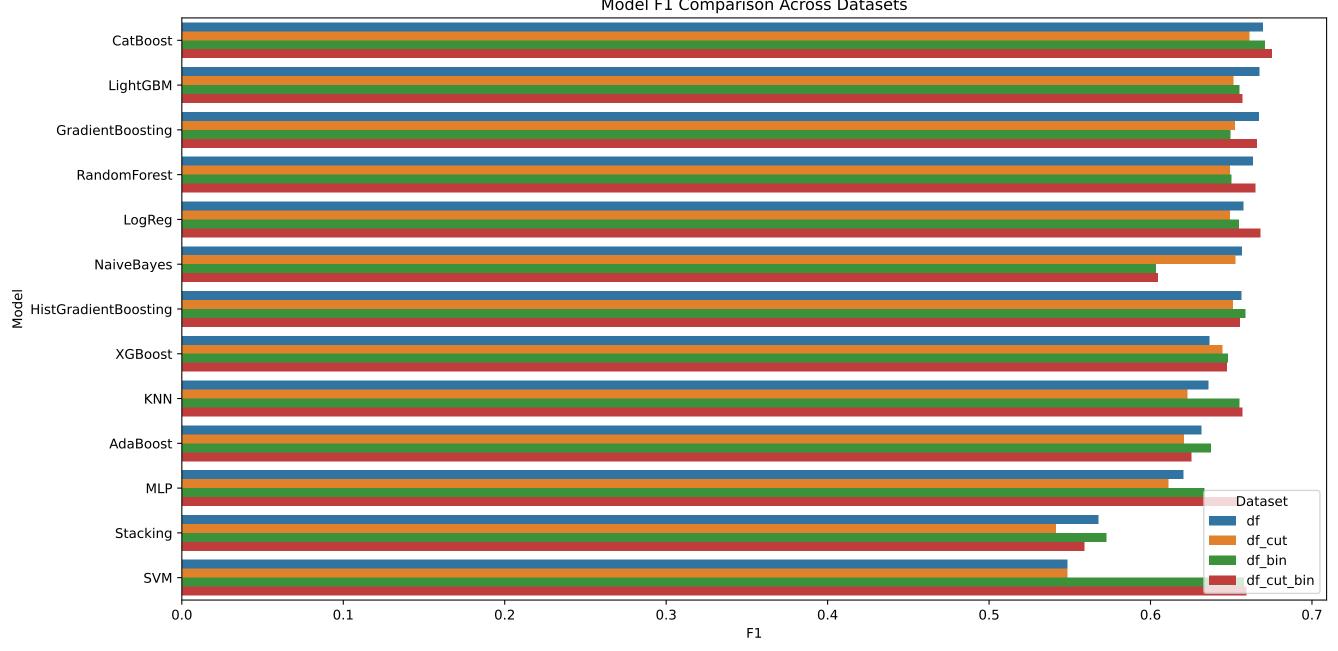
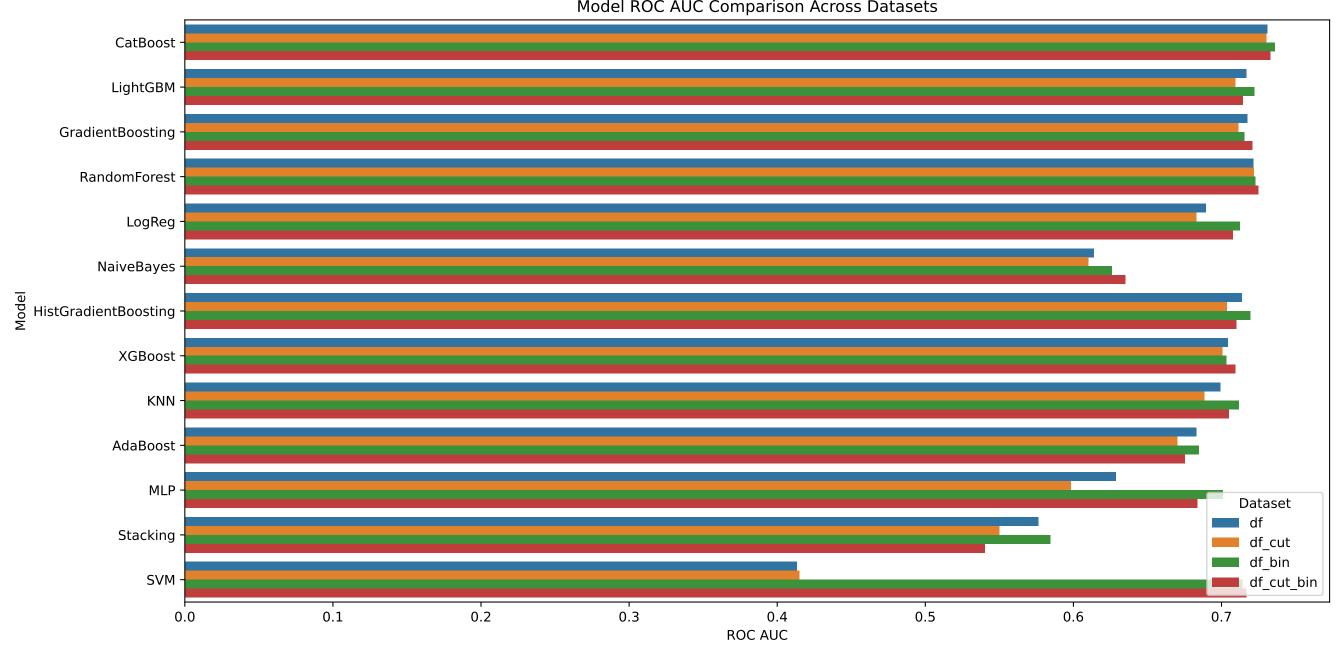
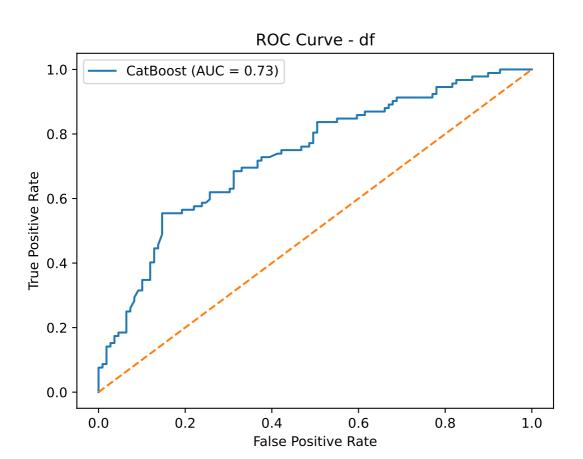
Model F1 Comparison Across Datasets

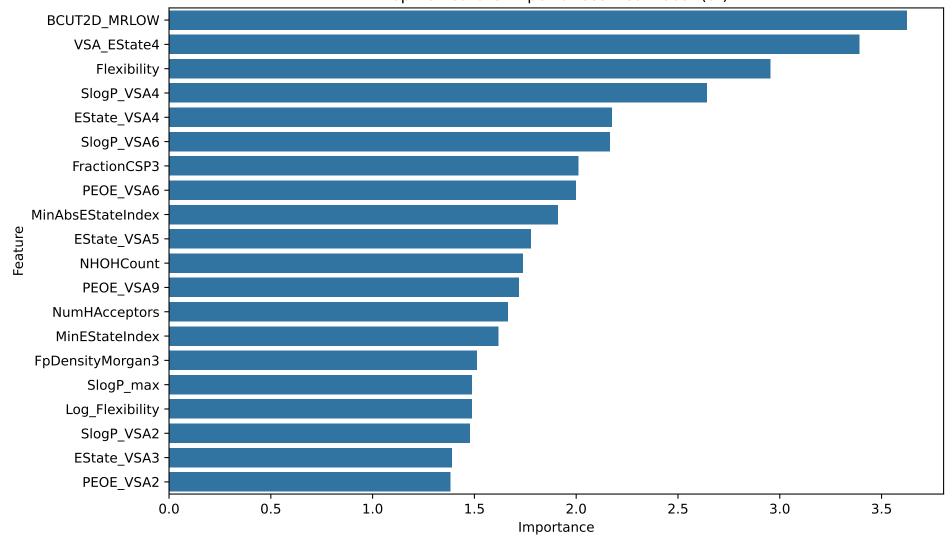


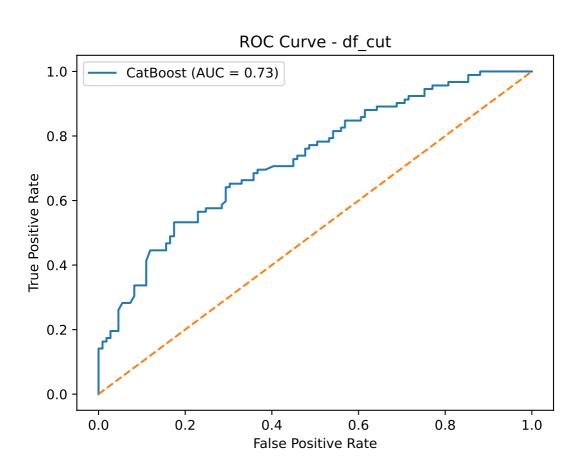




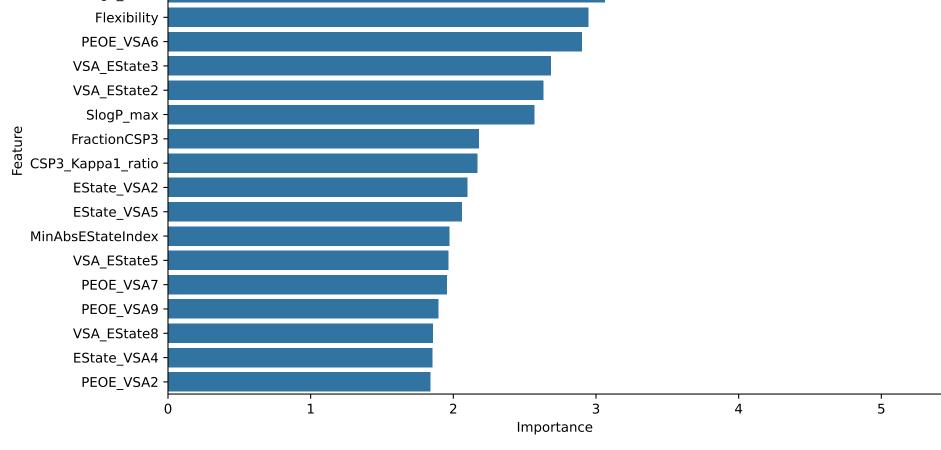


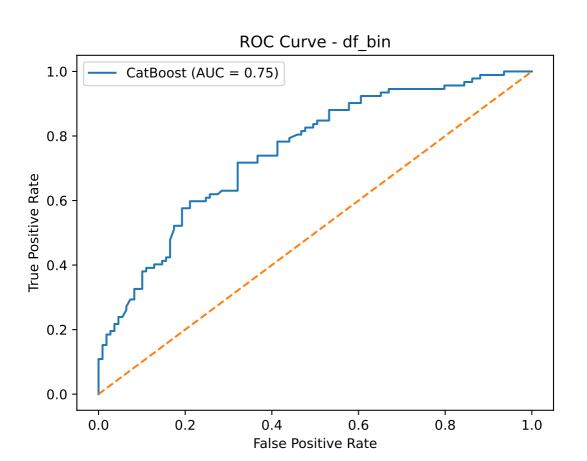
Top 20 Feature Importances - CatBoost (df)



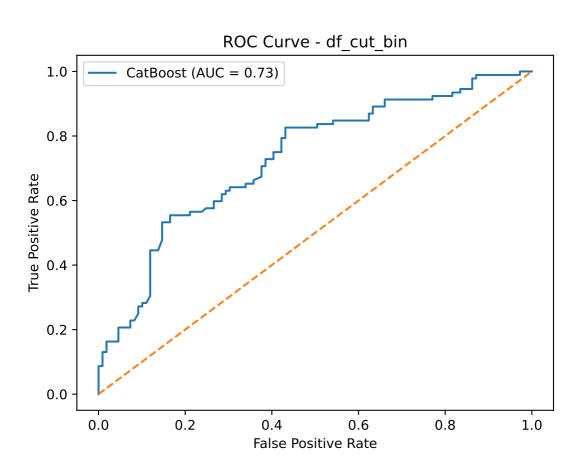


Top 20 Feature Importances - CatBoost (df cut) VSA_EState4 -BCUT2D_MRLOW -SMR_VSA7 -SlogP_VSA4 Flexibility -PEOE_VSA6 -VSA_EState3 -VSA_EState2 -SlogP_max -Feature FractionCSP3 -CSP3_Kappa1_ratio -EState_VSA2 -EState_VSA5 MinAbsEStateIndex -VSA_EState5 -PEOE_VSA7 -PEOE_VSA9 -





Top 20 Feature Importances - CatBoost (df bin) BCUT2D_MRLOW -VSA_EState3 -VSA_EState4 -Log_Flexibility -Ipc -FpDensityMorgan3 -NumSaturatedCarbocycles -PEOE_VSA_max -PEOE_VSA7 Feature PEOE_VSA8 -SlogP_VSA4 -NHOHCount -SlogP_std fr_bicyclic -SlogP_VSA6 -HallKierAlpha -Flexibility -MaxAbsPartialCharge -BCUT2D_LOGPHI -BCUT2D_CHGLO -2 4 5 Importance



Top 20 Feature Importances - CatBoost (df_cut_bin)

