

Leaf optical properties reflect variation in photosynthetic metabolism and its sensitivity to temperature

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Supplementary File S1

Specific details of the PLSR models

Below we provide specific details of each PLSR model developed in this study in tables S1-S4. This information includes the wavelengths selected in each two-stage PLSR model and corresponding regression coefficient, as well as the PLSR intercept value. In addition, we provide the results for the 70/30% cross validation for each trait examined. This information can be used to derive estimates of each trait based on the summation of the reflectance values at each wavelength, multiplied by the corresponding regression coefficients, and the intercept value. For example, to estimate V_{cmax} you would sum up the following:

$$V_{\text{cmax}} = \left[\begin{array}{l} (\lambda_{495} \times 2512.75) + (\lambda_{610} \times -3804.89) + (\lambda_{680} \times -9121.73) + (\lambda_{695} \times 8114.26) \\ + (\lambda_{710} \times -1281.10) + (\lambda_{1510} \times 4284.40) + (\lambda_{1680} \times 6566.05) + (\lambda_{1755} \times -9975.12) \\ + (\lambda_{1890} \times -5262.65) + (\lambda_{1935} \times 8315.75) + (\lambda_{2210} \times 7361.03) + (\lambda_{2405} \times -14208.39) \\ + (\lambda_{2490} \times 7473.89) \end{array} \right] - 105.10$$

where λ_{xxx} is the reflectance value at the specific wavelength. The summation of this equation would yield an estimated V_{cmax} value based on the PLSR model and spectral reflectance data. This can be done for each trait.

Table S1. Summary of the leaf nitrogen PLSR model wavelengths, coefficients, and jackknife statistics.

Leaf Nitrogen (%)

Parameter	Raw PLSR Coefficient
Intercept	3.948
<i>Wavelength</i>	
505	40.754
540	-102.288
590	323.029
630	-330.755
855	32.992
1690	-160.508
1765	197.576
1850	-111.713
1925	195.835
1995	-186.626
2115	121.167
2470	-180.068
2485	167.950
Jackknife statistics:	
Median R2 = 0.77	
Median RMSE = 0.32 %	

Table S2. Summary of the leaf mass per area PLSR model wavelengths, regression coefficients, and jackknife statistics.

Leaf mass per area (g m⁻²)

Parameter	Raw PLSR Coefficient
Intercept	41.829
<i>Wavelength</i>	
545	338.112
705	-246.133
885	-323.844
895	-287.7889
955	-53.214
1245	363.228
1250	341.854
1255	340.478
1260	344.962
1420	-166.532
1425	-185.984
1595	-546.692
1600	-518.648
1870	611.304
1875	494.976
1905	-1043.208
2040	791.886
2275	-367.818
2280	-420.966
2285	-431.731
2305	-189.182
2400	901.906
Jackknife statistics:	
Median R ² = 0.89	
Median RMSE = 3.77 g m ⁻²	

Table S3. Summary of the V_{cmax} PLSR model wavelengths, regression coefficients, and jackknife statistics.

V_{cmax} ($\mu\text{mol m}^{-2} \text{s}^{-1}$)

Parameter	Raw PLSR Coefficient
Intercept	-105.105
<i>Wavelength</i>	
495	2512.749
610	-3804.889
680	-9121.729
695	8114.260
710	-1281.079
1510	4284.383
1680	6566.049
1755	-9975.176
1890	-5262.651
1935	8315.752
2210	7361.025
2405	-14208.388
2490	7473.886
Jackknife statistics:	
Median $R^2 = 0.78$	
Median RMSE = 16.2	

Table S4. Summary of the J_{\max} PLSR model wavelengths, regression coefficients, and jackknife statistics.

J_{\max} ($\mu\text{mol m}^{-2} \text{s}^{-1}$)

Parameter	Raw PLSR Coefficient
Intercept	-20.650
<i>Wavelength</i>	
465	-274.189
485	3984.520
535	5125.756
550	-5721.735
615	4191.832
635	1109.040
670	-10882.564
710	-428.916
1095	-4967.966
1215	6337.985
1390	5793.293
1415	-5534.300
1575	4536.632
1580	4826.890
1710	-1167.044
1715	-1833.546
1720	-1927.169
1725	-2214.091
1730	-2548.040
1740	-1763.486
1880	-2488.854
1885	-1480.018
1890	-239.556
1895	837.299
1910	3433.131
1935	2952.828
1940	2893.471
1955	2376.691
1985	-271.257
1990	-1181.458
1995	-733.476
2000	-2350.489
2005	-1752.527

2265	1241.956
2270	581.440
2275	1592.081
2280	2434.431
2290	296.427
2295	316.057
2300	-2038.929
2305	-969.998
2450	2103.843
2460	-6022.569
2500	2491.480

Jackknife statistics:

Median $R^2 = 0.77$

Median RMSE = 20.1
