

Table S3-1. Machine learning models' hyperparameter tuning range

Hyperparameter Name	Range	LightGBM	XgBoost	CatBoost
max_depth	2~15	√	√	√
n_estimators(iterations)	40~640	√	√	√
learning_rate	[0.01, 0.02, 0.03, 0.04, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5]	√	√	√
gamma	[0.0, 0.1, 0.2, 0.3, 0.4]		√	
reg_alpha	[0.0001, 0.001, 0.01, 0.1, 1,10]	√	√	
reg_lambda (l2_leaf_reg)	[0.0001, 0.001, 0.01, 0.1, 1,10]		√	√
min_child_weight	1~8	√	√	
colsample_bytree	[0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1]		√	
subsample	[0.6, 0.7, 0.8, 0.9, 1]			
num_leaves	40~640	√		
min_child_samples	2~15	√		
bagging_fraction	[0.0001, 0.001, 0.01, 0.1, 1]	√		

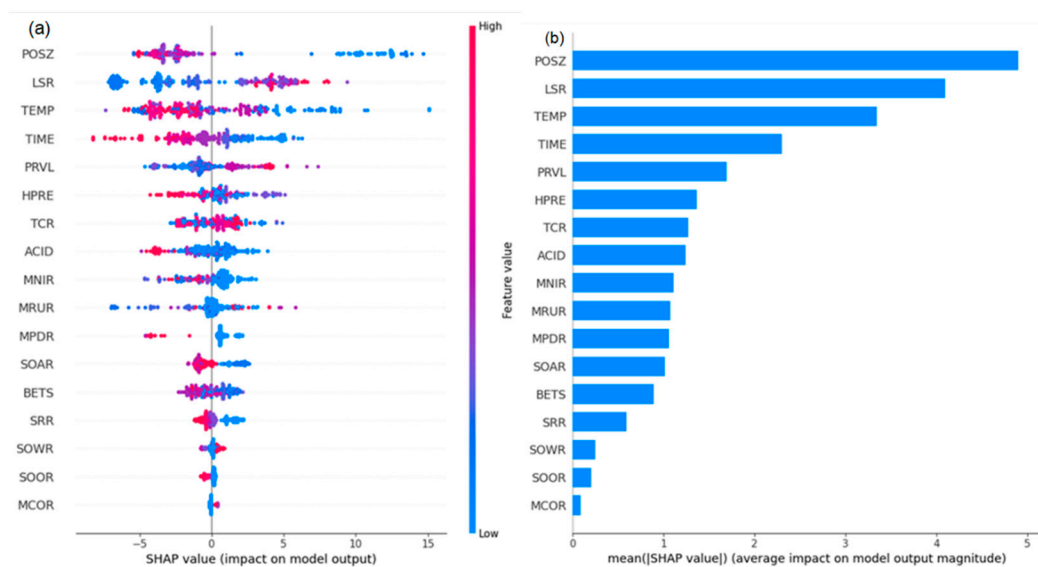


Figure S3-1. SHAP value (left) and feature importance (right) of LightGBM prediction on solid yield

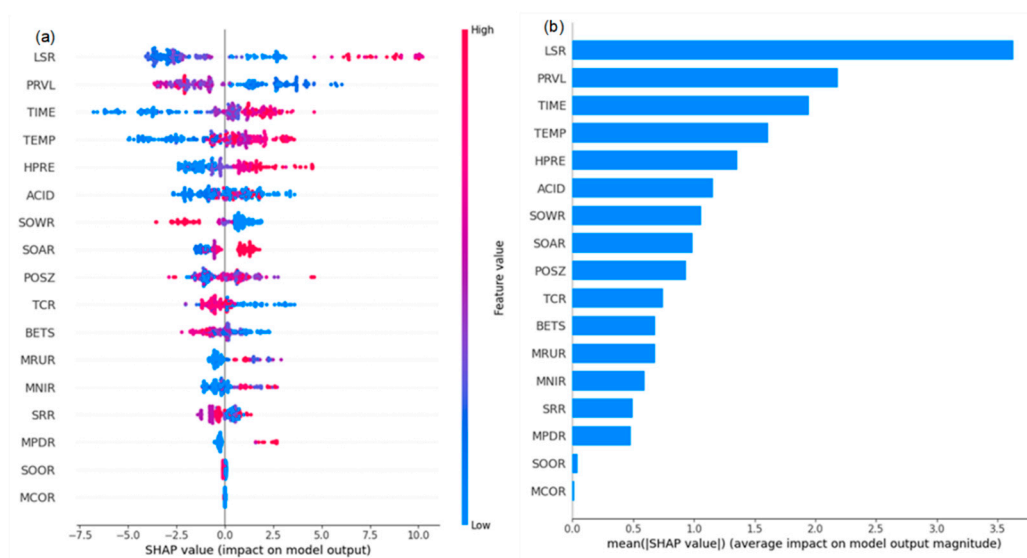


Figure S3-2. SHAP value (a) and feature importance (b) of LightGBM prediction on aromatics

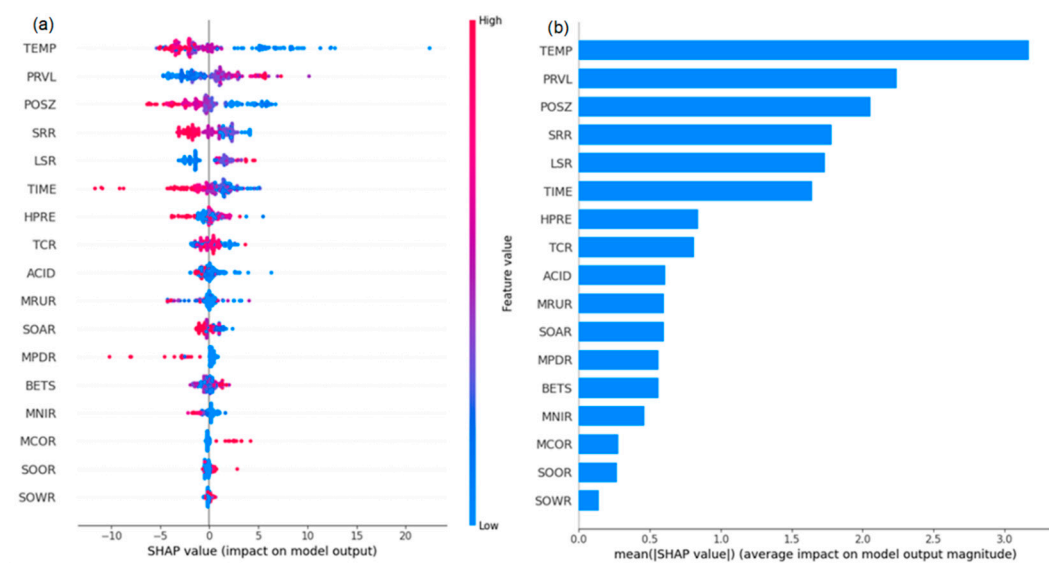


Figure S3-3. SHAP value (a) and feature importance (b) of CatBoost prediction on solid yield

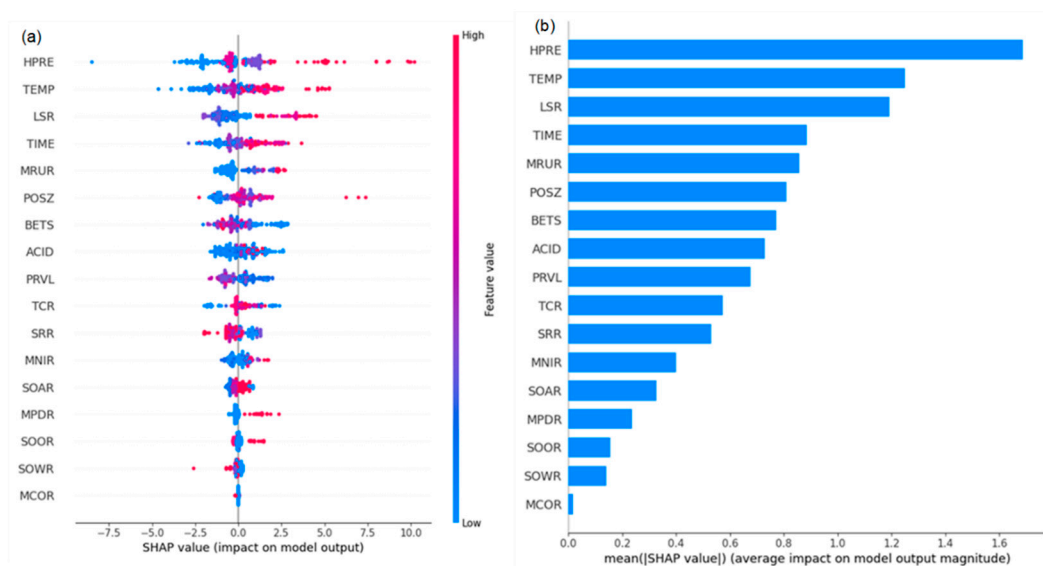


Figure S3-4. SHAP value (a) and feature importance (b) of CatBoost prediction on aromatics