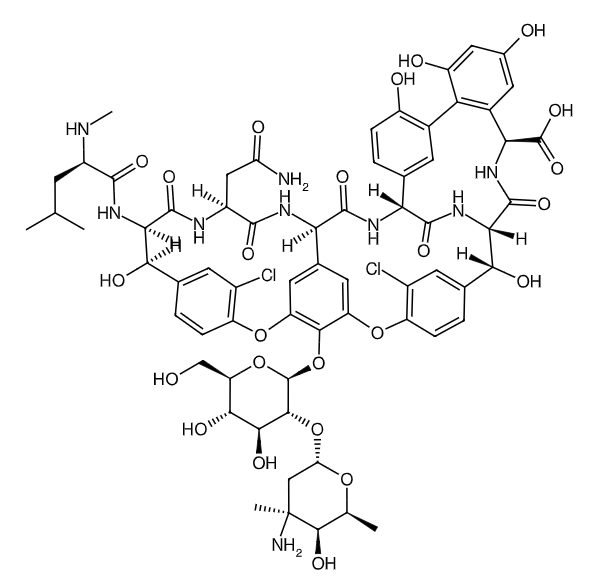
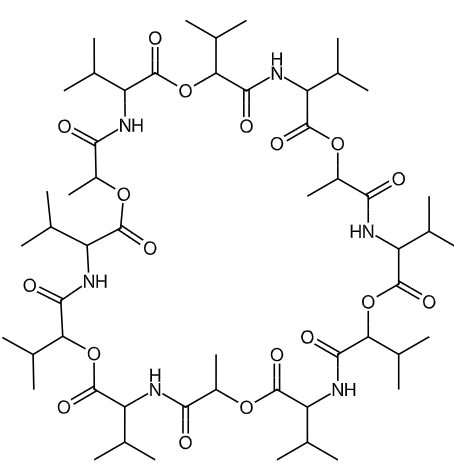
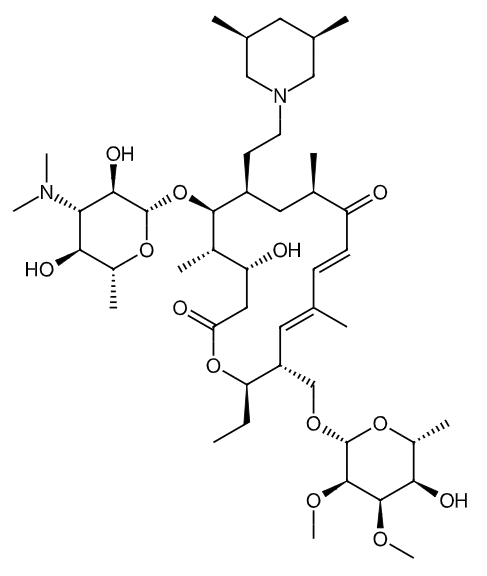
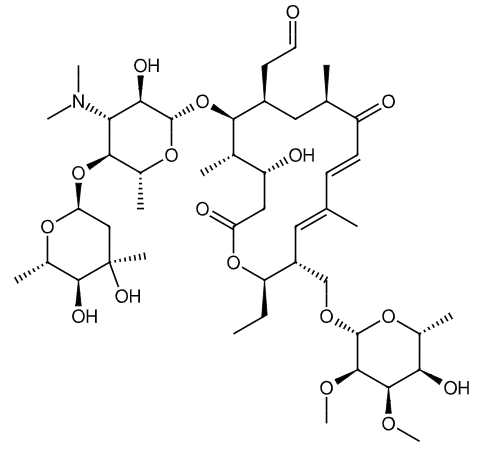
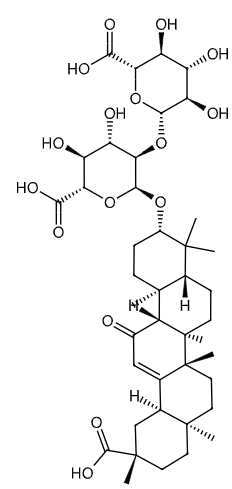
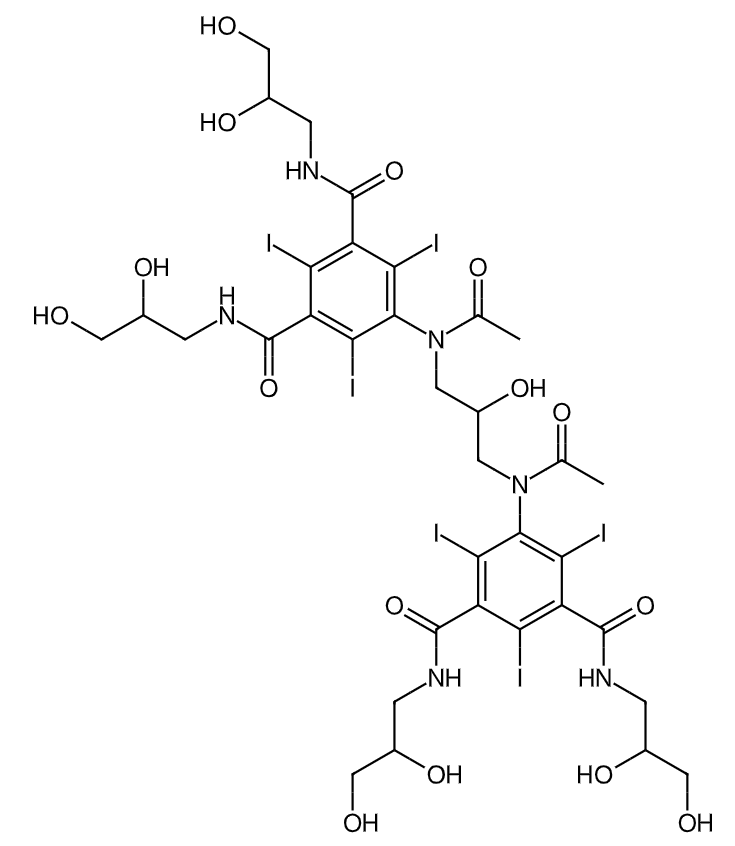
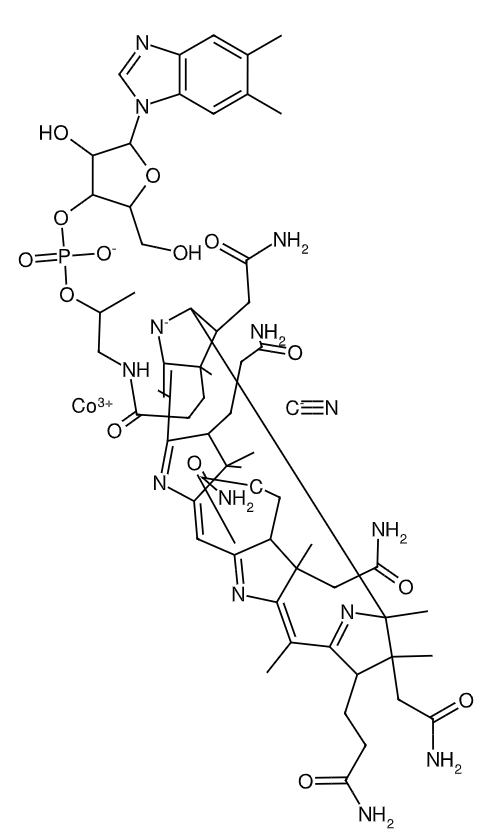
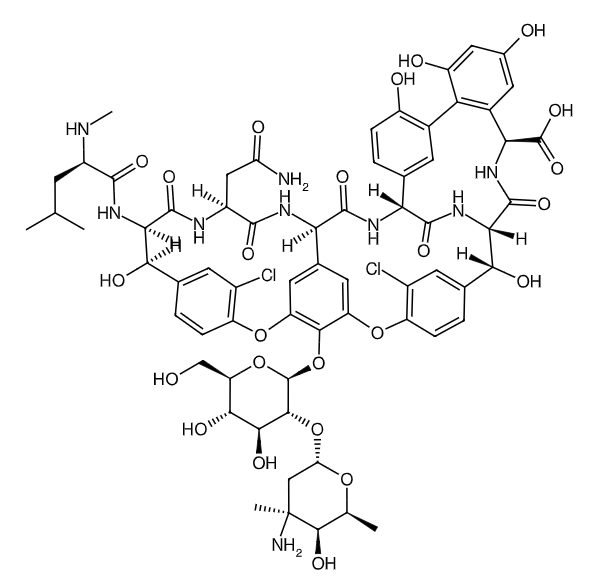
PCA Mordred No FS - outliers on PCA graph

Test Set Outliers (More Important for Analysis)

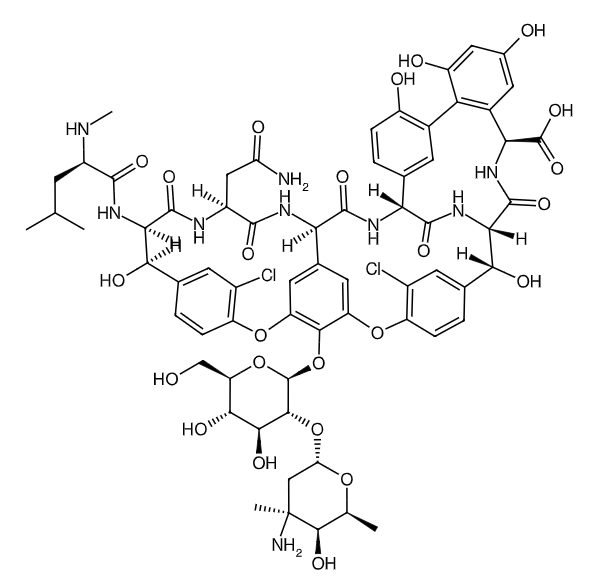
Training Set Outliers



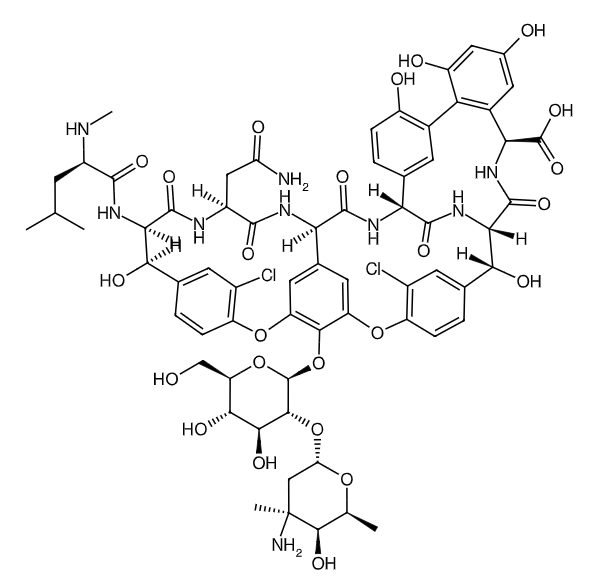


PCA Mordred with FS - Test Set Outliers

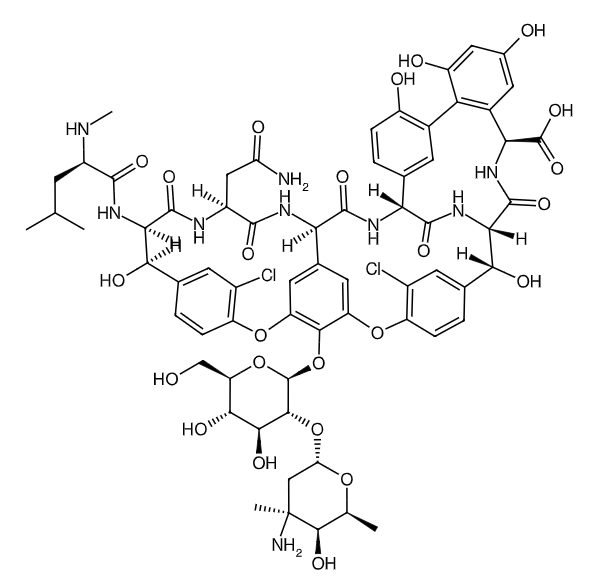
PCA Original - Test Set Outliers

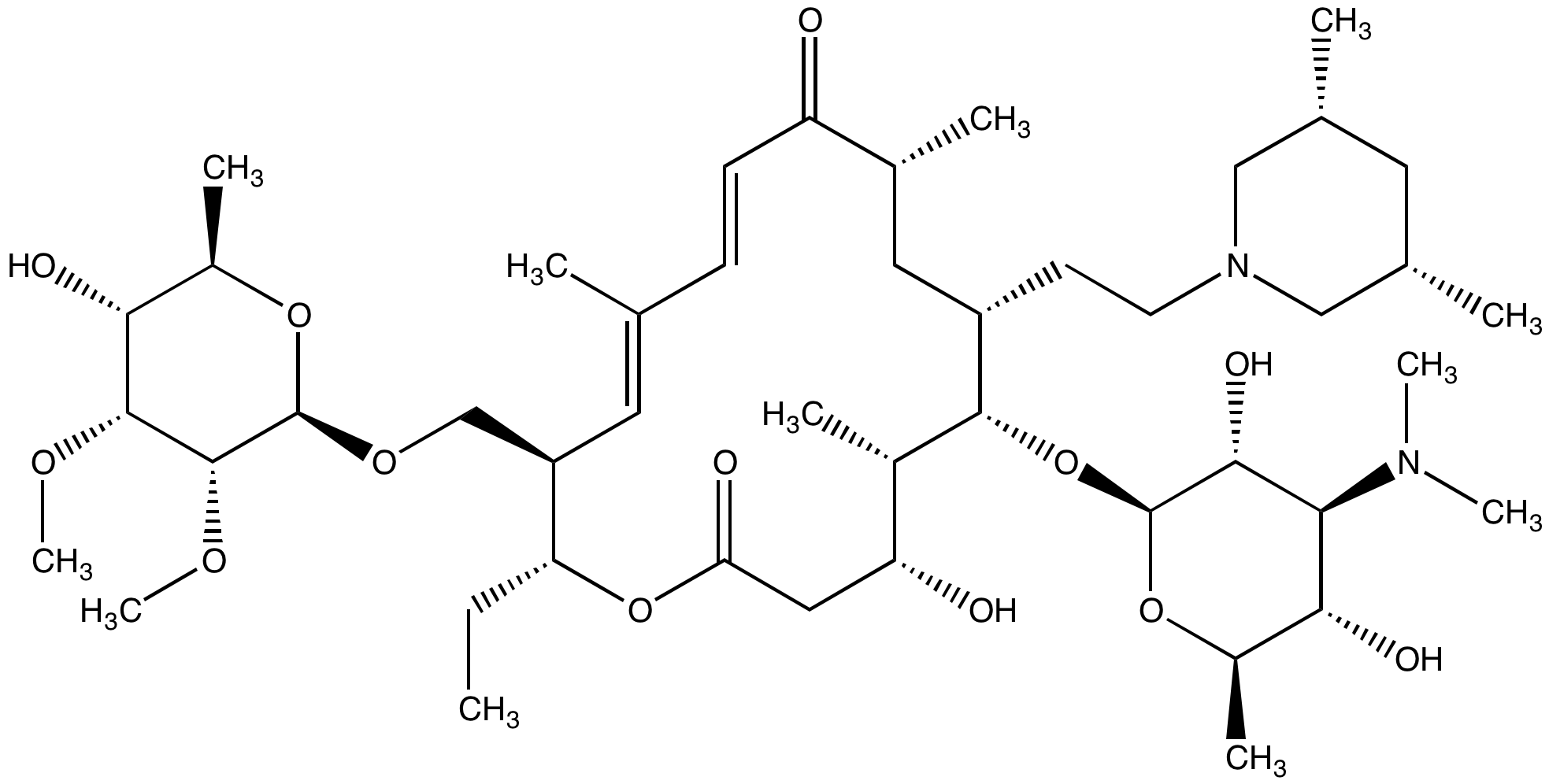


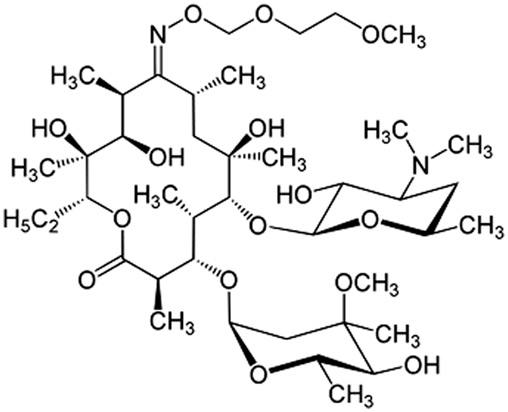
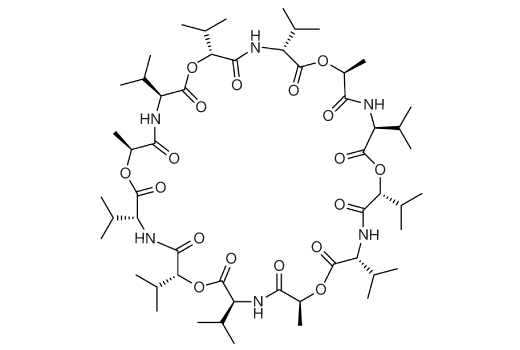
PCA Count Morgan - Test Set Outliers



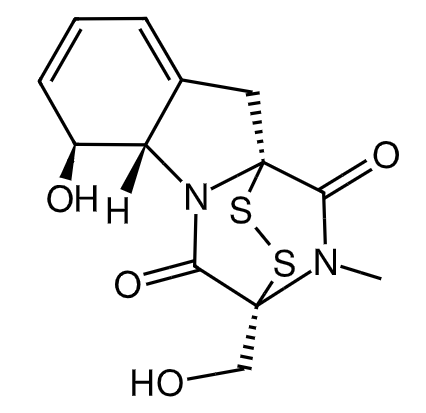
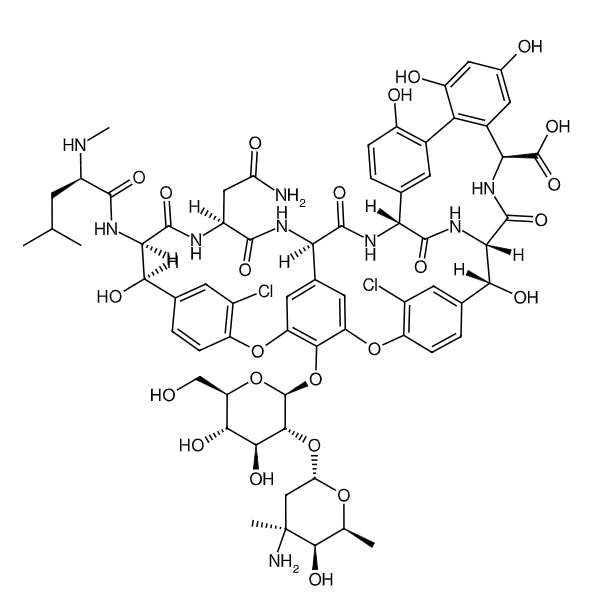
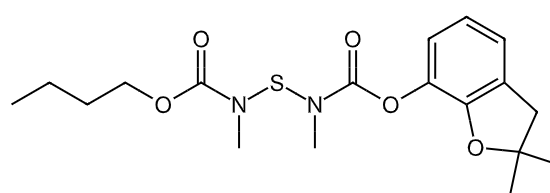
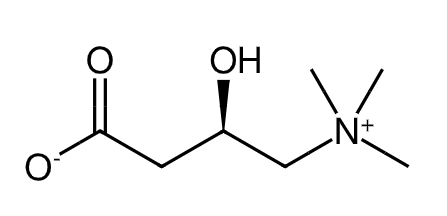
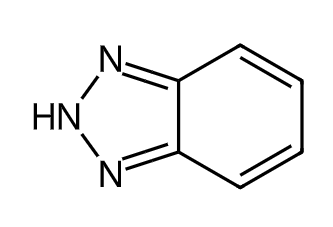
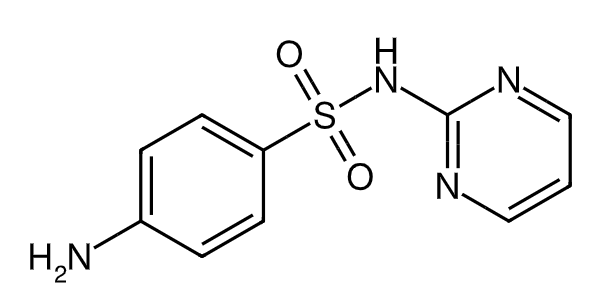
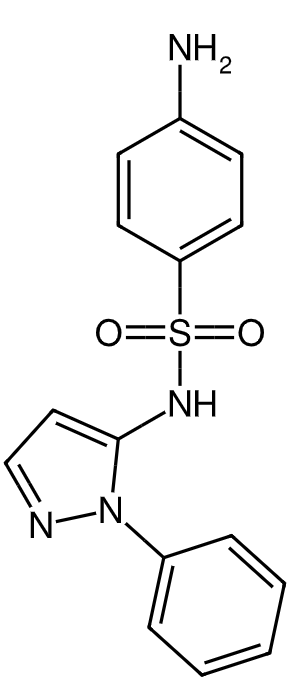
PCA Molecules Bit Morgan Test Set Outliers

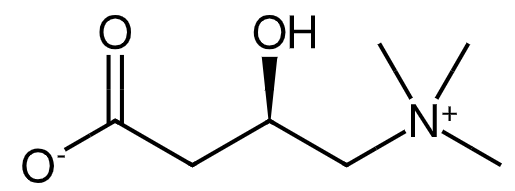


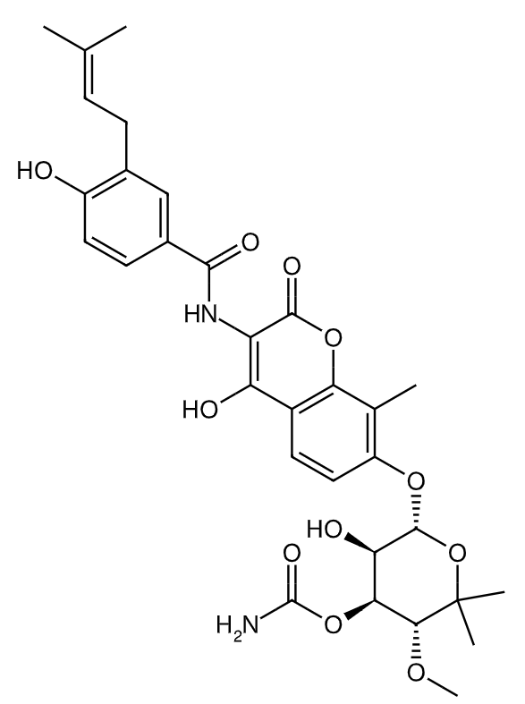
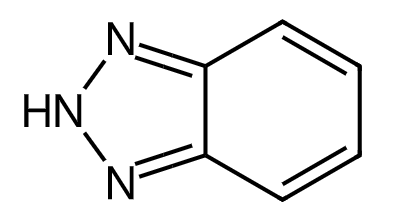
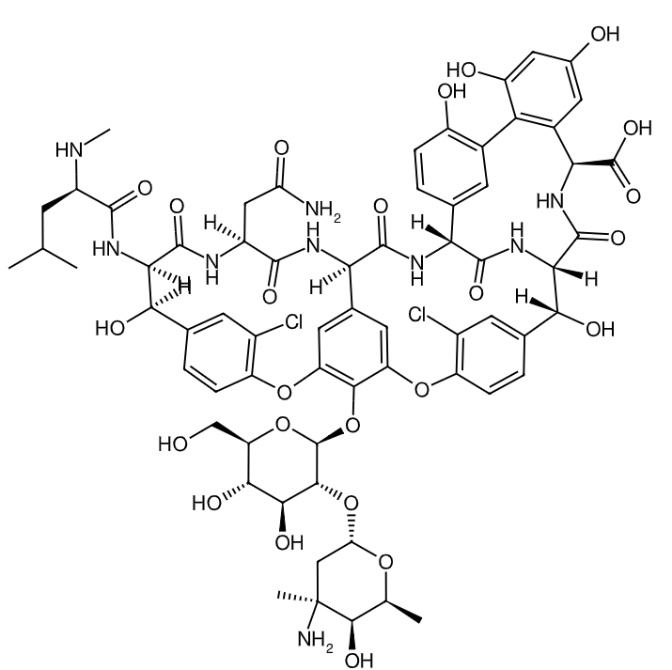
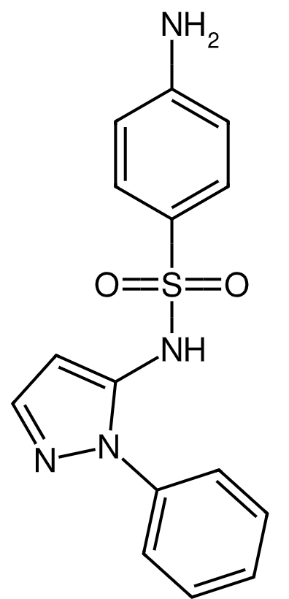
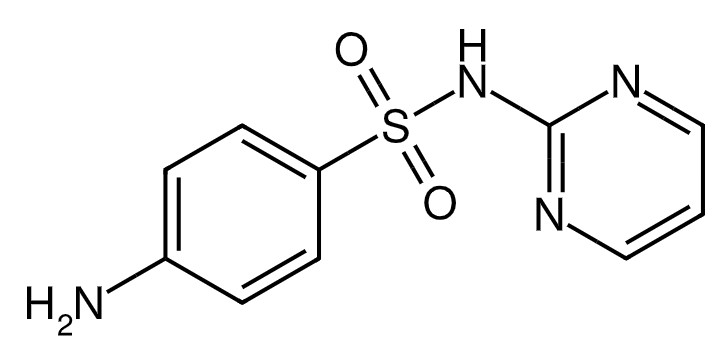
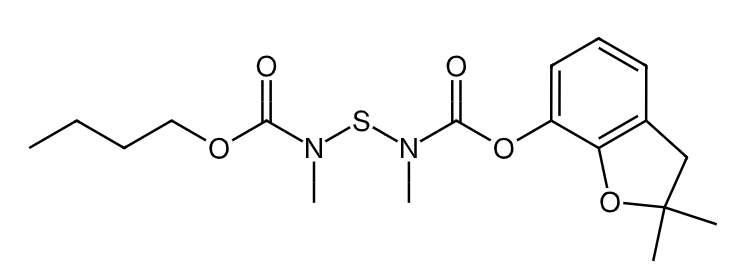
PCA Molecules

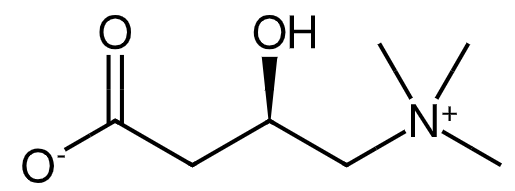


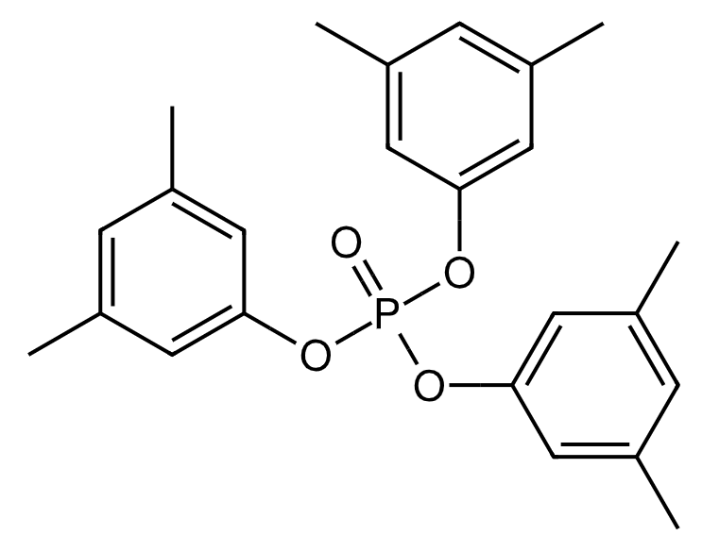
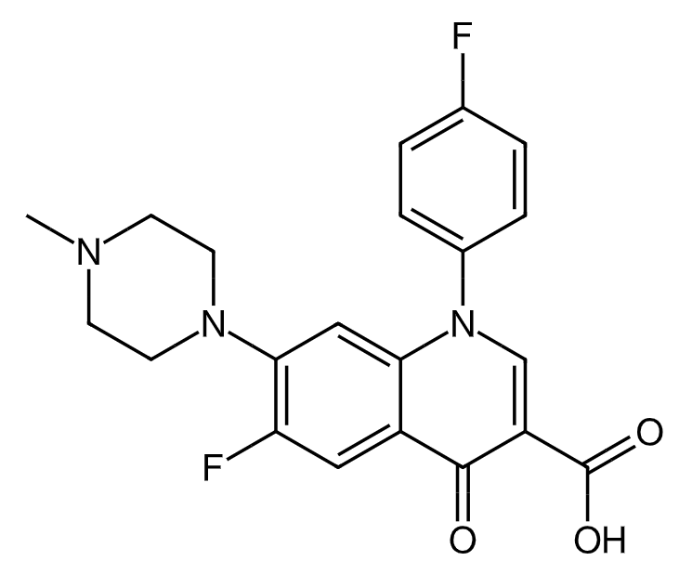
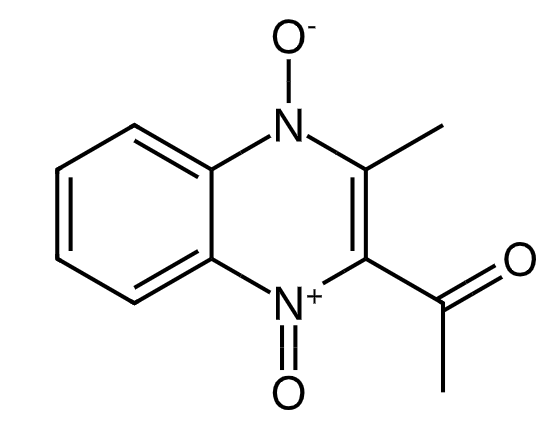
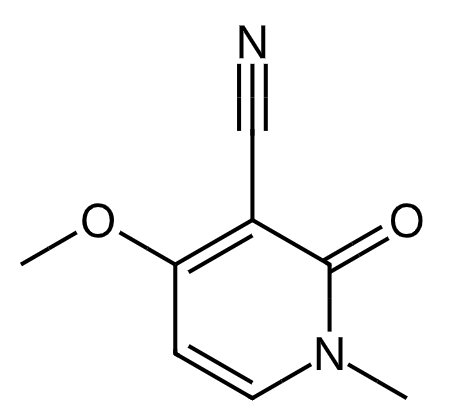
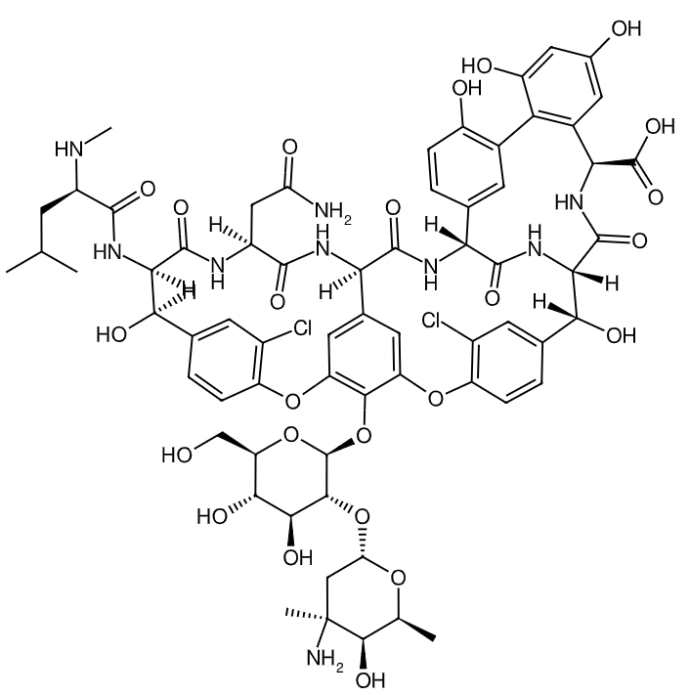
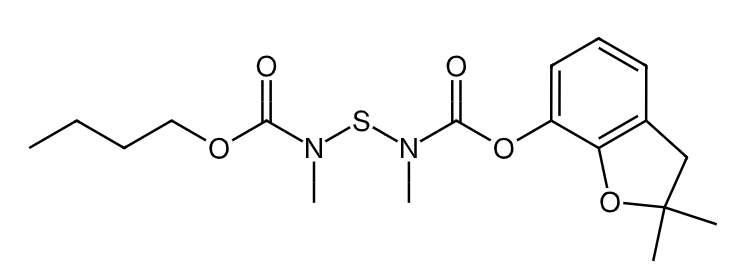
Outliers from Random Forest Random Search Original - bad error between predicted and actual retention times

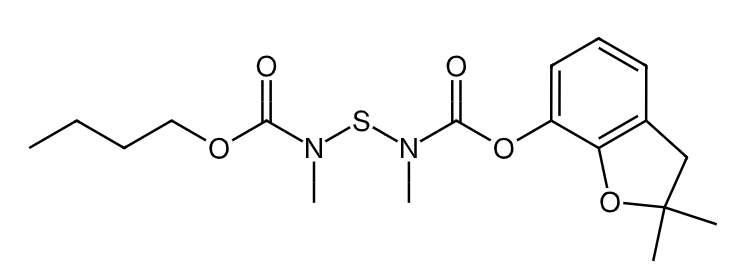


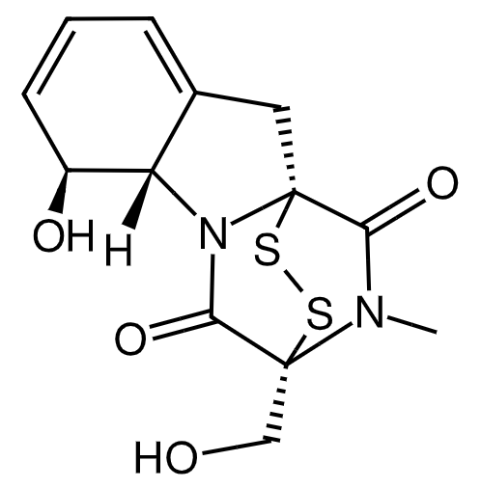
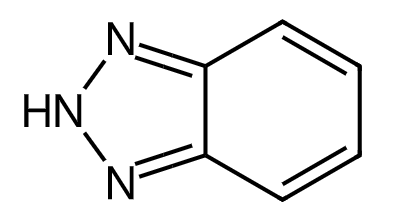
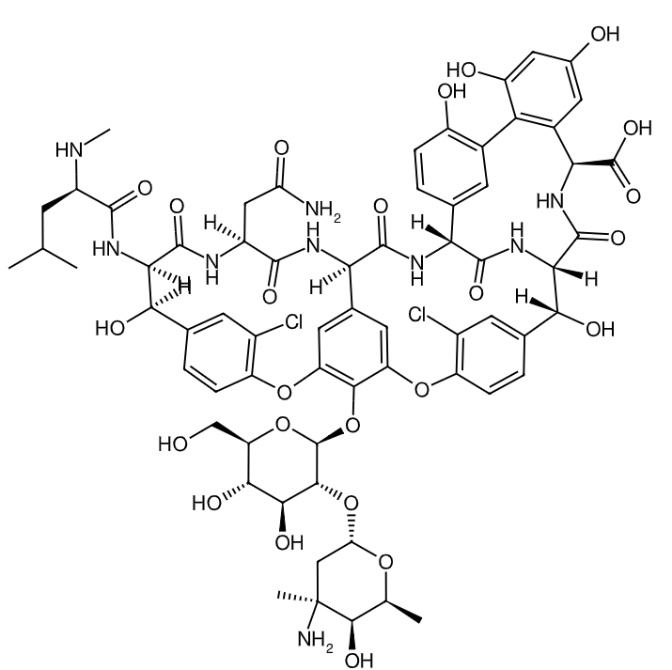
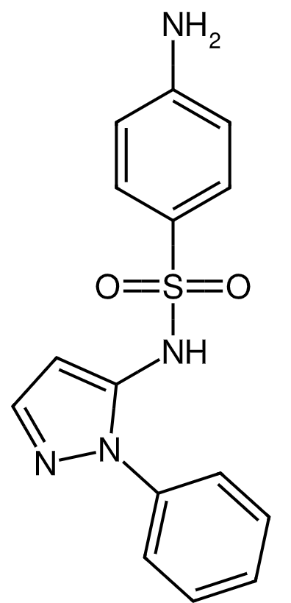
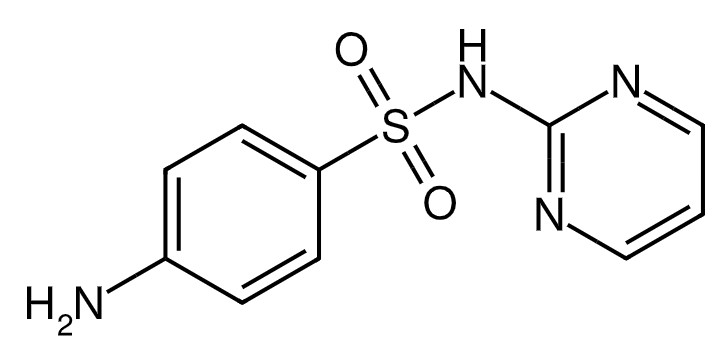
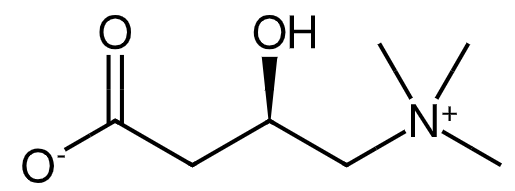
Outliers from Random Forest Random Search with Mordred No FS

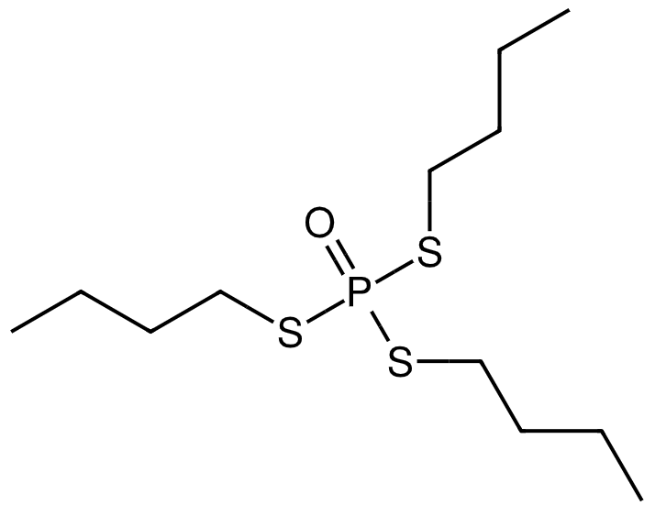
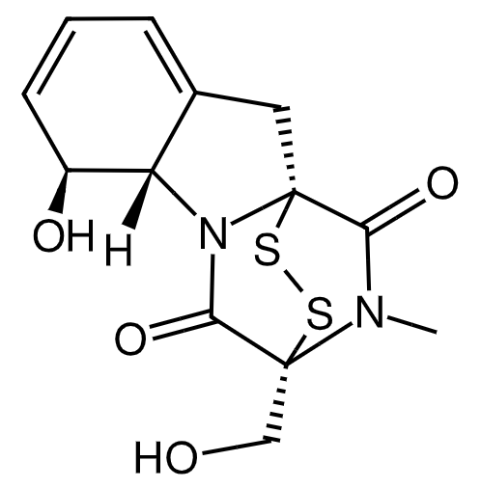
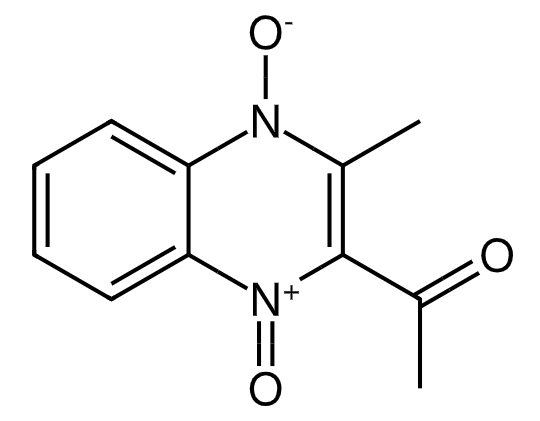
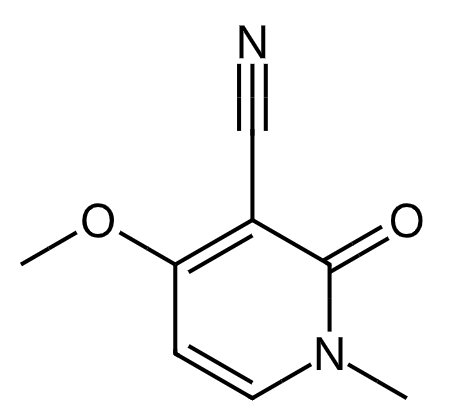
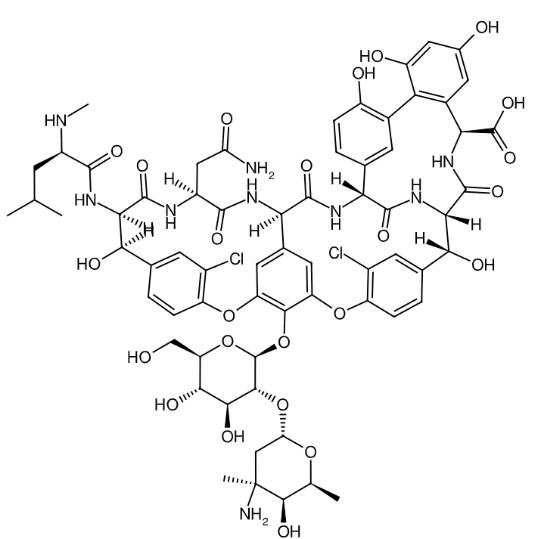
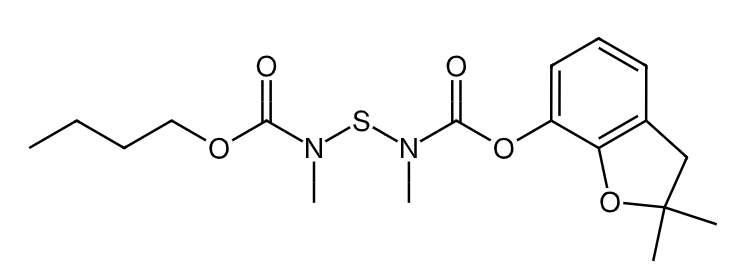
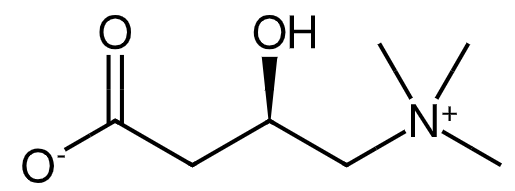


Outliers from SVR Random Search Original



Outliers from Random Forest Random Search with Mordred FS



Outliers using SVR Halving Search with Mordred No FS

3D Structure of furathiocarb (will try and find a reference for it)