

Reflectance Spectroscopy for the Classification and Prediction of Pigments in Agronomic Crops

Renan Falcioni ^{1,*}, Werner Camargos Antunes ¹, José Alexandre M. Demattê ² and Marcos Rafael Nanni ¹

¹ Graduate Program in Agronomy, Department of Agronomy, State University of Maringá, Av. Colombo, 5790, Maringá 87020-900, PR, Brazil; wcantunes@uem.br (W.C.A.); mrnanni@uem.br (M.R.N.)

² Department of Soil Science, Luiz de Queiroz College of Agriculture, University of São Paulo, Av. Pádua Dias, 11, Piracicaba 13418-260, SP, Brazil; jamdemat@usp.br

* Correspondence: renanfalcioni@gmail.com; Tel.: +55-44-3011-8940

Table S1. Vegetation indexes calculated from the hyperspectral reflectance of leaves.

| Index | Equation | Reference |
|---|---|-----------|
| NDVI ₇₅₀ = Normalized Difference Vegetation Index q750 | $(R_{750} - R_{705}) / (R_{750} + R_{705})$ | [52] |
| WBI = Water Band Index | $(R_{900}) / (R_{970})$ | [53] |
| RARS = Ratio Analysis of Reflectance Spectra | $(R_{746}) / (R_{513})$ | [53] |
| ARI1 = Anthocyanin Reflectance Index | $(1/R_{550}) - (1/R_{700})$ | [54] |
| PSND = Pigment Specific Normalized Difference | $(R_{800} - R_{470}) / (R_{800} + R_{470})$ | [55] |
| SIPI = Structurally Insensitive Pigment Index | $(R_{800} - R_{445}) / (R_{800} - R_{680})$ | [55] |
| PSRI = Plant Senescence Reflectance Index | $(R_{680} - R_{500}) / (R_{750})$ | [56] |
| PSRI2 = Plant Senescence Reflectance Index 2 | $(R_{672}) / (R_{550} + R_{708})$ | [56] |
| PSSRc = Pigment-specific Simple Ratio | $(R_{800}) / (R_{500})$ | [55] |
| VOG1 = Vogelmann Index 1 | $(R_{740}) / (R_{720})$ | [57] |
| VOG2 = Vogelmann Index 2 | $(R_{734} - R_{747}) / (R_{715} + R_{726})$ | [58] |
| MSI = Moisture Stress Index | (R_{1650} / R_{830}) | [59] |
| PRI = Photochemical Reflectance Index | $(R_{530} - R_{570}) / (R_{530} + R_{570})$ | [60] |
| PVR = Normalized Difference Photosynthetic | $(R_{550} - R_{650}) / (R_{550} + R_{650})$ | [61] |
| FR = Fluorescence Ratio | $(R_{690}) / (R_{740})$ | [62] |

Table S2. Descriptive analysis of pigment attribute-based area and mass. ($n = 360$).

| Attributes | Count (n) | Mean | Median | Minimum | Maximum | CV (%) |
|------------------------------|-----------|-------|--------|---------|---------|--------|
| Chla (mg m ⁻²) | 360 | 330.6 | 329.6 | 136.9 | 713.0 | 42.2 |
| Chlb (mg m ⁻²) | 360 | 210.1 | 154.2 | 61.0 | 994.4 | 69.7 |
| Chla+b (mg m ⁻²) | 360 | 540.7 | 475.5 | 197.9 | 1707.4 | 51.1 |
| Car (mg m ⁻²) | 360 | 122.3 | 116.6 | 52.4 | 287.8 | 41.3 |
| AnC (nmol m ⁻²) | 360 | 0.9 | 0.8 | 0.1 | 2.1 | 65.2 |
| Flv (nmol m ⁻²) | 360 | 73.4 | 68.9 | 15.8 | 116.8 | 37.1 |
| Chla (mg g ⁻¹) | 360 | 7.0 | 6.0 | 1.9 | 29.6 | 73.8 |
| Chlb (mg g ⁻¹) | 360 | 4.1 | 3.5 | 1.0 | 14.1 | 62.6 |
| Chla+b (mg g ⁻¹) | 360 | 11.1 | 9.7 | 3.1 | 41.1 | 66.6 |
| Car (mg g ⁻¹) | 360 | 2.5 | 2.3 | 0.7 | 9.4 | 61.3 |
| AnC (μmol g ⁻¹) | 360 | 0.2 | 0.1 | 0.0 | 0.7 | 93.4 |
| Flv (μmol g ⁻¹) | 360 | 11.9 | 11.3 | 3.5 | 20.4 | 33.4 |

Table S3. Simultaneous PLSR statistical models obtained by calibration and cross-validation phase by pigments for corn, sugarcane, coffee, canola, wheat, and tobacco crops. Model goodness-of-fit (R^2), offset, root mean square error (RMSE), ratio of performance to deviation (RPD), and bias parameters from UV-VIS-NIR-SWIR hyperspectral data. Abbreviation for attributes were indicate material and methods sections.

| PLSR Models | Attributes | PLSR Parameters | | | | | |
|------------------|--------------------------------|-----------------|-------|--------|-------|-----|------|
| | | r | R^2 | Offset | RMSE | RPD | Bias |
| Calibration | Chla (mg m^{-2}) | 0.92 | 0.85 | 48.8 | 54.3 | 2.6 | – |
| | Chlb (mg m^{-2}) | 0.91 | 0.83 | 33.3 | 51.3 | 2.4 | – |
| | Chla+b (mg m^{-2}) | 0.90 | 0.81 | 97.7 | 111.7 | 2.3 | – |
| | Car (mg m^{-2}) | 0.93 | 0.87 | 16.0 | 18.2 | 2.7 | – |
| | AnC (nmol m^{-2}) | 0.93 | 0.87 | 0.1 | 0.2 | 2.8 | – |
| | Flv (nmol m^{-2}) | 0.92 | 0.84 | 11.6 | 10.5 | 2.5 | – |
| | Chla (mg g^{-1}) | 0.90 | 0.81 | 1.4 | 2.4 | 2.3 | – |
| | Chlb (mg g^{-1}) | 0.88 | 0.78 | 1.3 | 1.4 | 2.1 | – |
| | Chla+b (mg g^{-1}) | 0.88 | 0.77 | 2.6 | 3.6 | 2.1 | – |
| | Car (mg g^{-1}) | 0.89 | 0.79 | 0.5 | 0.8 | 2.2 | – |
| | AnC ($\mu\text{mol g}^{-1}$) | 0.94 | 0.89 | 0.0 | 0.1 | 3.0 | – |
| | Flv ($\mu\text{mol g}^{-1}$) | 0.89 | 0.80 | 2.4 | 1.7 | 2.2 | – |
| Cross-Validation | Chla (mg m^{-2}) | 0.92 | 0.85 | 50.3 | 56.8 | 2.5 | – |
| | Chlb (mg m^{-2}) | 0.90 | 0.82 | 34.8 | 54.2 | 2.3 | – |
| | Chla+b (mg m^{-2}) | 0.90 | 0.81 | 99.9 | 114.4 | 2.3 | – |
| | Car (mg m^{-2}) | 0.93 | 0.86 | 16.0 | 18.8 | 2.7 | – |
| | AnC (nmol m^{-2}) | 0.93 | 0.87 | 0.1 | 0.2 | 2.7 | – |
| | Flv (nmol m^{-2}) | 0.92 | 0.85 | 12.2 | 10.9 | 2.6 | – |
| | Chla (mg g^{-1}) | 0.88 | 0.78 | 1.6 | 2.5 | 2.1 | – |
| | Chlb (mg g^{-1}) | 0.88 | 0.78 | 1.4 | 1.5 | 2.1 | – |
| | Chla+b (mg g^{-1}) | 0.88 | 0.77 | 2.6 | 3.8 | 2.1 | – |
| | Car (mg g^{-1}) | 0.88 | 0.77 | 0.6 | 0.7 | 2.1 | – |
| | AnC ($\mu\text{mol g}^{-1}$) | 0.94 | 0.88 | 0.0 | 0.0 | 2.9 | – |
| | Flv ($\mu\text{mol g}^{-1}$) | 0.89 | 0.79 | 2.5 | 1.7 | 2.2 | – |

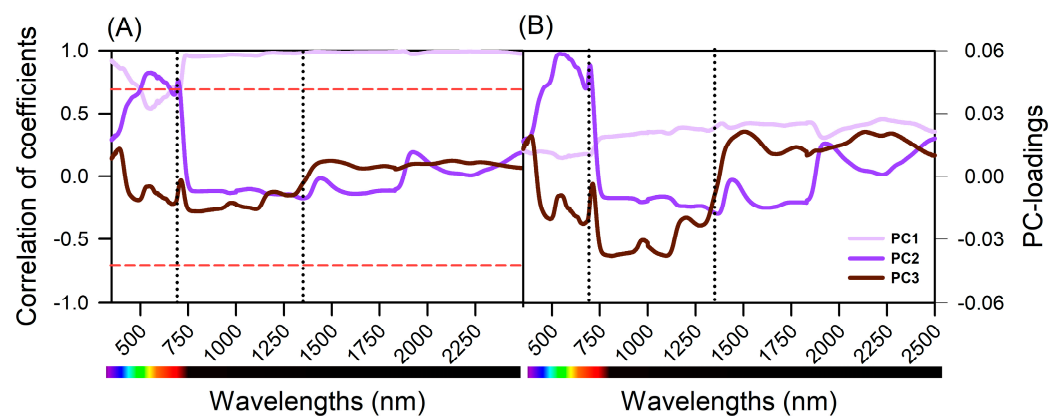


Figure S1. (A) Correlation coefficients and (B) PC loadings in the 350–2500 nm range, represented by light to dark purple lines for PC1, PC2, and PC3, respectively. The red line indicates the -0.70 to $+0.70$ correlation range, with dots marking the 700 and 1300 nm delimitations.

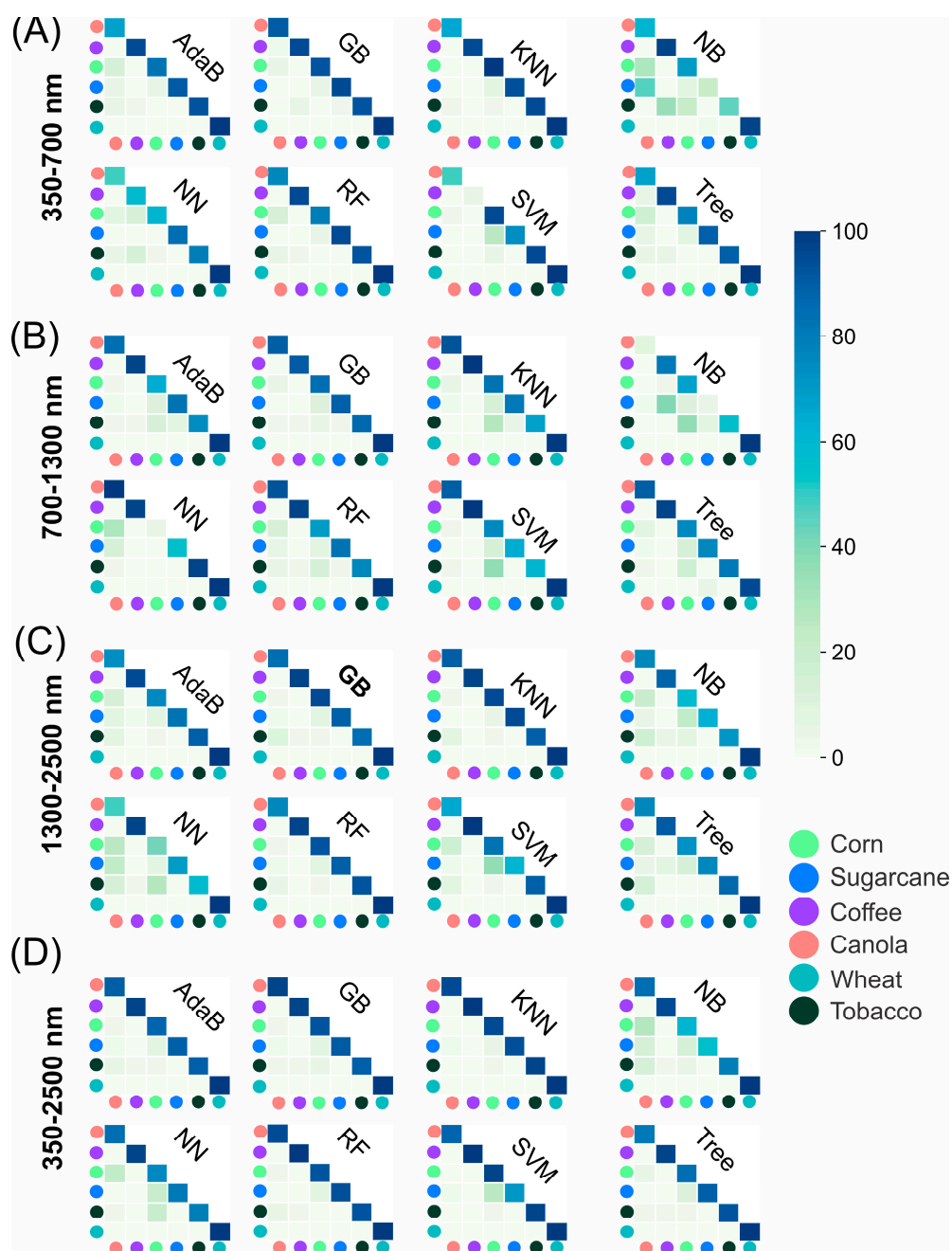


Figure S2. Matrix of correlation displayed accept and error frequency by model-based UV-VIS-NIR-SWIR comprising reflectance data to corn, sugarcane, coffee, canola, wheat, and tobacco plants. (A) 350–700 nm; (B) 700–1300 nm; (C) 1300–2500 nm; (D) 350–2500 nm. The correlation model test (frequency number) indicated a maximum simulation to correct classification-based independent data (scale 0 at 100; light green to dark blue). Abbreviation for models were indicate material and methods sections.

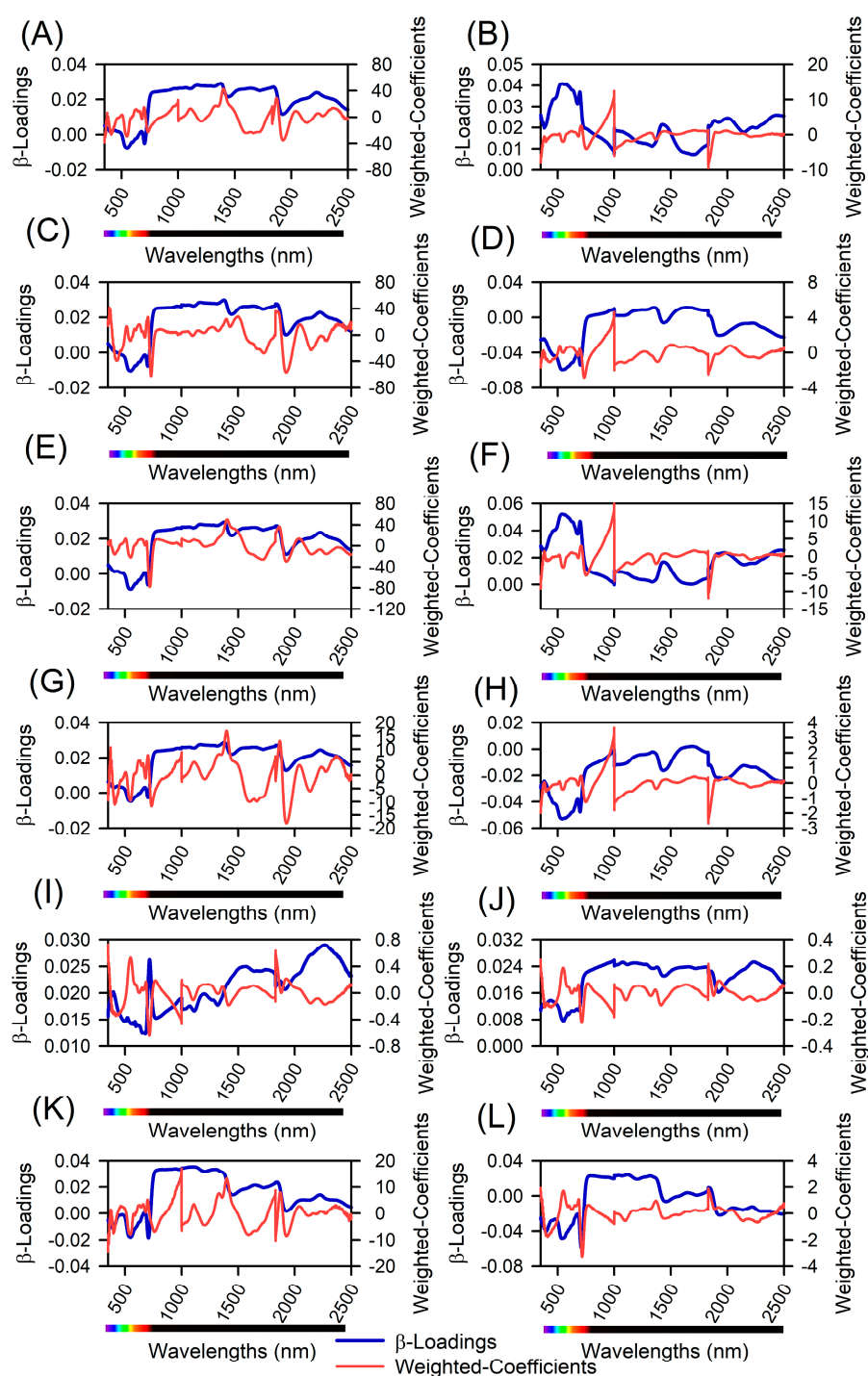


Figure S3. β -loadings and weighted-coefficients predicted PLSR method-based UV-VIS-NIR-SWIR hyperspectral data. (A) Chlorophyll *a* (Chl*a*; mg m⁻²); (B) Chlorophyll *b* (Chl*b*; mg m⁻²); (C) Chlorophyll *a+b* (Chl*a+b*; mg m⁻²); (D) Carotenoids (Car; mg m⁻²); (E) Anthocyanins (AnC; nmol cm⁻²); (F) Flavonoids (Flv; nmol cm⁻²); (G) Chlorophyll *a* (Chl*a*; mg g⁻¹); (H) Chlorophyll *b* (Chl*b*; mg g⁻¹); (I) Chlorophyll *a+b* (Chl*a+b*; mg g⁻¹); (J) Carotenoids (Car; mg g⁻¹); (K) Anthocyanins (AnC; μ mol g⁻¹); (L) Flavonoids (Flv; μ mol g⁻¹). Blue line (β -loadings) and red line (weighted-coefficients).

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