Table S1: List of the analyzed compounds and of the m/z ratio and mass spectra factor used for their integration.

Table S2: Source apportionment calculated using molecular, isotopic and elemental data.

Table S3: *p*-Values of the Student T-test comparing the source apportionment calculated using molecular data versus molecular, isotopic and elemental data. P-Values were higher than 0.05 then the differences were not significant.

Figure S1: Linear regression between measured $d^{13}C$ (Rowland et al., 2017) and modeled $d^{13}C$ from the source apportionment performed using moelcular data. The slope of the regression is 1.012 with a *p*-value < 0.0001 and R^2 is 0.59.

Figure S2: Linear regression between the sum of the concentrations of target compounds (µg/g of dry sample) and total organic carbon TOC from Rowland et al. (2017) (mg/g of dry sample). The slope of the regression is 1.70 E-03 with a *p*-value < 0.0001 and R^2 is 0.94.

Table S1. List of the analyzed compounds and of the m/z ratio and mass spectra factor used for their integration.

Compounds	m/z Int	MSF
Deoxyaldonic acids methyl ester produced by the THM of:		
pentose (2 peaks)	129	4
deoxyhexose (4 peaks)	129	4
hexose (4 peaks)	129	4
Low organic acid methyl esters		
2,4-Heptadienoic acid methyl ester	111	3.9
Succinic acid methyl ester	115	4.5
Fumaric acid methyl ester	113	3.3
Benzoic acid methyl ester	105	2.9
Fatty acid methyl esters		
$C_{6:0}$	74	3.1
$C_{7:0}$	74	3.1
$C_{8:0}$	74	3.0
$C_{9:0}$	74	3.6
$C_{10:0}$	74	3.0
a,*w*$C_{8:0}$	74	14.9
$C_{12:0}$	74	3.0
a,*w*$C_{9:0}$	74	10.2
i$C_{13:0}$	74	4.1
a$C_{13:0}$	74	4.1
$C_{13:0}$	74	4.1
br$C_{14:0}$	74	3.1
$C_{14:1}$	74	14.5
$C_{14:0}$	74	3.1
i$C_{15:0}$	74	3.3
a$C_{15:0}$	74	3.3
$C_{15:0}$	74	3.3
br$C_{16:0}$	74	4.9
$C_{16:1}$	74	14.5
$C_{16:0}$	74	4.9
i$C_{17:0}$	74	3.9
a$C_{17:0}$	74	3.9
$C_{17:1}$	74	14.5
$C_{17:0}$	74	3.9
$C_{18:1}$	74	14.6
$C_{18:0}$	74	4.5
wOH$C_{16:0}$	74	12.1
$C_{19:1}$	74	14.5
$C_{19:0}$	74	4.3
a,*w*$C_{16:0}$	74	11.3
$C_{20:0}$	74	4.9
wOH$C_{18:0}$	74	17.3
$C_{21:0}$	74	7.5

Table S1. continued.

Compounds	m/z Int	MSF
Fatty acid methyl esters		
a,*w*$C_{18:0}$	74	17.7
$C_{22:0}$	74	4.9
wOH$C_{20:0}$	74	12.9
$C_{23:0}$	74	8.4
a,*w*$C_{20:0}$	74	10.8
$C_{24:0}$	74	4.4
wOH$C_{22:0}$	74	13.5
$C_{25:0}$	74	7.7
a,*w*$C_{22:0}$	74	10.8
$C_{26:0}$	74	4.5
wOH$C_{24:0}$	74	13.5
$C_{27:0}$	74	5.1
a,*w*$C_{24:0}$	74	9.7
$C_{28:0}$	74	4.9
wOH$C_{26:0}$	74	14.4
$C_{29:0}$	74	4.9
a,*w*$C_{26:0}$	74	9.7
$C_{30:0}$	74	4.9
wOH$C_{28:0}$	74	14.4
$C_{31:0}$	74	4.9
a,*w*$C_{28:0}$	74	9.7
$C_{32:0}$	74	4.9
10,16-di$OHC_{16:0}$	71	7.4
9,10,18-tri$OHC_{18:0}$	71	8.6
Phenols		
1,4-Dimethoxybenzene	138	6.0
Dimethoxytoluene	152	5.7
Dimethoxytoluene	152	5.7
3-Methoxybenzoic acid methyl ester	135	3.9
4-Methoxybenzoic acid methyl ester	135	2.8
3-Methoxybenzaldehyde	136	4.3
4-Methoxybenzaldehyde	136	3.8
1,2,3-Trimethoxybenzene	168	3.8
1,2,4-Trimethoxybenzene	168	4.3
1,3,5-Trimethoxybenzene	168	3.0
Trimethoxytoluene (3 peaks)	167	7.0
dimethoxystyrene	164	3.9
1,2,3,4-Tetramethoxybenzene	198	3.5
1,2,3,5-Tetramethoxybenzene	198	13.5
3,4-Dimethoxybenzaldehyde	166	4.2
3,4-Dimethoxyacetophenone	165	2.8
2,3-Dimethoxybenzoic acid methyl ester	196	7.6
3,5-Dimethoxybenzoic acid methyl ester	196	5.1

Table S1. continued.

Compounds	m/z Int	MSF
Phenols		
3,4-Dimethoxybenzoic acid methyl ester	196	5.6
3,4,5-Trimethoxybenzaldehyde	196	6.7
3-(4-methoxyphenyl)prop-2-enoic acid methyl ester	192	6.7
3,4,5-Trimethoxyacetophenone	195	4.8
1,2-Dimethoxy-4-(1-methoxyethenyl)benzene	194	7.4
cis-1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	194	5.1
trans-1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	194	5.1
cis-1,2-Dimethoxy-4-(3-methoxy-1-propenyl)benzene	208	5.6
2,4,5-Trimethoxypropenylbenzene	208	4.4
1,2-Dimethoxy-4-(1-methoxy-1-propenyl)benzene	208	6.2
cis-1,2-Dimethoxy-4-(2-methoxy-1-propenyl)benzene	208	5.7
trans-1,2-Dimethoxy-4-(2-methoxy-1-propenyl)benzene	208	5.7
trans-1,2-Dimethoxy-4-(3-methoxy-1-propenyl)benzene	208	5.6
3,4,5-Trimethoxybenzoic acid emthyl ester	226	5.3
cis-1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene	224	7
trans-1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene	224	7
erythro-1,2-Dimethoxy-4-(1,2,3-trimethoxypropyl)benzene	181	3.6
threo-1,2-Dimethoxy-4-(1,2,3-trimethoxypropyl)benzene	181	3.6
3-(3,4-dimethoxyphenyl)prop-2-enoic acid methyl ester	222	3.7
cis-1,2,3-Trimethoxy-5-(2-methoxy-1-propenyl)benzene	238	7
trans-1,2,3-Trimethoxy-5-(2-methoxy-1-propenyl)benzene	238	7
cis-1,2-Dimethoxy-4-(2,3-dimethoxy-1-propenyl)benzene	238	8.5
trans-1,2-Dimethoxy-4-(2,3-dimethoxy-1-propenyl)benzene	238	8.5
erythro-1,2,3-Trimethoxy-5-(1,2,3-trimethoxypropyl)benzene	211	2.1
threo-1,2,3-Trimethoxy-5-(1,2,3-trimethoxypropyl)benzene	211	2.1

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Table S2. Source apportionment calculated using molecular, isotopic and elemental data.

		12 ha location			*79 ha location*		
		Li (%)	Sbed (%)	FH-W (%)	Li (%)	Sbed (%)	FH-W (%)
Event 1	C	97 ± 4	0 ± 1	2 ± 4	43 ± 8	57 ± 8	0 ± 0
May 1, 2014	M	75 ± 6	20 ± 4	4 ± 7	0 ± 0	98 ± 3	2 ± 3
	F	70 ± 10	16 ± 4	14 ± 12	43 ± 8	57 ± 8	0 ± 1
	POM	92 ± 7	4 ± 3	4 ± 8	40 ± 5	60 ± 6	0 ± 1
Event 2	C	97 ± 5	1 ± 2	2 ± 5	96 ± 5	1 ± 3	3 ± 5
Apr. 21, 2015	M	95 ± 6	1 ± 2	4 ± 7	52 ± 7	46 ± 6	2 ± 4
	F	64 ± 11	17 ± 5	19 ± 14	45 ± 8	52 ± 7	3 ± 5
	POM	85 ± 7	7 ± 3	9 ± 8	89 ± 7	8 ± 5	3 ± 5
Event 3	C	97 ± 4	2 ± 3	1 ± 2	45 ± 8	55 ± 8	0 ± 0
July 3, 2015	M	86 ± 4	12 ± 4	3 ± 5	39 ± 9	61 ± 9	0 ± 0
	F	58 ± 6	41 ± 6	1 ± 3	39 ± 9	53 ± 7	8 ± 7
	POM	80 ± 5	18 ± 4	2 ± 3	42 ± 8	55 ± 8	3 ± 2
Event 4	C	66 ± 14	0 ± 0	34 ± 14	fraction not available		
Sept. 30, 2015	M	63 ± 13	0 ± 0	37 ± 13	36 ± 8	0 ± 0	64 ± 8
	F	54 ± 10	1 ± 1	46 ± 10	68 ± 13	2 ± 3	29 ± 15
	POM	57 ± 12	0 ± 0	43 ± 12	-	-	-

Table S3. *p*-Values of the Student T-test comparing the source apportionment calculated using molecular data versus molecular, isotopic and elemental data. P-Values were higher than 0.05 then the differences were not significant.

		12 ha location			*79 ha location*		
		Li (%)	Sbed (%)	FH-W (%)	Li (%)	Sbed (%)	FH-W (%)
Event 1	C	0.37	0.25	0.45	0.27	0.27	*nc*
May 1, 2014	M	0.24	0.16	0.46	0.10	0.13	0.15
	F	0.14	0.11	0.34	0.10	0.11	0.17
Event 2	C	0.33	0.29	0.42	0.39	0.33	0.47
Apr. 21, 2015	M	0.44	0.31	0.49	0.10	0.18	0.09
	F	0.24	0.22	0.39	0.08	0.15	0.12
Event 3	C	0.27	0.37	0.33	0.23	0.23	*nc*
July 3, 2015	M	0.24	0.18	0.46	0.18	0.18	*nc*
	F	0.17	0.23	0.18	0.12	0.31	0.10
Event 4	C	0.20	0.19	0.17	fraction not available		
Sept. 30, 2015	M	0.19	*nc*	0.19	0.47	*nc*	0.47
	F	0.16	*nc*	0.20	0.15	0.30	0.19

nc. The calculation was not possible because the contributions were nul.

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Figure S1

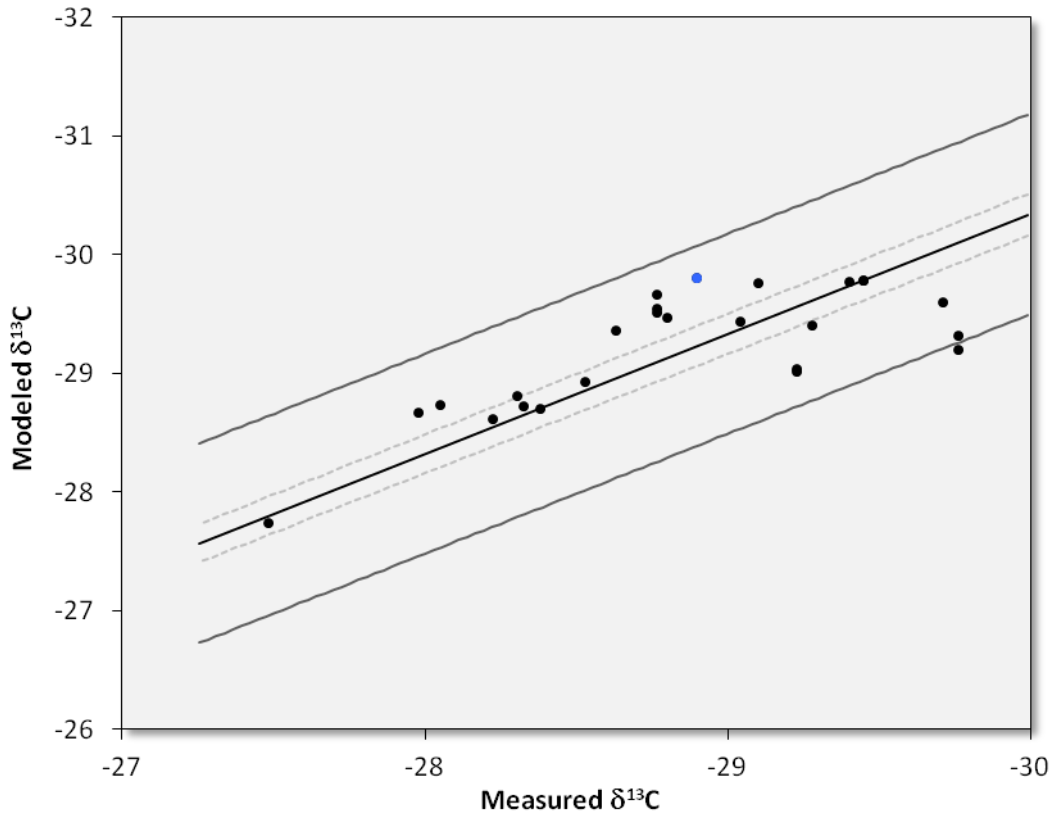
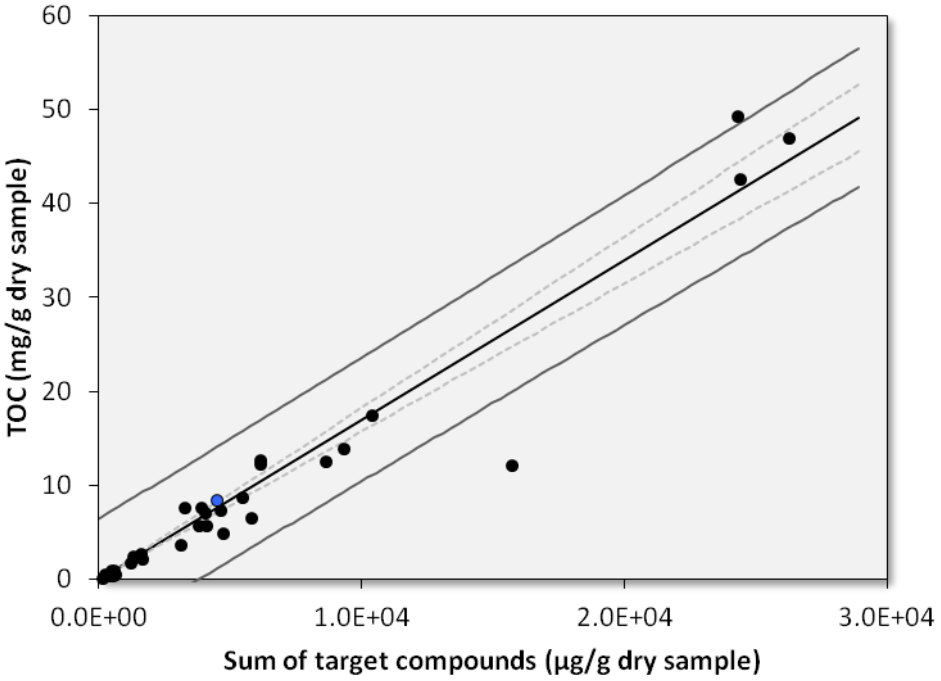


Figure S2


60
50
40
30
20
10
0
TOC (mg/g dry sample)
0.0E+00
1.0E+04
2.0E+04
3.0E+04
Sum of target compounds (µg/g dry sample)