Supplementary material

Disentangling the effects of parent material and litter input chemistry on molecular soil organic matter composition in converted forests in Western Europe

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Table S1: Lignin-derived compounds released upon THM

Code	Compound names	Fragment ion(s)/(M^+)	RT*
Guaiacyl structures			
G1	1,2-dimethoxybenzene	123/138	14.15
G2	3,4-dimethoxytoluene	137/152	16.12
G3	3,4-dimethoxystyrene	91/149/164	18.62
G4	3,4-dimethoxybenzaldehyde	151/165/166	20.63
G21	1-(3,4-dimethoxyphenyl)-1-propene	163/178	21.10
G5	3,4-dimethoxyacetophenone	137/165/180	22.15
G6	3,4-dimethoxybenzoic acid methyl ester	165/181/196	22.61
G24	3,4-dimethoxybenzeneacetic acid methyl ester	151/210	23.13
G7	cis-1-(3,4-dimethoxyphenyl)-2-methoxyethylene	151/179/194	23.22
G8	trans-1- (3,4-dimethoxyphenyl)-2-methoxyethylene	151/179/194	23.47
G9	cis-3-methoxy-1-(3,4-dimethoxyphenyl)-1-propene	177/193/208	23.53
G10	cis-1-(3,4-dimethoxyphenyl)-1-methoxy-1-propene	165/193/208	23.70
G11	trans-1-(3,4-dimethoxyphenyl)-1-methoxy-1-propene	165/193/208	23.88
G12	3-(3,4-dimethoxyphenyl) propanoic acid methyl ester	151/224	25.00
G13	trans-1-(3,4-dimethoxyphenyl)-3-methoxyprop-1-ene	91/177/208	25.09
G14	threo-1-(3,4-dimethoxyphenyl)-1,2,3-trimethoxypropane	166/181/270	25.94
G15	erythro-1-(3,4-dimethoxyphenyl)-1,2,3-trimethoxypropane	166/181/270	26.13
G18	trans-3-(3,4-dimethoxyphenyl)-3-propenoic acid methyl ester	191/207/222	27.16
G16	cis-1-(3,4-dimethoxyphenyl)-1,3-dimethoxyprop-1-ene	176/207/238	27.26
Syringyl structures			
S1	1,2,3-trimethoxybenzene	153/168	17.55
S2	3,4,5-trimethoxytoluene	139/167/182	19.90
S4	3,4,5-trimethoxybenzaldehyde	125/181/196	22.79
S5	3,4,5-trimethoxyacetophenone	139/195/210	24.09
S6	3,4,5-trimethoxybenzoic acid methyl ester	195/211/226	24.73
S7	cis-1-(3,4,5-trimethoxyphenyl)-2-methoxyethylene	181/209/224	25.60
S8	trans-1-(3,4,5-trimethoxyphenyl)-2-methoxyethylene	181/209/224	25.91
S14	threo-1-(3,4,5-trimethoxyphenyl)-1,2,3-trimethoxypropane	211/300	27.56
S15	erythro-1-(3,4,5-trimethoxyphenyl)-1,2,3-trimethoxypropane	211/300	27.72
p-Coumaryl structures			
P3	4-methoxystyrene	119/134	14.50
P4	4-methoxybenzaldehyde	92/135/136	15.36
P6	4-methoxybenzoic acid methyl ester	135/166	18.88
P22	1-(4-methoxyphenyl)-2-propanone	121/149/164	19.87

The compound names are from the methylated forms. The fragment ions that are underlined were used to distinguish between compounds with similar ion fragments. *RT = retention time.

Table S2: Cutin- and suberin-derived compounds released upon THM

Code	Fragment ion(s)/(M^+)	RT*
n-Alkanoic acid, methyl esters	*(74/87/143/M-15/M^+)*	
n-C14:0	199/242	25.10
n-C15:0	213/256	26.24
n-C16:0	227/270	28.11
n-C17:0	241/284	28.74
n-C18:1	264/296	30.51
n-C18:0	255/298	30.86
n-C18:2	262/294	33.28
n-C20:0	283/326	33.38
n-C22:0	311/354	35.68
n-C23:0	325/368	36.77
n-C24:0	339/382	37.82
n-C25:0	353/396	38.84
n-C26:0	367/410	39.81
n-C28:0	395/438	41.75
n-Alcohols, methyl ethers	*(55/57/83/M-32/M^+)*	
n-C22:0	308/340	34.64
n-C24:0	336/368	36.84
n-C26:0	364/396	38.90
n-C28:0	392/424	40.81
n-C30:0	420/452	42.87
ω-Methoxyalkanoic acid, methyl esters	*(74/87/98/143/M-64/M-47/M-32/M-15/M^+)*	
ω-C14:0	208/225/240/257/272	28.40
ω-C16:0	253/268/285/300	31.13
ω-C18:0	264/281/296/313/328	33.63
ω-C20:0	309/324/341/356	35.93
ω-C22:0	337/352/369/384	38.06
ω-C24:0	348/365/380/397/412	40.04
ω-C26:0	376/393/408/425/440	42.03
α,ω-Alkanedioic acid, dimethyl esters	(74/84/98/112/M-105/M-73/M-31/M^+)	
α,ω-C16:0	209/241/283/(314)	32.29
α,ω-C18:0	237/269/311/(342)	34.70
α,ω-C20:0	265/297/339/(370)	36.93
α,ω-C22:0	293/325/367/(398)	39.01
tri-methoxy fatty acid, methyl ester	(M^+)	
9,10,*ω*-trihydroxy C18:0	137/201/(388)	36.09
di-methoxy fatty acids, methyl ester	(M^+)	
x,ω-dihydroxy-C16:0	173/201/215/(330)	32.76

The compounds are listed in compound classes and sorted on their retention times. *RT = retention time.

Table S3: Summary of multi-factor Anova tests for all soil samples

Group	Data set	Gaume		Mullerthal		Combined
	Factors	Forest type	Substrate	Forest type	Substrate	Study area
Basic soil properties	pH	0.0027**	0.0051**	n.s.	<0.001	<0.001
	C/N (ratio)	<0.001	<0.001	n.s.	<0.001	n.s.
	SOC stocks	0.0072**	<0.001	n.s.	<0.001	<0.001
Lignin markers	ΛSG (yield)	0.0027**	0.0016**	n.s.	n.s.	<0.001
	ΓG (ratio)	0.0110*	n.s.	n.s.	0.0062**	<0.001
	S/G (ratio)	<0.001	n.s.	<0.001	n.s.	0.0107*
Aliphatic markers	Cutin yield	x	n.s.	x	0.0144*	n.s.
	Suberin yield	x	0.0065**	x	0.0011**	0.0435*
	Lig/Ali (ratio)	x	n.s.	x	n.s.	0.0148*

Significance levels used: * P <0.05, ** P <0.01, *** P <0.001 and n.s. = not significant. No values (x) are shown for forest type for the aliphatic markers because of the different calculation of both cutin and suberin yield for deciduous and coniferous forest (See manuscript: Table 2).

Table S4: Summary of the t-test results for lignin measured in the vegetation samples

Group	ΛSG yield	S/G ratio	Γ_G ratio
Deciduous roots (n = 5)	0.16	0.43	2.11
Deciduous leaves (n = 3)	0.06	0.82	2.82
P-value	0.0824 n.s.	0.3089 n.s.	0.6787 n.s.
Deciduous leaves/roots (n = 8)	0.12	0.58	2.62
Spruce needles/roots (n = 3)	0.17	0.06	8.76
P-value	0.4262 n.s.	0.0133*	0.27 n.s.

Significance levels used: * P <0.05 and n.s. = not significant. Statistical results are only shown for lignin as the vegetation data was used to designate the compounds used for the calculation of the cutin and suberin yields. ΛSG = lignin yield

Table S5: pH, C/N ratio and SOC stocks

Forest Type (Substrate) Soil Depth (cm)	pH (H_2O)		C/N ratio		SOC stocks ($t\ ha^{-1}$)	
Deciduous (Sandy)	Gaume	Mullerthal	Gaume	Mullerthal	Gaume	Mullerthal
0 - 5	3.9	4.1	13.6	15.6	11.6	15.1
5 - 10	3.9	3.9	13.3	15.1	8.1	7.5
10 - 15	4.0	4.0	13.6	14.5	7.1	6.5
15 - 20	4.2	4.2	12.9	12.9	5.0	5.0
Coniferous (Sandy)						
0 - 5	3.5	3.6	19.0	19.6	13.4	17.3
5 - 10	3.7	3.7	18.1	17.0	9.7	8.5
10 - 15	3.9	3.9	17.4	15.9	7.2	6.7
15 - 20	4.1	4.2	15.9	13.6	5.8	5.6
Deciduous (Loamy)						
0 - 5	4.2	5.6	11.5	13.0	7.3	22.5
5 - 10	4.1	5.5	11.6	11.6	6.2	16.5
10 - 15	4.3	5.6	10.6	10.3	4.3	10.8
15 - 20	4.2	5.6	10.7	9.4	4.1	9.1
Coniferous (Loamy)						
0 - 5	3.8	5.6	13.9	14.1	10.3	23.5
5 - 10	3.9	5.7	13.0	12.0	7.2	15.9
10 - 15	4.1	5.6	11.8	11.4	5.7	12.7
15 - 20	4.1	5.5	11.1	10.4	5.4	9.1

Values are averages of three plots.

Table S6: Lignin yield, S/G ratio and Γ_G ratio

Forest Type (Substrate) Soil Depth (cm)	Lignin yield Λ_{SG} (mg/100mg OC)		S/G ratio		Γ_G ratio	
Deciduous (Sandy)	Gaume	Mullerthal	Gaume	Mullerthal	Gaume	Mullerthal
0 - 5	0.4	0.6	0.22	0.17	12.97	5.65
5 - 10	0.1	0.4	0.16	0.16	5.84	4.49
10 - 15	0.2	0.3	0.15	0.33	4.15	3.27
15 - 20	0.1	0.3	0.15	0.35	6.27	8.78
Coniferous (Sandy)						
0 - 5	0.5	1.1	0.08	0.06	24.83	13.60
5 - 10	0.7	0.8	0.06	0.14	24.47	7.40
10 - 15	0.7	0.5	0.06	0.17	7.28	5.79
15 - 20	0.4	0.8	0.10	0.08	12.50	3.77
Deciduous (Loamy)						
0 - 5	0.1	0.8	0.16	0.29	8.87	2.11
5 - 10	0.1	0.7	0.25	0.33	7.06	3.51
10 - 15	0.1	0.4	0.24	0.18	4.98	3.31
15 - 20	0.0	0.1	0.22	0.49	-	4.28
Coniferous (Loamy)						
0 - 5	0.4	1.2	0.04	0.14	25.49	3.70
5 - 10	0.2	0.4	0.04	0.17	12.80	3.31
10 - 15	0.2	0.4	0.04	0.09	24.21	1.68
15 - 20	0.1	0.2	0.21	0.09	13.24	2.23

Values are averages of three plots. Values are missing when the ratio could not be calculated.

Table S7: Cutin yield, suberin yield and Lig/Ali ratio

Forest Type (Substrate) Soil Depth (cm)	Cutin yield (mg/100 mg OC)		Suberin Yield (mg/100 mg OC)		Lig/Ali ratio	
Deciduous (Sandy)	Gaume	Mullerthal	Gaume	Mullerthal	Gaume	Mullerthal
0 - 5	0.3	1.6	0.9	3.6	0.34	0.26
5 - 10	0.3	0.6	1.5	6.0	0.13	0.16
10 - 15	0.2	0.2	1.7	6.7	0.09	0.36
15 - 20	0.2	0.3	1.9	9.8	0.07	1.67
Coniferous (Sandy)						
0 - 5	1.2	1.8	0.6	0.3	0.32	0.71
5 - 10	2.5	7.9	1.3	1.5	0.26	0.42
10 - 15	3.1	5.7	0.6	0.5	0.17	0.61
15 - 20	4.0	6.8	0.5	0.4	0.33	0.71
Deciduous (Loamy)						
0 - 5	0.2	0.4	0.9	1.2	0.07	2.22
5 - 10	0.1	0.3	0.4	1.2	0.15	1.12
10 - 15	0.3	0.2	1.7	1.5	0.15	5.33
15 - 20	0.0	0.0	0.2	0.3	0.61	8.80
Coniferous (Loamy)						
0 - 5	3.4	0.7	1.0	0.1	0.09	4.11
5 - 10	2.4	0.5	0.3	0.0	0.10	1.85
10 - 15	0.3	0.7	0.1	0.1	0.58	1.67
15 - 20	1.0	0.1	0.1	0.0	0.19	1.52

Values are averages of three plots.