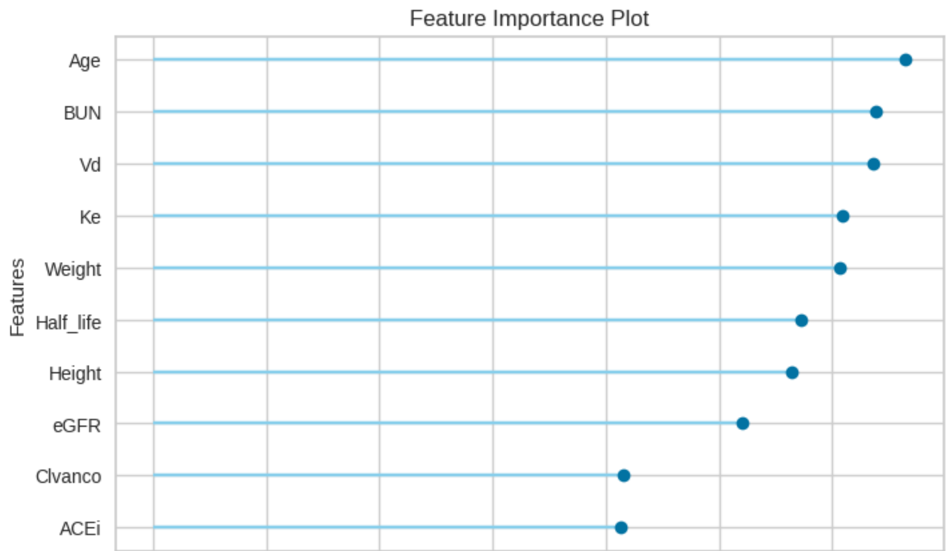
```
Fitting 5 folds for each of 10 candidates, totalling 50 fits
Original model was better than the tuned model, hence it will be returned. NOTE: The display metrics are for the tuned model (not the original o
```

Regression

```
1 # evaluate and make predictions with the best model
2 evaluate_model(best_tune)
```

Plot Type:

Pipeline Plot | Hyperparameters | Residuals | Prediction Error | Cooks Distance | Feature Selection
Learning Curve | Manifold Learning | Validation Curve | Feature Importance | Feature Importance... | Decision Tree
Interactive Residuals



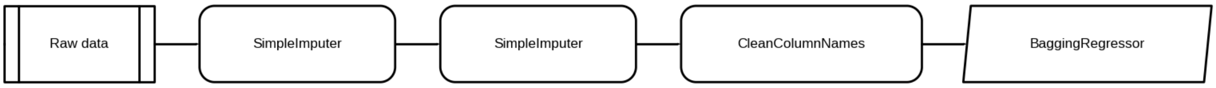

```
1 # assuming the data is already preprocessed and the setup is complete
2 ensemble = ensemble_model(best_tune, method = 'Bagging')
```

```
MAE MSE RMSE R2 RMSLE MAPE
```

```
# evaluate and make predictions with the bagging model
evaluate_model(ensemble)
```

Plot Type:

Pipeline Plot | Hyperparameters | Residuals | Prediction Error | Cooks Distance | Feature Selection
Learning Curve | Manifold Learning | Validation Curve | Feature Importance | Feature Importance… | Decision Tree
Interactive Residuals




```
predictions = predict_model(best_tune)
predictions2 = predict_model(ensemble)
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	Extra Trees Regressor	32.9447	8351.0648	91.3842	0.9653	0.0492	0.0165

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	Bagging Regressor	48.1688	9855.8595	99.2767	0.9591	0.0544	0.0250

```
predictions
```

	Gender	Age	Weight	Height	BMI	ICU	WBC	Hb	PLT	CRP	...	TZP	FLC	FQ	Crcl	Clvanco	Vd	Ke
145	0	75	70.0	150.0	31.100000	0	3.9	11.3	115	2.470000	...	0	0	0	79.000000	3.5	49.000000	0.070
280	0	79	48.0	157.0	19.500000	1	7.3	9.0	370	41.070000	...	0	0	0	93.400002	4.0	33.599998	0.082
175	1	57	43.0	172.0	14.500000	0	9.5	8.7	141	101.720001	...	0	0	0	190.699997	8.1	30.100000	0.163
373	1	65	70.0	170.0	24.200001	1	8.3	9.1	339	7.140000	...	0	0	0	98.500000	4.3	49.000000	0.086
420	1	87	55.0	170.0	19.000000	1	10.7	10.1	236	78.449997	...	0	0	0	63.299999	2.8	38.500000	0.057
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
57	0	75	60.0	162.0	22.900000	0	11.5	10.0	218	198.199997	...	0	0	0	86.900002	3.8	42.000000	0.077
415	1	66	75.0	178.0	23.700001	0	0.1	6.6	16	33.709999	...	0	0	0	89.599998	4.0	52.500000	0.079
24	0	58	60.0	160.0	23.400000	1	19.9	11.0	393	90.570000	...	0	0	0	98.400002	4.3	42.000000	0.086
17	0	82	51.0	135.0	28.000000	0	6.9	14.2	186	1.000000	...	0	0	0	57.200001	2.5	35.700001	0.052
66	0	82	51.0	135.0	28.000000	0	6.9	14.2	186	1.000000	...	0	0	0	57.200001	2.5	35.700001	0.052

```
# round off the prediction values to the nearest fifty
rounded_values = [round_to_nearest_fifty(num) for num in predictions['prediction_label']]

predictions["prediction_label"]= rounded_values

# create a dataframe to hold the true and predicted values
df_result = pd.DataFrame()
df_result['true'] = predictions['Initial VCM_daily_dose']
df_result['prediction'] = predictions['prediction_label']
```

```
predictions
```

	Gender	Age	Weight	Height	BMI	ICU	WBC	Hb	PLT	CRP	...	TZP	FLC	FQ	Crcl	Clvanco	Vd	Ke
145	0	75	70.0	150.0	31.100000	0	3.9	11.3	115	2.470000	...	0	0	0	79.000000	3.5	49.000000	0.070
280	0	79	48.0	157.0	19.500000	1	7.3	9.0	370	41.070000	...	0	0	0	93.400002	4.0	33.599998	0.082
175	1	57	43.0	172.0	14.500000	0	9.5	8.7	141	101.720001	...	0	0	0	190.699997	8.1	30.100000	0.163
373	1	65	70.0	170.0	24.200001	1	8.3	9.1	339	7.140000	...	0	0	0	98.500000	4.3	49.000000	0.086

```
df_result['prediction']
```

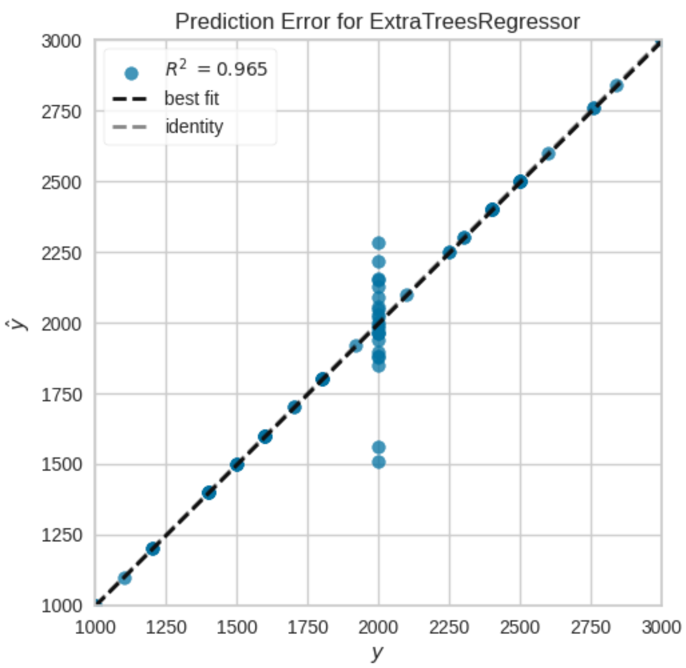
```
145    1950
280    1600
175    1200
373    2000
420    1900
       ...
57     2400
415    2100
24     1950
17     1500
66     1500
Name: prediction, Length: 85, dtype: int64
```

Results

```
df_result['accuracy'] = np.where(abs(df_result['true'] - df_result['prediction']) <= 50, 1, 0)
accuracy = round((len(df_result.loc[df_result['accuracy'] == 1])/ len(df_result)) * 100, 1)
print('Accuracy: ', accuracy, '%')

```

```
Accuracy:  85.9 %
```

```
plot_model(best_tune, plot = 'error')
```

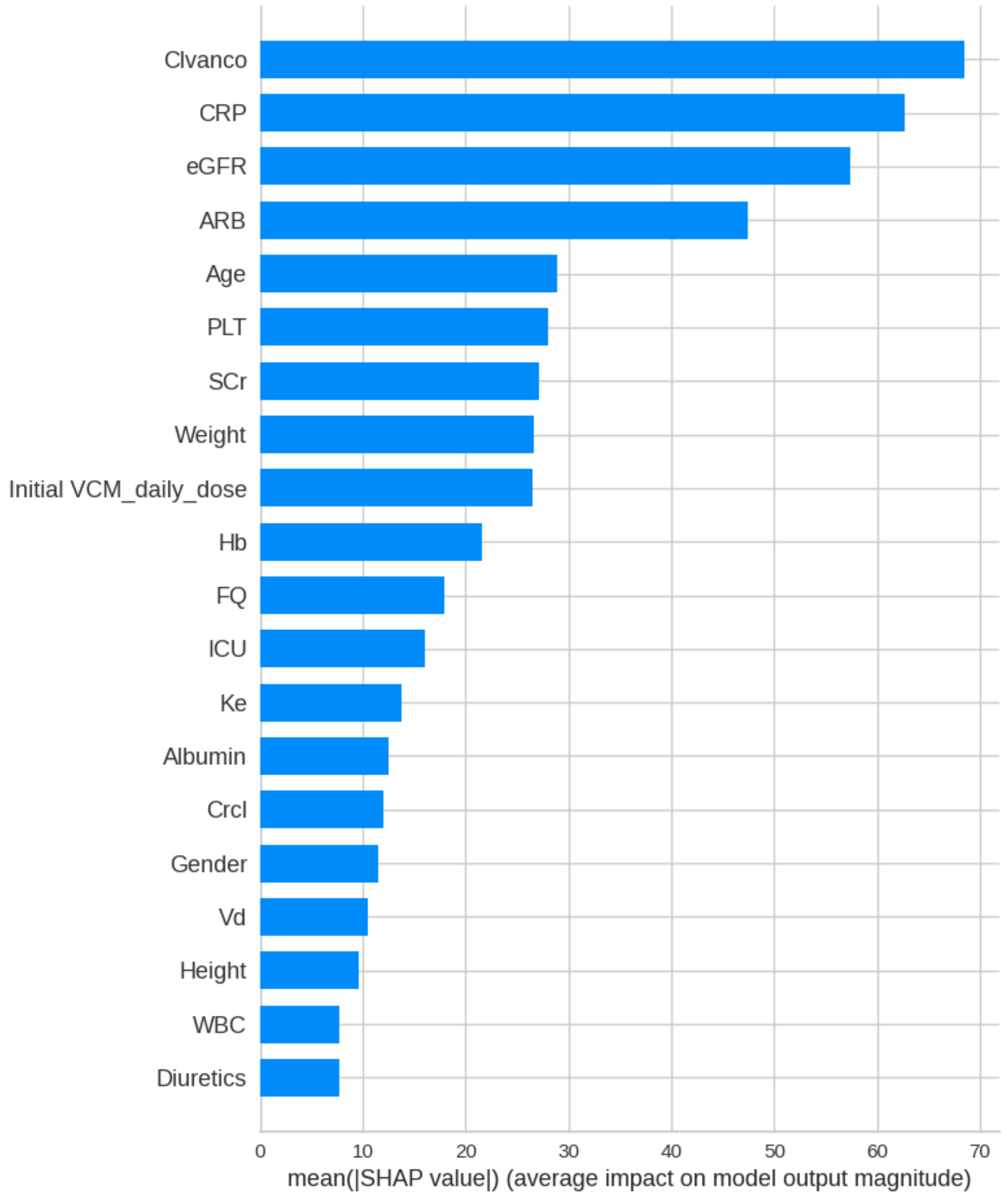


Feature engineering using SHAP

```
# create a shap explainer object
explainer = shap.Explainer(best_tune)
```

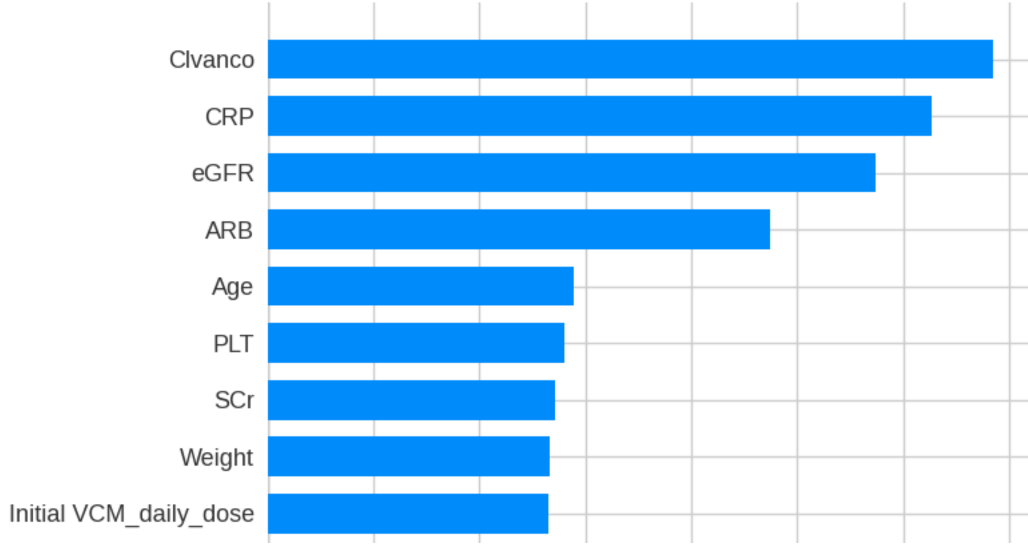
```
# calculate shap values on your data
shap_values = explainer.shap_values(df_D)
```

```
# plot the shap values
shap.summary_plot(shap_values, df_D, plot_type="bar" )
```




```
# get feature importance
feature_importance = np.abs(shap_values).mean(axis=0)
feature_importance = pd.Series(feature_importance, index=df_D.columns)

# get top 10 important features
top_10_features = feature_importance.sort_values(ascending=False)[:10].index

# create a new dataframe with only the top 10 important features
df_D_important = df_D[top_10_features]
```

```
# get indices of the selected features
selected_features_indices = [df_D.columns.tolist().index(feature) for feature in top_10_features]

# plot SHAP values of the selected features
shap.summary_plot(shap_values[:, selected_features_indices], df_D[top_10_features], plot_type="bar" )
```



Feature selection based on pycaret & SHAP feature importance

```
Pycaret_Feature_importance = ['Weight', 'Vd', 'Age', 'BUN', 'Half_life', 'eGFR', 'Height','Clvanco', 'I
SHAP_Feature_importance = ['Clvanco', 'CRP', 'eGFR', 'ARB', 'Age', 'PLT','SCr', 'Weight', 'Hb','Gender

# Convert the lists to sets and union them
union_set = set(Pycaret_Feature_importance) | set(SHAP_Feature_importance)

# Convert the result back to a list
union_list = list(union_set)
union_list
```

```
['Gender',
 'Clvanco',
 'BUN',
 'Half_life',
 'eGFR',
 'ACEi',
 'Hb',
 'Vd',
 'CRP',
 'PLT',
 'Height',
 'Ke',
 'Weight',
 'ARB',
 'Age',
 'SCr']
```

```
df_D2 = df_D[union_list].copy()
df_D2 = df_D2[['Gender', 'Age', 'Weight', 'Height', 'Hb', 'PLT', 'CRP', 'eGFR', 'BUN', 'SCr','ACEi', '.
df_D2['Initial VCM_daily_dose'] = df_D['Initial VCM_daily_dose']
df_D2
```

Gender	Age	Weight	Height	Hb	PLT	CRP	eGFR	BUN	SCr	ACEi	ARB	Clvanco	Vd	Ke	Half_life	Initial VCM_daily_dose

```
reg3 = setup(data=df_D2,
             target='Initial VCM_daily_dose',
             train_size=0.8,
             fold=5,
             fold_shuffle=True,
             use_gpu=True,
             session_id=42
            )

```

	Description	Value
0	Session id	42
1	Target	Initial VCM_daily_dose
2	Target type	Regression
3	Original data shape	(424, 17)
4	Transformed data shape	(424, 17)
5	Transformed train set shape	(339, 17)
6	Transformed test set shape	(85, 17)
7	Numeric features	16
8	Preprocess	True
9	Imputation type	simple
10	Numeric imputation	mean
11	Categorical imputation	mode
12	Fold Generator	KFold
13	Fold Number	5
14	CPU Jobs	-1
15	Use GPU	True
16	Log Experiment	False
17	Experiment Name	reg-default-name
18	USI	889d

```
best = compare_models(sort='mse')
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE	TT (Sec
et	Extra Trees Regressor	32.7330	8448.4357	90.6314	0.9624	0.0487	0.0164	0.36

```
best_tune = tune_model(best)
```

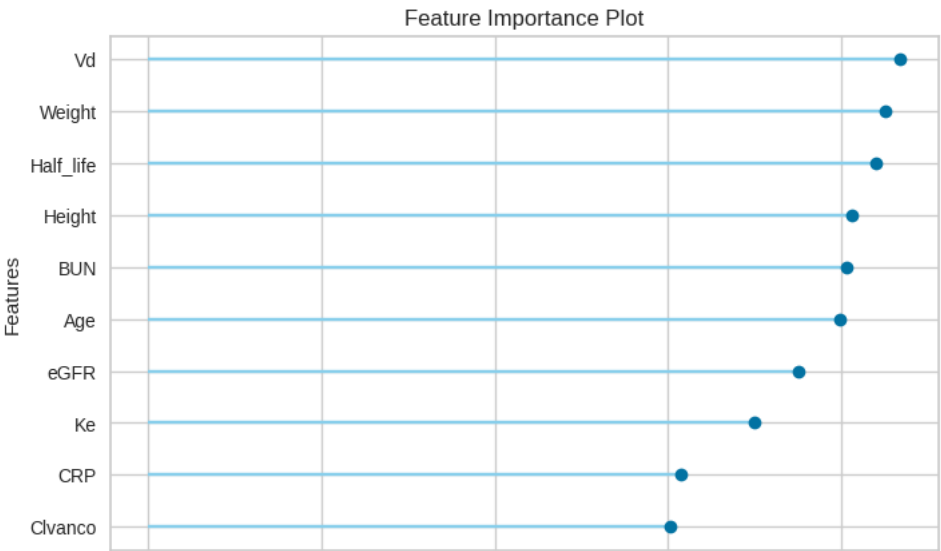
	MAE	MSE	RMSE	R2	RMSLE	MAPE
Fold						
0	138.4744	32343.0653	179.8418	0.8496	0.1018	0.0784
1	184.2888	61969.6985	248.9371	0.7501	0.1434	0.1076
2	153.4366	36494.7437	191.0360	0.8300	0.1198	0.0953
3	158.3576	37017.0786	192.3982	0.8218	0.1135	0.0925
4	140.5048	33288.2305	182.4506	0.8638	0.1026	0.0773
Mean	155.0125	40222.5633	198.9327	0.8231	0.1162	0.0902
Std	16.4606	11020.7179	25.4622	0.0393	0.0152	0.0113

```
Fitting 5 folds for each of 10 candidates, totalling 50 fits
Original model was better than the tuned model, hence it will be returned. NOTE: The display metrics are for the tuned model (not the original o
```

```
# evaluate and make predictions with the best model
evaluate_model(best_tune)
```

Plot Type:

Pipeline Plot	Hyperparameters	Residuals	Prediction Error	Cooks Distance	Feature Selection
Learning Curve	Manifold Learning	Validation Curve	Feature Importance	Feature Importance...	Decision Tree
Interactive Residuals					




```
predictions = predict_model(best_tune)
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	Extra Trees Regressor	28.5347	7675.5623	87.6103	0.9681	0.0476	0.0143

```
# round off the prediction values to the nearest fifty
rounded_values = [round_to_nearest_fifty(num) for num in df_result['prediction']]

predictions["prediction_label"]= rounded_values

# create a dataframe to hold the true and predicted values
df_result = pd.DataFrame()
df_result['true'] = predictions['Initial VCM_daily_dose']
df_result['prediction'] = predictions['prediction_label']
```

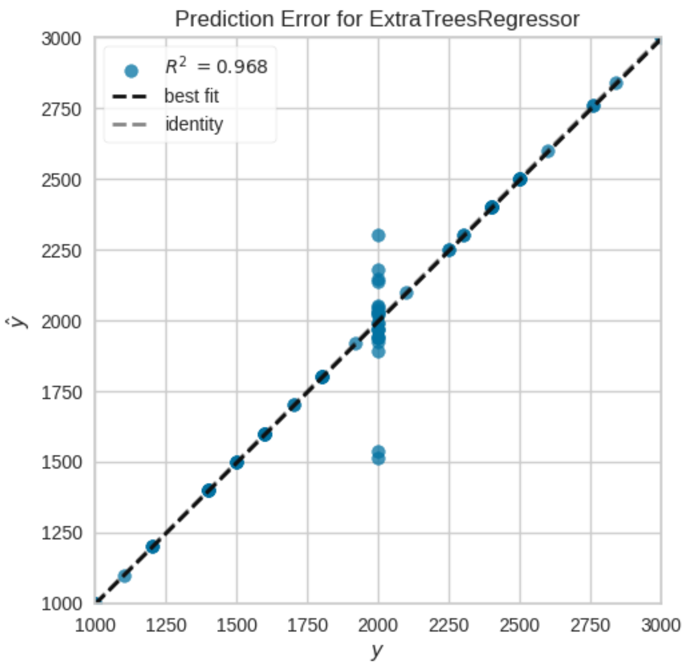
```
1 predictions
```

	Gender	Age	Weight	Height	Hb	PLT	CRP	eGFR	BUN	SCr	ACEi	ARB	Clvanco	Vd	Ke	Half_life	VCM_d
145	0	75	70.0	150.0	11.3	115	2.470000	84	14.800000	0.68	0	0	3.5	49.000000	0.070	9.9	
280	0	79	48.0	157.0	9.0	370	41.070000	90	11.700000	0.37	0	1	4.0	33.599998	0.082	8.5	
175	1	57	43.0	172.0	8.7	141	101.720001	90	3.900000	0.26	0	0	8.1	30.100000	0.163	4.3	
373	1	65	70.0	170.0	9.1	339	7.140000	90	10.200000	0.74	0	0	4.3	49.000000	0.086	8.0	
420	1	87	55.0	170.0	10.1	236	78.449997	90	19.799999	0.64	0	0	2.8	38.500000	0.057	12.2	
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	
57	0	75	60.0	162.0	10.0	218	198.199997	90	7.900000	0.53	0	0	3.8	42.000000	0.077	9.1	
415	1	66	75.0	178.0	6.6	16	33.709999	89	27.700001	0.86	0	0	4.0	52.500000	0.079	8.8	
24	0	58	60.0	160.0	11.0	393	90.570000	90	20.700001	0.59	0	1	4.3	42.000000	0.086	8.0	
17	0	82	51.0	135.0	14.2	186	1.000000	90	12.300000	0.61	0	0	2.5	35.700001	0.052	13.3	
66	0	82	51.0	135.0	14.2	186	1.000000	90	12.300000	0.61	0	0	2.5	35.700001	0.052	13.3	

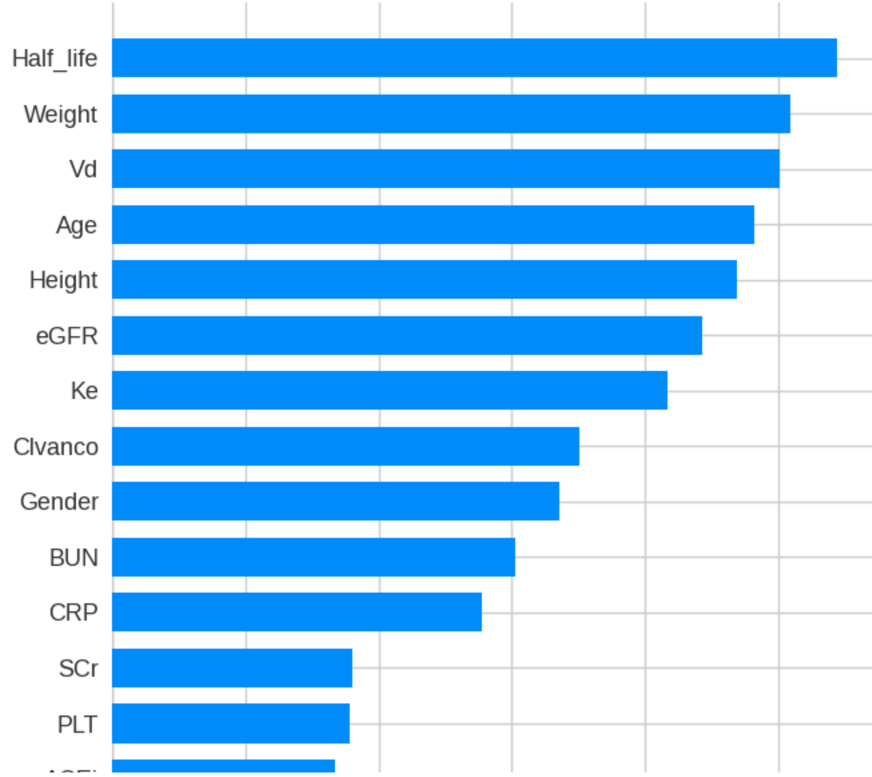
```
1 df_result['accuracy'] = np.where(abs(df_result['true'] - df_result['prediction']) <= 50, 1, 0)
2 accuracy = round((len(df_result.loc[df_result['accuracy'] == 1])/ len(df_result)) * 100, 1)
3 print('Accuracy: ', accuracy, '%')
4
```

```
Accuracy:  85.9 %
```

```
1 plot_model(best_tune, plot = 'error')
```




```
1 explainer = shap.Explainer(best_tune)
2 shap_values = explainer.shap_values(df_D2)
3 shap.summary_plot(shap_values, df_D2, plot_type="bar" )
```



Log Transformation of augmented dataset of 'Initial VCM_daily_dose'

```
1 df_D2['Initial VCM_daily_dose']
```

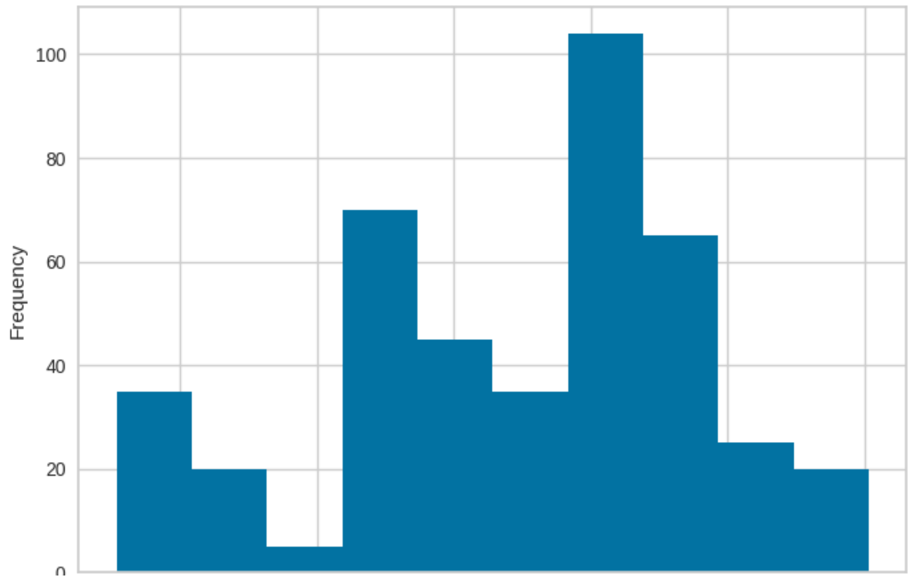
```
0      2300
1      2400
2      1380
3      1400
4      2750
       ...
419    2000
420    2000
421    1920
422    2400
423    2000
Name: Initial VCM_daily_dose, Length: 424, dtype: int64
```

```
1 df_D2['Initial VCM_daily_dose_log'] = df_D2['Initial VCM_daily_dose'].apply(lambda x: math.log(x))
2 df_D2
```

	Gender	Age	Weight	Height	Hb	PLT	CRP	eGFR	BUN	SCr	ACEi	ARB	Clvanco	Vd	Ke	Half_life	Initial VCM_daily_dose	VCM
0	1	48	80.0	171.0	10.1	396	113.99	90	6.7	0.67	0	0	6.6	56.0	0.131	5.3	2300	
1	1	55	85.0	180.0	8.5	501	84.08	82	10.4	0.95	0	0	4.7	59.5	0.092	7.5	2400	
2	0	91	41.0	148.0	7.4	159	34.18	52	32.3	1.00	0	0	1.1	28.7	0.024	28.8	1380	
3	0	82	50.0	150.0	10.4	228	159.65	90	10.3	0.40	0	1	3.7	35.0	0.075	9.2	1400	
4	1	59	53.0	165.0	10.7	271	94.45	90	7.7	0.65	0	0	4.0	37.1	0.081	8.6	2750	
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	
419	0	79	65.0	160.0	10.4	646	23.85	90	21.6	0.55	0	1	3.7	45.5	0.075	9.2	2000	
420	1	87	55.0	170.0	10.1	236	78.45	90	19.8	0.64	0	0	2.8	38.5	0.057	12.2	2000	
421	1	69	64.0	164.0	12.8	196	1.62	90	13.0	0.76	0	0	3.7	44.8	0.073	9.5	1920	
422	1	68	56.0	165.0	9.1	97	241.25	90	36.1	0.67	0	0	3.7	39.2	0.074	9.4	2400	
423	1	66	75.0	167.0	13.4	246	5.27	82	19.9	0.92	0	0	3.7	52.5	0.074	9.4	2000	

```
1 df_D2['Initial VCM_daily_dose_log'].plot.hist(bins=10)
```

```
&lt;Axes: ylabel='Frequency'&gt;
```




```
df_D3=df_D2.drop(columns='Initial VCM_daily_dose')
```

```
reg4 = setup(data=df_D3,
             target='Initial VCM_daily_dose_log',
             train_size=0.8,
             fold=5,
             fold_shuffle=True,
             use_gpu=True,
             session_id=42
            )

```

	Description	Value
0	Session id	42
1	Target	Initial VCM_daily_dose_log
2	Target type	Regression
3	Original data shape	(424, 17)
4	Transformed data shape	(424, 17)
5	Transformed train set shape	(339, 17)
6	Transformed test set shape	(85, 17)
7	Numeric features	16
8	Preprocess	True
9	Imputation type	simple
10	Numeric imputation	mean
11	Categorical imputation	mode
12	Fold Generator	KFold
13	Fold Number	5
14	CPU Jobs	-1
15	Use GPU	True
16	Log Experiment	False
17	Experiment Name	reg-default-name
18	USI	f142

```
best = compare_models(sort='mse')
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE	TT (Sec)
et	Extra Trees Regressor	0.0183	0.0032	0.0552	0.9572	0.0065	0.0024	0.3560
xgboost	Extreme Gradient Boosting	0.0232	0.0042	0.0631	0.9433	0.0074	0.0031	0.2180
catboost	CatBoost Regressor	0.0388	0.0043	0.0646	0.9422	0.0076	0.0051	15.5700
lightgbm	Light Gradient Boosting Machine	0.0475	0.0063	0.0783	0.9155	0.0092	0.0063	0.0840
rf	Random Forest Regressor	0.0474	0.0072	0.0821	0.9048	0.0097	0.0063	0.4780
gbr	Gradient Boosting Regressor	0.0538	0.0072	0.0840	0.9036	0.0099	0.0071	0.2040
dt	Decision Tree Regressor	0.0301	0.0098	0.0977	0.8651	0.0115	0.0040	0.0960
ada	AdaBoost Regressor	0.1153	0.0174	0.1319	0.7637	0.0155	0.0154	0.1640
lr	Linear Regression	0.1719	0.0433	0.2073	0.4174	0.0245	0.0230	0.1060
ridge	Ridge Regression	0.1737	0.0439	0.2088	0.4099	0.0248	0.0233	0.0920
knn	K Neighbors	0.1657	0.0477	0.2175	0.3479	0.0259	0.0223	0.1720

```
1 best_tune = tune_model(best)
```

Fold	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	0.0888	0.0129	0.1134	0.8039	0.0134	0.0118
1	0.1278	0.0263	0.1621	0.6808	0.0193	0.0172
2	0.1034	0.0167	0.1292	0.7658	0.0155	0.0140
3	0.0970	0.0142	0.1191	0.8096	0.0142	0.0130
4	0.0941	0.0153	0.1236	0.8003	0.0146	0.0125
Mean	0.1022	0.0171	0.1295	0.7721	0.0154	0.0137
Std	0.0136	0.0048	0.0171	0.0482	0.0021	0.0019

```
Fitting 5 folds for each of 10 candidates, totalling 50 fits
Original model was better than the tuned model, hence it will be returned. NOTE: The display metrics are for the tuned model (not the original o
```

```
1 # evaluate and make predictions with the best model
2 evaluate_model(best_tune)
```

Plot Type:

```
predictions = predict_model(best_tune)
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	Extra Trees Regressor	0.0162	0.0025	0.0497	0.9677	0.0058	0.0021

Vd

```
predictions
```

	Gender	Age	Weight	Height	Hb	PLT	CRP	eGFR	BUN	SCr	ACEi	ARB	Clvanco	Vd	Ke	Half_life	VCM_d:
145	0	75	70.0	150.0	11.3	115	2.470000	84	14.800000	0.68	0	0	3.5	49.000000	0.070	9.9	
280	0	79	48.0	157.0	9.0	370	41.070000	90	11.700000	0.37	0	1	4.0	33.599998	0.082	8.5	
175	1	57	43.0	172.0	8.7	141	101.720001	90	3.900000	0.26	0	0	8.1	30.100000	0.163	4.3	
373	1	65	70.0	170.0	9.1	339	7.140000	90	10.200000	0.74	0	0	4.3	49.000000	0.086	8.0	
420	1	87	55.0	170.0	10.1	236	78.449997	90	19.799999	0.64	0	0	2.8	38.500000	0.057	12.2	
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	
57	0	75	60.0	162.0	10.0	218	198.199997	90	7.900000	0.53	0	0	3.8	42.000000	0.077	9.1	
415	1	66	75.0	178.0	6.6	16	33.709999	89	27.700001	0.86	0	0	4.0	52.500000	0.079	8.8	
24	0	58	60.0	160.0	11.0	393	90.570000	90	20.700001	0.59	0	1	4.3	42.000000	0.086	8.0	
17	0	82	51.0	135.0	14.2	186	1.000000	90	12.300000	0.61	0	0	2.5	35.700001	0.052	13.3	
66	0	82	51.0	135.0	14.2	186	1.000000	90	12.300000	0.61	0	0	2.5	35.700001	0.052	13.3	

```
df_result = pd.DataFrame()
df_result['Initial VCM_daily_dose_log'] = predictions['Initial VCM_daily_dose_log']
df_result['prediction_label_log']=predictions['prediction_label']
```

```
index_list = [145, 280, 175, 373, 420, 73, 132, 137, 30, 72, 70, 94, 316, 90, 376, 416, 9, 247, 196, 2
index_series = pd.Series(index_list)  # Convert the list to a pandas Series

# List comprehension to store values
value_list = [df_D2.loc[index, 'Initial VCM_daily_dose'] for index in index_series]

print(value_list)


```

```
[2000, 1600, 1200, 2000, 2000, 1400, 2840, 2400, 1800, 1000, 2000, 2300, 1800, 1920, 1700, 3000, 2000, 1600, 2000, 1200, 1000, 1600, 2760, 1600,
```

```
df_result['Initial VCM_daily_dose']=value_list
df_result
```

```
df_result['prediction'] = np.exp(df_result['prediction_label_log'])
```

```
df_result
```

	Initial VCM_daily_dose_log	prediction_label_log	Initial VCM_daily_dose	prediction
145	7.600903	7.594826	2000	1987.884370
280	7.377759	7.377759	1600	1600.000115
175	7.090077	7.090077	1200	1200.000105
373	7.600903	7.630908	2000	2060.920649
420	7.600903	7.539718	2000	1881.298901
...	...	...	...	...
57	7.783224	7.783224	2400	2400.000215
415	7.600903	7.673586	2000	2150.780775
24	7.600903	7.616061	2000	2030.548697
17	7.313221	7.313221	1500	1500.000171
66	7.313221	7.313221	1500	1500.000171

85 rows × 4 columns

```
# round off the prediction values to the nearest fifty
rounded_values = [round_to_nearest_fifty(num) for num in df_result['prediction']]
df_result['prediction']= rounded_values
df_result
```

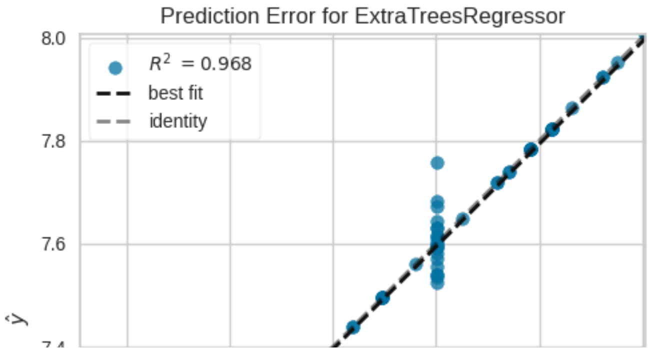
	Initial VCM_daily_dose_log	prediction_label_log	Initial VCM_daily_dose	prediction
145	7.600903	7.594826	2000	2000
280	7.377759	7.377759	1600	1600
175	7.090077	7.090077	1200	1200
373	7.600903	7.630908	2000	2050
420	7.600903	7.539718	2000	1900
...	...	...	...	...
57	7.783224	7.783224	2400	2400
415	7.600903	7.673586	2000	2150
24	7.600903	7.616061	2000	2050
17	7.313221	7.313221	1500	1500
66	7.313221	7.313221	1500	1500

85 rows × 4 columns

```
df_result['accuracy'] = np.where(abs(df_result['Initial VCM_daily_dose'] - df_result['prediction']) <
accuracy = round((len(df_result.loc[df_result['accuracy'] == 1])/ len(df_result)) * 100, 1)
print('Accuracy: ', accuracy, '%')
```

```
Accuracy:  87.1 %
```

```
plot_model(best_tune, plot = 'error')
```




```
final_VancoAI = finalize_model(estimator=best_tune)
```

```
save_model(model=final_VancoAI,
           model_name='final_VancoAI',
           verbose=False)
```

```
(Pipeline(memory=FastMemory(location=/tmp/joblib),
          steps=[('numerical_imputer',
                  TransformerWrapper(include=['Gender', 'Age', 'Weight',
                                              'Height', 'Hb', 'PLT', 'CRP',
                                              'eGFR', 'BUN', 'SCr', 'ACEi',
                                              'ARB', 'CIvanco', 'Vd', 'Ke',
                                              'Half_life'],
                                     transformer=SimpleImputer())),
                 ('categorical_imputer',
                  TransformerWrapper(include=[],
                                     transformer=SimpleImputer(strategy='most_frequent'))),
                 ('clean_column_names',
                  TransformerWrapper(transformer=CleanColumnNames())),
                 ('actual_estimator',
                  ExtraTreesRegressor(n_jobs=-1, random_state=42))]),
 'final_VancoAI.pkl')
```

```
from pycaret.regression import load_model
```

✓ 0초 오전 1:16에 완료됨