Using XGBoost to predict the ADMET

For this prediction challenge, we have use XGBoost library. This is optimized gradient boosting library for effective implementation of Gradient Boosting framework. Prior to modeling, the provided SMILES were curated by using workflow in KNIME. The curation protocol helps to removing any inorganics, salt, or mixture like compounds.   
Our combination of curation protocol and XGBoost gave us the best prediction for given endpoints.