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Plant spectral diversity integrates functional and phylogenetic components of biodiversity and predicts ecosystem function

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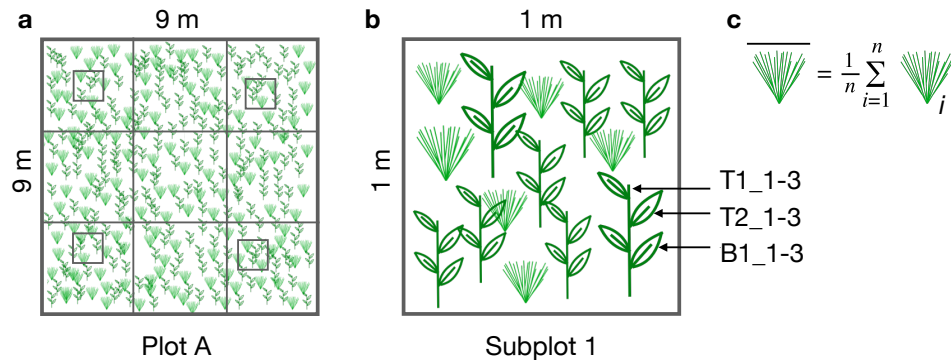
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Supplementary Methods

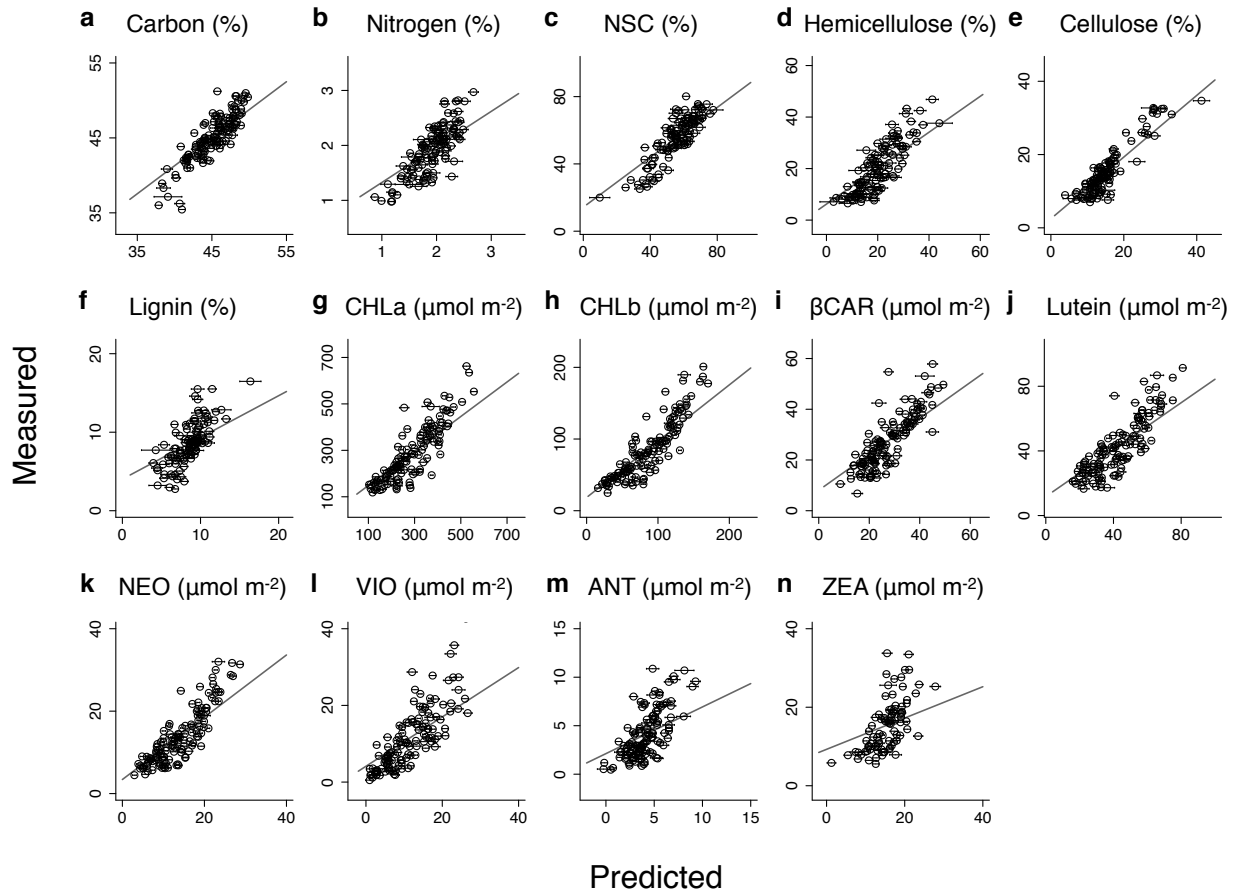
Phylogenetic signal

We estimated the phylogenetic signal of each spectral band using Blomberg's K^1 statistic as implemented in picante 1.6-22 in R³. Significance was tested by comparing the observed K value to the distribution of the K statistics estimated from both a white noise and a Brownian motion null model. If observed K values are not different ($P < 0.05$) from the random expectation (white noise null model), they can be considered labile. If observed K values are not different ($P < 0.05$) from the Brownian motion null model, they can be considered phylogenetically conserved. We estimated the Brownian motion null model based on 1,000 simulations of Brownian motion evolution and the white noise model by randomly permuting the reflectance values per band across the tips of the phylogeny 1,000 times.

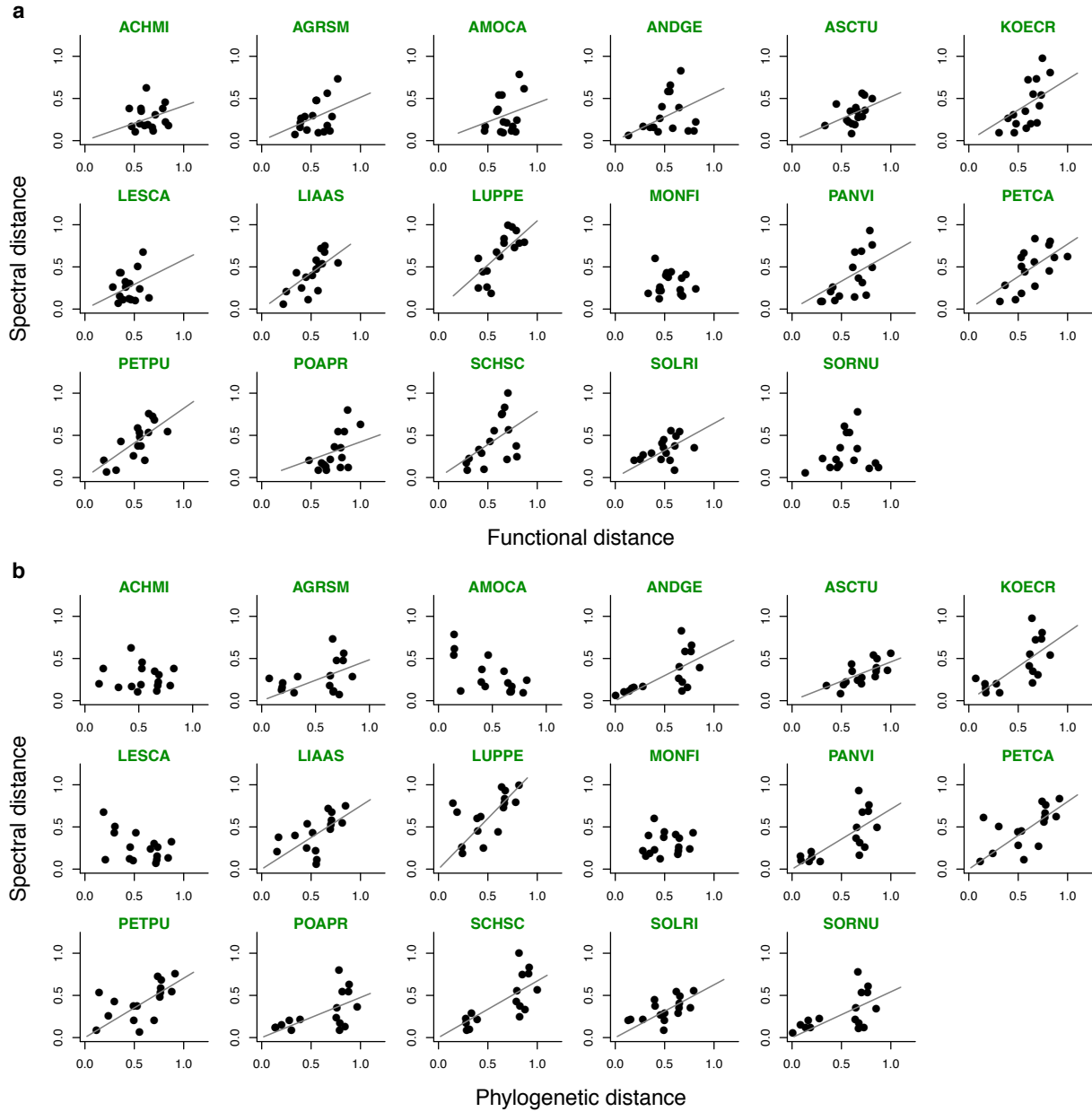
Supplementary Figures



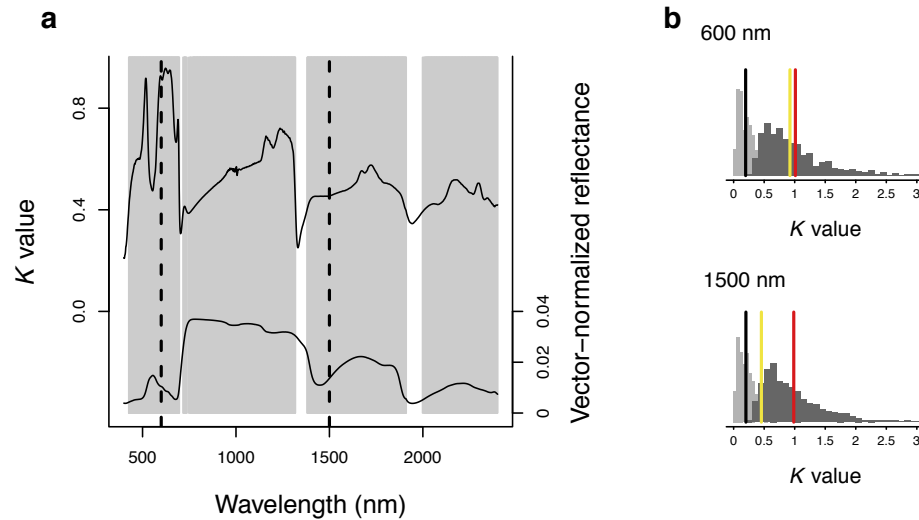
Supplementary Figure 1 | Sampling design and calculation of species mean spectra. a, In example plot A, two species, one forb and one grass species, are equally abundant. We collected spectral data in 4 to 8 1 m x 1 m subplots, depending on the number of species planted per plot. In monocultures and bicultures, we sampled the 4 corner subplots; in plots with 4 planted species, we sampled the 4 corner subplots and 2 additional outer subplots; in plots with 8 or 16 planted species, we sampled all 8 outer subplots. Within each subplot, we placed a 1 m x 1 m grid at random locations at least 50 cm away from the plot edges. **b,** We sampled a total of 4 individuals per subplot; the species were selected according to their abundance per plot. We selected the individuals per species at random and measured multiple individuals per species when the number of species per subplot was fewer than 4. For example, in each subplot of plot A we selected two individuals of the grass species and two individuals of the forb species. Depending on plant height, we measured either three (individuals < 30 cm in height) or five (individuals \geq 30 cm in height) leaves per individual. For individual 1 in plot A we measured three leaves, two from the top (T1, T2) and one from the bottom canopy layer (B1); we took three measurements per leaf (e.g., T1_1-3). **c,** Species' mean spectra are averaged spectra per species across plots.



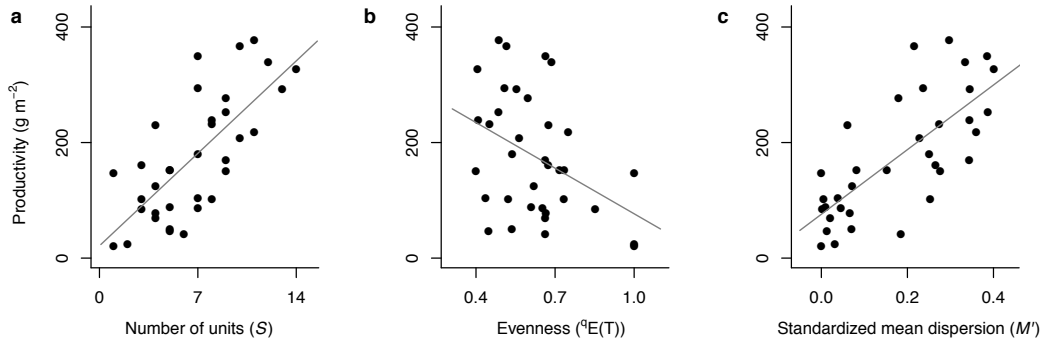
Supplementary Figure 2 | Partial least square regression models predicting 14 foliar traits from spectra. The lines in each panel indicate the mean fit of linear regression models between results from chemical assays and predicted values for **a**, carbon ($n = 127$, $r^2 = 0.75$, $b = 0.75$, $t_{125} = 19.48$, $P < 0.001$), **b**, nitrogen ($n = 119$, $r^2 = 0.65$, $b = 0.65$, $t_{117} = 14.77$, $P < 0.001$), **c**, non-structural carbohydrates (NSC, $n = 114$, $r^2 = 0.74$, $b = 0.74$, $t_{112} = 18.00$, $P < 0.001$), **d**, hemicellulose ($n = 113$, $r^2 = 0.71$, $b = 0.70$, $t_{111} = 16.35$, $P < 0.001$), **e**, cellulose ($n = 113$, $r^2 = 0.84$, $b = 0.84$, $t_{111} = 24.26$, $P < 0.001$) and **f**, lignin ($n = 112$, $r^2 = 0.53$, $b = 0.53$, $t_{110} = 11.22$, $P < 0.001$) concentration (%), **g**, chlorophyll a (CHLa, $n = 121$, $r^2 = 0.75$, $b = 0.74$, $t_{119} = 18.70$, $P < 0.001$), **h**, chlorophyll b (CHLb, $n = 124$, $r^2 = 0.79$, $b = 0.79$, $t_{122} = 21.24$, $P < 0.001$), **i**, β -carotene (β CAR, $n = 122$, $r^2 = 0.71$, $b = 0.71$, $t_{120} = 17.23$, $P < 0.001$), **j**, lutein ($n = 121$, $r^2 = 0.73$, $b = 0.73$, $t_{119} = 17.94$, $P < 0.001$), **k**, neoxanthin (NEO, $n = 125$, $r^2 = 0.76$, $b = 0.76$, $t_{123} = 19.60$, $P < 0.001$), **l**, violaxanthin (VIO, $n = 124$, $r^2 = 0.64$, $b = 0.64$, $t_{122} = 14.86$, $P < 0.001$), **m**, antheraxanthin (ANT, $n = 122$, $r^2 = 0.48$, $b = 0.48$, $t_{120} = 10.57$, $P < 0.001$) and **n**, zeaxanthin (ZEA, $n = 86$, $r^2 = 0.40$, $b = 0.40$, $t_{84} = 7.45$, $P < 0.001$) content ($\mu\text{mol m}^{-2}$). Whiskers indicate ± 1 standard deviation from the mean predicted value (circles). For model statistics, see Supplementary Table 1.



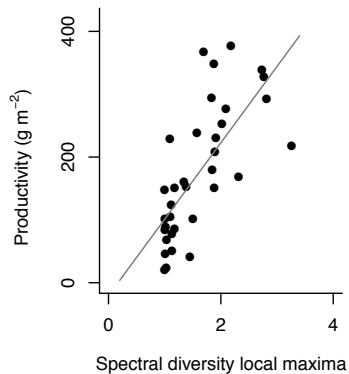
Supplementary Figure 3 | Spectral distance among species pairs increased with functional and phylogenetic distance for most focal species. Lines indicate the fitted linear regression models of a, functional and b, phylogenetic distance predicting spectral distance for individual 17 focal species paired with all other species. For species codes and statistics, see Supplementary Table 2.



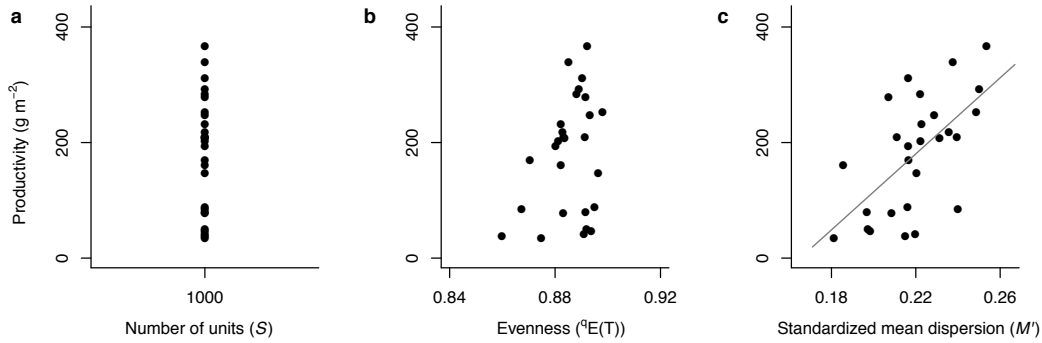
Supplementary Figure 4 | Phylogenetic signal (Blomberg's K) of mean spectra of 17 species measured at the Cedar Creek biodiversity experiment. a, The line on top indicates the mean estimate of the K statistic. Regions of the spectrum where K values are not different (Blomberg's K statistic, $P < 0.05$) from a Brownian motion model of evolution can be considered phylogenetically conserved and are shaded in grey. The average vector-normalized spectrum of all species is shown below. The dashed lines indicate the location of two example spectral bands at 600 and 1500 nm. **b**, The observed K value (yellow line) of two spectral bands, at 600 (top) and 1500 nm (bottom), relative to the mean (red line) of the Brownian motion null model distribution (dark grey bars), and the mean (black line) of the white noise model distribution (light grey bars).



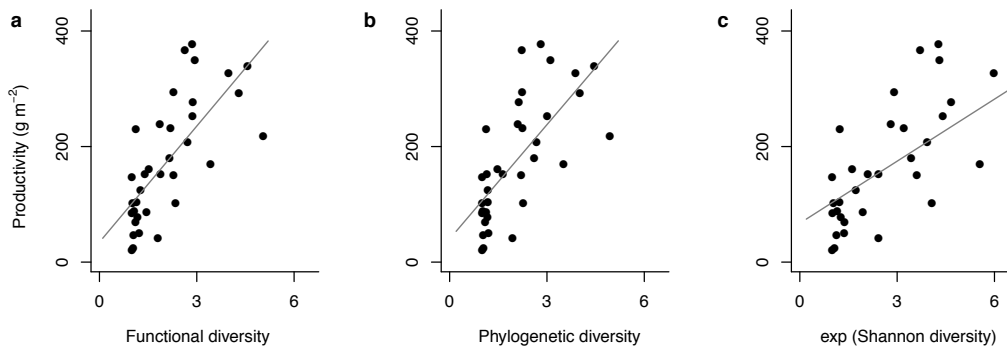
Supplementary Figure 5 | Relationships between the three components of leaf-level spectral diversity and productivity. More productive plant communities were generally characterised by **a**, a greater number ($n = 35$, $r^2 = 0.53$, $b = 22.86$, $t_{33} = 6.04$, $P < 0.001$) of **b**, more unevenly ($n = 35$, $r^2 = 0.16$, $b = -263.19$, $t_{33} = -2.53$, $P = 0.02$) and **c**, more widely dispersed ($n = 35$, $r^2 = 0.55$, $b = 559.36$, $t_{33} = 6.30$, $P < 0.001$) species mean spectra in spectral space. All relationships here and in similar subsequent figures are predicted from linear regression models, the line is the fitted regression line, and each point represents a single plot in the Cedar Creek biodiversity experiment.



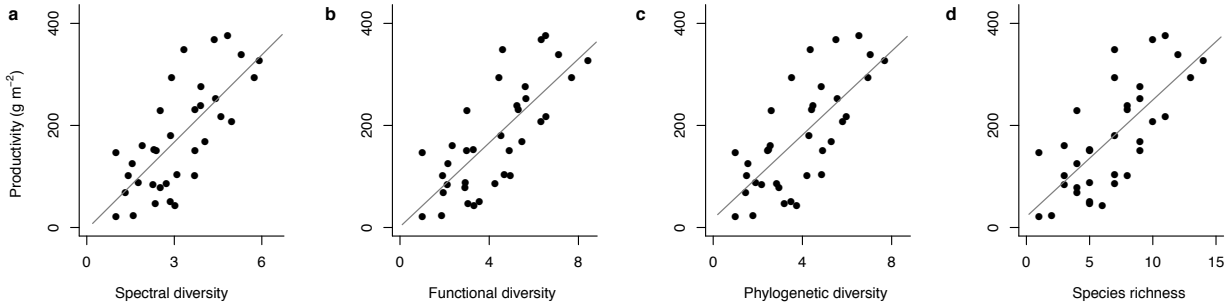
Supplementary Figure 6 | Relationship between leaf-level spectral diversity based on the most variable spectral bands and productivity. Aboveground productivity (g m^{-2}) increased with spectral diversity ($n = 35$, $r^2 = 0.51$, $b = 121.58$, $t_{33} = 5.88$, $P < 0.001$) using the spectral bands located at five local maxima of the coefficient of variation (at 429, 675, 1,451, 1,981, 2,360 nm; see Fig. 2) calculated per wavelength across spectra.



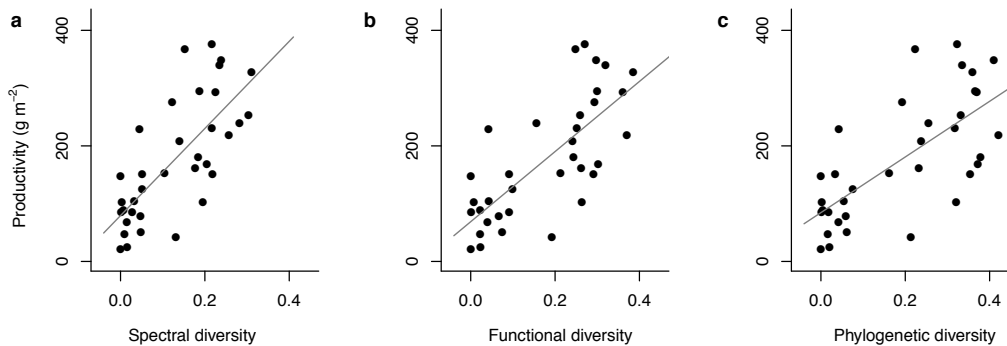
Supplementary Figure 7 | Relationships between the three components of remotely sensed spectral diversity and productivity. Spectral diversity was calculated based on **a**, 1,000 randomly extracted image pixels per plant community ($n = 27$). **b**, The evenness of the distribution of pixels in spectral space ($n = 27$, $r^2 = 0.09$, $b = 3250.0$, $t_{25} = 1.55$, $P = 0.13$) was not a significant predictor of aboveground productivity (g m^{-2}), but **c**, more productive plant communities were characterised by more widely dispersed pixels ($n = 27$, $r^2 = 0.37$, $b = 3289.9$, $t_{25} = 3.86$, $P < 0.001$).



Supplementary Figure 8 | Relationships between functional, phylogenetic, and taxonomic diversity and productivity. Aboveground productivity (g m^{-2}) increased with **a**, functional diversity ($n = 35$, $r^2 = 0.51$, $b = 66.96$, $t_{33} = 5.85$, $P < 0.001$) based on 14 leaf traits (see Methods, Supplementary Fig. 2, and Supplementary Table 1), **b**, phylogenetic diversity based on the molecular phylogeny published in ref. ⁴ ($n = 35$, $r^2 = 0.48$, $b = 65.95$, $t_{33} = 5.50$, $P < 0.001$) and **c**, effective Shannon diversity ($n = 35$, $r^2 = 0.47$, $b = 35.80$, $t_{33} = 5.38$, $P < 0.001$).



Supplementary Figure 9 | Relationships between non-abundance-weighted spectral, functional, phylogenetic, and taxonomic diversity and productivity. Aboveground productivity (g m^{-2}) increased with **a**, spectral diversity ($n = 35$, $r^2 = 0.53$, $b = 56.95$, $t_{33} = 6.04$, $P < 0.001$), **b**, functional diversity ($n = 35$, $r^2 = 0.56$, $b = 41.12$, $t_{33} = 6.54$, $P < 0.001$) based on 14 leaf traits (see Methods, Supplementary Fig. 2, and Supplementary Table 1), **c**, phylogenetic diversity based on the molecular phylogeny published in ref. ⁴ ($n = 35$, $r^2 = 0.52$, $b = 41.07$, $t_{33} = 5.94$, $P < 0.001$) and **d**, species richness ($n = 35$, $r^2 = 0.53$, $b = 22.86$, $t_{33} = 6.04$, $P < 0.001$).



Supplementary Figure 10 | Relationships between spectral, functional, and phylogenetic diversity calculated using functional dispersion (FDis)⁵ and productivity. Aboveground productivity (g m^{-2}) increased with **a**, spectral diversity ($n = 35$, $r^2 = 0.53$, $b = 753.92$, $t_{33} = 6.10$, $P < 0.001$), **b**, functional diversity ($n = 35$, $r^2 = 0.54$, $b = 606.82$, $t_{33} = 6.19$, $P < 0.001$) based on 14 leaf traits (see Methods, Supplementary Fig. 2, and Supplementary Table 1) and **c**, phylogenetic diversity based on the molecular phylogeny published in ref. ⁴ ($n = 35$, $r^2 = 0.49$, $b = 481.59$, $t_{33} = 5.59$, $P < 0.001$).

Supplementary Table 1 | Results of partial least squares regression (PLSR) models predicting 14 foliar traits from spectra.

Trait	<i>r</i>²	RMSEP	PLSR components	<i>n</i>	median	range
Carbon (%)	0.75	1.51	10	127	45.0	35.5-51.2
Nitrogen (%)	0.65	0.25	12	119	2.0	1.0-3.0
Non-structural carbohydrates (%)	0.74	6.61	12	114	57.0	20.0-80.2
Hemicellulose (%)	0.71	5.14	12	113	19.6	6.5-46.8
Cellulose (%)	0.84	2.61	11	113	13.8	7.0-34.7
Lignin (%)	0.53	1.78	11	112	8.6	2.8-16.5
Chlorophyll a (μmol m ⁻²)	0.75	60.60	5	121	270.5	118.6-662.5
Chlorophyll b (μmol m ⁻²)	0.79	18.60	6	124	79.3	24.8-201.0
β-carotene (μmol m ⁻²)	0.71	5.62	10	122	26.6	6.8-57.9
Lutein (μmol m ⁻²)	0.73	9.17	5	121	39.8	16.6-91.4
Neoxanthin (μmol m ⁻²)	0.76	3.28	6	125	12.5	4.5-32.0
Violaxanthin (μmol m ⁻²)	0.64	4.73	7	124	10.5	0.5-42.7
Antheraxanthin (μmol m ⁻²)	0.48	1.75	12	122	3.4	0.5-10.9
Zeaxanthin (μmol m ⁻²)	0.40	5.12	5	86	14.8	5.6-33.8

RMSEP = root mean square error of prediction

Supplementary Table 2 | Linear regression models between spectral distance, functional and phylogenetic distance for individual focal species paired with all other species.

Abbreviation	Species	Model	r^2	t (df)	P
ACHMI	<i>Achillea millefolium</i> L.	functional	0.12	52.61 (1,16)	<0.001
ACHMI		phylogenetic	-0.25	32.78 (1,16)	<0.001
AGRSM	<i>Agropyron smithii</i> Rydb.	functional	0.29	45.29 (1,16)	<0.001
AGRSM		phylogenetic	0.16	35.92 (1,16)	<0.001
AMOCA	<i>Amorpha canescens</i> Pursh	functional	0.20	35.84 (1,16)	<0.001
AMOCA		phylogenetic	-0.81	7.59 (1,16)	0.015
ANDGE	<i>Andropogon gerardii</i> Vitman	functional	0.12	28.76 (1,16)	<0.001
ANDGE		phylogenetic	0.47	56.65 (1,16)	<0.001
ASCTU	<i>Asclepias tuberosa</i> L.	functional	0.42	117.21 (1,16)	<0.001
ASCTU		phylogenetic	0.63	192.06 (1,16)	<0.001
KOECR	<i>Koeleria cristata</i> auct. non Pers. p.p.	functional	0.45	66.89 (1,16)	<0.001
KOECR		phylogenetic	0.54	82.05 (1,16)	<0.001
LESCA	<i>Lespedeza capitata</i> Michx.	functional	0.13	38.32 (1,16)	<0.001
LESCA		phylogenetic	-0.58	14.27 (1,16)	0.002
LIAAS	<i>Liatris aspera</i> Michx.	functional	0.61	150.56 (1,16)	<0.001
LIAAS		phylogenetic	0.43	96.88 (1,16)	<0.001
LUPPE	<i>Lupinus perennis</i> L.	functional	0.68	242.07 (1,16)	<0.001
LUPPE		phylogenetic	0.38	117.28 (1,16)	<0.001
MONFI	<i>Monarda fistulosa</i> L.	functional	-0.02	57.21 (1,16)	<0.001
MONFI		phylogenetic	0.02	59.66 (1,16)	<0.001
PANVI	<i>Panicum virgatum</i> L.	functional	0.48	61.57 (1,16)	<0.001
PANVI		phylogenetic	0.55	75.04 (1,16)	<0.001
PETCA	<i>Petalostemum candidum</i> (Willd.) Michx.	functional	0.54	123.83 (1,16)	<0.001
PETCA		phylogenetic	0.44	99.17 (1,16)	<0.001
PETPU	<i>Petalostemum purpureum</i> (Vent.) Rydb.	functional	0.64	156.64 (1,16)	<0.001
PETPU		phylogenetic	0.38	85.47 (1,16)	<0.001
POAPR	<i>Poa pratensis</i> L.	functional	0.33	44.70 (1,16)	<0.001
POAPR		phylogenetic	0.38	49.93 (1,16)	<0.001
SCHSC	<i>Schizachyrium scoparium</i> (Michx.) Nash	functional	0.38	59.90 (1,16)	<0.001
SCHSC		phylogenetic	0.60	99.50 (1,16)	<0.001
SOLRI	<i>Solidago rigida</i> L.	functional	0.31	102.70 (1,16)	<0.001
SOLRI		phylogenetic	0.44	130.04 (1,16)	<0.001
SORNU	<i>Sorghastrum nutans</i> (L.) Nash	functional	0.04	26.30 (1,16)	<0.001
SORNU		phylogenetic	0.36	47.09 (1,16)	<0.001

Supplementary Table 3 | Uni- and multivariate linear regression models using spectral (SDiv), phylogenetic (PDiv) and functional diversity (FDiv), and the effective Shannon index predicting aboveground productivity (g m⁻²).

Model	Variables	AIC	r²	F (df)	P
Univariate	SDiv	405.13	0.51	34.76 (1,33)	< 0.001
	FDiv	405.39	0.51	34.25 (1,33)	< 0.001
	PDiv	407.56	0.48	30.21 (1,33)	< 0.001
	Shannon	408.25	0.47	28.98 (1,33)	< 0.001
Multivariate	FDiv + Shannon	403.06	0.57	20.90 (2,32)	< 0.001
	SDiv + FDiv + Shannon	404.56	0.57	13.84 (3,31)	< 0.001
	PDiv + FDiv + Shannon	404.69	0.57	13.75 (3,31)	< 0.001
	SDiv + PDiv	405.00	0.54	18.91 (2,32)	< 0.001
	SDiv + PDiv + FDiv	406.35	0.55	12.64 (3,31)	< 0.001
	SDiv + Shannon	406.48	0.52	17.47 (2,32)	< 0.001
	SDiv + PDiv + Shannon	406.71	0.55	12.40 (3,31)	< 0.001
	SDiv + FDiv	406.98	0.52	16.99 (2,32)	< 0.001
	PDiv + FDiv	407.10	0.51	16.88 (2,32)	< 0.001
	PDiv + Shannon	409.47	0.48	14.72 (2,32)	< 0.001

Differences in Akaike's Information Criterion (AIC) < 3 when compared to the best univariate model SDiv are printed in bold.

Supplementary References

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