

Supporting Information

Transfer Learning-Enhanced Multi-Target QSRR Modeling

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Table S1: Hyperparameters for the MLP model

Hyperparameter	Value
FC layer	5
FC Units	1000, 500, 200, 100, 1
Dropout rate	0.1
Learning rate	1e-4

Based on the lipophilicity change over pH: we hv 2 groups of compounds (Group 1 having net charge and Group 2 , having no net charge). Below is their classification:

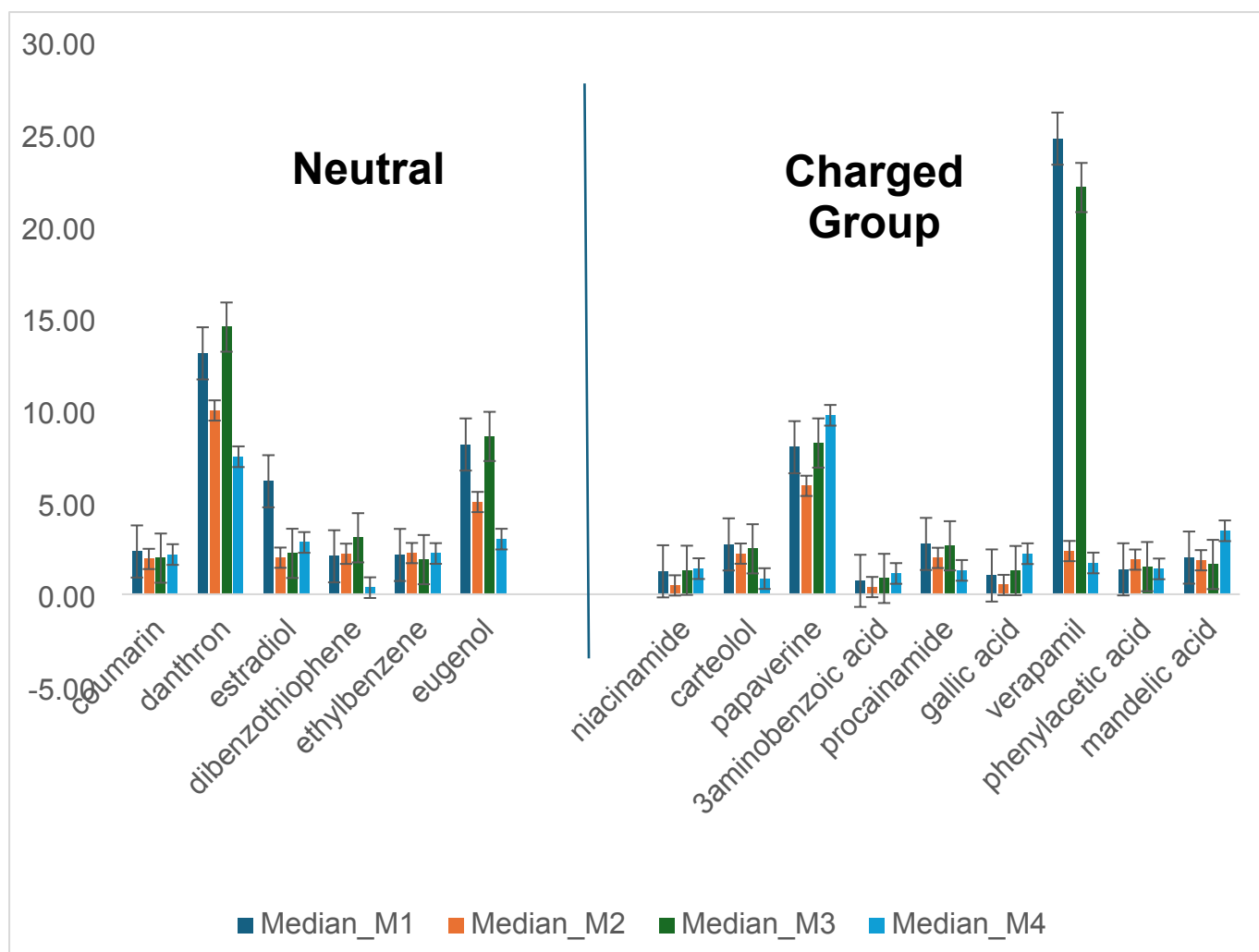


Figure S1 : Error Variations for group of compounds along the pH

x-axis: Specific compounds within each group , **y-axis:** The error values.

Different coloured bars (blue, orange, green, and light blue) represent different median values (Median_M1, Median_M2, Median_M3, and Median_M4) for each compound corresponding to four models(ST_WTL(M1), ST_TL(M2), MT_WTL(M3), MT_TL(M4)).

Error bars: the standard error in the measurements.

Table S3: Result comparison with SVM model

(Single target models for each target and calculated the mean)

Hyperparameter	Value
C	0.01

Degree	2
Model Performance	
MSE	48.45
R2	0.14

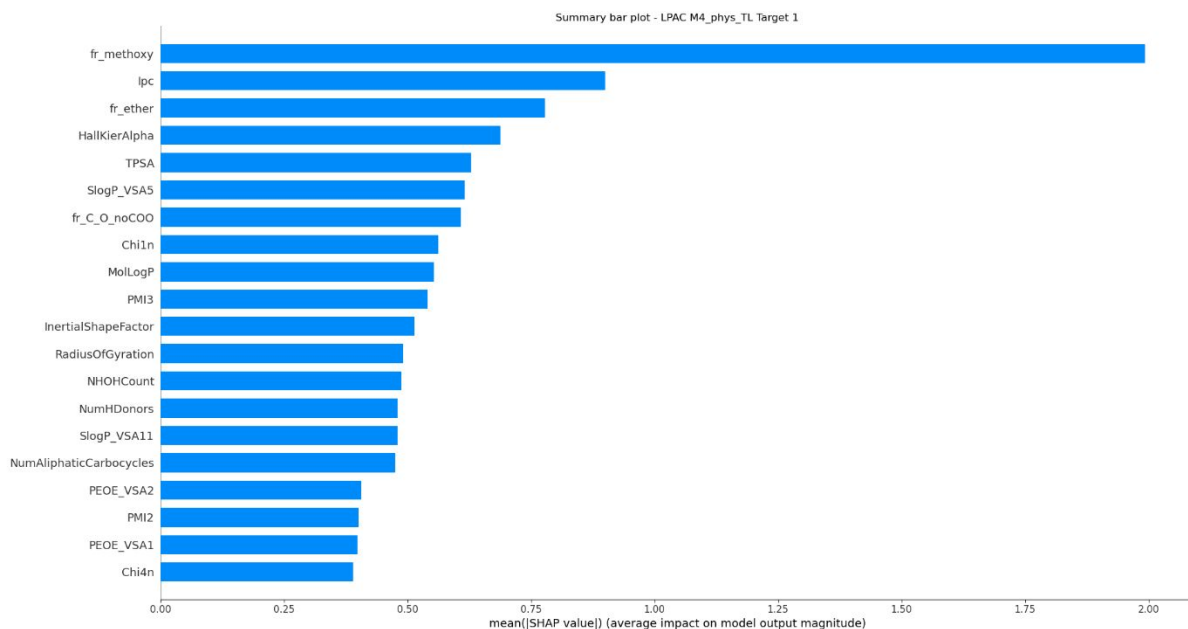


Figure S2: SHAP Summary plot for Multitarget QSRR(M4) for Target1- Retention time at pH 2.7

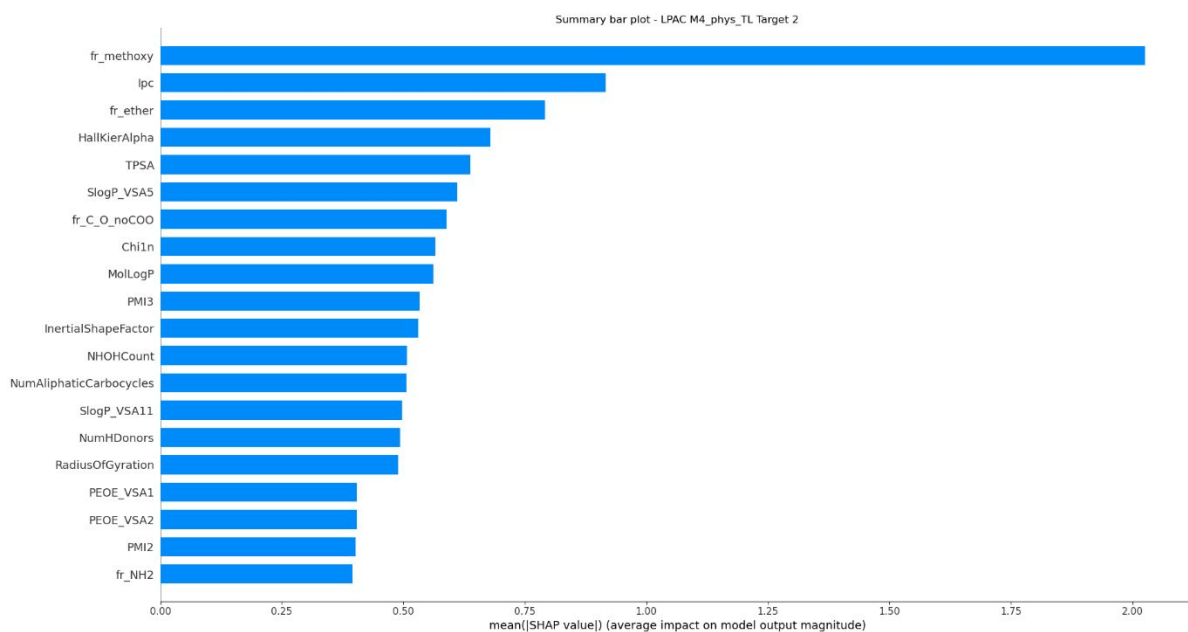


Figure S3: SHAP Summary plot for Multitarget QSRR(M4) for Target2- Retention time at pH 3.5

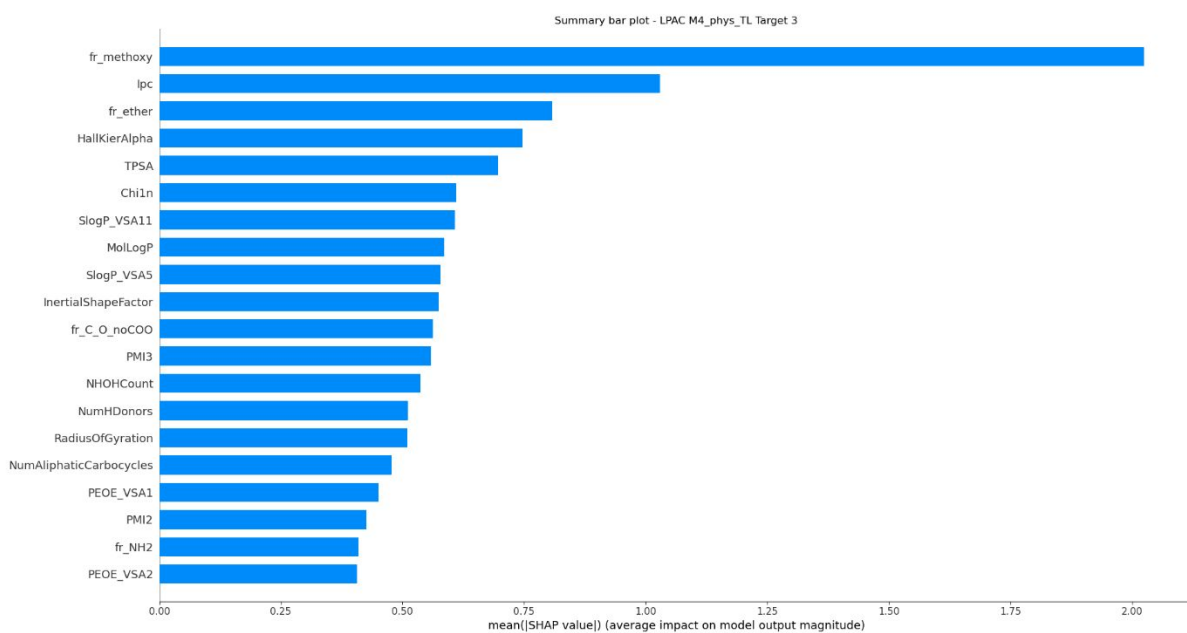


Figure S4: SHAP Summary plot for Multitarget QSRR(M4) for Target3- Retention time at pH 5.0

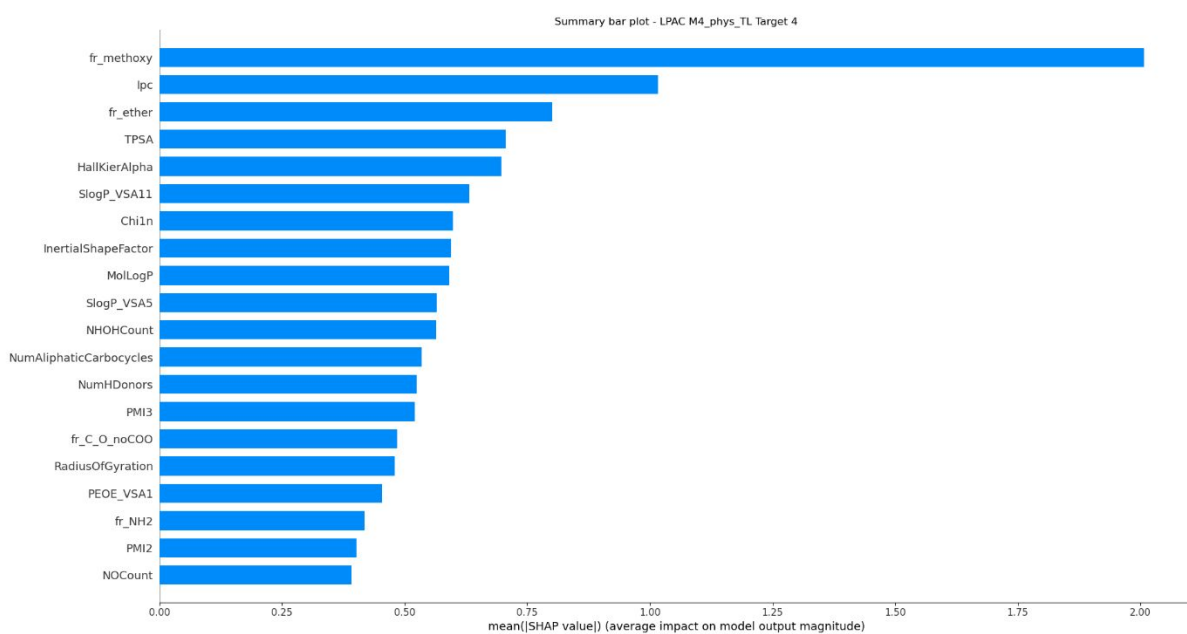


Figure S5: SHAP Summary plot for Multitarget QSRR(M4) for Target4- Retention time at pH 6.5

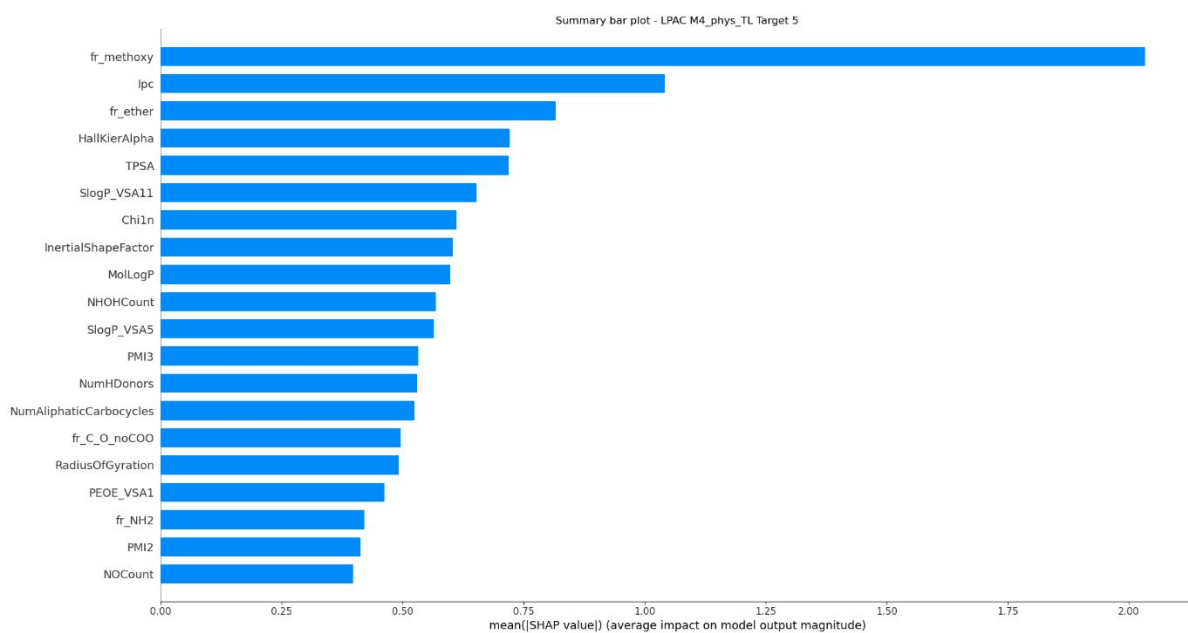


Figure S6: SHAP Summary plot for Multitarget QSRR(M4) for Target5- Retention time at pH 8.0