

A Multivariate Analysis-Driven Workflow to Tackle Uncertainties in Miniaturized NIR Data— Supplementary Materials



Figure S1. Example of configuration for spectral acquisitions.

Table S1. Descriptive statistics of spectra acquired with AvaSpec-Mini-NIR. Calculated on percentage reflectance data.

	Integrating sphere				Optical fiber			
	Sample 1	Sample 2	Sample 3	Sample 4	Sample 1	Sample 2	Sample 3	Sample 4
Relative standard deviation (%) – mean	6.06	3.96	2.20	1.57	126.99	73.39	9.42	10.05
RMS – mean	0.51	0.53	1.02	0.95	0.61	12.18	3.81	3.67
RMS – standard deviation	0.86	0.28	0.51	0.34	0.88	10.28	2.48	2.57
S/N mean	8.74	25.96	57.49	92.14	0.98	1.37	11.18	10.34
S/N standard deviation	0.33	4.38	25.29	46.31	0.41	0.07	2.24	1.87

Table S2. Descriptive statistics of spectra acquired with NeoSpectra Scanner. Calculated on percentage reflectance data.

	Sample 1	Sample 2	Sample 3	Sample 4
Relative stand deviation (%) – mean	17.39	30.09	2.36	2.51
RMS – mean	0.41	2.36	0.78	1.26
RMS – standard deviation	0.25	1.29	0.36	0.37
S/N mean	5.98	3.44	65.05	47.02
S/N standard deviation	1.21	0.71	44.10	18.05

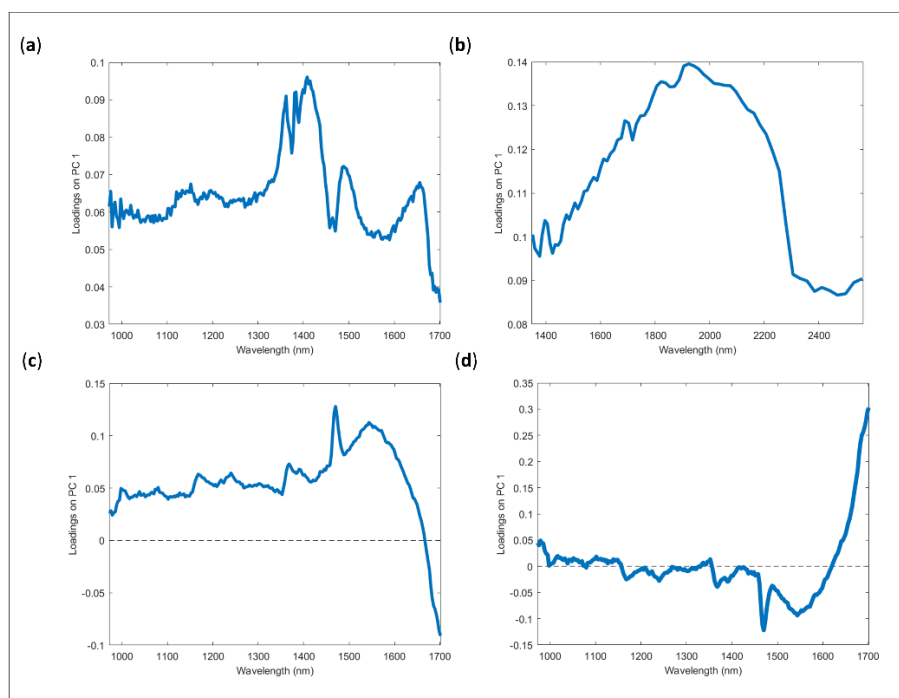


Figure S2. ASCA submodels examples. Loadings of the ASCA sub-model for the factor (a) session (b) replicates (c) and (d) timing of background. Instruments: (a) AvaSpec-Mini-NIR equipped with integrating sphere (b) NeoSpectra Scanner (c) and (d) AvaSpec-Mini-NIR equipped with optical fiber. Samples: (a) Sample 3 (b) Sample 2 (c) and (d) Sample 4.

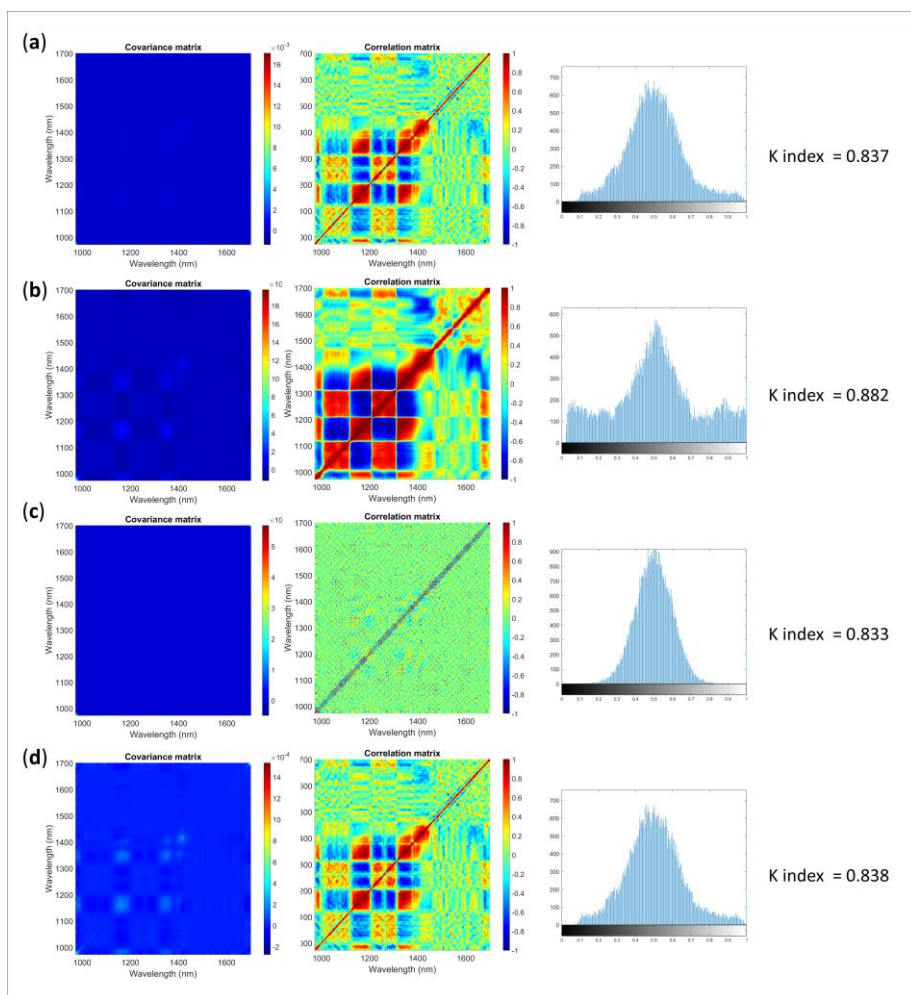


Figure S3. Multivariate error covariance matrix, correlation matrix, image histogram and K index for Sample 1 acquired with AvaSpec-Mini NIR with integrating sphere and preprocessed with first derivative (a) $w = 7, d = 1, p = 2$; (b) $w = 15, d = 1, p = 2$; (c) $w = 7, d = 2, p = 2$; (d) $w = 7, d = 1, p = 1$.

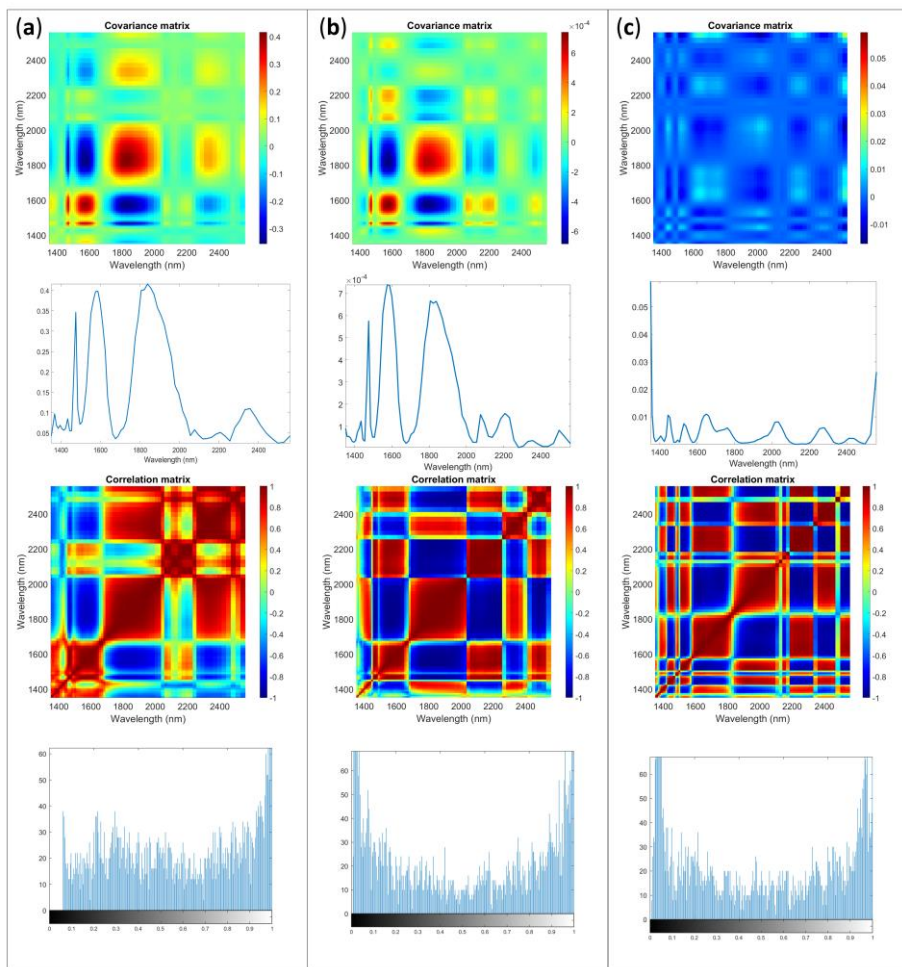


Figure S4. Multivariate error covariance matrix, error covariance matrix diagonal, correlation matrix and image histogram of the correlation matrix for Sample 3 acquired with NeoSpectra Scanner: (a) raw data (b) SNV (c) first derivative.

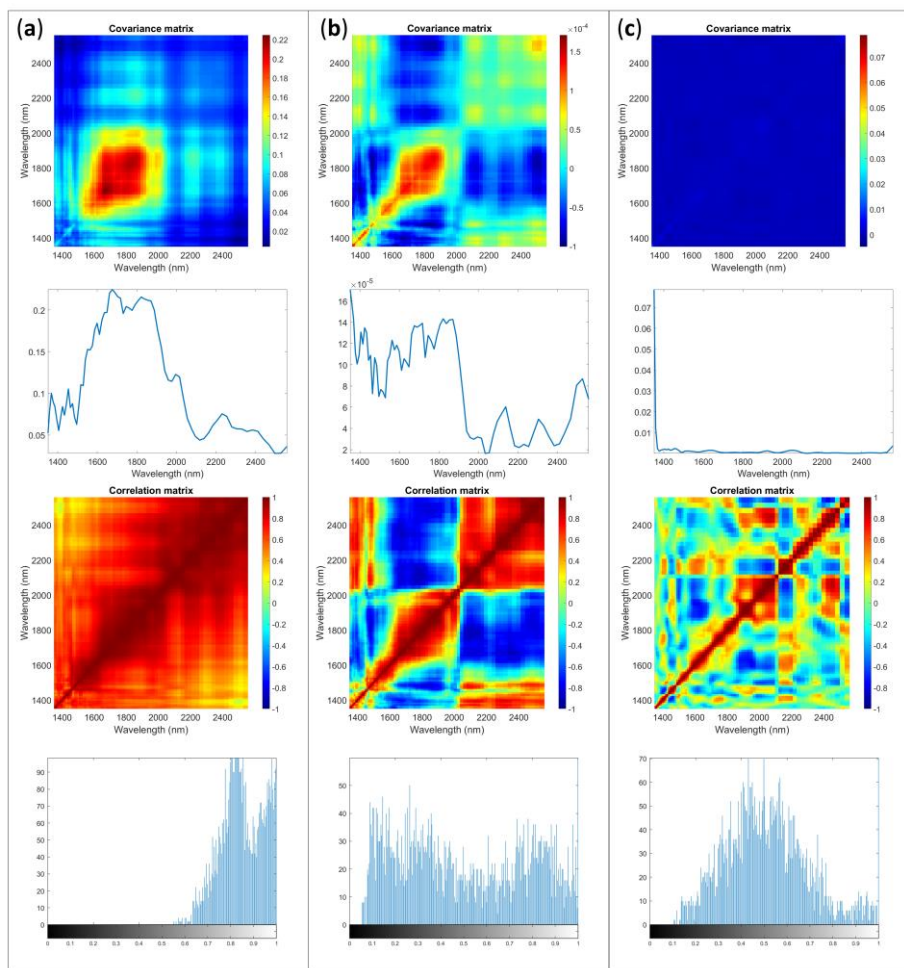


Figure S5. Multivariate error covariance matrix, error covariance matrix diagonal, correlation matrix and image histogram of the correlation matrix for Sample 4 acquired with NeoSpectra Scanner: (a) raw data (b) SNV (c) first derivative.