

Electronic Supplementary Information ESI 1: Needle chemical traits of the Scots pine trees grown at four post-mining sites (mean \pm standard deviation, range). Dump – abandoned dump, Mine – abandoned lignite mine, Sand – abandoned sand pit, Forest – control forest. * As content in the needles from the mine site were below the detection threshold for nine of the ten samples.) S.D. - Standard Deviation.

	Dump n =55	Mine n =19	Sand n =38	Forest n =38
Chlorophyll a+b [mg/g] dry weight	1.19 ± 0.450 0.54 - 2.64	3.21 ± 0.540 2.25 - 4.48	1.92 ± 0.480 1.04 - 2.86	2.96 ± 0.66 1.86 - 5.14
Total carotenoids [mg/g] dry weight	0.22 ± 0.068 0.13 - 0.42	0.48 ± 0.077 0.36 - 0.66	0.30 ± 0.076 0.17 - 0.47	0.46 ± 0.086 0.30 - 0.69
Carotenoids to Chlorophylls ratio [-]	0.20 ± 0.032 0.16 - 0.29	0.15 ± 0.006 0.13 - 0.16	0.15 ± 0.008 0.13 - 0.17	0.16 ± 0.010 0.13 - 0.18
Soluble phenolics [mg/g] fresh weight	132.05 ± 46.858 12.64 - 242.28	89.10 ± 20.544 59.64 - 150.93	87.28 ± 21.060 54.58 - 129.79	92.67 ± 30.390 55.3 - 166.75
Lignin [mg/g] dry weight	25.61 ± 3.736 19.30 - 38.44	27.11 ± 4.091 19.26 - 33.77	30.77 ± 3.797 21.95 - 42.24	28.96 ± 4.335 18.92 - 40.69
Relative water content [%]	52.27 ± 3.255 45.61 - 59.73	59.05 ± 2.322 55.32 - 62.83	59.11 ± 2.756 53.07 - 64.05	58.48 ± 3.623 51.79 - 65.18
As content * [mg/kg] dry weight	0.415 ± 0.2841 0.130 - 1.000	0.540 - -	1.034 ± 0.6996 0.570 - 2.900	0.418 ± 0.2367 0.140 - 0.780

Electronic Supplementary Information Table ESI 2: The results of the PLSR calibration and validation statistics (Cab – chlorophyll a + b content, Car – carotenoid content, RMSE – the root mean square error, R2 - coefficient of determination, RPD – the ratio of the standard error of prediction to sample standard deviation, A - absorbance defined as $1/\log(R)$, where R is spectral reflectance, and CR - continuum removal. The model quality was defined as in Brodský et al. (2012): * moderate (acceptable) quality with $R2 \geq 0.6$, $RPD \geq 1.5$; ** good quality with $R2 \geq 0.7$ and $RPD \geq 1.5$; *** the best quality with $R2 \geq 0.8$ and $RPD \geq 2.0$.)

Chemical traits / model statistics	Histogram normalization	RMSE – PLSR calibration	R ² – PLSR calibration	Number of factors	RMSE – PLSR validation	R ² – PLSR validation	RPD	Model quality
Cab (mg/g)	log	0.22 (5.56 %)	0.95	7	0.35 (15.28 %)	0.89	2.62	
Cab (mg/g) 400-1050 nm	log	0.27 (6.83 %)	0.92	5	0.37 (16.16 %)	0.81	2.05	
Cab (mg/g) A = 1/log(R)	log	0.33 (8.35 %)	0.88	13	0.41 (17.90 %)	0.75	2.08	
Cab (mg/g) CR	log	0.17 (4.30 %)	0.97	8	0.33 (14.41 %)	0.89	2.81	***
Car (mg/g)	log	0.08 (9.30 %)	0.66	10	0.07 (10.29 %)	0.67	1.95	**
Car (mg/g) 400-1050 nm	log	0.11 (12.79 %)	0.40	7	0.09 (13.24 %)	0.54	1.64	
Car (mg/g) A = 1/log(R)	log	0.10 (11.63 %)	0.51	6	0.08 (11.76 %)	0.58	1.71	
Car (mg/g) CR	log	0.08 (9.30 %)	0.64	7	0.09 (13.24 %)	0.55	1.49	
Car/Cab	-	0.08 (9.30 %)	0.74	10	0.07 (10.29 %)	0.57	2.25	
Car/Cab 400-1050 nm	-	0.08 (9.30 %)	0.70	10	0.06 (8.82 %)	0.65	2.52	
Car/Cab A = 1/log(R)	-	0.08 (9.30 %)	0.75	10	0.05 (7.35 %)	0.73	2.85	***
Car/Cab CR	-	0.09 (10.47 %)	0.64	6	0.07 (10.29 %)	0.55	2.20	
RWC (%)	sqrt	1.10	0.92	9	2.01	0.81	1.90	
RWC (%) 1050-2500 nm	sqrt	1.41	0.88	8	1.76	0.78	2.24	**
RWC (%) A = 1/log(R)	sqrt	1.20	0.91	7	1.94	0.74	2.04	
RWC (%) CR	sqrt	1.03	0.93	8	1.91	0.75	2.06	
Soluble phenolics (mg/g)	-	23.01 (13.46 %)	0.64	8	18.30 (15.51 %)	0.55	2.10	*
Soluble phenolics (mg/g) 1050-2500 nm	-	23.18 (13.56 %)	0.63	8	25.39 (21.52 %)	0.45	1.49	
Soluble phenolics (mg/g) 350-1050	-	18.67 (10.93 %)	0.76	9	20.00 (16.95 %)	0.46	1.89	
Soluble phenolics (mg/g) A = 1/log(R)	-	19.98 (11.69 %)	0.73	10	22.62 (19.18 %)	0.45	1.67	
Soluble phenolics (mg/g) CR	-	28.68 (16.78 %)	0.44	5	21.39 (18.13 %)	0.38	1.67	
Lignin (mg/g)	-	3.32 (18.17 %)	0.45	5	3.59 (24.24 %)	0.34	1.22	
Lignin (mg/g) 1050-2500 nm	-	3.43 (18.77 %)	0.40	4	3.62 (24.44 %)	0.23	1.20	
Lignin (mg/g) A = 1/log(R)	-	3.20 (17.52 %)	0.48	7	3.69 (24.92 %)	0.29	1.18	
Lignin (mg/g) CR	-	3.35 (18.34 %)	0.43	5	3.43 (23.16 %)	0.22	1.27	

Electronic Supplementary Information Figure ESI 3: Examples of the PLSR models of the VNIR spectra and needle chemical traits – chlorophyll a+b (Cab) and soluble phenolics. Chlorophylls: **A)** Loading plot, **B)** PLSR model calibration and validation. Soluble phenolics: **C)** Loading plot, **D)** PLSR model calibration and validation. Comp 1-3 denote the factor loading weight vectors. R-square cal. (R-square calibration), R-square val. (R-square validation), RMSE (Root mean square error). The PLSR Cab is modeled from the continuum-removed spectra. It is obvious from the spectral loading plots of chlorophyll and the soluble phenolics, the shapes of the curves of the first three components are similar but the loading values, i.e., the correlations between the spectra and needle parameters at specific wavelengths, are opposite.

Figure ESI 3:

