Comparison of different methods to determine the degree of peat decomposition in peat bogs

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Supplements

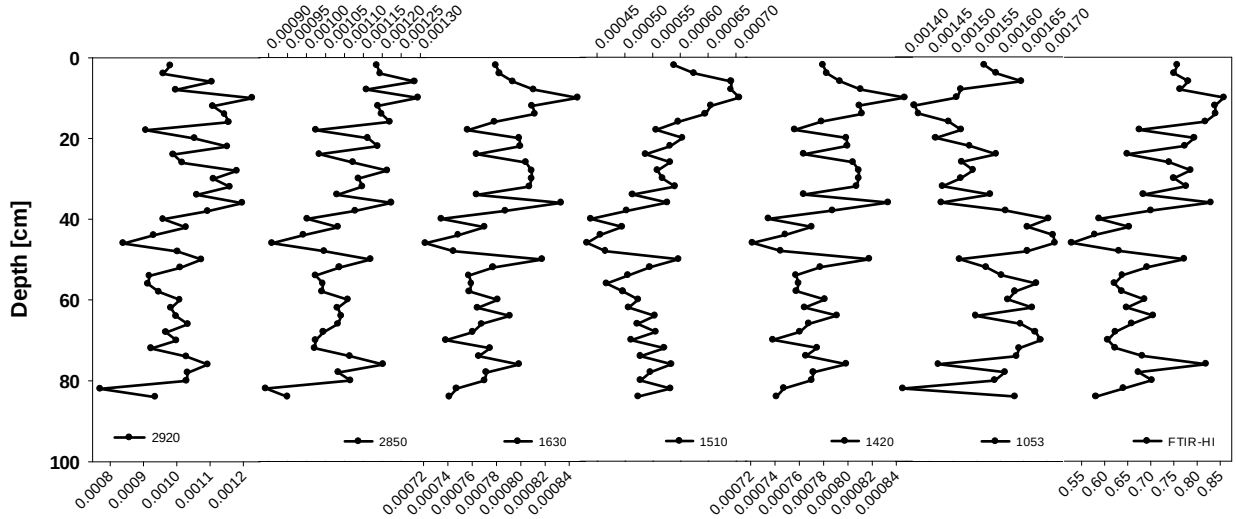

Figure S1: Records of selected FTIR band (cm^{-1}) intensities and FTIR humification index of KK peat.

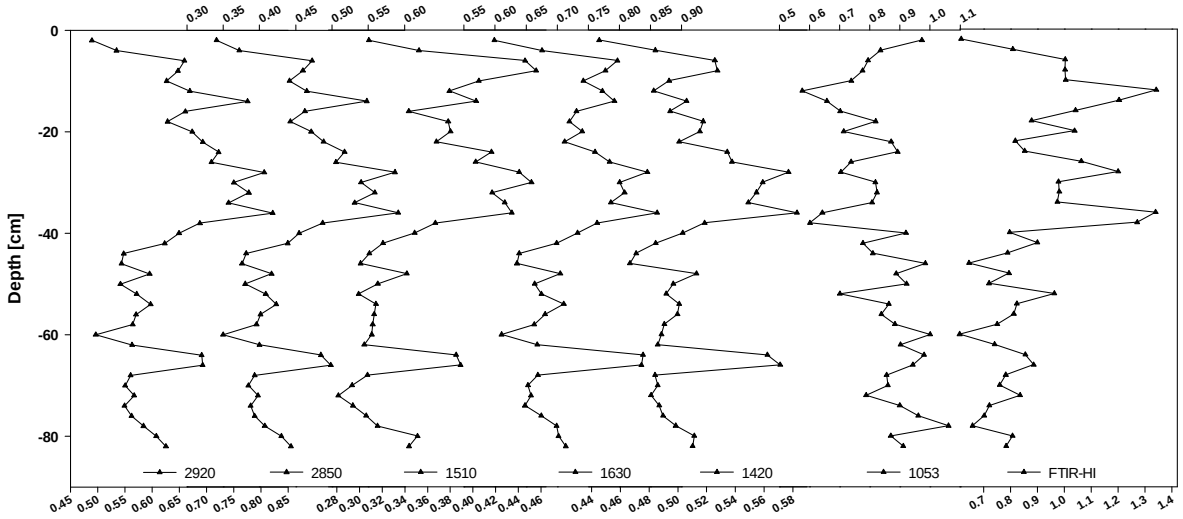

Figure S2: Records of selected FTIR band (cm^{-1}) intensities and FTIR humification index of KRB peat.

Table S1: Quantified pyrolysis products grouped according to origin and thereafter retention time. *m/z* typical mass; M molecular weight; RT retention time; ave. % TIC = mean values in the peat samples relative to the sum of all quantified pyrolysis products (*n* = 42); S.D. = standard deviation; Al aliphatic; Ps polysaccharide; K methylketone; Lg lignin; N N-compound; Ph phenol; F fatty acid; PA polyaromatics.

Code	Name	*m/z*	M	RT	TIC ave. %	S.D.
12-26	C_{12}-C_{26}*n*-alkanes	57, 71	-	-	-	-
12:1-26:1	C_{12}-C_{26}*n*-alkenes	55, 69	-	-	-	-
K21	*n*-C_{21}methylketone	58, 59	310	14.510	0.15	0.08
K22	*n*-C_{22}methylketone	58, 59	324	15.067	0.05	0.02
K23	*n*-C_{23}methylketone	58, 59	338	15.607	0.18	0.07
K24	*n*-C_{24}methylketone	58, 59	352	16.122	0.09	0.03
F16	*n*-C_{16}fattyaid	60, 73	256	12.477	0.40	0.23
F18	*n*-C_{18}fattyaid	60, 73	284	13.704	0.12	0.10
Al1	dodecanal	67, 82	184	8.292	0.27	0.19
Al2	branchedalkene	83, 280	280	14.729	0.08	0.03
Al3	pristene	55, 56	266	10.793	1.86	1.07
Lg1	4-vinylphenol	91, 120	120	6.722	2.46	0.92
Lg2	guaiacol	109, 124	124	5.401	1.21	0.53
Lg3	4-methylguaiacol	123, 138	138	6.401	0.93	0.54
Lg4	4-ethylguaiacol	137, 152	152	7.216	0.46	0.22
Lg5	4-vinylguaiacol	135, 150	150	7.554	2.50	1.15
Lg6	4-formylguaiacol	151, 152	152	8.432	0.26	0.09
Lg7	4-(prop-2-enyl)guaiacol, *trans*	164	164	8.734	0.21	0.10
Lg9	4-acetylguaiacol	151, 166	166	9.160	0.56	0.29
Lg10	4-(propan-2-one)guaiacol	137, 180	180	9.483	0.22	0.07
Lg11	syringol	139, 154	154	7.89	0.21	0.08
Lg12	4-methylsyringol	153, 168	168	8.71	0.22	0.11
Lg13	4-ethylsyringol	167, 182	182	9.347	0.11	0.04
Lg14	4-vinylsyringol	165, 180	180	9.685	0.30	0.13
Lg15	4-formylsyringol	181, 182	182	10.55	0.06	0.03
Lg16	4-(prop-2-enyl)syringol, *trans*	194	194	10.725	0.04	0.01
Lg17	4-acetylsyringol	181, 196	196	11.063	0.25	0.13
Lg18	4-(propan-3-one)syringol	181, 210	210	11.672	0.12	0.03
Ps5	4-hydroxy-5,6-dihydro-(2*H*)-pyran-2-one	58, 114	114	4.601	6.63	2.38
Ps6	dianhydrorhamnose	113, 128	128	4.980	0.85	0.38
Ps7	sugarcompound	72, 128	128	5.501	1.39	0.39
Ps8	C_1benzofuran	131, 132	132	5.573	0.17	0.04
Ps9	levoglucosenone	68, 98	126	5.718	7.39	2.18
Ps10	sugarcompound	57, 69, 82		6.566	2.62	0.74
Ps11	C_2benzofuran	145, 146	146	6.607	0.18	0.05
Ps12	1,4:3,6-dianhydro-alpha-D-glucose	57, 69	144	6.821	2.69	0.51
Ps13	levoglucosan	60, 73	162		37.44	8.15
Ph1	phenol	66, 94	94	4.398	7.18	2.47
Ph4	4-ethylphenol	107	108	6.181	0.84	0.23
Ph5	4-isopropenylphenol	119, 134	134	7.481	0.34	0.22
Ph6	3-methoxy-5-methylphenol	109, 138	138	7.658	0.05	0.03
Ph7	*p*-hydroxybiphenyl	141, 170	170	10.949	0.16	0.09
Ph8	ferulicestermethylester	145, 177, 208	208	11.802	0.01	0.01
Ph9	biphenylcompound	184	184	11.656	0.05	0.02
N1	C_1-pyrrole	80, 81	81	2.380	0.22	0.18

Table S1 (continued): Quantified pyrolysis products grouped according to origin and thereafter retention time. *m/z* typical mass; M molecular weight; RT retention time; ave. % TIC = mean values in the peat samples relative to the sum of all quantified pyrolysis products (*n*=42); S.D.= standard deviation. Al aliphatic; Ps polysaccharide; K methylketone; Lg lignin; N N-compound; Ph phenol; F fatty acid; PA polyaromatics.

Code	Name	m/z	M	RT	TIC ave. %	S.D.
N2	pyrrole	67	67	2.474	0.58	0.51
N3	pyridine	52, 79	79	2.474	1.01	0.79
N4	diketodipyrrole	93, 186	186	10.907	0.30	0.17
Ar1	benzene	78	78	2.068	1.03	0.89
Ar2	toluene	91, 92	92	2.531	4.31	3.22
PA1	naphthalene	128, 102	128	6.353	0.08	0.03
PA2	C_1-naphthalene	141, 142	141	7.398	0.10	0.03
St1	sequiterpene	161, 204	204	12.282	0.02	0.01
unkn1	Unidentified compound	137, 152	152	7.242	0.08	0.04
unkn2	Unidentified compound	80, 81		11.433	0.03	0.03
unkn3	Unidentified compound	86, 114, 210	210	14.115	0.19	0.30

Table S2: Results of Principal Component (Cp) analyses of KK and KRB peat decomposition proxy data (without pyrolysis GC-MS data) calculated separately and combined.

	KK			KRB		KRB-KK		
	Cp1	**Cp2**	**Cp3**	**Cp1**	**Cp2**	**Cp1**	**Cp2**	**Cp3**
C/N	**0.96**	0.002	0.11	**0.94**	-0.25	**0.94**	-0.15	0.12
OI	0.53	**-0.66**	-0.07	**0.86**	0.17	**0.72**	-0.14	-0.44
HI	**-0.91**	-0.20	-0.22	**-0.90**	-0.15	**-0.91**	0.17	0.12
$\delta^{13}C$	**0.79**	0.36	0.04	**0.72**	0.24	**0.74**	0.27	0.25
FTIR-HI	**-0.89**	0.20	0.3	**-0.83**	-0.13	**-0.86**	-0.29	-0.04
ABS	-0.19	0.17	**0.97**	**-0.17**	**-0.81**	-0.10	-0.54	**0.82**
$\delta^{15}N$	0.09	**0.78**	-0.15	-0.29	**0.64**	-0.12	**0.81**	0.42

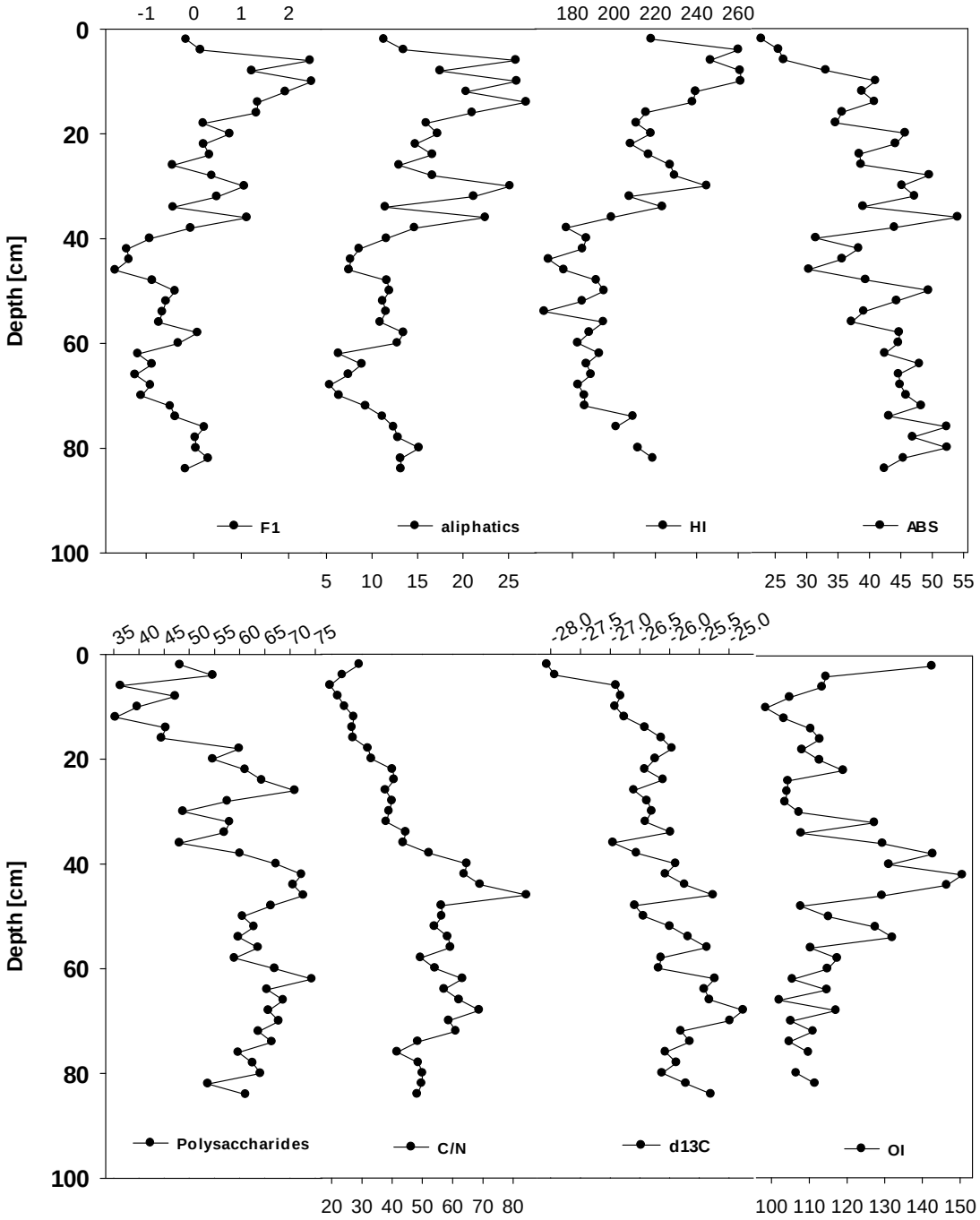

Figure S3: Records of decomposition proxies C/N ratios, $\delta^{13}C$ (‰) in bulk peat, oxygen and hydrogen indices (OI, HI, (mg CO_2 g^{-1}TOC)) determined by Rock Eval© analyses, UV-absorption of NaOH peat extracts compared to aliphatics and polysaccharides (ave. % TIC) and PCA factor F1 derived from Pyrolysis GC-MS analyses of KK peat.

Table S3. Correlation matrix of decomposition proxies. Negative correlations in italic; values < 0.30 are not indicated.

	CN	ABS	OI	HI	δ ^{13}C	δ ^{15}N	2850 cm^{-1}	2920 cm^{-1}	1630 cm^{-1}	1420 cm^{-1}	1053 cm^{-1}	FTIR-HI	Al (%)	Ps (%)	Lg (%)	F1	F2	Ph5 (%)	St1 (%)
CN	1			*0.74*	0.51		*0.44*	*0.36*	*0.51*	*0.40*	0.45	0.64	*0.71*	0.66		*0.74*		0.32	*0.66*
ABS		1																	
OI			1	*0.27*														0.37	
HI				1	*0.38*		0.32		0.37	0.30	*0.34*	0.45	0.58	*0.52*		0.60		*0.30*	0.63
δ ^{13}C					1		*0.20*		*0.43*		0.22	*0.42*	0.30	0.36		*0.32*			
δ ^{15}N						1													
2850 cm^{-1}							1		0.73	0.59	*0.32*	0.73	0.62	*0.29*		0.41		*0.38*	
2920 cm^{-1}								1	0.74	0.62		0.65	0.41			0.35			
1630 cm^{-1}									1	0.73		0.84	0.46	*0.41*		*0.48*		*0.33*	0.3
1420 cm^{-1}										1		0.82							0.3
1053 cm^{-1}											1	*0.61*	*0.38*	0.40		*0.43*		0.38	*0.38*
FTIR-HI												1	0.32	*0.55*				*0.48*	0.43
Al (%)													1	*0.68*		0.85		*0.31*	*0.73*
Ps (%)														1		*0.85*		0.32	*0.65*
Lg (%)															1		*0.74*		
F1																1		*0.45*	
F2																	1		
Ph5 (%)																		1	*0.35*
St1 (%)																			1

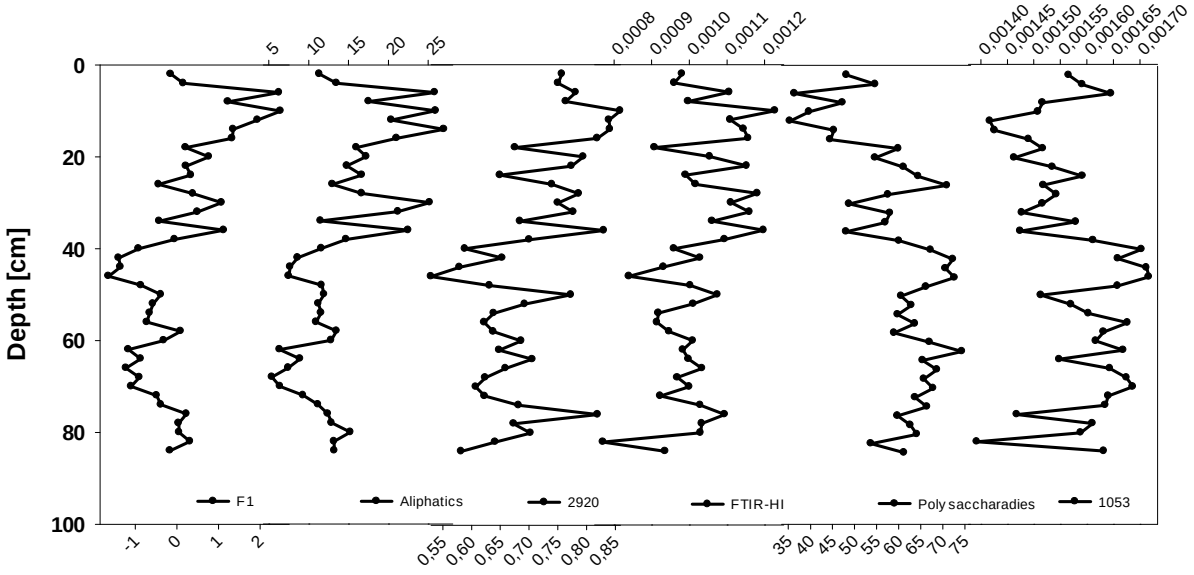

Figure S4: Depth profiles of the scores of F1 and F2, aliphatics, polysaccharides (Pyrolysis-GC-MS data), intensity records of FTIR bands 2920 cm^{-1} (aliphatic structures) and 1053 cm^{-1} (polysaccharides) and the record of the FTIR-humification index (ratio of bands 1630 cm^{-1} and 1053 cm^{-1}).