Regression Model Analysis of FDA Subset Data

- The Pycaret package will be utilized to first determine the best performing model on the data using the compare_models function.
- Then the model's model hyperparameters will be tuned using the tune_model function which uses cross-validation to test different combinations of hyperparameters.
- Followed by testing both bagging and boosting ensembles with the model.
- After the model with the maximum performance based on (R^2, RMSE, and MAPE) is chosen it will be finalized and saved.

In [1]:
```
import numpy as np
import pandas as pd
from sklearn import datasets, metrics
from pycaret.datasets import get_data
from pycaret.regression import *
import warnings
warnings.filterwarnings("ignore")
```

In [2]:
```
# set up PyCaret
data = pd.read_csv('D:/DataSets/FDA_1615.csv')
exclude_columns = ['zinc_id', 'smiles', 'Molecule Name', 'ROMol', 'Fingerprint'
target_column = 'similarity_mean'

# Create a new dataframe with the columns of interest
X = data.drop(exclude_columns + [target_column], axis=1)
y = data[target_column]
data = pd.concat([X, y], axis=1)

reg_model = setup(data, target=target_column, numeric_imputation="drop", catego

# Compare models using Pycaret
best_model = compare_models()

# Fine-tune the best model using Pycaret (RandomGridSearch, sklearn)
tuned_sk = tune_model(best_model, choose_better = True)

# tune model optuna
tuned_opt = tune_model(best_model, search_library = 'optuna', choose_better = T
```

. . .

Bagged Model

In [3]:
```python
# ensemble model
bagged_model = ensemble_model(best_model, choose_better = True)

type(bagged_model)
# >>> sklearn.ensemble._bagging.BaggingRegressor

print(bagged_model)
```

Fold	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	0.0031	0.0000	0.0043	0.9534	0.0039	0.0353
1	0.0037	0.0000	0.0052	0.9565	0.0048	0.0632
2	0.0035	0.0000	0.0049	0.9475	0.0044	0.0384
3	0.0033	0.0000	0.0048	0.9340	0.0044	0.0361
4	0.0033	0.0000	0.0047	0.9438	0.0042	0.0341
5	0.0033	0.0000	0.0046	0.9574	0.0042	0.0367
6	0.0034	0.0000	0.0045	0.9409	0.0041	0.0383
7	0.0034	0.0000	0.0047	0.9412	0.0043	0.0379
8	0.0028	0.0000	0.0039	0.9537	0.0036	0.0302
9	0.0033	0.0000	0.0043	0.9596	0.0039	0.0353
Mean	0.0033	0.0000	0.0046	0.9488	0.0042	0.0386
Std	0.0002	0.0000	0.0003	0.0081	0.0003	0.0085

```
Original model was better than the ensembled model, hence it will be returne
d. NOTE: The display metrics are for the ensembled model (not the original on
e).
LGBMRegressor(device='gpu', n_jobs=-1, random_state=158)
```

Boosted Model

In [4]:
```
# ensemble model
boosted_model = ensemble_model(best_model, method = 'Boosting', choose_better =

type(boosted_model)
# >>> sklearn.ensemble._weight_boosting.AdaBoostRegressor

print(boosted_model)
```

Fold	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	0.0026	0.0000	0.0036	0.9663	0.0033	0.0298
1	0.0031	0.0000	0.0042	0.9713	0.0039	0.0509
2	0.0031	0.0000	0.0043	0.9588	0.0039	0.0354
3	0.0031	0.0000	0.0045	0.9421	0.0041	0.0344
4	0.0029	0.0000	0.0043	0.9531	0.0039	0.0304
5	0.0030	0.0000	0.0043	0.9637	0.0039	0.0330
6	0.0029	0.0000	0.0043	0.9456	0.0039	0.0325
7	0.0033	0.0000	0.0047	0.9409	0.0043	0.0364
8	0.0026	0.0000	0.0036	0.9624	0.0032	0.0284
9	0.0029	0.0000	0.0040	0.9645	0.0037	0.0325
Mean	0.0030	0.0000	0.0042	0.9569	0.0038	0.0344
Std	0.0002	0.0000	0.0003	0.0102	0.0003	0.0060

```
AdaBoostRegressor(estimator=LGBMRegressor(device='gpu', n_jobs=-1,
                                          random_state=158),
                  n_estimators=10, random_state=158)
```

In [5]:
```
# Evaluate the transformed model on the original test data
evaluate_model(boosted_model)
```

```
interactive(children=(ToggleButtons(description='Plot Type:', icons=('',), op
tions=(('Pipeline Plot', 'pipelin…
```

In [6]:
```python
# Predict on hold-out
predict_model(boosted_model)
```

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	AdaBoost Regressor	0.0028	0.0000	0.0039	0.9612	0.0036	0.0312

Out[6]:

	feature_0	feature_1	feature_2	feature_3	feature_4	feature_5	feature_6	feature_7	feature
1128	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
865	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
1284	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
1261	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
399	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
...	...	...	...	...	...	...	...	...	
486	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
404	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
1606	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
327	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
1115	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

323 rows × 1617 columns

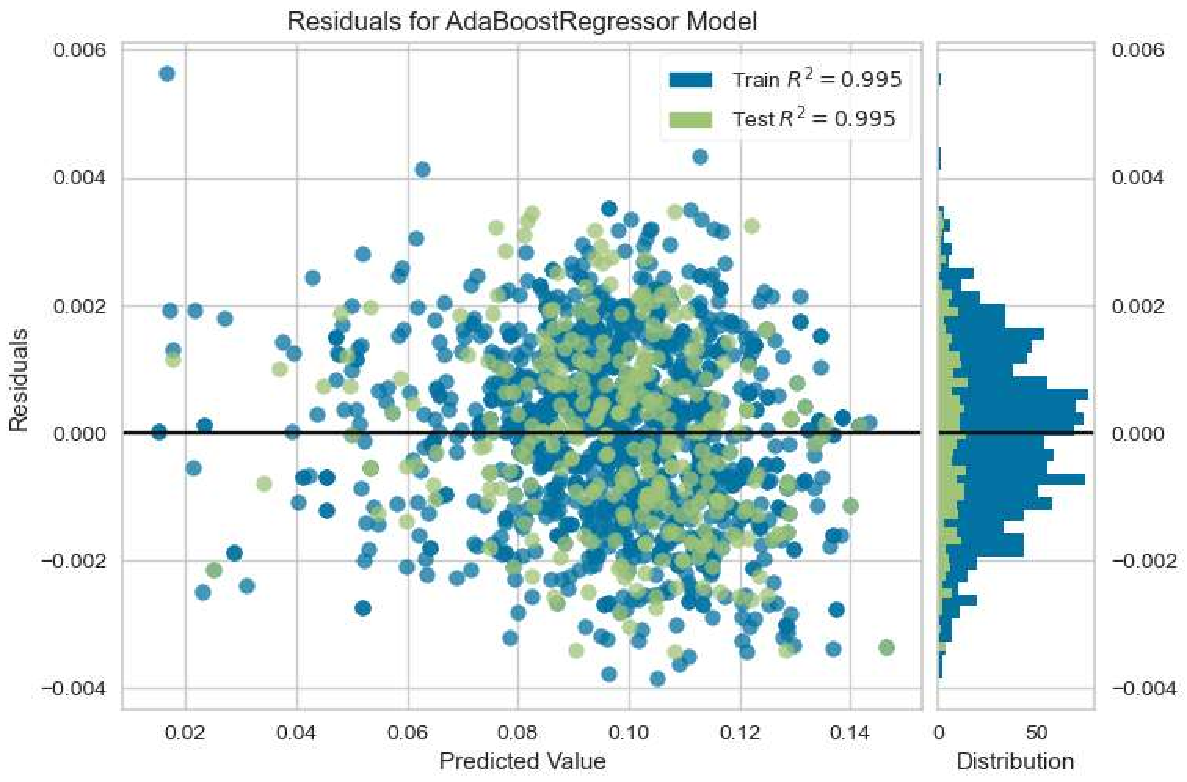
In [7]:
```python
# finalize and save the model, train model on entire dataset
final_model = finalize_model(boosted_model)

save_model(final_model, 'FDA_1615_Model_Boost')
```

```
Transformation Pipeline and Model Successfully Saved
```

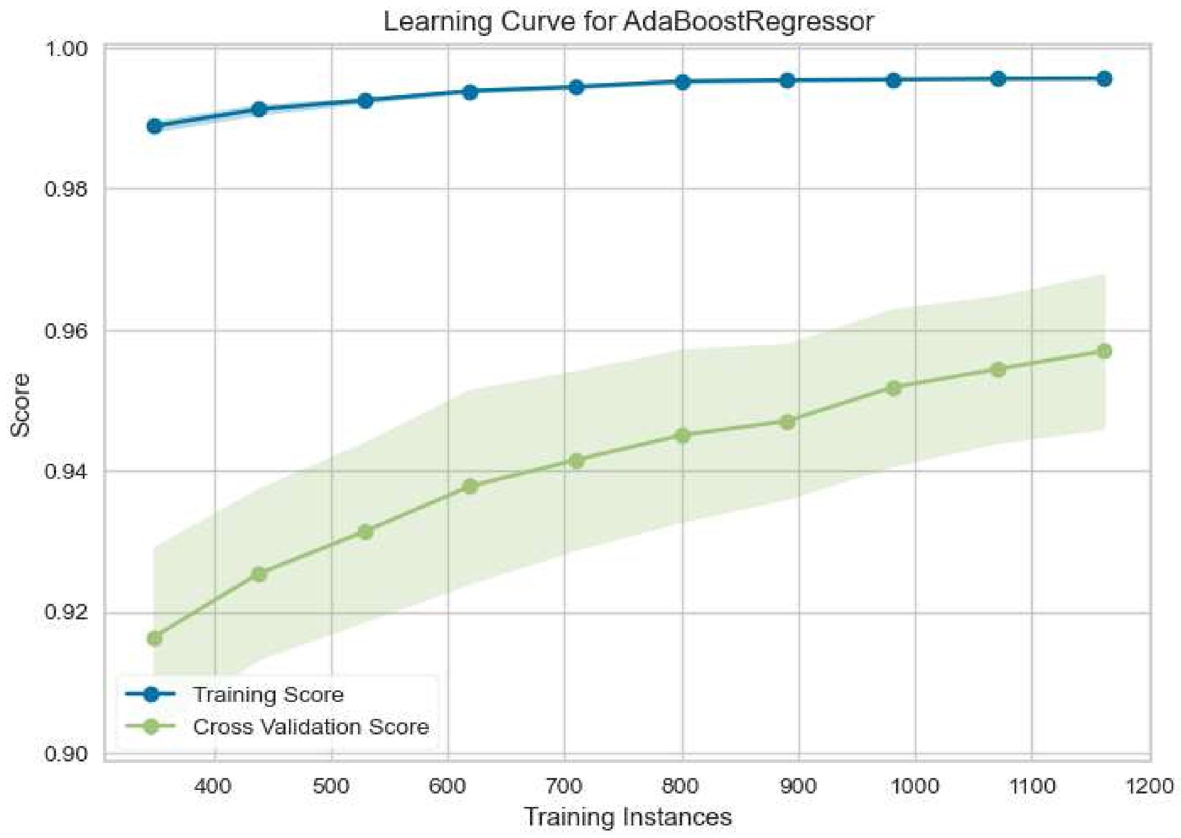
Out[7]:
```
(Pipeline(memory=FastMemory(location=C:\Users\jph41\AppData\Local\Temp\jobli
b),
          steps=[('placeholder', None),
                 ('actual_estimator',
                  AdaBoostRegressor(estimator=LGBMRegressor(device='gpu',
                                                             n_jobs=-1,
                                                             random_state=15
8),
                                    n_estimators=10, random_state=158))]),
 'FDA_1615_Model_Boost.pkl')
```

```
In [10]: plot_model(final_model, plot='residuals')
```



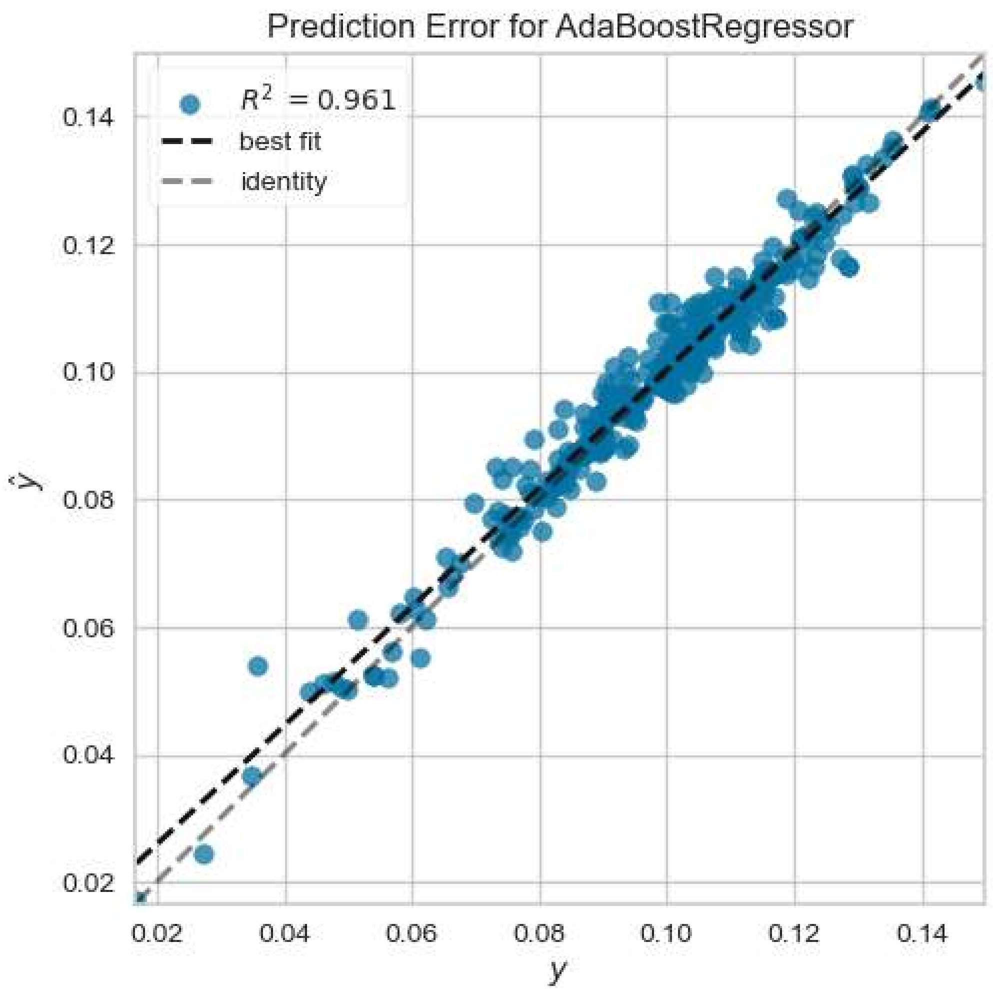
- In general a plot showing no clear pattern and some center bunching suggests that the model's performance is relatively good at predicting the mean value of the target variable, but may struggle to predict values that deviate significantly from the mean. This can be seen with several data points far from mean.

```
In [14]: plot_model(boosted_model, plot='learning')
```



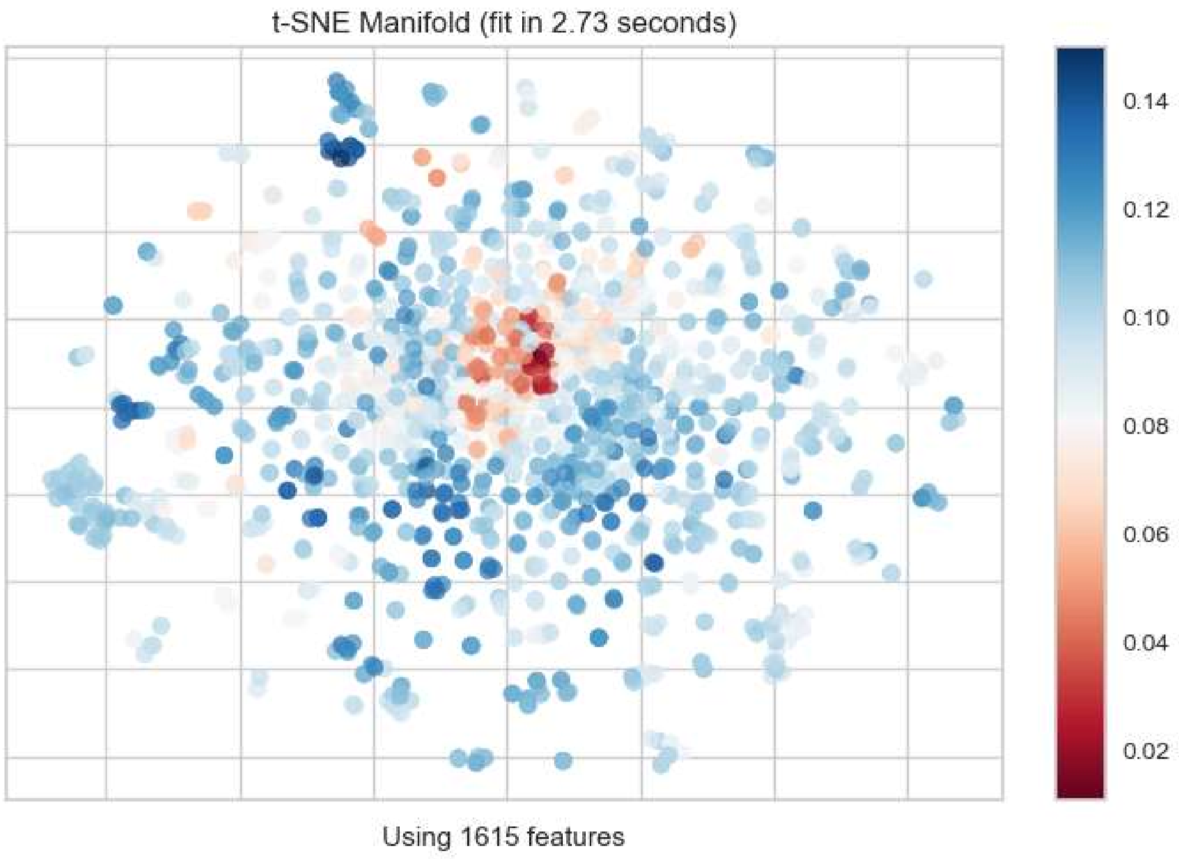
- The learning curve plot visualizes the performance of the algorithm as the training dataset increases.
- The training line has a slight rise and is above 0.98, indicating the model is able to learn from data well and can achieve a high training accuracy.
- The CV line rises from ~ 0.91 to 0.96, which means that as more training data is used, the performance of the model on the cross-validation data improves. An increasing CV line indicates that the model is generalizing well and will likely perform well on new data.

```
In [15]: plot_model(boosted_model, plot='error')
```



- A prediction plot is used to analyze the output of a model. In molecular similarity prediction, the plot displays the actual versus predicted values of molecular similarity scores. The plot shows some bunching in the upper right portion, this indicates that the model is slighlty overestimating the molecular similarity scores.

```
In [17]: plot_model(boosted_model, plot='manifold')
```



- The manifold plot shows the relationship between the instances in the high-dimensional space and how they are projected onto the lower-dimensional space.
- Clusters or patterns in the plot can indicate the presence of groups or subgroups within the data that may not be apparent in the higher-dimensional space. The dark cluster in the center would make sense for the data, molecules with structural elements in common should show as clusters.

LightGBM (Light Gradient Boosting Machine)

- A open-source, gradient-boosting framework that uses a tree-based learning algorithm. It uses the leaf-wise growth strategy that selects the leaf with the maximum delta loss to grow, which helps it to achieve higher accuracy.
- Each tree is trained on the error residuals of the previous trees, applying an iterative gradient descent process that progressively improves the model accuracy.

An ensemble method

- A process of combining multiple models to improve the accuracy and robustness of the predictions. They help in reducing overfitting, increasing stability, and improving generalization performance.

Boosting

- Is a type of ensemble method in which multiple weak models are combined to form a strong model. At each iteration, a new weak model is trained to correct the errors made by the previous models.

AdaBoost (Adaptive Boosting)

- An ensemble method that combines multiple weak learners to create a stronger and more accurate predictor.
- Each weak learner is trained using only a subset of the training data, and the weights of the training examples are adjusted to give more emphasis to the examples that are harder to predict.
- The final prediction is a weighted sum of all the weak learner predictions, where the weight of each weak learner reflects their predictive power.

Ensembling LigthGBM and AdaBoost

- This would combine the strengths of both algorithms and potentially improve the performance and stability of the overall model.
- Using LightGBM as the base model and employing AdaBoost to improve the predictions of the weaker learners.

- LightGBM is a popular gradient boosting algorithm known for its speed and scalability, AdaBoost is an adaptive boosting algorithm known for its ability to handle noisy data and reduce bias and variance.#

Model	Algorithm	MAE	MSE	RMSE	R2	RMSLE	MAPE	TT (Sec)
lightgbm	Light Gradient Boosting Machine	0.0032	0.0000	0.0044	0.9515	0.0041	0.0373	3.8900
catboost	CatBoost Regressor	0.0033	0.0000	0.0045	0.9509	0.0041	0.0387	12.3030
huber	Huber Regressor	0.0029	0.0000	0.0046	0.9481	0.0042	0.0377	4.4040
xgboost	Extreme Gradient Boosting	0.0032	0.0000	0.0048	0.9427	0.0044	0.0377	4.3310
ridge	Ridge Regression	0.0031	0.0000	0.0049	0.9426	0.0044	0.0393	2.8270
gbr	Gradient Boosting Regressor	0.0044	0.0000	0.0056	0.9232	0.0051	0.0503	4.6110
omp	Orthogonal Matching Pursuit	0.0042	0.0000	0.0057	0.9227	0.0052	0.0525	2.8140
rf	Random Forest Regressor	0.0040	0.0000	0.0057	0.9198	0.0052	0.0481	3.6490
br	Bayesian Ridge	0.0039	0.0000	0.0063	0.9017	0.0057	0.0460	4.3550
et	Extra Trees Regressor	0.0045	0.0001	0.0074	0.8631	0.0068	0.0548	3.6780
dt	Decision Tree Regressor	0.0047	0.0001	0.0078	0.8502	0.0071	0.0574	2.8390

Model	Algorithm	MAE	MSE	RMSE	R2	RMSLE	MAPE	TT (Sec)
ada	AdaBoost Regressor	0.0069	0.0001	0.0084	0.8296	0.0076	0.0804	4.1990
lar	Least Angle Regression	0.0103	0.0003	0.0147	0.3068	0.0133	0.1172	3.3470
knn	K Neighbors Regressor	0.0130	0.0003	0.0177	0.2249	0.0163	0.1438	2.8300
lasso	Lasso Regression	0.0154	0.0004	0.0204	-0.0019	0.0188	0.2132	2.7570
en	Elastic Net	0.0154	0.0004	0.0204	-0.0019	0.0188	0.2132	2.7950
llar	Lasso Least Angle Regression	0.0154	0.0004	0.0204	-0.0019	0.0188	0.2132	2.7810
dummy	Dummy Regressor	0.0154	0.0004	0.0204	-0.0019	0.0188	0.2132	2.7480
par	Passive Aggressive	0.0683	0.0049	0.0697	10.9370	0.0653	0.7056	2.7990

Ensemble Results

Fold	MAE	MSE	RMSE	R2	RMSLE	MAPE
0	0.0026	0.0000	0.0036	0.9663	0.0033	0.0298
1	0.0031	0.0000	0.0042	0.9713	0.0039	0.0509
2	0.0031	0.0000	0.0043	0.9588	0.0039	0.0354
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Std	0.0002	0.0000	0.0003	0.0102	0.0003	0.0060

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