# Predicting Antimicrobial Peptide Activity: A Machine Learning-Based Quantitative Structure–Activity Relationship Approach

**Eliezer I. Bonifacio-Velez de Villa, María E. Montoya-Alfaro, Luisa P. Negrón-Ballarte and Christian Solis-Calero ***

Faculty of Pharmacy and Biochemistry, Universidad Nacional Mayor de San Marcos, Lima 15001, Peru ; eliezerbvv1@gmail.com (E.I.B.-V); mmontoyaa@unmsm.edu.pe (M.E.M.-A.); lnegronb@unmsm.edu.pe (L.P.N.-B.)

*Correspondence: csolisc@unmsm.edu;

## Supplementary Materials

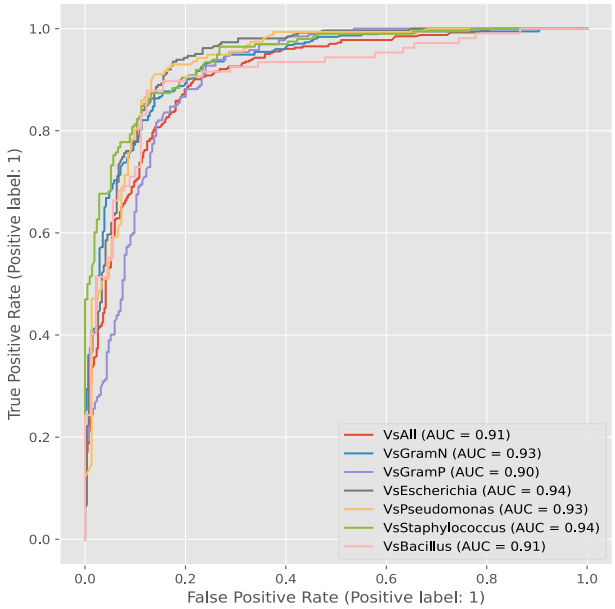



**Figure S1: ROC curve of the Random Forest -based classification models on the test dataset during validation.**

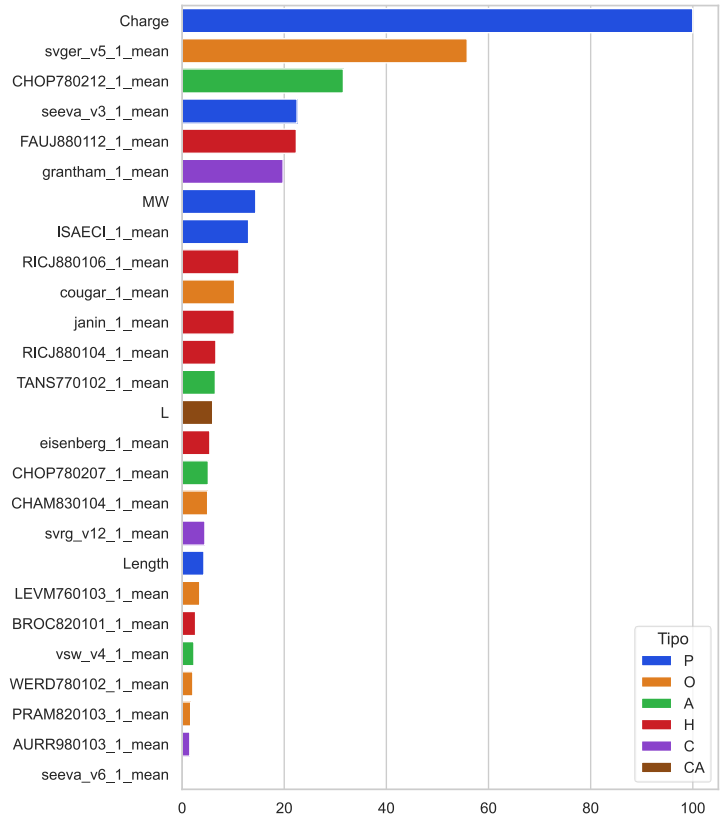



Figure S2: Importance of descriptors in the classification model against all microorganisms

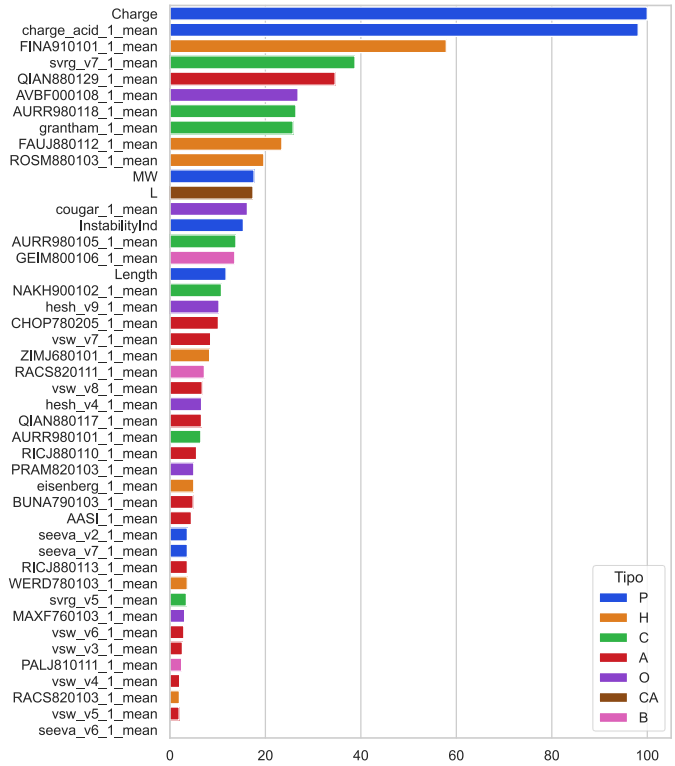



Figure S3: Importance of descriptors in the classification model against Gram-negative organisms

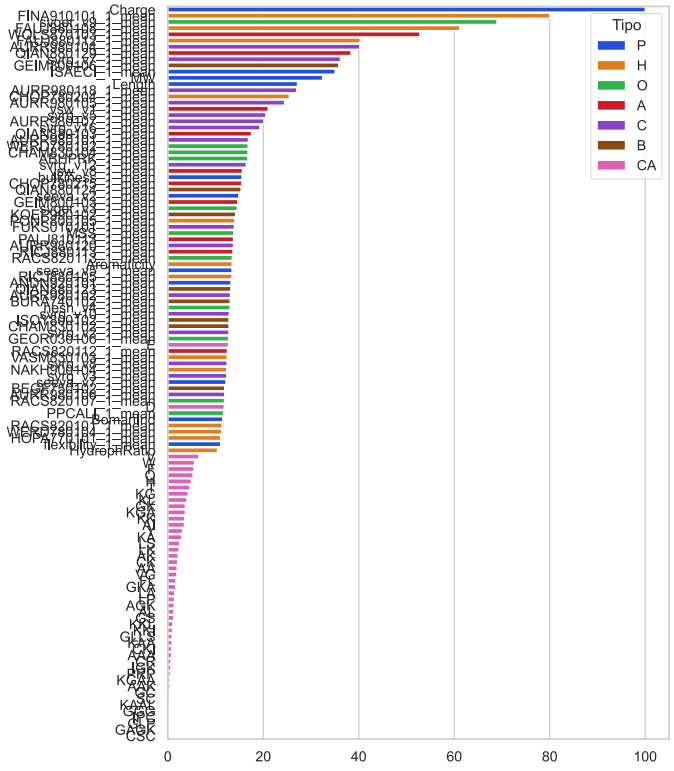



Figure S4: Importance of descriptors in the classification model against Gram-positive organisms

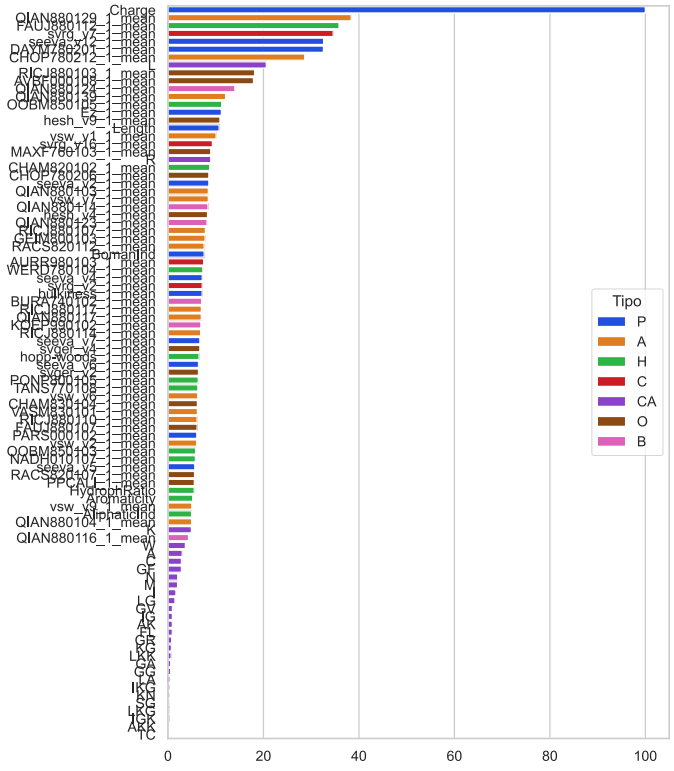



Figure S5: Importance of descriptors in the classification model against organisms of the genus *Escherichia*

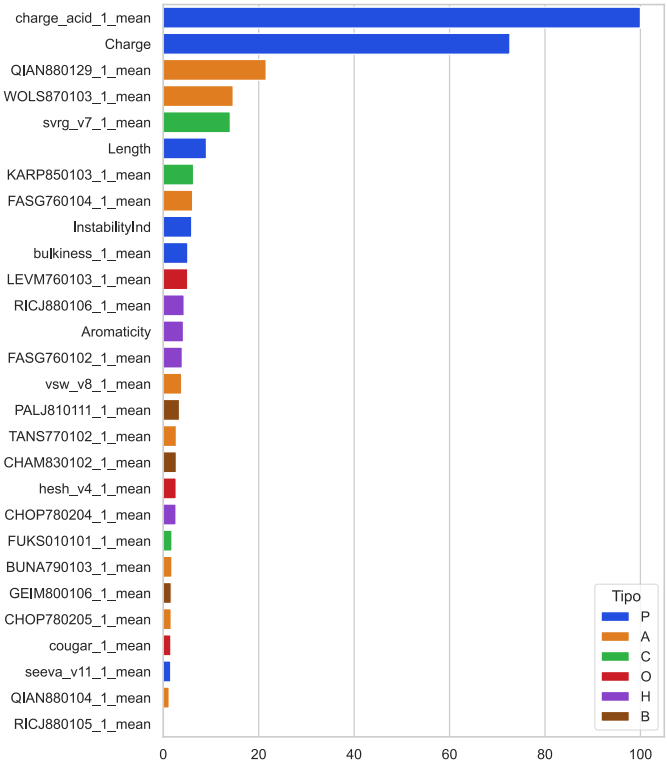



Figure S6: Importance of descriptors in the classification model against organisms of the genus *Pseudomonas*

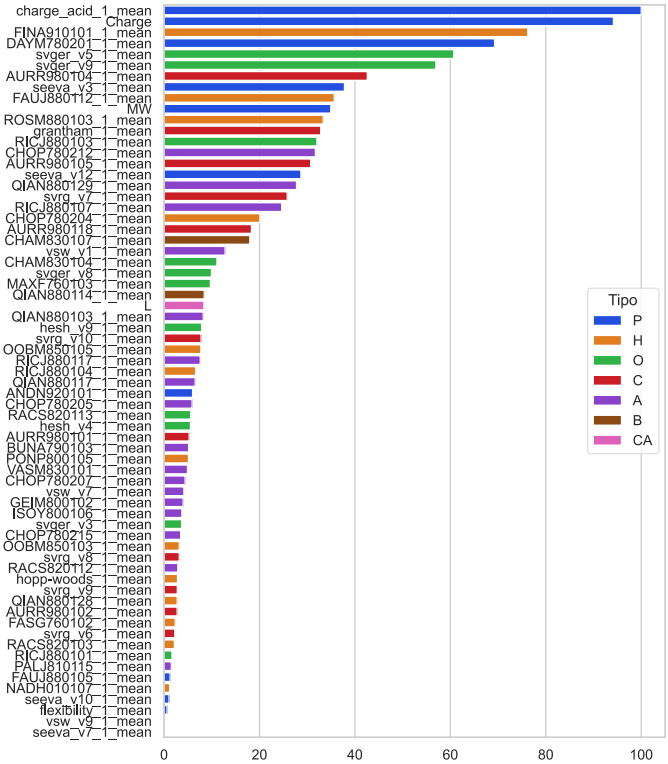



Figure S7: Importance of descriptors in the classification model against organisms of the genus *Staphylococcus*

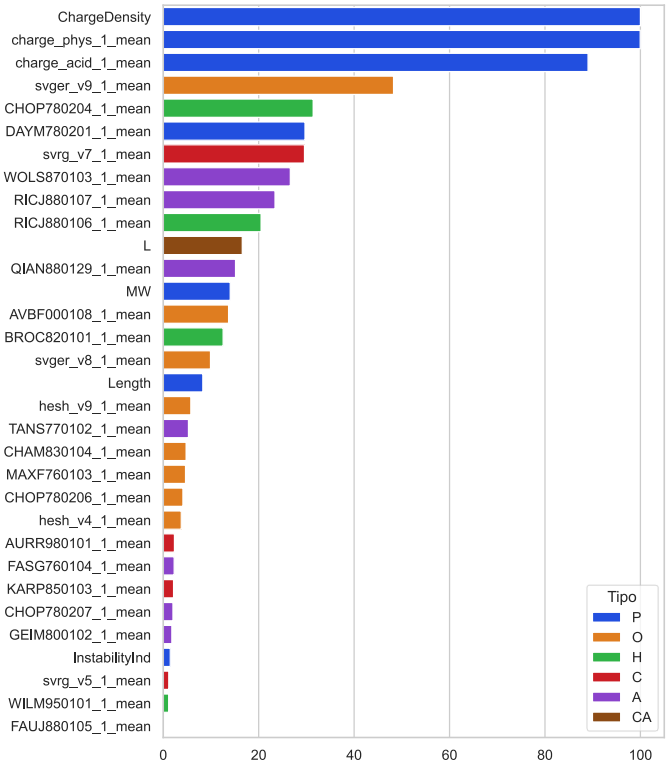



Figure S8: Importance of descriptors in the classification model against organisms of the genus *Bacillus*

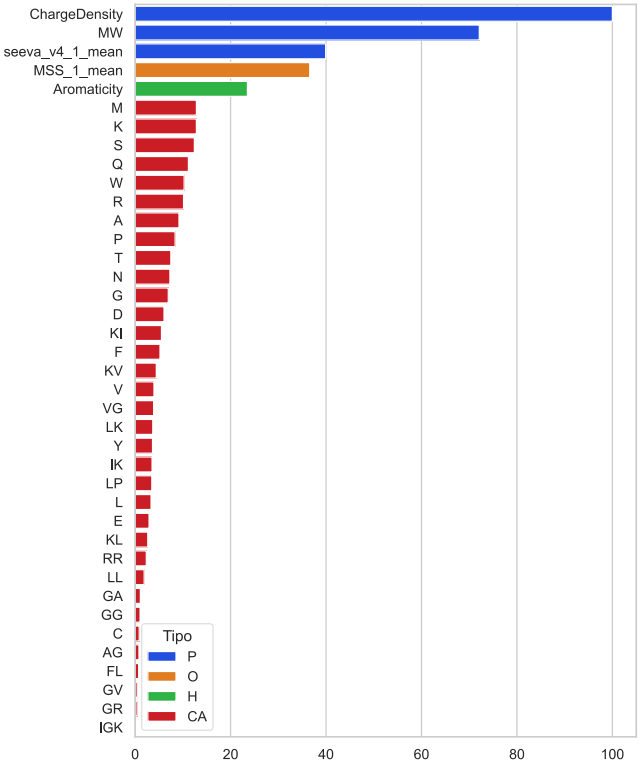



Figure S9: Importance of descriptors in the regression model against all microorganisms

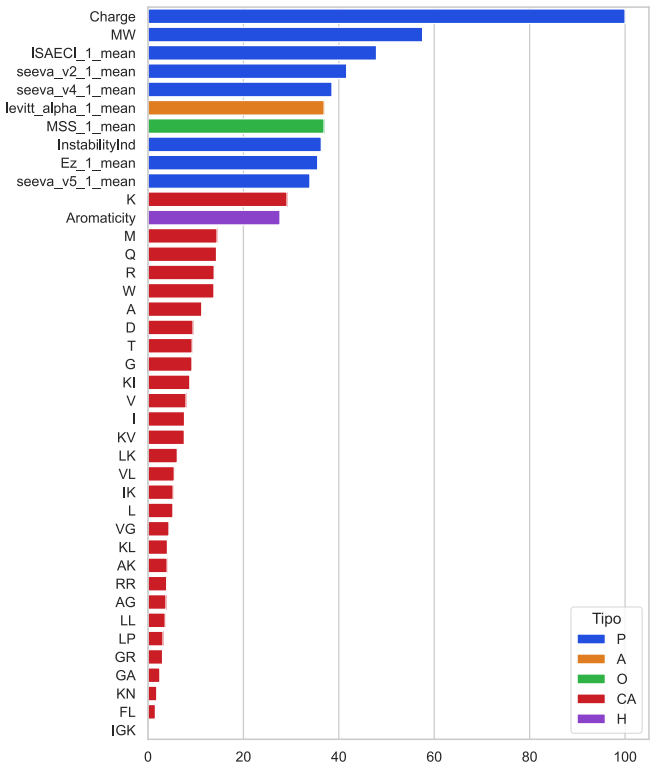



Figure S10: Importance of descriptors in the regression model against Gram-negative organisms

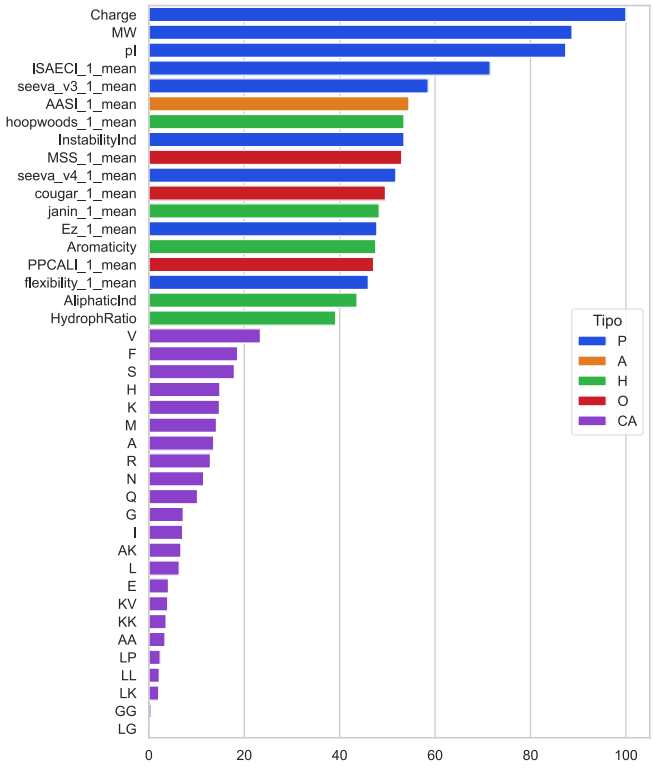



Figure S11: Importance of descriptors in the regression model against Gram-positive organisms

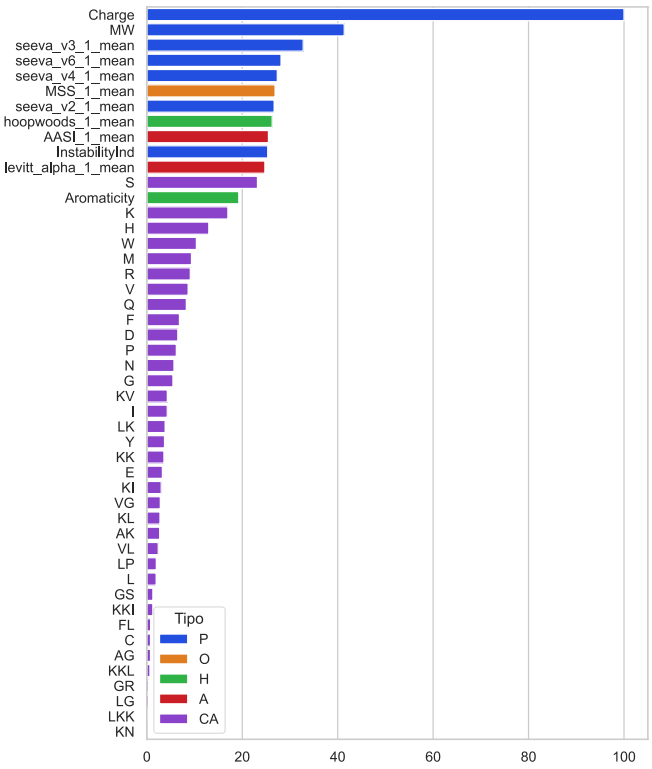



Figure S12: Importance of descriptors in the regression model against organisms of the genus *Escherichia*

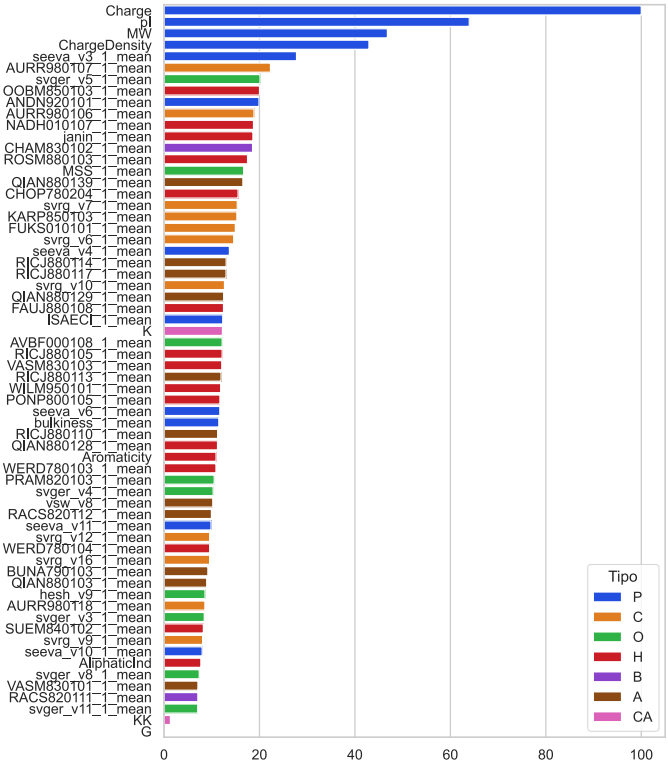



Figure S13: Importance of the descriptors in the regression model against organisms of the genus *Pseudomonas*

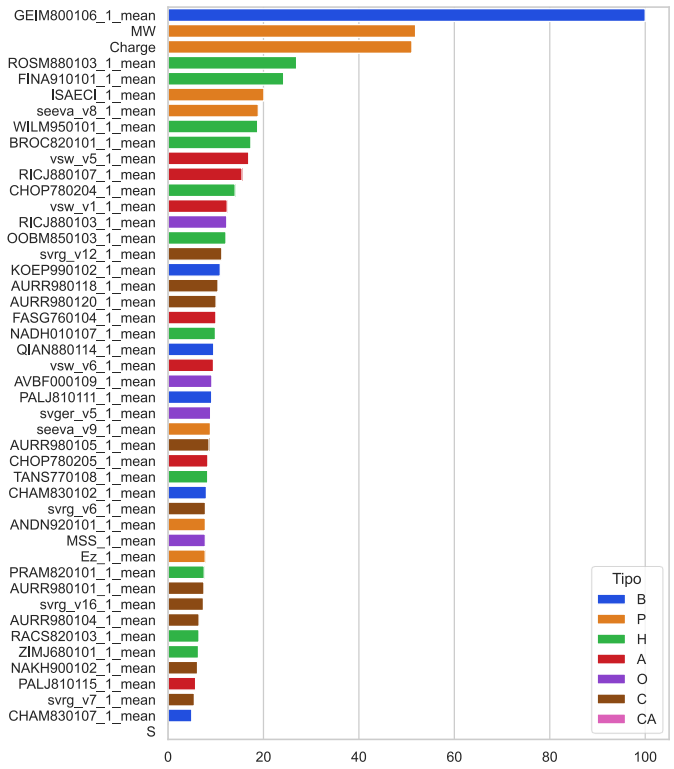



Figure S14: Importance of the descriptors in the regression model against organisms of the genus *Staphylococcus*

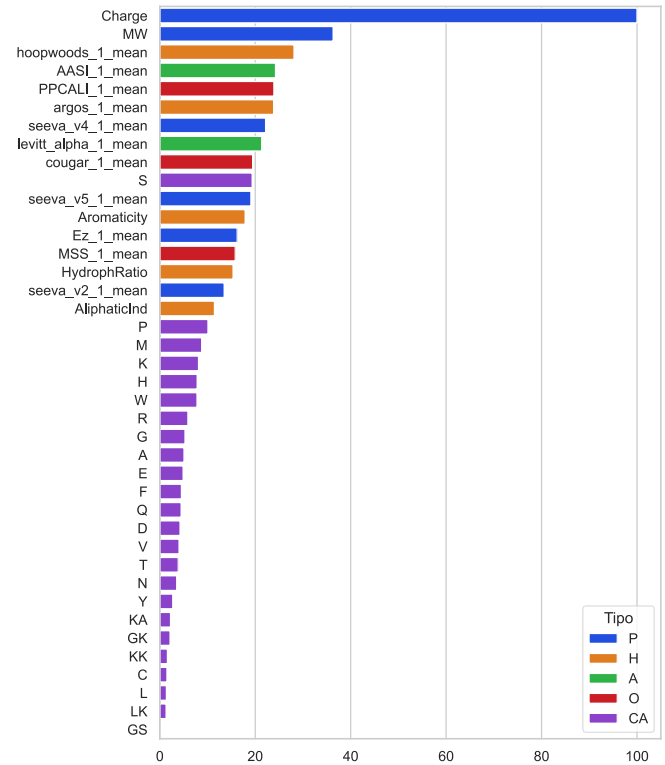



Figure S15: Importance of the descriptors in the regression model against organisms of the genus *Bacillus*.