

***New Phytologist* Supporting Information**

Article title: From the Arctic to the tropics: multi-biome prediction of leaf mass per area using leaf reflectance

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The following Supporting Information is available for this article:

Fig. S1 Comparison of the leaf mass per area (LMA) distribution in this article versus that found within the TRY global trait database (Kattge et al. 2011)

Fig. S2 Histogram distributions of the untransformed leaf mass per area (LMA) calibration and validation datasets used for model development and testing

Fig. S3 The coefficient of variation of the measured leaf mass per area (LMA) across the four main biomes included in this research

Fig. S4 The patterns of leaf reflectance across the four main biomes

Fig. S5 The relationship between leaf mass area (LMA) calculated from measured leaf area and dry mass and spectral reflectance within our model development dataset

Fig. S6 Model calibration and validation results for the leaf mass area (LMA) partial least squares regression (PLSR) model.

Fig. S7 Partial least squares regression (PLSR) model fit by biome.

Fig. S8 Combined calibration and validation partial least-squares regression (PLSR) model residuals by canopy position.

Fig. S9 Combined calibration and validation partial least-squares regression (PLSR) model residuals by leaf age.

Fig. S10 Evaluation of the leaf mass area (LMA) partial least squares regression (PLSR) model using the LOPEX and ANGERS foundational datasets (Hosgood et al., 1994; Jacquemoud et al., 2003; Feret et al., 2008).

Fig. S11 External validation of the leaf mass area (LMA) partial least squares regression (PLSR) model using data collected from NEON (National Ecological Observatory Network) sites.

Methods S1. An example R script illustrating the use of the multi-biome PLSR model to estimate leaf mass per area for LOPEX and Angers datasets, which are provided through the EcoSIS spectral library. Results of running the script are shown in Figure S10.

Table S1 Leaf spectra and LMA data sources.

Figure S1. Histogram of the full model development (combined calibration and validation data) leaf mass per area (LMA) dataset (top). Bottom: Comparison of the density of the distributions of LMA in this study to build and validate our spectra-trait model with the TRY global trait database (Kattge *et al.*, 2011). Note – the data range of the density plot was clipped to 400 g m^{-2} for display purposes since values in TRY can range up to 3007 g m^{-2} , though these extreme values are rare.

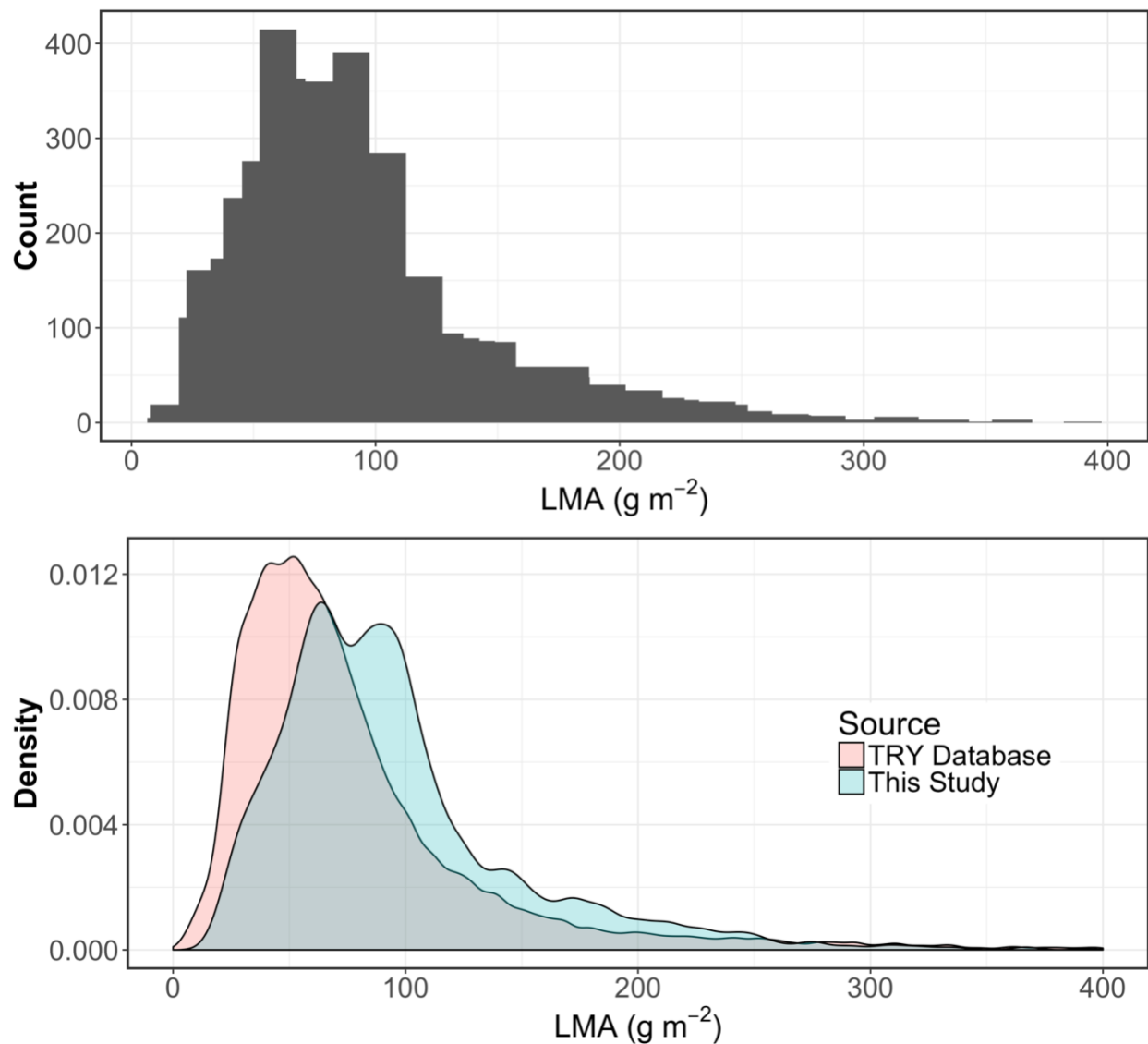


Figure S2. The untransformed distribution of calibration (top) and validation (bottom) samples used in the training (cal) and testing (val) of our LMA PLSR model. We split our original dataset (2,478 samples) into these different datasets (1,978 for calibration and 500 for validation) to train the model and ensure that both calibration and validation distributions covered a similar range of the full dataset.

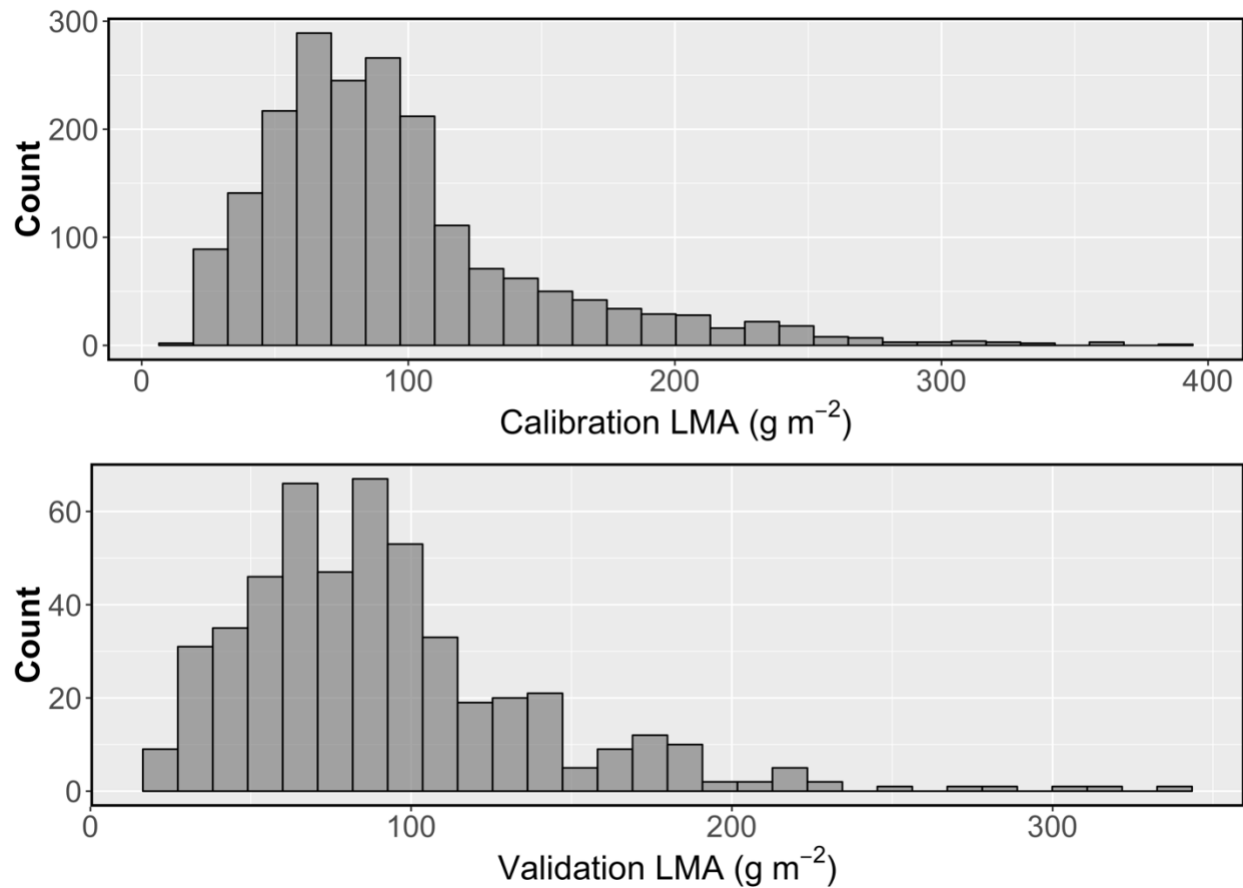


Figure S3. The coefficient of variation for leaf mass area (LMA) in the model development dataset calculated from measured leaf area and dry mass for the four biomes included in this study (boreal/temperate, $n= 935$, mean \pm S.D. 96 ± 62 gDW m^{-2} ; tropical, $n= 832$ 99 ± 38 gDW m^{-2} ; Mediterranean, $n= 102$ 160 ± 104 gDW m^{-2} ; Arctic, $n= 609$ 77 ± 20 gDW m^{-2}).

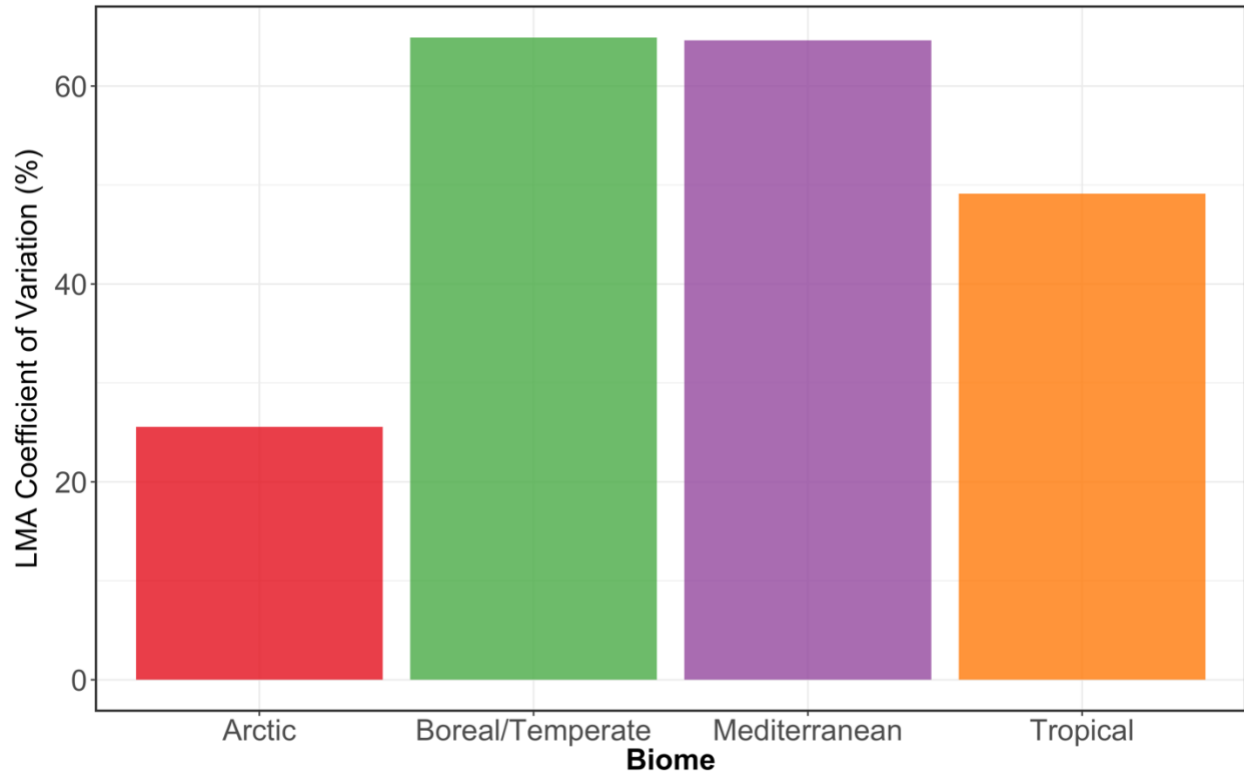


Figure S4. Leaf spectral reflectance patterns across each biome using the model development dataset (panel A, Arctic; panel B, boreal/temperate; panel C, Mediterranean; panel D, tropical). The type of instrumentation that was used to collect the data in each biome is provided in the top right section of the panels. Solid lines show mean values, the green shaded area is the 95% confidence interval of the data, and minimum and maximum values are indicated by dotted lines.

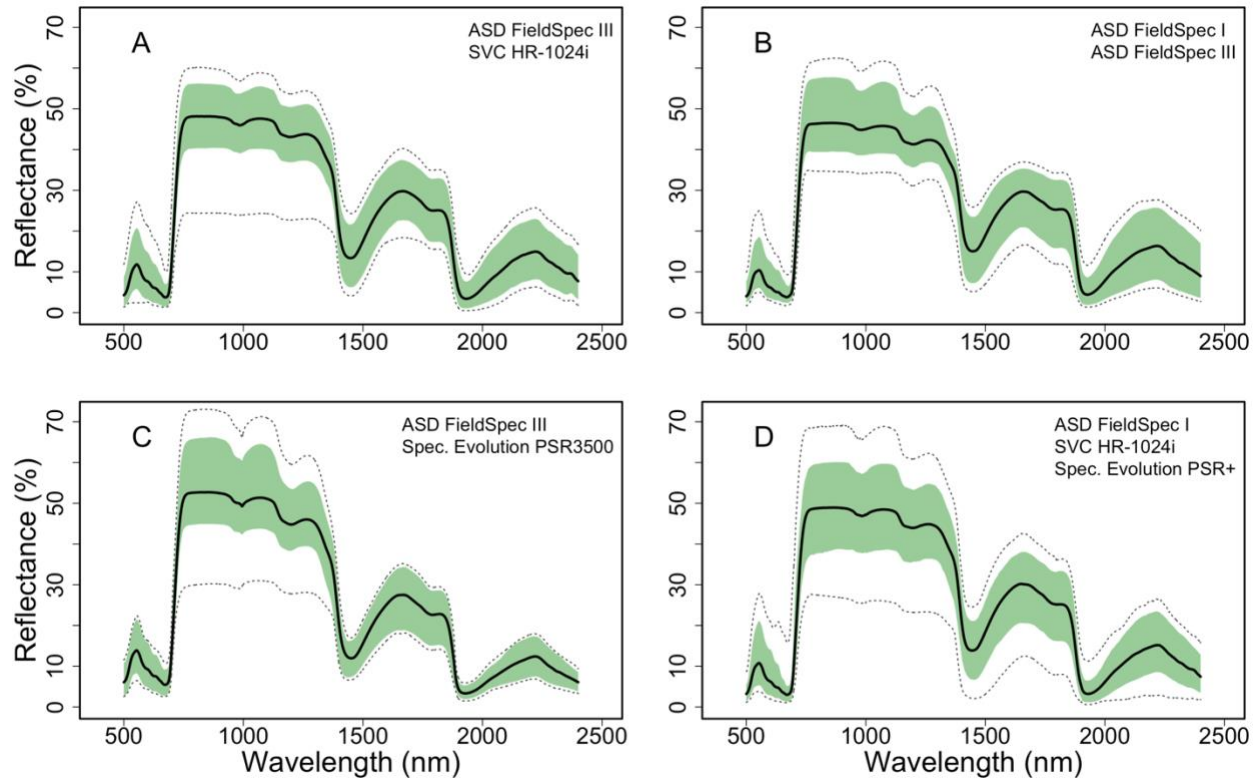


Figure S5. The relationship between leaf mass area (LMA) calculated from measured leaf area and dry mass and spectral reflectance within our model development dataset for different regions of the visible (550nm, panel A; 650nm, panel B), red-edge (750nm, panel C), NIR (800nm, panel D) and SWIR (1800nm, panel E; 2200nm, panel F).

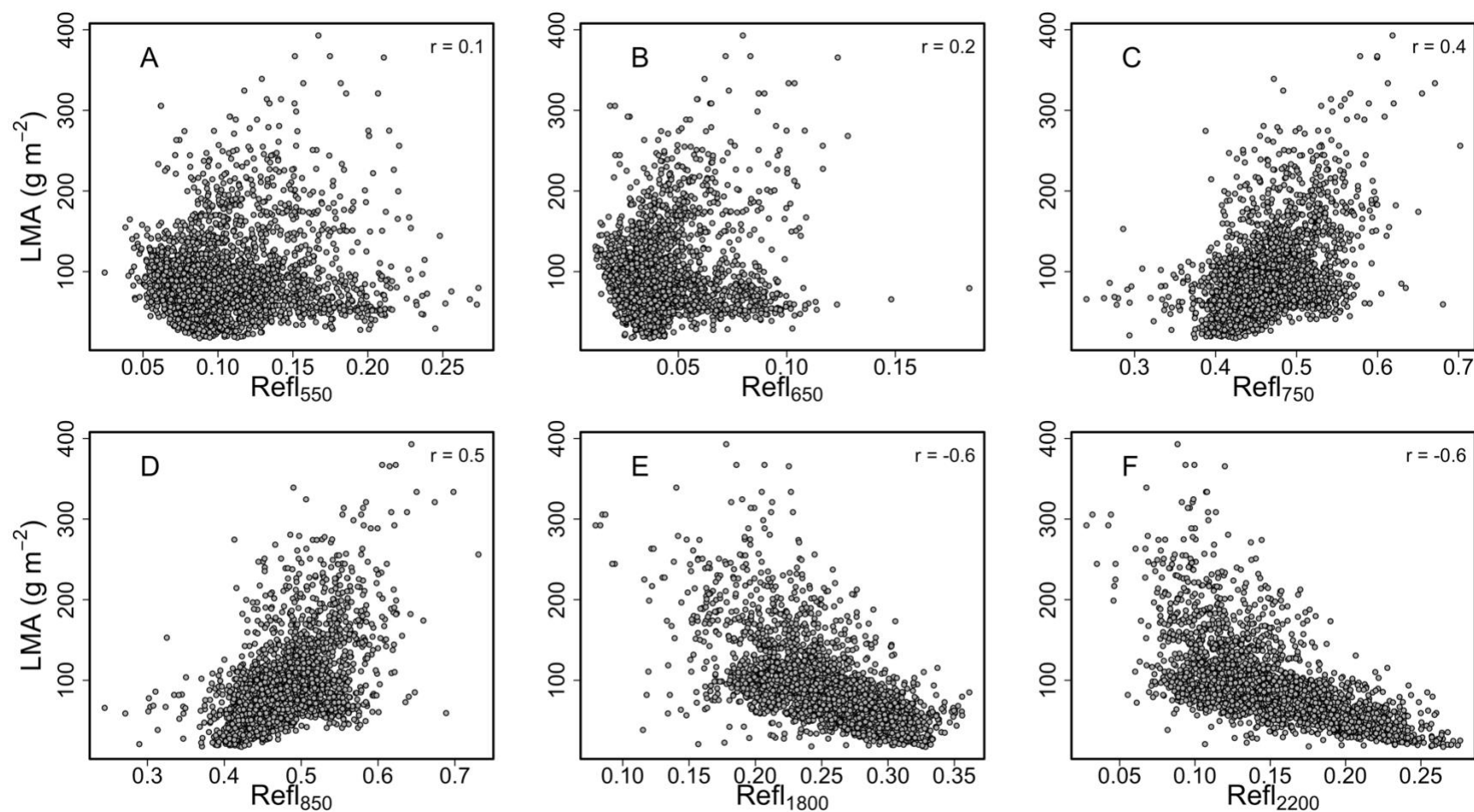


Figure S6. Calibration (panels A,C & E, n=1978) and validation (panels B,D & F, n=500) results for the spectra-leaf mass area (LMA) partial least squares regression (PLSR) model using the model development dataset. Panels A and B show the regression of observed LMA calculated from measured leaf area and dry mass versus the LMA predicted from the spectral model for the calibration data set (panel A) and the validation dataset (panel B). Statistics in panels A and B show the R^2 for the cross validation (panel A) and validation (panel B), the root mean square error (RMSE) and the average residual bias (Bias) of the regression. The 1:1 line is shown as a broken line. Panels C (calibration) and D (validation) show the residuals. Panels E and F show the frequency distribution for residuals of the predicted LMA.

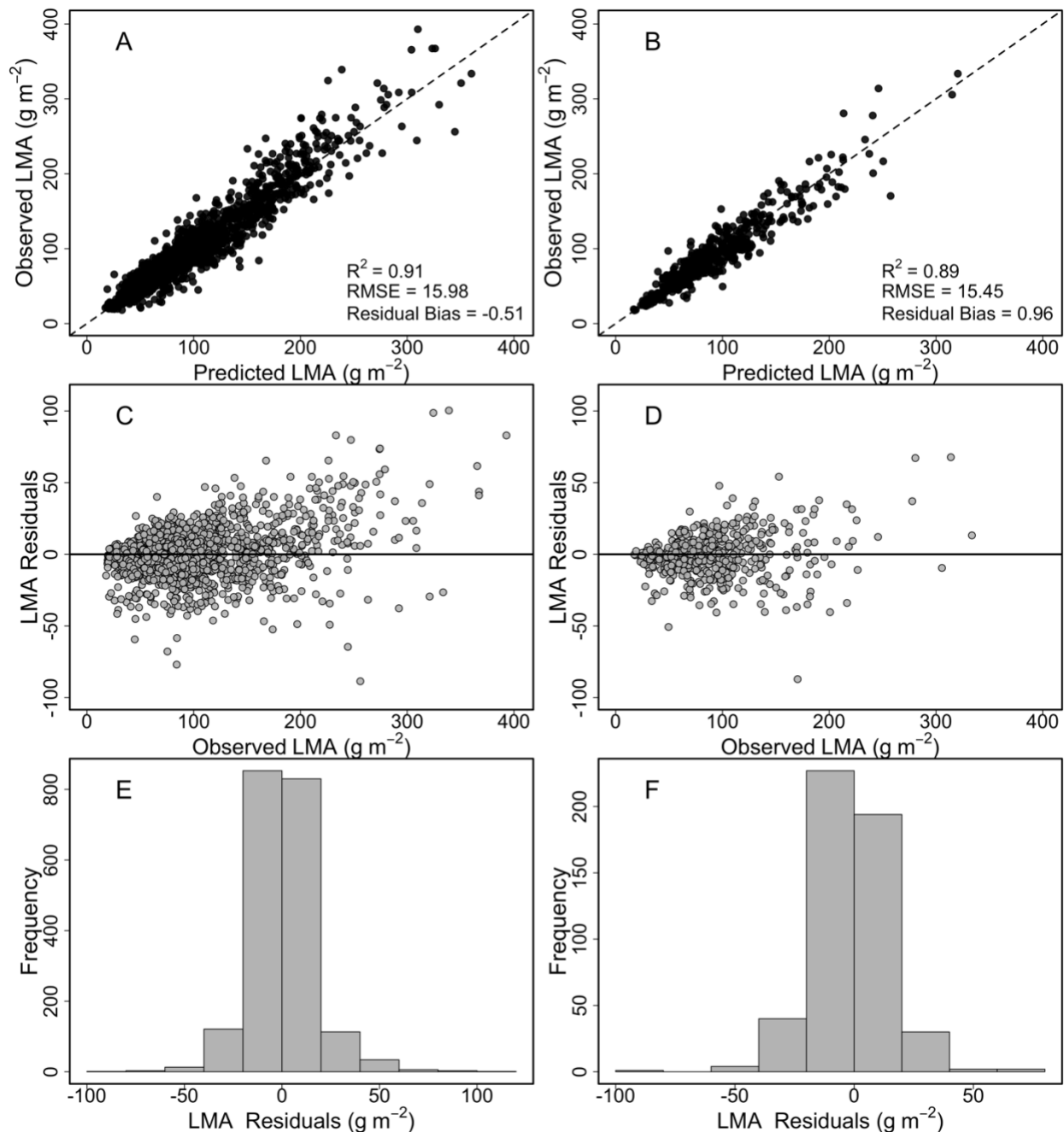


Figure S7. PLSR model fit by biome within the model development dataset. A- Arctic, B- Boreal/Temperate, C-Mediterranean, D-Tropical and Biosphere2. Black dots are calibration and grey are validation data points, respectively. Grey dot error bars are the 95% CI values for the predicted validation data points based on the PLSR model uncertainty analysis.

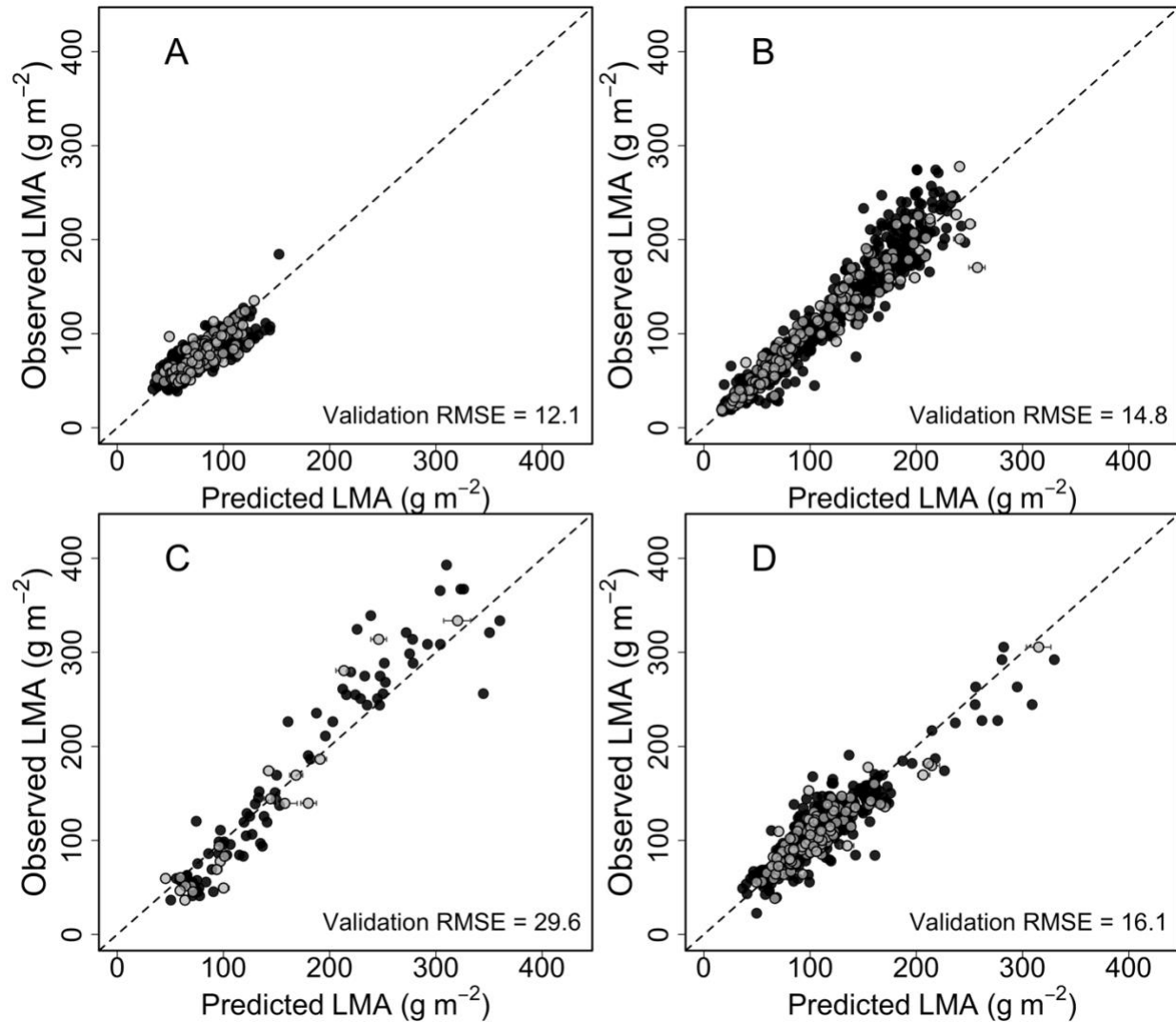


Figure S8. Combined calibration and validation PLSR model residuals by canopy position from shaded, bottom canopy leaves (Bot), mid-canopy (Mid), and top of canopy, fully sunlit foliage (Top).

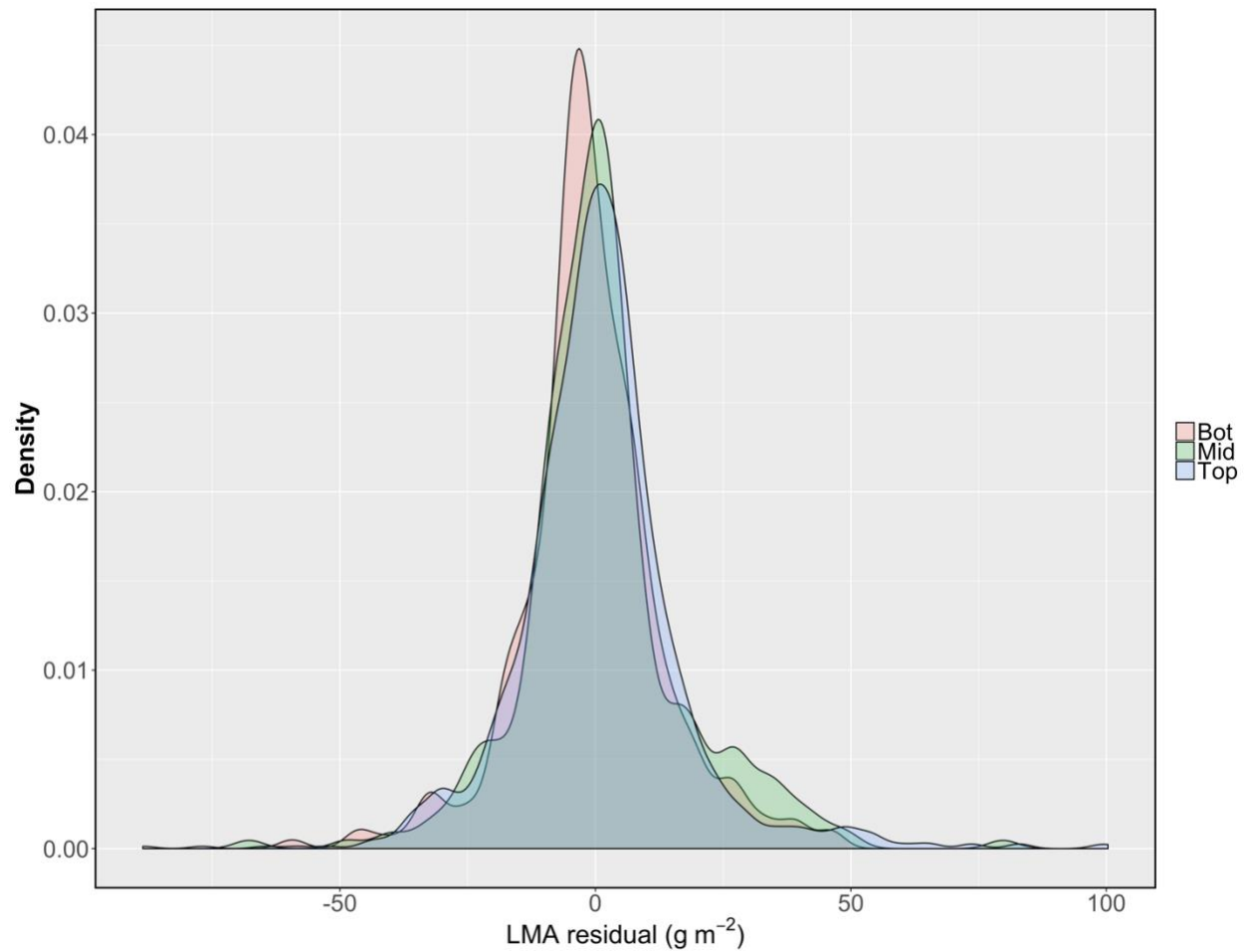


Figure S9. Combined calibration and validation PLSR model residuals by leaf age. Young represents expanding leaves or fully-expanded, current year cohorts for needle-leaf evergreen species, mature is the previous year's foliage for evergreen species and old represents leaves greater than one year old or senescent for evergreen broadleaf species, or needles greater than two years old for evergreen needle-leaf species. Broadleaf deciduous species are not included here. There were 1881 young leaves, 243 mature leaves, and 353 old leaves in the combined calibration and validation datasets.

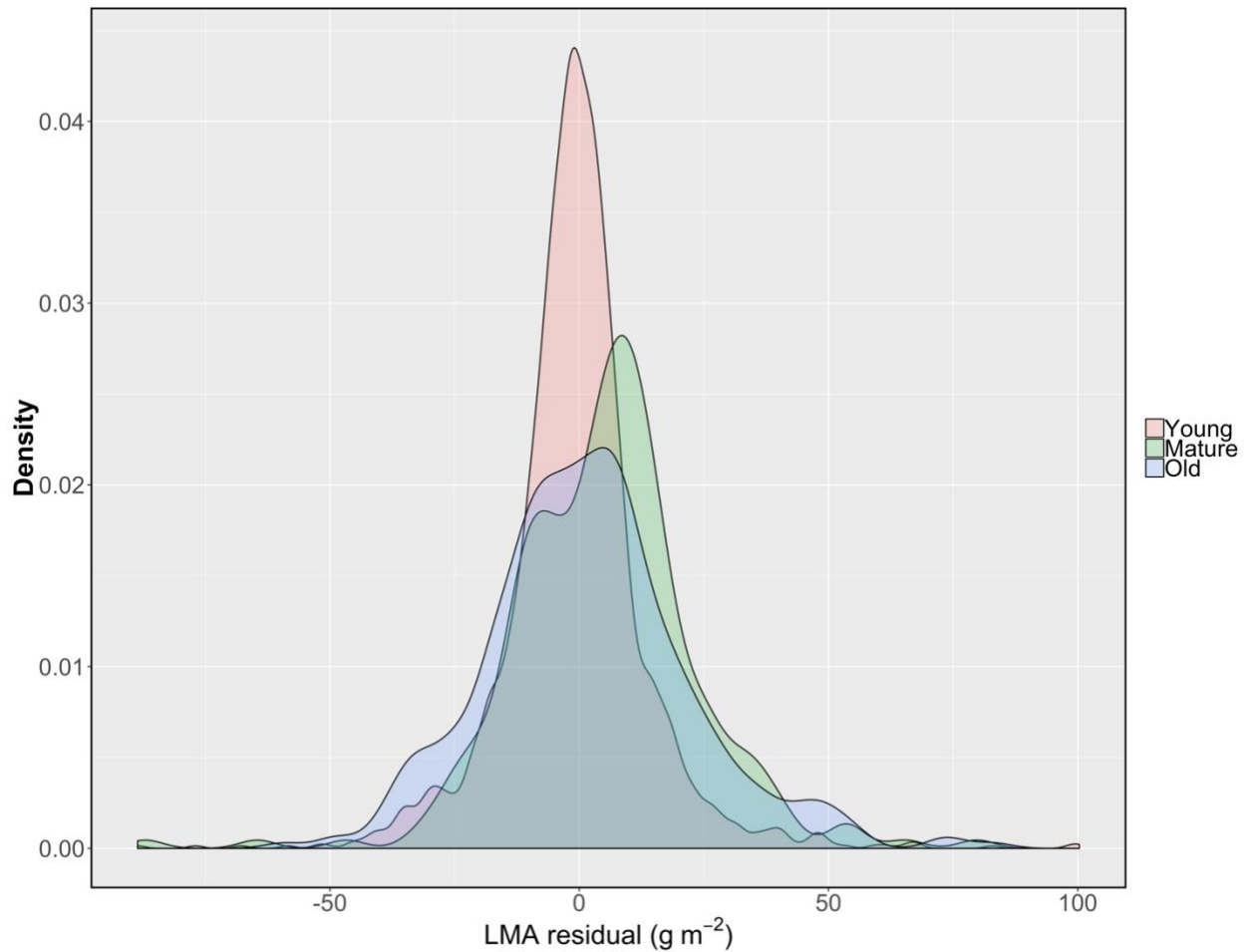
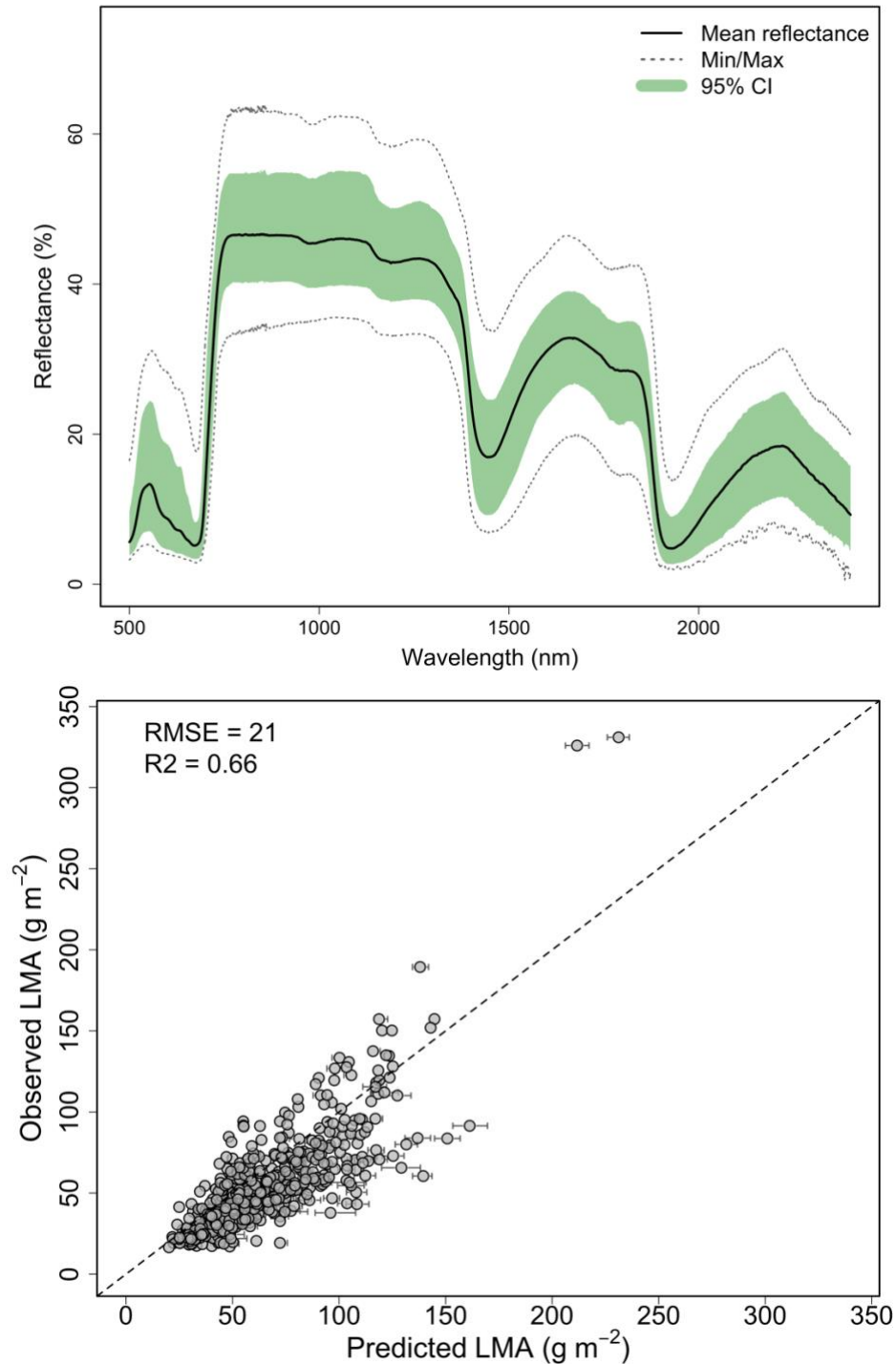


Figure S10. Top: leaf spectral reflectance extracted from the EcoSIS database (<https://ecosis.org>) for the LOPEX and ANGERS foundational spectra and leaf trait datasets (Hosgood *et al.*, 1994; Jacquemoud *et al.*, 2003; Feret *et al.*, 2008). Bottom: The results of applying our new global PLSR LMA model to the LOPEX and ANGERS spectra (predicted) and validation using the provided direct measurements of LMA (observed). A script to replicate these results is provided in a separate file (nph16123-sup-0002-MethodsS1.R).



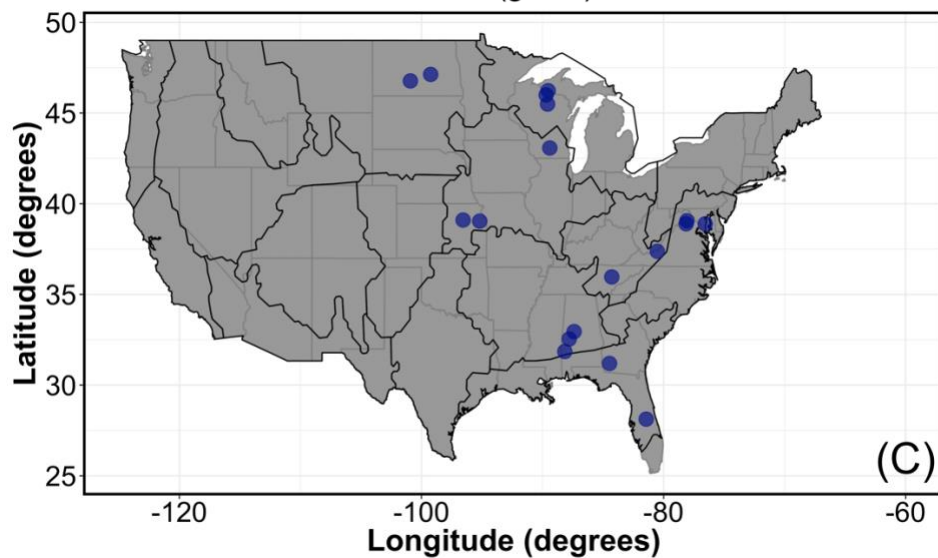
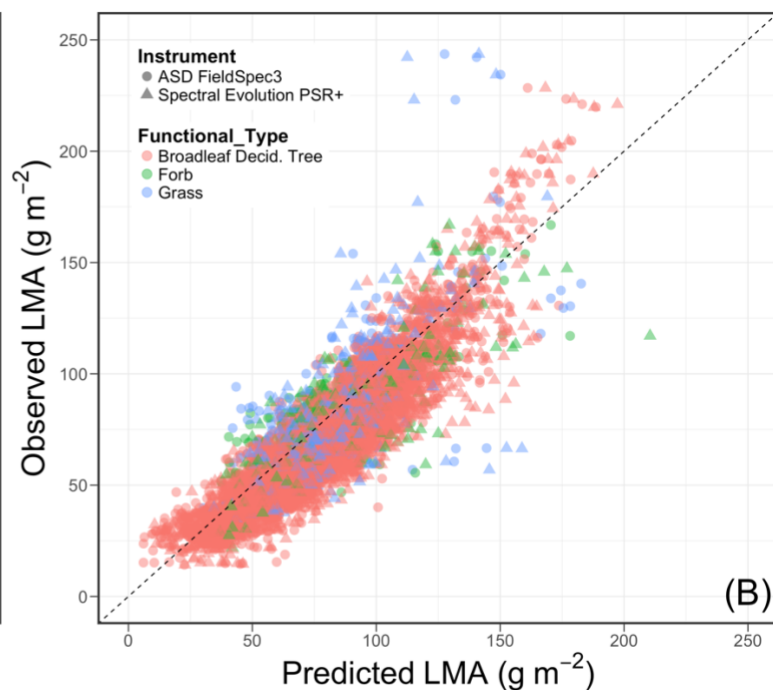
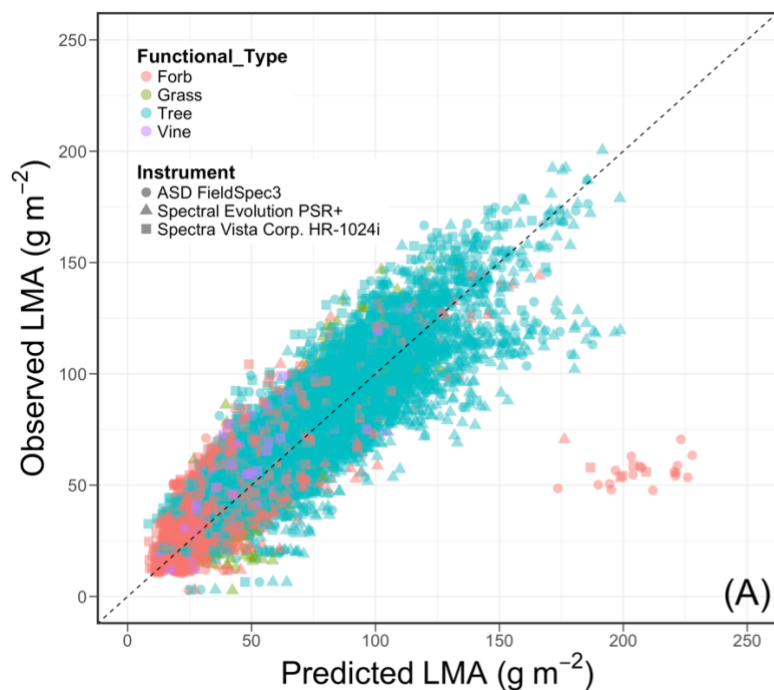


Figure S11. External validation of our global spectra-trait PLSR LMA model (A & B) using data collected from a range of NEON (National Ecological Observatory Network) sites representing seven NEON domains (C). Data were collected during the 2017 growing season, between the beginning of June to the end of September and represents tree, grass, forb, and vine vegetation functional types. Estimated LMA from the Madison and UNDERC, WI sites (A) had an RMSE of 16.1 while that from the remaining NEON sites (B) had an RMSE of 12.5 g m^{-2} , across species, sites, and instrumentation.

Methods S1. An example R script illustrating the use of the multi-biome PLSR model to estimate leaf mass per area for LOPEX and Angers datasets, which are provided through the EcoSIS spectral library. Results of running the script are shown in Figure S10.

Table S1. Leaf spectra and LMA data sources.

Biome	Dataset	Source	References
Arctic	Leaf Mass Area, Leaf Carbon and Nitrogen Content, Barrow, Alaska, 2012-2016	https://dx.doi.org/10.5440/1336812	Rogers <i>et al.</i> (2017)
	Leaf Spectral Reflectance, Barrow, Alaska 2013	https://doi.org/10.5440/1441203	Serbin <i>et al.</i> (2018b)
	NGEE Arctic Leaf Spectral Reflectance and Transmittance, Barrow, Alaska, 2014-2016	https://dx.doi.org/10.5440/1437044	Serbin <i>et al.</i> (2019a)
	Leaf Mass Area, Leaf Carbon and Nitrogen Content, Kougarok Road and Teller Road, Seward Peninsula, Alaska, 2016	https://dx.doi.org/10.5440/1430080	Rogers <i>et al.</i> (2016)
	NGEE Arctic Leaf Spectral Reflectance, Kougarok Road, Seward Peninsula, Alaska, 2016	https://dx.doi.org/10.5440/1430079	Serbin and Rogers (2019)
Boreal / Temperate	Fresh Leaf Spectra to Estimate Leaf Morphology and Biochemistry for Northern Temperate Forests	https://ecosis.org/#result/4a63d7ed-4c1e-40a7-8c88-ea0deea10072	Serbin (2012); (Serbin <i>et al.</i> , 2014)
Mediterranean	NASA HyspIRI Airborne Campaign Leaf and Canopy Spectra and Leaf Traits	https://ecosis.org/#result/dd94f09c-1794-44f4-82e9-a7ca707a1ec0	Serbin <i>et al.</i> (2015)
Temperate	Fresh leaf spectra and leaf mass per area (LMA) data collected from temperate trees, grasses, forbs, and vine species. Sites include NEON locations	http://ecosis.org/#result/7433af7d-fbbd-4617-8df4-4d892f0d4357	Chlus <i>et al.</i> , unpublished data,
		https://doi.org/doi:10.21232/9831-rq60	Wang <i>et al.</i> , unpublished data
Tropical	Leaf spectral reflectance of tropical plants growing in Biosphere 2	https://ecosis.org/#result/a0a81b5a-b808-479f-a910-687d95acb9ad	Wu <i>et al.</i> , unpublished data

Leaf Mass Area (LMA) and water content, March 2017, Puerto Rico	http://dx.doi.org/10.15486/ngt/1495202	Serbin <i>et al.</i> (2019b)
Puerto Rico leaf spectral reflectance (NGEE-Tropics), 2017	http://dx.doi.org/10.15486/ngt/1495204	Serbin <i>et al.</i> (2019c)
Leaf mass area, Feb2016-May2016, PA-SLZ, PA-PNM, PA-BCI: Panama	http://dx.doi.org/10.15486/ngt/1411973	Ely <i>et al.</i> (2018)
Leaf mass per area, by age, Feb2017, PA-SLZ: Panama	http://dx.doi.org/10.15486/ngt/1478532	Rogers <i>et al.</i> (2018)
Leaf spectra, Feb2016-April2016, PA-SLZ, PA-PNM, PA-BCI: Panama	http://dx.doi.org/10.15486/ngt/1478523	Serbin <i>et al.</i> (2018a)
Leaf spectra by leaf age, Feb2017, PA-SLZ: Panama	http://dx.doi.org/10.15486/ngt/1475180	Serbin <i>et al.</i> (2018c)
Tapajos, Brazil (Fluxnet BR-Sa1)	https://ecosis.org/#result/fa9163f1-425b-4890-b343-f07f63e37bc3	Wu <i>et al.</i> (2017)

References

- Ely K, Rogers A, Serbin SP, Wu J, Wolfe B, Dickman T, Collins A, Detto M, Grossiord C, McDowell N, et al. 2018. Leaf mass area, Feb2016-May2016, PA-SLZ, PA-PNM, PA-BCI: Panama. *NGEE Tropics Data Collection*.
- Feret JB, Francois C, Asner GP, Gitelson AA, Martin RE, Bidel LPR, Ustin SL, le Maire G, Jacquemoud S. 2008. PROSPECT-4 and 5: Advances in the leaf optical properties model separating photosynthetic pigments. *Remote Sensing of Environment* **112**(6): 3030-3043.
- Hosgood B, Jacquemoud S, Andreoli G, Verdebout J, Pedrini G, Schmuck G. 1994. Leaf Optical Properties EXperiment 93 (LOPEX93). Ispra, Italy: European Commission — Joint Research Centre.
- Jacquemoud S, Bidel L, Francois C, Pavan G 2003. ANGERS Leaf Optical Properties Database. <http://opticleaf.ipgp.fr/index.php?page=database>: OPTICLEAF.
- Kattge J, Díaz S, Lavorel S, Prentice IC, Leadley P, Bönsch G, Garnier E, Westoby M, Reich PB, Wright IJ, et al. 2011. TRY – a global database of plant traits. *Global Change Biology* **17**(9): 2905-2935.
- Rogers A, Ely K, Serbin SP, Wu J, Kinlock N 2018. Leaf mass per area, by age, Feb2017, PA-SLZ: Panama. *NGEE Tropics Data Collection*.
- Rogers A, Serbin SP, Ely K 2016. Leaf Mass Area, Leaf Carbon and Nitrogen Content, Kougark Road and Teller Road, Seward Peninsula, Alaska, 2016. *Next Generation Ecosystem Experiments Arctic Data Collection*. Oak Ridge National Laboratory: U.S. Department of Energy, Oak Ridge, Tennessee, USA.
- Rogers A, Serbin SP, Ely KS, Sloan VL, Wullschleger SD. 2017. Terrestrial biosphere models underestimate photosynthetic capacity and CO₂ assimilation in the Arctic. *New Phytologist* **216**(4): 1090-1103.
- Serbin SP. 2012. *Spectroscopic determination of leaf nutritional, morphological, and metabolic traits*. Ph.D. Forestry Ph.D. Dissertation, University of Wisconsin - Madison Madison, Wisconsin.
- Serbin SP, Ely K, Rogers A, Dickman T, Detto M, Wu J, Wolfe B, McDowell N, Grossiord C, Michaletz ST, et al. 2018a. Leaf spectra, Feb2016-April2016, PA-SLZ, PA-PNM, PA-BCI: Panama. *NGEE Tropics Data Collection*.
- Serbin SP, Lieberman-Cribbin W, Ely K, Rogers A 2019a. NGEE Arctic Leaf Spectral Reflectance and Transmittance, Barrow, Alaska, 2014-2016. *Next Generation Ecosystem Experiments Arctic Data Collection*. U.S. Department of Energy, Oak Ridge, Tennessee, USA.
- Serbin SP, Meng R, Wu J, Ely K 2019b. G-LiHT Campaign Leaf Mass Area and Water Content, Mar2017: Puerto Rico. *NGEE Tropics Data Collection*.
- Serbin SP, Meng R, Wu J, Ely K 2019c. G-LiHT Campaign Leaf Spectral Reflectance and Transmittance, Mar2017: Puerto Rico. *NGEE Tropics Data Collection*.
- Serbin SP, Rogers A 2019. NGEE Arctic Leaf Spectral Reflectance, Kougark Road, Seward Peninsula, Alaska, 2016. *Next Generation Ecosystem Experiments Arctic Data Collection*: U.S. Department of Energy, Oak Ridge, Tennessee, USA.
- Serbin SP, Rogers A, Liebig J 2018b. NGEE Arctic Leaf Spectral Reflectance, Barrow, Alaska 2013. *Next Generation Ecosystem Experiments Arctic Data Collection*. Oak Ridge National Laboratory.

- Serbin SP, Singh A, Desai AR, Dubois SG, Jablonski AD, Kingdon CC, Kruger EL, Townsend PA. 2015.** Remotely estimating photosynthetic capacity, and its response to temperature, in vegetation canopies using imaging spectroscopy. *Remote Sensing of Environment* **167**: 78-87.
- Serbin SP, Singh A, McNeil BE, Kingdon CC, Townsend PA. 2014.** Spectroscopic determination of leaf morphological and biochemical traits for northern temperate and boreal tree species. *Ecological Applications* **24**(7): 1651-1669.
- Serbin SP, Wu J, Ely K 2018c.** Leaf spectra by leaf age, Feb2017, PA-SLZ: Panama. *NGEE Tropics Data Collection*.
- Wu J, Chavana - Bryant C, Prohaska N, Serbin SP, Guan K, Albert LP, Yang X, Leeuwen WJD, Garnello AJ, Martins G, et al. 2017.** Convergence in relationships between leaf traits, spectra and age across diverse canopy environments and two contrasting tropical forests. *New Phytologist* **214**(3): 1033-1048.