

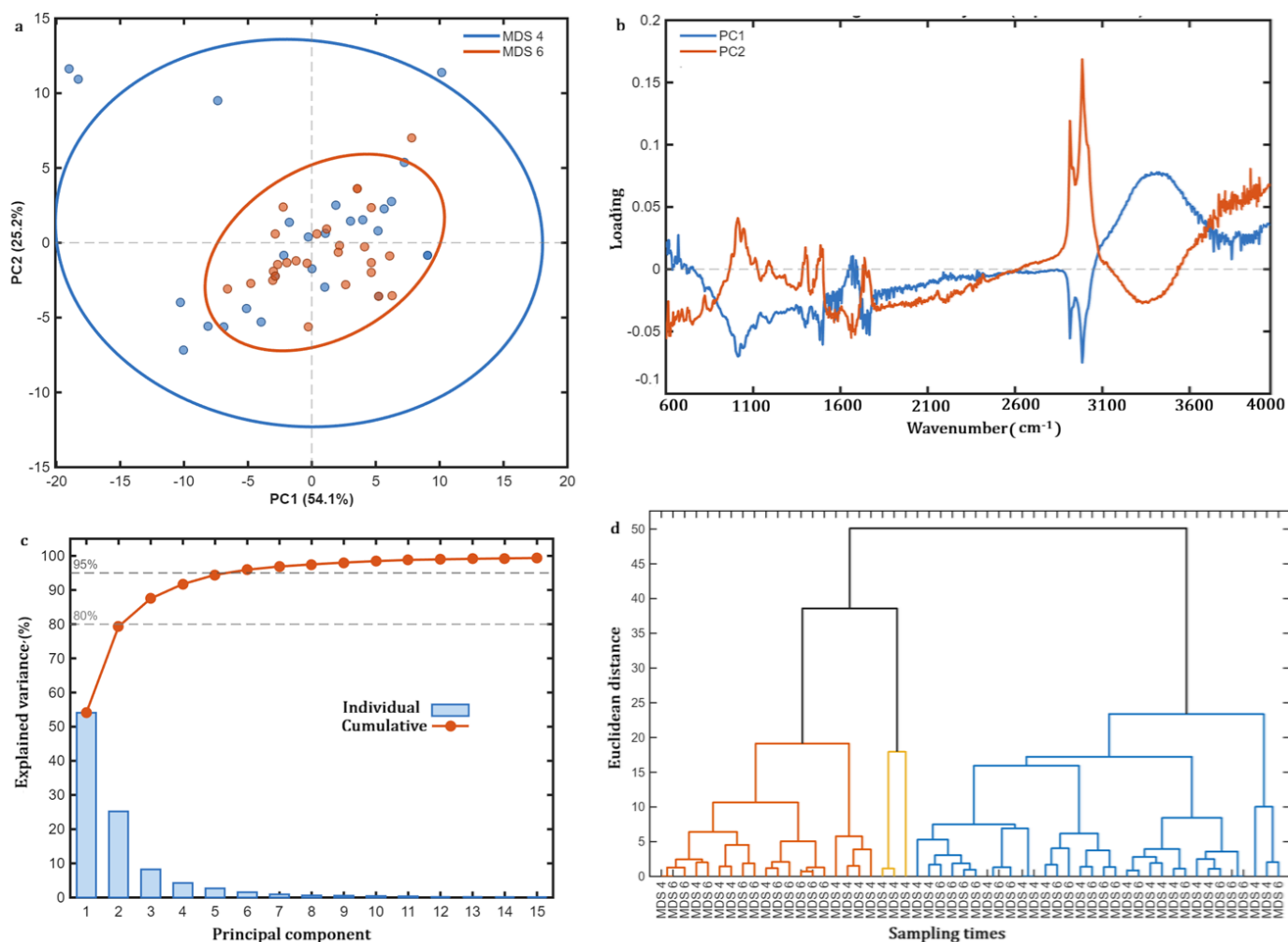


Figure S1. Multivariate analysis of MIR spectra from 4- and 6-month sampling times (MDS). **(a)** PCA scores plot (PC1 vs PC2) showing extensive overlap between sampling times. Ellipses represent the 95% confidence regions for each group. **(b)** PCA loading profiles for PC1 and PC2 across wavelengths. **(c)** Individual and cumulative explained variance of the principal components. **(d)** Ward hierarchical clustering based on PCA scores, showing no distinct clustering pattern according to sampling time.

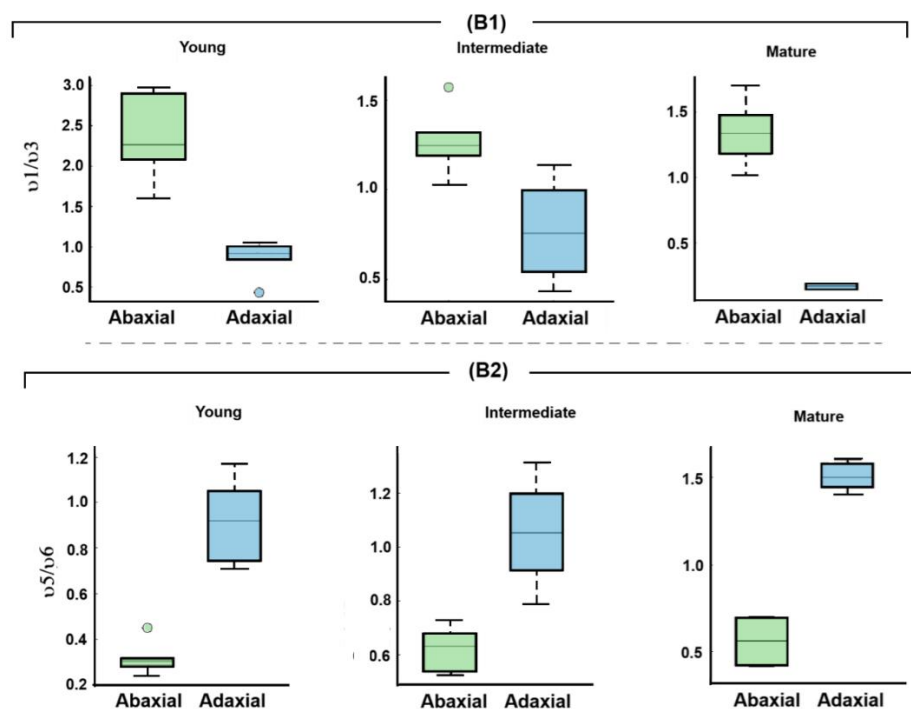


Figure S2. Box and whisker plot explaining the variation of the spectral ratios $v1/v3$ and $v5/v6$: Variation of the spectral ratios as a function of the adaxial and abaxial face (**B1** and **B2** correspond to the spectral ratios $v1/v3$ and $v5/v6$, respectively).

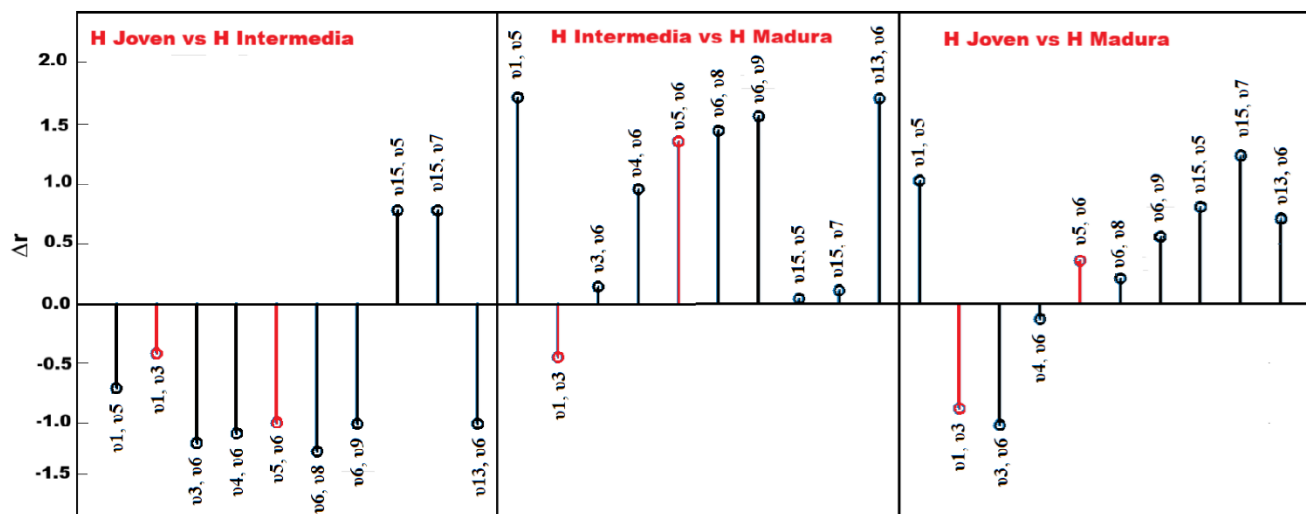


Figure S3. Differential correlation analysis (Δr) between characteristic FEDS-enhanced FT-MIR bands across cassava leaf ontogenetic stages. Positive Δr values indicate band-pair relationships that became more strongly correlated in the second ontogenetic group relative to the first, whereas negative values indicate a reduction in correlation strength. Only the band pairs exhibiting the largest changes in correlation are shown. Red markers highlight relationships involving the candidate spectral indexes selected for subsequent statistical evaluation. Band notation ($v1$ – $v15$) corresponds to the characteristic FT-MIR signals identified during the spectral characterization stage.

Table S1. Descriptive statistics (mean ± SD) of FT-MIR-derived spectral indices across ontogenetic stages (Joven, Intermedia, Madura).

Index	Young (mean ± SD)	Intermédiaire (mean ± SD)	Mature (mean ± SD)
IMIR1	0.967 ± 0.269	0.965 ± 0.217	0.735 ± 0.069
IMIR2	0.824 ± 0.219	0.804 ± 0.156	0.567 ± 0.035
IMIR3	1.163 ± 0.173	1.256 ± 0.147	1.494 ± 0.039
IMIR4	0.921 ± 0.109	0.973 ± 0.082	1.194 ± 0.046
IMIR5	0.991 ± 0.121	1.049 ± 0.097	1.154 ± 0.026
IMIR6	1.049 ± 0.080	1.059 ± 0.076	0.890 ± 0.030
IMIR7	1.049 ± 0.112	1.062 ± 0.083	0.896 ± 0.028
IMIR8	1.589 ± 0.172	1.316 ± 0.072	1.108 ± 0.025
IMIR9	1.883 ± 0.301	1.607 ± 0.078	1.349 ± 0.032
IMIR10	1.233 ± 0.191	1.089 ± 0.102	1.351 ± 0.051

Table S2. LMM results for spectral indices IMIR1–IMIR10 Linear Mixed-Effects Model: Index ~ Day + Ontogenetic Stage + (1 | Biological Replicate) · n = 72 (3 biological replicates × 3 ontogenetic stages × 8 sampling days).

Index	<i>p</i> -Value (Día)	<i>p</i> -Value (Ontogeny)	<i>p</i> -Value (Day × Stage)	AIC	BIC	R ² Marginal	Most Responsive Ontogenetic Stage
IMIR1	1.65 × 10 ⁻⁷ ***	7.60 × 10 ⁻⁸ ***	1.53 × 10 ⁻⁴ ***	−47.64	11.55	0.847	Mature
IMIR2	4.65 × 10 ⁻⁷ ***	1.45 × 10 ⁻¹⁰ ***	1.80 × 10 ⁻⁶ ***	−92.62	−33.42	0.817	Young
IMIR3	4.05 × 10 ⁻⁶ ***	1.68 × 10 ⁻⁶ ***	2.87 × 10 ⁻⁴ ***	−57.93	1.27	0.777	Mature
IMIR4	8.48 × 10 ⁻⁸ ***	3.09 × 10 ⁻⁴ ***	0.0029 **	−96.35	−37.16	0.745	Mature
IMIR5	1.30 × 10 ⁻¹¹ ***	0.0016 **	2.51 × 10 ⁻¹⁰ ***	−180.86	−121.67	0.884	Mature
IMIR6	1.48 × 10 ⁻⁷ ***	1.68 × 10 ⁻⁸ ***	0.0011 **	−181.63	−122.44	0.813	Mature
IMIR7	6.77 × 10 ⁻⁷ ***	1.34 × 10 ⁻⁸ ***	2.06 × 10 ⁻⁴ ***	−189.88	−130.68	0.817	Young
IMIR8	3.30 × 10 ⁻¹⁰ ***	2.67 × 10 ⁻¹⁷ ***	7.70 × 10 ⁻⁸ ***	10.87	70.06	0.909	Mature
IMIR9	1.20 × 10 ⁻⁶ ***	5.70 × 10 ⁻²² ***	4.85 × 10 ⁻⁸ ***	40.74	99.93	0.906	Mature
IMIR10	0.5534 ns	3.68 × 10 ⁻⁷ ***	0.2605 ns	−103.64	−44.44	0.607	Young

p-value (Day): significance of the temporal (day) fixed effect. *p*-value (Stage): significance of the ontogenetic stage fixed effect. *p*-value (Day × Stage): significance of the interaction between day and ontogenetic stage.

Significance codes: *** *p* < 0.001, ** *p* < 0.01, * *p* < 0.05, ns *p* ≥ 0.05.

R² marginal: variance explained by fixed effects only (Day + Stage ± Day × Stage), excluding the random intercept (1 | Replicate).

AIC / BIC: lower values indicate better model fit. Positive values for IMIR8 and IMIR9 reflect higher absolute residual variance in those indices.

Most sensitive stage: ontogenetic group with the steepest marginal temporal slope across days 1–16 (population-level linear fit).

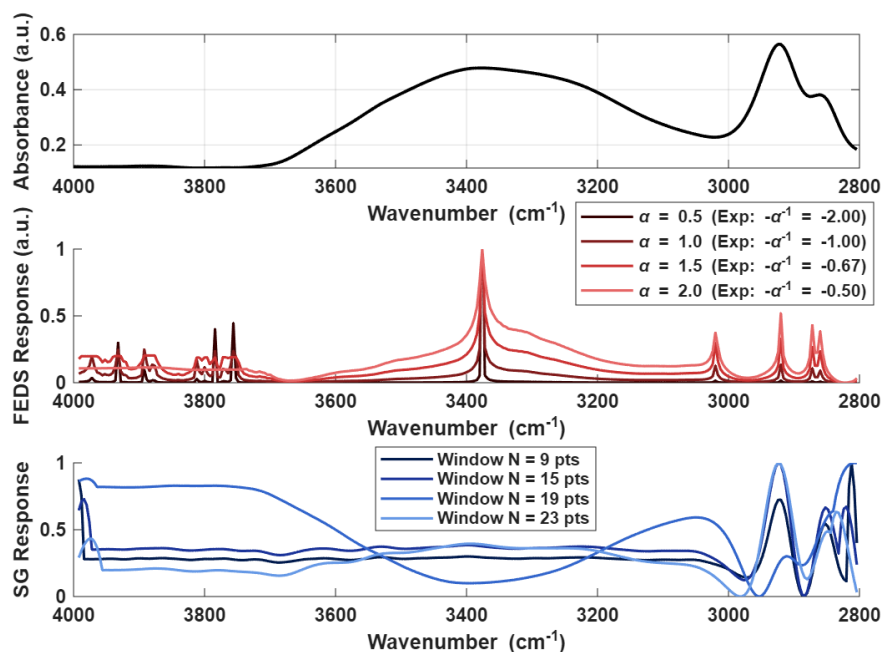


Figure S4. comparison between the original FT-MIR spectrum, the FEDS transformation, and the Savitzky–Golay second derivative in the 4000–2800 cm⁻¹ region (MIR1). The upper panel shows the original absorbance spectrum. The middle panel presents the FEDS responses obtained with different α values (0.5–2.0), illustrating the progressive enhancement and localization of spectral bands. The lower panel shows the Savitzky–Golay second-derivative responses calculated using different smoothing window sizes (9–23 points). FEDS produced sharp, positive, and well-localized responses for the broad O–H stretching band around 3400 cm⁻¹ and the partially overlapping C–H stretching bands near 2920 and 2850 cm⁻¹, whereas the Savitzky–Golay second derivative generated broader oscillatory derivative features that were strongly dependent on the selected window size.

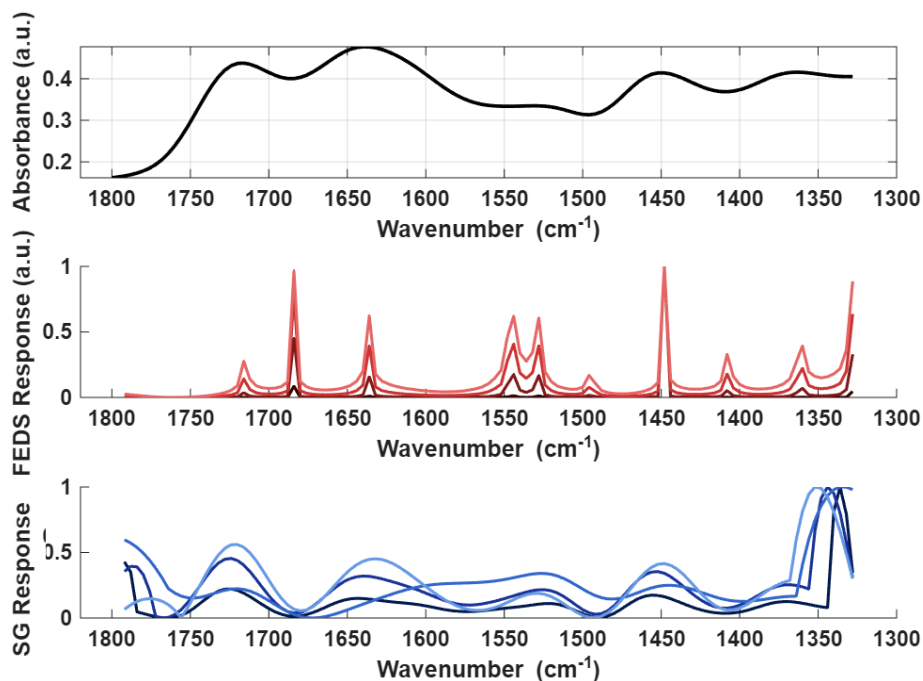


Figure S5. comparison between the original FT-MIR spectrum, the FEDS transformation, and the Savitzky–Golay second derivative in the 1800–1300 cm⁻¹ region (MIR2).

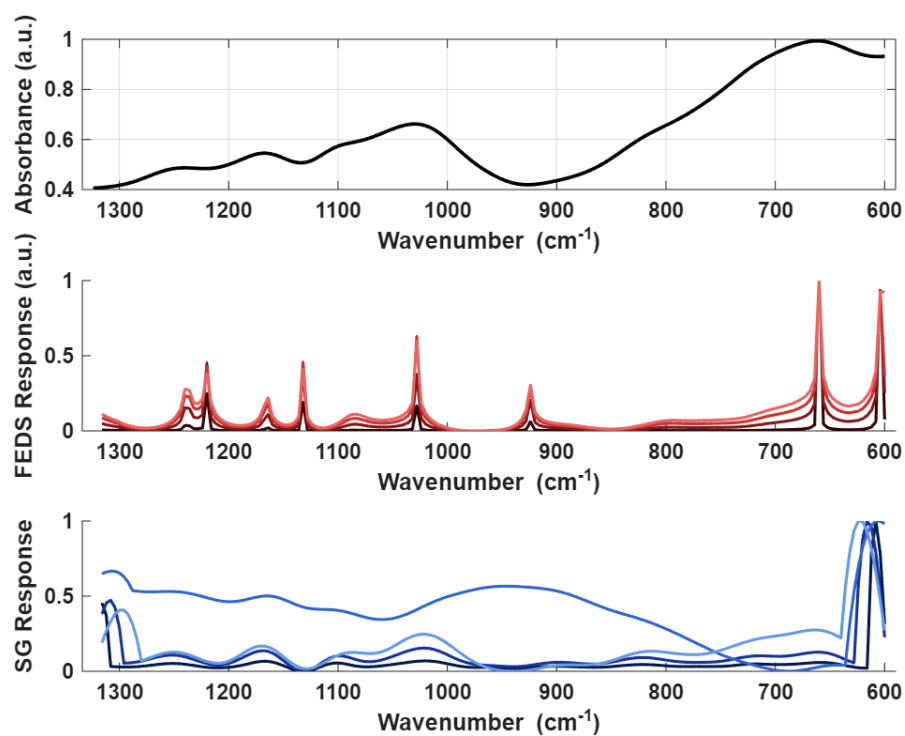


Figure S6. comparison between the original FT-MIR spectrum, the FEDS transformation, and the Savitzky-Golay second derivative in the 1300–600 cm^{-1} region (MIR3).