

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 $\delta^{13}\text{C}$ (Rowland et al., 2017) and modeled $\delta^{13}\text{C}$ from the source apportionment performed using molecular 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 ($\mu\text{g/g}$ of dry sample) and total organic carbon TOC from Rowland et al. (2017) (mg/g of dry sample). The slope of the regression is 1.70×10^{-3} 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. The 71 variables of the statistical treatment are identified with the symbol *

Compounds	m/z Int	MSF
<i>Deoxyaldonic acids methyl ester produced by the THM of:</i>		
pentose (2 peaks) *	129	4
deoxyhexose (4 peaks) *	129	4
hexose (4 peaks) *	129	4
<i>Low organic acid methyl esters</i>		
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
<i>Fatty acid methyl esters</i>		
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,wC _{8:0}	74	14.9
C _{12:0} *	74	3.0
a,wC _{9:0} *	74	10.2
iC _{13:0}	74	4.1
aC _{13:0}	74	4.1
C _{13:0} *	74	4.1
brC _{14:0} *	74	3.1
C _{14:1}	74	14.5
C _{14:0}	74	3.1
iC _{15:0}	74	3.3
aC _{15:0}	74	3.3
C _{15:0}	74	3.3
brC _{16:0} *	74	4.9
C _{16:1} *	74	14.5
C _{16:0} *	74	4.9
iC _{17:0} *	74	3.9
aC _{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
wOHC _{16:0} *	74	12.1
C _{19:1} *	74	14.5
C _{19:0}	74	4.3
a,wC _{16:0} *	74	11.3
C _{20:0}	74	4.9
wOHC _{18:0} *	74	17.3
C _{21:0}	74	7.5

Table S1. continued.

Compounds	m/z Int	MSF
<i>Fatty acid methyl esters</i>		
<i>a,w</i> C _{18:0}	74	17.7
C _{22:0} *	74	4.9
<i>wOHC</i> _{20:0} *	74	12.9
C _{23:0}	74	8.4
<i>a,w</i> C _{20:0} *	74	10.8
C _{24:0} *	74	4.4
<i>wOHC</i> _{22:0} *	74	13.5
C _{25:0}	74	7.7
<i>a,w</i> C _{22:0} *	74	10.8
C _{26:0}	74	4.5
<i>wOHC</i> _{24:0} *	74	13.5
C _{27:0} *	74	5.1
<i>a,w</i> C _{24:0} *	74	9.7
C _{28:0} *	74	4.9
<i>wOHC</i> _{26:0} *	74	14.4
C _{29:0} *	74	4.9
<i>a,w</i> C _{26:0}	74	9.7
C _{30:0}	74	4.9
<i>wOHC</i> _{28:0}	74	14.4
C _{31:0} *	74	4.9
<i>a,w</i> C _{28:0}	74	9.7
C _{32:0}	74	4.9
10,16-diOHC _{16:0} *	71	7.4
9,10,18-triOHC _{18:0} *	71	8.6
<i>Phenols</i>		
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
<i>Phenols</i>		
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
<i>cis</i> -1,2-Dimethoxy-4-(2-methoxyethenyl)benzene *	194	5.1
<i>trans</i> -1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	194	5.1
<i>cis</i> -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
<i>cis</i> -1,2-Dimethoxy-4-(2-methoxy-1-propenyl)benzene	208	5.7
<i>trans</i> -1,2-Dimethoxy-4-(2-methoxy-1-propenyl)benzene *	208	5.7
<i>trans</i> -1,2-Dimethoxy-4-(3-methoxy-1-propenyl)benzene *	208	5.6
3,4,5-Trimethoxybenzoic acid methyl ester *	226	5.3
<i>cis</i> -1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene	224	7
<i>trans</i> -1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene *	224	7
<i>erythro</i> -1,2-Dimethoxy-4-(1,2,3-trimethoxypropyl)benzene *	181	3.6
<i>threo</i> -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
<i>cis</i> -1,2,3-Trimethoxy-5-(2-methoxy-1-propenyl)benzene *	238	7
<i>trans</i> -1,2,3-Trimethoxy-5-(2-methoxy-1-propenyl)benzene	238	7
<i>cis</i> -1,2-Dimethoxy-4-(2,3-dimethoxy-1-propenyl)benzene	238	8.5
<i>trans</i> -1,2-Dimethoxy-4-(2,3-dimethoxy-1-propenyl)benzene	238	8.5
<i>erythro</i> -1,2,3-Trimethoxy-5-(1,2,3-trimethoxypropyl)benzene	211	2.1
<i>threo</i> -1,2,3-Trimethoxy-5-(1,2,3-trimethoxypropyl)benzene *	211	2.1

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

		<i>12 ha location</i>			<i>79 ha location</i>		
		Li (%)	Sbed (%)	FH-W (%)	Li (%)	Sbed (%)	FH-W (%)
Event 1	C	97 ± 4	0 ± 1	2 ± 4	43 ± 8	57 ± 8	0 ± 0
<i>May 1, 2014</i>	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
<i>Apr. 21, 2015</i>	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
<i>July 3, 2015</i>	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		
<i>Sept. 30, 2015</i>	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.

		<i>12 ha location</i>			<i>79 ha location</i>		
		Li (%)	Sbed (%)	FH-W (%)	Li (%)	Sbed (%)	FH-W (%)
Event 1 <i>May 1, 2014</i>	C	0.37	0.25	0.45	0.27	0.27	<i>nc</i>
	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 <i>Apr. 21, 2015</i>	C	0.33	0.29	0.42	0.39	0.33	0.47
	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 <i>July 3, 2015</i>	C	0.27	0.37	0.33	0.23	0.23	<i>nc</i>
	M	0.24	0.18	0.46	0.18	0.18	<i>nc</i>
	F	0.17	0.23	0.18	0.12	0.31	0.10
Event 4 <i>Sept. 30, 2015</i>	C	0.20	0.19	0.17	fraction not available		
	M	0.19	<i>nc</i>	0.19	0.47	<i>nc</i>	0.47
	F	0.16	<i>nc</i>	0.20	0.15	0.30	0.19

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

Figure S1

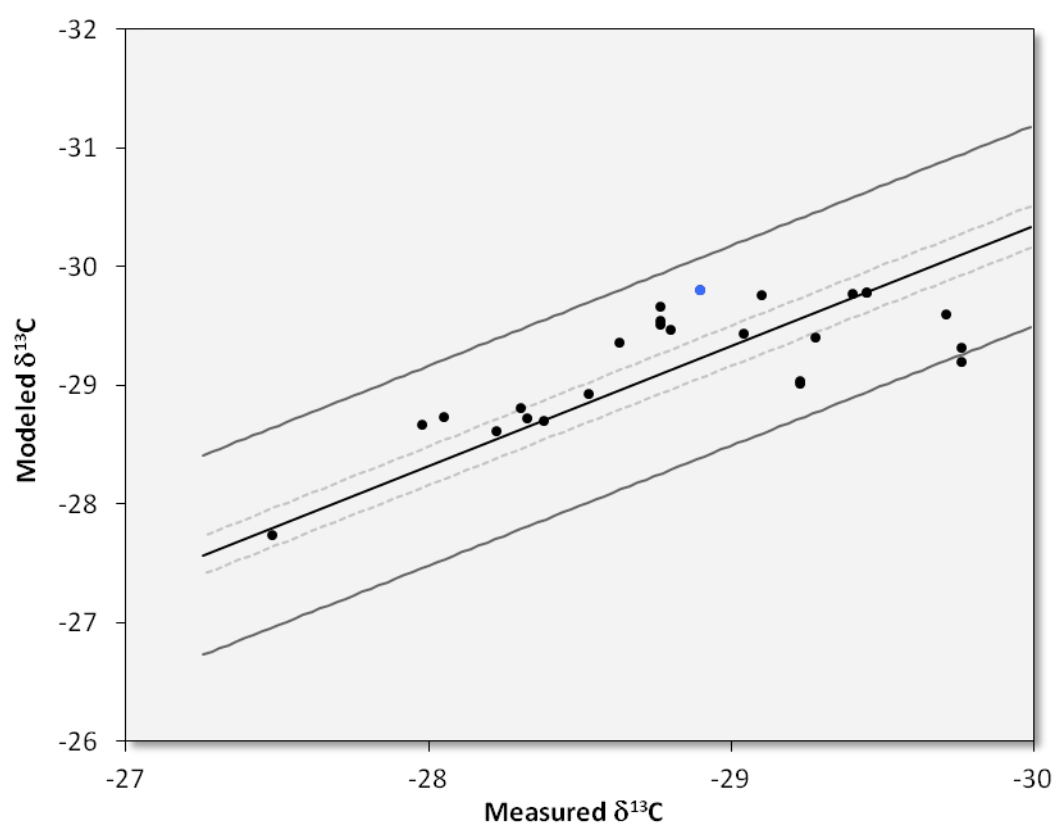


Figure S2

