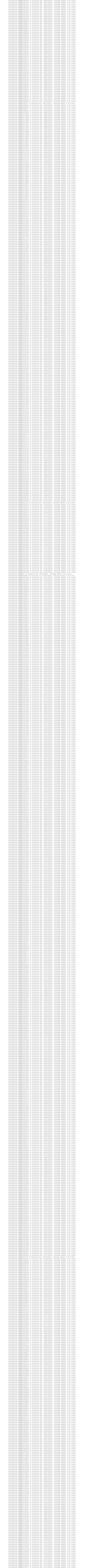
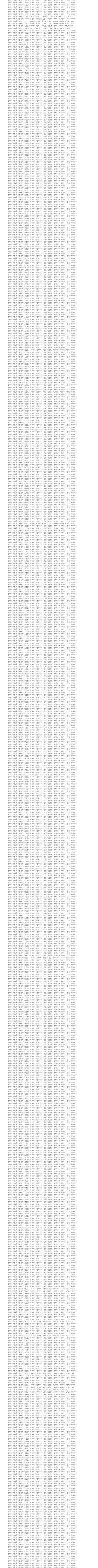
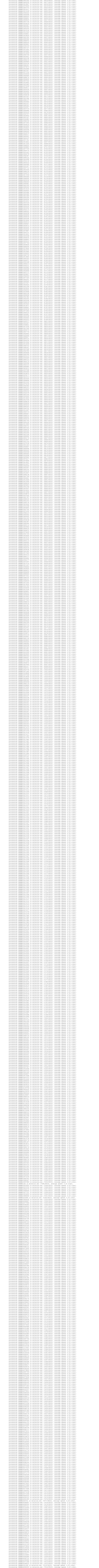


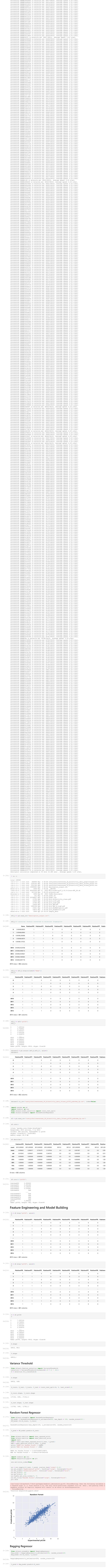
Processing CHEMBL2442324 in molecule.smi (4802/8915). Average speed: 0.22 s/mol. Processing CHEMBL2442320 in molecule.smi (4803/8915). Average speed: 0.22 s/mol. Processing CHEMBL2442319 in molecule.smi (4804/8915). Average speed: 0.22 s/mol. Processing CHEMBL3086102 in molecule.smi (4805/8915). Average speed: 0.22 s/mol. Processing CHEMBL3086104 in molecule.smi (4806/8915). Average speed: 0.22 s/mol. Processing CHEMBL3086103 in molecule.smi (4807/8915). Average speed: 0.22 s/mol. Processing CHEMBL3086105 in molecule.smi (4808/8915). Average speed: 0.22 s/mol. Processing CHEMBL3086106 in molecule.smi (4809/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087194 in molecule.smi (4810/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087195 in molecule.smi (4811/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087196 in molecule.smi (4813/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087197 in molecule.smi (4813/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087197 in molecule.smi (4814/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087198 in molecule.smi (4814/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087198 in molecule.smi (4814/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087198 in molecule.smi (4815/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087198 in molecule.smi (4815/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087198 in molecule.smi (4815/8915). Average speed: 0.22 s/mol. Processing CHEMBL3087198 in molecule.smi (4815/8915). Average speed: 0.22 s/mol.











In [129	<pre>print('RMSE for print('MAE for) RMSE for Bagging MAE for Bagging import seaborn i import matplotl. sns.set(color_color) ax = sns.regplor ax.set_xlabel(') ax.set_ylabel(') ax.set_ylabel(') ax.set_ylim(0, ax.figure.set_s.ax.set_title('Baplt.show /usr/local/lib/ps keyword args:</pre>	ib.pyplot as plt codes=True) ct(Y_test, Y_pred, scatter_kws={'alpha':0.4}) Experimental pIC50', fontsize='large', fontweight='bold') Predicted pIC50', fontsize='large', fontweight='bold') 12) 12) cize_inches(7, 7) cagging', fontsize='large', fontweight='bold') cython3.7/dist-packages/seaborn/_decorators.py:43: FutureWarning: Pass the following variables x, y. From version 0.12, the only valid positional argument will be `data`, and passing other
Out[129	s keyword args: rguments without FutureWarning	bythons.//dist-packages/seaporn/_decorators.py:43: Futurewarning: Pass the following variables x, y. From version 0.12, the only valid positional argument will be `data`, and passing other an explicit keyword will result in an error or misinterpretation. Stlib.pyplot.show> Bagging
In [130 Out[130	ABR_model = Adal ABR_model.fit(X	Experimental pIC50 egressor semble import AdaBoostRegressor BoostRegressor(n_estimators=100, learning_rate=0.1, random_state=123) c_train, Y_train) or(learning_rate=0.1, n_estimators=100, random_state=123)
In [131 In [132	RMSE = math.sqr MAE = mean_abso print('RMSE for print('MAE for a RMSE for AdaBoost MAE for AdaBoost import seaborn import matploth sns.set(color_co	ib.pyplot as plt codes=True)
Out[133	ax.set_xlabel('!ax.set_ylabel('!ax.set_xlim(0, ax.set_ylim(0, ax.figure.set_s.ax.set_title('Adplt.show /usr/local/lib/ps keyword args: rguments without FutureWarning	12) dize_inches(7, 7) daBoost',fontsize='large', fontweight='bold') bython3.7/dist-packages/seaborn/_decorators.py:43: FutureWarning: Pass the following variables x, y. From version 0.12, the only valid positional argument will be `data`, and passing other t an explicit keyword will result in an error or misinterpretation.
	10 8 8 4 2	
	0 0 2	4 6 8 10 12 Experimental pIC50