

Article

Canopy-Level Estimation of Photosynthetic Phenotypic Parameters in Winter Wheat Using VIS–NIR–SWIR Hyperspectral Regions

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Abstract

Photosynthetic phenotypic parameters of winter wheat are important indicators of canopy physiological status, photosynthetic function, and crop growth. However, canopy-scale hyperspectral estimation of these parameters remains affected by canopy structural heterogeneity, environmental variation, and mixed spectral signals. This study evaluated the contribution of visible (VIS), near-infrared (NIR), and shortwave infrared (SWIR) regions and their combinations to estimating photosynthetic phenotypic parameters of winter wheat. Field experiments were conducted under three nitrogen application levels and 65 winter wheat genotypes, and a total of 507 valid canopy-level samples were used for model development and validation. Competitive adaptive reweighted sampling (CARS) was used to select characteristic wavelengths, and partial least squares regression (PLSR), Bayesian ridge regression (BR), and backpropagation neural network (BPNN) were applied to construct estimation models. Model performance was assessed using R^2 , RMSE, and RPD. Results showed that NIR-based models achieved the best overall performance, with the highest validation R^2 of 0.828 for photosynthetic rate. The VIS + NIR combination showed stable predictive ability across multiple parameters, whereas SWIR-only models showed limited performance, with R^2 values below 0.5 for most parameters. Photosynthetic rate, intercellular CO_2 concentration, performance index on an absorption basis, and chlorophyll a content were predicted more accurately than the other traits. These findings indicate that canopy hyperspectral data can support quantitative monitoring of photosynthetic phenotypic parameters, and that NIR-related structural and scattering information plays a key role in winter wheat canopy phenotyping.

Keywords: winter wheat; photosynthesis traits; hyperspectral sensing; VIS–NIR–SWIR; canopy estimation

Academic Editor: Dariusz Gozdowski

Received: 2 June 2026

Revised: 23 July 2026

Accepted: 27 July 2026

Published: 29 July 2026

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1. Introduction

Winter wheat is one of the most important staple crops worldwide, playing a critical role in global food security and agricultural sustainability [1]. Its productivity is closely linked to photosynthetic processes, which determine biomass accumulation and final yield formation. Photosynthetic phenotypic parameters, including photosynthetic rate, chlorophyll fluorescence, and pigment content, are key indicators of crop physiological status and photosynthetic efficiency [2–4]. However, monitoring these parameters under field conditions remains challenging, as conventional measurement methods such as gas exchange systems and fluorescence instruments are labor-intensive, time-consuming, and limited in spatial representativeness [4,5]. Therefore, efficient, non-destructive, and field-scale monitoring approaches are needed to support precision agriculture and crop phenotyping applications [5,6].

In recent years, hyperspectral remote sensing has been widely adopted for crop physiological monitoring due to its continuous spectral information and sensitivity to biochemical and structural characteristics [6–9]. Numerous studies have demonstrated that hyperspectral reflectance can be used to estimate photosynthetic parameters, chlorophyll fluorescence, and pigment content across different crops [3,7,10]. Recent advances have further confirmed the potential of hyperspectral techniques for high-throughput phenotyping under field conditions [11,12]. In winter wheat studies, hyperspectral data combined with machine learning methods have shown potential for estimating physiological traits and improving the use of spectral information in modeling [13–15].

However, most existing approaches rely on full-spectrum modeling or predefined spectral indices, which may introduce redundant information and reduce model efficiency [8,16]. At the canopy scale, hyperspectral signals are affected by structural heterogeneity, soil background interference, and illumination variability [17]. These factors increase the complexity of spectral responses and make it more difficult to accurately estimate photosynthetic phenotypic parameters under field conditions.

Different spectral regions provide distinct but complementary information for crop physiological monitoring. The visible (VIS) region is mainly related to pigment absorption, the near-infrared (NIR) region reflects canopy structure and multiple scattering, and the shortwave infrared (SWIR) region is sensitive to water status and biochemical composition [16,18,19]. However, the relative contributions of VIS, NIR, SWIR, and their combinations to canopy-level photosynthetic phenotyping remain insufficiently quantified, particularly across gas-exchange, chlorophyll-fluorescence, and pigment-related traits. Therefore, the novelty of this study is the systematic comparison of individual and combined VIS–NIR–SWIR spectral regions for canopy-level estimation of winter wheat photosynthetic phenotypic parameters, together with CARS-based wavelength selection and both linear and nonlinear modeling approaches. We hypothesized that different spectral regions would contribute unequally to canopy-level photosynthetic phenotyping, with NIR and VIS + NIR expected to provide more stable estimation performance than SWIR alone because of their stronger association with canopy structural and pigment-related information. Based on this hypothesis, the objectives of this study were to: (1) develop canopy-level estimation models for photosynthetic phenotypic parameters of winter wheat using different VIS, NIR, SWIR, and combined spectral inputs; (2) evaluate whether NIR and VIS + NIR spectral configurations provide more stable model performance than SWIR-only inputs; and (3) identify optimal spectral configurations for different types of photosynthetic phenotypic parameters.

2. Materials and Methods

The overall workflow of this study is shown in Figure 1. The methodological framework was designed to evaluate the contribution of VIS–NIR–SWIR spectral regions to canopy-level estimation of photosynthetic phenotypic parameters in winter wheat. The workflow included a field experiment and data collection, canopy hyperspectral data acquisition and preprocessing, spectral region construction, CARS-based characteristic wavelength selection, model development, and performance evaluation. Additional methodological details are provided in Appendix A.

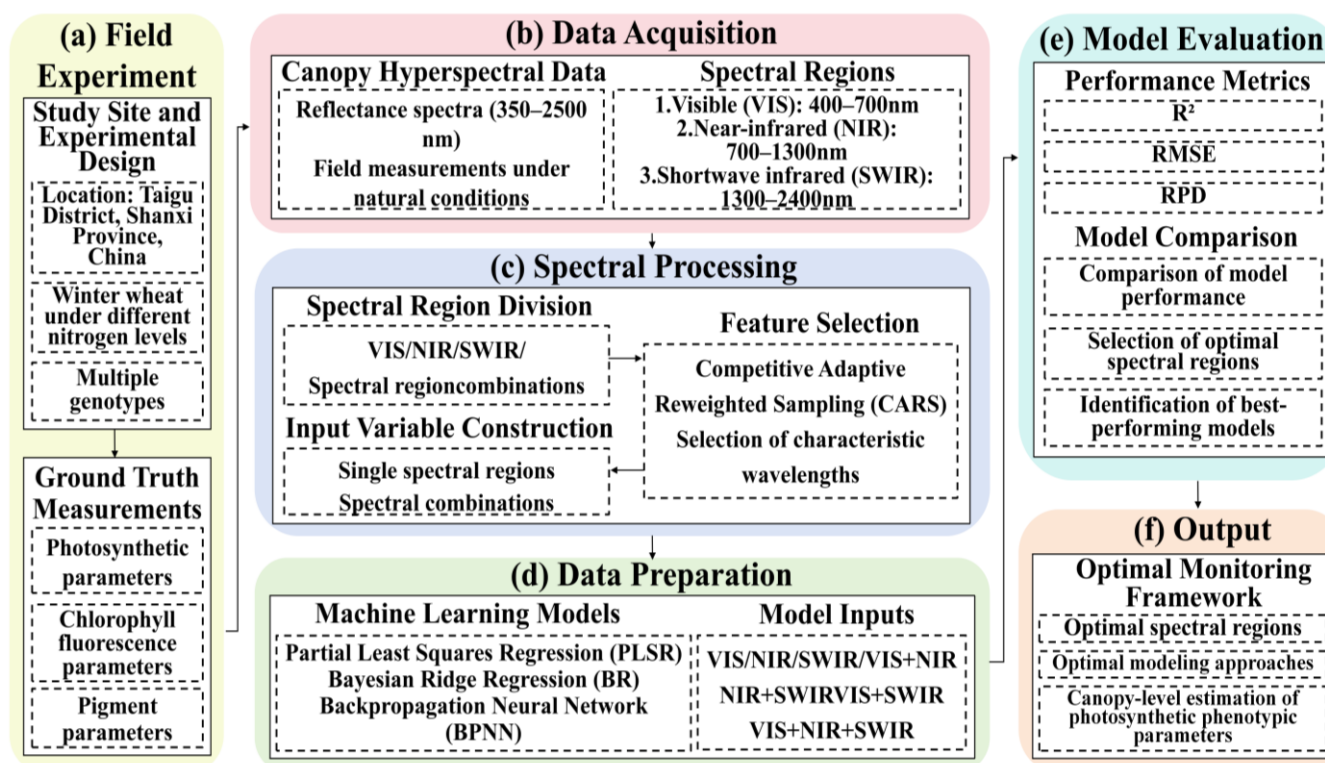


Figure 1. The workflow of this study.

2.1. Study Sites and Experimental Design

The experiment was conducted in Mengjiazhuang Village, Taigu District, Jinzhong City, Shanxi Province, China (37°44' N, 112°59' E), at an elevation of approximately 840 m. Field experiments were carried out from October 2022 to June 2023. A nitrogen gradient experiment was established with three nitrogen application levels: 0, 100, and 200 kg·hm^{−2}. Under each nitrogen level, 65 winter wheat genotypes, including landraces, cultivated varieties, and breeding lines, were planted, resulting in 195 plots. Each plot had an area of 3 m² (1.5 m × 2 m). Phosphorus and potassium fertilizers were applied as basal fertilizers at 120 kg·hm^{−2}, and other field management practices followed local conventional practices. The geographical location and field layout of the experimental site are shown in Figure 2.

Canopy hyperspectral data and photosynthetic phenotypic parameters were measured at five growth stages, including the jointing, booting, flowering, grain-filling, and maturity stages. For model construction, the booting, flowering, and grain-filling stages were used because sufficient valid paired spectral and physiological observations were available for these stages after quality control. In total, 585 potential plot-level observations were expected from 195 plots across these three stages. After applying the quality-control criteria described in Sections 2.2.1 and 2.2.3, 507 valid paired observations were retained, indicating that 78 observations were excluded. The valid samples were distrib-

uted across the booting, flowering, and grain-filling stages, with 180, 174, and 153 samples, respectively. It should be noted that the experiment was conducted at one site during the 2022–2023 growing season; therefore, further validation across different years, sites, and management conditions is needed to evaluate the broader applicability of the models.

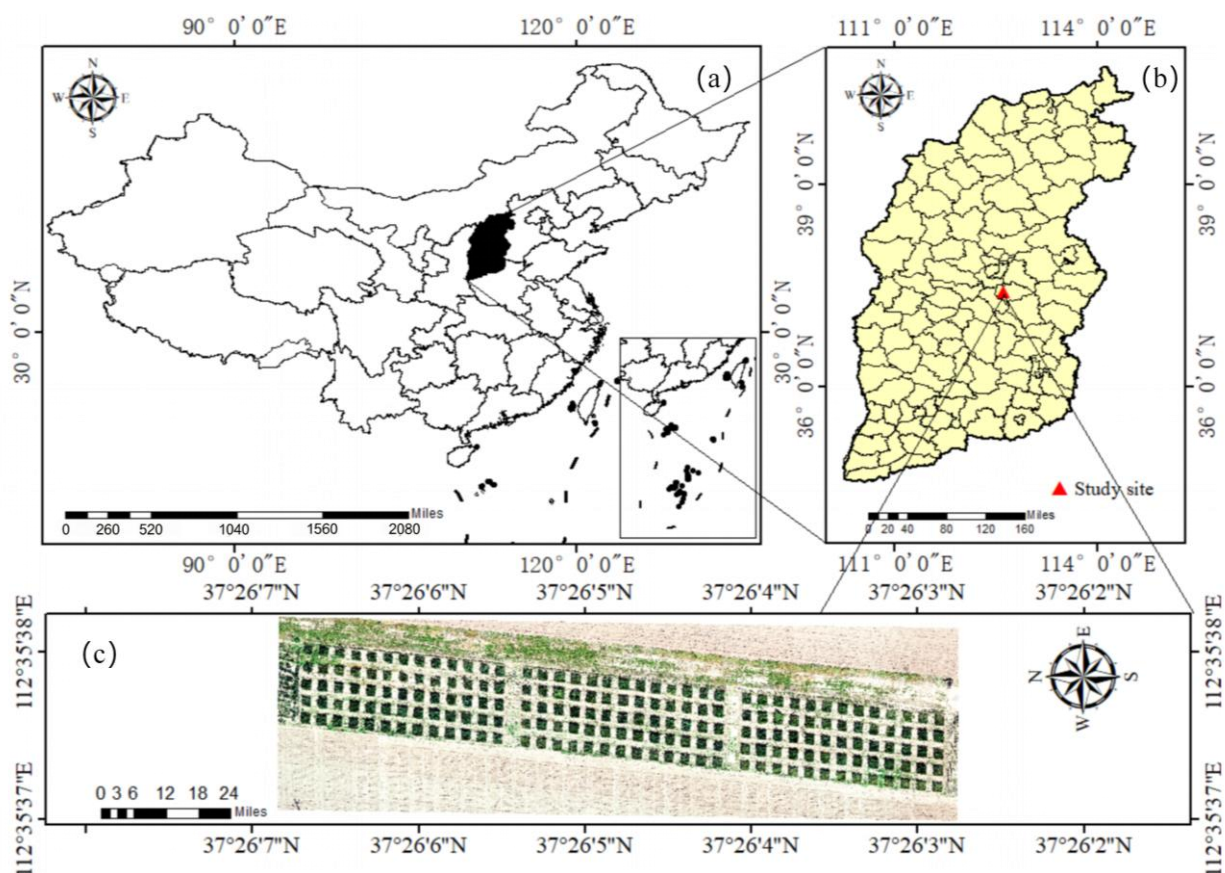


Figure 2. Experimental design: (a,b) geographical location of Taigu District; (c) experimental area.

2.2. Data Collection and Preprocessing

2.2.1. Measurement of Photosynthetic Phenotypic Parameters

Photosynthetic phenotypic parameters were measured at key growth stages of winter wheat. Gas-exchange parameters, including photosynthetic rate (Photo), stomatal conductance (Cond), transpiration rate (Trmmol), and intercellular CO₂ concentration (Ci), were measured using a LI-6400 portable gas-exchange system (LI-COR Biosciences, Lincoln, NE, USA) on clear and windless days between 9:00 and 11:00, following established procedures for minimizing measurement errors in leaf gas-exchange analysis [20]. Representative plants were selected within each plot, and the first fully expanded leaf or flag leaf was used for measurement. Repeated measurements were averaged to obtain one plot-level value.

Chlorophyll fluorescence parameters, including the maximum quantum efficiency of photosystem II (Fv/Fm) and the performance index on an absorption basis (PI abs), were measured using a Handy PEA plant efficiency analyzer (Hansatech Instruments Ltd., King's Lynn, Norfolk, UK). Representative flag leaves were dark-adapted for 30 min before measurement. Both Fv/Fm and PI abs are commonly used to characterize photosystem II performance and plant photosynthetic status under field conditions [21]. Photosynthetic pigment parameters, including chlorophyll a content (Ca), chlorophyll b content (Cb), and carotenoid content (Cc), were determined using the 95% ethanol (Sinopharm Chemical Reagent Co., Ltd., Shanghai, China) extraction method. Absorbance was meas-

ured at 665, 649, and 470 nm using a UV-1800 ultraviolet–visible spectrophotometer (Shimadzu Corporation, Kyoto, Japan), and pigment contents were calculated using established spectrophotometric equations [22].

For physiological-data quality control, samples with missing measurements, unstable instrument readings, abnormal physiological values, or severe lodging were excluded. Spectral quality-control procedures are described separately in Section 2.2.3. Only samples with valid paired physiological and canopy hyperspectral observations were retained for model construction and validation.

2.2.2. Canopy Hyperspectral Data Acquisition

Canopy hyperspectral reflectance was measured using a FieldSpec3 portable spectrometer (Analytical Spectral Devices, Boulder, CO, USA), covering a spectral range of 350–2500 nm. This spectral range is widely used in crop hyperspectral studies because it contains information related to pigment absorption, canopy structure, water status, and biochemical characteristics [23–25].

Spectral measurements were conducted between 10:00 and 14:00 local time under clear, cloud-free, and low-wind conditions. Before each measurement, the spectrometer was calibrated using a standard white-reference panel to ensure spectral consistency [25]. During data acquisition, the sensor probe was held vertically approximately 80 cm above the canopy surface. For each plot, three representative sampling points with relatively uniform growth were selected, and three spectral measurements were collected at each point. After abnormal spectra were removed, the remaining measurements were averaged to obtain one representative plot-level canopy reflectance curve. This strategy was used to reduce random measurement error and improve the representativeness and reproducibility of field spectral observations [26–28].

2.2.3. Spectral Data Preprocessing

The original spectral data were preprocessed before model construction. Abnormal spectral curves were removed using ViewSpec Pro 6.20 (ASD Inc., Boulder, CO, USA) software, and repeated measurements were averaged for each sample. The bands of 350–400 nm and 2400–2500 nm were removed because of low detector sensitivity and high noise levels. The wavelength ranges of 1300–1400 nm and 1800–1950 nm were also excluded because they are strongly affected by water absorption and may cause unstable spectral fluctuations. Similar preprocessing procedures have been widely used in hyperspectral studies to reduce noise and improve model stability and robustness [23,29,30].

2.3. Spectral Region Construction and Feature Wavelength Selection

2.3.1. Spectral Region Construction

To evaluate the contribution of different spectral regions, the preprocessed spectra were divided into visible (VIS, 400–700 nm), near-infrared (NIR, 700–1300 nm), and shortwave infrared (SWIR, 1300–2400 nm) regions according to the agricultural remote sensing standard (NY/T 4370-2023) and previous hyperspectral studies. The VIS region mainly reflects pigment absorption features, the NIR region characterizes canopy structure and scattering information, and the SWIR region is sensitive to water status and biochemical components [16,18,19,29].

In addition to the individual spectral regions, four combined spectral inputs were constructed: VIS + NIR, NIR + SWIR, VIS + SWIR, and VIS + NIR + SWIR. These individual and combined spectral regions were used as model inputs to compare their performance in estimating canopy-level photosynthetic phenotypic parameters. The corresponding wavelength ranges are listed in Table 1.

Table 1. Nominal wavelength ranges of the individual and combined spectral regions.

Spectral Regions and Combinations of Regions	Band Range (nm)
VIS	400–700
NIR	700–1300
SWIR	1300–2400
VIS + NIR	400–1300
NIR + SWIR	700–2400
VIS + SWIR	400–700,1300–2400
VIS + NIR + SWIR	400–2400

Note: The wavelength ranges of 1300–1400 and 1800–1950 nm were excluded during spectral pre-processing because of strong water absorption.

2.3.2. Feature Wavelength Selection

To reduce spectral redundancy and retain informative wavelengths, characteristic wavelength selection was performed for each spectral input and target parameter using competitive adaptive reweighted sampling (CARS). CARS determines the optimal wavelength subset according to the minimum root mean square error of cross-validation (RMSECV) [29,31]. Previous studies have shown that reducing hyperspectral dimensionality can improve modeling efficiency while retaining useful spectral information [32–34]. CARS has been widely used for hyperspectral feature selection because of its ability to reduce dimensionality while preserving key spectral information [34,35]. In this study, CARS was used to select characteristic wavelengths for canopy-level photosynthetic phenotypic parameters under different spectral regions.

To quantitatively evaluate the contribution of different spectral regions, the number of wavelengths selected by CARS was counted separately for each target parameter in the VIS, NIR, and SWIR regions. Because the optimal wavelength subsets were independently selected for different target parameters, the same wavelength selected for different parameters was counted separately. The total number, mean, and standard deviation of selected wavelengths were calculated for each spectral region. In addition, an exploratory Spearman rank correlation analysis was performed to determine whether the number of selected wavelengths was associated with predictive performance. For each target parameter–spectral region combination, the selected wavelength number was related to the mean validation R^2 obtained across the three modeling methods and 30 repeated calibration–validation partitions. A separate correlation analysis was also conducted for the nine SWIR-based combinations. Statistical significance was determined at $p < 0.05$.

2.4. Model Development and Evaluation

2.4.1. Model Development

Three modeling methods were used to estimate canopy-level photosynthetic phenotypic parameters: partial least squares regression (PLSR), Bayesian ridge regression (BR), and backpropagation neural network (BPNN). PLSR was used as a baseline linear model because it is suitable for high-dimensional and collinear spectral variables [10,12,31]; BR was selected as a regularized linear model because it can improve model stability and generalization when dealing with noisy and highly collinear hyperspectral variables [25,36]. BPNN was selected as a nonlinear model to characterize complex relationships between hyperspectral inputs and target variables [13,36]. Previous studies have also shown that neural network models can effectively capture nonlinear spectral features and improve the prediction of crop physiological traits [26,36]. All models were trained and validated using the same dataset partitioning and preprocessing procedures to ensure comparability among spectral inputs and modeling methods.

To improve model reproducibility, the key parameter settings of PLSR, BR, and BPNN were specified in detail. For PLSR, candidate numbers of latent variables ranging from 1 to 20 were evaluated using five-fold cross-validation within the calibration set. The number of latent variables corresponding to the minimum root mean square error of cross-validation (RMSECV) was selected, after which the model was refitted using the complete calibration set.

BR was implemented in Python 3.8 using the BayesianRidge class from the scikit-learn library. Gamma prior distributions were assigned to the precision parameters of the regression coefficients and observation noise. The prior hyperparameters were set to $\alpha_1 = 1 \times 10^{-6}$, $\alpha_2 = 1 \times 10^{-6}$, $\lambda_1 = 1 \times 10^{-6}$, and $\lambda_2 = 1 \times 10^{-6}$. The maximum number of iterations was set to 300, and model convergence was defined using a tolerance of 1×10^{-3} .

For BPNN, a single-hidden-layer feedforward neural network was constructed in MATLAB R2018b. The hidden layer contained 10 neurons and used the hyperbolic tangent sigmoid transfer function (tansig), whereas the output layer used a linear transfer function (purelin). The network was trained using the Levenberg–Marquardt backpropagation algorithm (trainlm). Because trainlm performs batch optimization using the complete calibration dataset, conventional learning-rate and mini-batch-size parameters were not specified. The maximum number of training epochs was set to 1000, and the performance goal was set to 5×10^{-3} . Before network training, the input and output variables were normalized using the mapminmax function. The normalization parameters were estimated using the calibration set only and were subsequently applied to the corresponding validation set. Predicted values were transformed back to their original measurement scales before model evaluation.

2.4.2. Model Evaluation

Model performance was evaluated using the coefficient of determination (R^2), root mean square error (RMSE), and ratio of performance to deviation (RPD). These metrics are commonly used in hyperspectral crop modeling to characterize model fit, prediction error, and predictive ability [26,37]. All evaluation metrics were calculated using the validation set.

The evaluation metrics were calculated as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^n (Y_i - Y'_i)^2}{\sum_{i=1}^n (Y_i - \bar{Y})^2} \quad (1)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (Y_i - Y'_i)^2} \quad (2)$$

$$RPD = \frac{SD}{RMSE} \quad (3)$$

where n represents the number of samples; Y_i and Y'_i represent the measured and predicted values of the i -th sample, respectively; $\bar{Y}$ represents the mean measured value; and SD represents the standard deviation of the measured values.

2.4.3. Statistical Significance Analysis

To quantitatively compare the performance of different spectral regions and modeling methods, the complete dataset was randomly divided into calibration and validation

sets at a ratio of 3:1, and this procedure was repeated 30 times using random seeds ranging from 1 to 30. Within each repetition, identical calibration and validation samples were used for all seven spectral-region configurations and the three modeling methods to ensure paired and directly comparable evaluations.

Validation-set R^2 , RMSE, and RPD were calculated for each repetition, and RMSE was selected as the primary metric for statistical inference because it directly represents prediction error in the original measurement units. A blocked two-way analysis of variance was conducted separately for each photosynthetic phenotypic parameter, with spectral region, modeling method, and their interaction as fixed factors and repetition as a blocking factor. Because the interaction effects were significant, paired Wilcoxon signed-rank tests were subsequently conducted among the 21 spectral region–model combinations. The Holm method was used to adjust the p -values for multiple comparisons and control the family-wise error rate [38]. Differences were considered statistically significant at an adjusted p -value of less than 0.05. Repeated modeling results are reported as the mean $\pm$ standard deviation.

3. Results

3.1. Descriptive Statistics of Photosynthetic Phenotypic Parameters of Winter Wheat

The descriptive statistics of canopy-level photosynthetic phenotypic parameters are summarized in Table 2. A total of 507 valid samples were obtained and divided into a calibration set ($n = 380$) and a validation set ($n = 127$) at a ratio of 3:1.

Table 2. Descriptive statistical analysis of photosynthetic phenotypic parameters.

Parameters	Data	N	Min	Max	Average	Range	SD	Skewness	Kurtosis
Photo	C	380	4.092	43.973	20.010	39.881	10.844	0.940	−0.431
	V	127	6.169	43.754	20.261	37.585	10.959	0.935	−0.487
	T	507	4.092	43.973	20.026	39.881	10.822	0.944	−0.430
Cond	C	380	0.045	0.594	0.244	0.549	0.103	1.115	1.225
	V	127	0.090	0.591	0.248	0.501	0.106	1.214	1.385
	T	507	0.045	0.594	0.245	0.549	0.103	1.124	1.236
Trmmol	C	380	1.539	13.792	5.869	12.253	2.346	0.911	0.709
	V	127	2.304	13.355	5.940	11.051	2.397	0.968	0.773
	T	507	1.539	13.792	5.872	12.253	2.336	0.908	0.690
Ci	C	380	0.627	347.498	210.287	346.870	77.507	−1.190	0.598
	V	127	4.595	344.329	212.499	339.734	76.468	−1.168	0.635
	T	507	0.627	347.498	210.577	346.870	77.027	−1.194	0.611
Fv/Fm	C	380	0.691	0.850	0.802	0.159	0.025	−0.763	0.989
	V	127	0.735	0.849	0.802	0.114	0.024	−0.469	−0.124
	T	507	0.691	0.850	0.802	0.159	0.024	−0.708	0.769
PI abs	C	380	0.768	4.571	2.408	3.803	0.756	0.181	−0.539
	V	127	0.990	4.508	2.433	3.517	0.765	0.277	−0.449
	T	507	0.768	4.571	2.410	3.803	0.753	0.184	−0.556
Ca	C	380	0.934	4.730	2.665	3.795	0.605	0.052	−0.032
	V	127	1.279	4.657	2.691	3.378	0.614	0.314	0.148
	T	507	0.934	4.730	2.668	3.795	0.601	0.072	−0.085
Cb	C	380	0.292	1.769	0.865	1.476	0.242	0.429	0.123
	V	127	0.397	1.610	0.873	1.213	0.245	0.537	0.102
	T	507	0.292	1.769	0.866	1.476	0.241	0.429	0.064
Cc	C	380	0.118	0.975	0.426	0.856	0.136	0.818	1.056
	V	127	0.160	0.899	0.431	0.739	0.138	0.946	1.081
	T	507	0.118	0.975	0.426	0.856	0.135	0.817	0.984

Note: C represents the calibration set, V represents the validation set, and T represents the total sample. Photo: photosynthetic rate; Cond: stomatal conductance; Trmmol: transpiration rate; Ci: intercellular CO₂ concentration; Fv/Fm: maximum photochemical efficiency; PI abs: performance index on absorption basis; Ca, Cb, and Cc represent chlorophyll a, chlorophyll b, and carotenoid contents, respectively.

The photosynthetic phenotypic parameters showed different degrees of variability. Photosynthetic parameters such as Photo, Trmmol, and Ci had relatively large standard deviations, indicating greater variation. In contrast, chlorophyll fluorescence parameters and pigment-related parameters showed relatively smaller ranges of variation.

In terms of distribution characteristics, Ci and Fv/Fm showed negative skewness, whereas most other parameters showed positive skewness. The value ranges of the calibration set generally covered those of the validation set, indicating that the dataset partitioning was reasonable and suitable for subsequent modeling analysis.

3.2. Correlation Analysis Among Photosynthetic Phenotypic Parameters of Winter Wheat

Pearson correlation analysis was performed to evaluate the relationships among photosynthetic phenotypic parameters using all 507 valid samples. The significance of each correlation coefficient was tested using a two-tailed test. No multiple-comparison correction was applied because this analysis was mainly used for descriptive exploration of trait relationships. The correlation results are shown in Figure 3.

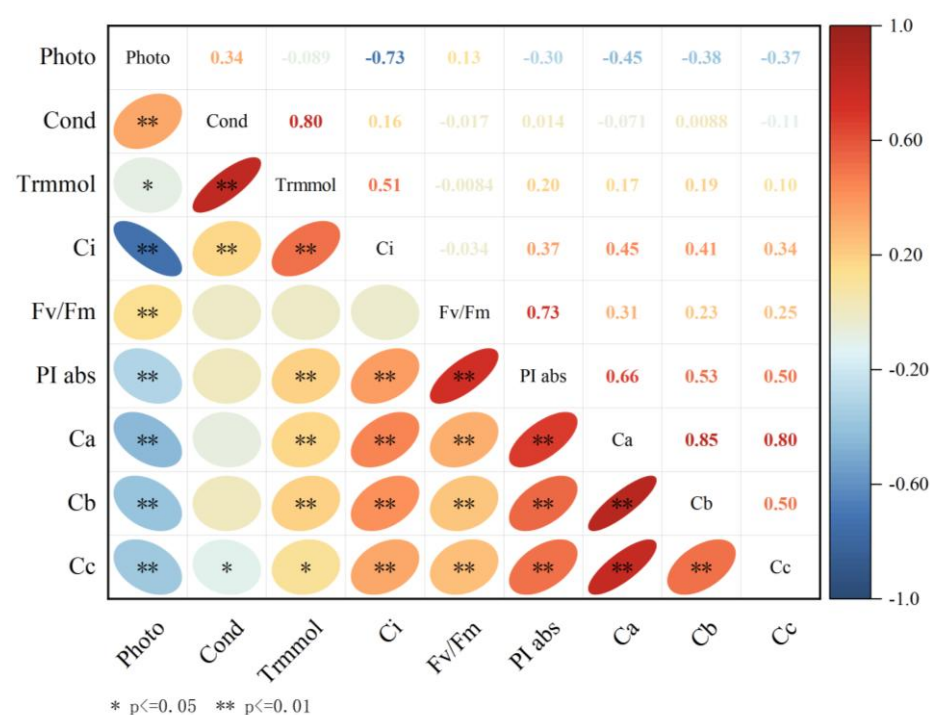


Figure 3. Pearson correlation analysis among photosynthetic phenotypic parameters based on 507 valid samples. Significance levels were determined using a two-tailed test. * and ** indicate significance at $p < 0.05$ and $p < 0.01$, respectively. No multiple-comparison correction was applied.

Several photosynthetic phenotypic parameters showed different degrees of correlation. Photosynthetic rate (Photo) was strongly negatively correlated with intercellular CO₂ concentration (Ci) ($r = -0.73$), while transpiration rate (Trmmol) was strongly positively correlated with stomatal conductance (Cond) ($r = 0.80$). The maximum photochemical efficiency (Fv/Fm) also showed a strong positive correlation with the performance index on an absorption basis (PI abs) ($r = 0.73$).

The photosynthetic pigment parameters, including chlorophyll a content (Ca), chlorophyll b content (Cb), and carotenoid content (Cc), were also highly correlated with each other ($r = 0.80\text{--}0.85$), indicating consistent variation patterns among pigment-related traits. These results suggest close interrelationships among different photosynthetic phenotypic parameters.

3.3. Canopy-Scale Monitoring of Photosynthetic Phenotypic Parameters Under Different Spectral Regions

To evaluate the role of spectral-region information in canopy-level estimation, model performance was compared across individual spectral regions and their combinations. An overall spectral-region-dependent pattern was observed, although the magnitude and ranking of model performance varied among target parameters and modeling methods. Overall, NIR-based models provided the strongest performance, SWIR-based models showed the weakest performance, and VIS + NIR combinations produced relatively stable results across multiple photosynthetic phenotypic parameters.

The numbers of characteristic wavelengths selected from different spectral regions are summarized in Table 3. Detailed model performances for photosynthetic parameters, chlorophyll fluorescence parameters, and pigment-related parameters are provided in Appendix B (Tables A1–A3).

Table 3. Number of wavelengths selected by CARS from different spectral regions for each photosynthetic phenotypic parameter.

Parameter	VIS	NIR	SWIR
Photo	18	55	8
Cond	27	57	6
Trmmol	17	45	18
Ci	54	22	19
Fv/Fm	6	11	5
PI abs	14	24	14
Ca	9	9	12
Cb	8	12	4
Cc	7	12	20
Total	160	247	106
Mean $\pm$ SD	17.8 $\pm$ 15.2	27.4 $\pm$ 19.6	11.8 $\pm$ 6.3

Note: CARS wavelength selection was conducted independently for each target parameter. Therefore, the total represents the sum of the parameter-specific wavelength counts, and wavelengths selected for different parameters were counted separately. SD represents the standard deviation across the nine target parameters.

3.3.1. Characteristic Wavelength Distribution Selected by CARS

The characteristic wavelengths selected using CARS for different photosynthetic phenotypic parameters are shown in Figure 4.

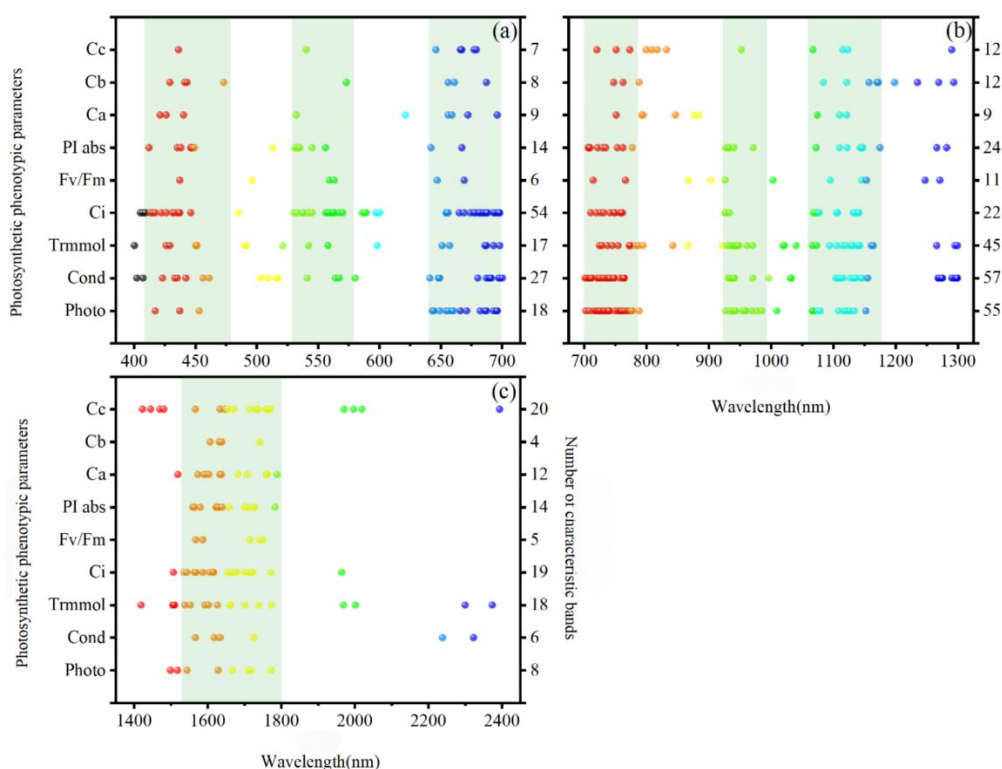


Figure 4. Feature wavelength selection results for photosynthetic phenotypic parameters based on the CARS method at the canopy scale. Panels (a–c) show the distributions of characteristic wavelengths selected in the visible, near-infrared, and shortwave-infrared spectral regions, respectively. The colored dots indicate the characteristic wavelengths selected by CARS for each photosynthetic phenotypic parameter, with colors changing from red to blue as the wavelength increases. The green shaded areas highlight the wavelength ranges in which the selected characteristic wavelengths are concentrated.

The number of wavelengths selected by CARS differed considerably among spectral regions and target parameters (Table 3). Across the nine photosynthetic phenotypic parameters, CARS selected a total of 160 VIS, 247 NIR, and 106 SWIR wavelengths. These values corresponded to 17.8 ± 15.2 , 27.4 ± 19.6 , and 11.8 ± 6.3 wavelengths per parameter for VIS, NIR, and SWIR, respectively. NIR contained the largest number of selected wavelengths for six of the nine parameters, whereas SWIR contained the smallest or joint-smallest number for six parameters.

However, the smaller number of SWIR wavelengths did not fully explain its inferior predictive performance. Across the 27 target parameter–spectral region combinations, the number of CARS-selected wavelengths was not significantly correlated with mean validation R^2 (Spearman's $\rho = 0.199$, $p = 0.319$). The relationship also remained nonsignificant when only the nine SWIR combinations were considered ($\rho = 0.250$, $p = 0.516$). For example, 20, 19, and 18 SWIR wavelengths were selected for Cc, Ci, and Trmmol, respectively, but the corresponding SWIR-based models still showed limited predictive performance. Therefore, the relatively poor performance of SWIR could not be attributed solely to the number of wavelengths retained by CARS.

The selected wavelengths were mainly concentrated in the ranges of 400–450 nm, 530–570 nm, 665–780 nm, 1066–1141 nm, and 1537–1658 nm. This distribution indicates that canopy-level photosynthetic phenotyping depends on information from multiple spectral domains, but the NIR region contained a larger absolute number of selected wavelengths.

3.3.2. Effects of Spectral Regions on Model Performance

Across the evaluated parameters, the NIR region showed the most consistent predictive advantage. For several parameters, including Photo, Cond, Fv/Fm, PI abs, and Cb, the best-performing models were derived from the NIR region. Photo achieved the highest overall accuracy using the NIR-based BPNN model, with $R^2 = 0.828$, RMSE = 4.531, and RPD = 2.409. PI abs also showed strong performance with the NIR-based BR model, reaching $R^2 = 0.649$ and RPD = 1.689.

The VIS + NIR combination provided the most stable performance among combined spectral inputs. It achieved the best or near-best performance for several parameters, including Ci, PI abs, and Cc. For Ci, the VIS + NIR-based BR model produced the highest accuracy, with $R^2 = 0.710$, RMSE = 41.051, and RPD = 1.855. This result suggests that combining pigment-related information from VIS with structural information from NIR can improve prediction stability for some canopy-level traits.

In contrast, SWIR-only models generally showed weaker performance. For most parameters, models based solely on SWIR had lower R^2 and RPD values than those based on NIR or VIS + NIR. This indicates that SWIR information alone was less effective for canopy-level estimation of photosynthetic phenotypic parameters under the field conditions of this study.

3.3.3. Statistical Comparison of Spectral Regions and Modeling Methods

The blocked two-way analysis of variance showed that spectral region, modeling method, and their interaction significantly affected validation RMSE for all nine photosynthetic phenotypic parameters (all $p \leq 0.003$; Table 4). The significant interaction effects indicated that the relative performance of the modeling methods depended on both the spectral region and the target parameter.

Table 4. Effects of spectral region, modeling method, and their interaction on validation RMSE based on 30 repeated calibration–validation partitions.

Parameter	Spectral Region, F	<i>p</i> -Value	Modeling Method, F	<i>p</i> -Value	Region × Method, F	<i>p</i> -Value
Photo	1024.84	<0.001	2529.55	<0.001	46.75	<0.001
Cond	8.63	<0.001	17.43	<0.001	3.81	<0.001
Trmmol	18.31	<0.001	6.50	0.002	4.57	<0.001
Ci	142.26	<0.001	447.82	<0.001	16.28	<0.001
Fv/Fm	75.44	<0.001	264.91	<0.001	17.89	<0.001
PI abs	229.54	<0.001	201.49	<0.001	8.95	<0.001
Ca	375.38	<0.001	77.89	<0.001	32.88	<0.001
Cb	625.63	<0.001	16.24	<0.001	6.90	<0.001
Cc	20.05	<0.001	7.84	<0.001	2.50	0.003

Note: Validation RMSE was used as the response variable. Spectral region, modeling method, and their interaction were treated as fixed factors, and repetition was included as a blocking factor. The degrees of freedom for spectral region, modeling method, and their interaction were 6, 2, and 12, respectively.

Holm-adjusted paired comparisons showed that VIS + NIR–BR achieved the lowest mean RMSE for Photo and significantly outperformed most of the alternative combinations. (adjusted $p < 0.05$). For the remaining parameters, although specific combinations produced the lowest mean RMSE, their differences from one or more of the other top-performing combinations were not statistically significant after Holm adjustment. Therefore, numerical superiority was not interpreted as statistically significant superiority unless it was supported by the Holm-adjusted pairwise comparisons.

3.3.4. Parameter-Dependent Predictability at the Canopy Scale

Prediction performance differed strongly among target parameters. Photo, Ci, PI abs, and Ca were relatively well predicted, with optimal R^2 values greater than 0.6 and RPD values exceeding 1.4. These parameters are more closely related to canopy structural status, pigment information, or integrated photosynthetic performance, and therefore were more readily captured by canopy hyperspectral signals.

In contrast, Cond and Fv/Fm showed limited predictive performance. The optimal R^2 values for these parameters were only 0.264 and 0.267, respectively, with RPD values close to 1.0. This is an important result because it indicates that not all photosynthetic phenotypic parameters can be reliably estimated from canopy hyperspectral reflectance alone. Parameters strongly affected by instantaneous physiological regulation or weak canopy-level spectral expression may require additional structural, environmental, or temporal information for accurate estimation.

Cb and Cc showed intermediate to limited predictability. Although NIR or VIS + NIR produced the best results for these parameters, their overall accuracy remained lower than that of Photo, Ci, PI abs, and Ca. These differences indicate that target parameter type had a strong influence on model performance, and this effect was more apparent than the difference among PLSR, BR, and BPNN in several cases.

3.4. Optimal Models and Validation Plots

The repeated statistical analysis confirmed that prediction performance was jointly affected by spectral region, modeling method, and target parameter characteristics. The significant spectral region $\times$ modeling method interactions indicated that the relative advantage of each modeling method varied among spectral inputs and photosynthetic phenotypic parameters. Among the nine photosynthetic phenotypic parameters, NIR or VIS + NIR was selected as the optimal or near-optimal spectral input for most parameters. BR achieved the best performance for several parameters, BPNN was optimal for Photo and Cb, and PLSR was optimal only for Trmmol. This indicates that model choice affected performance, but the dominant pattern was determined by spectral-region information and target parameter characteristics. The optimal spectral configurations and corresponding model performance for all nine photosynthetic phenotypic parameters are summarized in Table 5.

Table 5. Summary of optimal spectral configurations and model performance for canopy-level photosynthetic phenotypic parameters.

Parameter	Best Spectral Input	Best Model	R^2	RMSE	RPD	Predictability
Photo	NIR	BPNN	0.828	4.531	2.409	High
Cond	NIR	BR	0.264	0.091	1.165	Low
Trmmol	VIS + NIR + SWIR	PLSR	0.428	1.774	1.322	Moderate
Ci	VIS + NIR	BR	0.710	41.051	1.855	High
Fv/Fm	NIR	BR	0.267	0.020	1.168	Low
PI abs	NIR	BR	0.649	0.451	1.689	High
Ca	VIS + NIR + SWIR	BR	0.642	0.366	1.672	High
Cb	NIR	BPNN	0.437	0.183	1.333	Moderate
Cc	VIS + NIR	BR	0.387	0.108	1.277	Low

Note: High: $R^2 > 0.6$ and $RPD > 1.4$; Moderate: $0.4 \leq R^2 \leq 0.6$; Low: $R^2 < 0.4$.

The 1:1 validation plots of the optimal models are shown in Figure 5.

Photo, Ci, PI abs, and Ca showed relatively good agreement between measured and predicted values in both calibration and validation sets. Their data points were distributed closer to the 1:1 line, indicating that these parameters were more predictable at the canopy

scale. In contrast, parameters such as Cond and Fv/Fm showed weaker predictive performance, consistent with their lower R^2 and RPD values. This further supports the conclusion that canopy hyperspectral monitoring is more reliable for parameters linked to canopy structure, pigment status, or integrated photosynthetic performance, but less reliable for parameters with weak canopy-level spectral expression.

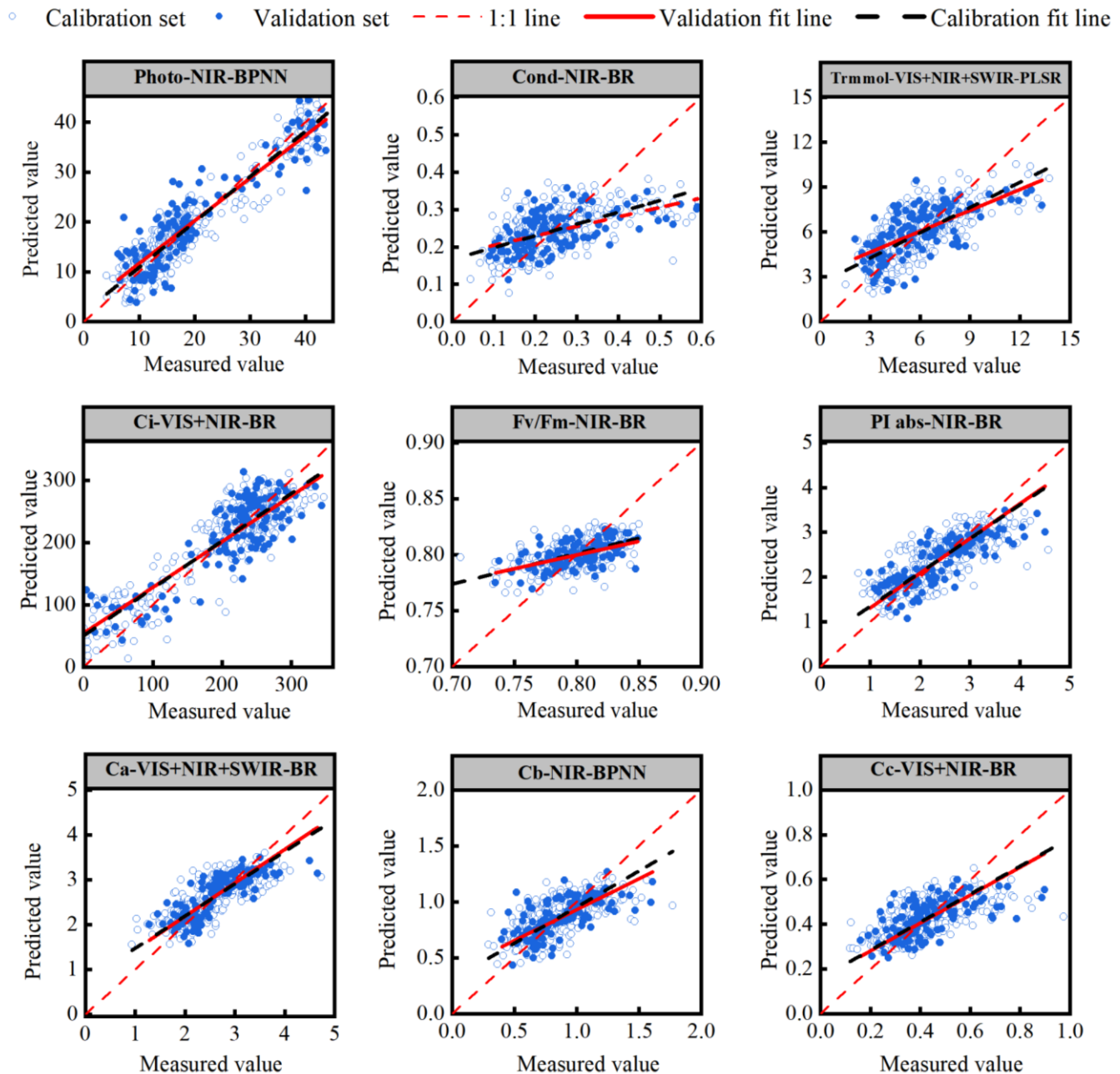


Figure 5. 1:1 fitting plots of the optimal models for photosynthetic phenotypic parameters at the canopy scale.

4. Discussion

4.1. Effects of Spectral Regions at Canopy Scale

The central finding of this study is that canopy-level prediction of photosynthetic phenotypic parameters was largely driven by canopy structural information captured in the NIR region. Different spectral regions contributed unequally to model performance, with NIR generally providing higher prediction accuracy for several parameters. This re-

sult suggests that, at the canopy scale, hyperspectral estimation is strongly influenced by structural and scattering-related signals rather than by direct retrieval of all physiological processes.

The dominant role of NIR can be explained from structural and radiative transfer perspectives. NIR reflectance is strongly affected by multiple scattering within the canopy and is closely related to structural traits such as canopy density, leaf area index, and biomass accumulation [16,27,39]. These structural attributes are closely associated with canopy photosynthetic capacity, which strengthens the relationship between NIR signals and photosynthetic phenotypic parameters. Compared with short-term physiological fluctuations, canopy structural information tends to represent cumulative growth status and is therefore more stable under field conditions. This helps explain why NIR-based models showed relatively robust performance across several parameters. In addition, NIR wavelengths are less affected by atmospheric water absorption than SWIR, which further improves their stability under field observation conditions [40,41].

In contrast, SWIR showed limited applicability in this study. Although SWIR reflectance is sensitive to vegetation water status and several biochemical constituents [19], its effectiveness at the canopy scale can be reduced by strong water absorption, exposed soil background, soil-moisture variation, canopy structural heterogeneity, and within-canopy shading [40–42]. Previous canopy-level studies in wheat have shown that wavelengths sensitive to leaf water status are distributed mainly in the NIR and SWIR regions, supporting the interpretation that SWIR primarily captures water-related variation rather than direct photosynthetic information [43]. When the winter wheat canopy is not completely closed, exposed soil contributes to the measured reflectance, and changes in soil moisture alter the SWIR background signal. Overlapping leaves and vertical canopy heterogeneity also reduce the spectral contribution from lower canopy layers and increase within-canopy variability. Consequently, canopy SWIR reflectance represents a mixture of leaf water status, soil background, shaded leaves, and canopy structure, weakening its direct relationship with the investigated photosynthetic phenotypic parameters. These factors partly explain the relatively low R^2 values of the SWIR-only models. Similar limitations have been reported in previous field hyperspectral studies [8,10].

The VIS + NIR combination showed relatively stable performance across multiple parameters. VIS mainly provides pigment-related absorption information, whereas NIR provides canopy structural and scattering information [16,18]. Their combination therefore integrates biochemical and structural information, improving model stability and reducing prediction uncertainty. This result supports the use of spectral-region-based modeling rather than relying only on full-spectrum inputs, especially when the objective is to identify efficient and interpretable spectral configurations for canopy-level monitoring [6,27].

4.2. Scale Effects on Hyperspectral Monitoring

Several key references cited in this study were based on leaf-level measurements, whereas the present study focused on canopy-level estimation under field conditions. Compared with leaf spectra, canopy reflectance represents an integrated signal from multiple leaves and vertical canopy layers and is more strongly affected by canopy architecture, soil background, illumination variation, viewing geometry, occlusion, and within-canopy shadowing. A recent multi-environment study in spring wheat showed that canopy spectra were more effective for predicting leaf area index and grain yield, whereas leaf spectra performed better for chlorophyll-fluorescence traits, demonstrating that spectral predictability depends on both observation scale and target-trait characteristics [44]. At the leaf level, spectral measurements provide more direct information on pigment absorption, leaf water status, and biochemical composition because interference from can-

opy structure and soil background is limited. In contrast, the present canopy-level results showed that NIR and VIS + NIR generally provided more stable predictive performance, whereas SWIR-only models showed relatively limited performance for most parameters. This contrast indicates that spectral–physiological relationships identified at the leaf level cannot be transferred directly to canopy-scale observations.

The relatively low prediction accuracy of some parameters indicates that not all photosynthetic phenotypic parameters can be effectively captured at the canopy scale. Canopy hyperspectral reflectance is determined by multiple interacting factors, including canopy structure, soil background, and illumination conditions [17,42]. Field measurements in winter wheat have also demonstrated that canopy reflectance contains a variable contribution from the soil background and that the magnitude of this contribution changes with crop development stage [45]. The observed signal is mainly dominated by the upper canopy structure, while occlusion effects reduce the spectral contribution from other canopy components [40,46]. Moreover, high-resolution hyperspectral imaging has revealed distinct spectral signatures between sunlit and shaded wheat canopy components, confirming that within-canopy illumination heterogeneity can substantially alter the measured spectral signal [47].

Clear vertical structural heterogeneity exists within the canopy, which weakens the direct relationship between spectral signals and physiological parameters. Under field conditions, physiological changes are not always directly reflected in spectral variation, and environmental fluctuations further increase observational uncertainty [17,42]. This effect is especially important for parameters that are weakly linked to canopy structure or are strongly affected by instantaneous physiological responses.

These factors help explain why parameters such as Cond and Fv/Fm showed relatively limited predictive performance. Nevertheless, canopy hyperspectral indices and PLSR have been successfully used to estimate wheat chlorophyll fluorescence traits under simulated salinity gradients, suggesting that the predictability of fluorescence parameters may improve when physiological variation is sufficiently large and systematically induced [48]. Their weak performance does not simply reflect model limitations; it also indicates that some physiological processes are difficult to infer from canopy reflectance alone. In contrast, parameters more closely associated with canopy structure, pigment status, or integrated photosynthetic performance were more readily captured by hyperspectral signals.

Therefore, the key limitation is not only the modeling algorithm, but also the scale mismatch between canopy-level spectral observations and the physiological processes represented by some target variables. Future improvement may require integrating structural information, environmental variables, or temporal features to better represent canopy heterogeneity and physiological dynamics.

4.3. Influence of Modeling Approaches

Model performance varied across modeling approaches, and the significant spectral region × modeling method interactions indicated that the effect of each modeling method depended on the spectral input and target parameter. Bayesian ridge regression (BR) showed stable performance across multiple parameters, which can be attributed to its regularization mechanism for handling multicollinearity in high-dimensional hyperspectral data [33]. This makes BR suitable for spectral datasets with strong correlations among bands.

Backpropagation neural network (BPNN) performed better for specific parameters, such as Photo and Cb, suggesting that nonlinear relationships existed between spectral inputs and these target variables. Neural networks can capture complex nonlinear patterns in hyperspectral data and have been used for crop physiological trait estimation un-

der field conditions [26,36]. In this study, the advantage of BPNN for selected parameters indicates that nonlinear modeling can be useful when the spectral–parameter relationship is complex.

Partial least squares regression (PLSR), as a linear method, performed well only for specific cases such as Trmmol. This suggests that PLSR may be suitable when the relationship between spectral variables and target parameters is relatively linear, but its predictive ability may be limited for parameters with indirect or nonlinear spectral responses [32].

Overall, model selection should consider both the structure of hyperspectral data and the physiological nature of the target parameter. More importantly, advanced modeling methods cannot fully compensate for weak spectral sensitivity at the canopy scale. For parameters that are not well represented in canopy reflectance, improving input information may be more important than increasing model complexity.

The repeated-partition analysis provided more rigorous evidence for the differences among spectral regions and modeling methods. Significant spectral region $\times$ modeling method interactions were observed for all nine parameters, indicating that no single modeling method consistently performed best across all spectral inputs and target traits. The numerical ranking obtained from a single calibration–validation partition was therefore sensitive to data partitioning in some cases. This finding highlights the importance of repeated model evaluation and paired statistical comparisons when identifying reliable spectral region–model combinations. Accordingly, combinations with the lowest mean RMSE were not interpreted as statistically superior unless the corresponding Holm-adjusted pairwise comparisons were significant.

4.4. Implications and Limitations

The results of this study indicate that spectral region selection is critical for canopy-level hyperspectral monitoring of photosynthetic phenotypic parameters. The strong performance of NIR and the stable performance of VIS + NIR suggest that effective monitoring at the canopy scale depends largely on capturing structural and pigment-related information. This finding is useful for simplifying spectral inputs, reducing redundant bands, and supporting the design of efficient field monitoring sensors [36]. Previous research on field-grown durum wheat also showed that selecting a small subset of relevant canopy spectral features could improve trait-estimation accuracy compared with broader spectral representations, further supporting the practical value of targeted wavelength selection [49].

A key implication is that canopy hyperspectral monitoring is more reliable for parameters that are structurally or integratively expressed at the canopy scale. Parameters directly or indirectly linked to canopy structure, pigment status, or integrated photosynthetic performance can be estimated with relatively higher accuracy. In contrast, parameters controlled by instantaneous physiological regulation or weak canopy-level spectral expression are more difficult to estimate accurately.

Several limitations should be acknowledged. As the data were collected from one experimental site during the 2022–2023 growing season, the robustness and transferability of the models still need to be further validated across different geographical regions, climatic years, and management conditions. In addition, canopy spectra are affected by soil background, illumination variability, canopy architecture, and environmental conditions, which were not fully modeled in this study [42]. The moderate or limited accuracy observed for some parameters also indicates that hyperspectral data alone may not fully capture complex physiological processes at the canopy scale [10].

In addition, because alternative SWIR-oriented preprocessing methods, continuum-based features, and feature-selection algorithms were not systematically compared, the

present analysis cannot completely separate intrinsic SWIR information limitations from methodological effects. The nonsignificant relationship between the number of selected wavelengths and predictive performance did not support feature quantity alone as the primary explanation for the weak SWIR results.

4.5. Future Work

Future research should focus on two aspects: improving model generalization and enhancing canopy information representation. The stability of NIR and VIS + NIR configurations should be further validated across different years, ecological regions, and cultivation conditions. This would help determine whether the structural dominance observed in this study is consistent under broader field conditions.

To address the influence of canopy structural heterogeneity, hyperspectral data could be integrated with LiDAR-derived structural information and thermal infrared data reflecting canopy temperature. Such multi-source information may improve the representation of canopy architecture, physiological status, and environmental stress responses [50].

From the modeling perspective, ensemble learning and deep learning methods could be further compared for different photosynthetic phenotypic parameters [51,52]. Incorporating time-series information across growth stages may also help characterize dynamic changes in photosynthetic function. Based on the key spectral regions identified in this study, future work could optimize sensor band configurations and develop more efficient and cost-effective crop hyperspectral monitoring systems.

5. Conclusions

This study evaluated the contribution of VIS, NIR, SWIR, and their combinations to canopy-level estimation of photosynthetic phenotypic parameters in winter wheat. The results showed that spectral region selection had a clear influence on model performance. NIR provided the most consistent contribution, indicating that canopy structural and scattering information plays an important role in estimating photosynthetic-related traits at the canopy scale. The VIS + NIR combination also showed stable performance, suggesting that integrating pigment absorption information from VIS with structural information from NIR can improve the reliability of canopy-level monitoring.

The predictability of different parameters varied substantially. Photosynthetic rate, intercellular CO₂ concentration, performance index on an absorption basis, and chlorophyll a content were more reliably estimated, whereas stomatal conductance, maximum photochemical efficiency, chlorophyll b content, and carotenoid content showed limited or moderate predictability. This indicates that canopy hyperspectral reflectance is more suitable for traits closely related to canopy structure, pigment status, or integrated photosynthetic performance, but less effective for parameters strongly affected by instantaneous physiological regulation.

These findings provide practical guidance for spectral-region selection and sensor-band optimization in field phenotyping. For efficient canopy-level monitoring of winter wheat photosynthetic phenotypic parameters, NIR bands should be prioritized, while VIS bands can be incorporated to enhance pigment-related information. SWIR-only models generally showed limited performance, and the number of CARS-selected wavelengths alone did not explain this limitation, indicating that SWIR performance was jointly affected by trait-spectral relationships, canopy-scale interference, and potential methodological constraints.

However, because the experiment was conducted at a single site during one growing season, the identified spectral configurations and model performance require further val-

idation across multiple years, geographical regions, genotypes, and management conditions before broader application.

Author Contributions: Conceptualization, S.G. and C.W.; methodology, S.G., D.W., R.H., B.S., W.Y. and C.W.; validation, S.G., D.W., R.H., B.S. and L.X.; formal analysis, S.G., D.W. and B.S.; investigation, S.G., D.W., R.H., T.L., L.G., Y.Z., C.Y., H.S. and L.X.; resources, W.Y., H.S., M.F., X.J. and C.W.; data curation, S.G., D.W., R.H., T.L., L.G., Y.Z., C.Y., H.S., M.F. and L.X.; writing—original draft preparation, S.G. and D.W.; writing—review and editing, S.G., D.W., B.S., X.Q., W.Y., L.X., M.F., X.J. and C.W.; visualization, S.G., D.W. and M.F.; supervision, W.Y., M.F., X.J. and C.W.; project administration, W.Y., M.F., X.J. and C.W.; funding acquisition, H.S., M.F., X.J. and C.W. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the Basic Research Program of Shanxi Province (202303021212090, 202203021221231, 202303021212260), the Research Project Supported by Shanxi Scholarship Council of China (2025-022), the Earmarked Fund for Modern Agro-industry Technology Research System (2026CYJSTX02-23), and the National Natural Science Foundation of China (31871571, 31371572).

Institutional Review Board Statement: Not applicable.

Data Availability Statement: The raw data supporting the conclusions of this article will be made available by the authors on request.

Acknowledgments: The authors would like to thank the staff of the College of Agriculture, Shanxi Agricultural University, and the collaborators involved in field management, sample collection, and data acquisition for their assistance during the experiment.

Conflicts of Interest: The authors declare no conflicts of interest.

Appendix A. Methods

Appendix A.1 Additional Details of Field Spectral Acquisition

During canopy spectral acquisition, the sensor probe was kept vertically above the winter wheat canopy, with an approximate distance of 80 cm from the canopy surface. For each plot, three representative sampling points with relatively uniform growth were selected, and three spectral measurements were collected at each point. After abnormal spectra were removed, the remaining repeated measurements were averaged to obtain one representative canopy reflectance curve for each plot.

This repeated measurement strategy was used to reduce random measurement errors and improve plot-level spectral representativeness in field hyperspectral observations [15,16].

Appendix A.2 Additional Details of Spectral Preprocessing

After spectral acquisition, abnormal spectral curves were removed using View-SpecPro software. The repeated spectral measurements of each sample were averaged before subsequent spectral region division and feature selection.

The bands of 350–400 nm and 2400–2500 nm were removed because of relatively low detector sensitivity and high noise levels at the two ends of the spectral range. The wavelength ranges of 1300–1400 nm and 1800–1950 nm were also excluded because they are strongly affected by water absorption and may cause unstable spectral fluctuations. Similar preprocessing procedures have been used in hyperspectral studies to reduce noise and improve model stability [13,18,19].

Appendix A.3 Additional Details of CARS Feature Selection

Competitive adaptive reweighted sampling (CARS) was applied separately to each spectral input and each target parameter. During the CARS procedure, wavelength subsets were generated through repeated sampling. Variables with relatively low contributions were gradually removed, and the optimal wavelength subset was selected according to the minimum root mean square error of cross-validation (RMSECV) [18,22].

This procedure was used to reduce spectral redundancy while retaining informative wavelengths for model construction. Previous studies have shown that CARS is effective for hyperspectral feature selection and dimensionality reduction [26,27].

Appendix A.4 Additional Details of Model Implementation

For model comparison, all spectral inputs and target parameters used the same dataset partitioning strategy. The calibration set was used for model training, and the validation set was used for independent performance evaluation. The same preprocessing results and CARS-selected feature variables were used within each corresponding spectral input to ensure comparability among modeling methods.

PLSR, BR, and BPNN were selected to represent linear baseline modeling, regularized linear modeling, and nonlinear modeling, respectively. This design allowed the study to compare whether model performance was mainly affected by spectral region selection or by model type.

Appendix A.5 Additional Details of Model Evaluation

All evaluation metrics were calculated using the validation set. R^2 was used to assess the explanatory ability of the model, RMSE was used to quantify prediction error, and RPD was used to evaluate predictive reliability. The same evaluation procedure was applied to all spectral regions, spectral combinations, and modeling methods to ensure consistent comparison.

Appendix B. Tables

Table A1. Model performance for canopy-level photosynthetic parameters under different spectral regions and their combinations.

Variables	Spectral Region	PLSR			BR			BPNN		
		R^2	RMSE	RPD	R^2	RMSE	RPD	R^2	RMSE	RPD
Photo	VIS	0.663	6.298	1.723	0.624	6.690	1.632	0.611	6.811	1.603
	NIR	0.799	4.860	2.233	0.825	4.568	2.390	0.828	4.531	2.409
	SWIR	0.430	8.189	1.325	0.422	8.300	1.315	0.458	8.035	1.358
	VIS + NIR	0.790	4.973	2.182	0.801	4.864	2.244	0.693	6.043	1.806
	NIR + SWIR	0.742	5.516	1.967	0.718	5.792	1.885	0.775	5.174	2.110
	VIS + SWIR	0.644	6.474	1.676	0.348	8.811	1.239	0.672	6.256	1.745
	VIS + NIR + SWIR	0.779	5.095	2.130	0.680	6.171	1.769	0.793	4.962	2.200
Cond	VIS	0.065	0.102	1.038	0.013	0.105	1.007	0.207	0.094	1.123
	NIR	0.157	0.097	1.093	0.264	0.091	1.165	0.221	0.093	1.133
	SWIR	0.006	0.102	1.003	0.018	0.105	1.009	0.195	0.095	1.114
	VIS + NIR	0.216	0.094	1.134	0.259	0.091	1.162	0.243	0.092	1.149
	NIR + SWIR	0.044	0.103	1.027	0.206	0.094	1.122	0.236	0.092	1.144
	VIS + SWIR	0.009	0.102	1.004	0.018	0.105	1.009	0.161	0.097	1.092
	VIS + NIR + SWIR	0.152	0.097	1.090	0.140	0.098	1.078	0.219	0.093	1.132
Trmmol	VIS	0.235	2.050	1.144	0.075	2.296	1.040	0.123	2.236	1.068
	NIR	0.382	1.842	1.272	0.417	1.824	1.309	0.312	1.981	1.205
	SWIR	0.139	2.175	1.078	0.245	2.074	1.151	0.274	2.034	1.174
	VIS + NIR	0.421	1.784	1.314	0.390	1.865	1.280	0.372	1.891	1.262

	NIR + SWIR	0.301	1.959	1.196	0.395	1.858	1.285	0.310	1.983	1.204
	VIS + SWIR	0.371	1.859	1.261	0.079	2.291	1.042	0.144	2.210	1.081
	VIS + NIR + SWIR	0.428	1.774	1.322	0.362	1.907	1.252	0.334	1.948	1.226
	VIS	0.486	54.625	1.394	0.544	51.457	1.480	0.664	44.149	1.725
	NIR	0.651	45.014	1.692	0.654	44.820	1.699	0.667	43.959	1.733
	SWIR	0.295	63.950	1.191	0.145	70.438	1.081	0.339	61.934	1.230
Ci	VIS + NIR	0.661	44.358	1.717	0.710	41.051	1.855	0.542	51.563	1.477
	NIR + SWIR	0.048	75.433	1.025	0.557	50.712	1.502	0.522	52.658	1.446
	VIS + SWIR	0.085	73.958	1.045	0.594	31.077	1.569	0.572	49.830	1.529
	VIS + NIR + SWIR	0.677	43.309	1.759	0.356	61.147	1.246	0.293	64.034	1.189

Note: The best result for each metric is shown in bold.

Table A2. Model performance for canopy-level chlorophyll fluorescence parameters under different spectral regions and their combinations.

Variables	Spectral Region	PLSR			BR			BPNN		
		R ²	RMSE	RPD	R ²	RMSE	RPD	R ²	RMSE	RPD
Fv/Fm	VIS	0.021	0.023	1.011	0.077	0.023	1.041	0.052	0.023	1.027
	NIR	0.019	0.023	1.009	0.267	0.020	1.168	0.193	0.021	1.113
	SWIR	0.029	0.023	1.015	0.068	0.023	1.036	0.094	0.023	1.050
	VIS + NIR	0.081	0.023	1.043	0.252	0.020	1.156	0.207	0.021	1.123
	NIR + SWIR	0.037	0.024	0.982	0.080	0.023	1.047	0.026	0.023	1.013
	VIS + SWIR	0.042	0.023	1.021	0.027	0.023	1.018	0.136	0.022	1.076
	VIS + NIR + SWIR	0.052	0.023	1.027	0.046	0.023	1.028	0.054	0.023	1.028
PI abs	VIS	0.546	0.514	1.483	0.558	0.507	1.504	0.480	0.550	1.386
	NIR	0.604	0.480	1.588	0.649	0.451	1.689	0.463	0.559	1.364
	SWIR	0.395	0.593	1.285	0.299	0.638	1.194	0.472	0.554	1.376
	VIS + NIR	0.563	0.504	1.513	0.640	0.458	1.666	0.528	0.524	1.456
	NIR + SWIR	0.561	0.505	1.510	0.587	0.490	1.556	0.522	0.527	1.446
	VIS + SWIR	0.522	0.527	1.447	0.544	0.515	1.481	0.496	0.541	1.408
	VIS + NIR + SWIR	0.5110	0.5330	1.429	0.603	0.480	1.588	0.462	0.559	1.363

Note: The best result for each metric is shown in bold.

Table A3. Model performance for canopy-level photosynthetic pigment parameters under different spectral regions and their combinations.

Variables	Spectral Region	PLSR			BR			BPNN		
		R ²	RMSE	RPD	R ²	RMSE	RPD	R ²	RMSE	RPD
Ca	VIS	0.610	0.382	1.602	0.607	0.383	1.596	0.559	0.406	1.505
	NIR	0.621	0.377	1.623	0.615	0.379	1.612	0.590	0.392	1.561
	SWIR	0.281	0.519	1.179	0.437	0.459	1.333	0.461	0.449	1.363
	VIS + NIR	0.665	0.354	1.728	0.627	0.373	1.638	0.610	0.382	1.602
	NIR + SWIR	0.658	0.358	1.71	0.624	0.375	1.632	0.600	0.387	1.581
	VIS + SWIR	0.435	0.460	1.330	0.553	0.409	1.496	0.582	0.395	1.547
	VIS + NIR + SWIR	0.582	0.395	1.547	0.642	0.366	1.672	0.618	0.378	1.619
Cb	VIS	0.188	0.220	1.110	0.339	0.198	1.230	0.317	0.201	1.210
	NIR	0.381	0.192	1.271	0.395	0.190	1.285	0.437	0.183	1.333
	SWIR	0.139	0.226	1.078	0.148	0.225	1.083	0.349	0.197	1.24
	VIS + NIR	0.408	0.188	1.299	0.412	0.187	1.304	0.374	0.193	1.264
	NIR + SWIR	0.327	0.200	1.219	0.407	0.188	1.299	0.373	0.193	1.263
	VIS + SWIR	0.270	0.208	1.170	0.388	0.191	1.278	0.234	0.213	1.143
	VIS + NIR + SWIR	0.371	0.193	1.261	0.399	0.189	1.290	0.411	0.187	1.303
Cc	VIS	0.031	0.136	1.016	0.288	0.116	1.185	0.302	0.115	1.197
	NIR	0.019	0.136	1.010	0.360	0.110	1.250	0.380	0.108	1.270

SWIR	0.061	0.133	1.032	0.287	0.116	1.185	0.273	0.117	1.173
VIS + NIR	0.031	0.136	1.016	0.387	0.108	1.277	0.380	0.108	1.270
NIR + SWIR	0.054	0.134	1.028	0.341	0.112	1.232	0.263	0.118	1.165
VIS + SWIR	0.061	0.133	1.032	0.311	0.114	1.205	0.287	0.116	1.184
VIS + NIR + SWIR	0.042	0.135	1.022	0.366	0.110	1.256	0.329	0.113	1.221

Note: The best result for each metric is shown in bold.

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