Supporting information

Estimation of pigment concentration in LDPE *via* in-line hyperspectral imaging and machine learning

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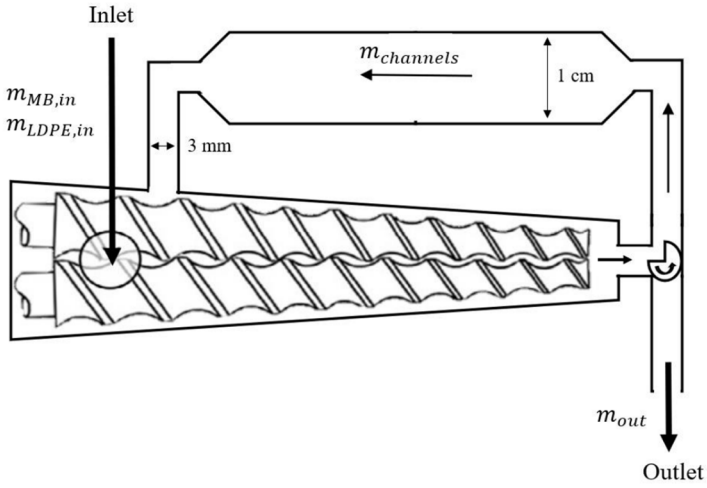
Content

S1. Samples preparation

Schematic of the twin-screw extruder for compounding of the samples. The inlet and outlet are marked.



Concentration calculation

Assumptions: The concentration in the channels was always equal to the concentration out (x_{out}) of the extruder, and the pigment concentration of the pure LDPE was zero. The calculation of the concentration assumes homogenic mixing and no effect from dead zones in the compounder both in the feeding zone, screw zone, channels, and recycling chamber.

Mass balance equations:

Initial run:

$$m_{total,in} = m_{MB,in} + m_{LDPE,in} \quad \text{(S1)}$$

$$m_{channels} = m_{total,in} - m_{out} \quad \text{(S2)}$$

$$x_{out_{n=1\ and\ 2}} = \frac{m_{MB,in} \cdot x_{MB} + m_{LDPE,in} \cdot x_{LDPE}}{m_{total,in}} \quad \text{(S3)}$$

When new LDPE is added:

$$x_{channels} = x_{out_{n-1}} \quad \text{(S4)}$$

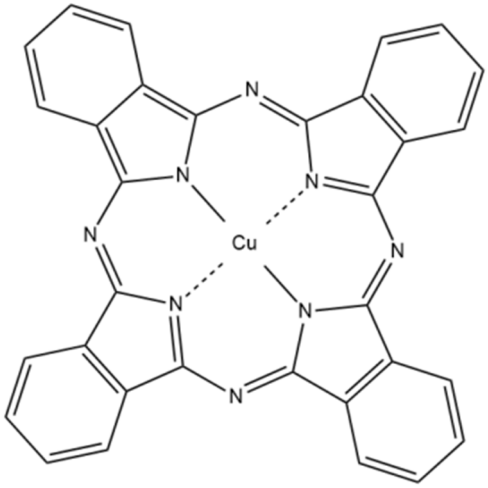
$$m_{channels} = m_{channels_{n-1}} + m_{LDPE,in} - m_{out} \quad \text{(S5)}$$

$$x_{out} = \frac{m_{channels} \cdot x_{channels} + m_{LDPE,in} \cdot x_{LDPE}}{m_{LDPE,in} + m_{channels}} \quad \text{(S6)}$$

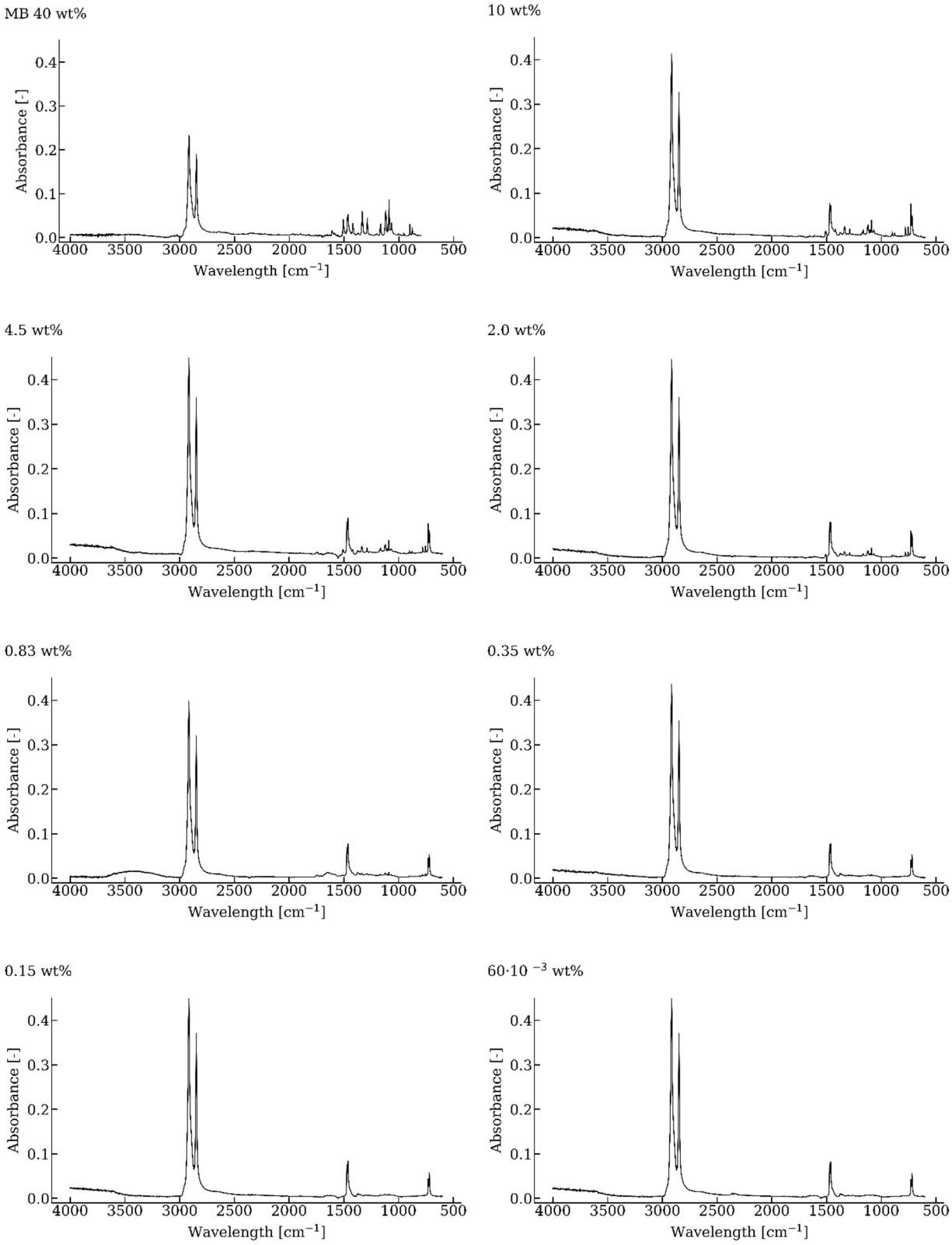
Where, x: pigment concentration in wt%, m_{in}: mass going into the extruder of either MB, LDPE or total, $m_{channels}$: total mass in channels and recycling chamber, n: the cycle number.

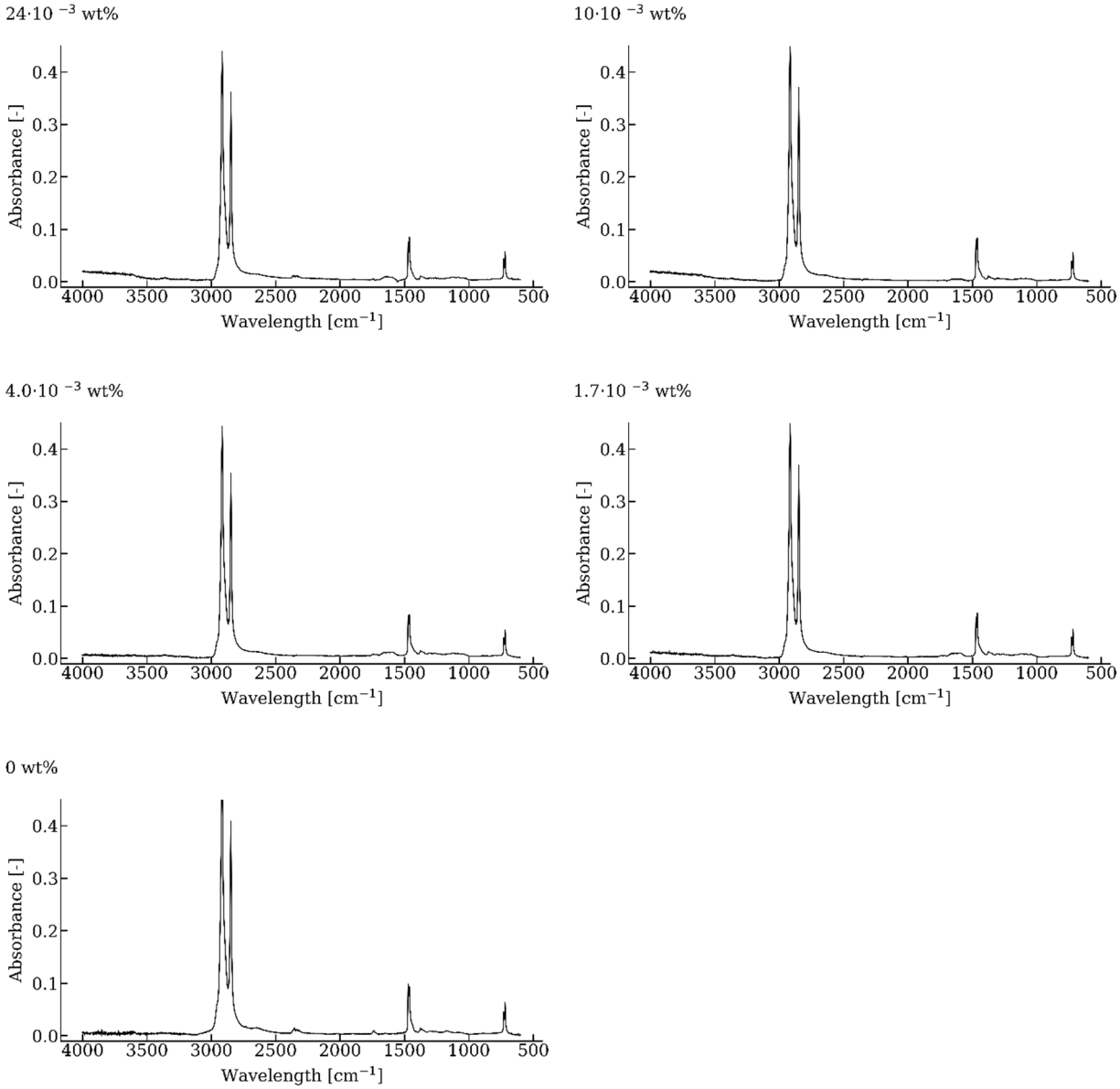
Pigment Blue 15:3

Molecular structure of Pigment Blue 15:3 (Copper (II) phthalocyanine, $C_{32}H_{16}CuN_8$, CAS 147-14-8) pigment.



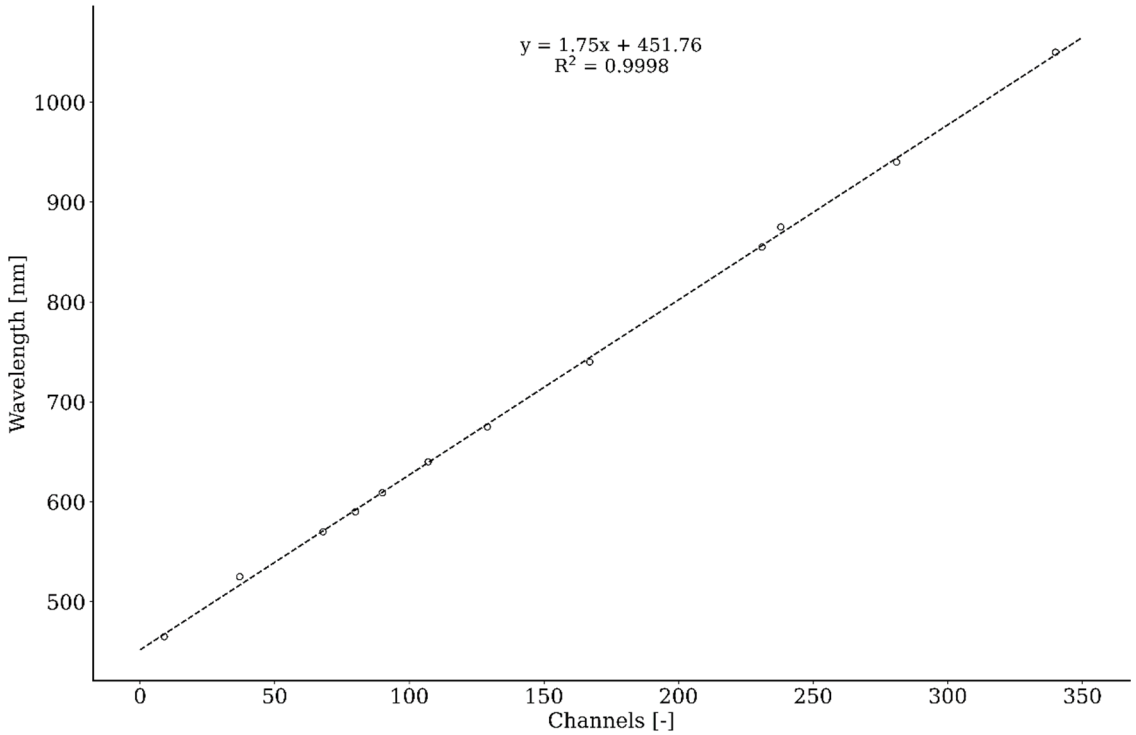
S2. ATR FTIR spectra of all materials

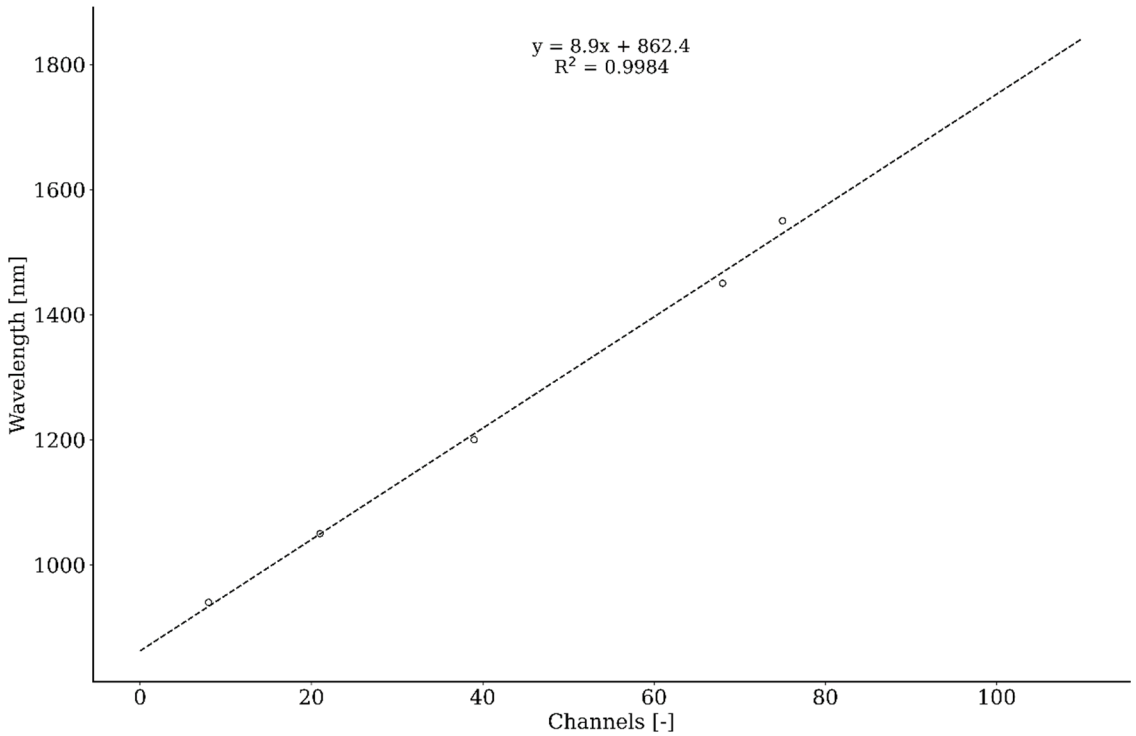



24·10 −3 wt%
10·10 −3 wt%
4.0·10 −3 wt%
1.7·10 −3 wt%
0 wt%
Absorbance [-]
Wavelength [cm−1]
0.0
0.1
0.2
0.3
0.4
4000
3500
3000
2500
2000
1500
1000
500

S3. Hyperspectral camera calibration

Spectral calibration of Vis/NIR and SWIR regions

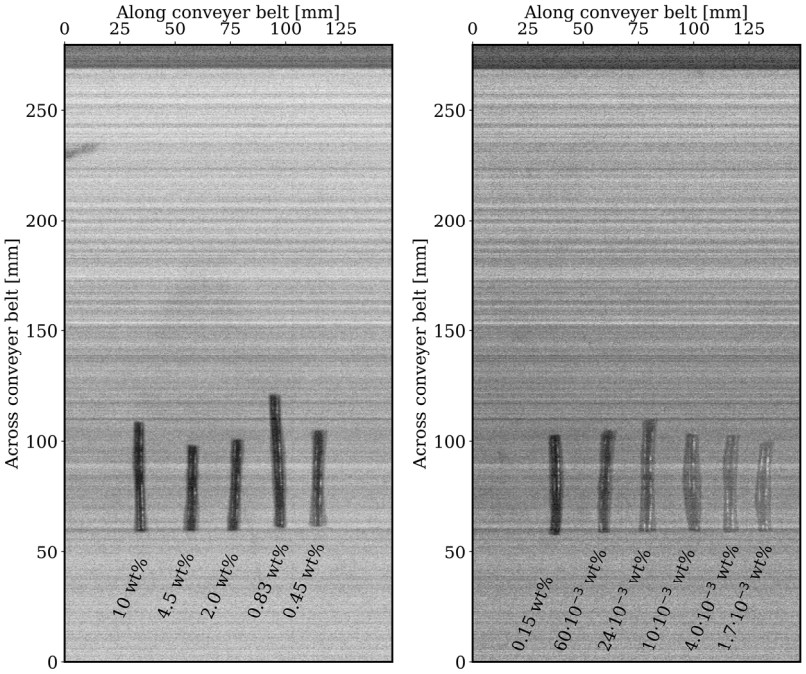




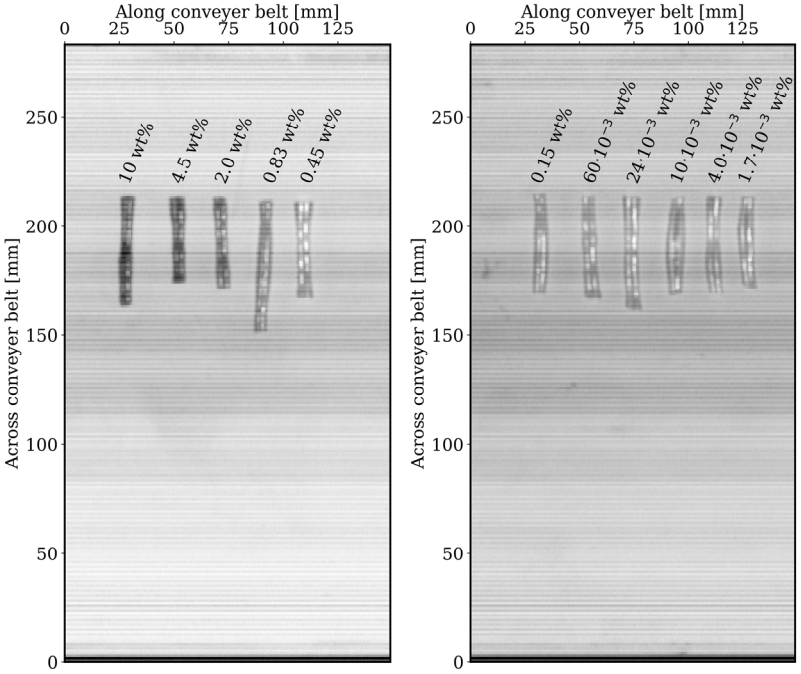
S4. Hyperspectral camera spectra of all components

Combined, individual and detailed spectra, extracted from the data cube obtained from the hyper spectral camera, of all the samples in the study.

Images of the hyperspectral samples at 504 nm (Vis/NIR).

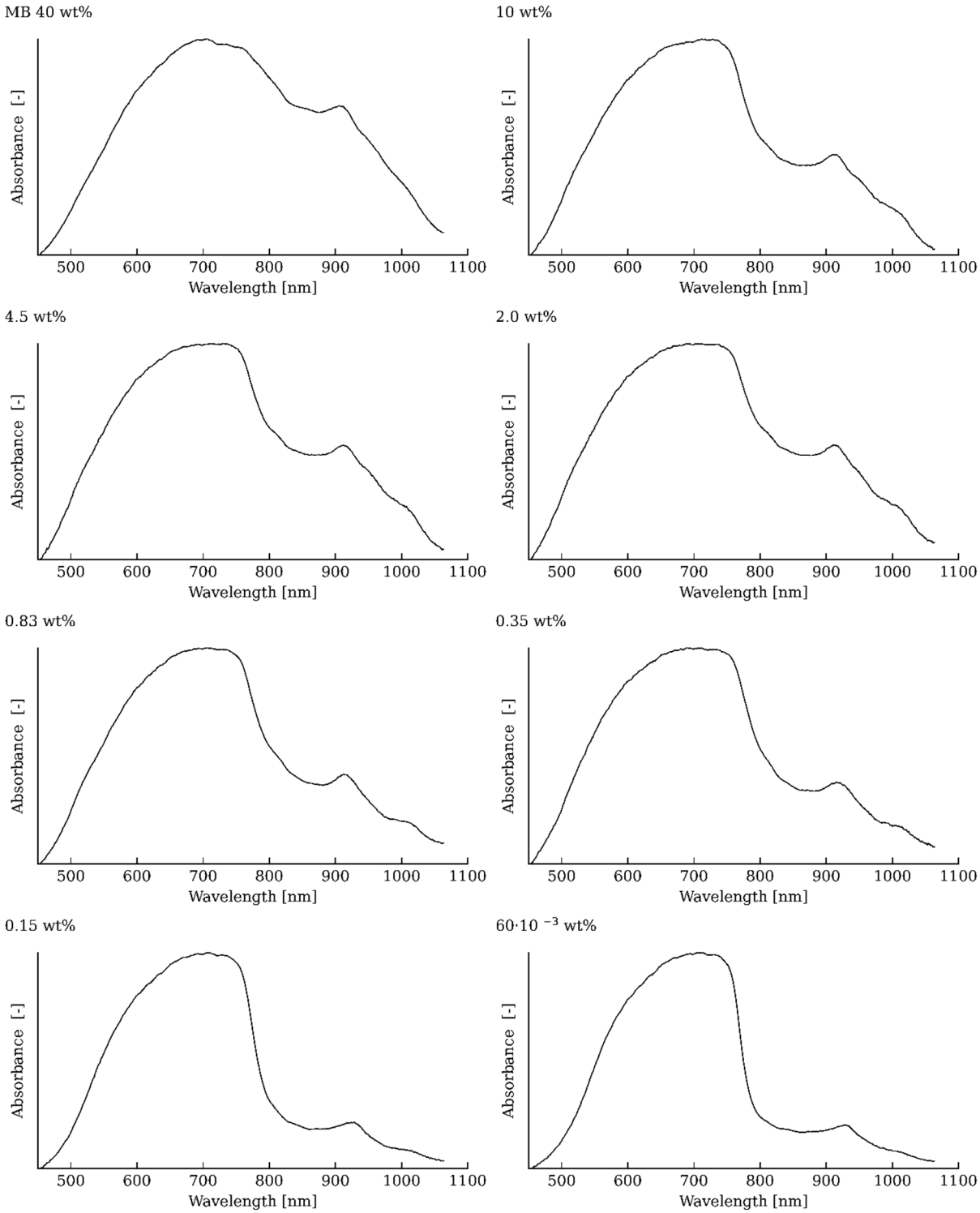


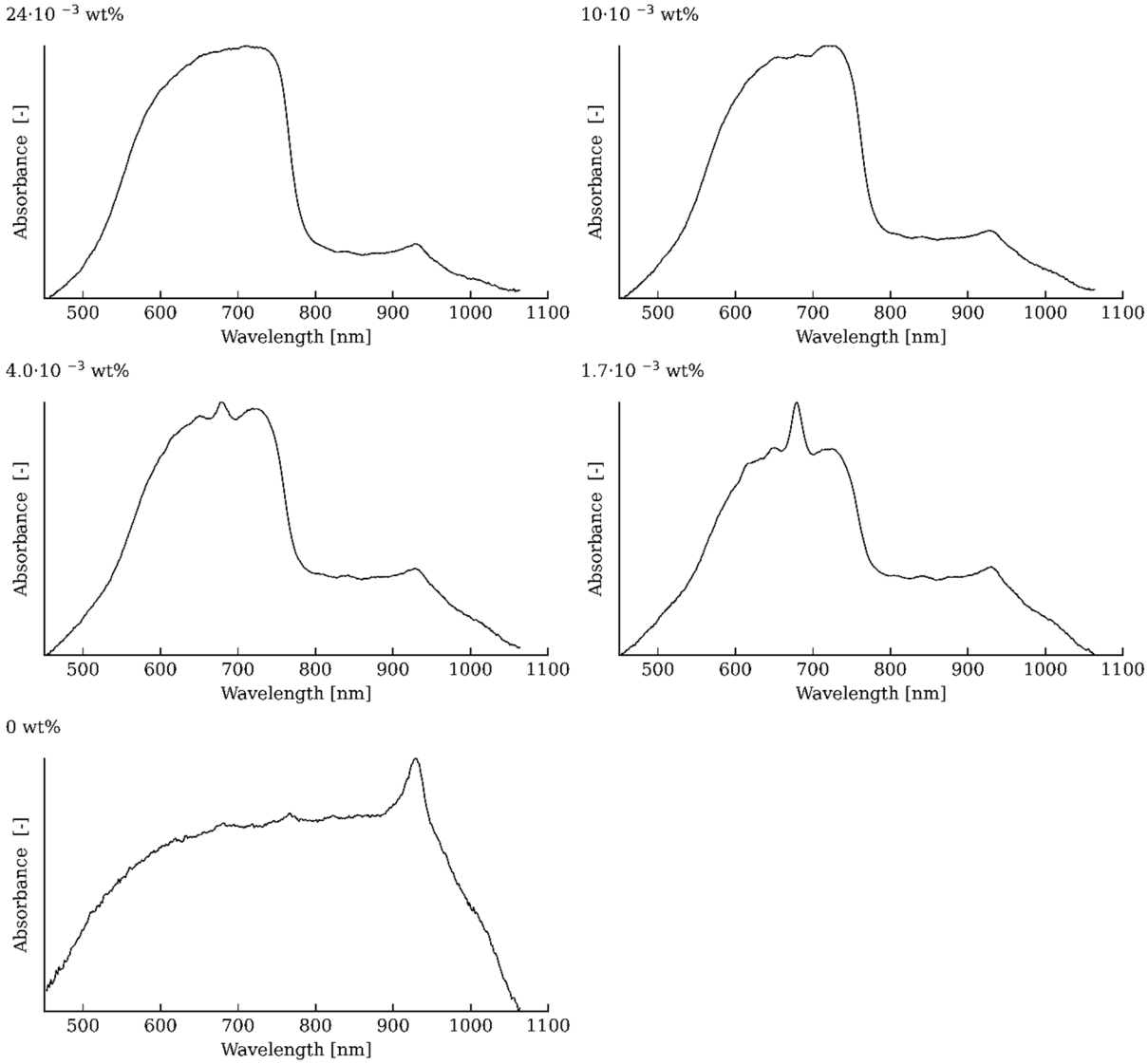
Images of the hyperspectral samples at 1129 nm (SWIR).



Individual Vis/NIR Spectra

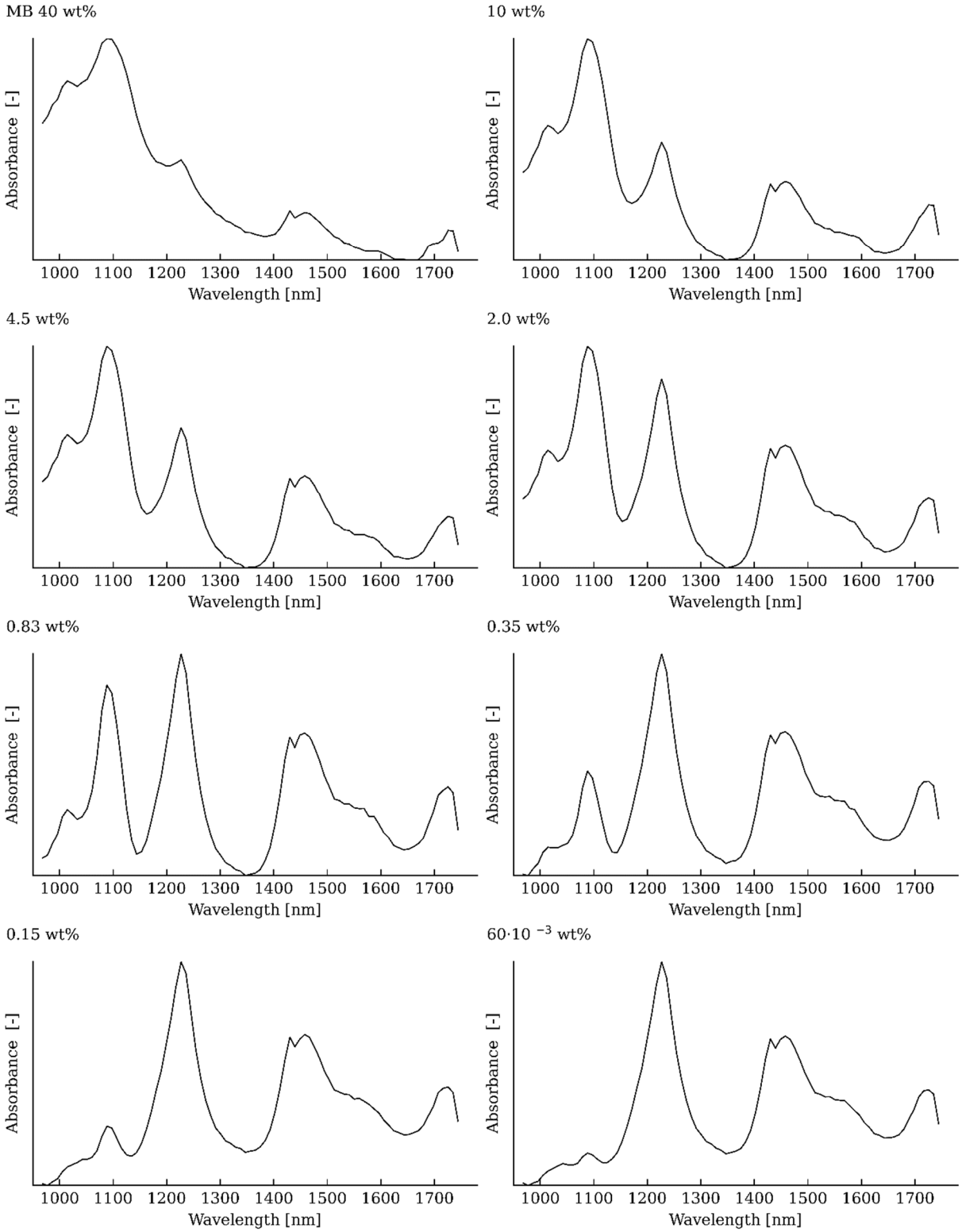
Individual accumulated spectra of the Vis spectral range extracted from the hyper cube.

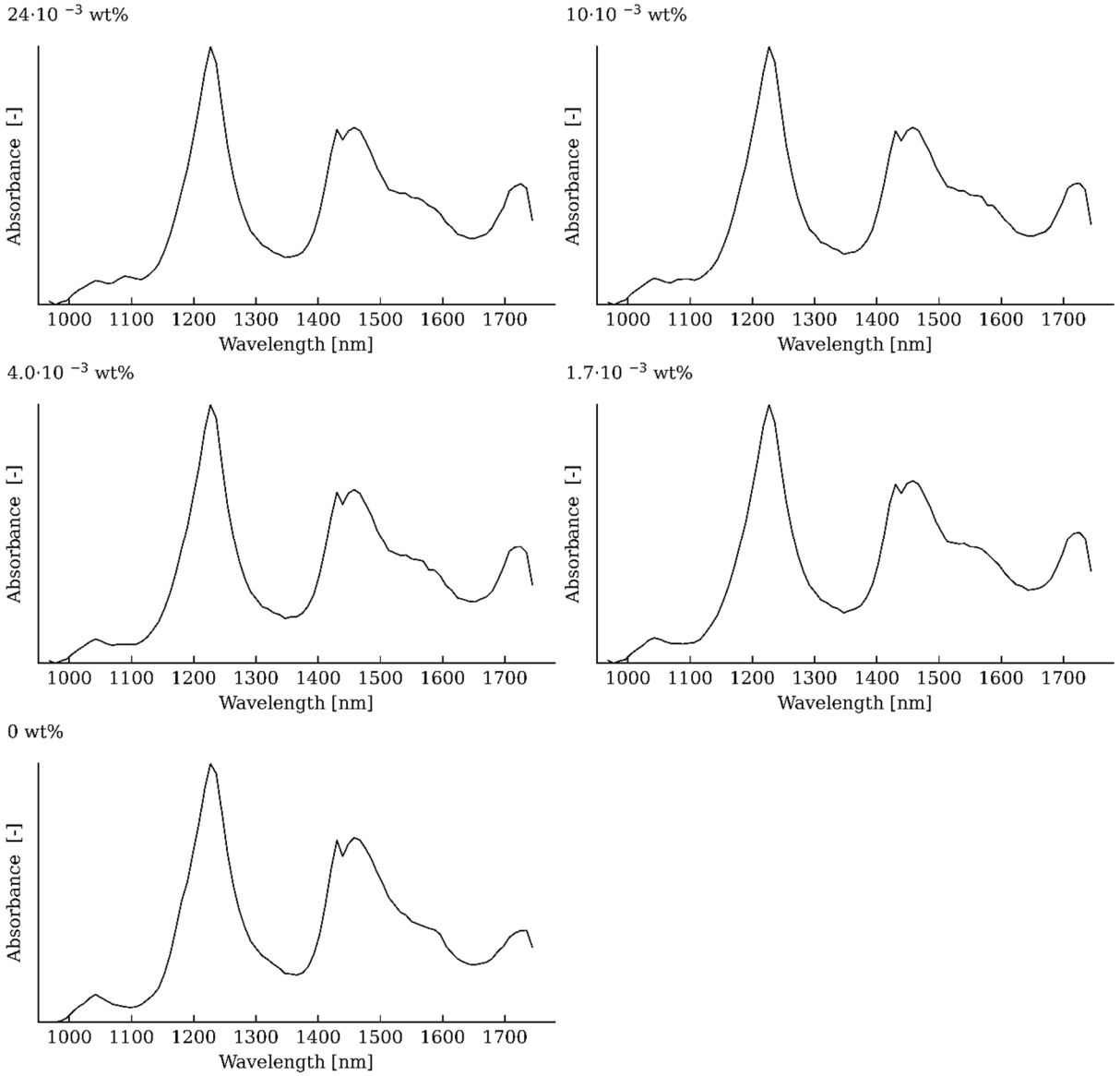



24·10 −3 wt%
10·10 −3 wt%
4.0·10 −3 wt%
1.7·10 −3 wt%
0 wt%
Absorbance [-]
Wavelength [nm]
500
600
700
800
900
1000
1100

Individual SWIR spectra

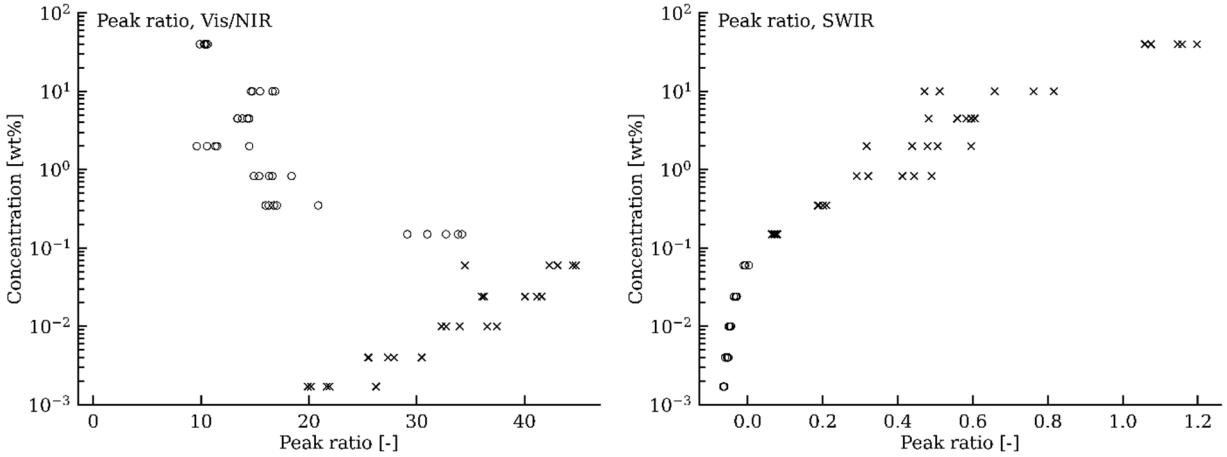
Individual accumulated and normalized spectra of the SWIR spectral range extracted from the hyper cube.




24·10 −3 wt%
10·10 −3 wt%
4.0·10 −3 wt%
1.7·10 −3 wt%
0 wt%
Absorbance [-]
1000 1100 1200 1300 1400 1500 1600 1700
Wavelength [nm]

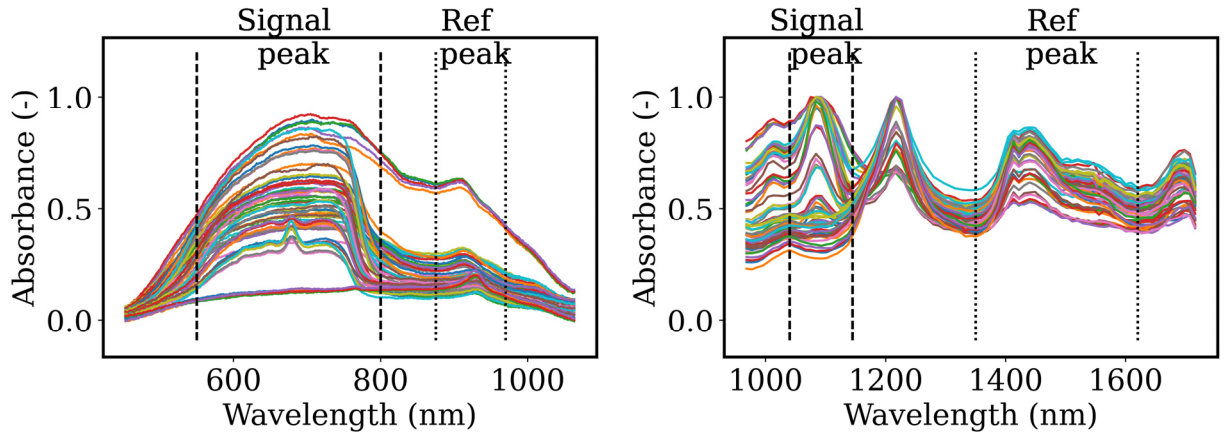
S5. Peak ratio analysis and concentration modelling

Detection limit Vis/NIR and SWIR



Symbol times = included and circle = not included.

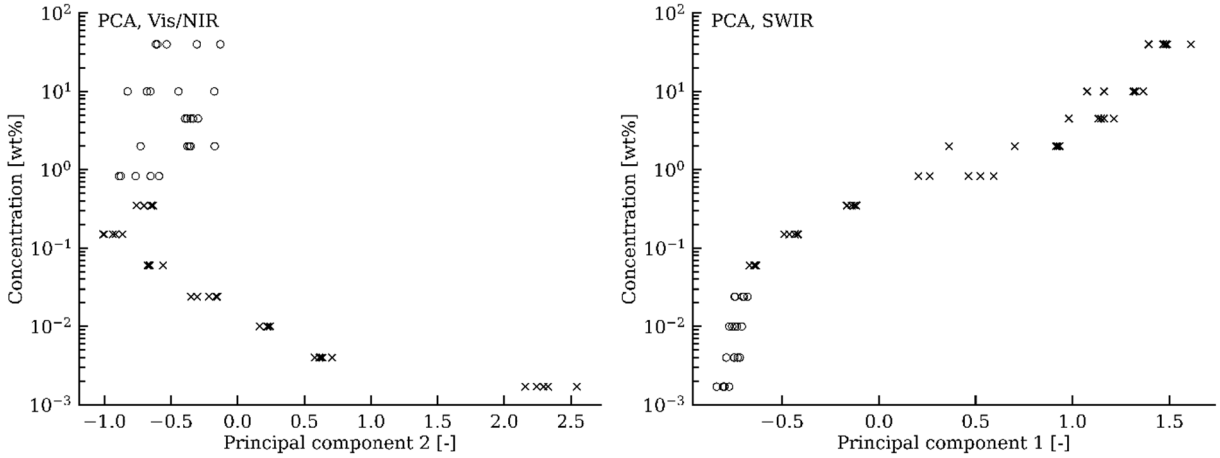
Integration limit Vis/NIR and SWIR



All the individual spectra can be seen in section S4.

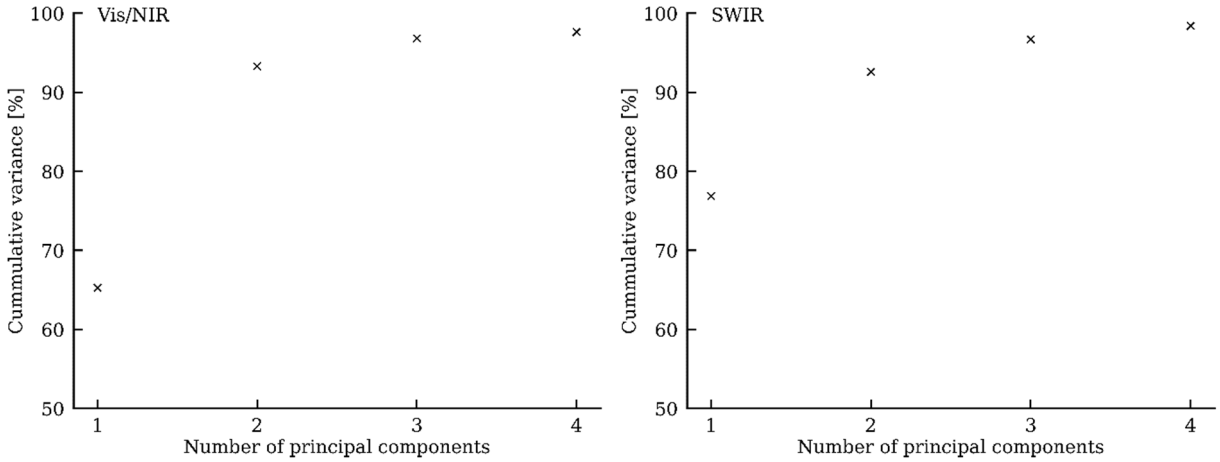
S6. PCA analysis and concentration modelling

Detection limit Vis/NIR and SWIR



Symbol times = included and circle = not included.

Scree plot on optimized Vis/NIR and SWIR



Loading plots on optimized Vis-NIR and SWIR