SUPPLEMENTARY INFORMATION

Detection and classification of fentanyl and its precursors by surface enhanced Raman spectroscopy

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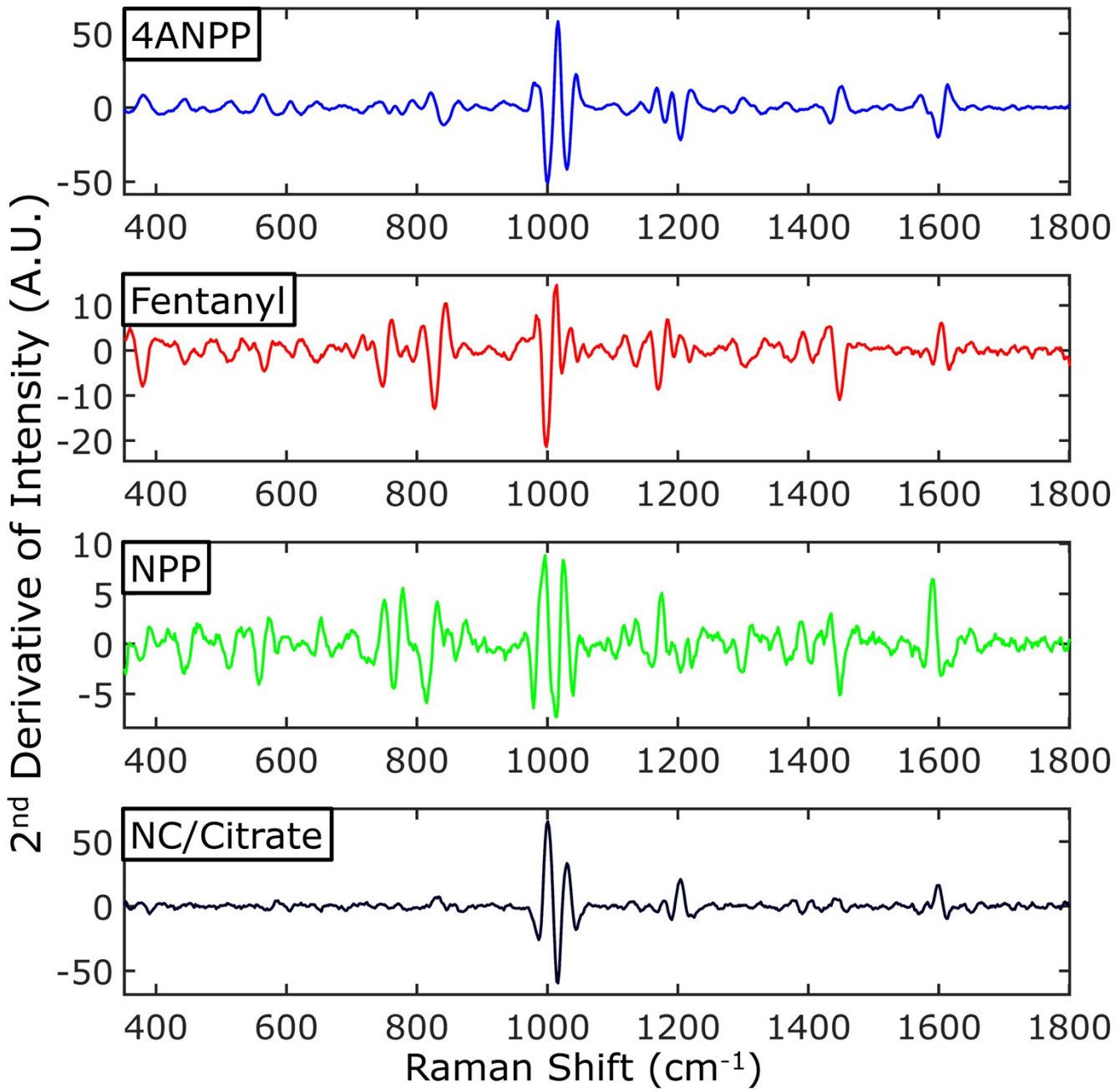

Figure S1: Preprocessed spectra of respective averaged spectra from figure 1. Preprocessing methods are identical for each analyte. Preprocessing applied in order of application: multiplicative signal correction with median ratio normalization (MSC), smoothing via Savitzky–Golay (SavGol) filter with 15 point filter width, 2nd order polynomial, and 2nd derivative, and lastly mean centering.

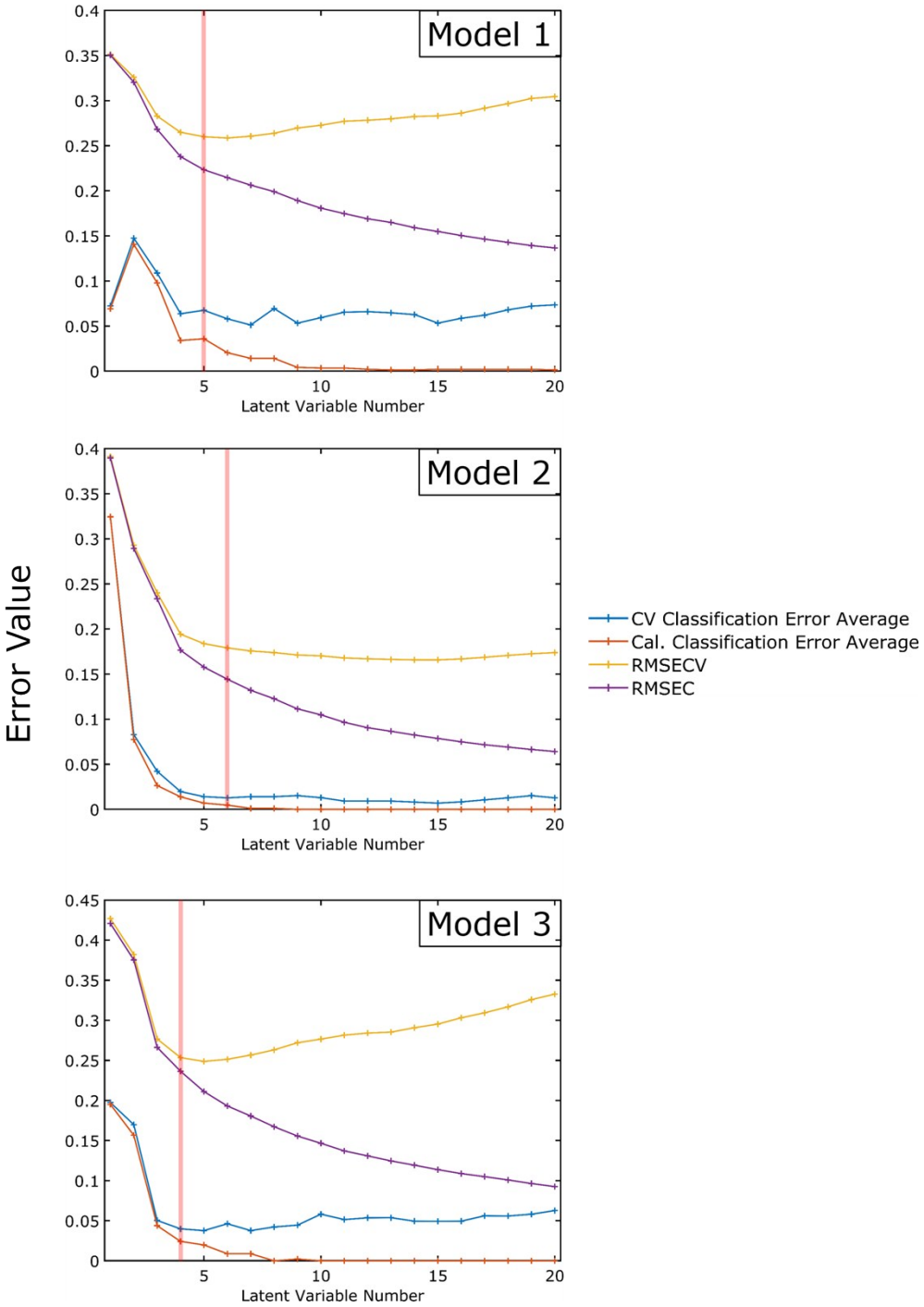

Figure S2: Error plots based on number of latent variables (LV) used. Plots for each model calibration are shown. Blue lines indicate average error in classification from cross validation (CV) results. Orange lines indicate average error in classification from calibration (Cal) results. Blue lines indicate root mean square error (RMSE) in CV results. Purple lines indicate root mean square error (RMSE) in Cal results. Vertical red line indicates number of LVs used.

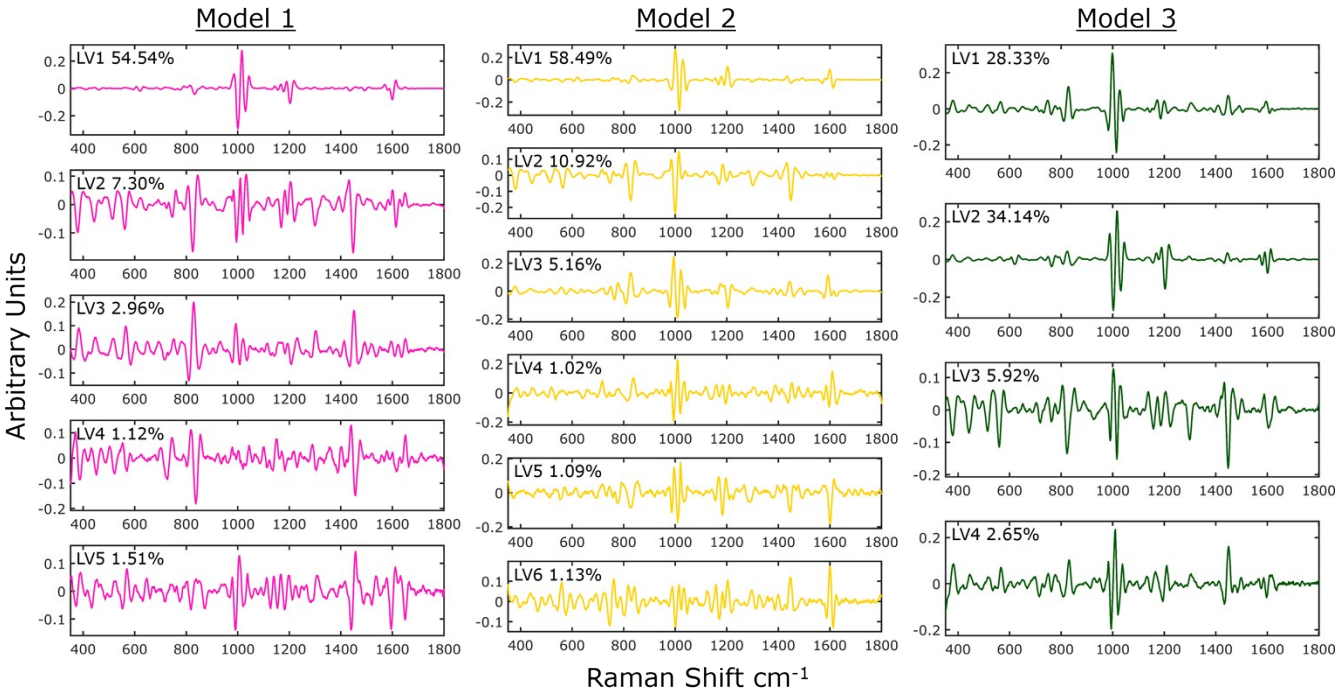

Figure S3: Loadings plots for each model used in the hierarchical PLSDA approach presented in the manuscript. Number of latent variables per model were selected using information in figure S2. Criteria for number of LVs used were based on the lowest classification error, discrepancy between Cal and CV error, and an error reduction threshold of 20%.

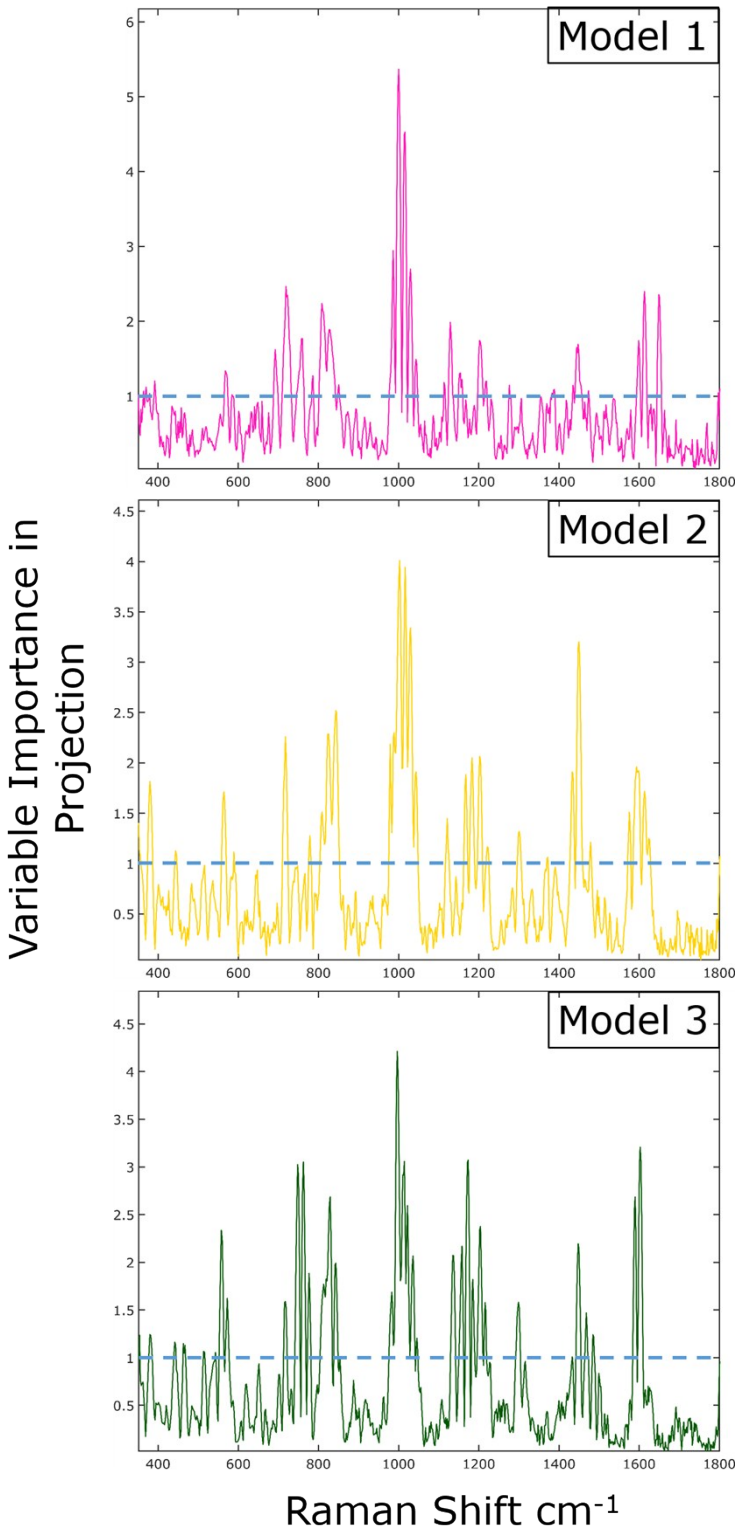

Figure S4: Plots of variable importance in projection (VIP) based on Raman Shift. Blue dashed line indicates VIP score of 1, which is the threshold for importance determination. Scores above 1 indicate

Raman Shift of importance to model. The regions above threshold were used to identify bands that were used for discriminating

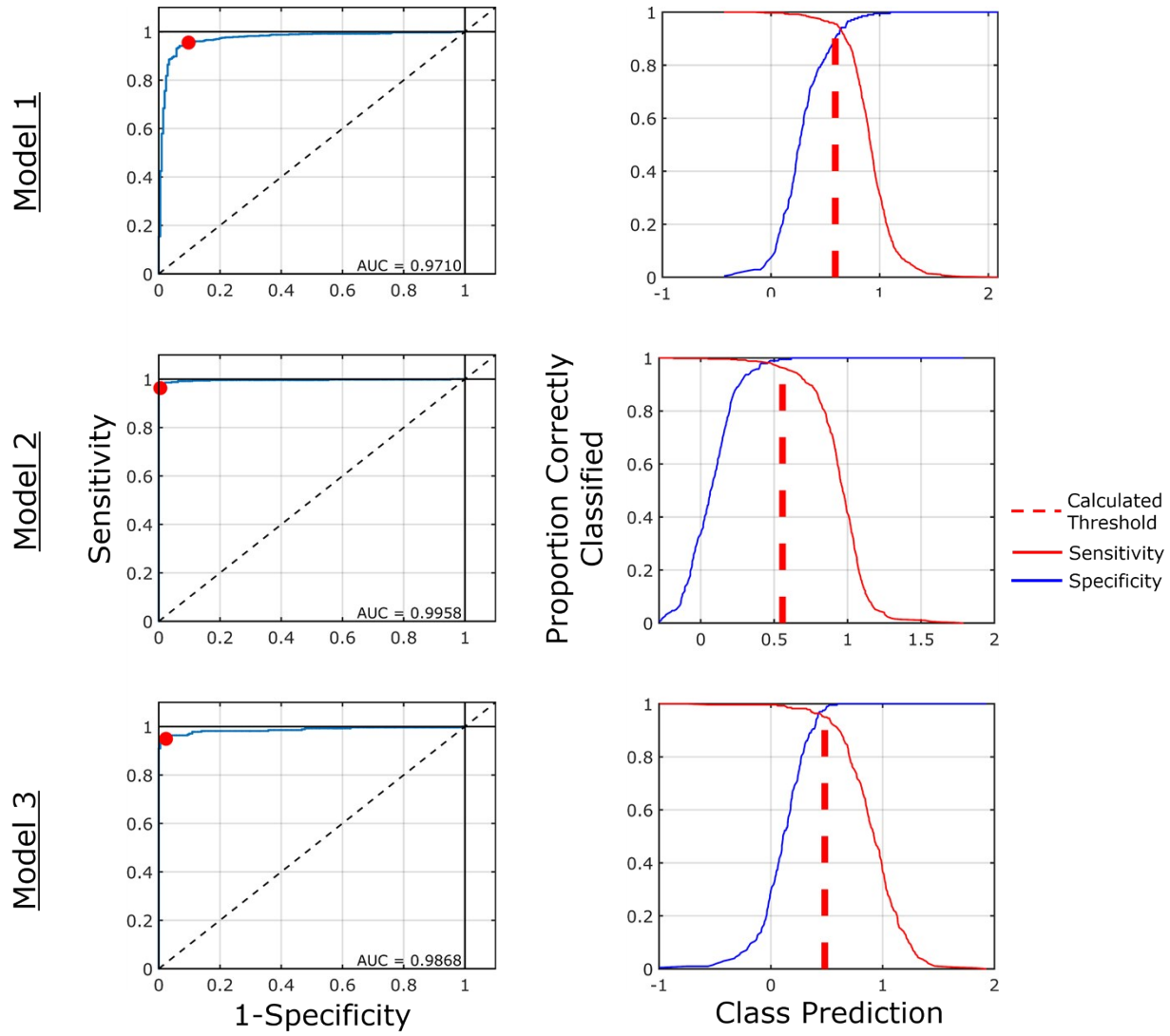

Figure S5: Receiver operating characteristic curves for each model (rows) in the hierarchical PLSDA (left column) and sensitivity and specificity curves derived from logistic regression for each model (right column). The vertical dashed red line indicates the calculated threshold from the PLSDA model. Solid red and blue curves indicate sensitivity and specificity, respectively. For each model class prediction values are dummy variables. For model 1, 2, and 3 a class prediction value of 1 corresponds to the class Negative Control, 4ANPP, and fentanyl, respectively and a class prediction value of 0 corresponds to the class 4ANPP or fentanyl or NPP, fentanyl or NPP, and NPP, respectively.

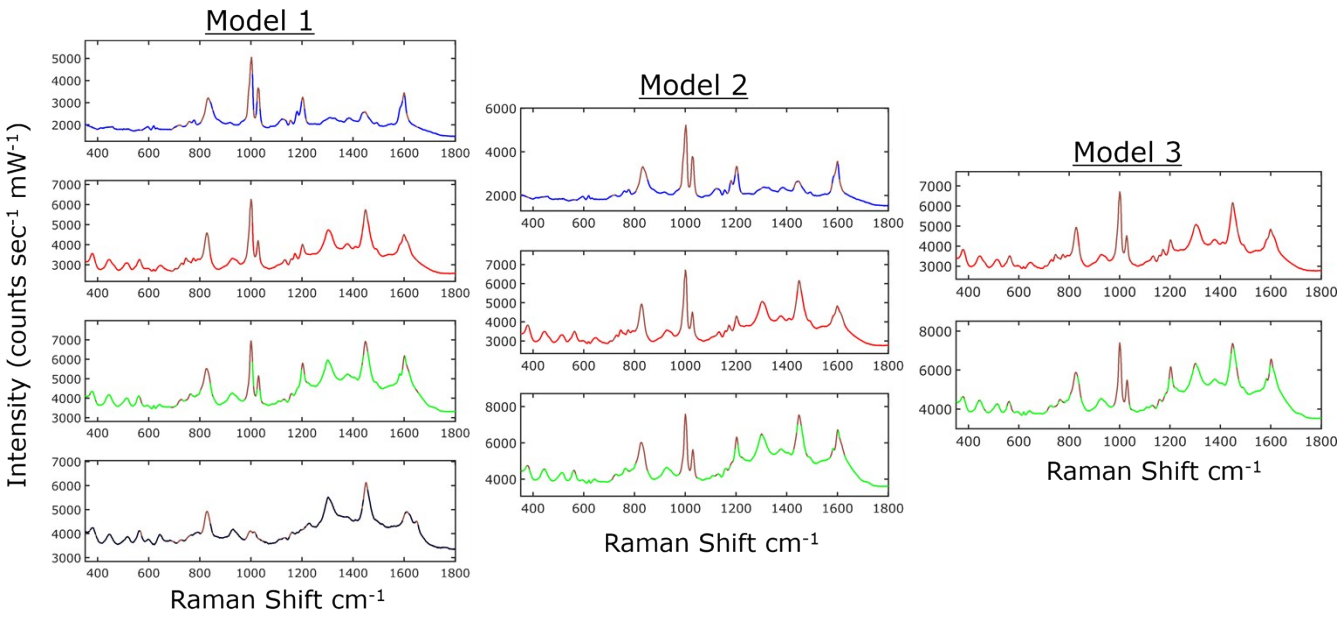

Figure S6: Spectral regions indicated as important by VIP scores. Each model step has different regions determined as important by VIP indicated with brown highlighting. The major regions to the models are the peaks at 800, 1000, 1030, 1200, 1450, and 1600 cm^{-1}.