

# SUPPLEMENTARY MATERIAL

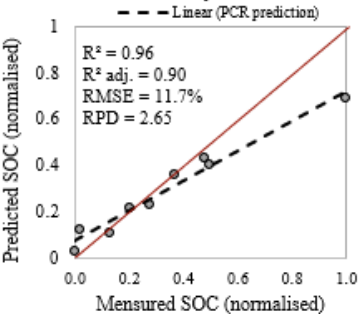
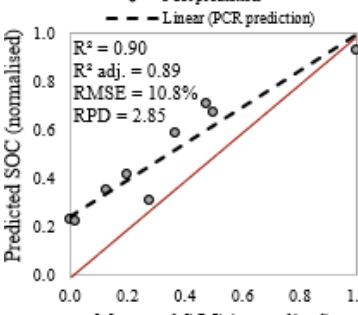
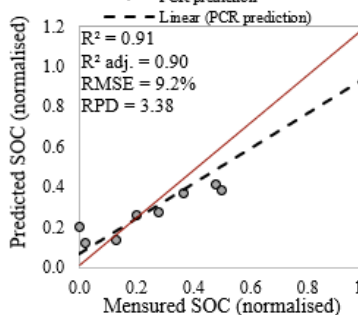
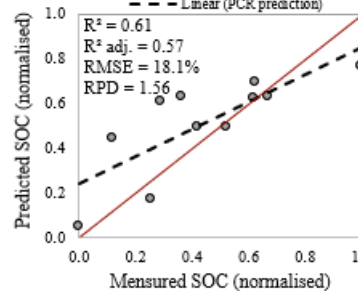
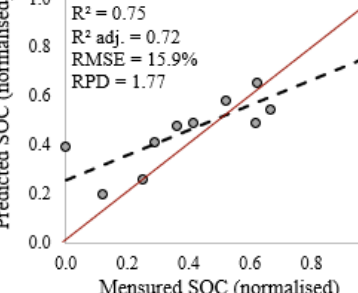
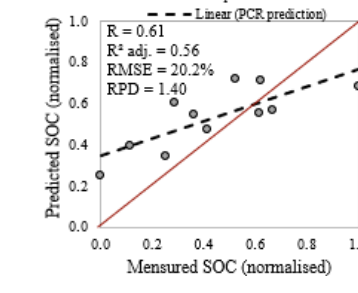
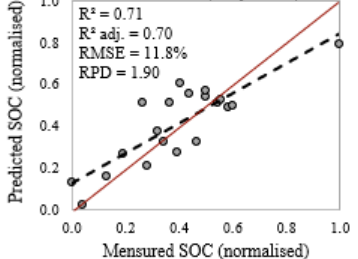
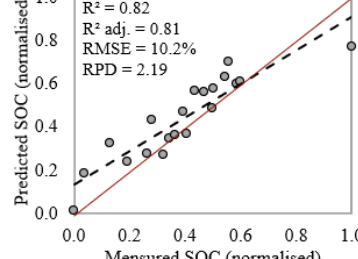
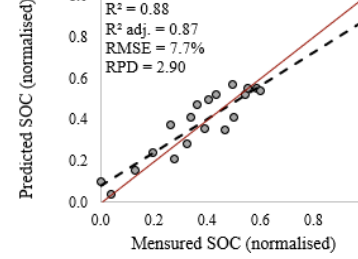
Table S1. Validation results of the PCR models for estimating SOC using the 350-2500 nm spectrum.

PCR	Untransformed Full Spectrum	First Derivative Full Spectrum	Smoothed Full Spectrum
A1	<p><b>A1 - Untransformed spectrum (11 factors)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.86</math> <math>R^2 \text{ adj.} = 0.84</math> RMSE = 15.2% RPD = 2.03</p>	<p><b>A1 - 1<sup>st</sup> derivative (17 factors)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.91</math> <math>R^2 \text{ adj.} = 0.90</math> RMSE = 17.6% RPD = 1.76</p>	<p><b>A1 - Smoothed reflectance (11 factors)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.86</math> <math>R^2 \text{ adj.} = 0.84</math> RMSE = 15.0% RPD = 2.06</p>
A2	<p><b>A2 - Untransformed spectrum (19 factors)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.40</math> <math>R^2 \text{ adj.} = 0.34</math> RMSE = 21.7% RPD = 1.30</p> <p><b>A1 &amp; A2 - Untransformed spectrum (26 factors)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.77</math> <math>R^2 \text{ adj.} = 0.76</math> RMSE = 10.6% RPD = 2.11</p>	<p><b>A2 - 1<sup>st</sup> derivative (5 factors)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.13</math> <math>R^2 \text{ adj.} = 0.03</math> RMSE = 25.7% RPD = 1.10</p>	<p><b>A2 - Smoothed reflectance (20 factors)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.39</math> <math>R^2 \text{ adj.} = 0.32</math> RMSE = 22.1% RPD = 1.28</p>
A1&A2	<p><b>A1 &amp; A2 - Untransformed spectrum (26 factors)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.77</math> <math>R^2 \text{ adj.} = 0.76</math> RMSE = 10.6% RPD = 2.11</p>	<p><b>A1 &amp; A2 - 1<sup>st</sup> derivative (1 factor)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.17</math> <math>R^2 \text{ adj.} = 0.13</math> RMSE = 29.2% RPD = 0.77</p>	<p><b>A1 &amp; A2 - Smoothed reflectance (20 factors)</b></p> <p>Predicted SOC (normalised)</p> <p>Measured SOC (normalised)</p> <p>PCR prediction Linear (PCR prediction)</p> <p><math>R^2 = 0.73</math> <math>R^2 \text{ adj.} = 0.72</math> RMSE = 11.6% RPD = 1.93</p>

**Table S2. Validation results of the PLSR models for estimating SOC using the 350-2500 nm spectrum**

PLSR	Untransformed Full Spectrum	First Derivative Full Spectrum	Smoothed Full Spectrum
A1	<p><b>A1 - Untransformed spectrum (8 factors)</b></p> <p> <math>R^2 = 0.81</math>  <math>R^2 \text{ adj.} = 0.78</math>  <math>\text{RMSE} = 15.0\%</math>  <math>\text{RPD} = 2.07</math> </p>	<p><b>A1 - 1<sup>st</sup> derivative (6 factors)</b></p> <p> <math>R^2 = 0.88</math>  <math>R^2 \text{ adj.} = 0.86</math>  <math>\text{RMSE} = 16.0\%</math>  <math>\text{RPD} = 1.93</math> </p>	<p><b>A1 - Smoothed reflectance (7 factors)</b></p> <p> <math>R^2 = 0.84</math>  <math>R^2 \text{ adj.} = 0.81</math>  <math>\text{RMSE} = 15.1\%</math>  <math>\text{RPD} = 2.04</math> </p>
A2	<p><b>A2 - Untransformed spectrum (11 factors)</b></p> <p> <math>R^2 = 0.44</math>  <math>R^2 \text{ adj.} = 0.38</math>  <math>\text{RMSE} = 22.3\%</math>  <math>\text{RPD} = 1.27</math> </p>	<p><b>A2 - 1<sup>st</sup> derivative (1 factor)</b></p> <p> <math>R^2 = 0.07</math>  <math>R^2 \text{ adj.} = 0.02</math>  <math>\text{RMSE} = 29.2\%</math>  <math>\text{RPD} = 0.97</math> </p>	<p><b>A2 - Smoothed reflectance (11 factors)</b></p> <p> <math>R^2 = 0.47</math>  <math>R^2 \text{ adj.} = 0.41</math>  <math>\text{RMSE} = 21.8\%</math>  <math>\text{RPD} = 1.29</math> </p>
A1&A2	<p><b>A1 &amp; A2 - Untransformed spectrum (12 factors)</b></p> <p> <math>R^2 = 0.73</math>  <math>R^2 \text{ adj.} = 0.71</math>  <math>\text{RMSE} = 11.9\%</math>  <math>\text{RPD} = 1.88</math> </p>	<p><b>A1 &amp; A2 - 1<sup>st</sup> derivative (1 factor)</b></p> <p> <math>R^2 = 0.19</math>  <math>R^2 \text{ adj.} = 0.14</math>  <math>\text{RMSE} = 30.2\%</math>  <math>\text{RPD} = 0.74</math> </p>	<p><b>A1 &amp; A2 - Smoothed reflectance (20 factors)</b></p> <p> <math>R^2 = 0.76</math>  <math>R^2 \text{ adj.} = 0.75</math>  <math>\text{RMSE} = 11.2\%</math>  <math>\text{RPD} = 1.99</math> </p>

Table S3. Validation results of the PCR models for SOC prediction after selecting the spectral bands.

PCR	Untransformed Selected Bands	First Derivative Selected Bands	Smoothed Selected Bands
A1	<b>A1 - Untransformed spectrum (10 factors)</b> 	<b>A1 - 1<sup>st</sup> derivative (10 factors)</b> 	<b>A1 - Smoothed reflectance (9 factors)</b> 
A2	<b>A2 - Untransformed spectrum (5 factors)</b> 	<b>A2 - 1<sup>st</sup> derivative (10 factors)</b> 	<b>A2 - Smoothed reflectance (4 factors)</b> 
A1&A2	<b>A1&amp;A2 - Untransformed spectrum (6 factors)</b> 	<b>A1&amp;A2 - 1<sup>st</sup> derivative (11 factors)</b> 	<b>A1&amp;A2 - Smoothed reflectance (13 factors)</b> 

**Table S4.** Validation results of the PLSR models for SOC prediction after selecting the spectral bands.

PLSR	Untransformed Selected Bands	First Derivative Selected Bands	Smoothed Selected Bands
A1	<p><b>A1 - Untransformed spectrum (9 factors)</b></p> <p> <math>R^2 = 0.95</math>  <math>R^2 \text{ adj.} = 0.95</math>  <math>\text{RMSE} = 14.1\%</math>  <math>\text{RPD} = 2.19</math> </p>	<p><b>A1 - 1<sup>st</sup> derivative (9 factors)</b></p> <p> <math>R^2 = 0.90</math>  <math>R^2 \text{ adj.} = 0.89</math>  <math>\text{RMSE} = 10.9\%</math>  <math>\text{RPD} = 2.85</math> </p>	<p><b>A1 - Smoothed reflectance (8 factors)</b></p> <p> <math>R^2 = 0.92</math>  <math>R^2 \text{ adj.} = 0.91</math>  <math>\text{RMSE} = 8.7\%</math>  <math>\text{RPD} = 3.56</math> </p>
A2	<p><b>A2 - Untransformed spectrum (5 factors)</b></p> <p> <math>R^2 = 0.61</math>  <math>R^2 \text{ adj.} = 0.57</math>  <math>\text{RMSE} = 18.2\%</math>  <math>\text{RPD} = 1.56</math> </p>	<p><b>A2 - 1<sup>st</sup> derivative (7 factors)</b></p> <p> <math>R^2 = 0.74</math>  <math>R^2 \text{ adj.} = 0.71</math>  <math>\text{RMSE} = 15.9\%</math>  <math>\text{RPD} = 1.78</math> </p>	<p><b>A2 - Smoothed reflectance (4 factors)</b></p> <p> <math>R^2 = 0.61</math>  <math>R^2 \text{ adj.} = 0.56</math>  <math>\text{RMSE} = 20.2\%</math>  <math>\text{RPD} = 1.40</math> </p>
A1&A2	<p><b>A1&amp;A2 - Untransformed spectrum (6 factors)</b></p> <p> <math>R^2 = 0.71</math>  <math>R^2 \text{ adj.} = 0.70</math>  <math>\text{RMSE} = 11.8\%</math>  <math>\text{RPD} = 1.90</math> </p>	<p><b>A1&amp;A2 - 1<sup>st</sup> derivative (7 factors)</b></p> <p> <math>R^2 = 0.86</math>  <math>R^2 \text{ adj.} = 0.85</math>  <math>\text{RMSE} = 9.7\%</math>  <math>\text{RPD} = 2.30</math> </p>	<p><b>A1&amp;A2 - Smoothed reflectance (9 factors)</b></p> <p> <math>R^2 = 0.88</math>  <math>R^2 \text{ adj.} = 0.87</math>  <math>\text{RMSE} = 7.9\%</math>  <math>\text{RPD} = 2.85</math> </p>