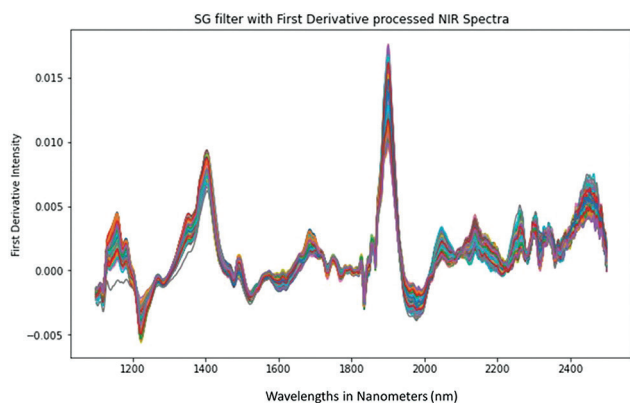
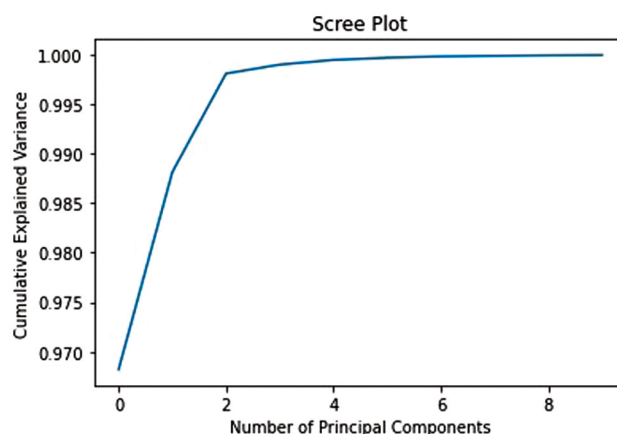


Supplementary Table 1 PC-wise factor loadings

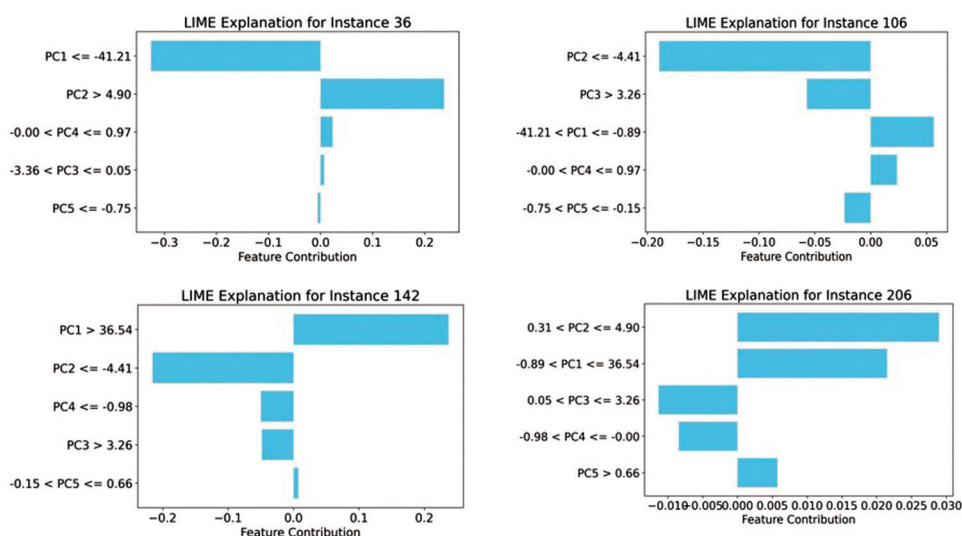
Feature variables	Principal Components (PCs)				
	0	1	2	3	4
1100.0	0.011388	0.016778	0.029197	0.009896	0.019866
1100.5	0.011396	0.017317	0.031234	0.010117	0.020452
1101.0	0.011435	0.018007	0.033755	0.010409	0.021206
1101.5	0.011217	0.018415	0.035985	0.010516	0.021617
1102.0	0.010625	0.018186	0.037178	0.010337	0.021388
...
2497.5	0.013726	0.010146	0.039042	0.009447	0.009032
2498.0	0.014998	0.010780	0.037795	0.011178	0.008612
2498.5	0.015934	0.011155	0.035587	0.012860	0.008114
2499.0	0.016697	0.011421	0.033186	0.014362	0.007571
2499.5	0.016688	0.011182	0.029605	0.015122	0.006758



Supplementary Fig. 1 SNV and SG pre-processed spectra graph plot.



Supplementary Fig. 2 Scree Plot of PCA.



Supplementary Fig. 3 Feature contribution interpretation using the local interpretable model-agnostic explanations (LIME explanation) method on random five instances of testing dataset.