Supplementary Information

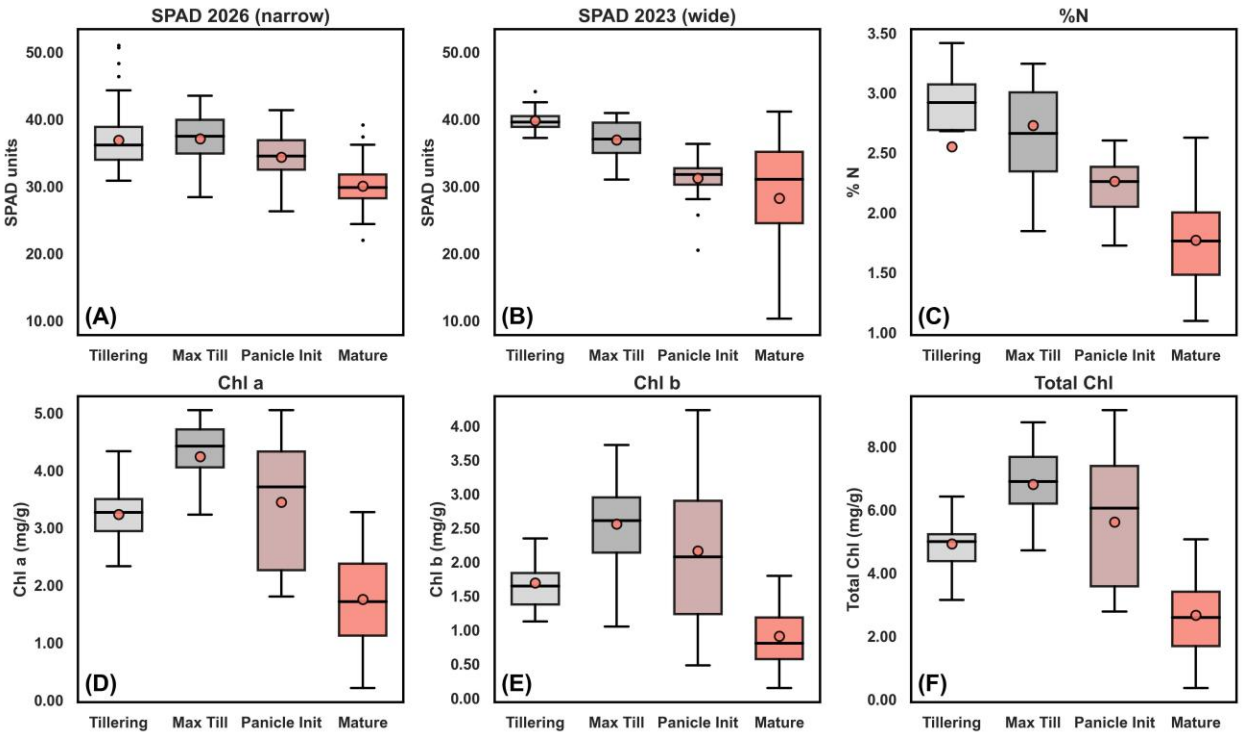


Figure S1. Reference measurements across four growth stages: SPAD in (a) the 2026 narrow-geometry experiment (n = 228) and (b) the 2023 wide-geometry experiment (n = 140); (c) %N, (d) chlorophyll a, (e) chlorophyll b and (f) total chlorophyll in the 2023 experiment (n = 140). Boxes show the interquartile range, lines the median and circles the mean; outliers are shown for SPAD only. Chlorophyll is expressed in mg g^{-1} fresh weight.

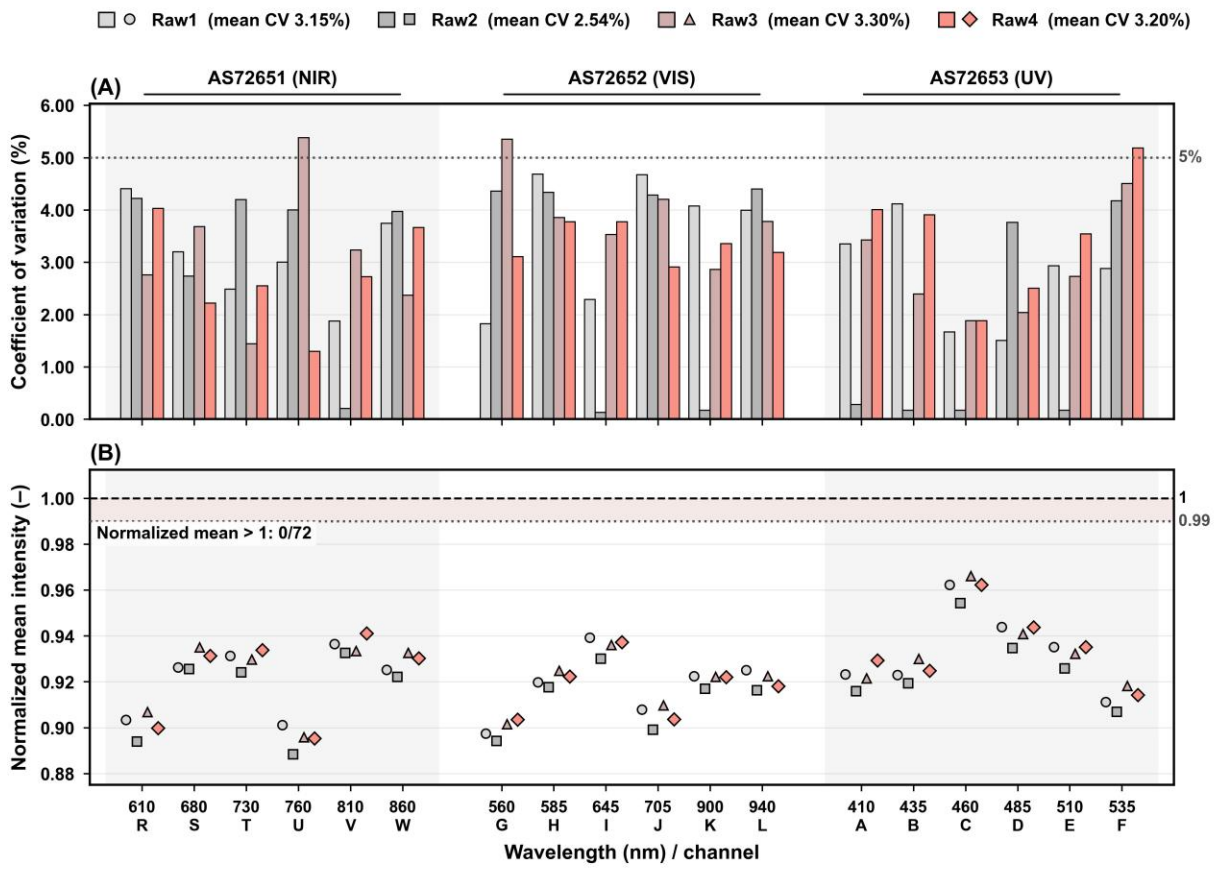


Figure S2. Sensor quality check using a Spectralon white reference. Stability of the AS7265x sensor response under the wide-geometry configuration was evaluated across four measurement periods corresponding to tillering, maximum tillering, panicle initiation, and mature stages (Raw1–Raw4). Channels are grouped by sensor die (AS72651, NIR; AS72652, VIS; AS72653, UV). (A) Channel-wise CV of raw sensor counts ranged from 0.13% to 5.38%, with mean CV of 2.54%–3.30%; the dotted line indicates 5%. (B) Mean responses normalized to the per-channel maximum ranged from 0.888 to 0.966 (overall mean = 0.923), indicating relatively consistent sensor response across measurement periods.

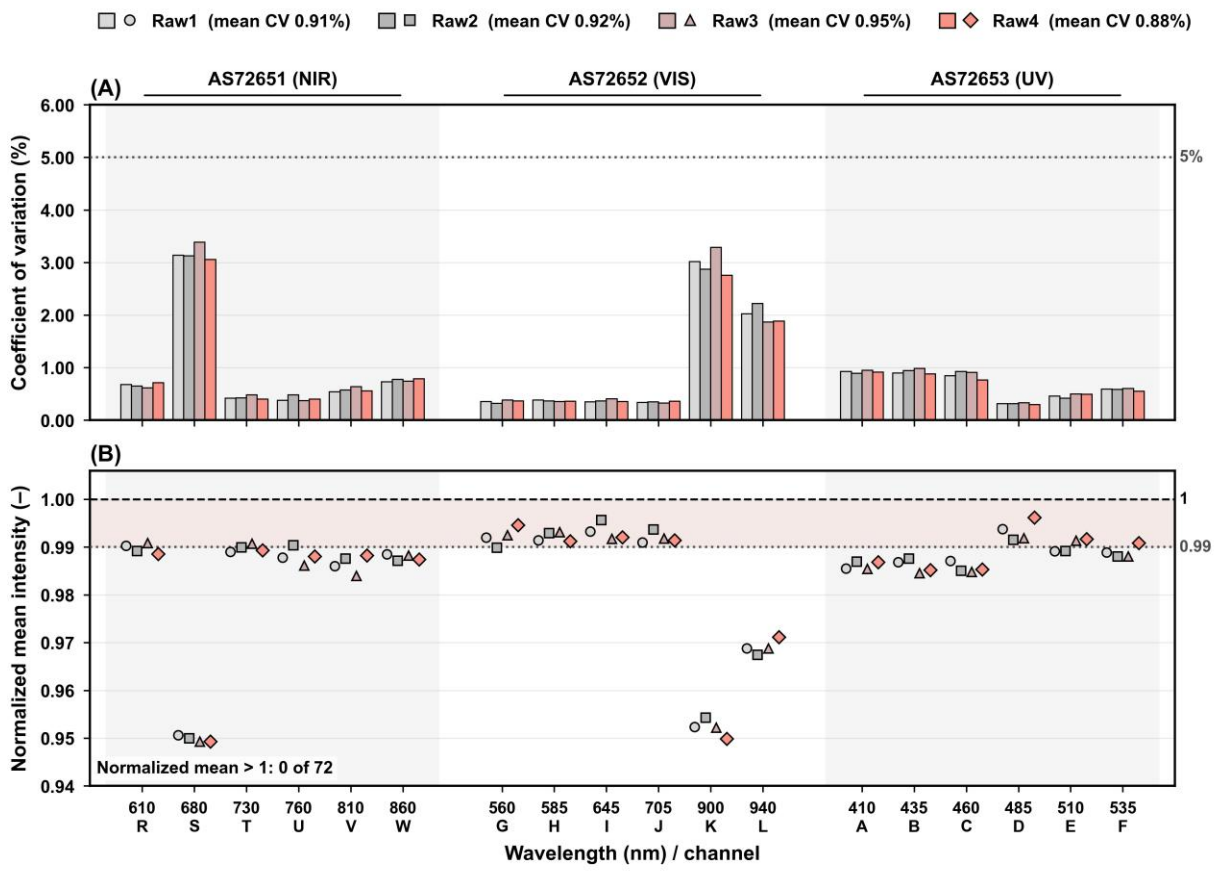


Figure S3. Sensor stability check using a Spectralon white reference. Stability of the AS7265x sensor response under the narrow-geometry configuration was evaluated across four measurement periods (Raw1–Raw4). Channels are grouped by sensor die (AS72651, NIR; AS72652, VIS; AS72653, UV). (A) Channel-wise CV of raw sensor counts ranged from 0.29% to 3.39%, with mean CV of 0.88%–0.95%; the dotted line indicates 5%. (B) Mean responses normalized to the per-channel maximum ranged from 0.949 to 0.996 (overall mean = 0.984).

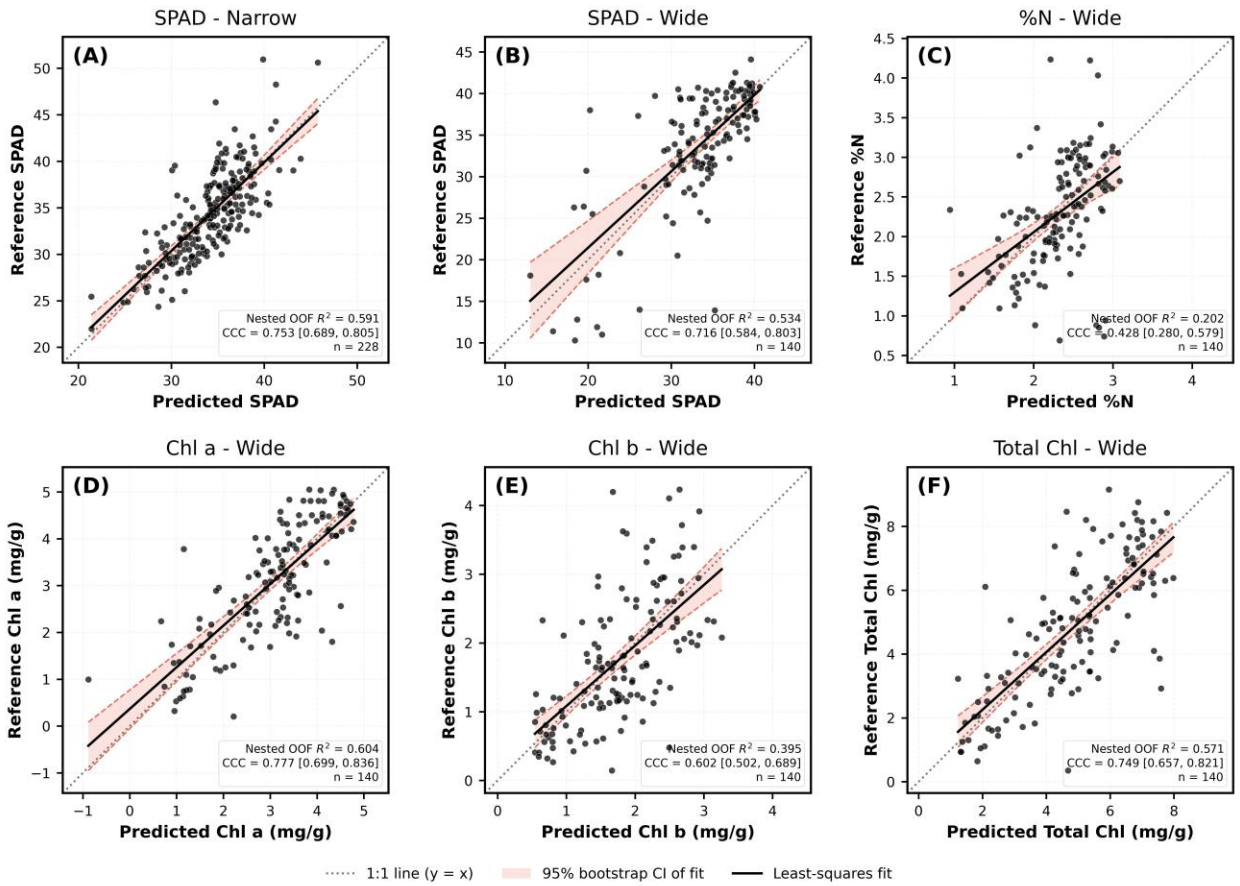


Figure S4. Agreement between reference values and nested out-of-fold predictions using all RF-Selected channels. Panel (a) shows SPAD under the narrow geometry. Panels (b–f) show the wide geometry with a black background: (b) SPAD, (c) %N, (d) chlorophyll a, (e) chlorophyll b, and (f) total chlorophyll. Dotted lines indicate 1:1 agreement; solid lines show ordinary least-squares fits, and shaded bands show their 95% bootstrap confidence intervals.

Table S1. Repeat-level quality control and biological-sample averaging for the wide and narrow-geometry dataset.

Background	Growth stage	Biological samples, initial	Reflectance repeats, initial	Repeats removed by QC	Repeats retained	Biological samples after QC	Mean retained repeats/ sample
Wide-White	Tillering	30	135	0	135	30	4.5
Wide-White	Maximum tillering	40	200	4	196	40	4.9
Wide-White	Panicle initiation	25	107	0	107	25	4.28
Wide-White	Mature	46	258	4	254	46	5.52
Wide-White total	—	141	700	8	692	141	4.91
Wide-Black	Tillering	30	127	0	127	30	4.23
Wide-Black	Maximum tillering	40	186	0	186	40	4.65
Wide-Black	Panicle initiation	24	101	0	101	24	4.21
Wide-Black	Mature	46	216	0	216	46	4.7
Wide-Black total	—	140	630	0	630	140	4.50
Narrow	Tillering	70	350	0	350	70	5
Narrow	Maximum tillering	49	245	0	245	49	5
Narrow	Panicle initiation	40	200	0	200	40	5
Narrow	Mature	69	339	0	339	69	4.91
Narrow total	—	228	1134	0	1134	228	4.97

Note : Each biological sample was measured repeatedly for leaf reflectance. Quality control was applied at the repeat level, whereby an entire repeat was excluded if any of the 18 normalized spectral channels exceeded 1.0. No repeat was excluded from the narrow-geometry dataset; therefore, all 1,134 measurements were retained and averaged into 228 biological-sample spectra.

Table S2. Datasets, inputs and nested validation design.

Item	Specified setting	Role in the analysis
Biological samples	BLACK wide: n = 140; WHITE wide: n = 141; NARROW: n = 228.	One row and one Sample_ID per independent biological sample in each input table.
Targets	BLACK and WHITE: SPAD, %N, chlorophyll a, chlorophyll b, total chlorophyll; NARROW: SPAD.	Separate nested search for every dataset and target.
Spectral input	18 AS7265x channels, 410–940 nm.	Full 18 retains all channels; RF Selected searches k = 2–18.
Upstream preparation	Spectralon normalized, sample averaged inputs are supplied to the code.	No second Spectralon normalization or averaging is performed in the model run; complete biological samples enter CV.
Fold design	Outer five folds; inner three folds; random seed 42; no fixed holdout.	Shuffled StratifiedKFold by growth stage when feasible; otherwise shuffled KFold. Growth stage is splitting metadata, not a predictor.
Matched scenarios	Full 18 and RF Selected have independent inner searches on identical outer partitions.	Each sample receives one OOF prediction per scenario and target. An outer validation fold is never used for tuning.
Pipeline order	Full: all channels → StandardScaler → regressor. Selected: RFTopKSelector → StandardScaler → regressor.	Both selector and scaler are fitted within training data presented to each CV fit.

Note : The 18 nominal wavelengths (nm) are 410, 435, 460, 485, 510, 535, 560, 585, 610, 645, 680, 705, 730, 760, 810, 860, 900, and 940. OOF denotes out of fold.

Table S3. Hyperparameter grids of the seven regression model families evaluated within the inner cross-validation folds.

Model	Searched model hyperparameters	Full 18 grid size
Linear regression (LR)	No model hyperparameter grid; LinearRegression defaults.	1
Ridge	alpha ∈ {0.001, 0.01, 0.1, 1, 10, 100}.	6
Lasso	alpha ∈ {0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1.0}. Fixed: max_iter = 500000, tol = 10^{-4}, selection = random, random_state = 42.	7
Support vector regression (SVR)	C ∈ {0.1, 1, 10, 100}; kernel ∈ {linear, rbf}; gamma ∈ {scale, auto}.	16
k-nearest neighbors (KNN)	n_neighbors ∈ {3, 5, 7, 9}; weights ∈ {uniform, distance}; metric ∈ {euclidean, manhattan}.	16
Random forest regressor	n_estimators ∈ {50, 100, 200}; max_depth ∈ {None, 10, 20}; min_samples_split ∈ {2, 5}; min_samples_leaf ∈ {1, 2}. Fixed: random_state = 42, n_jobs = 1.	36
Gradient boosting regressor	n_estimators ∈ {50, 100, 200}; learning_rate ∈ {0.01, 0.05, 0.1}; max_depth ∈ {2, 3, 5}. Fixed: random_state = 42.	27

Note : Full 18 evaluates 109 parameter combinations in total across the seven model families for each inner search (provided the KNN neighbor values fit the smallest inner training fold). RF Selected instead evaluates 120 jointly sampled configurations per family and search. The gamma choices are included in the coded SVR grid even when the linear kernel makes gamma inactive. Unlisted settings use the estimator defaults of the original scikit-learn environment.

Table S4. Configuration of the random forest-based channel selector and the joint sampled search used in the RF Selected scenario.

Component	Implemented setting	Operational rule
RF ranker	RandomForestRegressor fitted in the selector; n_jobs = 1.	Mean decrease in impurity (feature_importances_) ranks channels in stable descending order.
Ranker grid	n_estimators = {50, 100, 200}; max_depth = {None, 10, 20, 30}; min_samples_split = {2, 5, 10}; min_samples_leaf = {1, 2, 4}; max_features = {sqrt, log2, None}.	3 × 4 × 3 × 3 × 3 = 324 possible RF ranker combinations.
Number of channels	$k \in \{2, 3, \ldots, 18\}$; 17 candidate sizes.	Select the top k ranked channels. k = 1 is excluded; k = 18 retains the full channel set.
Joint sampled search	120 configurations per regression family per inner search, sampling the product of ranker settings and that family's model grid.	Every k is represented: 16 sizes receive seven draws and one size receives eight draws, with the extra draw assigned by the seeded permutation.
Channel ordering	The chosen channel identities are restored to canonical input order before scaling and prediction.	RF importance determines membership, not predictor column order; k = 18 therefore contains the Full 18 feature matrix.
Fold-local fitting	RF ranking, StandardScaler and regression model are fitted in each inner training fold; the chosen pipeline is refitted on its outer training fold.	No globally ranked wavelength list is computed from all samples for OOF evaluation.

Table S5. Model-selection and assessment rules in the nested cross-validation: inner scoring, one-standard-error criterion, simplicity order, and outer-fold refitting.

Decision point	Exact rule	Data available to the decision
Inner scoring	For every candidate calculate mean RMSE across three inner validation folds; R^2 and MAE are also recorded.	Only the current outer training subset is split into inner train and validation folds.
Best candidate and one-SE set	Identify the lowest mean inner RMSE across all seven families within a scenario. Retain candidates with mean RMSE ≤ that minimum + SE of the minimum-RMSE candidate; SE = sample SD of its three fold RMSE values / √3.	Only inner validation scores from the current scenario and outer training subset.
Simplicity order	Within the one-SE set: fewer channels; lower model complexity rank (LR 1, Ridge/Lasso 2, KNN 3, SVR 4, RF 5, GB 6); then lower mean RMSE, mean MAE, RMSE SD, R^2 SD, model name, and candidate index.	Prespecified deterministic tie order; outer validation results play no role.
Scenario separation	Choose one Full 18 winner and one RF Selected winner independently. The scenarios do not compete in the inner search.	Exactly the same outer train/validation IDs are used in both scenarios within each dataset.
Refit and assessment	Fit the selected selector/scaler/regressor pipeline on the whole outer training subset; predict the untouched outer validation subset once.	No estimator uses outer validation observations while fitting, scaling, ranking, or tuning.
Diagnostic flags	Underfit, overfit, unstable and large inner-to-outer R^2 drop labels are reported but never filter candidates or remove folds.	All outer validation predictions are retained in pooled OOF performance.
Final full-data fit	After nested OOF evaluation, repeat scenario-specific inner search and fit a deployable estimator on all samples.	This full-data fit does not provide the reported generalization estimates.

Table S6. OOF metrics, bootstrap comparisons and computational settings.

Output or setting	Definition or code setting	Interpretation
Pooled OOF metrics	R^2, RMSE, MAE, and Lin's concordance correlation coefficient (CCC) on the pooled outer validation predictions; RPIQ = interquartile range of observed values / pooled OOF RMSE.	One observed–predicted pair per biological ID, scenario, dataset and target.
CCC calculation	$CCC = 2\,cov(y, \hat{y}) / [var(y) + var(\hat{y}) + (mean(y) - mean(\hat{y}))^2]$, with population moments (ddof = 0).	Agreement combines precision and location/scale bias.
Metric intervals	2,000 percentile bootstrap resamples of fixed observed–OOF prediction pairs; 2.5th and 97.5th percentiles; base seed 42.	Descriptive uncertainty conditional on saved OOF predictions; models and folds are not retrained per resample.
Selected − Full	Within each dataset, resample matched biological IDs and subtract Full from RF Selected for R^2, RMSE, MAE and CCC.	Scenarios use the same outer fold per ID; positive ΔR^2/ΔCCC and negative ΔRMSE/ΔMAE favor Selected.
WHITE − BLACK	For the wide measurements, use 140 matched biological IDs per target/scenario and resample each pair together. The one unmatched WHITE ID is excluded only from this contrast.	The color-specific outer fold labels need not match; matching is by biological ID and reference value.
CI and zero	The 95% CI for a metric difference is compared with zero; the code supplies above_zero, below_zero, or includes_zero labels.	No separate paired p-value is calculated. A CI including zero does not establish a directional difference.
Fitting environment	Recorded original model-fit versions: Python 3.8.19; NumPy 1.22.4; pandas 2.0.3; scikit-learn 1.3.2.	The verification-only requirements may use newer versions without refitting models.
Compute controls	search_n_jobs = 2; pre_dispatch = 2; numeric_threads = 1; nominal figure_dpi = 600.	Search candidates are deterministic under recorded seeds and software versions.

Table S7. Nested out-of-fold prediction performance for SPAD, leaf nitrogen, and chlorophyll traits using full-spectrum and RF-selected predictors under different sensor aperture and background configurations.

Narrow sensor aperture							
Target	**Scenario**	**Biological IDs (n)**	**R^2 [95% CI]**	**RMSE [95% CI]**	**MAE [95% CI]**	**CCC [95% CI]**	**RPIQ [95% CI]**
SPAD	Full 18	228	0.665 [0.573, 0.737]	2.720 [2.453, 2.984]	2.122 [1.909, 2.350]	0.810 [0.756, 0.849]	2.340 [2.006, 2.767]
SPAD	RF Selected	228	0.591 [0.490, 0.670]	3.005 [2.673, 3.358]	2.302 [2.055, 2.573]	0.753 [0.688, 0.806]	2.118 [1.797, 2.528]
Wide sensor aperture -Black Background							
Target	**Scenario**	**Biological IDs (n)**	**R^2 [95% CI]**	**RMSE [95% CI]**	**MAE [95% CI]**	**CCC [95% CI]**	**RPIQ [95% CI]**
SPAD	Full 18	140	0.620 [0.426, 0.754]	4.432 [3.589, 5.319]	3.154 [2.686, 3.709]	0.778 [0.667, 0.859]	1.737 [1.406, 2.244]
SPAD	RF Selected	140	0.534 [0.311, 0.679]	4.909 [4.077, 5.832]	3.575 [3.061, 4.162]	0.716 [0.587, 0.806]	1.568 [1.257, 1.968]
%N	Full 18	140	0.262 [0.060, 0.439]	0.593 [0.480, 0.705]	0.410 [0.342, 0.485]	0.470 [0.312, 0.618]	1.680 [1.319, 2.109]
%N	RF Selected	140	0.202 [0.003, 0.380]	0.616 [0.504, 0.725]	0.442 [0.375, 0.516]	0.428 [0.276, 0.574]	1.616 [1.264, 1.989]
Chl a	Full 18	140	0.619 [0.496, 0.711]	0.774 [0.682, 0.866]	0.607 [0.529, 0.690]	0.765 [0.686, 0.824]	2.569 [2.081, 3.066]
Chl a	RF Selected	140	0.604 [0.447, 0.715]	0.789 [0.679, 0.904]	0.612 [0.531, 0.697]	0.777 [0.696, 0.837]	2.520 [2.019, 3.092]
Chl b	Full 18	140	0.486 [0.341, 0.592]	0.677 [0.596, 0.764]	0.535 [0.470, 0.610]	0.664 [0.569, 0.738]	1.810 [1.538, 2.349]
Chl b	RF Selected	140	0.395 [0.241, 0.519]	0.735 [0.639, 0.835]	0.573 [0.500, 0.655]	0.602 [0.497, 0.686]	1.668 [1.454, 2.178]
Total Chl	Full 18	140	0.567 [0.425, 0.671]	1.398 [1.224, 1.578]	1.085 [0.944, 1.243]	0.734 [0.645, 0.800]	2.321 [1.947, 2.784]
Total Chl	RF Selected	140	0.571 [0.408, 0.692]	1.391 [1.172, 1.601]	1.062 [0.922, 1.223]	0.749 [0.654, 0.823]	2.333 [1.936, 2.848]
Wide sensor aperture -White Background							
Target	**Scenario**	**Biological IDs (n)**	**R^2 [95% CI]**	**RMSE [95% CI]**	**MAE [95% CI]**	**CCC [95% CI]**	**RPIQ [95% CI]**
SPAD	Full 18	141	0.580 [0.426, 0.684]	4.661 [4.080, 5.253]	3.577 [3.118, 4.103]	0.753 [0.669, 0.817]	1.673 [1.397, 2.010]
SPAD	RF Selected	141	0.521 [0.353, 0.638]	4.979 [4.264, 5.670]	3.712 [3.183, 4.272]	0.703 [0.612, 0.776]	1.566 [1.275, 1.920]
%N	Full 18	141	0.371 [0.207, 0.518]	0.545 [0.442, 0.639]	0.394 [0.332, 0.459]	0.562 [0.441, 0.682]	1.822 [1.414, 2.256]
%N	RF Selected	141	0.233 [0.073, 0.383]	0.602 [0.507, 0.695]	0.453 [0.389, 0.522]	0.469 [0.340, 0.595]	1.650 [1.287, 2.027]
Chl a	Full 18	141	0.440 [0.248, 0.576]	0.944 [0.828, 1.053]	0.760 [0.669, 0.851]	0.648 [0.530, 0.741]	2.110 [1.764, 2.522]
Chl a	RF Selected	141	0.313 [0.123, 0.464]	1.045 [0.939, 1.149]	0.854 [0.754, 0.953]	0.554 [0.441, 0.654]	1.905 [1.588, 2.244]
Chl b	Full 18	141	0.265 [0.090, 0.403]	0.824 [0.722, 0.925]	0.648 [0.564, 0.735]	0.479 [0.365, 0.579]	1.483 [1.303, 1.960]
Chl b	RF Selected	141	0.167 [-0.019, 0.328]	0.878 [0.756, 1.005]	0.673 [0.583, 0.773]	0.401 [0.263, 0.532]	1.393 [1.226, 1.844]
Total Chl	Full 18	141	0.408 [0.215, 0.550]	1.652 [1.453, 1.844]	1.325 [1.163, 1.491]	0.621 [0.502, 0.715]	1.960 [1.679, 2.334]
Total Chl	RF Selected	141	0.352 [0.175, 0.484]	1.729 [1.525, 1.926]	1.406 [1.242, 1.578]	0.552 [0.434, 0.650]	1.873 [1.614, 2.225]

Table S8. Paired comparison of out-of-fold prediction performance between the Full 18-channel and RF-selected predictor scenarios

Dataset	Target	n	Full R^2	Selected R^2	ΔR^2 [95% CI]	Full RMSE	Selected RMSE	ΔRMSE [95% CI]	Full MAE	Selected MAE	ΔMAE [95% CI]	Full CCC	Selected CCC	ΔCCC [95% CI]
Black	SPAD	140	0.6	0.534	−0.086 [−0.160, −0.024]	4.432	4.909	0.477 [0.135, 0.857]	3.15	3.575	0.420 [0.101, 0.771]	0.778	0.716	−0.062 [−0.112, −0.016]
Black	N (%)	140	0.3	0.202	−0.060 [−0.170, 0.034]	0.593	0.616	0.024 [−0.014, 0.065]	0.41	0.442	0.032 [−0.001, 0.066]	0.47	0.428	−0.042 [−0.114, 0.026]
Black	Chl a	140	0.6	0.604	−0.015 [−0.119, 0.075]	0.774	0.789	0.015 [−0.078, 0.112]	0.61	0.612	0.005 [−0.073, 0.085]	0.765	0.777	0.013 [−0.041, 0.067]
Black	Chl b	140	0.5	0.395	−0.091 [−0.204, 0.022]	0.677	0.735	0.058 [−0.014, 0.127]	0.54	0.573	0.038 [−0.011, 0.088]	0.664	0.602	−0.063 [−0.136, 0.012]
Black	Total Chl	140	0.6	0.571	0.004 [−0.101, 0.115]	1.398	1.391	−0.007 [−0.182, 0.161]	1.09	1.062	−0.023 [−0.158, 0.107]	0.734	0.749	0.015 [−0.049, 0.081]
White	SPAD	141	0.6	0.521	−0.059 [−0.166, 0.035]	4.661	4.979	0.318 [−0.183, 0.882]	3.58	3.712	0.135 [−0.297, 0.593]	0.753	0.703	−0.050 [−0.119, 0.013]
White	N (%)	141	0.4	0.233	−0.138 [−0.240, −0.044]	0.545	0.602	0.057 [0.018, 0.098]	0.39	0.453	0.060 [0.024, 0.095]	0.562	0.469	−0.094 [−0.165, −0.029]
White	Chl a	141	0.4	0.313	−0.127 [−0.232, −0.020]	0.944	1.045	0.101 [0.016, 0.182]	0.76	0.854	0.094 [0.021, 0.168]	0.648	0.554	−0.094 [−0.161, −0.025]
White	Chl b	141	0.3	0.167	−0.098 [−0.204, 0.025]	0.824	0.878	0.053 [−0.013, 0.114]	0.65	0.673	0.025 [−0.034, 0.081]	0.479	0.401	−0.078 [−0.160, 0.012]
White	Total Chl	141	0.4	0.352	−0.056 [−0.144, 0.037]	1.652	1.729	0.076 [−0.050, 0.201]	1.33	1.406	0.081 [−0.016, 0.182]	0.621	0.552	−0.068 [−0.132, −0.010]
Narrow	SPAD	228	0.7	0.591	−0.074 [−0.143, −0.006]	2.72	3.005	0.285 [0.025, 0.558]	2.12	2.302	0.180 [−0.021, 0.378]	0.81	0.753	−0.057 [−0.106, −0.014]

Table S9. Paired comparison of out-of-fold prediction performance between black and white backgrounds under the wide sensor aperture

Dataset	Target	n	Full R^2	Selected R^2	ΔR^2 [95% CI]	Full RMSE	Selected RMSE	ΔRMSE [95% CI]	Full MAE	Selected MAE	ΔMAE [95% CI]	Full CCC	Selected CCC	ΔCCC [95% CI]
SPAD	Full 18	140	0.6	0.588	−0.032 [−0.170, 0.130]	4.432	4.613	0.181 [−0.653, 0.977]	3.15	3.536	0.382 [−0.176, 0.925]	0.778	0.759	−0.019 [−0.101, 0.078]
	RF Selected	140	0.5	0.522	−0.012 [−0.199, 0.194]	4.909	4.973	0.063 [−0.955, 1.059]	3.58	3.697	0.122 [−0.564, 0.766]	0.716	0.704	−0.012 [−0.129, 0.112]
N (%)	Full 18	140	0.3	0.371	0.109 [−0.045, 0.256]	0.593	0.547	−0.046 [−0.105, 0.018]	0.41	0.396	−0.014 [−0.071, 0.041]	0.47	0.562	0.092 [−0.027, 0.205]
	RF Selected	140	0.2	0.235	0.033 [−0.163, 0.218]	0.616	0.603	−0.013 [−0.083, 0.063]	0.44	0.454	0.012 [−0.045, 0.072]	0.428	0.469	0.041 [−0.109, 0.179]
Chl a	Full 18	140	0.6	0.434	−0.186 [−0.367, −0.035]	0.774	0.944	0.170 [0.032, 0.312]	0.61	0.759	0.152 [0.037, 0.273]	0.765	0.646	−0.119 [−0.230, −0.021]
	RF Selected	140	0.6	0.312	−0.293 [−0.466, −0.123]	0.789	1.041	0.252 [0.097, 0.385]	0.61	0.849	0.237 [0.115, 0.349]	0.777	0.556	−0.221 [−0.324, −0.121]
Chl b	Full 18	140	0.5	0.267	−0.219 [−0.377, −0.074]	0.677	0.809	0.132 [0.043, 0.218]	0.54	0.638	0.103 [0.028, 0.180]	0.664	0.487	−0.177 [−0.286, −0.074]
	RF Selected	140	0.4	0.182	−0.213 [−0.379, −0.050]	0.735	0.854	0.119 [0.027, 0.213]	0.57	0.66	0.087 [0.003, 0.176]	0.602	0.418	−0.183 [−0.311, −0.058]
Total Chl	Full 18	140	0.6	0.399	−0.168 [−0.326, −0.022]	1.398	1.647	0.248 [0.035, 0.453]	1.09	1.318	0.233 [0.053, 0.412]	0.734	0.618	−0.116 [−0.215, −0.021]
	RF Selected	140	0.6	0.363	−0.208 [−0.394, −0.037]	1.391	1.695	0.304 [0.050, 0.559]	1.06	1.385	0.323 [0.129, 0.513]	0.749	0.564	−0.185 [−0.302, −0.072]