**Table S1.** Prediction results of pigments using different pre-processing methods.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Pigments** | **Pretreatment** | **Calibration set** |  | **Prediction set** | **RPD** |
| **Rc2** | **RMSEc** |  | **Rp2** | **RMSEp** |
| Chla | Raw | 0.7632 | 1.97 |  | 0.7976 | 1.53 | 2.22 |
| S-G | 0.7645 | 1.97 |  | 0.7781 | 1.55 | 2.12 |
| SNV | 0.8002 | 1.83 |  | 0.7171 | 1.75 | 1.88 |
| S-G+SNV | 0.7877 | 1.88 |  | 0.8064 | 1.49 | 2.27 |
| Chlb | Raw | 0.7863 | 0.78 |  | 0.7831 | 0.56 | 2.15 |
| S-G | 0.7790 | 0.79 |  | 0.8286 | 0.54 | 2.42 |
| SNV | 0.8036 | 0.73 |  | 0.8223 | 0.59 | 2.37 |
| S-G+SNV | 0.7944 | 0.75 |  | 0.8156 | 0.60 | 2.33 |
| Chll | Raw | 0.7863 | 2.60 |  | 0.7369 | 2.46 | 1.95 |
| S-G | 0.7772 | 2.67 |  | 0.7646 | 2.29 | 2.06 |
| SNV | 0.7964 | 2.53 |  | 0.7776 | 2.25 | 2.12 |
| S-G+SNV | 0.7982 | 2.53 |  | 0.7677 | 2.29 | 2.07 |
| Caro | Raw | 0.6827 | 0.35 |  | 0.6912 | 0.29 | 1.80 |
| S-G | 0.6710 | 0.36 |  | 0.6828 | 0.29 | 1.78 |
| SNV | 0.6768 | 0.35 |  | 0.7294 | 0.29 | 1.92 |
| S-G+SNV | 0.6689 | 0.36 |  | 0.7213 | 0.28 | 1.89 |

**Table S2.** Classification of variables screened by the CARS algorithm using the IRIV algorithm.

|  |  |  |
| --- | --- | --- |
| **Pigment****s** | **Variable classification** | **Spectral variables (nm)** |
| Chla | Strong information | 473, 504, 672, 698, 702 |
| Weak information | 506, 691, 692, 715, 716, 730, 731, 745, 760, 821, 831 |
| Chlb | Strong information | 439, 497, 667, 689, 691, 702, 703, 715, 716 |
| Weak information | 734, 736, 737, 760, 761, 864, 895 |
| Chll | Strong information | 473, 502, 670, 692, 702, 703, 745 |
| Weak information | 506, 672, 691, 715, 716, 731, 733, 736, 737, 760, 821, 832 |
| Caro | Strong information | 468, 473, 506, 761, 890 |
| Weak information | 510, 671, 691, 694, 699, 700, 715, 716, 730, 731, 733, 821, 823 |

**Table S3.** The key wavelengths screened by CARS and CARS-IRIV algorithms for Chla, Chlb, Chll, and Caro.

|  |  |  |  |
| --- | --- | --- | --- |
| **Pigment****s** | **VSMa** | **NVb** | **Key spectral variables (nm)** |
| Chla | CARS | 16 | 473, 504, 506, 672, 691, 692, 698, 702, 715, 716, 730, 731, 745, 760, 821, 831 |
| CARS-IRIV | 12 | 473, 506, 672, 692, 698, 702, 715, 731, 745, 760, 821, 831 |
| Chlb | CARS | 16 | 439, 497, 667, 689, 691,702, 703, 715, 716, 734, 736, 737, 760, 761, 864, 895 |
| CARS-IRIV | 10 | 439, 497, 667, 691, 702, 715, 736, 760, 864, 895 |
| Chll | CARS | 19 | 473, 502, 506, 670, 672, 691, 692, 702, 703, 715, 716, 731, 733, 736, 737, 745, 760, 821, 832 |
| CARS-IRIV | 12 | 473, 506, 672, 691, 702, 715, 731, 736, 745, 760, 821, 832 |
| Caro | CARS | 18 | 468, 473, 506, 510, 671, 691, 694, 699, 700, 715, 716, 730, 731, 733, 761,821, 823, 890 |
| CARS-IRIV | 11 | 473, 506, 510, 671, 691, 699, 715, 730, 761, 821, 890 |

aVSM: variables selection methods; bNV: number of variables.

**Table S4.** Fertilizer (mg/L), EC, and pH with different nitrogen concentrations.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Fertilizer** | **N20** | **N40** | **N60** | **N80** | **N100** | **N120** | **N140** | **N160** | **N180** | **N200** |
| Calcium nitrate | 0 | 307.48 | 605.68 | 913.15 | 1216 | 1216 | 1216 | 1216 | 1216 | 1216 |
| Calcium fertilizer | 491.57 | 367.27 | 246.72 | 122.43 | 0 | 0 | 0 | 0 | 0 | 0 |
| Urea | 0 | 0 | 0 | 0 | 0 | 131.67 | 262.34 | 395.01 | 526.68 | 658.35 |
| Calcium ammonium nitrate | 42.1 | 42.1 | 42.1 | 42.1 | 42.1 | 42.1 | 42.1 | 42.1 | 42.1 | 42.1 |
| Potassium nitrate | 395 | 395 | 395 | 395 | 395 | 395 | 395 | 395 | 395 | 395 |
| Potassium phosphate monobasic | 208 | 208 | 208 | 208 | 208 | 208 | 208 | 208 | 208 | 208 |
| Potassium sulphate | 393 | 393 | 393 | 393 | 393 | 393 | 393 | 393 | 393 | 393 |
| Magnesium sulphate | 466 | 466 | 466 | 466 | 466 | 466 | 466 | 466 | 466 | 466 |
| Nitrogen concentration | 59.64 | 121.14 | 181.7 | 242.27 | 302.84 | 363.41 | 423.98 | 484.54 | 545.54 | 605.68 |
| EC | 2.49 | 2.42 | 2.40 | 2.30 | 2.29 | 2.33 | 2.43 | 2.50 | 2.53 | 2.56 |
| pH | 6.88 | 6.84 | 6.80 | 6.95 | 6.99 | 7.05 | 7.00 | 6.95 | 6.96 | 6.98 |



**Figure S1.** The changes in sample variables (NSV), RMSEcv, and regression coefficient paths (RCs) in a subset of CARS arithmetic for Chla.



**Figure S2.** The changes in sample variables (NSV), RMSEcv, and regression coefficient paths (RCs) in a subset of CARS arithmetic for Chlb.



**Figure S3.** The changes in sample variables (NSV), RMSEcv, and regression coefficient paths (RCs) in a subset of CARS arithmetic for Chll.



**Figure S4.** The changes in sample variables (NSV), RMSEcv, and regression coefficient paths (RCs) in a subset of CARS arithmetic for Caro.