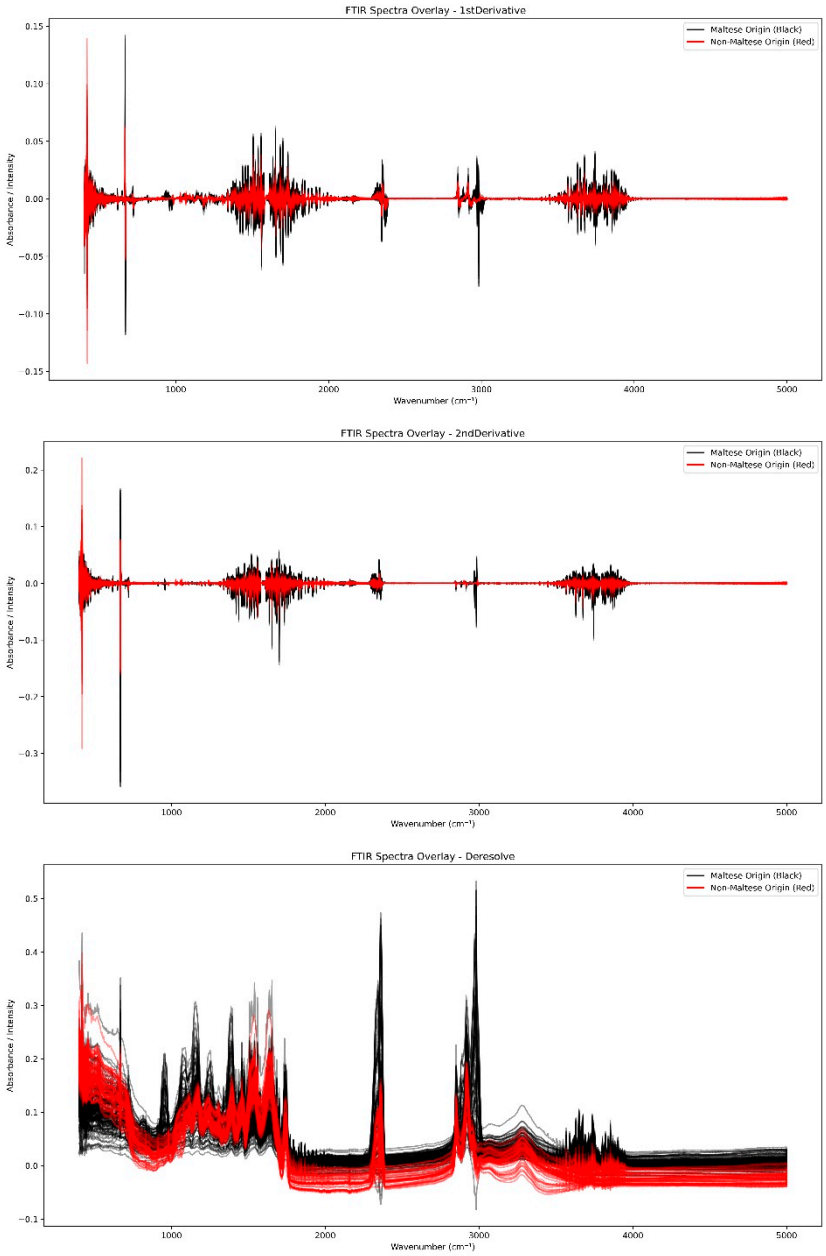
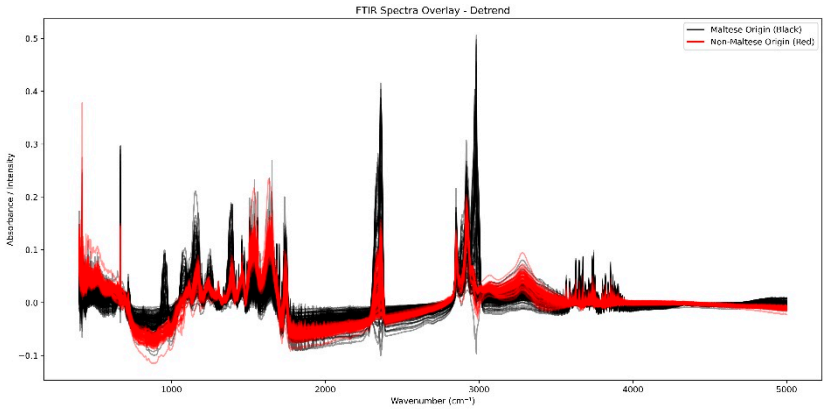
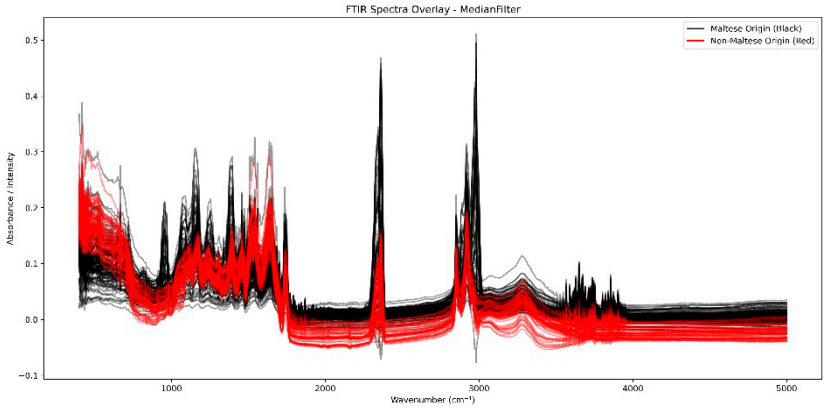
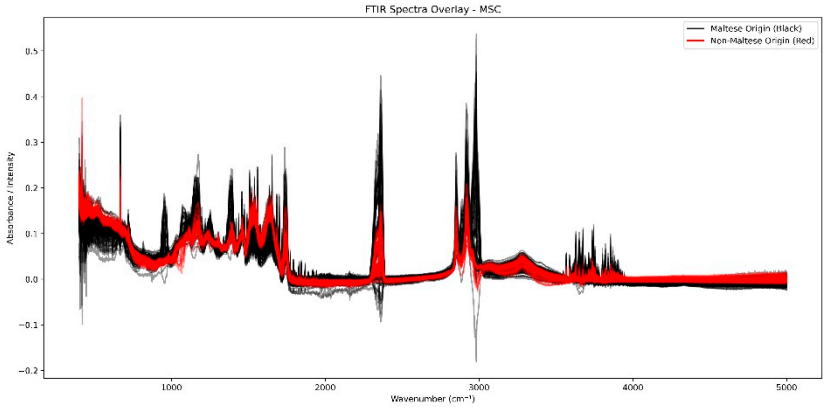
Supplementary material

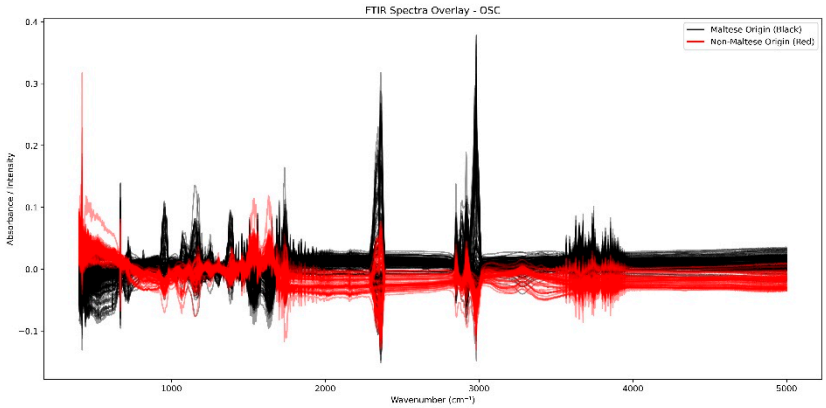
Figure S1: Representative ATR-FTIR spectra of Maltese pork (black) and non-Maltese pork (red) after applying different spectral transformations. Rows correspond to preprocessing methods: Raw, 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Standard Normal Variate (SNV), and SNV+Detrend.

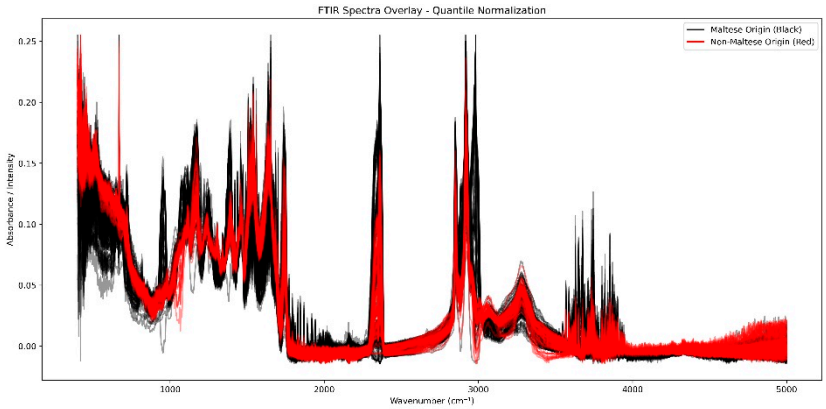


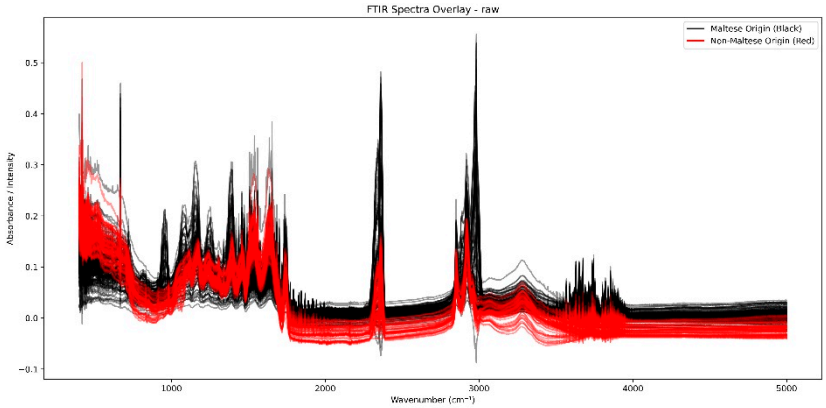

FTIR Spectra Overlay - Detrend
Maltese Origin (Black)
Non-Maltese Origin (Red)
Absorbance / Intensity
Wavenumber (cm⁻¹)

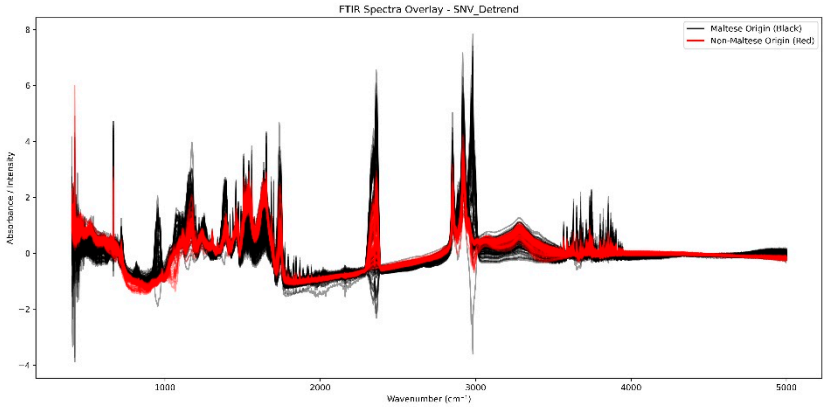

FTIR Spectra Overlay - MedianFilter
Maltese Origin (Black)
Non-Maltese Origin (Red)
Absorbance / Intensity
Wavenumber (cm⁻¹)


FTIR Spectra Overlay - MSC
Maltese Origin (Black)
Non-Maltese Origin (Red)
Absorbance / Intensity
Wavenumber (cm⁻¹)


FTIR Spectra Overlay - OSC
Maltese Origin (Black)
Non-Maltese Origin (Red)
Absorbance / Intensity
Wavenumber (cm⁻¹)


FTIR Spectra Overlay - Quantile Normalization
Maltese Origin (Black)
Non-Maltese Origin (Red)
Absorbance / Intensity
Wavenumber (cm⁻¹)


FTIR Spectra Overlay - raw
Maltese Origin (Black)
Non-Maltese Origin (Red)
Absorbance / Intensity
Wavenumber (cm⁻¹)


FTIR Spectra Overlay - SNV_Detrend
Maltese Origin (Black)
Non-Maltese Origin (Red)
Absorbance / Intensity
Wavenumber (cm⁻¹)

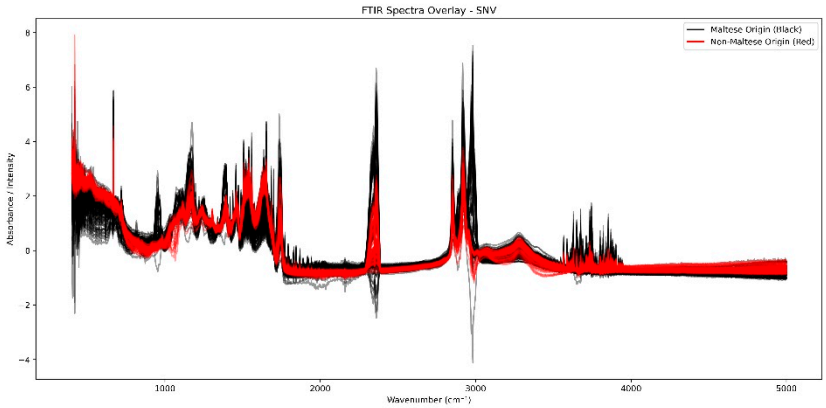
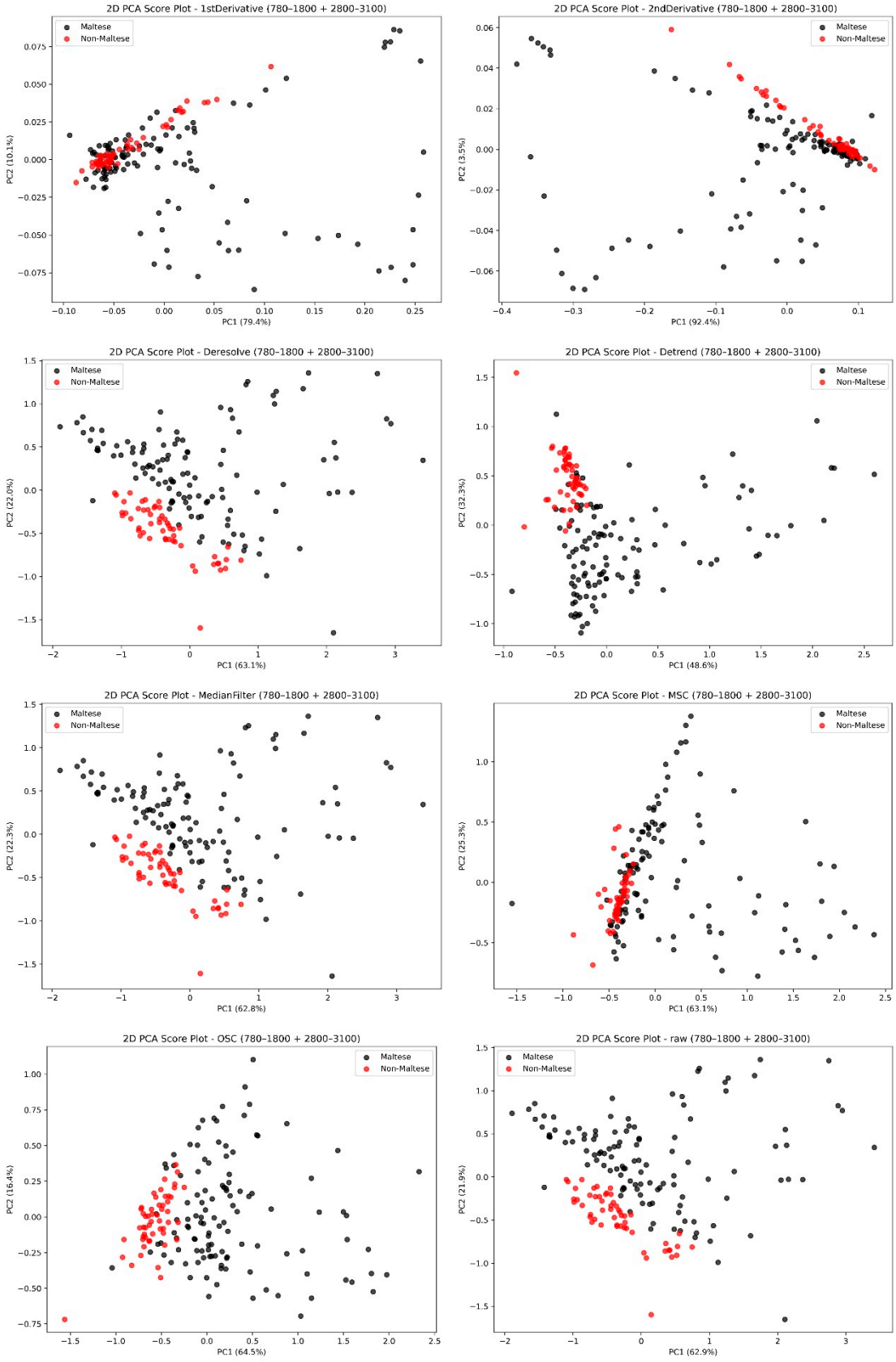
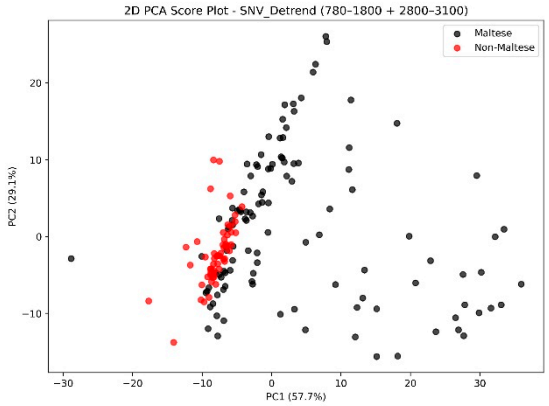

FTIR Spectra Overlay - SNV
Maltese Origin (Black)
Non-Maltese Origin (Red)
Absorbance / Intensity
Wavenumber (cm⁻¹)

Figure S2: PCA score plots of the full spectrum (4000–400 cm^{-1}) for all spectral transformations. Rows correspond to preprocessing methods: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend




2D PCA Score Plot - SNV_Detrend (780–1800 + 2800–3100)
Maltese
Non-Maltese
PC2 (29.1%)
PC1 (57.7%)
20
10
0
−10
−30
−20
−10
0
10
20
30

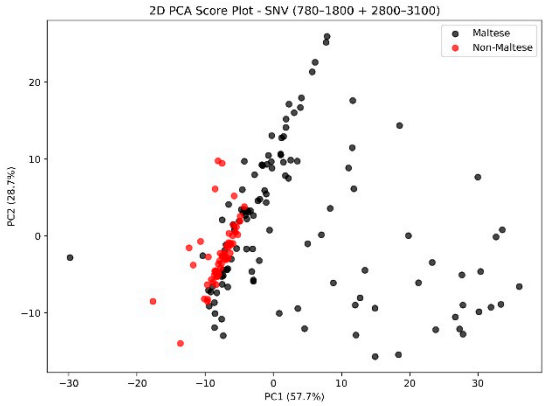
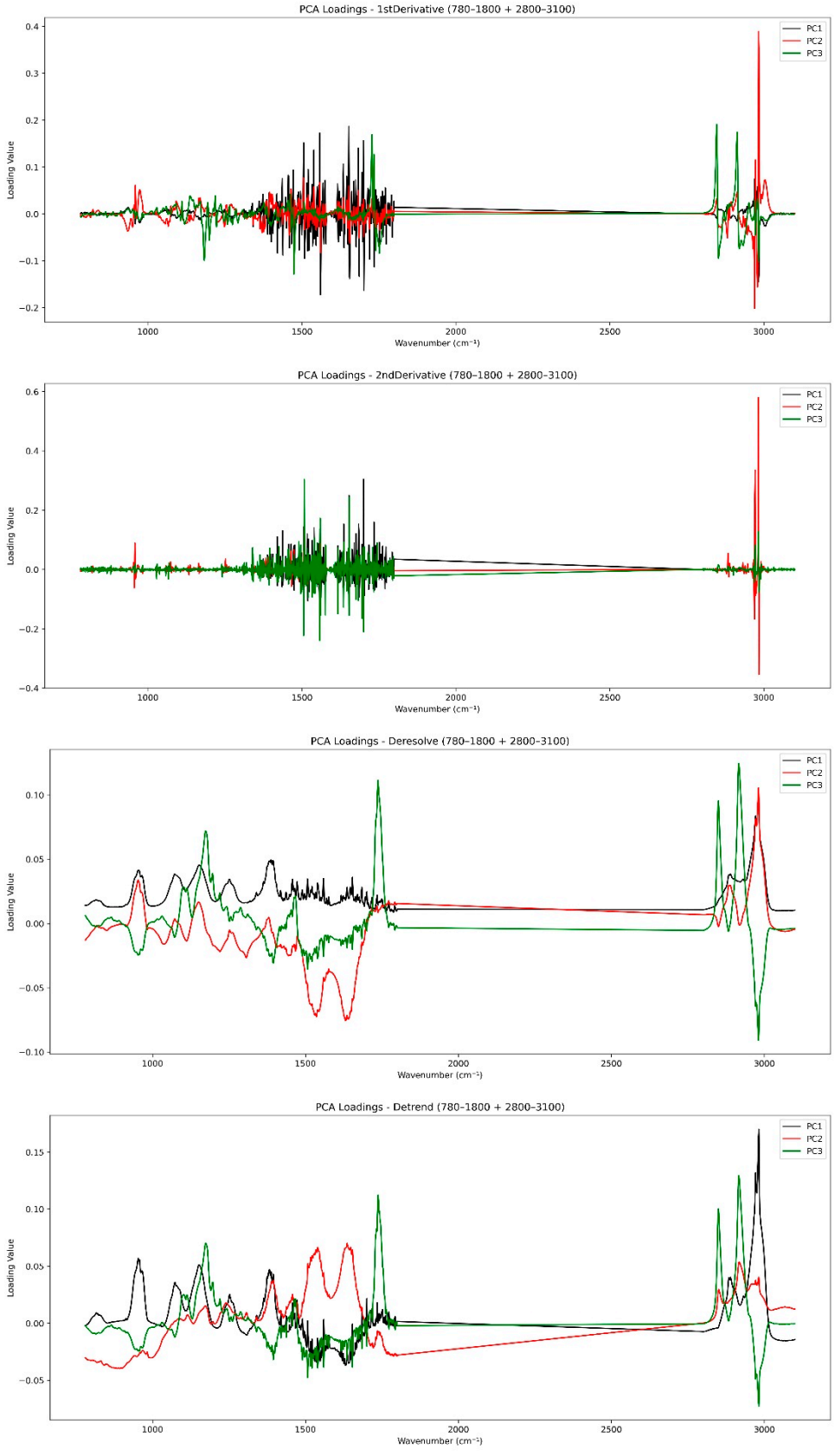
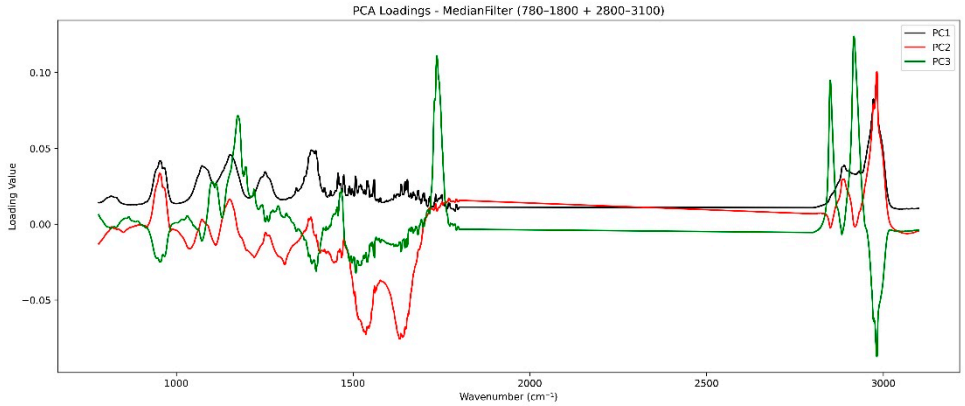
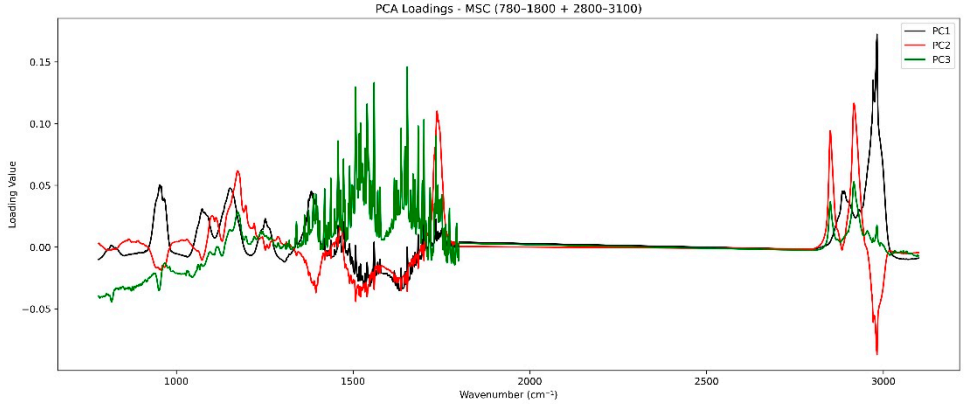
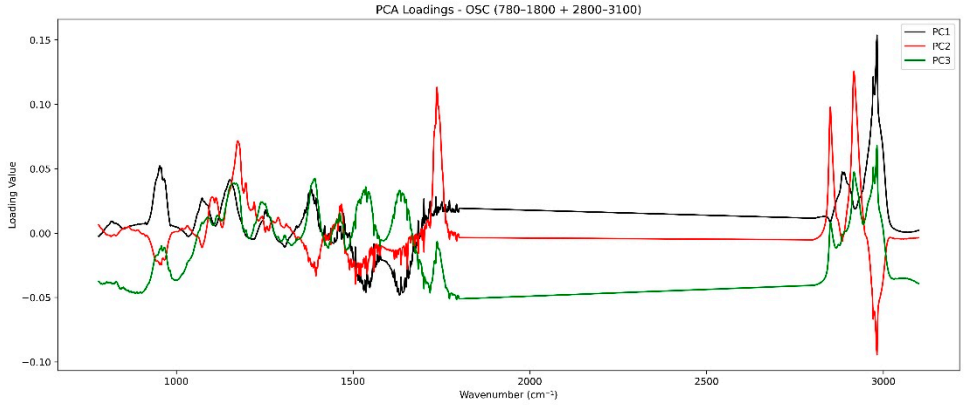

2D PCA Score Plot - SNV (780–1800 + 2800–3100)
Maltese
Non-Maltese
PC2 (28.7%)
PC1 (57.7%)
20
10
0
−10
−30
−20
−10
0
10
20
30

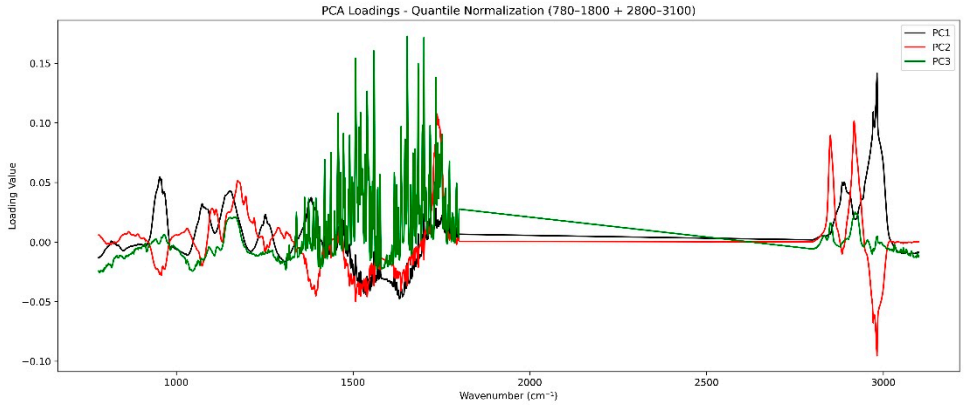
Figure S3: PCA loading plots of the full spectrum (4000–400 cm^{-1}) for all applied spectral transformations. Rows correspond to preprocessing methods: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend.

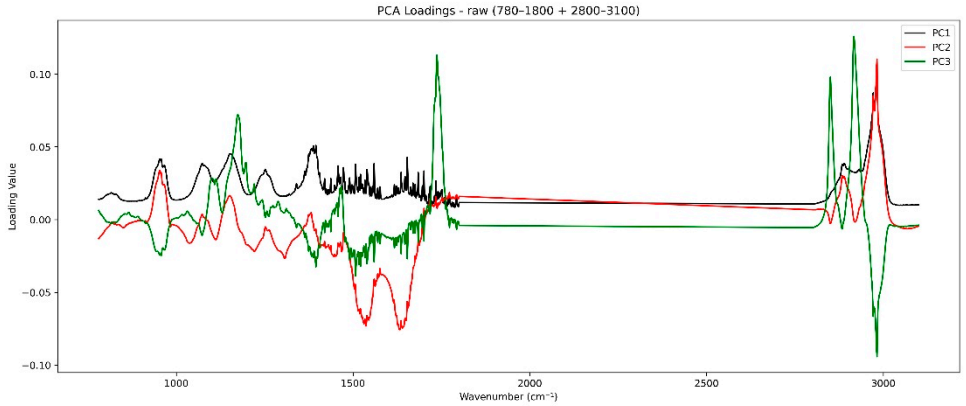


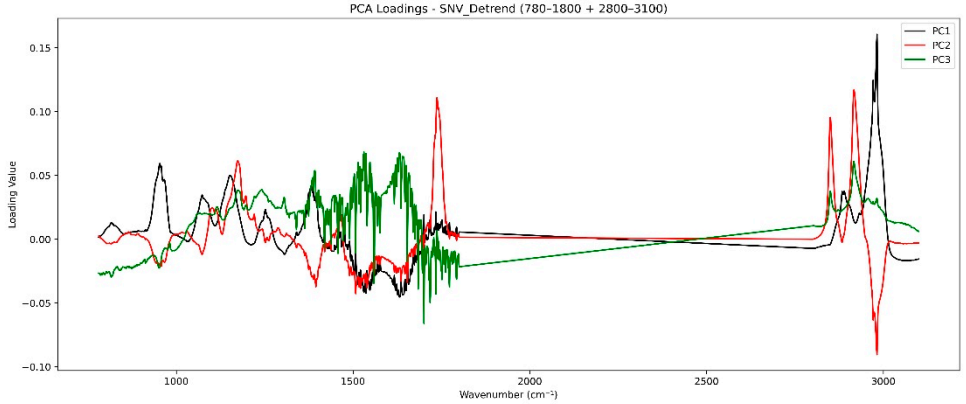

PCA Loadings - MedianFilter (780–1800 + 2800–3100)
PC1
PC2
PC3
Loading Value
0.10
0.05
0.00
−0.05
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)


PCA Loadings - MSC (780–1800 + 2800–3100)
PC1
PC2
PC3
Loading Value
0.15
0.10
0.05
0.00
−0.05
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)


PCA Loadings - OSC (780–1800 + 2800–3100)
PC1
PC2
PC3
Loading Value
0.15
0.10
0.05
0.00
−0.05
−0.10
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)


PCA Loadings - Quantile Normalization (780–1800 + 2800–3100)
PC1
PC2
PC3
Loading Value
0.15
0.10
0.05
0.00
−0.05
−0.10
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)


PCA Loadings - raw (780–1800 + 2800–3100)
PC1
PC2
PC3
Loading Value
0.10
0.05
0.00
−0.05
−0.10
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)


PCA Loadings - SNV_Detrend (780–1800 + 2800–3100)
PC1
PC2
PC3
Loading Value
0.15
0.10
0.05
0.00
−0.05
−0.10
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)

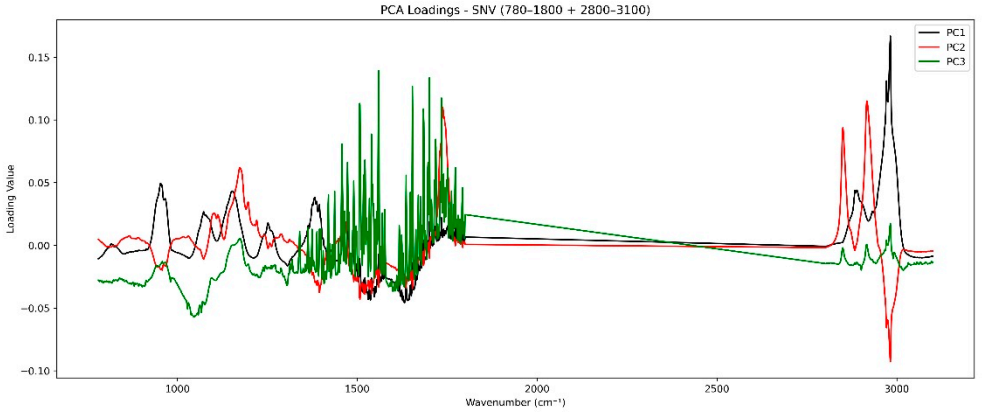
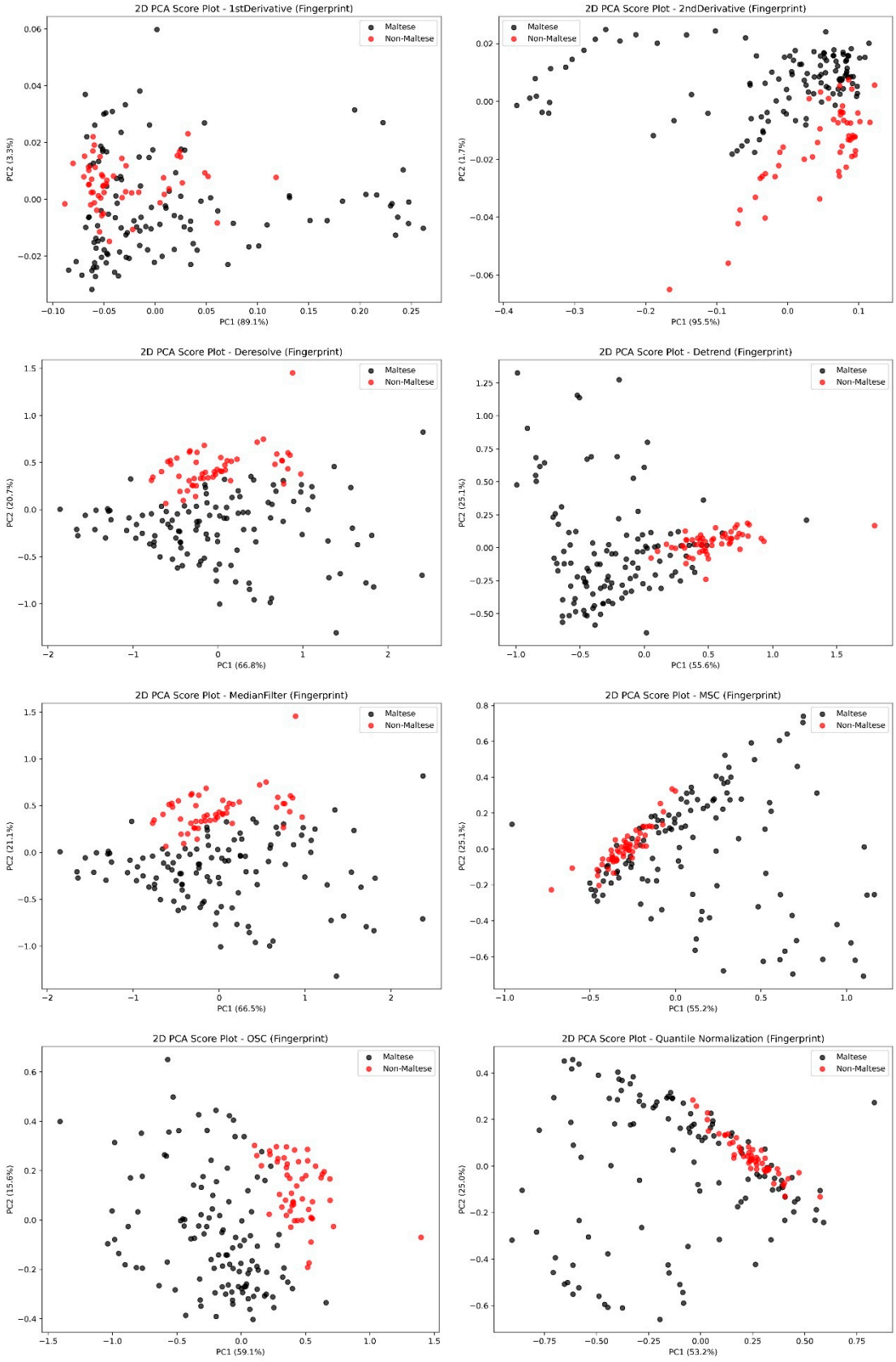
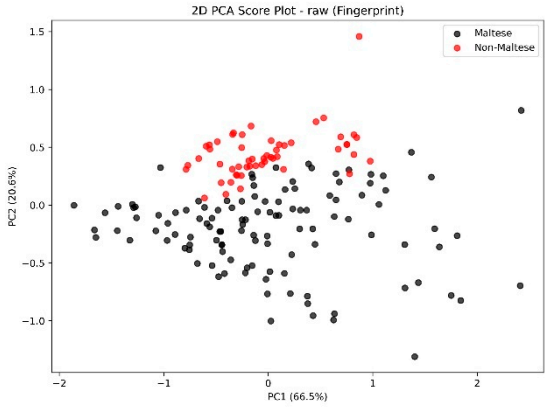
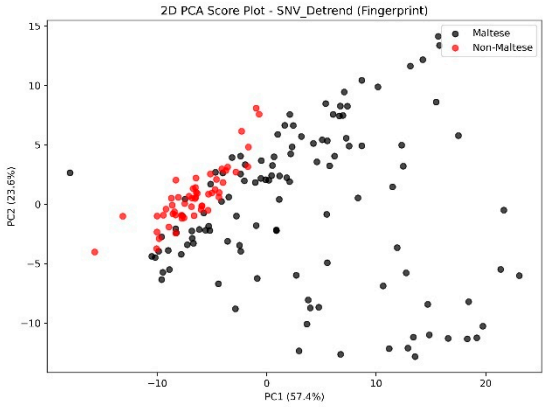

PCA Loadings - SNV (780–1800 + 2800–3100)
PC1
PC2
PC3
Loading Value
0.15
0.10
0.05
0.00
−0.05
−0.10
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)

Figure S4: PCA score plots of the fingerprint region (1800–850 cm^{-1}) for all spectral transformations. Rows correspond to the different preprocessing methods applied: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend




2D PCA Score Plot - raw (Fingerprint)
Maltese
Non-Maltese
PC2 (20.6%)
PC1 (66.5%)


2D PCA Score Plot - SNV_Detrend (Fingerprint)
Maltese
Non-Maltese
PC2 (23.6%)
PC1 (57.4%)

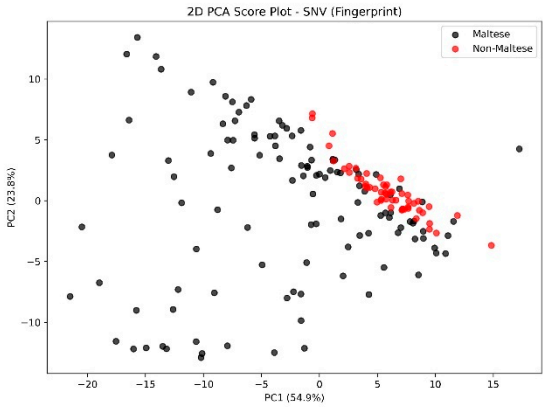
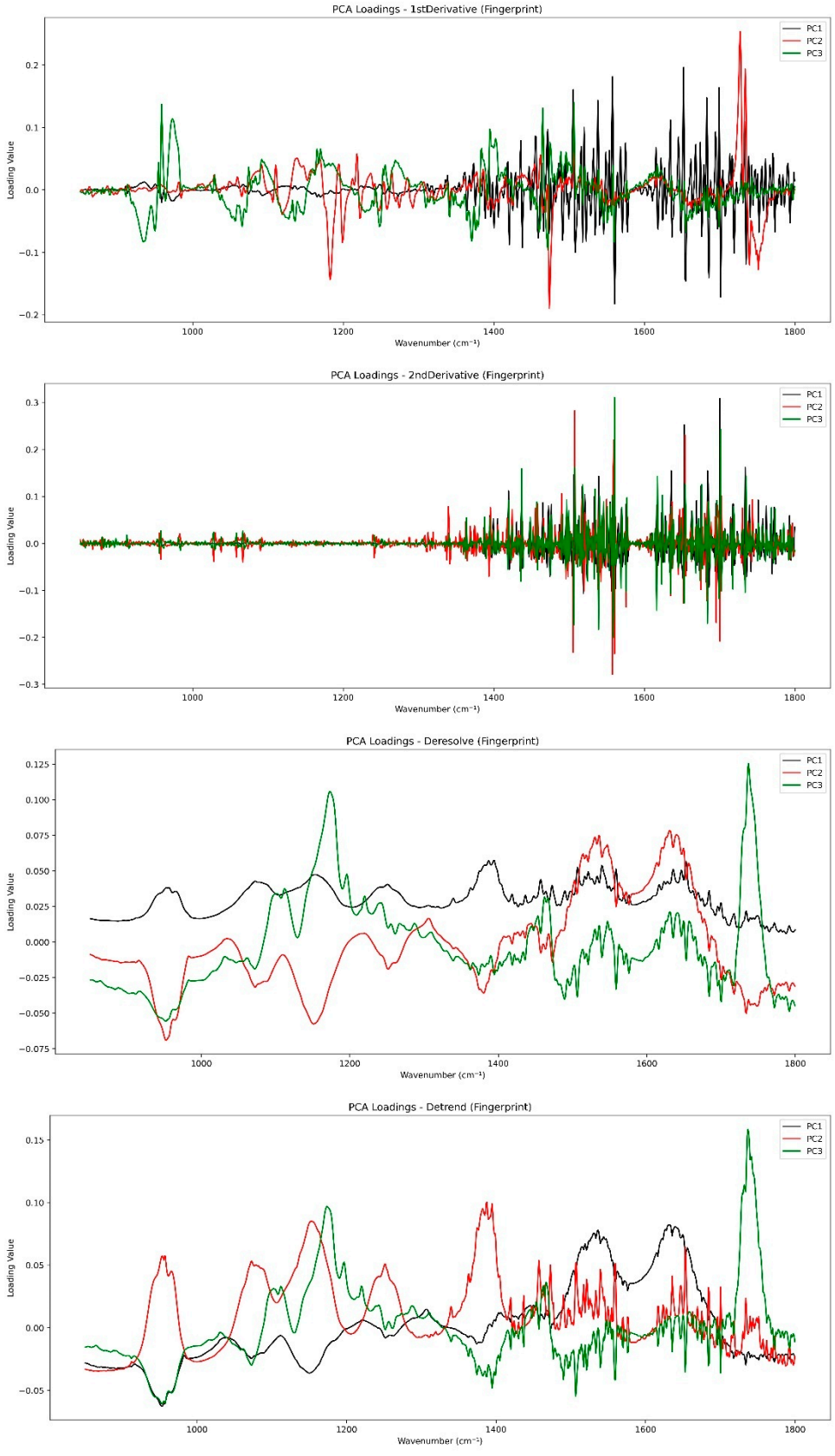
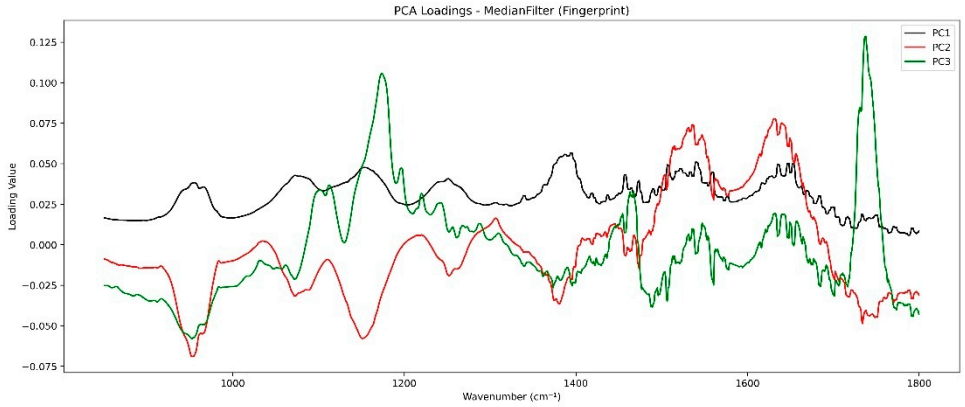
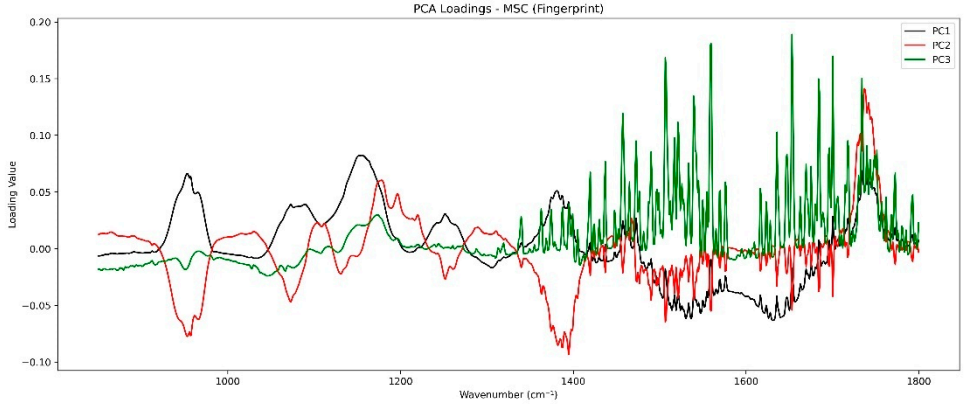
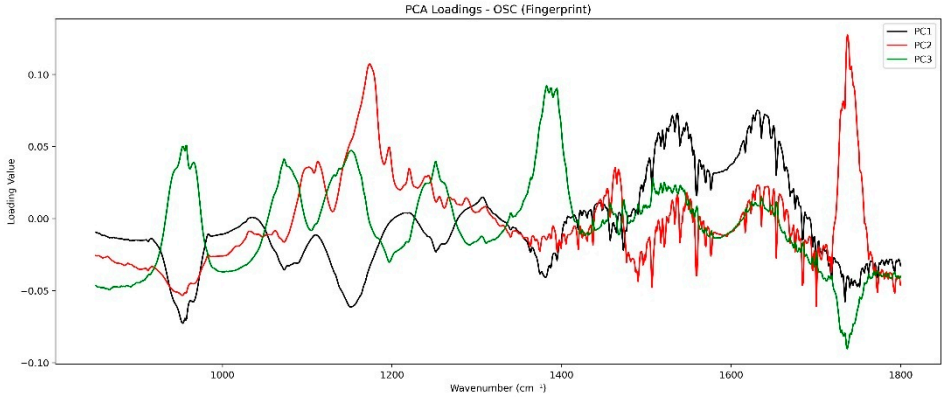

2D PCA Score Plot - SNV (Fingerprint)
Maltese
Non-Maltese
PC2 (23.8%)
PC1 (54.9%)

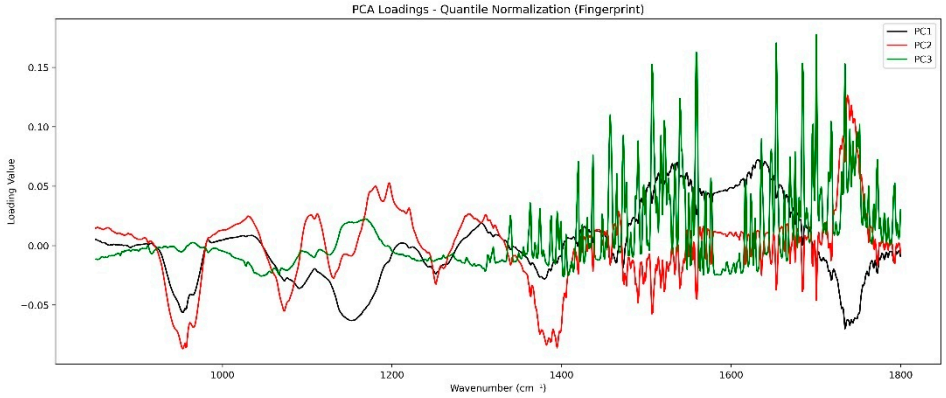
Figure S5: PCA loading plots of the fingerprint region (1800–850 cm^{-1}) for all applied spectral transformations. Rows correspond to preprocessing methods: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend

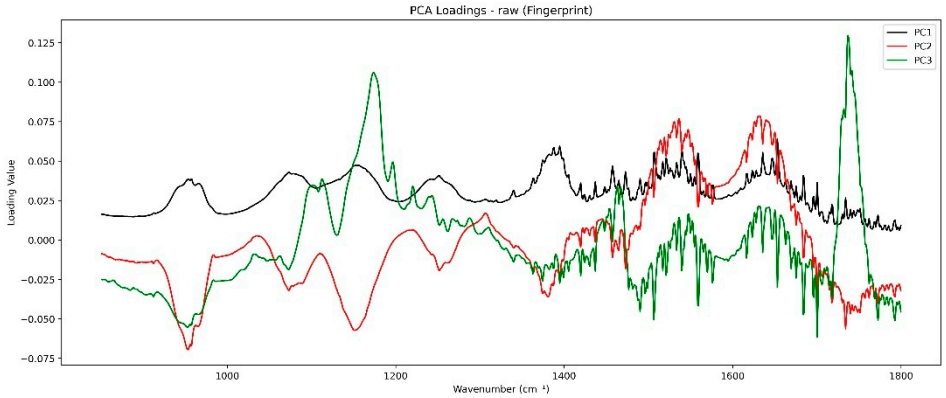


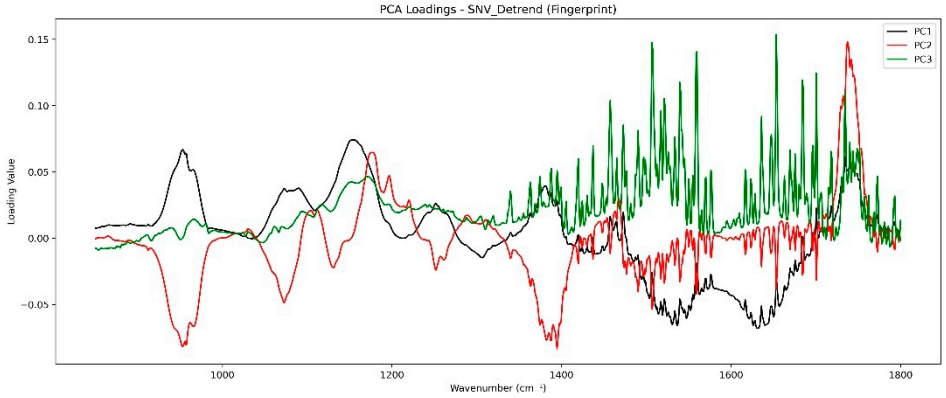

PCA Loadings - MedianFilter (Fingerprint)
PC1
PC2
PC3
Loading Value
Wavenumber (cm⁻¹)


PCA Loadings - MSC (Fingerprint)
PC1
PC2
PC3
Loading Value
Wavenumber (cm⁻¹)


PCA Loadings - OSC (Fingerprint)
PC1
PC2
PC3
Loading Value
Wavenumber (cm ⁻¹)


PCA Loadings - Quantile Normalization (Fingerprint)
PC1
PC2
PC3
Loading Value
Wavenumber (cm ⁻¹)


PCA Loadings - raw (Fingerprint)
PC1
PC2
PC3
Loading Value
0.125
0.100
0.075
0.050
0.025
0.000
−0.025
−0.050
−0.075
1000
1200
1400
1600
1800
Wavenumber (cm ⁻¹)


PCA Loadings - SNV_Detrend (Fingerprint)
PC1
PC2
PC3
Loading Value
0.15
0.10
0.05
0.00
−0.05
1000
1200
1400
1600
1800
Wavenumber (cm ⁻¹)

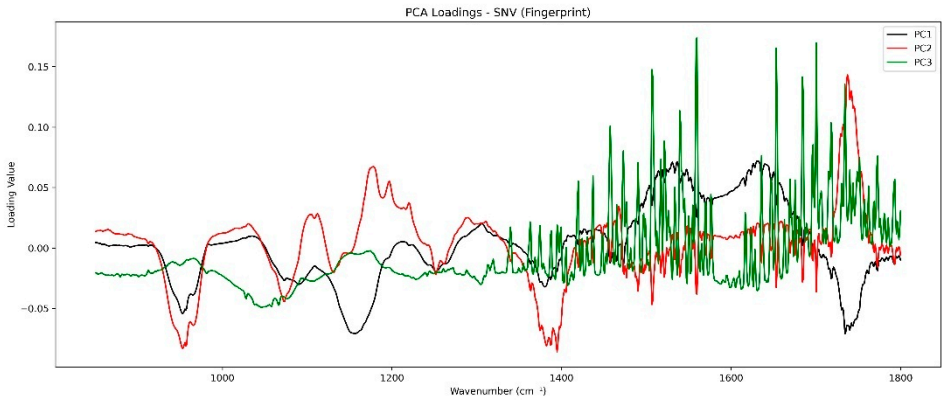
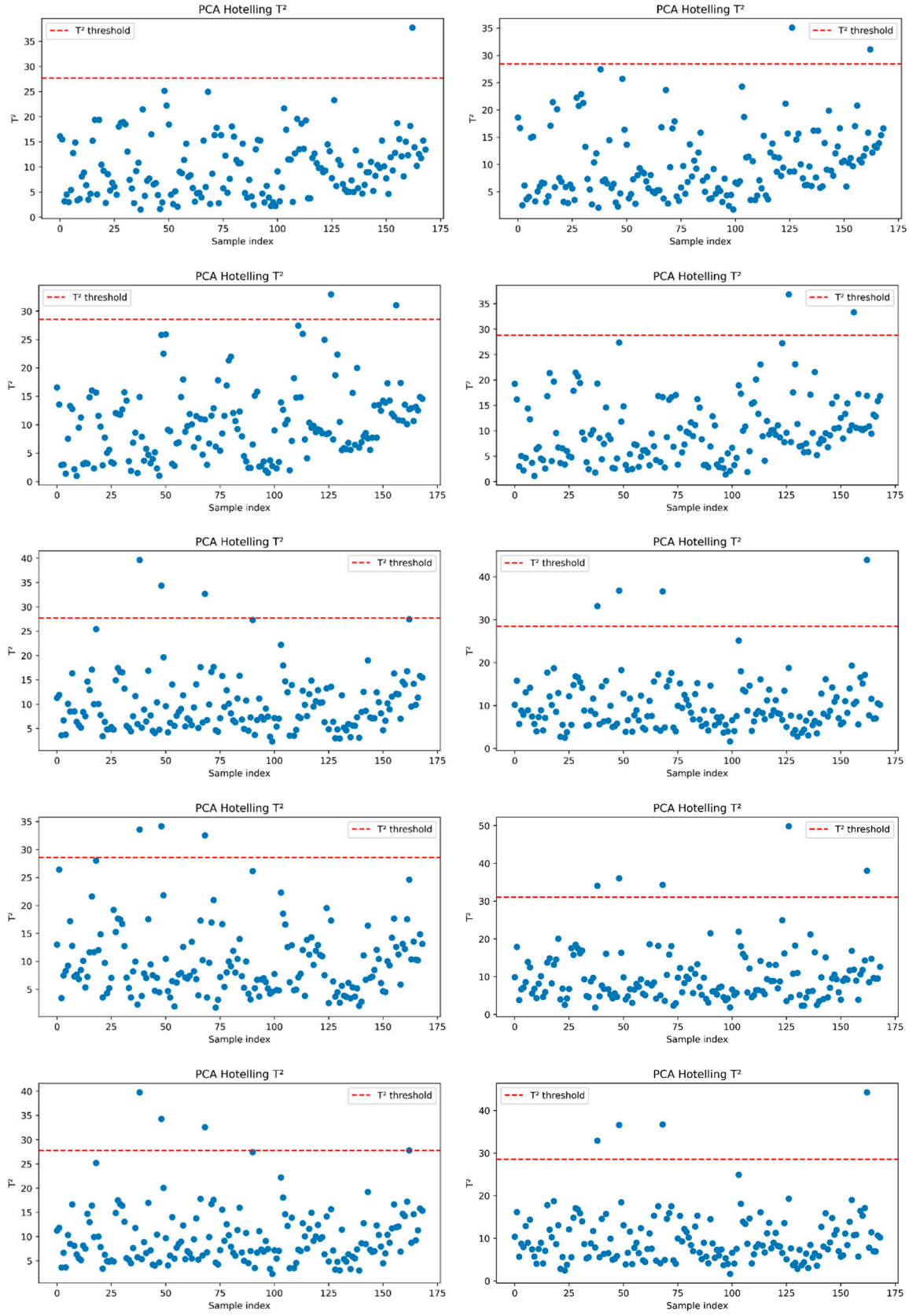
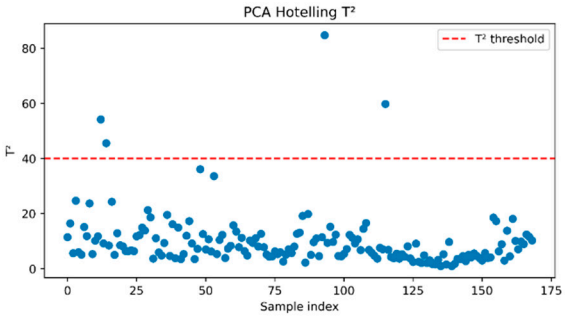
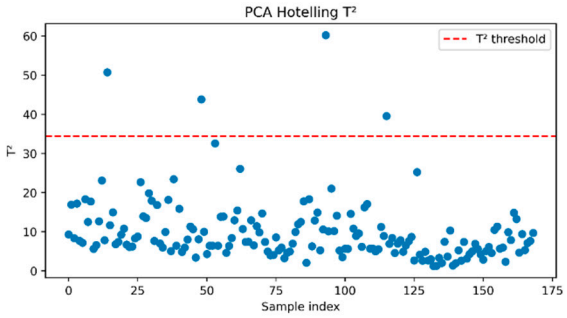
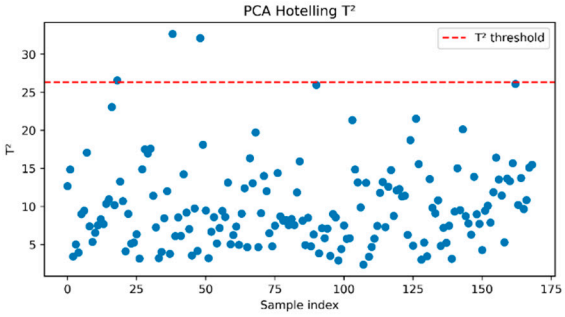

PCA Loadings - SNV (Fingerprint)
PC1
PC2
PC3
Loading Value
0.15
0.10
0.05
0.00
−0.05
1000
1200
1400
1600
1800
Wavenumber (cm ⁻¹)

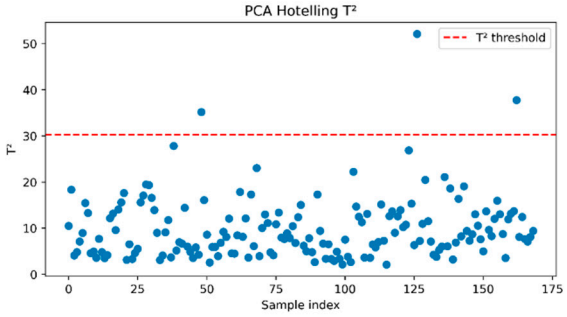
Figure S6: . Outlier analysis using Hotelling's T^2 plots for all spectral transformations comparing the whole spectrum (right panels) and the fingerprint region (left panels). Rows correspond to different preprocessing methods applied to the ATR-FTIR pork dataset: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, MSC, OSC, Quantile Normalization, Raw, SNV, and SNV+Detrend.

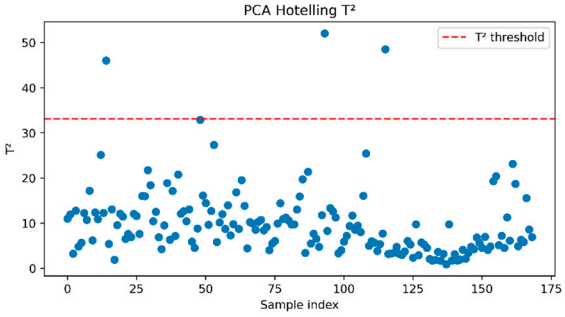


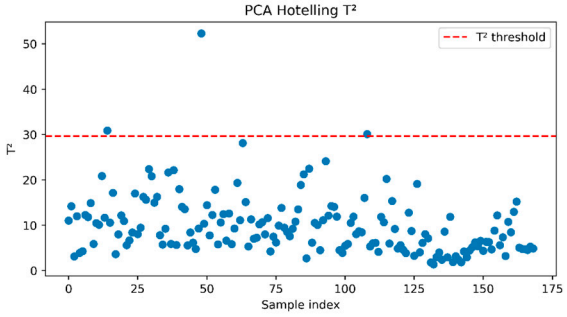

PCA Hotelling T²
T² threshold
T²
Sample index

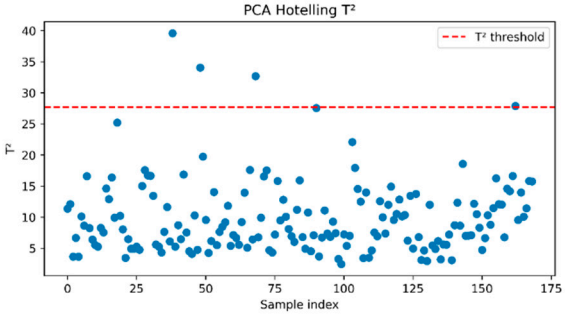

PCA Hotelling T²
T² threshold
T²
Sample index

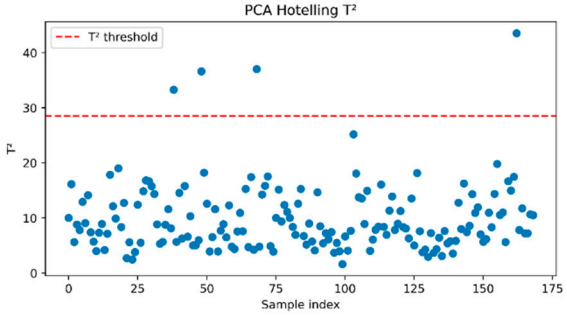

PCA Hotelling T²
T² threshold
T²
Sample index

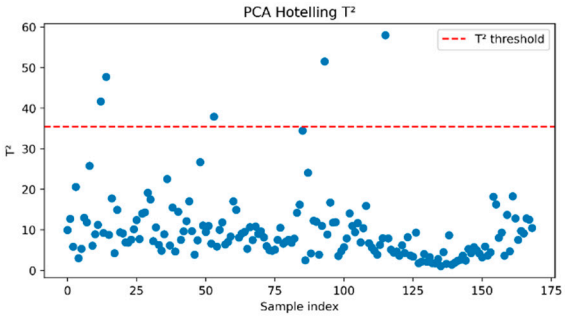

PCA Hotelling T²
T² threshold
T²
Sample index

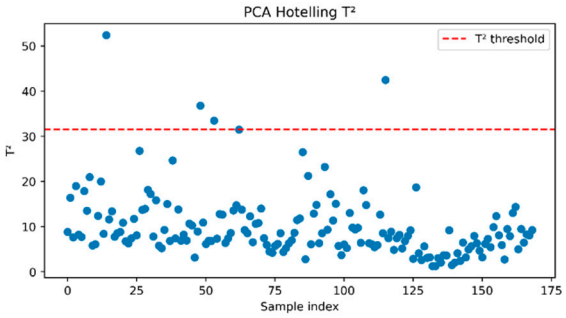

PCA Hotelling T²
T² threshold
T²
Sample index

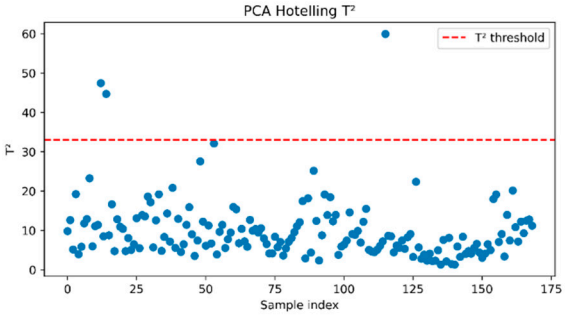

PCA Hotelling T²
T² threshold
T²
Sample index


PCA Hotelling T²
T² threshold
T²
Sample index


PCA Hotelling T²
T² threshold
T²
Sample index


PCA Hotelling T²
T² threshold
T²
Sample index


PCA Hotelling T²
T² threshold
T²
Sample index


PCA Hotelling T²
T² threshold
T²
Sample index

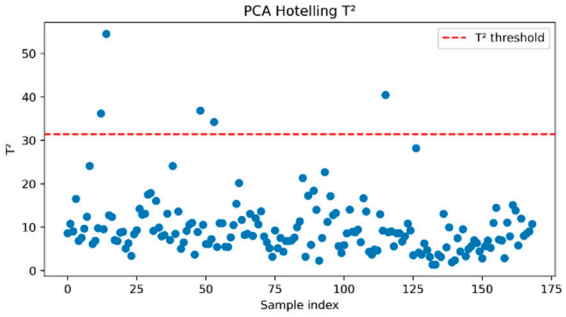
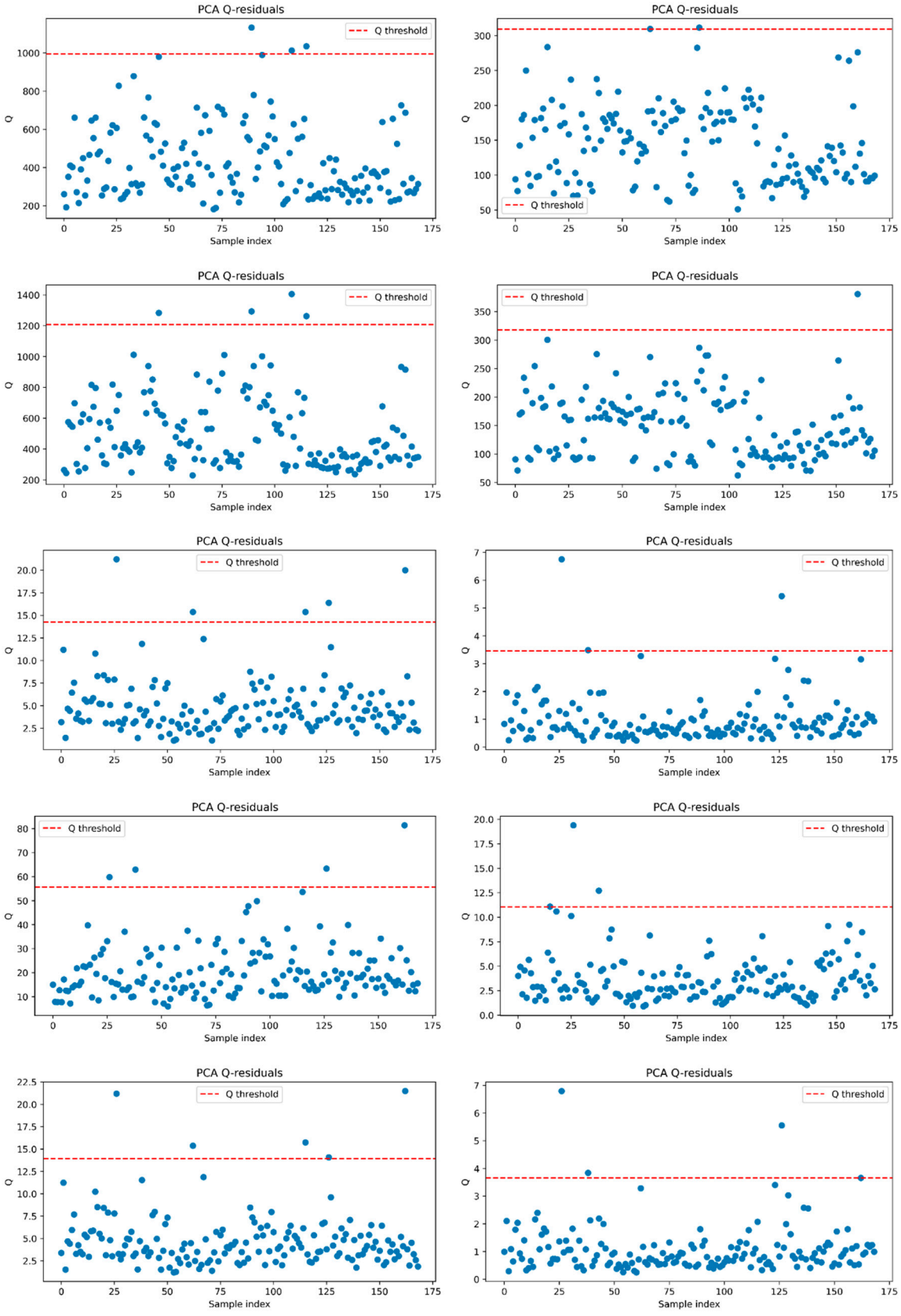
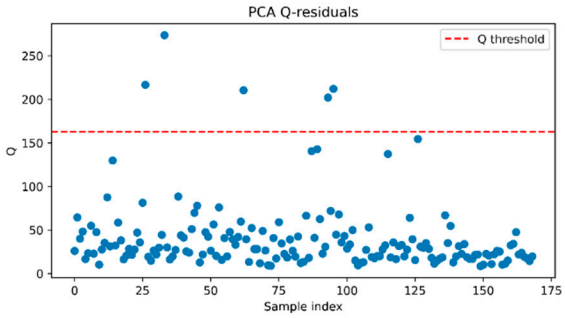
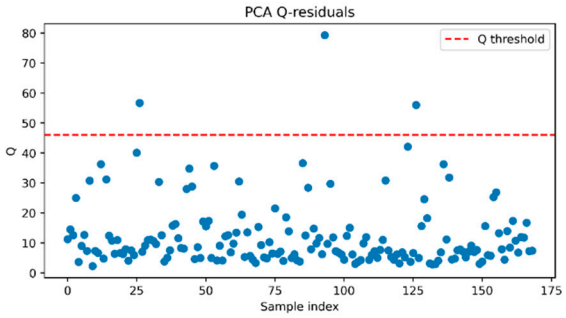
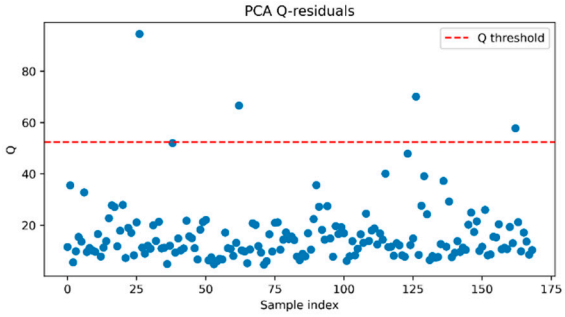

PCA Hotelling T²
T² threshold
T²
Sample index

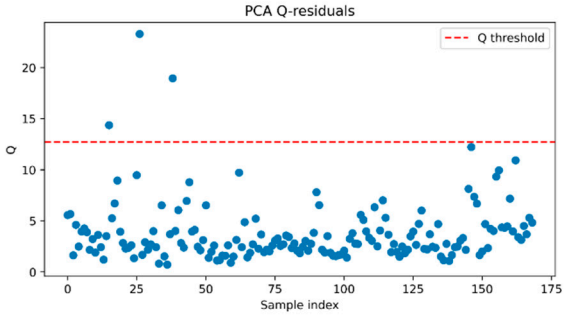
Figure S7: . Q resdiual plots for all spectral transformations comparing the whole spectrum (right panels) and the fingerprint region (left panels). Rows correspond to different preprocessing methods applied to the ATR-FTIR pork dataset: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, MSC, OSC, Quantile Normalization, Raw, SNV, and SNV+Detrend.

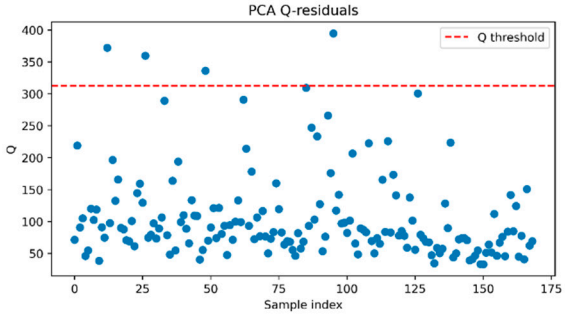


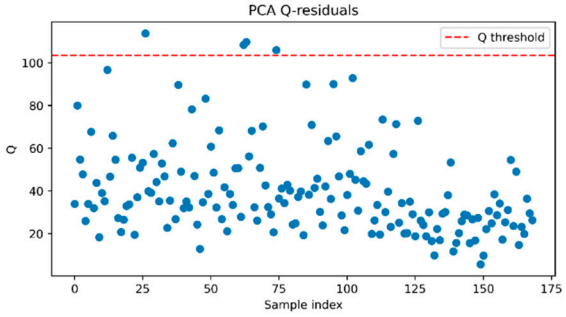

PCA Q-residuals
Q threshold
Q
Sample index

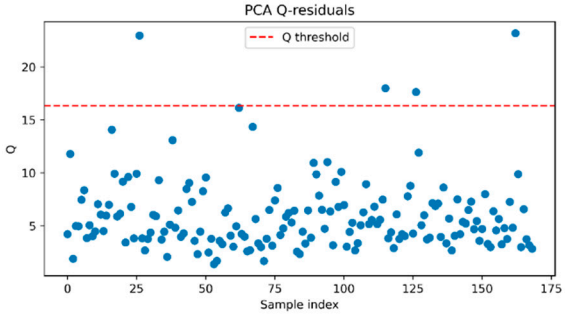

PCA Q-residuals
Q threshold
Q
Sample index

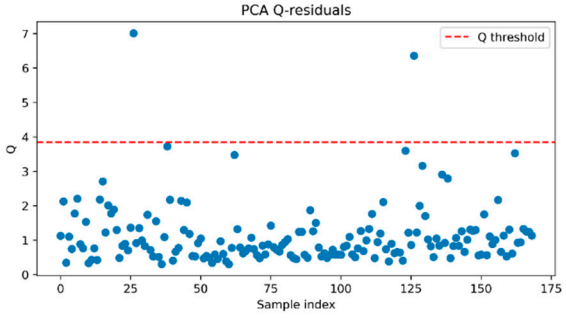

PCA Q-residuals
Q threshold
Q
Sample index

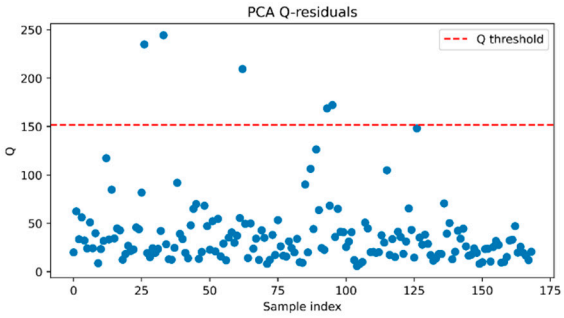

PCA Q-residuals
Q threshold
Q
Sample index

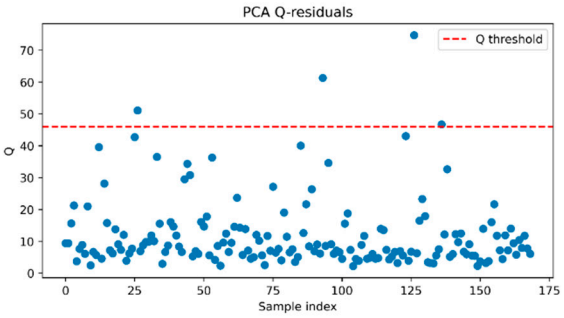

PCA Q-residuals
Q threshold
Q
Sample index

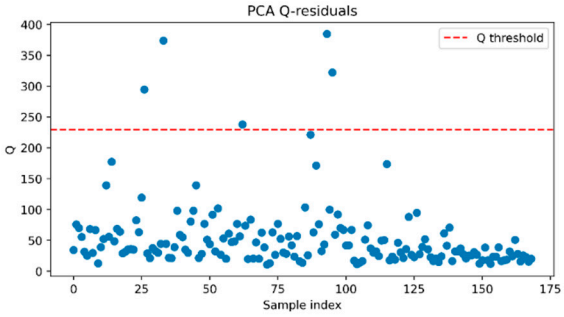

PCA Q-residuals
Q threshold
Q
Sample index


PCA Q-residuals
Q threshold
Q
Sample index


PCA Q-residuals
Q threshold
Q
Sample index


PCA Q-residuals
Q threshold
Q
Sample index


PCA Q-residuals
Q threshold
Q
Sample index


PCA Q-residuals
Q threshold
Q
Sample index

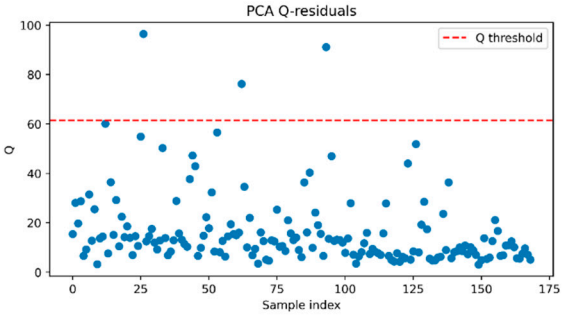
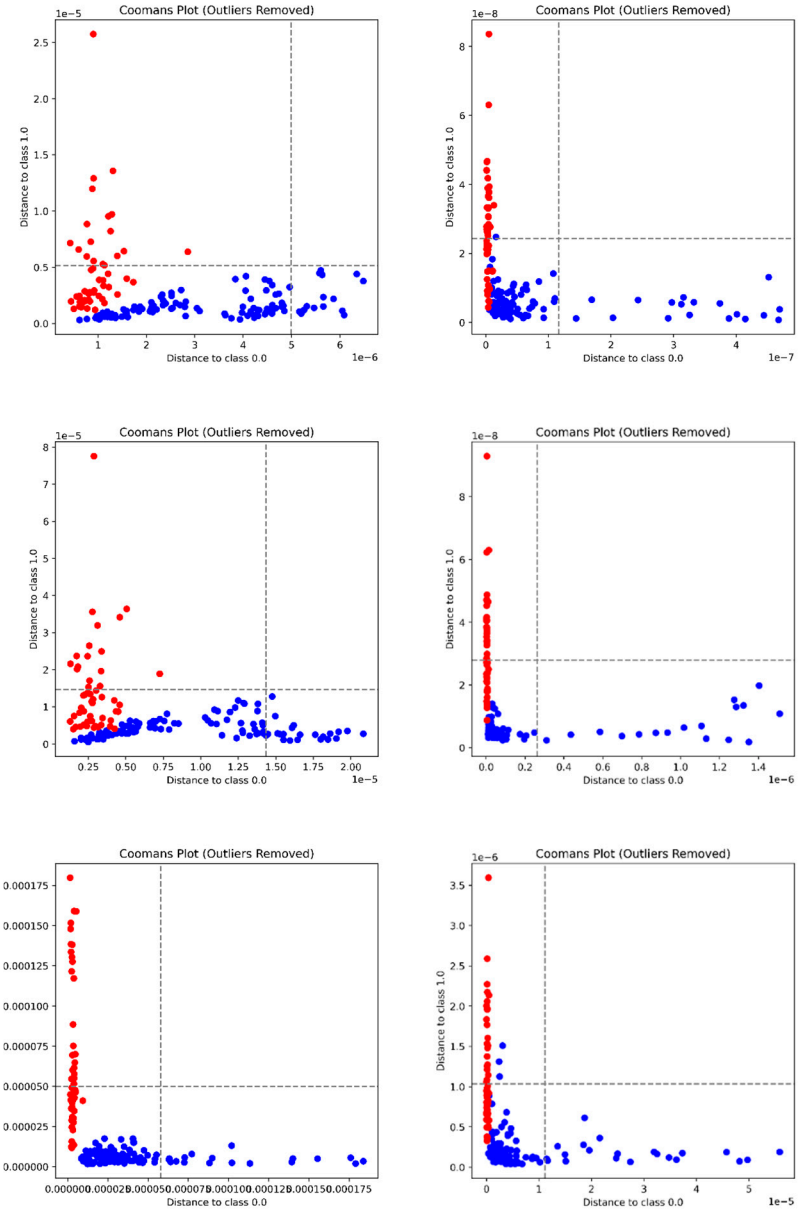
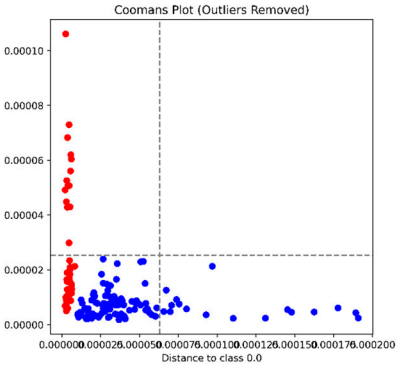
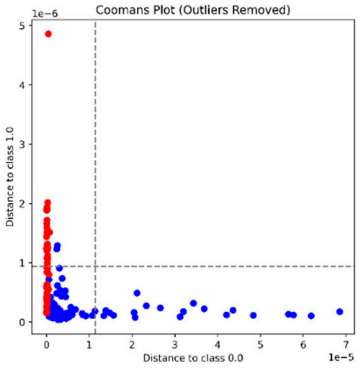
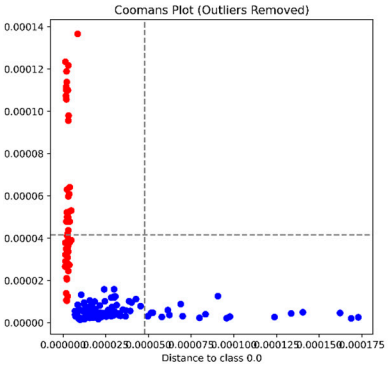

PCA Q-residuals
Q threshold
Q
Sample index

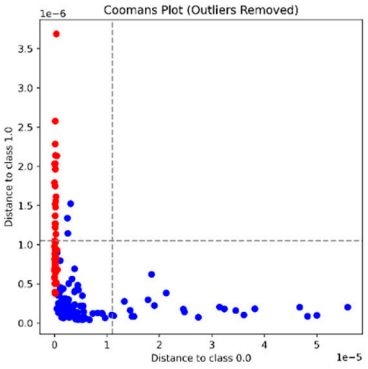
Figure S8: . Coomans plots (Q-residuals vs Hotelling's T^2) for all spectral transformations, comparing the *whole spectrum* (right panels) and the *fingerprint region* (left panels). Rows correspond to different preprocessing methods applied to the ATR-FTIR pork dataset: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend.

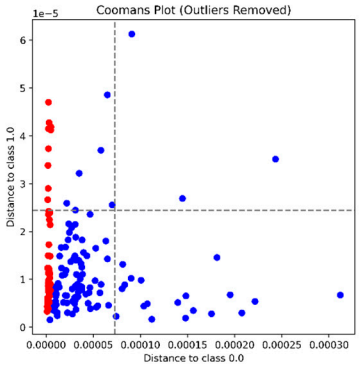


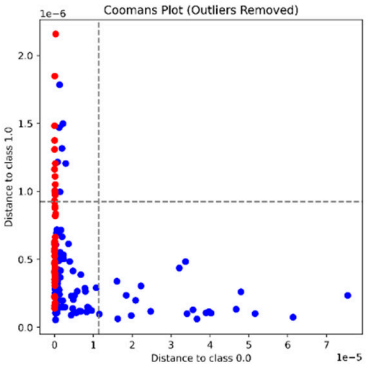

Coomans Plot (Outliers Removed)
Distance to class 0.0

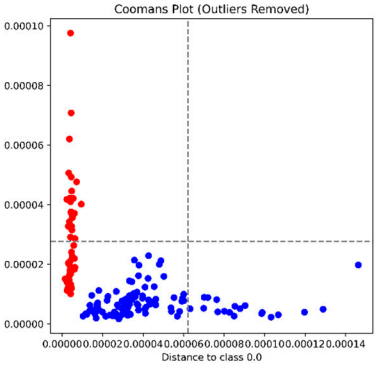

Coomans Plot (Outliers Removed)
1e−6
Distance to class 1.0
Distance to class 0.0
1e−5

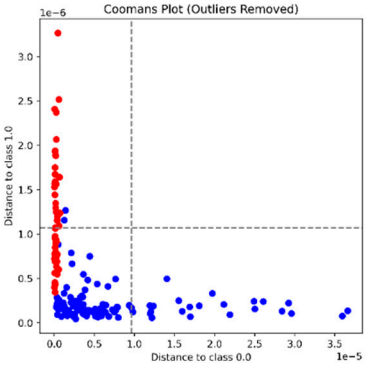

Coomans Plot (Outliers Removed)
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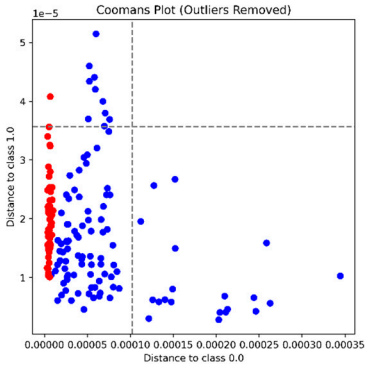

Coomans Plot (Outliers Removed)
1e−6
Distance to class 1.0
Distance to class 0.0
1e−5

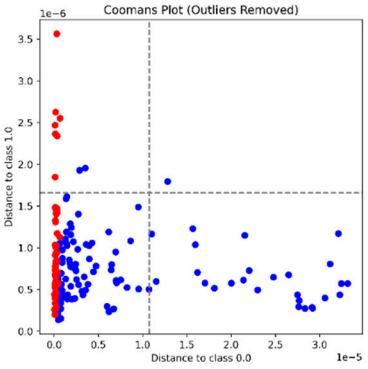

Coomans Plot (Outliers Removed)
1e−5
Distance to class 1.0
Distance to class 0.0

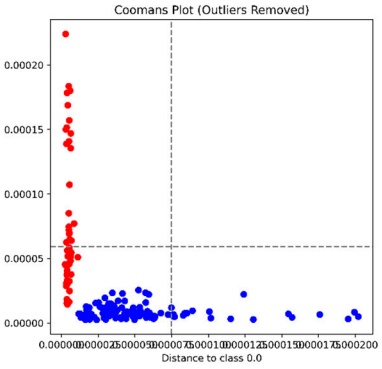

Coomans Plot (Outliers Removed)
1e−6
Distance to class 1.0
Distance to class 0.0
1e−5

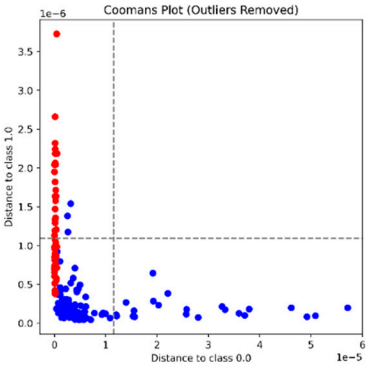

Coomans Plot (Outliers Removed)
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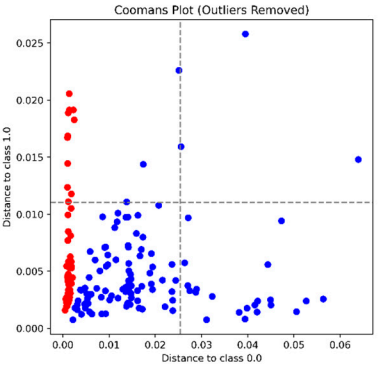

Coomans Plot (Outliers Removed)
1e−6
Distance to class 1.0
Distance to class 0.0
1e−5

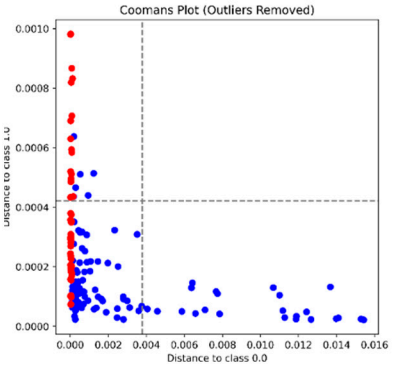

Coomans Plot (Outliers Removed)
1e−5
Distance to class 1.0
Distance to class 0.0

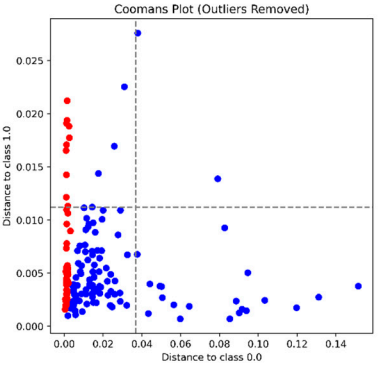

Coomans Plot (Outliers Removed)
1e−6
Distance to class 1.0
Distance to class 0.0
1e−5


Coomans Plot (Outliers Removed)
Distance to class 1.0
Distance to class 0.0


Coomans Plot (Outliers Removed)
1e−6
Distance to class 1.0
Distance to class 0.0
1e−5


Coomans Plot (Outliers Removed)
Distance to class 1.0
Distance to class 0.0


Coomans Plot (Outliers Removed)
Distance to class 0.0


Coomans Plot (Outliers Removed)
Distance to class 1.0
Distance to class 0.0

Coomans Plot (Outliers Removed)
Distance to class 1.0
Distance to class 0.0

Coomans Plot (Outliers Removed)
Distance to class 0.0

Figure S9. SIMCA classification performance metrics (Accuracy and Specificity) comparing the *whole spectrum* and the *fingerprint region* across different spectral transformations: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Multiplicative Scatter Correction (MSC), Median Filter, Orthogonal Signal Correction (OSC), Quantile Normalization, Standard Normal Variate (SNV), SNV+Detrend, and Raw. Bars represent classification accuracy (blue = whole spectrum; orange = fingerprint) and specificity (green = whole spectrum; pink = fingerprint).

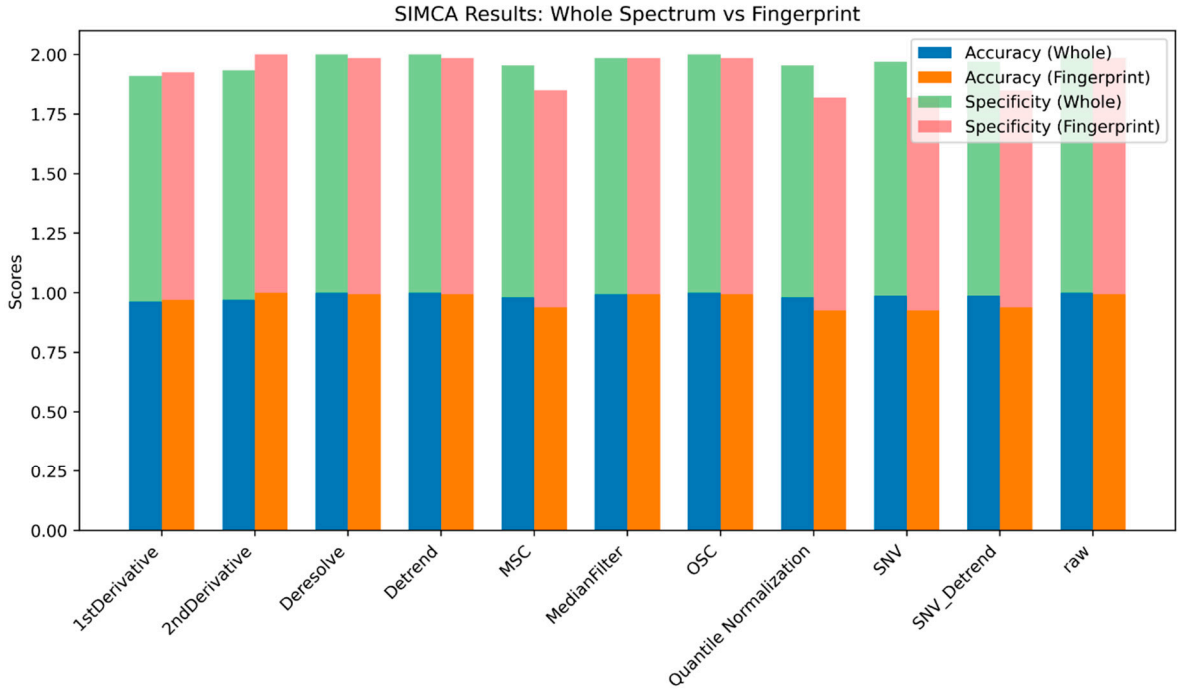
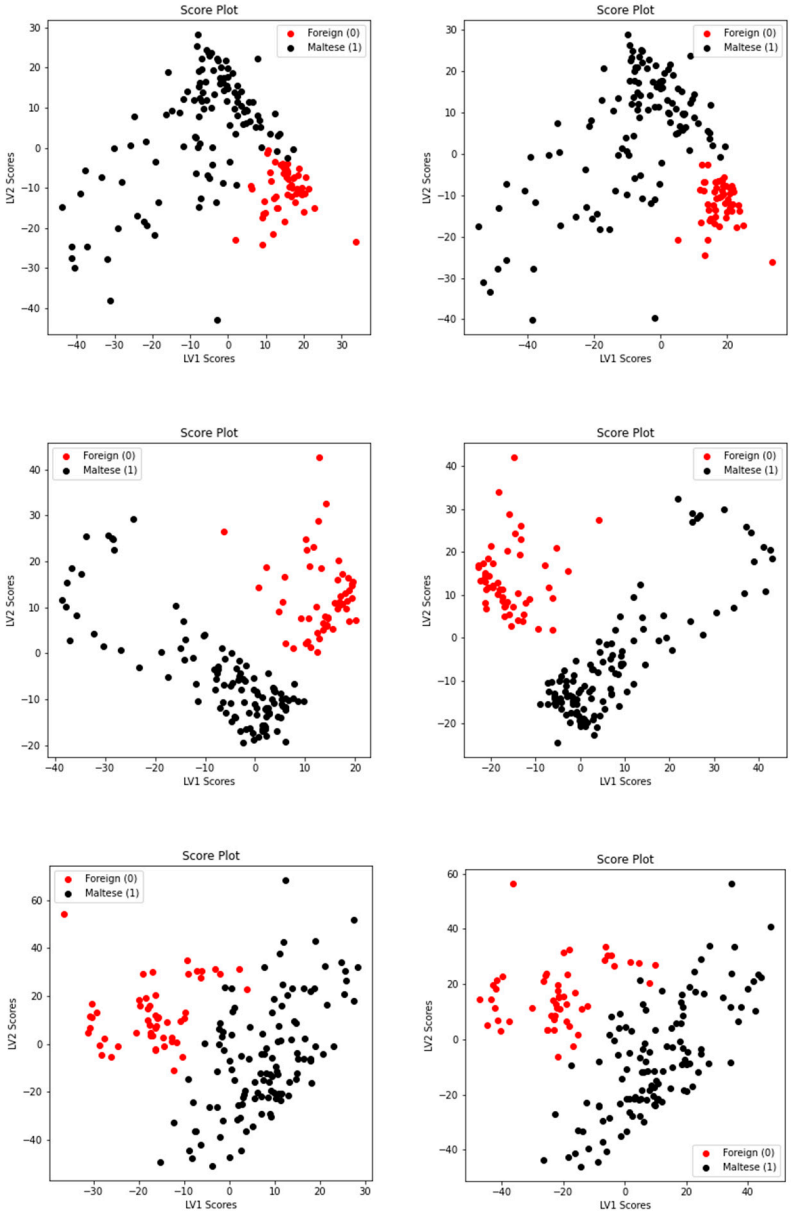
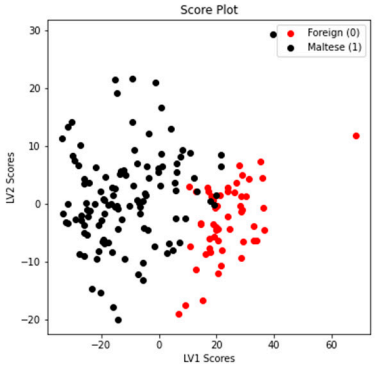
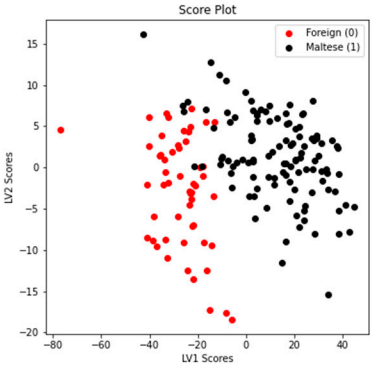
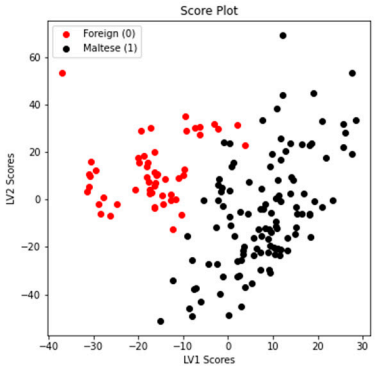


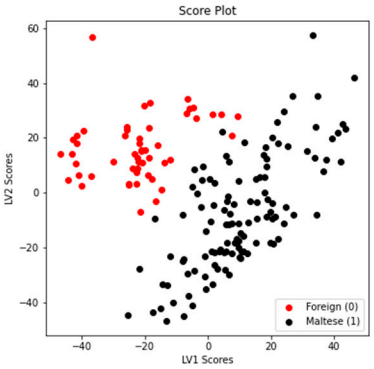
Figure S10: . PLS-DA score plots for all spectral transformations, comparing the *whole spectrum* (right panels) and the *fingerprint region* (left panels). Rows correspond to different preprocessing methods applied to the ATR-FTIR pork dataset: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend.

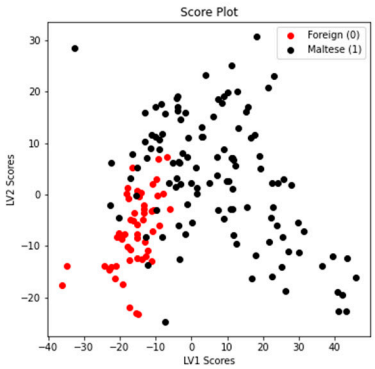


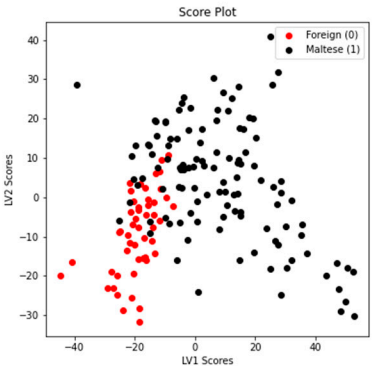

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

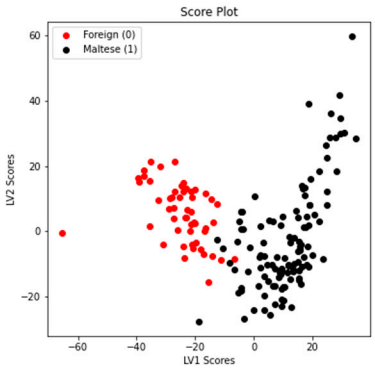

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

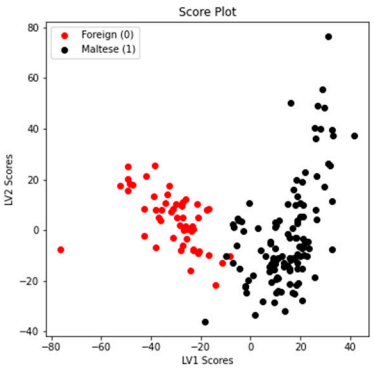

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

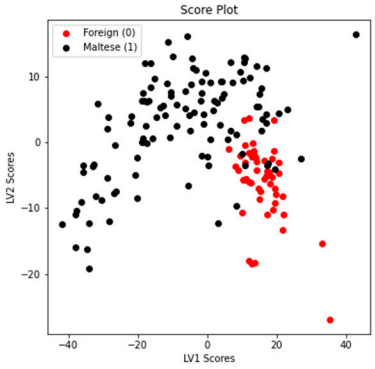

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

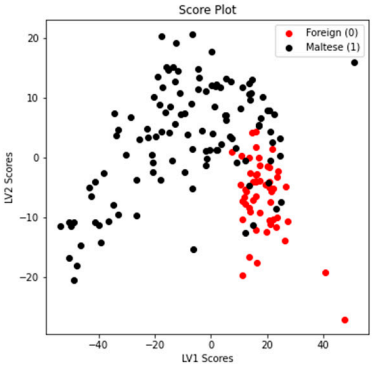

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

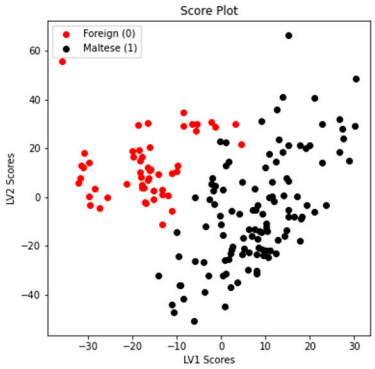

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

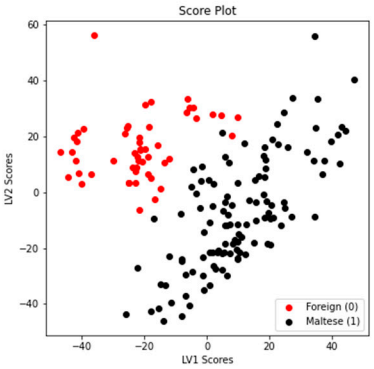

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

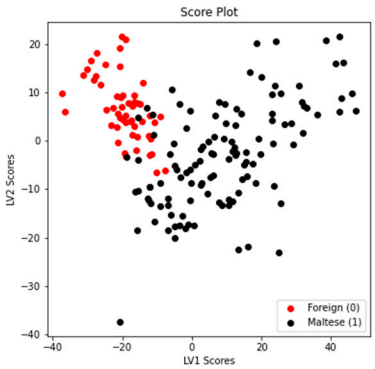

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

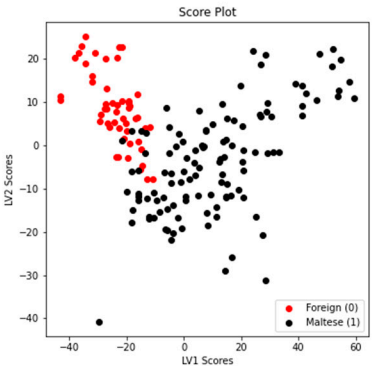

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

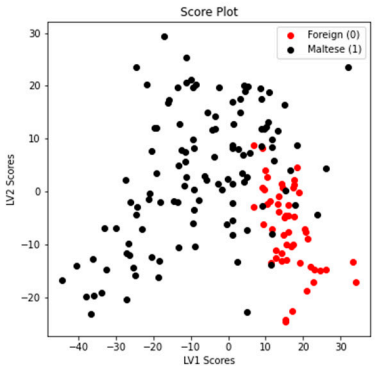

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores


Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores


Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores


Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores


Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores


Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

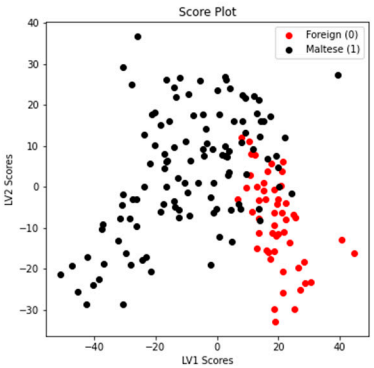
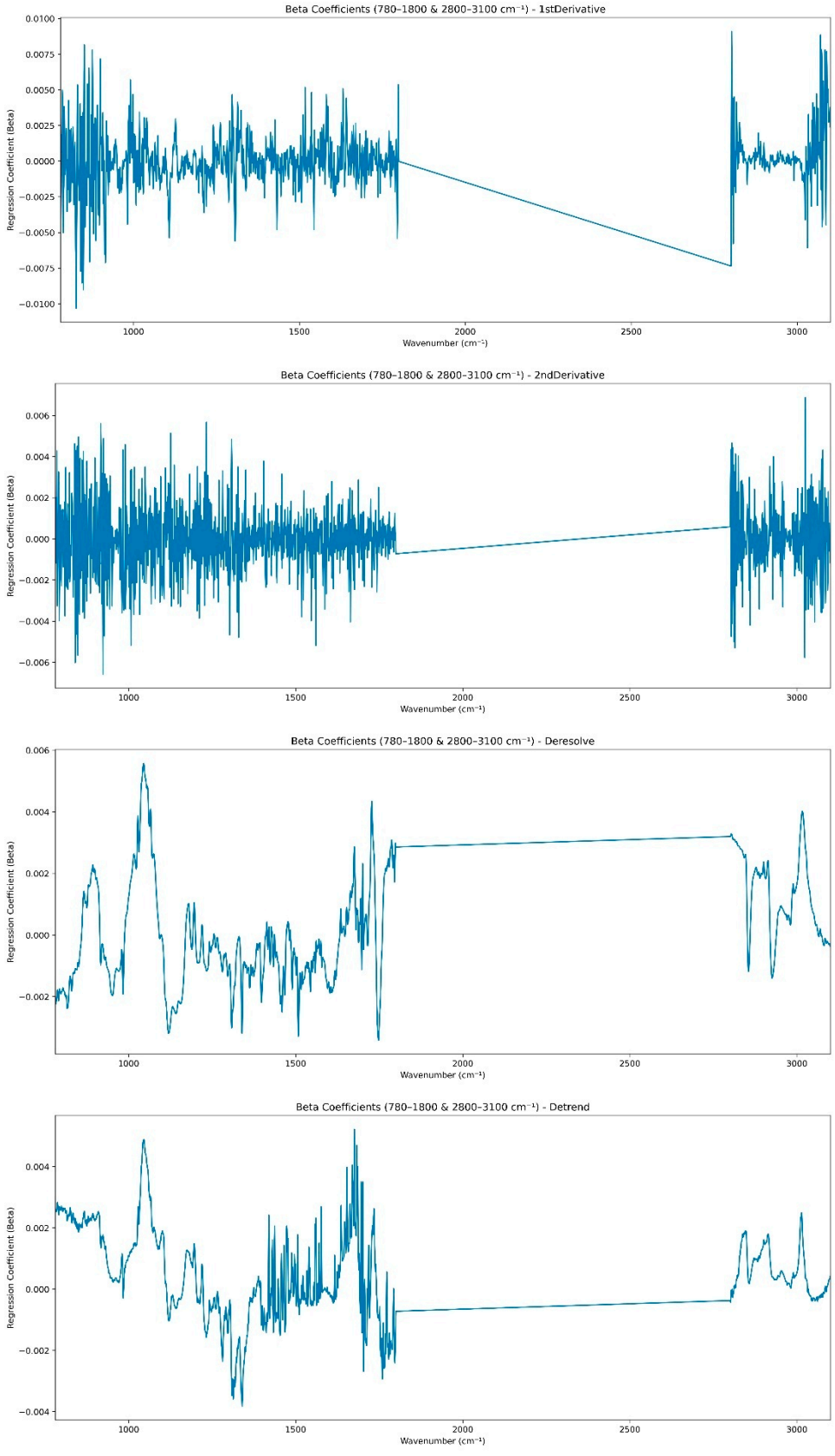
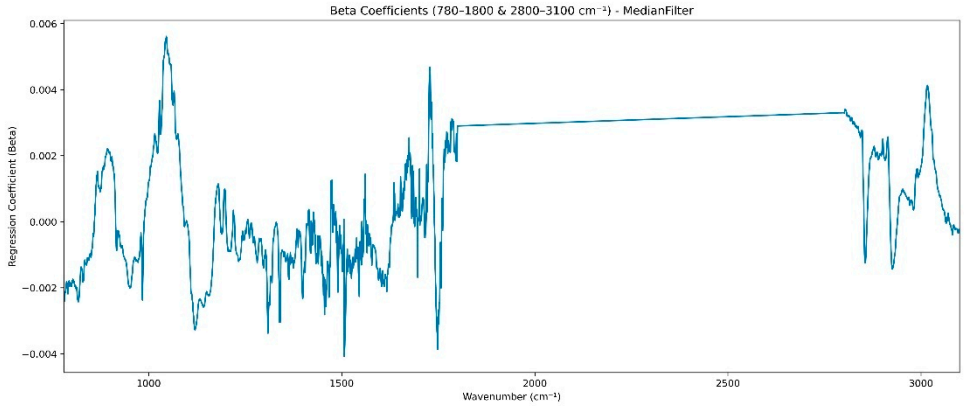
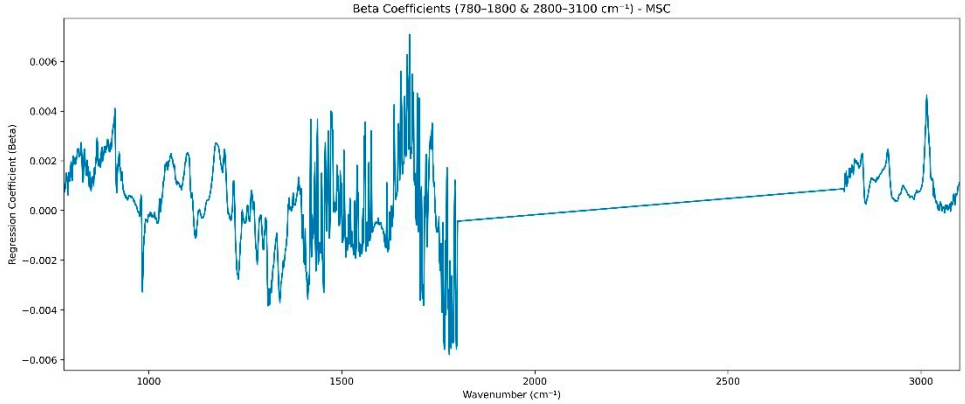
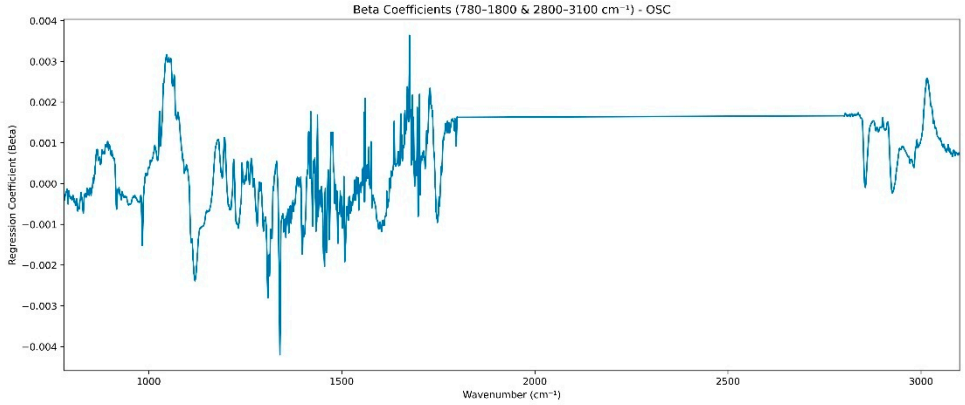

Score Plot
Foreign (0)
Maltese (1)
LV2 Scores
LV1 Scores

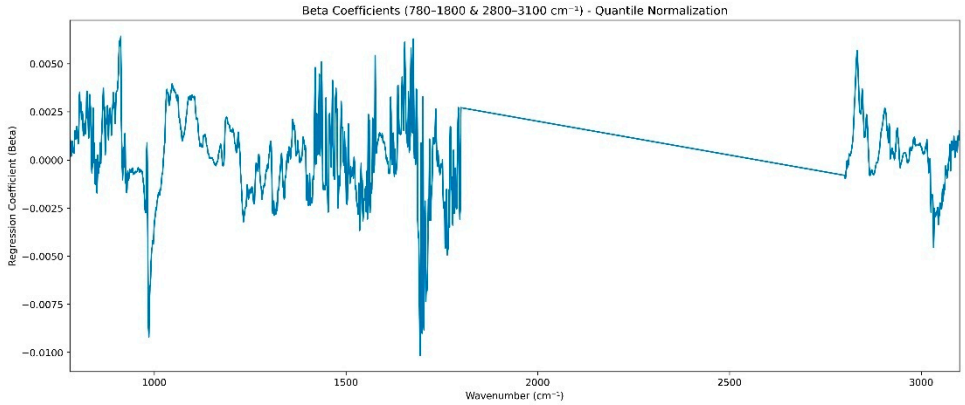
Figure S11: β-regression coefficient plots of the full spectrum (4000–400 cm^{-1}) for all applied spectral transformations. Rows correspond to preprocessing methods: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend.

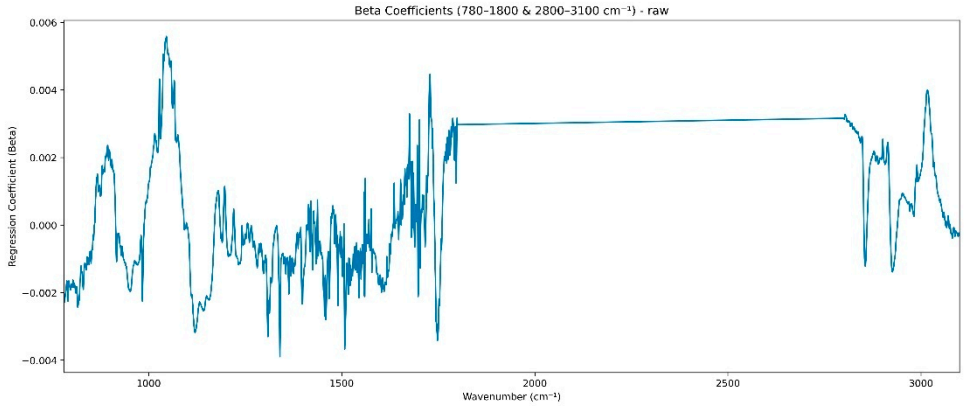


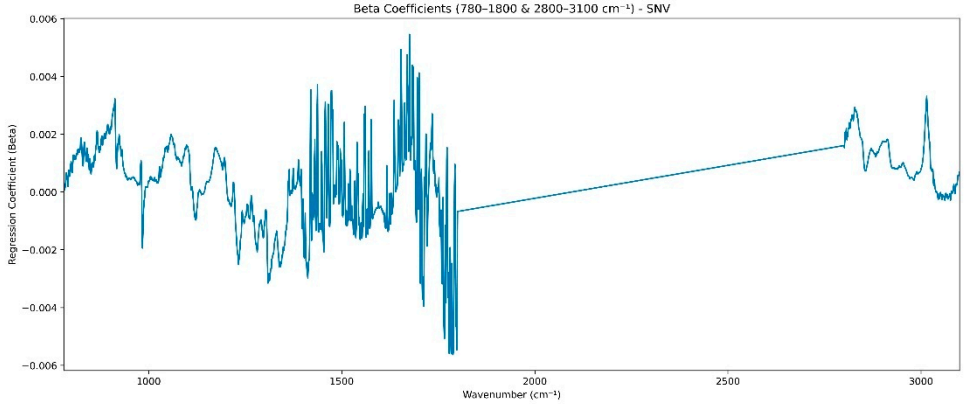

Beta Coefficients (780–1800 & 2800–3100 cm⁻¹) - MedianFilter
Regression Coefficient (Beta)
Wavenumber (cm⁻¹)


Beta Coefficients (780–1800 & 2800–3100 cm⁻¹) - MSC
Regression Coefficient (Beta)
Wavenumber (cm⁻¹)


Beta Coefficients (780–1800 & 2800–3100 cm⁻¹) - OSC
Regression Coefficient (Beta)
Wavenumber (cm⁻¹)


Beta Coefficients (780–1800 & 2800–3100 cm⁻¹) - Quantile Normalization
Regression Coefficient (Beta)
Wavenumber (cm⁻¹)


Beta Coefficients (780–1800 & 2800–3100 cm⁻¹) - raw
Regression Coefficient (Beta)
0.006
0.004
0.002
0.000
−0.002
−0.004
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)


Beta Coefficients (780–1800 & 2800–3100 cm⁻¹) - SNV
Regression Coefficient (Beta)
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)

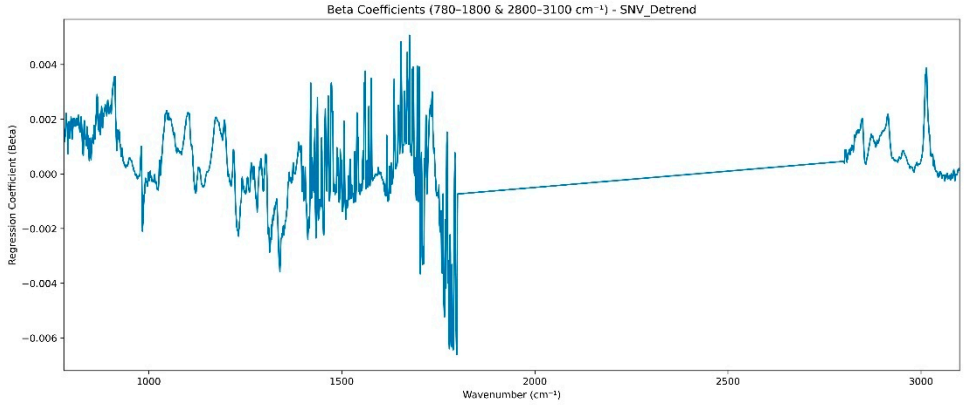
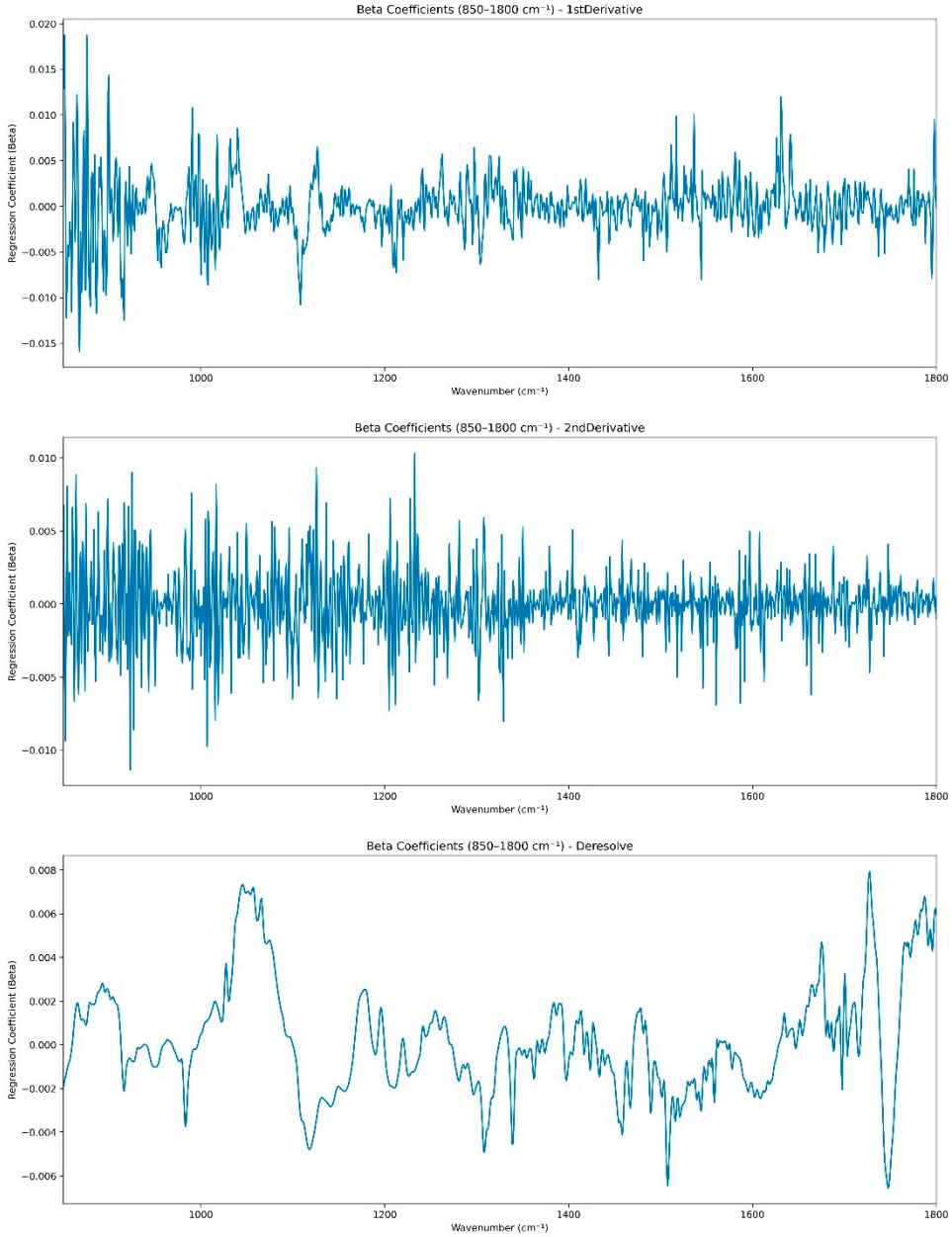
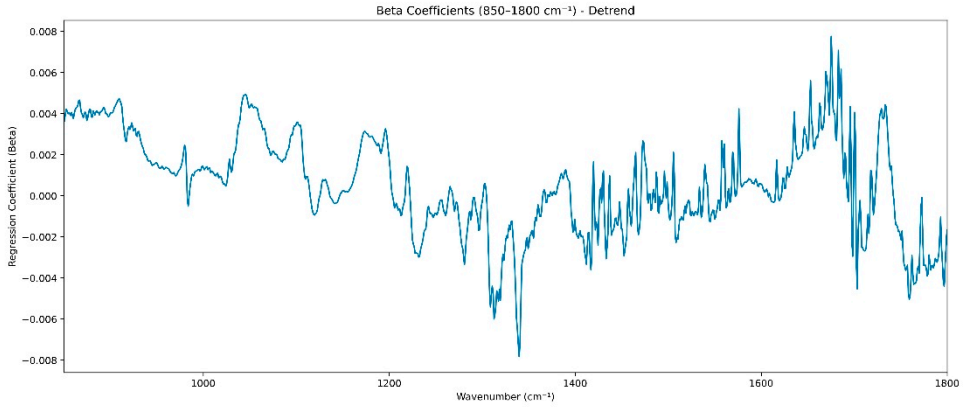
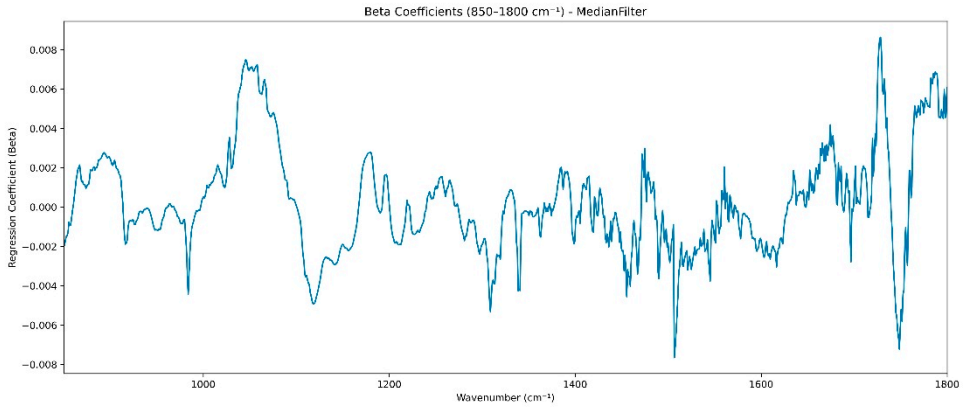
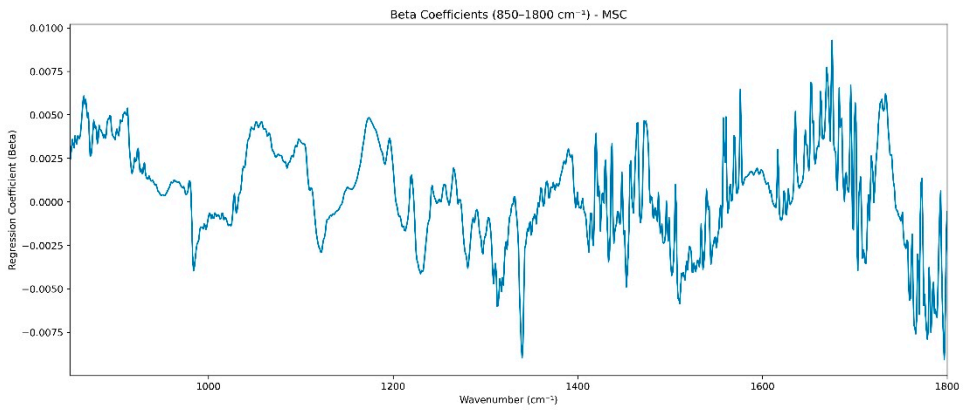

Beta Coefficients (780–1800 & 2800–3100 cm⁻¹) - SNV_Detrend
Regression Coefficient (Beta)
0.004
0.002
0.000
−0.002
−0.004
−0.006
1000
1500
2000
2500
3000
Wavenumber (cm⁻¹)

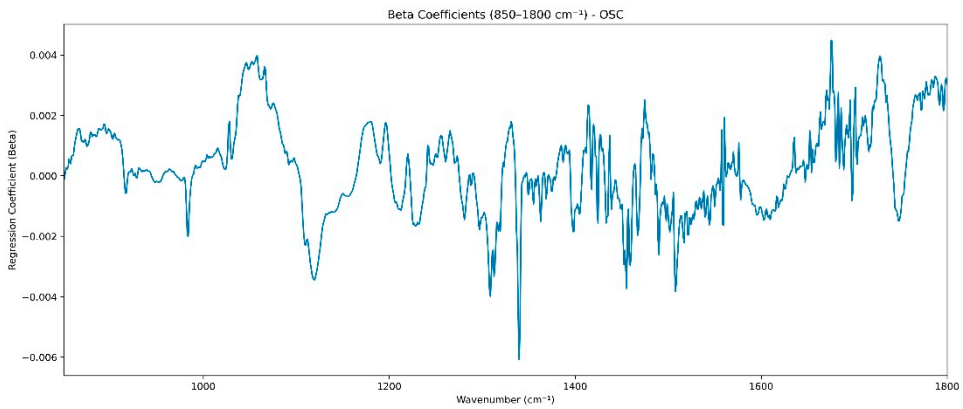
Figure S12: β-regression coefficient plots of the fingerprint region for all applied spectral transformations. Rows correspond to preprocessing methods: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend.

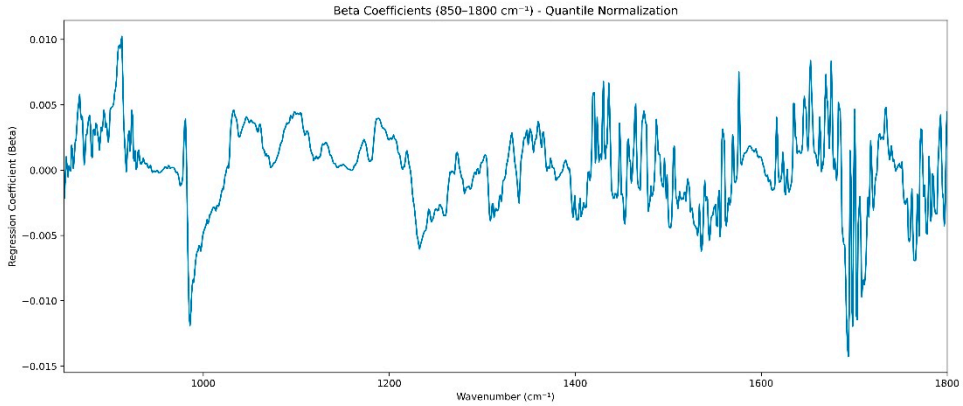


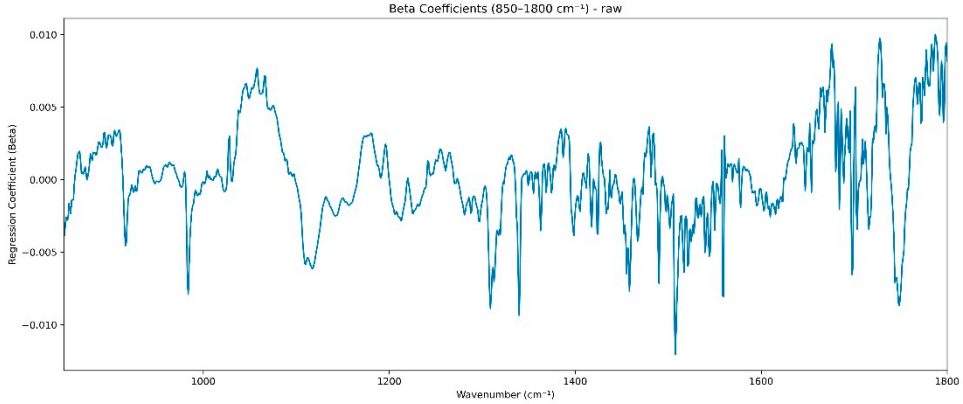

Beta Coefficients (850–1800 cm⁻¹) - Detrend
Regression Coefficient (Beta)
Wavenumber (cm⁻¹)

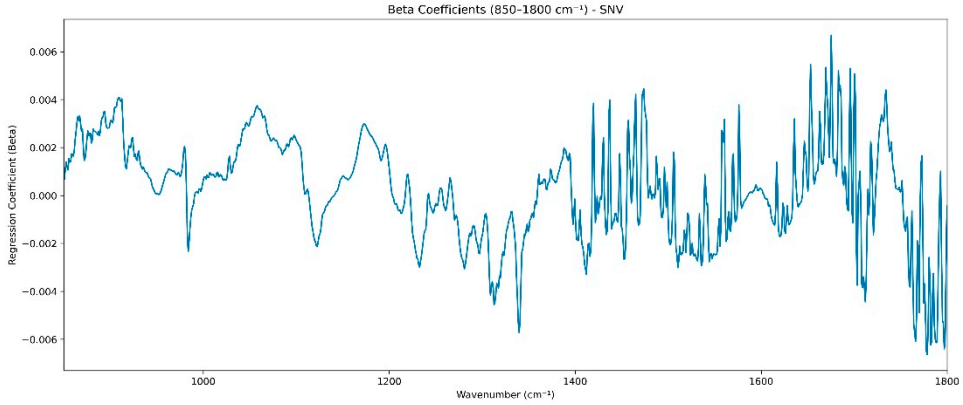

Beta Coefficients (850–1800 cm⁻¹) - MedianFilter
Regression Coefficient (Beta)
Wavenumber (cm⁻¹)


Beta Coefficients (850–1800 cm⁻¹) - MSC
Regression Coefficient (Beta)
Wavenumber (cm⁻¹)


Beta Coefficients (850–1800 cm⁻¹) - OSC
Regression Coefficient (Beta)
Wavenumber (cm⁻¹)


Beta Coefficients (850–1800 cm⁻¹) - Quantile Normalization
Regression Coefficient (Beta)
0.010
0.005
0.000
−0.005
−0.010
−0.015
1000
1200
1400
1600
1800
Wavenumber (cm⁻¹)


Beta Coefficients (850–1800 cm⁻¹) - raw
Regression Coefficient (Beta)
0.010
0.005
0.000
−0.005
−0.010
1000
1200
1400
1600
1800
Wavenumber (cm⁻¹)


Beta Coefficients (850–1800 cm⁻¹) - SNV
Regression Coefficient (Beta)
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
1000
1200
1400
1600
1800
Wavenumber (cm⁻¹)

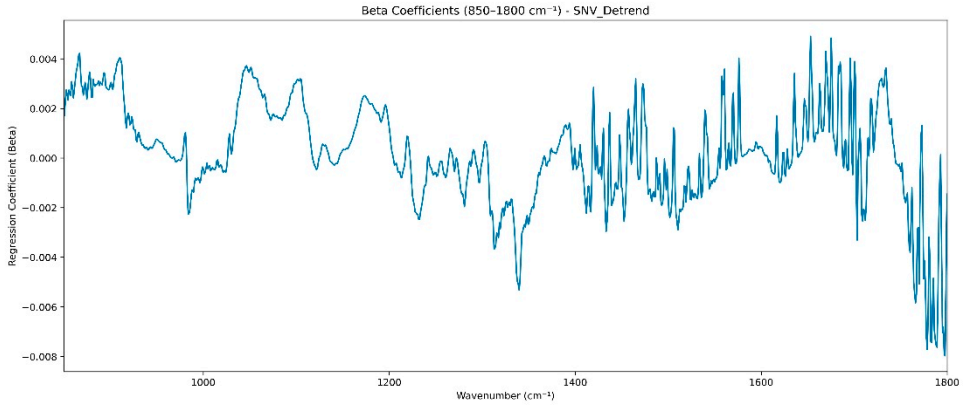
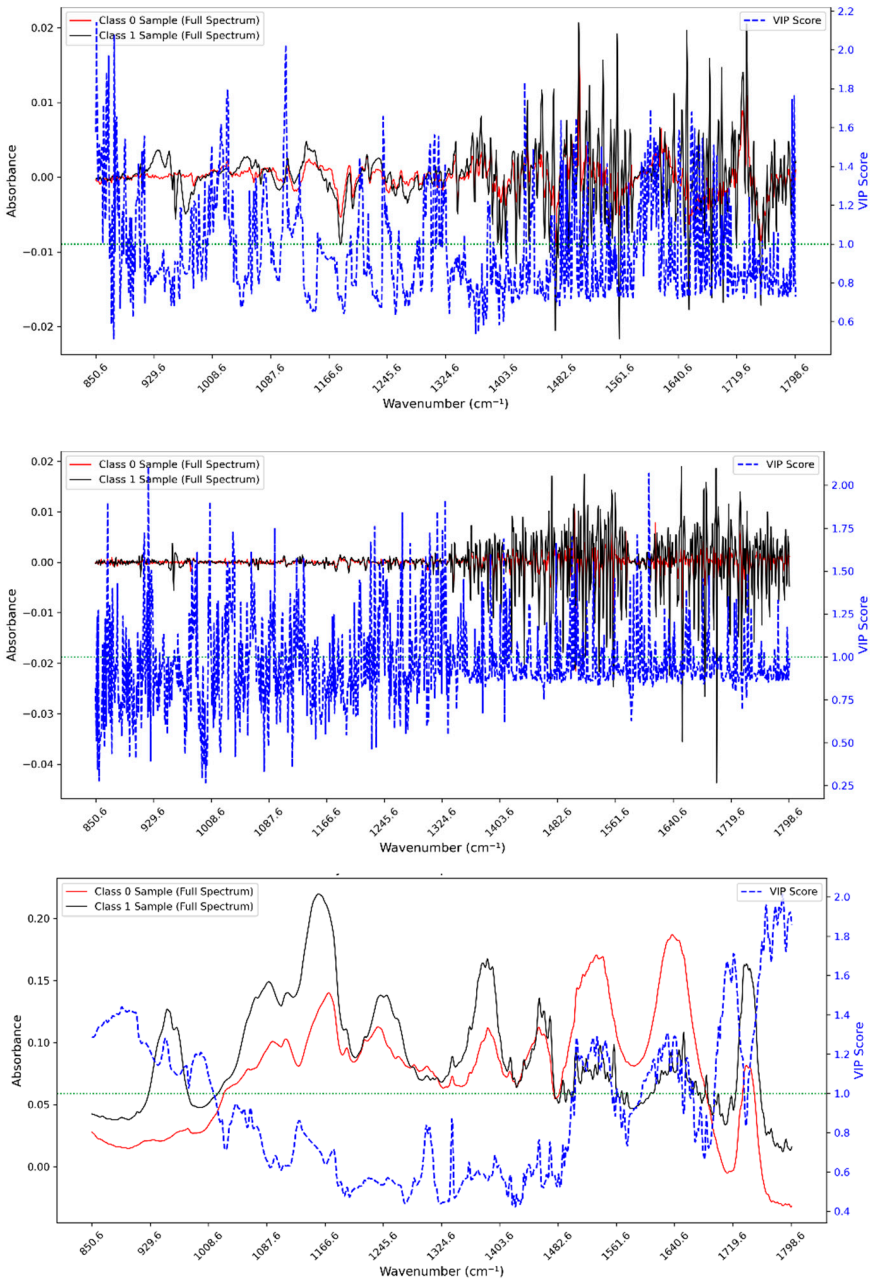
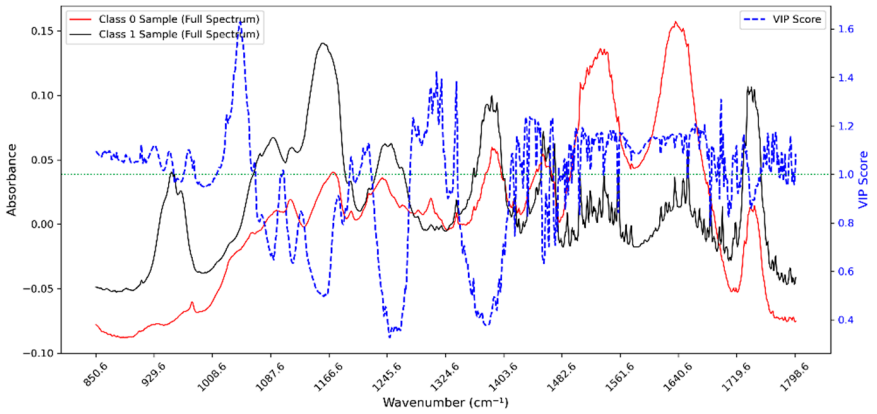
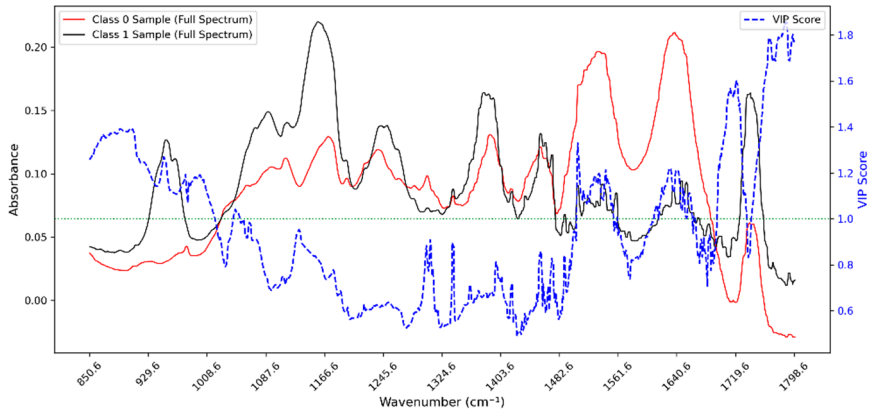
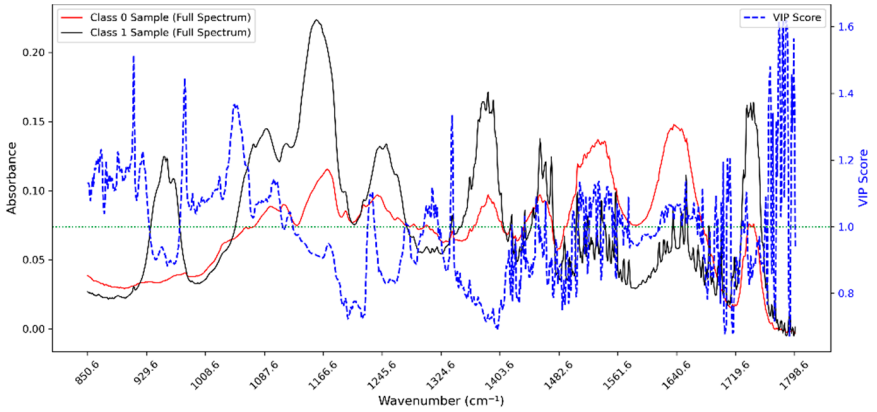

Beta Coefficients (850–1800 cm⁻¹) - SNV_Detrend
Regression Coefficient (Beta)
0.004
0.002
0.000
−0.002
−0.004
−0.006
−0.008
1000
1200
1400
1600
1800
Wavenumber (cm⁻¹)

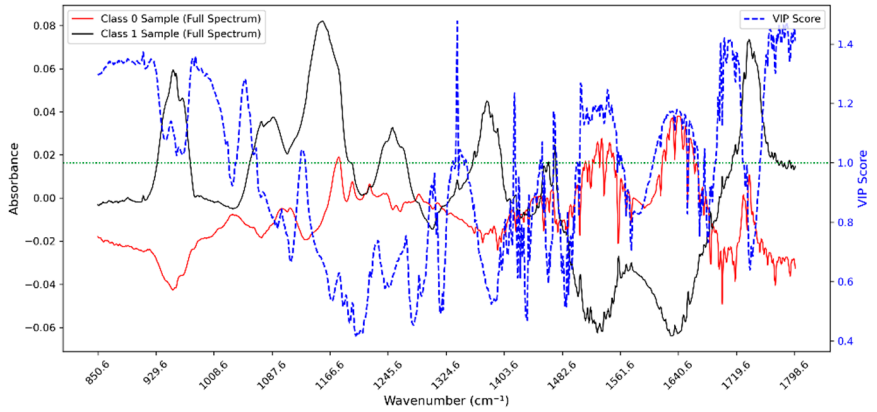
Figure S13. VIP plots (blue) of the fingerprint region for all applied spectral transformations. Rows correspond to preprocessing methods: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend for the local (Black) and foreign (Red)

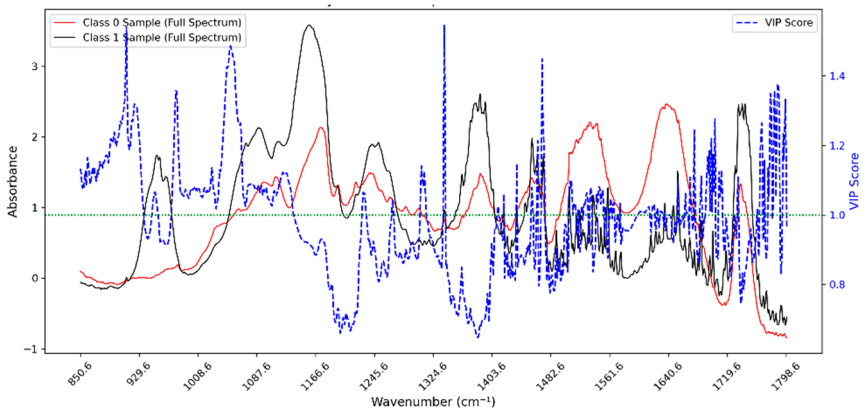


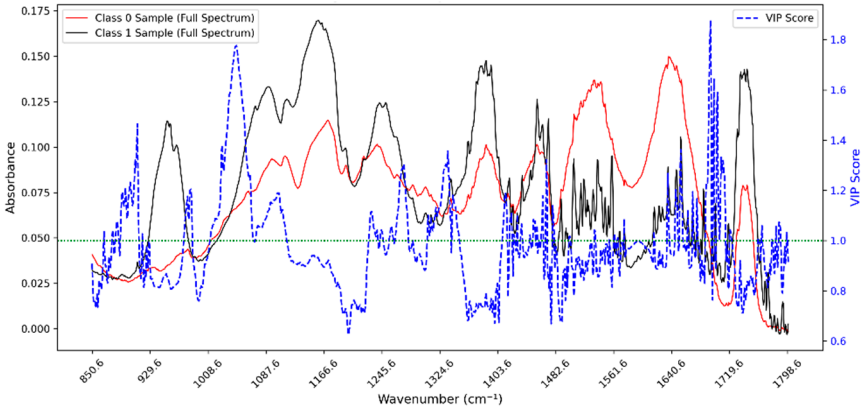

Class 0 Sample (Full Spectrum)
Class 1 Sample (Full Spectrum)
VIP Score
Absorbance
VIP Score
Wavenumber (cm⁻¹)
850.6
929.6
1008.6
1087.6
1166.6
1245.6
1324.6
1403.6
1482.6
1561.6
1640.6
1719.6
1798.6

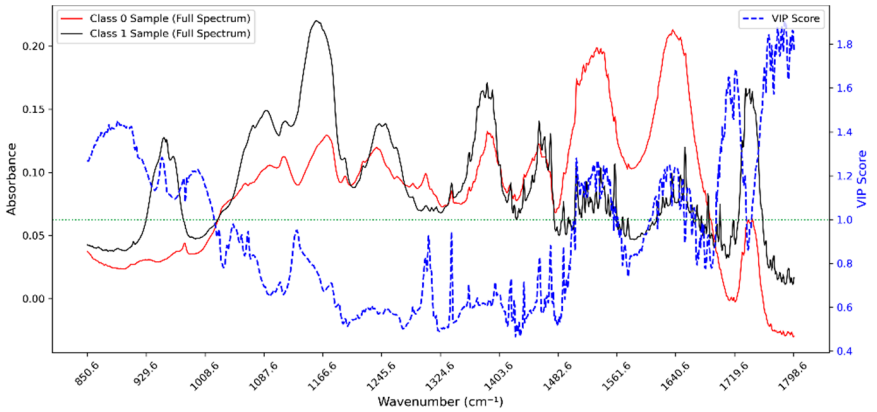

Class 0 Sample (Full Spectrum)
Class 1 Sample (Full Spectrum)
VIP Score
Absorbance
VIP Score
Wavenumber (cm⁻¹)
850.6
929.6
1008.6
1087.6
1166.6
1245.6
1324.6
1403.6
1482.6
1561.6
1640.6
1719.6
1798.6


Class 0 Sample (Full Spectrum)
Class 1 Sample (Full Spectrum)
VIP Score
Absorbance
VIP Score
Wavenumber (cm⁻¹)
850.6
929.6
1008.6
1087.6
1166.6
1245.6
1324.6
1403.6
1482.6
1561.6
1640.6
1719.6
1798.6


Class 0 Sample (Full Spectrum)
Class 1 Sample (Full Spectrum)
VIP Score
Absorbance
VIP Score
Wavenumber (cm⁻¹)
850.6
929.6
1008.6
1087.6
1166.6
1245.6
1324.6
1403.6
1482.6
1561.6
1640.6
1719.6
1798.6


Class 0 Sample (Full Spectrum)
Class 1 Sample (Full Spectrum)
VIP Score
Absorbance
VIP Score
Wavenumber (cm⁻¹)
850.6
929.6
1008.6
1087.6
1166.6
1245.6
1324.6
1403.6
1482.6
1561.6
1640.6
1719.6
1798.6


Class 0 Sample (Full Spectrum)
Class 1 Sample (Full Spectrum)
VIP Score
Absorbance
VIP Score
Wavenumber (cm⁻¹)
850.6
929.6
1008.6
1087.6
1166.6
1245.6
1324.6
1403.6
1482.6
1561.6
1640.6
1719.6
1798.6


Class 0 Sample (Full Spectrum)
Class 1 Sample (Full Spectrum)
VIP Score
Absorbance
VIP Score
Wavenumber (cm⁻¹)
850.6
929.6
1008.6
1087.6
1166.6
1245.6
1324.6
1403.6
1482.6
1561.6
1640.6
1719.6
1798.6

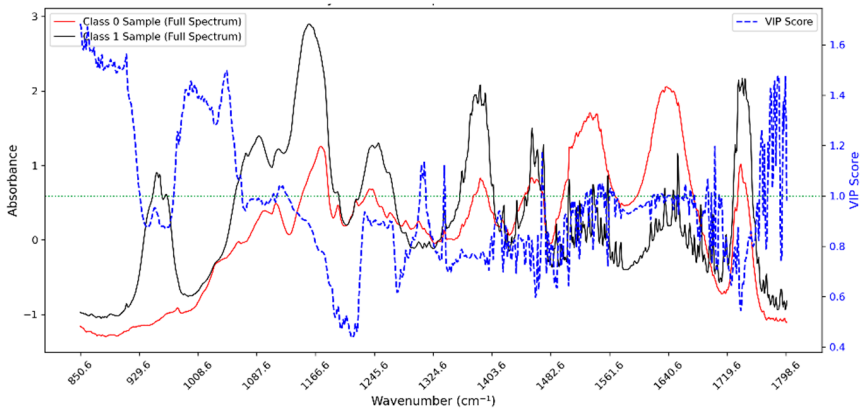
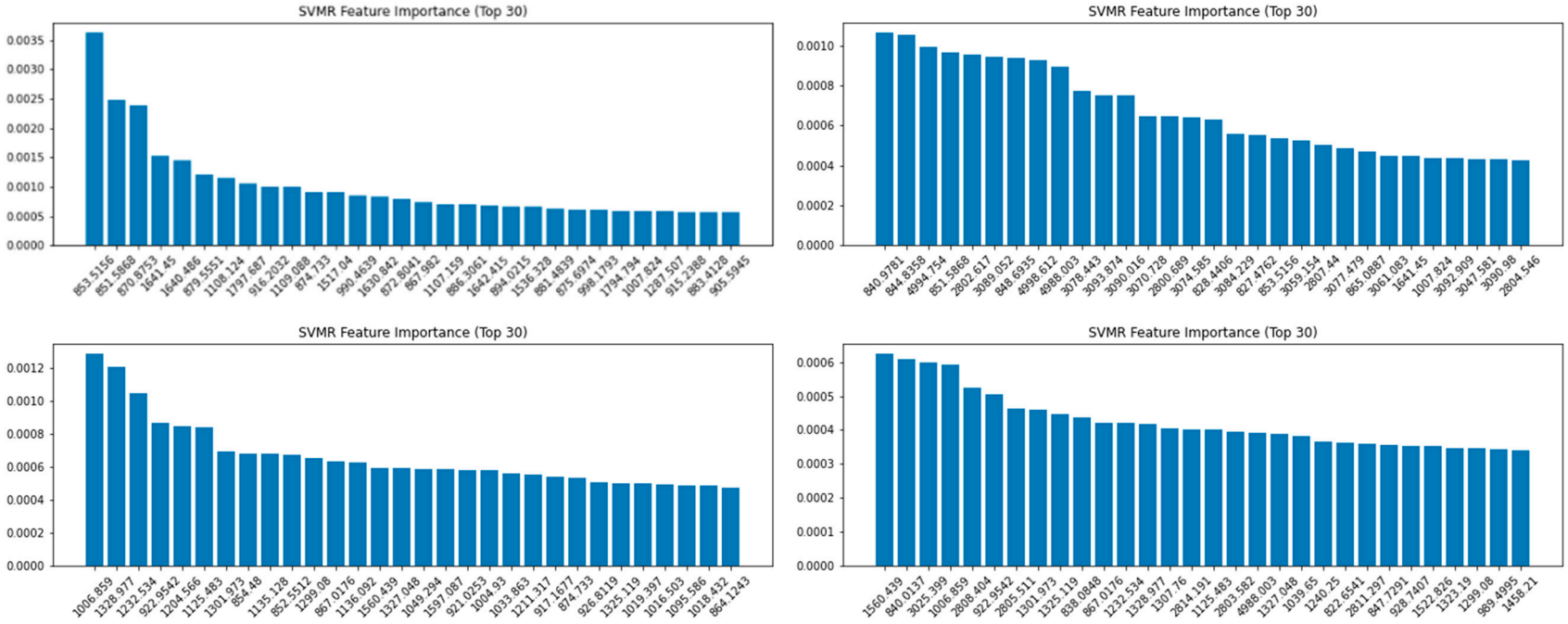
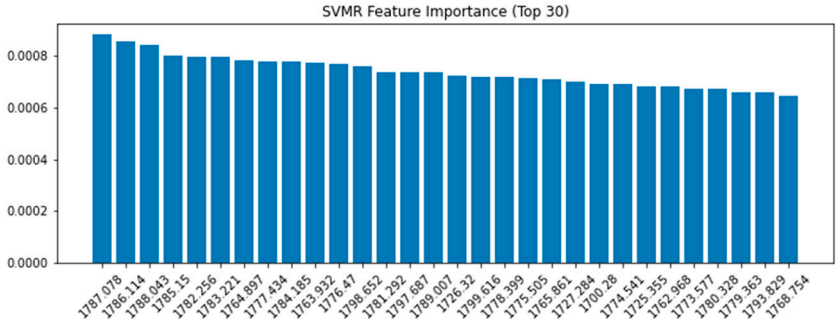
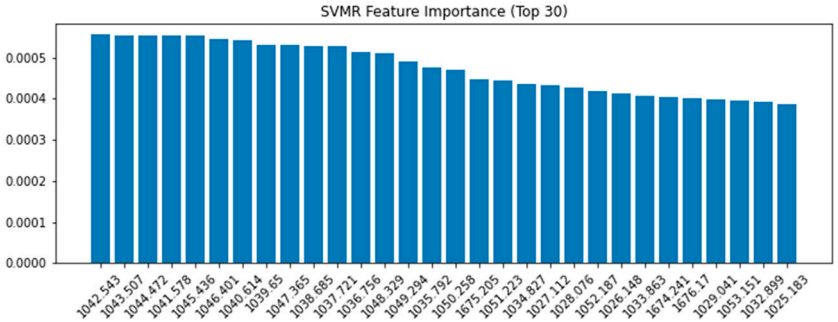
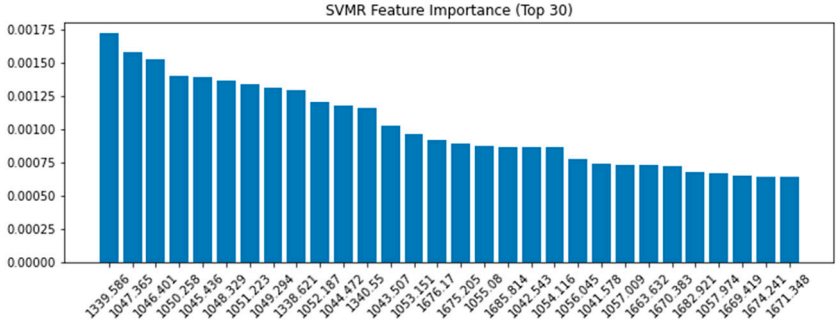

Class 0 Sample (Full Spectrum)
Class 1 Sample (Full Spectrum)
VIP Score
Absorbance
VIP Score
Wavenumber (cm⁻¹)
850.6
929.6
1008.6
1087.6
1166.6
1245.6
1324.6
1403.6
1482.6
1561.6
1640.6
1719.6
1798.6

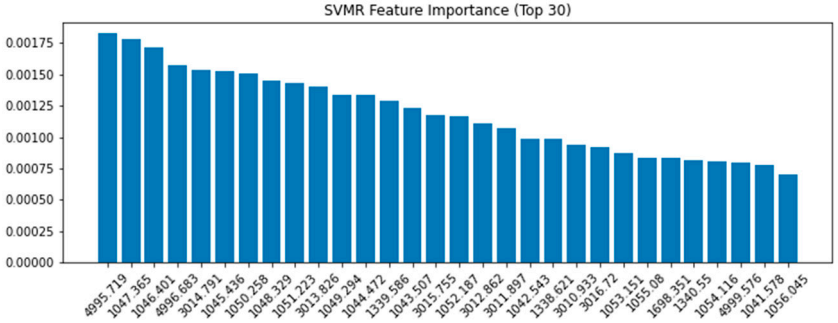
Figure S14: . Top 30 feature importance plots for all spectral transformations, comparing the *whole spectrum* (left panels) and the *fingerprint region* (right panels). Rows correspond to different preprocessing methods applied to the ATR-FTIR pork dataset: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend.

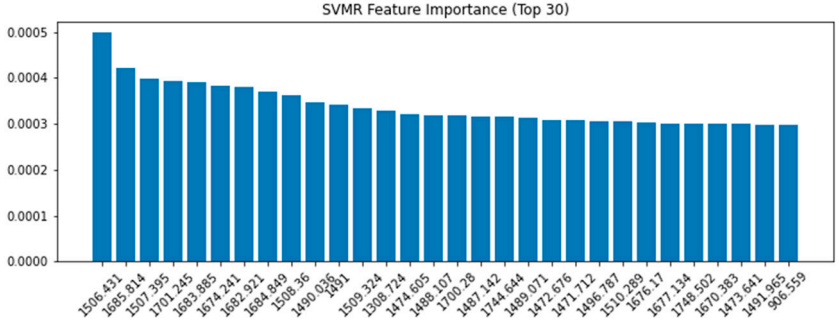


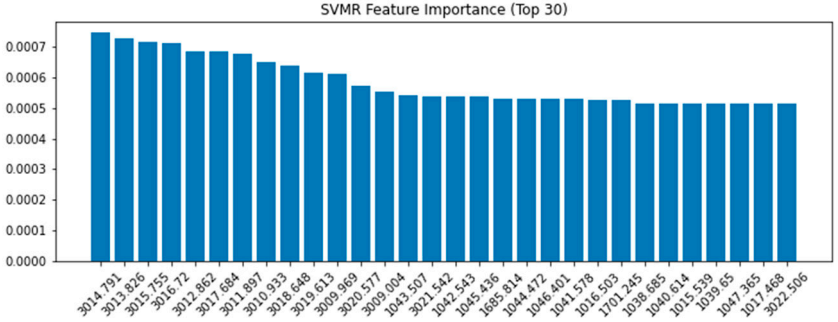

SVMR Feature Importance (Top 30)
0.0008
0.0006
0.0004
0.0002
0.0000
1787.078
1786.114
1788.643
1785.15
1782.256
1783.221
1764.897
1777.434
1784.185
1763.932
1776.47
1798.652
1781.292
1797.687
1789.007
1726.32
1799.616
1778.399
1775.505
1765.861
1727.284
1700.28
1774.541
1725.355
1762.968
1773.577
1780.328
1779.363
1793.829
1768.754

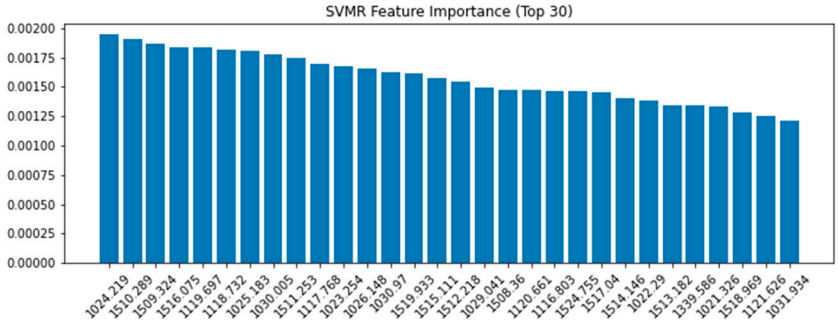

SVMR Feature Importance (Top 30)
0.0005
0.0004
0.0003
0.0002
0.0001
0.0000
1042.543
1043.507
1044.472
1041.578
1045.436
1046.401
1040.614
1039.65
1047.365
1038.685
1037.721
1036.756
1048.329
1049.294
1035.792
1050.258
1675.205
1051.223
1034.827
1027.112
1028.076
1052.187
1026.148
1033.863
1674.241
1676.17
1029.041
1053.151
1032.899
1025.183

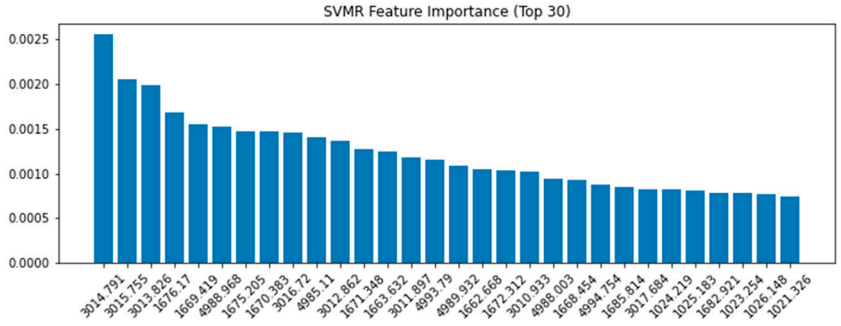

SVMR Feature Importance (Top 30)
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
1339.586
1047.365
1046.401
1050.258
1045.436
1048.329
1051.223
1049.294
1338.621
1052.187
1044.472
1340.55
1043.507
1053.151
1676.17
1675.205
1055.08
1685.814
1042.543
1054.116
1056.045
1041.578
1057.009
1663.632
1670.383
1682.921
1057.974
1669.419
1674.241
1671.348

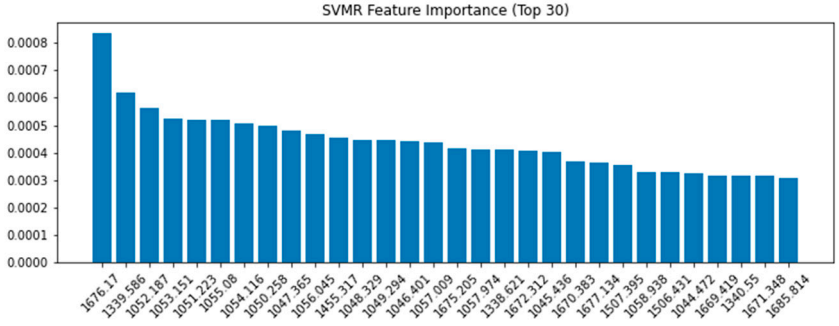

SVMR Feature Importance (Top 30)
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
4995.719
1047.365
1046.401
4996.683
3014.791
1045.436
1050.258
1048.329
1051.223
3013.826
1049.294
1044.472
1339.586
1043.507
3015.755
1052.187
3012.862
3011.897
1042.543
1338.621
3010.933
3016.72
1053.151
1055.08
1698.351
1340.55
1054.116
4999.576
1041.578
1056.045

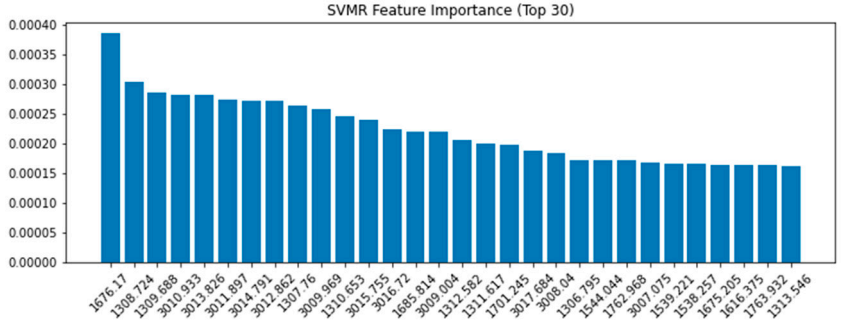

SVMR Feature Importance (Top 30)
0.0005
0.0004
0.0003
0.0002
0.0001
0.0000
1506.431
1685.814
1507.395
1701.245
1683.885
1674.241
1682.921
1684.849
1508.36
1490.036
1491
1509.324
1308.724
1474.605
1488.107
1700.28
1487.142
1744.644
1489.071
1472.676
1471.712
1496.787
1510.289
1676.17
1677.134
1748.502
1670.383
1473.641
1491.965
906.559

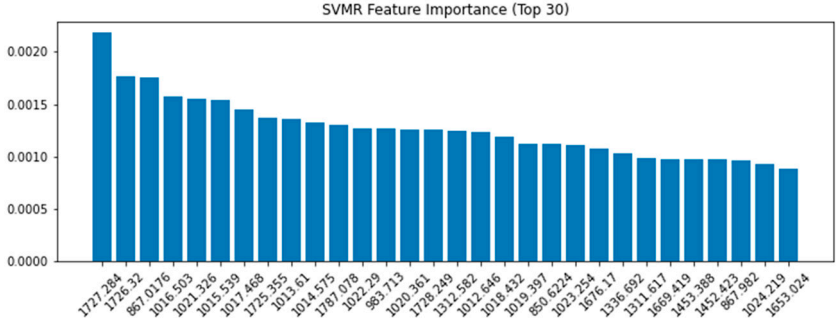

SVMR Feature Importance (Top 30)
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0.0000
3014.791
3013.826
3015.755
3016.72
3012.862
3017.684
3011.897
3010.933
3018.648
3019.613
3009.969
3020.577
3009.004
1043.507
3021.542
1042.543
1045.436
1685.814
1044.472
1046.401
1041.578
1016.503
1701.245
1038.685
1040.614
1015.539
1039.65
1047.365
1017.468
3022.506

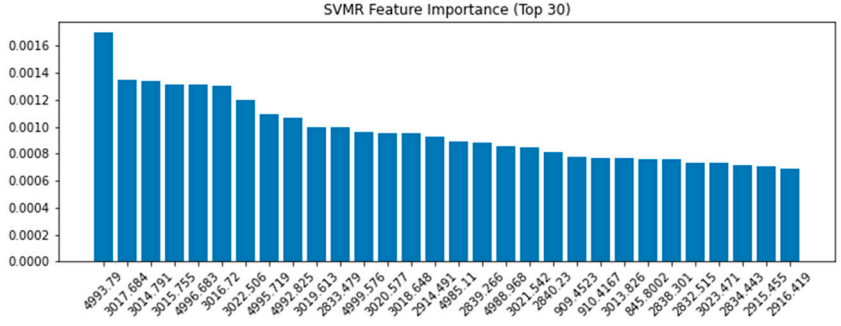

SVMR Feature Importance (Top 30)
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0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
1024.219
1510.289
1509.324
1516.075
1119.697
1118.732
1025.183
1030.005
1511.253
1117.768
1023.254
1026.148
1030.97
1519.933
1515.111
1512.218
1029.041
1508.36
1120.661
1116.803
1524.755
1517.04
1514.146
1022.29
1513.182
1339.586
1021.326
1518.969
1121.626
1031.934

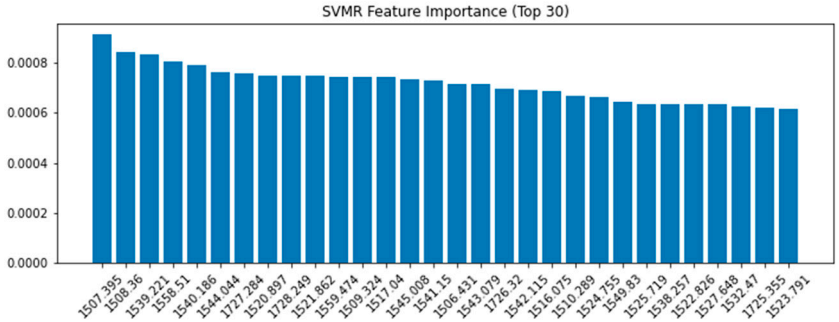

SVMR Feature Importance (Top 30)
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
3014.791
3015.755
3013.826
1676.17
1669.419
4988.968
1675.205
1670.383
3016.72
4985.11
3012.862
1671.348
1663.632
3011.897
4993.79
4989.932
1662.668
1672.312
3010.933
4988.003
1668.454
4994.754
1685.814
3017.684
1024.219
1025.183
1682.921
1023.254
1026.148
1021.326

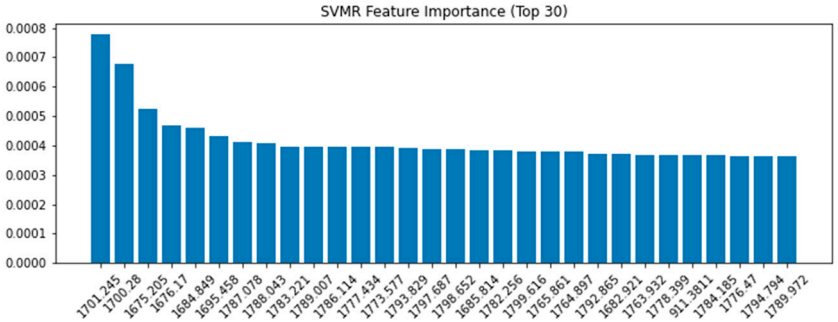

SVMR Feature Importance (Top 30)
0.0008
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0.0000
1676.17
1339.586
1052.187
1053.151
1051.223
1055.08
1054.116
1050.258
1047.365
1056.045
1455.317
1048.329
1049.294
1046.401
1057.009
1675.205
1057.974
1338.621
1672.312
1045.436
1670.383
1677.134
1507.395
1058.938
1506.431
1044.472
1669.419
1340.55
1671.348
1685.814

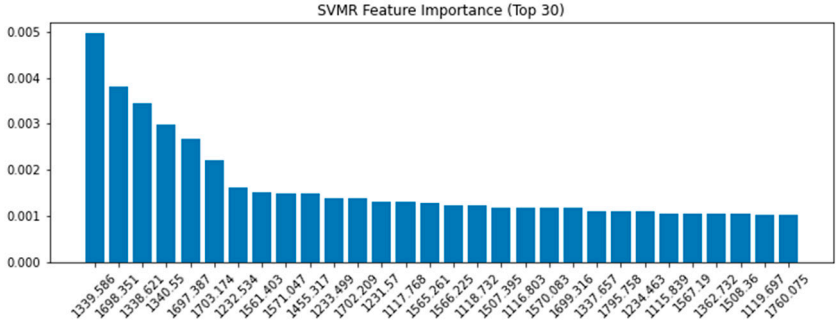

SVMR Feature Importance (Top 30)
0.00040
0.00035
0.00030
0.00025
0.00020
0.00015
0.00010
0.00005
0.00000
1676.17
1308.724
1309.688
3010.933
3013.826
3011.897
3014.791
3012.862
1307.76
3009.969
1310.653
3015.755
3016.72
1685.814
3009.004
1312.582
1311.617
1701.245
3017.684
3008.04
1306.795
1544.044
1762.968
3007.075
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1675.205
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1763.932
1313.546

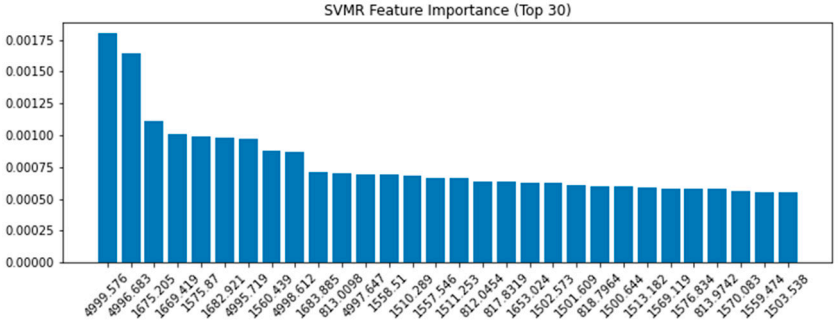

SVMR Feature Importance (Top 30)
0.0020
0.0015
0.0010
0.0005
0.0000
1727.284
1726.32
867.0176
1016.503
1021.326
1015.539
1017.468
1725.355
1013.61
1014.575
1787.078
1022.29
983.713
1020.361
1728.249
1312.582
1012.646
1018.432
1019.397
850.6224
1023.254
1676.17
1336.692
1311.617
1669.419
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1024.219
1653.024

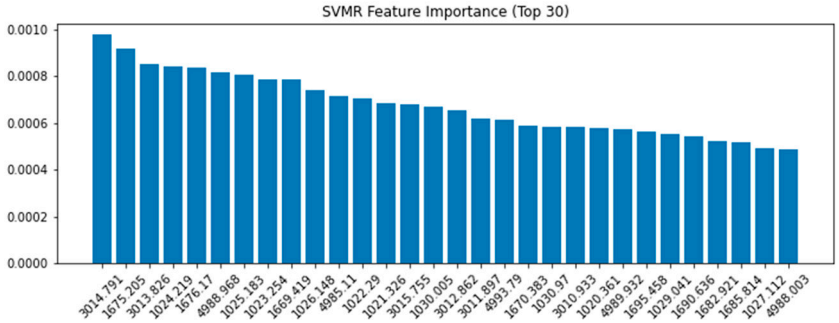

SVMR Feature Importance (Top 30)
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
4993.79
3017.684
3014.791
3015.755
4996.683
3016.72
3022.506
4995.719
4992.825
3019.613
2833.479
4999.576
3020.577
3018.648
2914.491
4985.11
2839.266
4988.968
3021.542
2840.23
909.4523
910.4167
3013.826
845.8002
2838.301
2832.515
3023.471
2834.443
2915.455
2916.419


SVMR Feature Importance (Top 30)
0.0008
0.0006
0.0004
0.0002
0.0000
1507.395
1508.36
1539.221
1558.51
1540.186
1544.044
1727.284
1520.897
1728.249
1521.862
1559.474
1509.324
1517.04
1545.008
1541.15
1506.431
1543.079
1726.32
1542.115
1516.075
1510.289
1524.755
1549.83
1525.719
1538.257
1522.826
1527.648
1532.47
1725.355
1523.791


SVMR Feature Importance (Top 30)
0.0008
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0.0000
1701.245
1700.28
1675.205
1676.17
1684.849
1695.458
1787.078
1788.043
1783.221
1789.007
1786.114
1777.434
1773.577
1793.829
1797.687
1798.652
1685.814
1782.256
1799.616
1765.861
1764.897
1792.865
1682.921
1763.932
1778.399
911.3811
1784.185
1776.47
1794.794
1789.972


SVMR Feature Importance (Top 30)
0.005
0.004
0.003
0.002
0.001
0.000
1339.586
1698.351
1338.621
1340.55
1697.387
1703.174
1232.534
1561.403
1571.047
1455.317
1233.490
1702.209
1231.57
1117.768
1565.261
1566.225
1118.732
1507.395
1116.803
1570.083
1699.316
1337.657
1795.758
1234.463
1115.839
1567.19
1362.732
1508.36
1119.697
1760.075


SVMR Feature Importance (Top 30)
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
4999.576
4996.683
1675.205
1669.419
1575.87
1682.921
4995.719
1560.439
4998.612
1683.885
813.0098
4997.647
1558.51
1510.289
1557.546
1511.253
812.0454
817.8319
1653.024
1502.573
1501.609
818.7964
1500.644
1513.182
1569.119
1576.834
813.9742
1570.083
1559.474
1503.538


SVMR Feature Importance (Top 30)
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
3014.791
1675.205
3013.826
1024.219
1676.17
4988.968
1025.183
1023.254
1669.419
1026.148
4985.11
1022.29
1021.326
3015.755
1030.005
3012.862
3011.897
4993.79
1670.383
1030.97
3010.933
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1029.041
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1682.921
1685.814
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4988.003

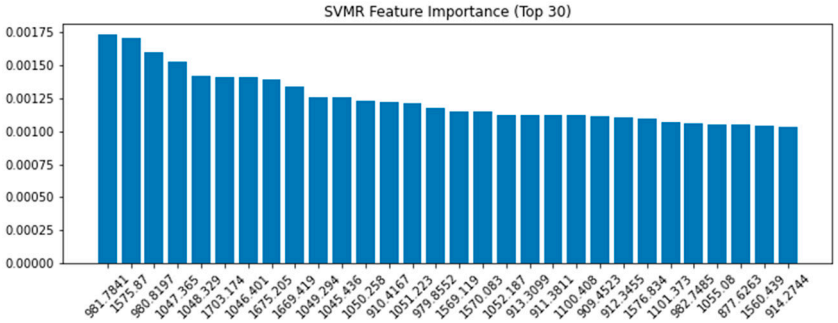
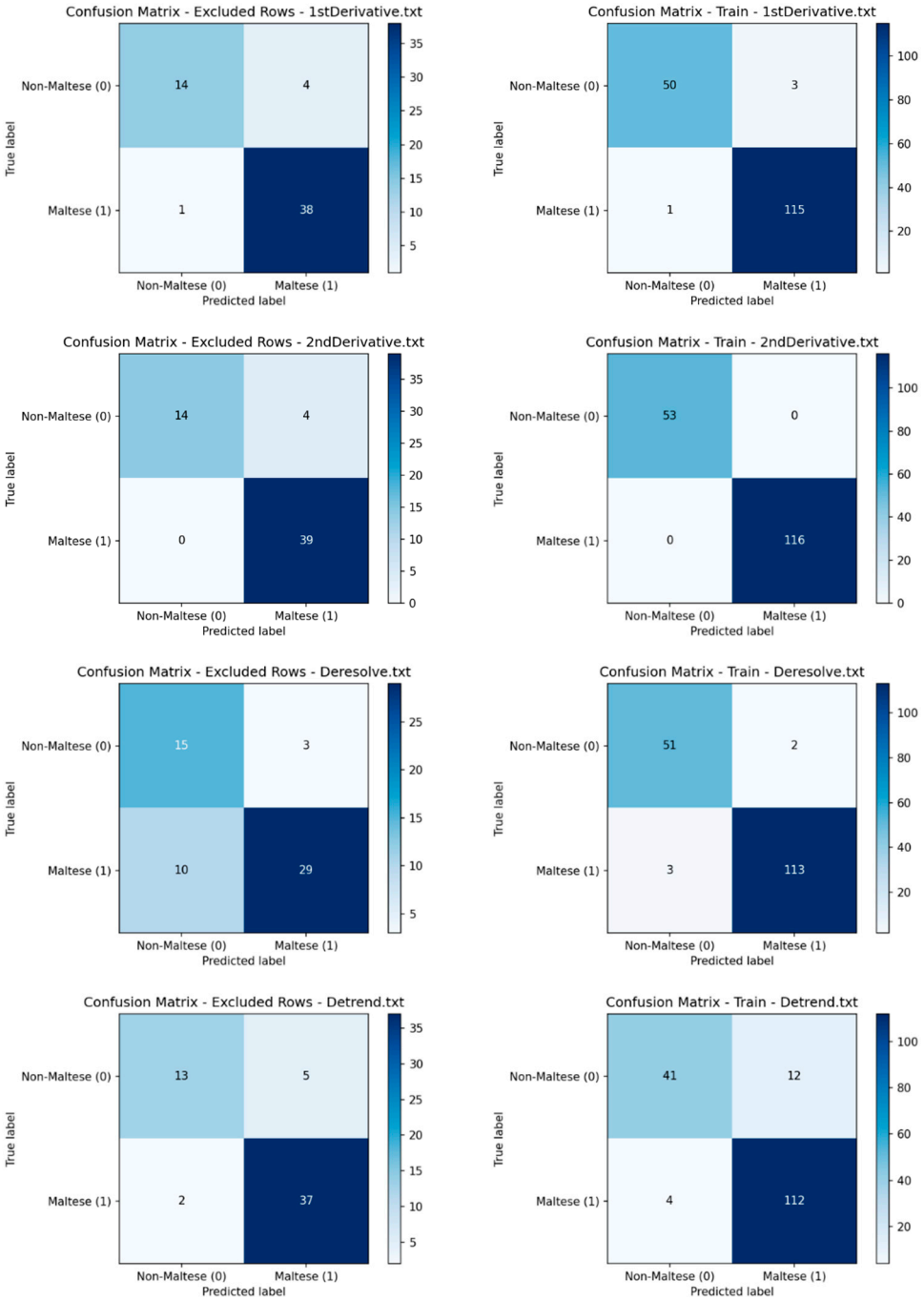
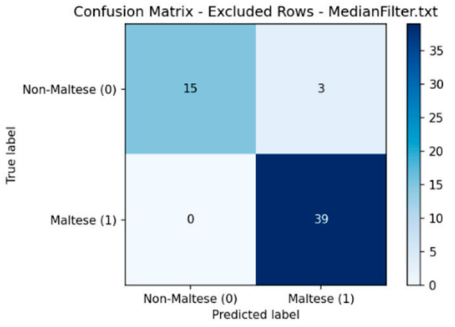
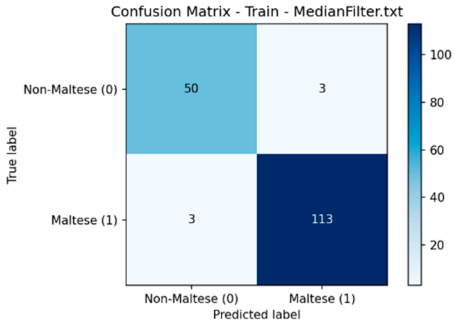
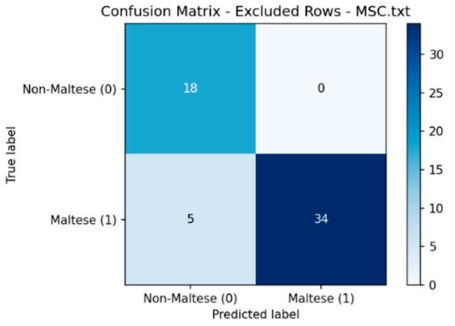

SVMR Feature Importance (Top 30)
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0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
981.7841
1575.87
980.8197
1047.365
1048.329
1703.174
1046.401
1675.205
1669.419
1049.294
1045.436
1050.258
910.4167
1051.223
979.8552
1569.119
1570.083
1052.187
913.3099
911.3811
1100.408
909.4523
912.3455
1576.834
1101.373
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1055.08
877.6263
1560.439
914.2744

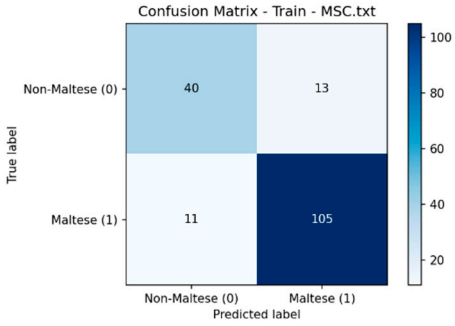
Figure S15. Confusion matrices for classification of Maltese and non-Maltese pork using ANN models with different preprocessing methods: Rows correspond to different preprocessing methods applied to the ATR-FTIR pork dataset: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend. Left panels represent results from excluded rows (external validation), while right panels represent results from training datasets. Correct classifications are indicated along the diagonal, with misclassifications off-diagonal.

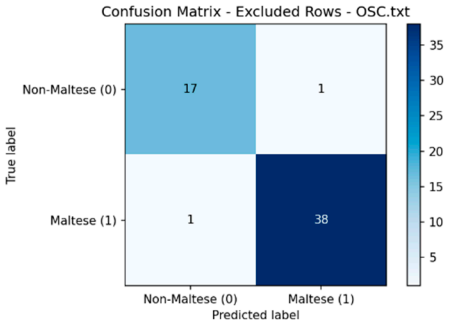


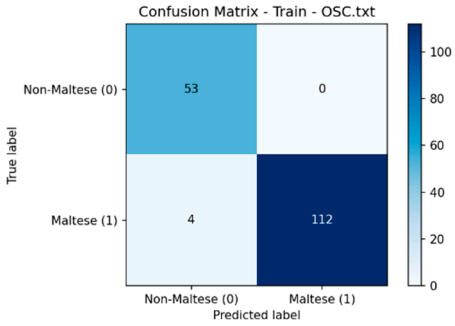

Confusion Matrix - Excluded Rows - MedianFilter.txt
Non-Maltese (0)
Maltese (1)
True label
15
3
0
39
Non-Maltese (0)
Maltese (1)
Predicted label
35
30
25
20
15
10
5
0

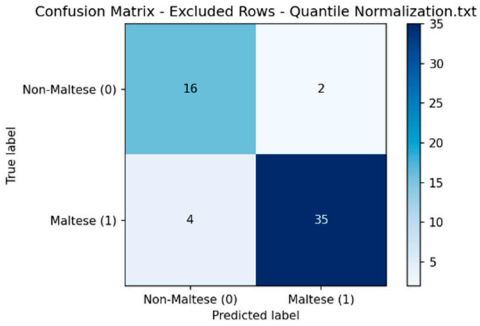

Confusion Matrix - Train - MedianFilter.txt
Non-Maltese (0)
Maltese (1)
True label
50
3
3
113
Non-Maltese (0)
Maltese (1)
Predicted label
100
80
60
40
20

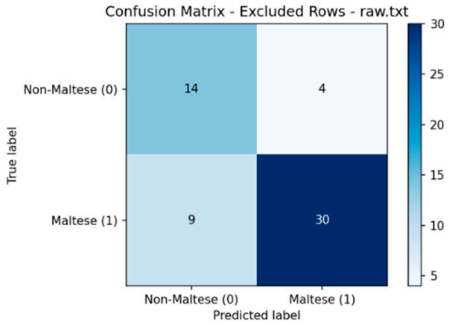

Confusion Matrix - Excluded Rows - MSC.txt
Non-Maltese (0)
Maltese (1)
True label
18
0
5
34
Non-Maltese (0)
Maltese (1)
Predicted label
30
25
20
15
10
5
0

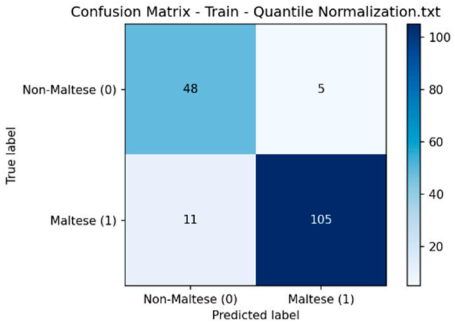

Confusion Matrix - Train - MSC.txt
Non-Maltese (0)
Maltese (1)
True label
40
13
11
105
Non-Maltese (0)
Maltese (1)
Predicted label
100
80
60
40
20

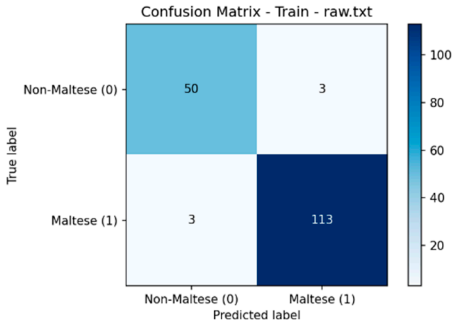

Confusion Matrix - Excluded Rows - OSC.txt
Non-Maltese (0)
Maltese (1)
True label
17
1
1
38
Non-Maltese (0)
Maltese (1)
Predicted label
35
30
25
20
15
10
5

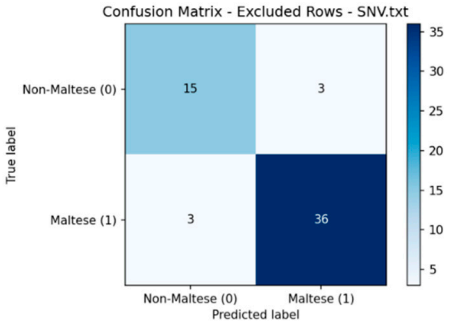

Confusion Matrix - Train - OSC.txt
Non-Maltese (0)
Maltese (1)
True label
53
0
4
112
Non-Maltese (0)
Maltese (1)
Predicted label
100
80
60
40
20
0

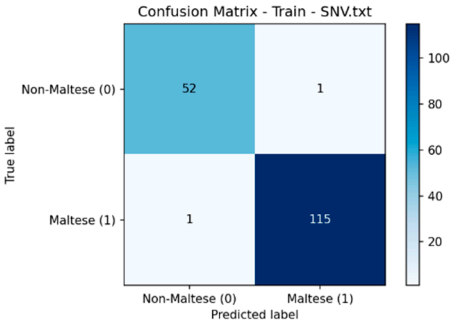

Confusion Matrix - Excluded Rows - Quantile Normalization.txt
Non-Maltese (0)
Maltese (1)
True label
16
2
4
35
Non-Maltese (0)
Maltese (1)
Predicted label
35
30
25
20
15
10
5

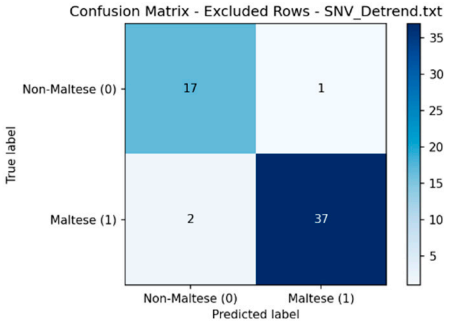

Confusion Matrix - Excluded Rows - raw.txt
Non-Maltese (0)
Maltese (1)
True label
14
4
9
30
Non-Maltese (0)
Maltese (1)
Predicted label
30
25
20
15
10
5


Confusion Matrix - Train - Quantile Normalization.txt
Non-Maltese (0)
Maltese (1)
True label
48
5
11
105
Non-Maltese (0)
Maltese (1)
Predicted label
100
80
60
40
20


Confusion Matrix - Train - raw.txt
Non-Maltese (0)
Maltese (1)
True label
50
3
3
113
Non-Maltese (0)
Maltese (1)
Predicted label
100
80
60
40
20


Confusion Matrix - Excluded Rows - SNV.txt
Non-Maltese (0)
Maltese (1)
True label
15
3
3
36
Non-Maltese (0)
Maltese (1)
Predicted label
35
30
25
20
15
10
5


Confusion Matrix - Train - SNV.txt
Non-Maltese (0)
Maltese (1)
True label
52
1
1
115
Non-Maltese (0)
Maltese (1)
Predicted label
100
80
60
40
20


Confusion Matrix - Excluded Rows - SNV_Detrend.txt
Non-Maltese (0)
Maltese (1)
True label
17
1
2
37
Non-Maltese (0)
Maltese (1)
Predicted label
35
30
25
20
15
10
5

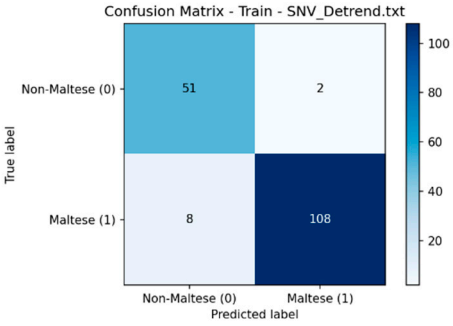
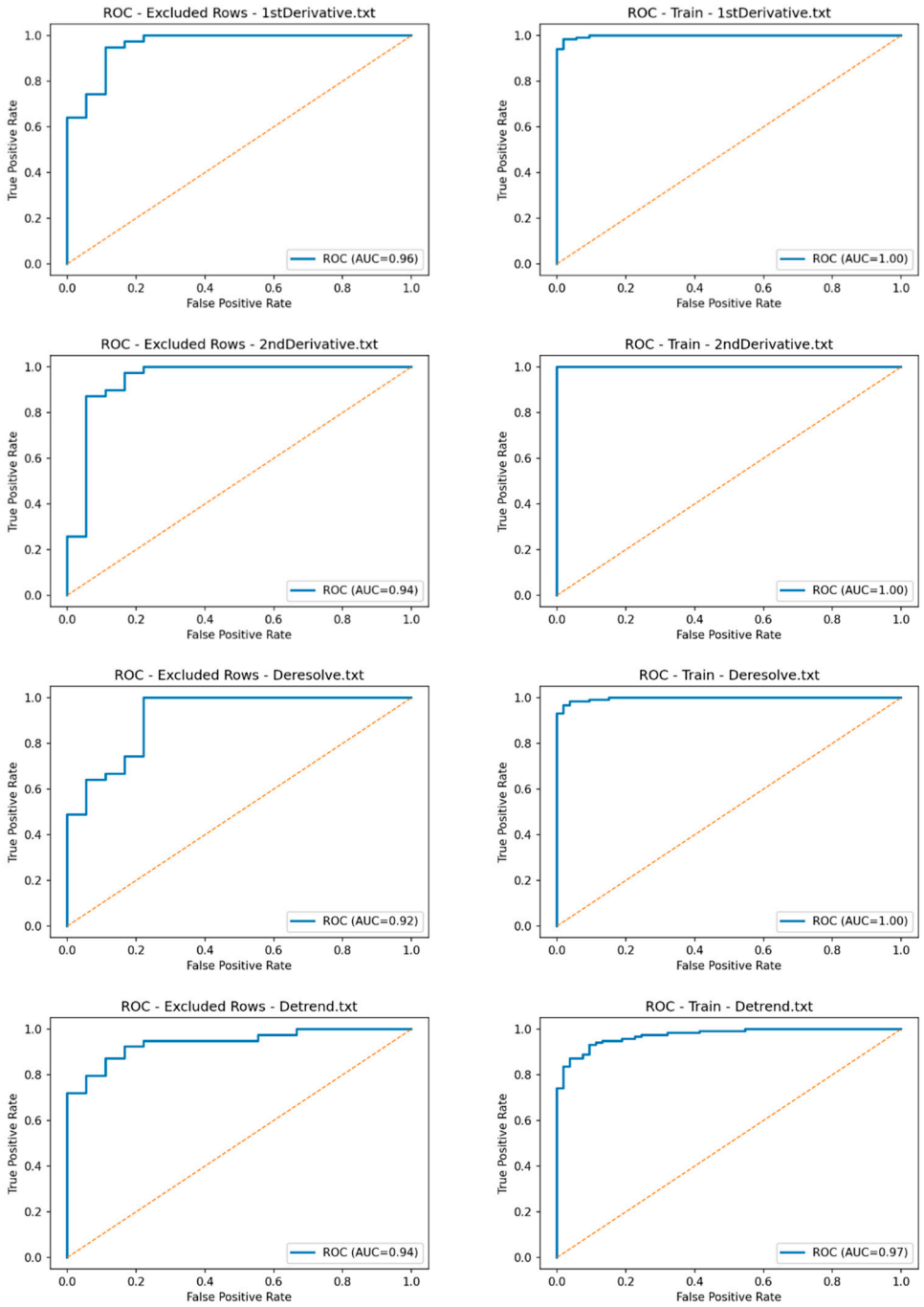
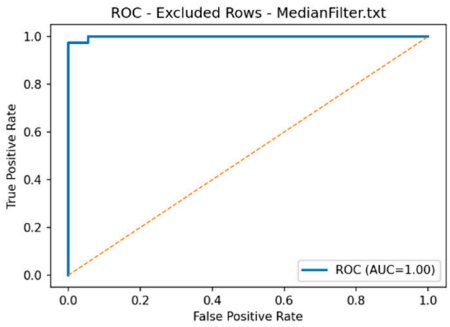
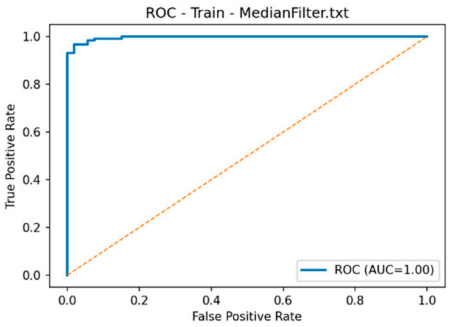
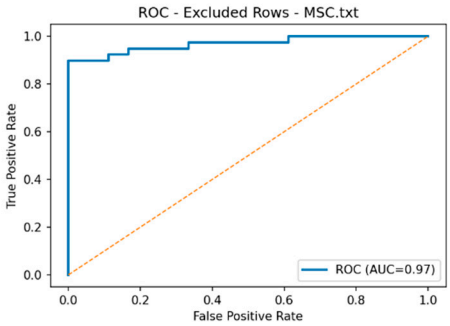

Confusion Matrix - Train - SNV_Detrend.txt
Non-Maltese (0)
Maltese (1)
True label
51
2
8
108
Non-Maltese (0)
Maltese (1)
Predicted label
100
80
60
40
20

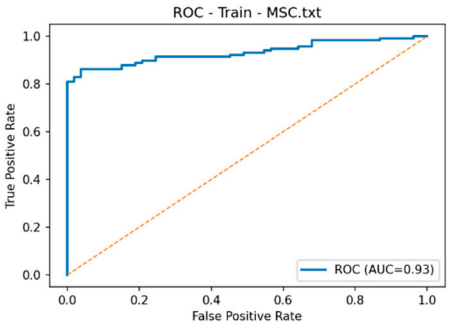
Figure S16. Receiver Operating Characteristic (ROC) curves for classification of Maltese and non-Maltese pork using ANN models with different preprocessing methods: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend. Left panels represent excluded rows (external validation), while right panels represent training datasets. The area under the curve (AUC) is shown for each model, with values close to 1.0 indicating strong classification performance.

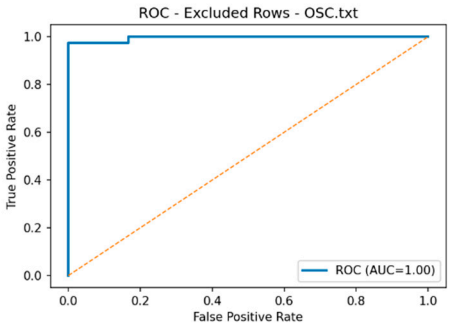


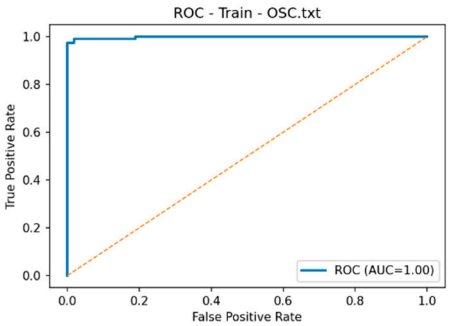

ROC - Excluded Rows - MedianFilter.txt
True Positive Rate
False Positive Rate
ROC (AUC=1.00)

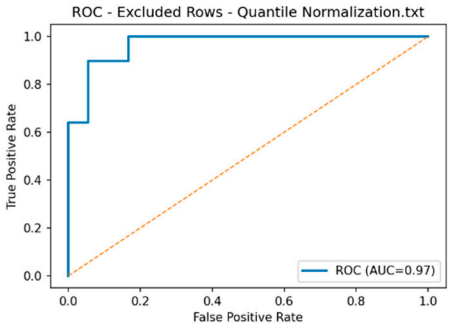

ROC - Train - MedianFilter.txt
True Positive Rate
False Positive Rate
ROC (AUC=1.00)

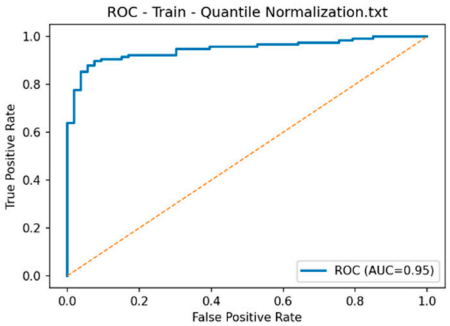

ROC - Excluded Rows - MSC.txt
True Positive Rate
False Positive Rate
ROC (AUC=0.97)

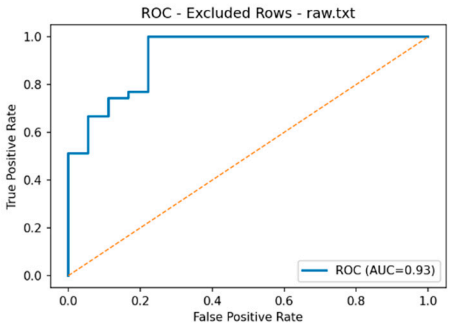

ROC - Train - MSC.txt
True Positive Rate
False Positive Rate
ROC (AUC=0.93)

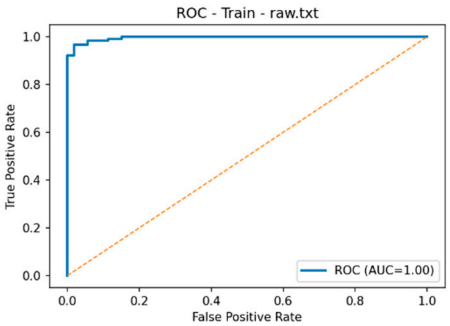

ROC - Excluded Rows - OSC.txt
True Positive Rate
False Positive Rate
ROC (AUC=1.00)

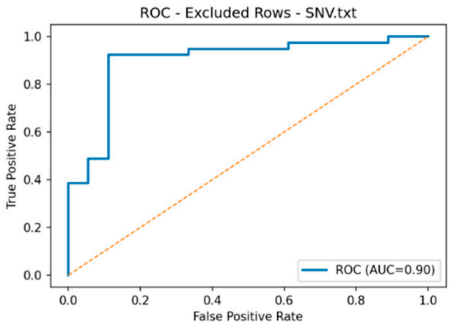

ROC - Train - OSC.txt
True Positive Rate
False Positive Rate
ROC (AUC=1.00)

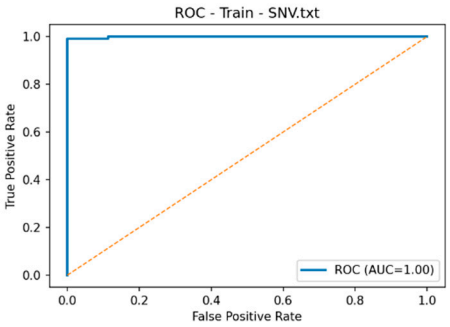

ROC - Excluded Rows - Quantile Normalization.txt
True Positive Rate
False Positive Rate
ROC (AUC=0.97)

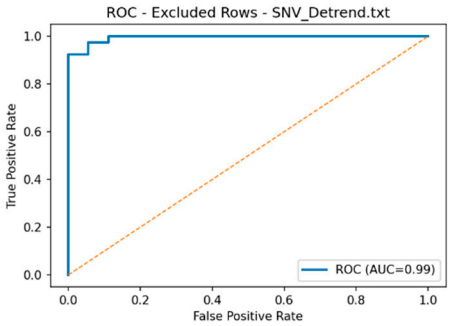

ROC - Train - Quantile Normalization.txt
True Positive Rate
False Positive Rate
ROC (AUC=0.95)


ROC - Excluded Rows - raw.txt
True Positive Rate
False Positive Rate
ROC (AUC=0.93)


ROC - Train - raw.txt
True Positive Rate
False Positive Rate
ROC (AUC=1.00)


ROC - Excluded Rows - SNV.txt
True Positive Rate
False Positive Rate
ROC (AUC=0.90)
0.0
0.2
0.4
0.6
0.8
1.0


ROC - Train - SNV.txt
True Positive Rate
False Positive Rate
ROC (AUC=1.00)
0.0
0.2
0.4
0.6
0.8
1.0


ROC - Excluded Rows - SNV_Detrend.txt
True Positive Rate
False Positive Rate
ROC (AUC=0.99)
0.0
0.2
0.4
0.6
0.8
1.0

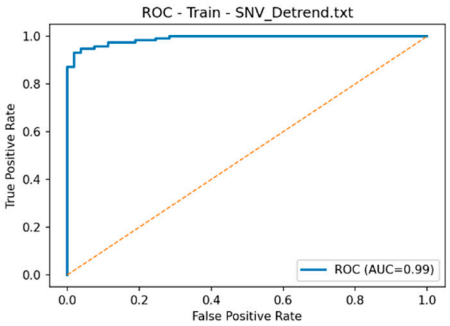
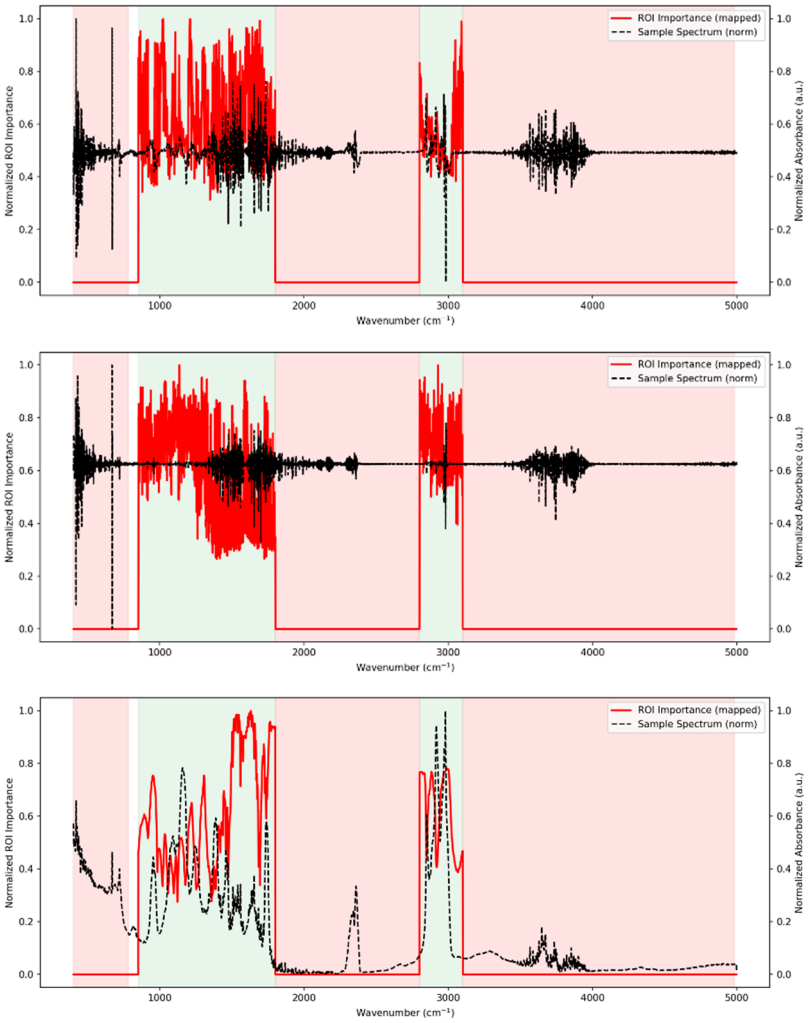
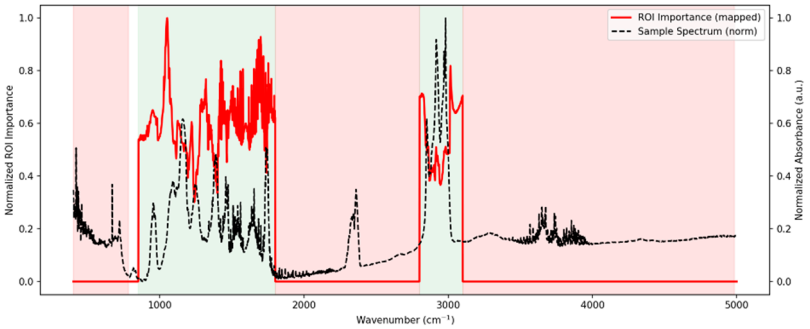
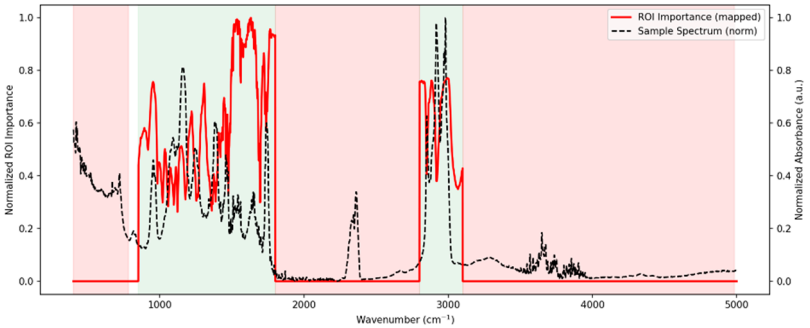
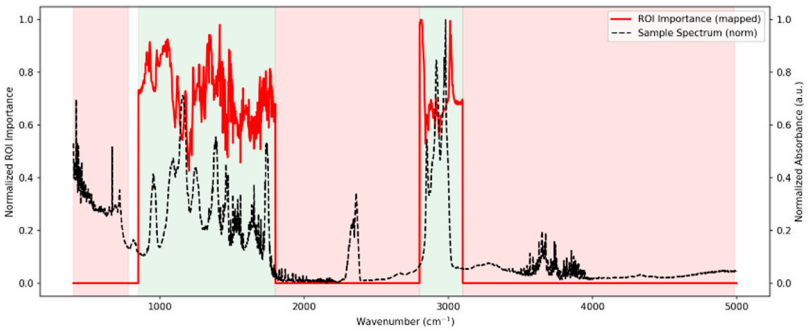

ROC - Train - SNV_Detrend.txt
True Positive Rate
False Positive Rate
ROC (AUC=0.99)
0.0
0.2
0.4
0.6
0.8
1.0

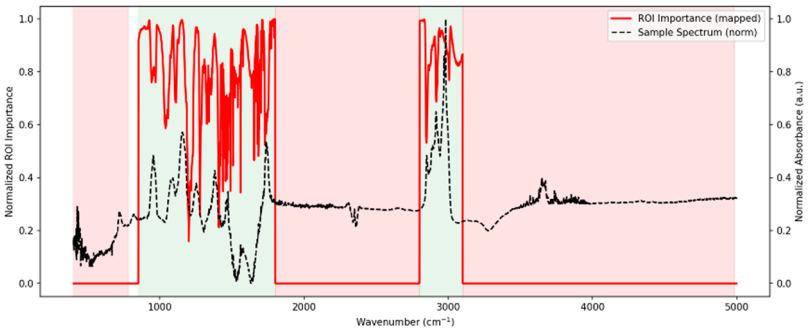
Figure S17. Region of Importance (ROI) plots showing the most influential wavenumber regions for discrimination between Maltese and non-Maltese pork. The black dashed line represents the normalized ATR-FTIR spectrum, while the red trace indicates the ROI importance values identified by chemometric modelling with different preprocessing methods: 1st Derivative, 2nd Derivative, Deresolve, Detrend, Median Filter, Multiplicative Scatter Correction (MSC), Orthogonal Signal Correction (OSC), Quantile Normalization, Raw, Standard Normal Variate (SNV), and SNV+Detrend. Shaded areas highlight spectral intervals consistently selected as informative across preprocessing strategies.

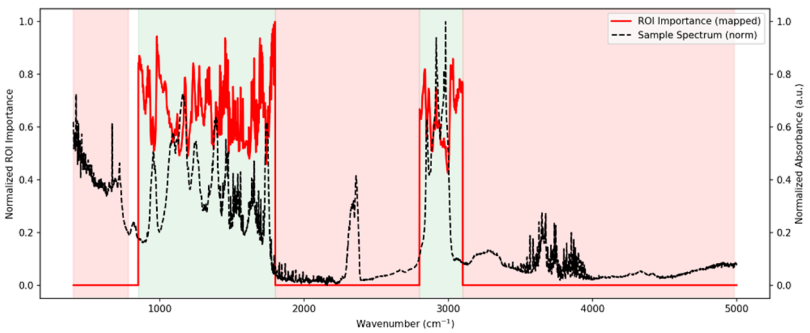


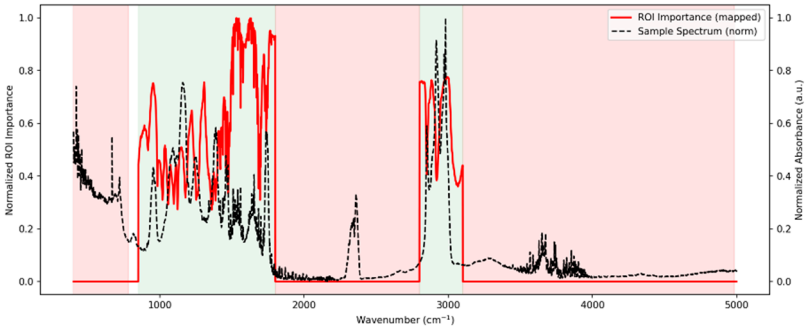

ROI Importance (mapped)
Sample Spectrum (norm)
Normalized ROI Importance
Normalized Absorbance (a.u.)
Wavenumber (cm⁻¹)

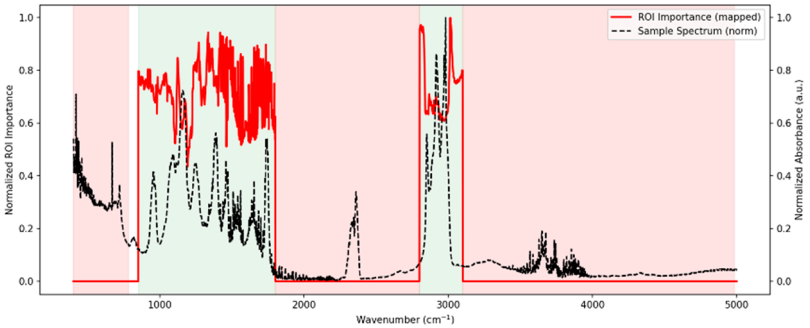

ROI Importance (mapped)
Sample Spectrum (norm)
Normalized ROI Importance
Normalized Absorbance (a.u.)
Wavenumber (cm⁻¹)

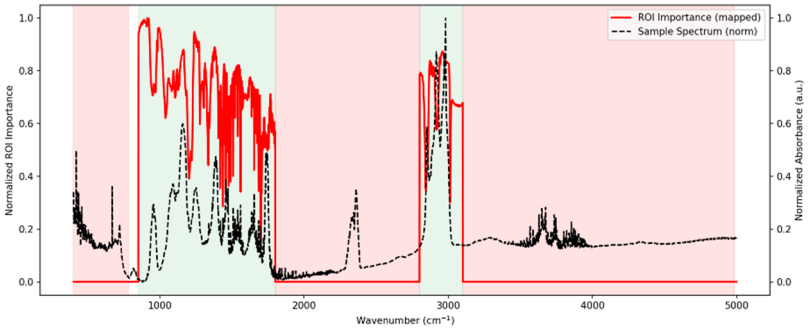

ROI Importance (mapped)
Sample Spectrum (norm)
Normalized ROI Importance
Normalized Absorbance (a.u.)
Wavenumber (cm⁻¹)


ROI Importance (mapped)
Sample Spectrum (norm)
Normalized ROI Importance
Normalized Absorbance (a.u.)
Wavenumber (cm⁻¹)


ROI Importance (mapped)
Sample Spectrum (norm)
Normalized ROI Importance
Normalized Absorbance (a.u.)
Wavenumber (cm⁻¹)


ROI Importance (mapped)
Sample Spectrum (norm)
Normalized ROI Importance
Normalized Absorbance (a.u.)
Wavenumber (cm⁻¹)


ROI Importance (mapped)
Sample Spectrum (norm)
Normalized ROI Importance
Normalized Absorbance (a.u.)
Wavenumber (cm⁻¹)


ROI Importance (mapped)
Sample Spectrum (norm)
Normalized ROI Importance
Normalized Absorbance (a.u.)
Wavenumber (cm⁻¹)