Supplementary material

A multi-analytical approach to studying the chemical composition of typical carbon sink samples

Maria Luisa Astolfi[1,2,*], Lorenzo Massimi[3,4], Mattia Rapa[5], Rita Rosa Plà[6], Raquel Clara Jasan[6], Mabel Tudino[7], Silvia Canepari[3,4], Marcelo Enrique Conti[5]

[1] Department of Chemistry, Sapienza University of Rome, P.le Aldo Moro 5, 00185, Rome, Italy

[2] CIABC, Sapienza University of Rome, P.le Aldo Moro 5, 00185 Rome, Italy

[3] Department of Environmental Biology, Sapienza University of Rome, P.le Aldo Moro 5, Rome, 00185, Italy

[4] C.N.R. Institute of Atmospheric Pollution Research, Via Salaria, Km 29,300, Monterotondo St., Rome, 00015, Italy

[5] Department of Management, Sapienza University of Rome, Via del Castro Laurenziano 9, 00161 Rome, Italy

[6] Departamento Química Nuclear, Gerencia Química Nuclear y Ciencias de la Salud (GAATN), Centro Atómico Ezeiza, Comisión Nacional de Energía Atómica (CNEA), Av. Presbítero J. González y Aragón 15 (CP B1802AYA), Ezeiza, Buenos Aires, Argentina

[7] INQUIMAE, Departamento de Química Inorgánica, Analítica y Química Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Buenos Aires, Argentina

*Corresponding author: marialuisa.astolfi@uniroma1.it

Table S1. Data obtained from the analysis of certified materials using INAA (n=3).

	Certified value		Experimental value		
Element	**concentration**	**uncertainty/ confidence interval**	**concentration**	**uncertainty**	**Certified reference material**
	mg kg^{-1}		**mg kg^{-1}**		
As	412	16	430	7	Soil[a]
Br	24.2	1.6	24.1	1.6	Grass[b]
Ca	5,453	251	5,200	800	Grass[b]
Ce	68.4	6.6	63.5	4.8	Andesite[b]
Co	18.8	1.1	19.6	0.9	Andesite[b]
Cr	198	5	212	10	Coal[c]
Cs	1.35	0.12	1.3	0.2	Andesite[b]
Eu	1.3	0.2	1.2	0.06	Andesite[b]
Fe	37,546	1,645	37,000	800	Andesite[b]
Hf	6.80	-	6.99	0.80	Coal[c]
K	25,870	1,330	25,000	5,400	Grass[b]
La	34.8	2.3	34.1	0.6	Andesite[b]
Lu	0.42	0.05	0.432	0.042	Soil[a]
Na	3,293	227	3,270	220	Grass[b]
Rb	117	6	118	14	Soil[a]
Sb	0.049	0.042	0.047	0.009	Grass[b]
Sc	12.9	0.4	12.6	0.1	Andesite[b]
Sm	4.86	0.61	4.83	0.50	Andesite[b]
Tb	0.014	0.012 - 0.016	0.0141	0.0075	Lichen[d]
Th	6.81	0.48	6.55	0.17	Andesite[b]
Yb	2.8	0.4	2.51	0.38	Soil[a]
Zn	210	-	259	8	Coal[c]

[a] Soil, GBW 07405

[b] Andesite ACH-1 and Grass (Poaceae) from Wepal 2011-4

[c] Coal Fly Ash (NIST-1633b)

[d] RM IAEA Lichen 336

Table S2. Results [mean and standard deviation (SD); mg kg^{-1} d.w.] from INAA of the elements also analyzed by ICP-MS and ICP-OES (n=16).

			As	Ce	Co	Cr	Cs	Fe	La	Rb	Sb	Zn
Sample	**Site**	**LOD[a]**	1	0.5	0.2	0.5	0.1	200	0.2	2	0.03	2
P	**A**	Mean	<1	1.94	0.51	1.81	<0.1	851	1.01	<2	<0.03	6.5
		SD	-	0.54	0.01	0.53	-	18	0.20	-	-	1.2
	B	Mean	<1	8.8	1.36	<0.5	<0.1	3,620	4.35	<2	<0.03	3.1
		SD	-	2.3	0.37	-	-	190	0.89	-	-	3.0
	C	Mean	<1	3.16	0.76	1.43	<0.1	1,230	1.03	<2	<0.03	3.5
		SD	-	0.40	0.01	1.66	-	200	0.18	-	-	3.5
	D	Mean	<1	1.0	0.69	<0.5	<0.1	1,460	0.73	<2	<0.03	<2
		SD	-	1.1	0.15	-	-	95	0.03	-	-	-
	E	Mean	16.7	13.26	12.3	<0.5	<0.1	16,900	4.73	<2	<0.03	<2
		SD	1.3	0.64	0.5	-	-	620	0.42	-	-	-
	F	Mean	<1	0.51	0.50	<0.5	<0.1	792	0.29	<2	<0.03	3.1
		SD	-	0.36	0.04	-	-	77	0.03	-	-	0.9
	G	Mean	<1	1.25	0.47	1.73	<0.1	832	0.58	<2	<0.03	3.9
		SD	-	0.02	0.01	0.31	-	25	0.05	-	-	0.5
	H	Mean	<1	0.64	0.36	0.51	<0.1	427	0.30	<2	<0.03	3.3
		SD	-	0.19	0.06	0.36	-	26	0.06	-	-	0.9
	All	Mean	2.6	3.8	2.1	0.81	<0.1	3260	1.6	<2	<0.03	3.2
		SD	5.5	4.6	4.0	0.83	-	5400	1.8	-	-	2.1
S	**A**	Mean	4.1	27.6	2.92	15.3	1.32	<200	9.86	22.7	0.637	33.8
		SD	0.3	0.8	0.08	1.2	0.12	-	0.43	1.1	0.019	0.5
	B	Mean	<1	1.16	0.36	<0.5	<0.1	744	0.49	<2	<0.03	7.3
		SD	-	0.31	0.01	-	-	16	0.09	-	-	0.3
	C	Mean	3.1	9.6	1.71	10.2	0.69	<200	3.44	15.5	0.181	18.2
		SD	0.1	1.4	0.10	0.01	0.09	-	0.35	0.6	0.025	2.2
	D	Mean	<1	3.44	1.51	2.02	0.30	2240	1.47	5.8	<0.03	16.7
		SD	-	0.01	0.26	0.49	0.03	300	0.15	2.5	-	2.0
	E	Mean	3.8	8.78	3.77	4.44	0.30	<200	2.80	<2	0.255	22.1
		SD	0.4	0.20	0.12	1.50	0.03	-	0.09	-	0.005	0.1
	F	Mean	<1	0.40	<0.2	<0.5	<0.1	<200	<0.2	<2	<0.03	7.8
		SD	-	0.21	-	-	-	-	-	-	-	0.2
	G	Mean	1.7	12.0	2.59	7.06	0.80	<200	4.19	11.6	0.175	17.3
		SD	0.7	2.6	0.55	2.32	0.31	-	0.96	3.7	0.047	6.9
	H	Mean	<1	3.76	0.50	2.80	0.28	<200	1.41	3.5	<0.03	7.7
		SD	-	0.26	0.06	0.69	0.08	-	0.20	3.5	-	2.2
	All	Mean	1.9	8.3	1.7	5.3	0.47	448	3.0	7.9	0.16	16.4
		SD	1.5	8.6	1.3	5.2	0.43	736	3.0	7.9	0.21	8.9

[a] LOD, limit of determination.

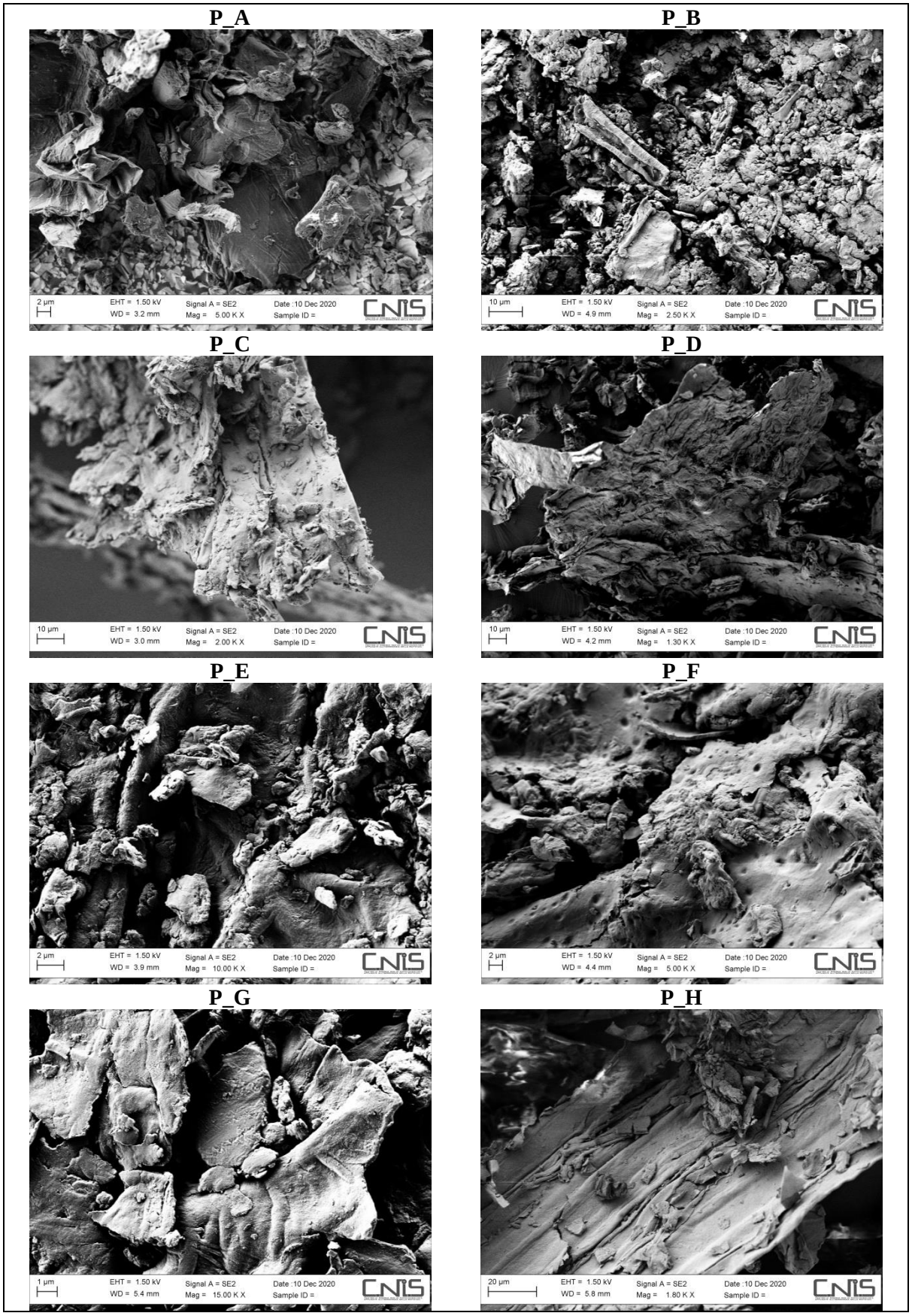

Fig. S1. Micrographs (from 1 to 20 µm) of peat (P) surface from each site (A, B, C, D, E, F, G, H) obtained by HRFESEM.

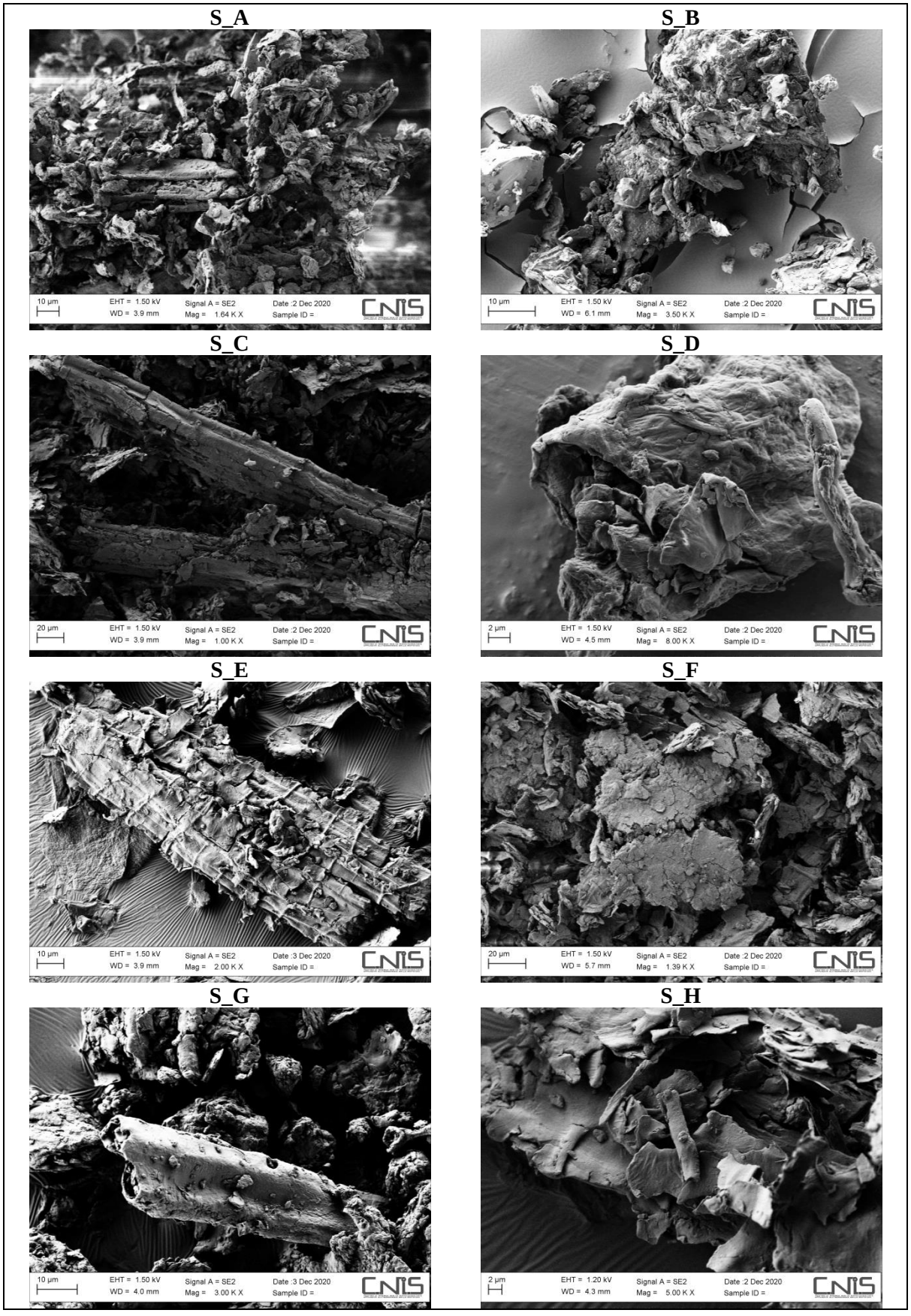

Fig. S2. Micrographs (from 2 to 20 µm) of *Sphagnum* moss (S) surface from each site (A, B, C, D, E, F, G, H) obtained by HRFESEM.

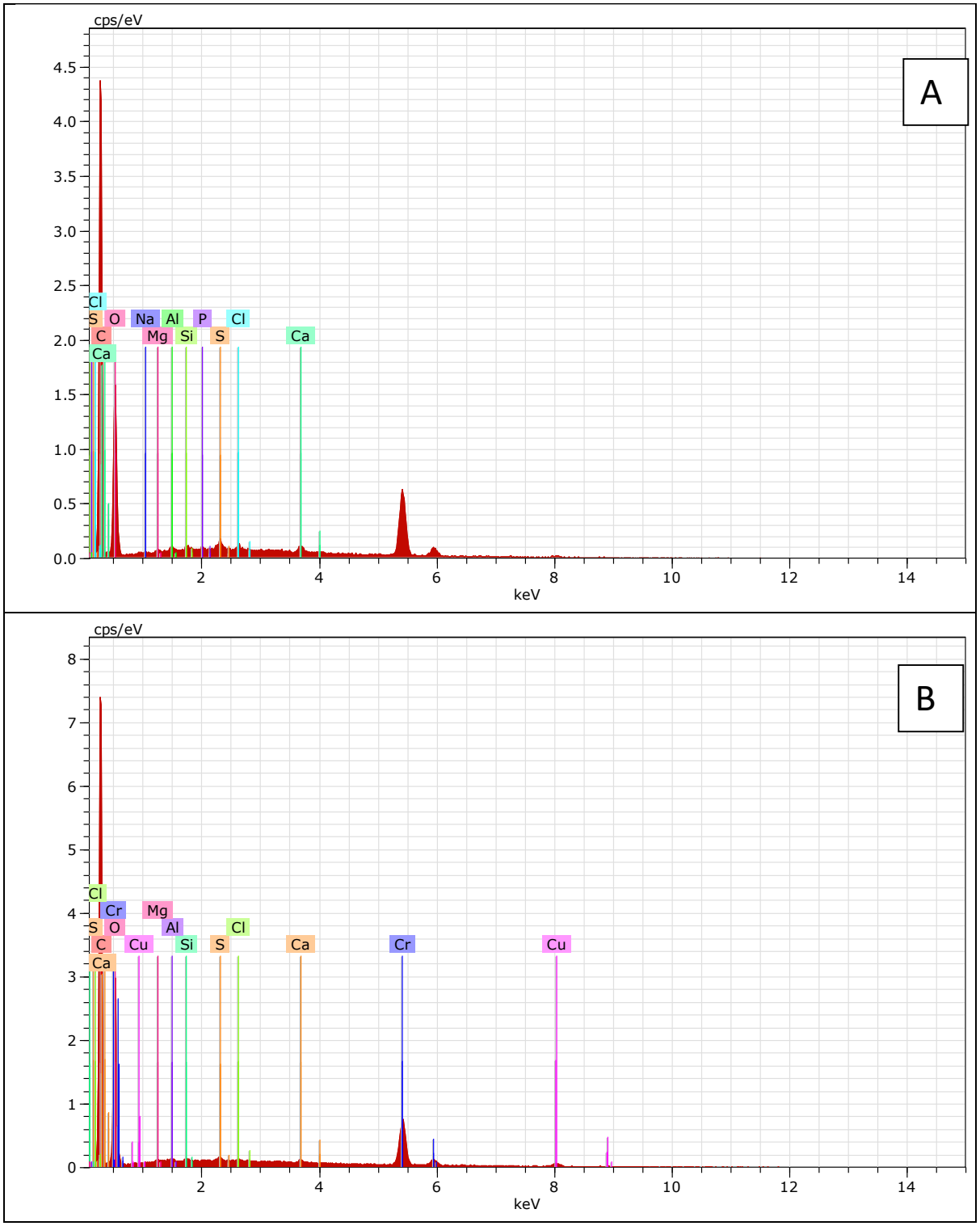

Fig. S3. Two typical spectra of peat samples obtained by XEDS microanalysis.

Table S3. Elemental percentage contents (wt.%) in peat samples (range, minimum - maximum) by XEDS microanalysis (n=16).

Element	Minimum	Error (1σ)	Maximum	Error (1σ)
Al	0.04	0.03	0.35	0.06
Ca	0.03	0.03	16.9	0.5
Cl	0.01	0.03	0.27	0.04
Cr	-	-	12.0	0.3
Cu	-	-	2.80	0.13
Mg	0.03	0.03	0.14	0.04
Na	0.01	0.03	0.24	0.05
O	25.8	3.7	45.6	5.3
P	0.01	0.03	0.06	0.03
S	0.12	0.03	0.99	0.08
Si	0.08	0.03	1.33	0.11

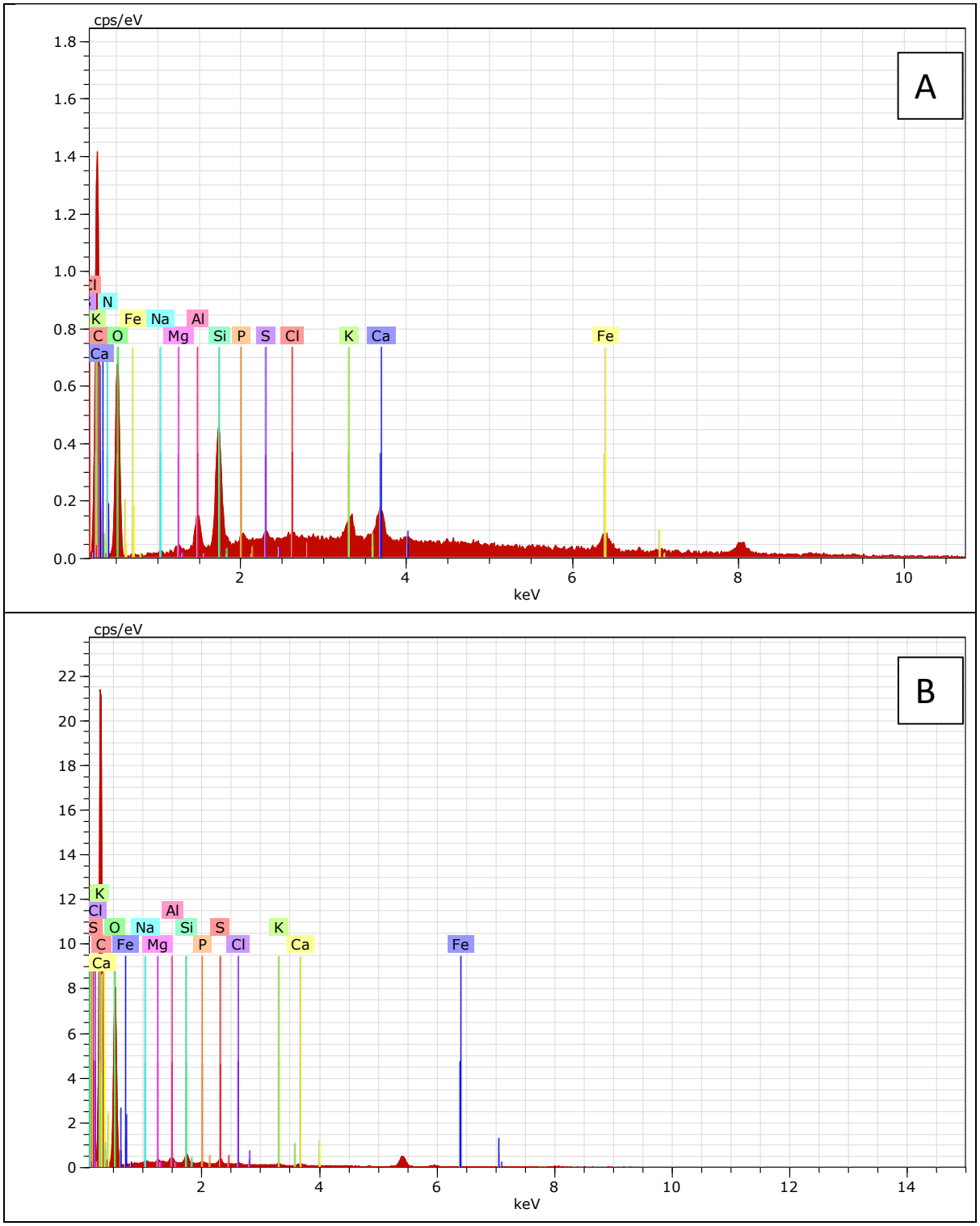

Fig. S4. Two typical spectra of *Sphagnum* moss sample obtained by XEDS microanalysis.

Table S4. Elemental percentage contents in *Sphagnum* moss samples (range, minimum - maximum) by XEDS microanalysis (n=16).

Element	Minimum	Error (1σ)	Maximum	Error (1σ)
Al	0.01	0.03	2.31	0.07
Ca	0.09	0.03	2.03	0.07
Cl	0.02	0.03	0.23	0.04
Fe	0.01	0.03	3.52	0.07
K	0.09	0.03	1.36	0.07
Mg	0.08	0.03	0.78	0.08
N	0.41	0.13	3.85	0.71
Na	0.03	0.03	0.48	0.05
O	29.7	3.7	44.5	5.3
P	0.02	0.03	0.35	0.04
S	0.01	0.03	0.41	0.04
Si	0.13	0.04	7.44	0.13

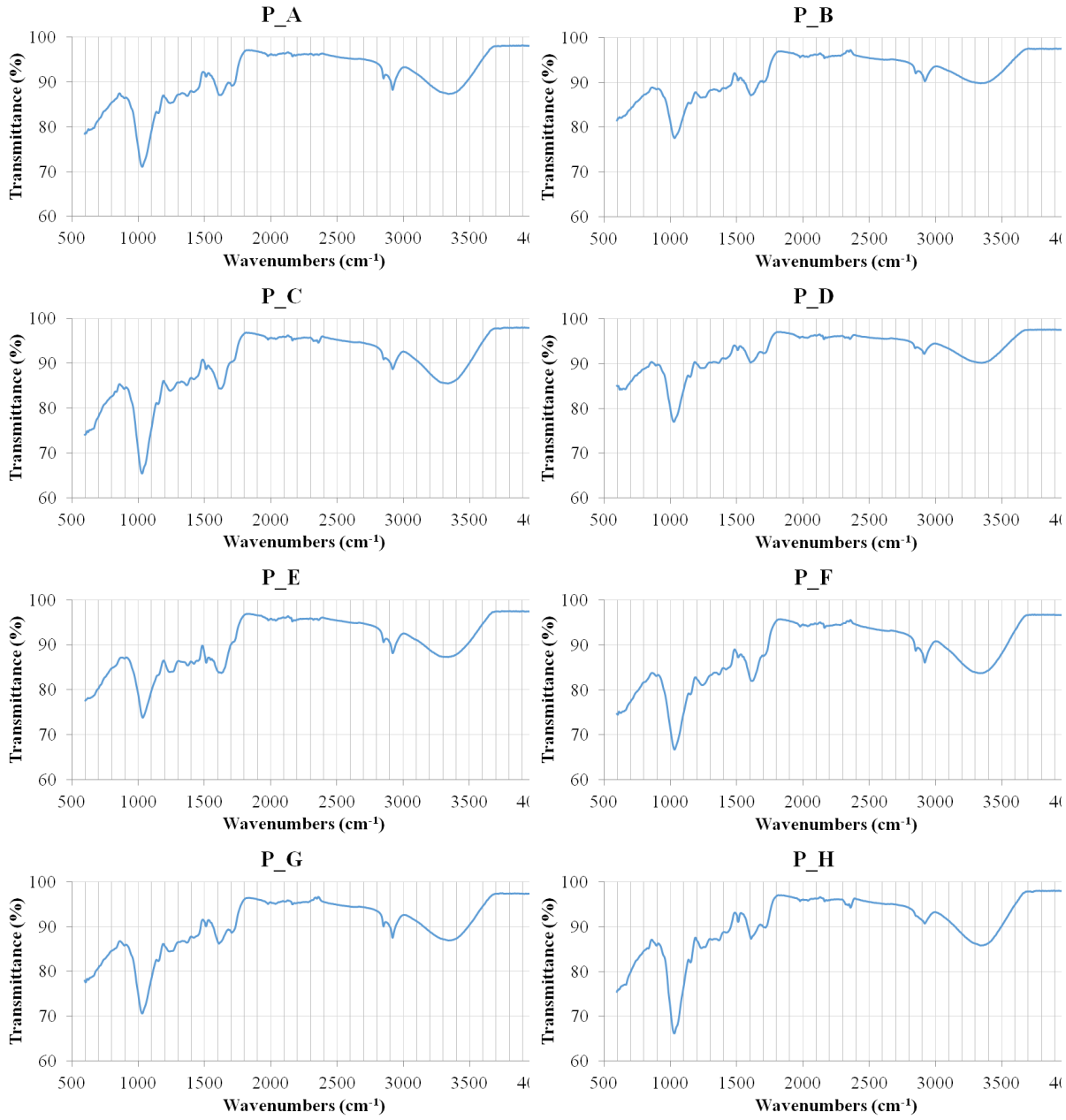

Fig. S5. FTIR spectra of peat (P) from all sites (A, B, C, D, E, F, G, and H).

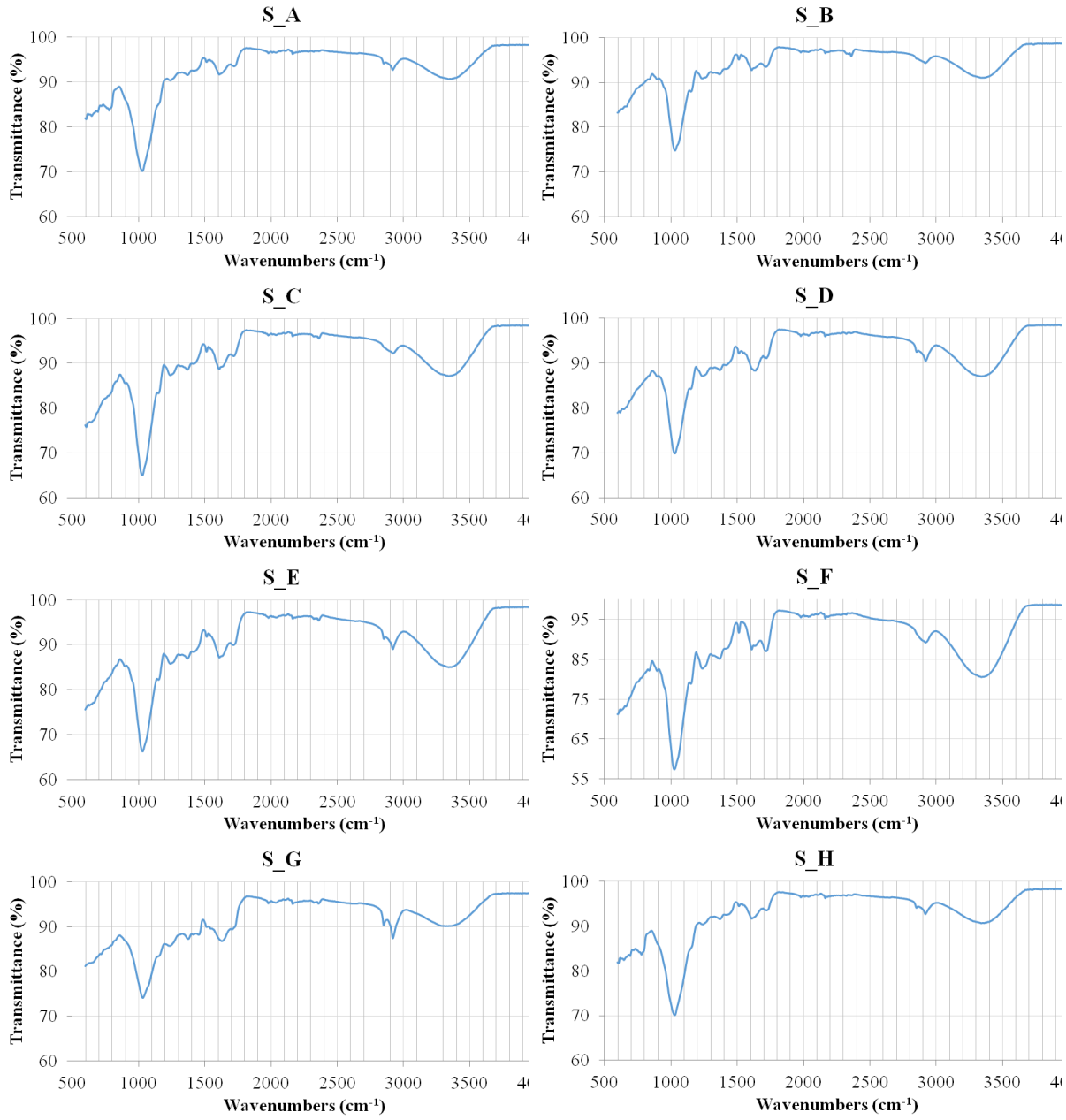

Fig. S6. FTIR spectra of *Sphagnum* moss (S) from all sites (A, B, C, D, E, F, G, and H).

Table S5. Main IR absorption bands in peat samples with associated functional groups.

Wavenumber (cm^{-1})	Functional groups; characterization
3,440-3,320	-O-H stretching; cellulose[1,2]
2,920	Antisymmetric CH_2; fats, wax, lipids[1,3,4]
2,850	Symmetric CH_2; fats, wax, lipids[1,3,4]
1,720	C=O stretch of COOH or COOR; carboxylic acids, aromatic esters[1,3,5,6]
1,710-1,707	C=O stretch of COOH; free organic acids[6]
1,653	Amide I (C=O); proteinaceous origin[7,8]
1,650-1,600	Aromatic C=C stretching and/or asymmetric C-O stretch in COO-, NH bend; lignin and other aromatics, or aromatic or aliphatic carboxylates[1,3,9]
1,626	Aromatic C=C stretching[4]
1,550	Amide II (N-H in plane); proteinaceous origin[7,8]
1,515-1,513	Aromatic C=C stretching; lignin/phenolic backbone[1]
1,426	Symmetric C-O stretch from COO- and OH deformation (COOH); carboxylate, carboxylic structures (humic acids)[10]
1,450, 1,370	C-H deformations; phenolic (lignin) and aliphatic structures[10]
1,265	Aromatic CO- and phenolic -OH stretching; lignin[11,12]
1,237	C-N; secondary amides[13]
1,160	Polysaccharides, alcoholic groups[14,15]
1,100	Amide III, carbohydrates, aromatic ethers, Si-O-C groups[16]
~1,080	Si-O stretching[4,17]
1,080-1,030	combination of C-O stretching and O-H deformation; polysaccharides[12,18,19,20,21]
1,000	Antisymmetric stretching vibration of Si-O[22,23]
916	Clay minerals; kaolinite doublet and smectite[15]
835	Aromatic CH out of plane; lignin[8]
698, 770-790	Si-O-H vibrations; clays, quartz[24,25]

Table S6. Results of the total elemental content [mean and standard deviation (SD); mg kg^{-1} d.w.] in peat for each site by AMA, ICP-MS, ICP-OES, and INAA (n=16).

	Site																
	A		B		C		D		E		F		G		H		
Element	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	p-value
Al	1,170	320	2,120	93	1,700	160	752	170	1,450	400	438	41	594	45	536	45	ns
As	0.37	0.23	1.1	0.2	0.42	0.13	0.46	0.05	13.0	1.0	0.37	0.17	<0.2	0.11	<0.2	0.14	ns
B	<5	-	<5	-	<5	-	<5	-	<5	-	7.3	2.7	<5	-	<5	-	-
Ba	25.9	6.5	57.1	7.2	27.5	0.6	15.2	1.6	85.2	14	11.8	1.7	20.7	4.6	9.2	0.2	ns
Be	0.027	0.008	0.100	0.006	0.060	0.003	0.030	0.002	0.166	0.019	<0.02	-	0.030	0.003	<0.02	-	ns
Bi	<0.01	-	<0.01	-	0.011	0.002	<0.01	-	0.015	0.002	<0.01	-	<0.01	-	<0.01	-	-
Ca	1,120	200	3,770	240	3,300	20	760	80	2,530	410	3,180	180	1,190	46	796	32	ns
Cd	0.072	0.002	0.133	0.031	0.064	0.003	0.042	0.001	0.149	0.026	0.045	0.002	0.036	0.002	0.050	0.002	ns
Ce	1.58	0.30	7.93	0.98	2.07	0.08	1.25	0.14	10.5	0.6	0.47	0.03	1.12	0.03	0.46	0.12	ns
Co	0.45	0.02	1.18	0.03	0.58	0.06	0.57	0.10	9.64	0.38	<0.4	-	0.45	0.01	<0.4	-	ns
Cr	2.4	1.1	1.5	1.5	2.28	0.25	1.96	0.50	2.76	0.69	6.4	4.1	3.56	0.65	4.88	0.16	ns
Cs	0.044	0.011	0.029	0.006	0.091	0.011	0.064	0.002	0.066	0.004	0.016	0.004	0.044	0.004	0.021	0.004	ns
Cu	1.86	0.24	6.03	0.24	2.37	0.09	1.38	0.19	4.33	0.75	2.18	0.50	1.69	0.06	0.89	0.11	ns
Eu	<0.06	-	0.19	0.01	<0.06	-	<0.06	-	0.36	0.03	<0.06	-	<0.06	-	<0.06	-	-
Fe	731	36	3,360	190	1,150	31	1,230	160	13,000	240	603	18	870	1	406	39	ns
Ga	0.375	0.094	0.458	0.002	0.478	0.055	0.252	0.005	0.246	0.026	0.130	0.025	0.303	0.002	0.147	0.021	ns
Hf	4.8	3.8	3.8	2.6	2.5	1.9	2.4	0.1	9.4	9.6	1.0	0.7	2.2	0.1	5.4	1.7	ns
Hg	0.0744	0.0026	0.0274	0.0034	0.0719	0.0045	0.0299	0.0026	0.0382	0.0040	0.0601	0.0031	0.0284	0.0009	0.0198	0.0009	ns
K	324	120	207	31	397	28	243	46	177	50	155	29	159	7	101	9	ns
La	0.791	0.147	3.84	0.42	0.923	0.033	0.577	0.046	3.67	0.35	0.194	0.022	0.501	0.003	0.226	0.052	ns
Li	0.148	0.017	0.165	0.016	0.185	0.025	0.048	0.003	0.122	0.019	0.058	0.025	0.254	0.001	0.027	0.009	ns
Lu	0.024	0.012	0.055	0.006	0.016	0.016	<0.01	-	0.115	0.001	<0.01	-	<0.01	-	<0.01	-	ns
Mg	984	7	526	40	689	18	1,240	21	565	25	1,400	10	130	55	916	14	ns
Mn	25.3	5.2	33.4	0.8	15.2	1.5	6.6	3.7	733	8	33.6	3.5	23.1	1.0	5.5	0.5	ns
Mo	0.18	0.03	0.44	0.02	<0.1	-	<0.1	-	0.17	0.03	0.64	0.01	<0.1	-	<0.1	-	ns
Na	665	44	399	44	564	49	306	40	255	66	542	24	401	14	176	13	ns
Nb	0.158	0.058	0.259	0.001	0.291	0.028	0.137	0.010	0.171	0.018	0.055	0.015	0.137	0.003	0.057	0.007	ns
Ni	0.70	0.11	1.87	0.10	1.22	0.13	0.68	0.11	7.44	0.48	0.42	0.11	0.73	0.04	0.55	0.07	ns
P	149	16	370	74	299	12	113	23	573	65	304	24	142	4	62	2	ns
Pb	0.96	0.11	0.81	0.12	1.19	0.12	0.63	0.03	0.71	0.21	0.26	0.05	0.61	0.02	0.52	0.04	ns
Rb	0.87	0.24	0.54	0.12	1.00	0.22	0.59	0.02	1.72	0.04	0.36	0.06	0.57	0.08	0.28	0.04	ns
S	1,720	280	2,870	190	3,260	91	1,450	160	2,320	300	2,190	5	2,450	140	1,290	97	ns
Sb	<0.2	-	<0.2	-	<0.2	-	<0.2	-	<0.2	-	<0.2	-	<0.2	-	<0.2	-	-
Sc	0.79	0.16	1.13	0.09	0.94	0.13	0.390	0.044	1.34	0.23	0.162	0.024	0.453	0.005	0.157	0.009	ns
Se	<0.5	-	0.77	0.09	0.48	0.14	0.67	0.49	<0.5	-	<0.5	-	0.94	0.04	<0.5	-	-
Si	6,860	2,400	3,680	1,140	7,440	560	3,340	860	2,700	840	2,230	100	3,200	140	1,200	160	ns
Sm	0.200	0.036	0.87	0.12	0.275	0.040	0.129	0.004	1.66	0.13	0.066	0.013	0.106	0.011	0.059	0.006	ns
Sn	0.103	0.015	0.041	0.014	0.075	0.005	0.061	0.009	0.032	0.005	0.034	0.008	0.051	0.025	<0.02	-	ns
Sr	21.2	1.9	52.5	0.2	15.8	0.8	23.7	1.5	52.9	1.9	36.2	1.2	21.1	0.5	14.3	0.9	ns

Te	<0.02	-	<0.02	-	<0.02	-	<0.02	-	<0.02	-	<0.02	-	<0.02	-	<0.02	-	-
Th	0.281	0.052	0.755	0.078	0.521	0.058	0.269	0.014	1.68	0.07	0.12	0.14	0.256	0.007	0.075	0.070	ns
Ti	125	45	98.8	7.5	158	15	65	12	45	14	25.2	4.0	74.8	0.2	28.3	5.0	ns
Tl	0.008	0.001	0.007	0.000	0.031	0.001	0.009	0.002	0.031	0.002	0.007	0.001	0.009	0.000	0.005	0.002	ns
U	0.093	0.027	0.163	0.004	0.083	0.003	0.039	0.004	0.121	0.020	0.025	0.002	0.046	0.003	0.017	0.002	ns
V	2.62	0.80	4.21	0.47	3.60	0.01	1.50	0.20	3.00	0.11	0.74	0.16	2.22	0.22	0.75	0.07	ns
W	<0.1	-	<0.1	-	<0.1	-	<0.1	-	<0.1	-	<0.1	-	<0.1	-	<0.1	-	-
Yb	0.14	0.04	0.34	0.05	<0.1	-	<0.1	-	0.86	0.08	<0.1	-	<0.1	-	<0.1	-	-
Zn	<1	-	2.4	5.3	<1	-	<1	-	6.2	0.7	<1	-	2.1	0.4	<1	-	ns
Zr	8,950	7,800	4,500	2,900	7,290	5,200	4,480	250	17,300	18,000	1,740	1,300	3,790	1,200	10,900	3,300	ns

[a] Non-parametric Kruskal-Wallis test was applied: "-" = not determined; "ns" = not significant at $p > 0.05$.

Table S7. Results of the total elemental content [mean and standard deviation (SD); mg kg^{-1} d.w.] in *Sphagnum* moss for each site by AMA, ICP-MS, ICP-OES, and INAA (n=16).

	Site																
	A		B		C		D		E		F		G		H		
Element	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	p-value
Al	7,780	12	633	10	1,590	30	1,180	440	1,390	290	296	45	5,100	600	1,170	2	ns
As	2.67	0.27	0.32	0.03	2.03	0.42	0.46	0.10	2.56	0.20	<0.2	0.11	1.25	0.01	0.47	0.07	ns
B	<5	-	<5	-	<5	-	<5	-	<5	-	<5	-	<5	-	<5	-	-
Ba	80.7	2.3	22.2	0.7	61.5	6.2	24.9	1.6	32.1	6.0	3.3	0.8	67	15	27.0	0.1	ns
Be	0.160	0.030	<0.02	-	0.086	0.005	0.026	0.001	0.060	0.002	<0.02	-	0.154	0.025	0.020	0.002	ns
Bi	0.062	0.007	<0.01	-	0.022	0.001	0.006	0.001	0.031	0.004	<0.01	-	0.037	0.009	<0.01	-	-
Ca	1,940	48	2,800	28	3,190	240	1,040	29	1,920	290	1,260	180	5,960	340	2,680	79	ns
Cd	0.259	0.037	0.033	0.010	0.140	0.017	0.206	0.017	0.165	0.051	0.032	0.003	0.144	0.017	0.058	0.005	ns
Ce	18.4	2.8	1.15	0.24	6.87	0.27	3.16	0.20	6.42	0.21	0.20	0.02	9.14	2.28	1.62	0.07	ns
Co	5.24	0.10	0.53	0.01	2.64	0.29	1.74	0.22	3.41	0.65	<0.4	-	3.26	0.70	0.50	0.07	ns
Cr	11.7	0.53	0.47	0.07	7.7	1.3	1.41	0.04	2.08	0.58	0.11	0.19	4.7	1.2	1.18	0.14	ns
Cs	0.550	0.091	0.055	0.008	0.387	0.006	0.233	0.008	0.130	0.002	0.010	0.000	0.40	0.11	0.081	0.007	ns
Cu	9.25	0.17	1.15	0.19	3.24	0.05	1.82	0.33	6.01	0.17	0.59	0.03	5.5	1.2	1.24	0.03	ns
Eu	0.47	0.06	<0.06	-	0.15	0.01	<0.06	-	0.16	0.01	<0.06	-	0.21	0.04	0.07	0.01	-
Fe	7,680	470	734	140	4,630	5	1,920	104	5,840	180	125	2	4,840	1,400	781	31	ns
Ga	2.57	0.30	0.207	0.033	1.34	0.06	0.339	0.030	0.735	0.002	0.048	0.003	1.36	0.32	0.316	0.023	ns
Hf	58.7	29.8	2.8	0.3	13.7	7.7	6.0	0.5	22.8	15.2	11.6	4.0	7.4	5.2	16.7	4.4	ns
Hg	0.0720	0.0057	0.0417	0.0001	0.0417	0.0001	0.101	0.009	0.0706	0.0015	0.0239	0.0020	0.115	0.001	0.0380	0.0038	ns
K	3,560	16	690	4	2,640	230	1,300	96	944	200	1,730	270	1,800	600	1,200	100	ns
La	7.62	1.19	0.424	0.095	2.61	0.10	1.08	0.01	2.19	0.07	0.076	0.007	3.40	0.78	0.616	0.031	ns
Li	3.71	0.26	0.487	0.046	1.64	0.07	0.189	0.066	0.703	0.054	0.034	0.007	2.2	1.2	0.226	0.014	ns
Lu	0.174	0.008	<0.01	-	0.072	0.003	0.016	0.016	0.052	0.007	<0.01	-	0.082	0.008	0.037	0.001	ns
Mg	1,920	29	1,200	170	2,400	98	1,380	120	1,340	41	446	19	1,150	280	703	24	ns
Mn	452	138	187	4	200	11	21	8	473	26	249	19	371	227	168	3	ns
Mo	0.16	0.01	<0.1	-	<0.1	-	<0.1	-	<0.1	-	<0.1	-	0.25	0.05	<0.1	-	ns
Na	3,630	62	726	15	1,340	160	694	130	790	79	546	90	1,350	380	713	8	ns
Nb	0.337	0.031	0.101	0.016	0.426	0.002	0.171	0.017	0.168	0.002	0.010	0.001	0.398	0.030	0.127	0.003	ns
Ni	5.27	0.12	0.53	0.09	3.29	0.09	0.92	0.03	3.39	0.14	0.09	0.07	3.86	0.81	0.66	0.04	ns
P	458	10	230	15	395	35	623	11	370	33	473	66	777	20	152	19	ns
Pb	7.48	0.16	0.732	0.054	5.47	0.52	1.56	0.01	10.2	0.1	0.140	0.014	4.3	1.8	0.873	0.016	ns
Rb	9.1	1.2	1.18	0.20	5.09	0.22	2.18	0.07	3.12	0.29	0.93	0.04	4.9	1.8	1.40	0.24	ns
S	531	54	361	14	541	36	1,190	36	537	66	276	53	2,020	120	316	38	ns
Sb	<0.2	-	<0.2	-	<0.2	-	<0.2	-	<0.2	-	<0.2	-	<0.2	-	<0.2	-	-
Sc	5.39	0.18	0.231	0.028	2.22	0.24	0.657	0.080	1.31	0.01	0.095	0.003	2.38	0.43	0.83	0.03	ns
Se	<0.5	-	<0.5	-	<0.5	-	<0.5	-	<0.5	-	<0.5	-	<0.5	-	<0.5	-	-
Si	95,800	6,300	4,340	290	29,300	2,900	7,840	1,500	15,000	290	919	200	28,800	10,600	8,770	680	ns
Sm	2.35	0.16	0.106	0.008	0.80	0.12	0.263	0.042	0.710	0.005	0.048	0.017	0.81	0.28	0.321	0.003	ns
Sn	0.407	0.063	0.065	0.009	0.217	0.007	0.071	0.011	0.197	0.001	<0.02	-	0.189	0.022	0.050	0.012	ns
Sr	28.3	2.7	17.4	2.9	28.5	0.7	29.1	3.5	25.7	0.1	11.0	0.9	51.4	5.9	13.2	1.0	ns
Te	<0.02	-	<0.02	-	<0.02	-	<0.02	-	<0.02	-	<0.02	-	<0.02	-	<0.02	-	-

Th	2.91	0.13	0.202	0.001	1.23	0.19	0.404	0.071	1.01	0.04	0.074	0.069	1.76	0.28	0.600	0.014	ns
Ti	1,042	28	58.1	3.4	388	31	130	27	208	8	13.7	0.5	416	120	156	21	ns
Tl	0.078	0.014	0.0048	0.0014	0.0836	0.0017	0.0524	0.0073	0.0371	0.0007	0.0016	0.0001	0.056	0.012	0.0146	0.0010	ns
U	0.307	0.037	0.028	0.019	0.119	0.001	0.062	0.001	0.129	0.001	0.006	0.001	0.170	0.009	0.028	0.001	ns
V	18.4	3.0	1.18	0.19	8.21	0.26	2.12	0.12	6.08	0.17	0.38	0.11	8.26	1.31	2.07	0.20	ns
W	<0.1	-	<0.1	-	<0.1	-	<0.1	-	<0.1	-	<0.1	-	<0.1	-	<0.1	-	-
Yb	1.05	0.10	<0.1	-	0.43	0.08	<0.1	-	0.26	0.05	<0.1	-	0.49	0.05	0.17	0.04	-
Zn	37.8	3.8	9.8	1.5	24.0	1.0	17.0	3.7	26.8	1.0	9.2	0.7	21.5	7.7	8.8	1.3	ns
Zr	2,200	1,100	111	5	587	220	292	23	890	620	434	130	277	220	655	270	ns

[a] Non-parametric Kruskal-Wallis test was applied: "-" = not determined; "ns" = not significant at $p > 0.05$.

Table S8. Threshold and guideline values (mg kg^{-1}) for the dangerous elements in soils.

Elements	Legislative Decree 152/2006 and subsequent amendments and additions			Ministry of the Environment, Finland 2007		
	Agricultural soil contamination threshold[a]	Sites for public, private and residential green areas	Sites for commercial and industrial use	Threshold value	Lower guideline value[b]	Higher guideline value[b]
As	30	20	50	5	50 (e)	100 (e)
Be	7	2	10	NG[c]	NG[c]	NG[c]
Cd	5	2	15	1	10 (e)	20 (e)
Co	30	20	250	20	100 (e)	250 (e)
Cr	150	150	800	100	200 (e)	300 (e)
Cu	200	120	600	100	150 (e)	200 (e)
Hg	1	1	5	0.5	2 (e)	5 (e)
Ni	120	120	500	50	100 (e)	150 (e)
Pb	100	100	1,000	60	200 (t)	250 (e)
Sb	10	10	30	2	10 (t)	50 (e)
Se	3	3	15	NG[c]	NG[c]	NG[c]
Sn	NG[c]	1	350	NG[c]	NG[c]	NG[c]
Tl	1	1	10	NG[c]	NG[c]	NG[c]
V	90	90	250	100	150 (e)	250 (e)
Zn	300	150	1,500	200	250 (e)	400 (e)

[a] Ministerial Degree 46/2019 Annex 2, Article 3.

[b] The guideline values have been defined on the basis of either ecological risks (e) or health risks (t).

[c] NG stands for Not Given.

Table S9. Stepwise variables result for C, H, N, O and S contents.

Step	Variables	SP[a]	SSS[b]	R^{2c}	Cp[d]	n[e]	AICc[f]	BIC[g]
1	% C	0.0013	2.145046	0.5363	36.03	2	18.9304	19.2481
2	O/C	0.0026	0.954894	0.7750	13.305	3	10.9963	10.4503
3	H/C	0.0705	0.222394	0.8306	9.5466	4	10.819	8.68195
4	% S	0.0824	0.168899	0.8728	7.1734	5	11.5657	6.86793
5	C/N	0.1515	0.098871	0.8975	6.6133	6	14.775	6.18313
6	% H	0.1615	0.084221	0.9186	6.4326	7	19.6664	5.27564
7	% O*	0.2977	0.04372	0.9295	7.3006	8	28.7885	5.7418
8	% N	0.6006	0.011609	0.9324	9	9	44.1158	7.84169
	Best	.	.	0.9186	6.4326	7	19.6664	5.27564

[a] SP, significant probability. [b] SSS, sequential sum of squares. [c] R^2, coefficient of determination. [e] n, number of parameters in the model, including the intercept. [f] AICc, corrected akaike's information criterion. [g] BIC, Bayesan information criterion.

Table S10. Stepwise variables result for infrared spectra.

Step	Variables	SP[a]	SSS[b]	R^{2c}	Cp[d]	n[e]	AICc[f]	BIC[g]
1	1489	0.0343	1.128127	0.2820	.	2	25.924	26.2418
2	1662.6	0.0061	1.295054	0.6058	.	3	19.9675	19.4215
3	3194.1	0.0848	0.35835	0.6954	.	4	20.2061	18.0691
4	2306.9	0.0392	0.404905	0.7966	.	5	19.0767	14.3789
5	3437.2	0.1722	0.144609	0.8328	.	6	22.612	14.0201
6	1562.3	0.2312	0.103593	0.8587	.	7	28.4914	14.1007
7	3425.6	0.4497	0.041363	0.8690	.	8	38.7044	15.6577
8	1566.2	0.6589	0.01543	0.8729	.	9	54.2262	17.9521
9	1577.8	0.7830	0.006938	0.8746	.	10	78.0064	20.5049
10	1558.5	0.9087	0.001457	0.8750	.	11	117.96	23.2309
11	3190.3	0.9751	0.000138	0.8750	.	12	197.955	25.9991
12	2823.8	0.9889	3.768e-5	0.8750	.	13	437.954	28.7705
13	2962.7	0.9998	1.975e-8	0.8750	.	14	.	31.5431
14	1681.9	1.0000	7.16e-13	0.8750	.	15	.	34.3157
	Best	.	.	0.8328	.	6	22.612	14.0201

[a] SP, significant probability. [b] SSS, sequential sum of squares. [c] R^2, coefficient of determination. [e] n, number of parameters in the model, including the intercept. [f] AICc, corrected akaike's information criterion. [g] BIC, Bayesan information criterion.

Table S11. Stepwise variables result for multi-elemental analysis.

Step	Variables	SP[a]	SSS[b]	R^{2c}	Cp[d]	n[e]	AICc[f]	BIC[g]
1	S	0.0000	4.511415	0.5827	.	2	24.7614	28.1745
2	Ca	0.0000	1.574923	0.7862	.	3	6.68807	10.8856
3	Hg	0.0004	0.630972	0.8677	.	4	-5.3253	-0.5553
4	Mo	0.0044	0.279373	0.9037	.	5	-12.094	-6.9905
5	P	0.0117	0.17017	0.9257	.	6	-16.76	-11.592
6	Zr	0.0005	0.231136	0.9556	.	7	-29.019	-24.093
7	As	0.0376	0.060089	0.9633	.	8	-30.946	-26.611
8	Hf	0.0337	0.053686	0.9703	.	9	-33.016	-29.676
9	Be	0.3423	0.009902	0.9715	.	10	-29.485	-27.606
10	La	0.0263	0.049239	0.9779	.	11	-31.889	-32.015
11	U	0.0185	0.044304	0.9836	.	12	-35.105	-37.875
12	Al	0.2379	0.009693	0.9849	.	13	-30.734	-36.908
13	Ce	0.2219	0.01011	0.9862	.	14	-25.785	-36.275
14	Ba	0.2950	0.0073	0.9871	.	15	-19.12	-35.033
15	Mn	0.1989	0.010707	0.9885	.	16	-12.425	-35.124
16	Ni	0.1763	0.011251	0.9900	.	17	-4.6952	-35.883
17	Sm	0.0698	0.017931	0.9923	.	18	1.25832	-40.587
18	Th	0.2502	0.006479	0.9931	.	19	14.6082	-40.712
19	Pb	0.3299	0.004597	0.9937	.	20	32.4764	-40.076
20	Cr	0.3337	0.004551	0.9943	.	21	55.2654	-39.687
21	Si	0.2711	0.005843	0.9951	.	22	84.074	-40.659
22	Lu	0.1923	0.007737	0.9961	.	23	121.357	-44.227
23	Ti	0.3297	0.004137	0.9966	.	24	178.843	-45.307
24	Sn	0.2742	0.00513	0.9973	.	25	265.143	-48.574
25	Cu	0.2570	0.005242	0.9979	.	26	411.366	-53.917
26	Rb	0.3660	0.003299	0.9984	.	27	714.216	-57.633
27	Ga	0.1975	0.006051	0.9991	.	28	1624.2	-74.218
28	Zn	0.3886	0.002493	0.9995	.	29	.	-85.296
29	Bi	0.4865	0.002176	0.9997	.	30	.	-104.69
	Best	.	.	0.9997	.	30	.	-104.69

[a] SP, significant probability. [b] SSS, sequential sum of squares. [c] R^2, coefficient of determination. [e] n, number of parameters in the model, including the intercept. [f] AICc, corrected akaike's information criterion. [g] BIC, Bayesan information criterion.

References

1. Cocozza, C., D'orazio, V., Miano, T.M. & Shotyk, W. Characterization of solid and aqueous phases of a peat bog profile using molecular fluorescence spectroscopy, ESR and FT-IR, and comparison with physical properties. Org. Geochem. 34(1), 49-60 (2003).
2. Kloprogge, J.T., Hickey, L. & Frost, R.L. FT-Raman and FT-IR spectroscopic study of synthetic Mg/Zn/Al-hydrotalcites. J. Raman Spectros. 35(11), 967-974 (2004).
3. Niemeyer, J., Chen, Y., & Bollag, J.M. Characterization of humic acids, composts, and peat by diffuse reflectance Fourier-transform infrared spectroscopy. Soil Sci. Soc. Am. J. 56(1), 135-140 (1992).
4. Romão, L.P. et al. Structure and properties of Brazilian peat: analysis by spectroscopy and microscopy. J. Braz. Chem. Soc. 18, 714-720 (2007).
5. Haberhauer, G., Rafferty, B., Strebl, F. & Gerzabek, M.H. Comparison of the composition of forest soil litter derived from three different sites at various decompositional stages using FTIR spectroscopy. Geoderma 83(3-4), 331-342 (1998).
6. Gondar, D., Lopez, R., Fiol, S., Antelo, J.M. & Arce, F. Characterization and acid–base properties of fulvic and humic acids isolated from two horizons of an ombrotrophic peat bog. Geoderma 126, 367–374 (2005).
7. Ibarra, J.V., Munoz, E. & Moliner, R. FTIR study of the evolution of coal structure during the coalification process. Org. Geochem. 24, 725–735 (1996).
8. Zaccheo, P., Cabassi, G., Ricca, G. & Crippa, L. Decomposition of organic residues in soil: experimental technique and spectroscopic approach. Org. Geochem. 33, 327–345 (2002).
9. Coates, J.P. The interpretation of infrared spectra: Published reference sources. Appl. Spectros. Rev. 31(1-2), 179-192 (1996).
10. Parker, F. Applications of infrared spectroscopy in biochemistry, biology, and medicine (Springer Science & Business Media, 2012).

11. Guo, Y. & Bustin, R.M. FTIR spectroscopy and reflectance of modern charcoals and fungal decayed woods: implications for studies of inertinite in coals. Int. J. Coal Geol. 37(1-2), 29-53 (1998).
12. González, J.A. et al. Preferential accumulation of selectively preserved biomacromolecules in the humus fractions from a peat deposit as seen by analytical pyrolysis and spectroscopic techniques. J. Anal. Appl. Pyrolysis 68, 287-298 (2003).
13. Smith, B. Infrared spectral interpretation: a systematic approach (CRC press, 2018).
14. Zaccone, C., Miano, T.M. & Shotyk, W. Qualitative comparison between raw peat and related humic acids in an ombrotrophic bog profile. Org. Geochem. 38(1), 151-160 (2007).
15. Rossel, R.V. & Behrens, T. Using data mining to model and interpret soil diffuse reflectance spectra. Geoderma 158(1-2), 46-54 (2010).
16. Hafidi, M., Amir, S., Revel, J.C. Structural characterization of olive mill waster-water after aerobic digestion using elemental analysis, FTIR and 13C NMR. Process Biochem. 40(8), 2615-2622 (2005).
17. Poppi, N.R. & Talamoni, J. Estudo dos ácidos húmico e fúlvico, extraídos de solos, por espectroscopia de infravermelho. Quím. Nova 15(4), 281-285 (1992).
18. Marchessault, R.H. Application of infra-red spectroscopy to cellulose and wood polysaccharides. Pure Appl. Chem. 5(1-2), 107-130 (1962).
19. Hergert, L. in: Infrared spectra, Lignins (eds. Sarkanen, K., Ludwin, C.). (Wiley Interscience, 1974).
20. Painter, P., Starsinic, M. & Coleman, M. Determination of functional groups in coal by Fourier transform interferometry. Fourier Transform Infrared Spectros. 4, 169-240 (2012).
21. Grube, M., Lin, J.G., Lee, P.H. & Kokorevicha, S. Evaluation of sewage sludge-based compost by FT-IR spectroscopy. Geoderma 130(3-4), 324-333 (2006).
22. Geiger, C.A. A powder infrared spectroscopic investigation of garnet binaries in the system Mg3Al2Si3O12-Fe3Al2O12-Mn3Al2Si3O12-Ca3Al2Si3O12 (1998).
23. Saikia, B.J., Parthasarathy, G. & Sarmah, N.C. Fourier transform infrared spectroscopic estimation of crystallinity in SiO2 based rocks. Bull. Mater. Sci. 31(5), 775-779 (2008).

24. Orlov, D.S. Humus Acids of Soils, Russian Translation Series 35. A. A. Balkema: Rotterdam, The Netherlands, 35-70 (1985).

25. Haberhauer, G., Feigl, B., Gerzabek, M.H. & Cerri, C. FT-IR spectroscopy of organic matter in tropical soils: changes induced through deforestation. Appl. Spectros. 54(2), 221-224 (2000).