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Environmental Chemistry

Supplementary Material

Exploration of changes in the chemical composition of sedimentary organic matter and the underlying processes during biodegradation through advanced analytical techniques

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Table S1. Percentages of removal or production of organic carbon in the artificial sediments ($\Delta\%_{OC}$) and in the porewaters ($\Delta\%_{DOC}$) (data from Derrien *et al*. 2019) after 60 days of incubation for both oxygen conditions.

	$\Delta\%_{OC}$		$\Delta\%_{DOC}$	
Mixing ratios	Oxic	Anoxic	Oxic	Anoxic
S:A, 100:0	17.1 ± 3.6	–16.0 ± 5.3	–9.1 ± 19.0	–38.4 ± 8.2
S:A, 75:25	38.1 ± 62.0	–15.3 ± 32.4	41.6 ± 13.7	60.6 ± 1.7
S:A, 50:50	28.1 ± 3.1	42.1 ± 88.2	–32.2 ± 8.6	10.5 ± 15.3
S:A, 25:75	28.7 ± 16.9	–19.1 ± 34.7	22.5 ± 45.0	112.4
S:A, 0:100	17.9 ± 2.8	–2.6 ± 14.4	33.5 ± 1.5	51.6 ± 3.4

Table S2. Characteristics of compound classes used for categorizing FT-ICR MS molecular formulas.

Compound class	Criterion
Aromatic formula	AImod = 0.5–0.67
Condensed aromatic structure	$0.2 \leq H/C \leq 0.7$; $0 \leq O/C \leq 0.67$
Lignin–CRAM	$0.7 \leq H/C \leq 1.5$; $0.1 \leq O/C \leq 0.67$
Protein	$1.5 \leq H/C \leq 2.2$; $0.3 \leq O/C \leq 0.67$
Carbohydrate & aminosugar	$1.5 \leq H/C \leq 2.4$; $0.67 \leq O/C \leq 1.2$
Lipid	$1.5 \leq H/C \leq 2.0$ $0 \leq O/C \leq 0.3$
Unsaturated hydrocarbon	$0.7 \leq H/C \leq 1.5$; $0 \leq O/C \leq 0.1$
Tannin	$0.5 \leq H/C \leq 1.5$; $0.65 \leq O/C \leq 1$

CRAM, carboxylic rich alicyclic molecules.

Table S3. List of the all the identified compounds by THM-GC/MS, their associated *m*/*z* and mass spectra factor (MSF).

Compounds name	***m*/*z***	**MSF**
Small organic acids (SOAc)		
fumaric acid methyl ester	113	3.3
succinic acid	115	4.5
2,4-heptadienoic acid methyl ester	111	3.9
methyl succinic acid methyl ester	59	4.1
glutaconic acid methyl ester	59	8.5
glutaric acid methyl ester	59	6.2
Phenols (PHE)		
benzoic acid methyl ester	105	2.9
1,2-dimethoxybenzene	138	4.7
1,3-dimethoxybenzene	138	3.9
1,4-dimethoxybenzene	138	6.0
4-methyl-1,2-dimethoxybenzene	152	5.7
2-methyl-1,4-dimethoxybenzene	152	6.1
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 (2,4,6-trimethoxytoluene)	167	7.0
trimethoxytoluene	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
3,5-dimethoxybenzoic acid methyl ester	196	5.1
3,4-dimethoxybenzoic acid methyl ester	196	5.6
3,4,5-trimethoxybenzaldehyde (syringaldehyde)	196	6.7
3-(4-methoxyphenyl)prop-2-enoic acid methyl ester (Z,E)	192	6.7
3,4,5-trimethoxyacetophenone (acetosyringone)	195	4.8
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 (Z,E)	222	3.7
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
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
Carbohydrates (Car)		
C5 (xylose)	129	4
C5 (xylose)	129	4
deoxyC6-1 (rhamnose)	129	4
deoxyC6-2 (Fucose)	129	4
deoxyC6-3 (Rhamnose)	129	4
deoxyC6-4 (Fucose)	129	4
C6-1 (Glucose)	129	4
C6-2 (Galactose)	129	4
C6-3 (Glucose)	129	4
C6-4 (Galactose)	129	4
Fatty acids		
$C_{8:0}$	74	3.0
$C_{9:0}$	74	3.6
$C_{10:0}$	74	3.0
$C_{12:0}$	74	3
α,ω-diacid C9:0	74	10.2
$C_{13:0}$	74	4.1
***br*$C_{14:0}$**	74	3.1
$C_{14:0}$	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
10Me16:O	74	3.9
***i*$C_{17:0}$**	74	3.9
a$C_{17:0}$	74	3.9
$C_{17:0}$	74	3.9
10Me17:0	74	4.5
C18:1	74	14.6
C18:1	74	14.6
C18:0	74	4.5
***ωOH*$C_{16:0}$**	74	12.1
10Me18:0	74	8
$C_{19:1}$	74	14.5
***α,ω*$C_{16:0}$**	74	11.3
$C_{20:0}$	74	4.9
$C_{22:0}$	74	4.9
ωOH$C_{20:0}$	74	12.9
$C_{23:0}$	74	8.4

$\alpha,\omega C_{20:0}$	74	10.8
$C_{24:0}$	74	4.4
$\omega OHC_{22:0}$	74	13.5
$C_{25:0}$	74	7.7
$\alpha,\omega C_{22:0}$	74	10.8
$C_{26:0}$	74	4.5
$\omega OHC_{24:0}$	74	13.5
$C_{27:0}$	74	5.1
$\alpha,\omega C_{24:0}$	74	9.7
$C_{28:0}$	74	4.9
$\omega OHC_{26:0}$	74	14.4
$C_{29:0}$	74	4.9
$\alpha,\omega C_{26:0}$	74	9.7
$C_{30:0}$	74	4.9
$\omega OHC_{28:0}$	74	14.4
$C_{31:0}$	74	4.9
$\alpha,\omega C_{28:0}$	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
$C_{16:2}$	67	9.5
$C_{16:2}$	67	9.5
$C_{16:2}$	67	9.5
$C_{16:2}$	67	9.5
$C_{18:2}$	67	9.5
$C_{18:2}$	67	9.5
$C_{18:2}$	67	9.5
$C_{18:2}$	67	9.5
Fatty alcohols (Falcohol)		
C18:0	83	10
C20:0	83	10
C22:0	83	10
C24:0	83	10
C26:0	83	10
C28:0	83	10
C30:0	83	10
C32:0	83	10
Chlrorophyll markers (Phytol)		
Phytol	71	11
Neophytadiene	68	55
N-containing compounds (Ncompound)		
2-pyrrolidone-5-carboxylic acid, N-methyl, methyl ester	98	4
Uracil, 1,3-dimethyl (base azotée ARN)	140	10
Adenine trimethyl	148	9
Hypoxanthine	164	3
Thymine dimethyl	154	27
1-Methylindole	131	3
1,3-Dimethylindole	144	3

Bold formatting indicates the molecules selected for the statistical analysis (PCA with 67 variables).

Table S4. LDI FT-ICR MS data of the different artificial sediments including intensity-weighted average molecular masses, elemental ratios, DBE, AI_{mod}, MLB_L and distribution in CHO, CHON, CHOS, and CHONS elemental formulas and selected compound classes at day 0 and day 60 in oxic conditions.

Parameter	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
Number of formula	0	2818	1408	3348	1522	1653
	60	3052	1430	2417	1221	731
m/*z*	0	358.3	370.2	378.8	363.8	464.4
	60	352.2	363.2	359.0	407.4	470.8
C	0	22.5	21.1	21.8	21.2	29.1
	60	20.9	20.6	20.8	22.3	29.6
H	0	15.8	20.8	22.0	21.8	25.0
	60	17.0	20.9	22.1	27.0	26.4
O	0	3.7	4.2	4.1	3.7	2.3
	60	4.1	4.1	3.7	4.3	2.2
N	0	0.7	1.5	1.5	1.5	3.8
	60	1.0	1.4	1.5	2.0	3.9
S	0	0.1	0.3	0.3	0.3	0.0
	60	0.2	0.3	0.2	0.5	0.0
H/C	0	0.8	1.0	1.1	1.1	0.8
	60	0.9	1.1	1.1	1.3	0.9
O/C	0	0.2	0.2	0.2	0.2	0.1
	60	0.2	0.2	0.2	0.2	0.1
N/C	0	0.0	0.1	0.1	0.1	0.1
	60	0.1	0.1	0.1	0.1	0.1
S/C	0	0.0	0.0	0.0	0.0	0.0
	60	0.0	0.0	0.0	0.0	0.0
DBE	0	16.0	12.4	12.6	12.1	19.5
	60	13.8	11.9	11.5	10.8	19.3
AI_{mod}	0	0.61	0.42	0.45	0.45	0.69
	60	0.56	0.45	0.44	0.28	0.67
MLB_L (%)	0	11.7	19.8	18.2	20.4	2.9
	60	13.8	17.6	19.5	27.6	4.4
CHO (%)	0	55.2	38.5	32.6	37.0	0.0
	60	43.5	36.1	30.5	14.8	0.0
CHON (%)	0	33.6	35.4	40.0	38.4	98.9
	60	38.9	38.2	45.3	40.1	98.9
CHOS (%)	0	3.8	11.8	13.3	13.8	1.1
	60	8.0	10.5	10.1	12.3	1.1
CHONS (%)	0	7.5	14.3	14.1	10.8	0.0
	60	9.6	15.2	14.1	32.8	0.0
Aromatic formula (%)	0	20.2	21.4	18.7	20.8	30.5
	60	21.8	22.1	20.0	17.5	34.2
Condensed aromatic structure (%)	0	51.2	28.9	28.0	30.2	30.1
	60	38.9	27.1	28.8	18.2	23.1
Lignin/CRAM (%)	0	31.1	39.7	39.6	38.6	30.7
	60	37.7	43.6	39.0	39.0	25.3

Parameter	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
Protein (%)	0	2.8	4.9	5.4	5.1	1.0
	60	2.7	4.7	5.4	8.7	1.6
Carbohydrate and aminosugar (%)	0	1.7	2.6	2.0	1.3	0.0
	60	2.3	1.5	1.8	3.7	0.0
Lipid (%)	0	7.1	12.0	10.3	13.8	2.0
	60	8.6	10.6	11.9	14.2	2.8
Unsaturated hydrocarbon (%)	0	4.8	9.0	12.2	10.9	36.3
	60	6.8	8.7	12.0	14.2	47.1
Tannin (%)	0	1.3	2.8	2.4	0.2	0.0
	60	3.1	3.7	1.1	2.0	0.0

Table S5. LDI FT-ICR MS data of the different artificial sediments including intensity-weighted average molecular masses, elemental ratios, DBE, AI_{mod}, MLB_L and distribution in CHO, CHON, CHOS, and CHONS elemental formulas and selected compound classes at day 0 and day 60 in anoxic conditions.

Parameter	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
Number of formula	0	1949	2263	2885	1667	1503
	60	2258	1271	2641	801	238
m/*z*	0	365.6	354.2	377.4	368.6	466.1
	60	357.8	466.5	371.6	446.0	484.0
C	0	20.4	20.1	21.7	21.3	29.1
	60	20.2	27.1	21.3	25.8	30.3
H	0	17.2	19.8	22.5	24.8	25.2
	60	16.9	27.1	23.4	29.6	28.0
O	0	5.0	4.2	3.9	3.5	2.4
	60	4.9	3.2	3.8	3.8	2.3
N	0	1.2	1.6	1.7	1.8	3.8
	60	1.1	3.9	1.6	1.9	4.0
S	0	0.3	0.1	0.3	0.2	0.0
	60	0.2	0.3	0.3	0.6	0.0
H/C	0	0.9	1.0	1.1	1.2	0.9
	60	0.9	1.1	1.1	1.2	0.9
O/C	0	0.3	0.2	0.2	0.2	0.1
	60	0.3	0.1	0.2	0.2	0.1
N/C	0	0.1	0.1	0.1	0.1	0.1
	60	0.1	0.2	0.1	0.1	0.1
S/C	0	0.0	0.0	0.0	0.0	0.0
	60	0.0	0.0	0.0	0.0	0.0
DBE	0	13.4	12.0	12.3	10.8	19.5
	60	13.3	16.5	11.4	12.9	19.3
AI_{mod}	0	0.51	0.53	0.49	0.43	0.68
	60	0.57	0.41	0.44	0.40	0.64
MLB_L (%)	0	14.5	16.4	15.6	20.9	4.9
	60	12.3	17.1	18.2	19.1	8.8
CHO (%)	0	39.3	36.1	29.0	26.5	0.4
	60	44.3	0.0	27.2	16.0	0.0
CHON (%)	0	38.4	47.4	42.9	49.2	96.5
	60	39.5	72.3	43.6	29.4	100.0
CHOS (%)	0	9.7	9.9	16.8	16.4	3.1
	60	9.2	3.9	15.2	24.7	0.0
CHONS (%)	0	12.6	6.6	11.3	7.9	0.0
	60	7.1	23.8	14.1	29.9	0.0
Aromatic formula (%)	0	23.1	21.7	20.2	15.6	30.3
	60	25.0	24.6	20.7	17.7	45.8
Condensed aromatic	0	37.2	27.7	27.0	22.2	27.2
structure (%)	60	37.9	19.8	24.8	19.2	6.1
Lignin/CRAM (%)	0	38.2	42.0	44.2	39.2	30.4
	60	41.6	30.8	42.8	33.0	26.1

Protein (%)	0	3.6	3.3	3.7	4.9	1.7
	60	2.0	10.2	4.6	3.0	3.7
Carbohydrate and	0	3.5	1.4	0.8	0.0	0.3
aminosugar (%)	60	2.1	1.1	1.3	2.7	0.0
Lipid (%)	0	7.3	11.4	10.8	15.5	2.9
	60	8.2	4.5	12.0	12.9	4.9
Unsaturated	0	4.9	12.0	12.5	17.9	37.5
hydrocarbon (%)	60	4.6	33.7	13.6	28.3	59.2
Tannin (%)	0	5.2	2.3	1.0	0.3	0.0
	60	4.2	0.0	0.8	1.0	0.0

Table S6. Relative distributions of the target compounds (biomarkers) identified by THM-GC-MS in the artificial sediments at day 0 and day 60 in oxic conditions.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
Small organic acids (SOAc)						
fumaric acid methyl ester	0	0.55 ± 0.14	0.40 ± 0.07	0.26 ± 0.04	0.14 ± 0.00	0.07 ± 0.02
	60	0.57 ± 0.20	0.28 ± 0.02	0.06 ± 0.03	0.12 ± 0.01	0.18 ± 0.14
succinic acid	0	0.95 ± 0.15	1.15 ± 0.25	1.39 ± 0.08	1.05 ± 0.03	2.11 ± 0.30
	60	1.17 ± 0.36	0.52 ± 0.03	0.18 ± 0.01	0.22 ± 0.00	4.27 ± 1.47
2,4-heptadienoic acid methyl ester	0	1.02 ± 0.12	0.83 ± 0.01	0.19 ± 0.07	0.18 ± 0.00	n.d.
	60	0.86 ± 0.04	0.47 ± 0.06	0.14 ± 0.08	0.19 ± 0.00	n.d.
methyl succinic acid methyl ester	0	0.32 ± 0.04	0.18 ± 0.04	0.15 ± 0.04	0.07 ± 0.00	n.d.
	60	0.40 ± 0.12	0.16 ± 0.00	0.03 ± 0.01	0.13 ± 0.02	n.d.
glutaconic acid methyl ester	0	0.20 ± 0.06	0.34 ± 0.22	0.54 ± 0.02	0.41 ± 0.02	n.d.
	60	0.36 ± 0.01	0.23 ± 0.08	0.05 ± 0.06	0.12 ± 0.05	n.d.
glutaric acid methyl ester	0	0.17 ± 0.01	0.17 ± 0.04	0.14 ± 0.01	0.07 ± 0.01	n.d.
	60	0.24 ± 0.02	0.12 ± 0.01	0.03 ± 0.00	0.13 ± 0.05	n.d.
Phenols (PHE)						
benzoic acid methyl ester	0	0.44 ± 0.04	0.41 ± 0.04	0.27 ± 0.01	0.18 ± 0.04	n.d.
	60	0.59 ± 0.12	0.32 ± 0.01	0.08 ± 0.03	0.23 ± 0.15	n.d.
1,2-dimethoxybenzene	0	0.17 ± 0.03	0.15 ± 0.01	0.11 ± 0.01	0.04 ± 0.01	n.d.
	60	0.39 ± 0.15	0.12 ± 0.02	0.03 ± 0.02	0.03 ± 0.00	n.d.
1,3-dimethoxybenzene	0	0.22 ± 0.05	0.18 ± 0.02	0.15 ± 0.00	0.06 ± 0.01	n.d.
	60	0.31 ± 0.06	0.15 ± 0.02	0.04 ± 0.02	0.05 ± 0.01	n.d.
1,4-dimethoxybenzene	0	0.07 ± 0.03	0.04 ± 0.00	0.08 ± 0.04	0.01 ± 0.00	n.d.
	60	0.08 ± 0.00	0.01 ± 0.02	0.02 ± 0.02	n.d.	n.d.
4-methyl-1,2-dimethoxybenzene	0	0.19 ± 0.05	0.26 ± 0.09	0.22 ± 0.05	0.09 ± 0.03	n.d.
	60	0.49 ± 0.10	0.20 ± 0.09	0.05 ± 0.03	0.03 ± 0.01	n.d.
2-methyl-1,4-dimethoxybenzene	0	0.08 ± 0.03	0.07 ± 0.00	0.04 ± 0.01	0.01 ± 0.00	n.d.
	60	0.10 ± 0.01	0.04 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	n.d.
3-methoxybenzoic acid methyl ester	0	0.18 ± 0.01	0.12 ± 0.00	0.07 ± 0.02	0.04 ± 0.01	n.d.
	60	0.18 ± 0.02	0.08 ± 0.00	0.03 ± 0.01	0.03 ± 0.00	n.d.
4-methoxybenzoic acid methyl ester	0	0.30 ± 0.01	0.24 ± 0.01	0.14 ± 0.01	0.08 ± 0.02	n.d.
	60	0.36 ± 0.01	0.14 ± 0.02	0.05 ± 0.02	0.09 ± 0.03	n.d.
3-methoxybenzaldehyde	0	0.19 ± 0.10	0.12 ± 0.01	0.15 ± 0.13	0.03 ± 0.00	n.d.
	60	0.25 ± 0.08	0.09 ± 0.02	0.04 ± 0.00	0.03 ± 0.00	n.d.
4-methoxybenzaldehyde	0	0.11 ± 0.01	0.15 ± 0.01	0.12 ± 0.03	0.15 ± 0.01	n.d.
	60	0.16 ± 0.00	0.08 ± 0.01	0.05 ± 0.02	0.08 ± 0.02	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
1,2,3-trimethoxybenzene	0	0.05 ± 0.01	0.04 ± 0.00	0.03 ± 0.00	0.01 ± 0.00	n.d.
	60	0.07 ± 0.01	0.03 ± 0.00	0.02 ± 0.01	0.01 ± 0.00	n.d.
1,2,4-trimethoxybenzene	0	0.49 ± 0.07	0.37 ± 0.00	0.23 ± 0.03	0.08 ± 0.00	n.d.
	60	0.63 ± 0.06	0.25 ± 0.02	0.13 ± 0.06	0.07 ± 0.02	n.d.
1,3,5-trimethoxybenzene	0	0.09 ± 0.02	0.09 ± 0.02	0.05 ± 0.00	0.02 ± 0.00	n.d.
	60	0.15 ± 0.01	0.06 ± 0.01	0.02 ± 0.01	0.01 ± 0.00	n.d.
trimethoxytoluene (2,4,6-trimethoxytoluene)	0	0.08 ± 0.02	0.05 ± 0.00	0.04 ± 0.02	0.01 ± 0.00	n.d.
	60	0.07 ± 0.02	0.04 ± 0.00	0.02 ± 0.01	0.01 ± 0.00	n.d.
trimethoxytoluene	0	0.06 ± 0.00	0.06 ± 0.00	0.05 ± 0.00	0.01 ± 0.01	n.d.
	60	0.14 ± 0.03	0.05 ± 0.01	0.02 ± 0.00	0.01 ± 0.00	n.d.
dimethoxystyrene	0	0.17 ± 0.01	0.18 ± 0.06	0.10 ± 0.02	0.04 ± 0.00	n.d.
	60	0.40 ± 0.14	0.14 ± 0.05	0.04 ± 0.02	0.02 ± 0.00	n.d.
1,2,3,4-tetramethoxybenzene	0	0.06 ± 0.00	0.04 ± 0.00	0.03 ± 0.00	0.01 ± 0.00	n.d.
	60	0.10 ± 0.02	0.04 ± 0.01	0.01 ± 0.00	n.d.	n.d.
1,2,3,5-tetramethoxybenzene	0	0.15 ± 0.01	0.11 ± 0.00	0.06 ± 0.01	0.01 ± 0.01	n.d.
	60	0.22 ± 0.01	0.07 ± 0.01	0.03 ± 0.01	0.01 ± 0.00	n.d.
3,4-dimethoxybenzaldehyde	0	0.44 ± 0.07	0.34 ± 0.03	0.11 ± 0.01	0.08 ± 0.03	n.d.
	60	0.57 ± 0.13	0.25 ± 0.00	0.08 ± 0.02	0.06 ± 0.01	n.d.
3,4-dimethoxyacetophenone	0	0.22 ± 0.01	0.21 ± 0.01	0.12 ± 0.02	0.06 ± 0.01	n.d.
	60	0.42 ± 0.10	0.17 ± 0.03	0.04 ± 0.03	0.03 ± 0.01	n.d.
3,5-dimethoxybenzoic acid methyl ester	0	0.03 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	n.d.	n.d.
	60	0.04 ± 0.01	0.02 ± 0.00	0.01 ± 0.00	n.d.	n.d.
3,4-dimethoxybenzoic acid methyl ester	0	2.57 ± 0.14	1.86 ± 0.08	1.00 ± 0.14	0.34 ± 0.07	n.d.
	60	3.57 ± 0.79	1.31 ± 0.10	0.36 ± 0.17	0.21 ± 0.00	n.d.
3,4,5-trimethoxybenzaldehyde (syringaldehyde)	0	0.21 ± 0.06	0.17 ± 0.01	0.05 ± 0.02	0.03 ± 0.01	n.d.
	60	0.27 ± 0.08	0.13 ± 0.01	0.04 ± 0.01	0.02 ± 0.01	n.d.
3-(4-methoxyphenyl)prop-2-enoic acid methyl ester (Z,E)	0	0.50 ± 0.02	0.37 ± 0.03	0.22 ± 0.02	0.10 ± 0.00	n.d.
	60	0.61 ± 0.03	0.31 ± 0.04	0.10 ± 0.05	0.06 ± 0.01	n.d.
3,4,5-trimethoxyacetophenone (acetosyringone)	0	0.13 ± 0.01	0.12 ± 0.01	0.07 ± 0.01	0.02 ± 0.00	n.d.
	60	0.22 ± 0.06	0.09 ± 0.01	0.02 ± 0.02	0.01 ± 0.00	n.d.
cis-1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	0	0.36 ± 0.02	0.28 ± 0.00	0.12 ± 0.03	0.05 ± 0.00	n.d.
	60	0.38 ± 0.04	0.17 ± 0.01	0.08 ± 0.00	0.03 ± 0.00	n.d.
trans-1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	0	0.28 ± 0.01	0.23 ± 0.01	0.10 ± 0.02	0.04 ± 0.00	n.d.
	60	0.32 ± 0.04	0.14 ± 0.00	0.06 ± 0.00	0.02 ± 0.00	n.d.
cis-1,2-Dimethoxy-4-(3-methoxy-1-propenyl)benzene	0	0.03 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	n.d.	n.d.
	60	0.03 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	n.d.	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
2,4,5-Trimethoxypropenylbenzene	0	0.03 ± 0.01	0.03 ± 0.00	0.02 ± 0.00	n.d.	n.d.
	60	0.07 ± 0.03	0.03 ± 0.00	0.01 ± 0.00	n.d.	n.d.
1,2-Dimethoxy-4-(1-methoxy-1-propenyl)benzene	0	0.03 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	n.d.	n.d.
	60	0.03 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	n.d.	n.d.
cis-1,2-Dimethoxy-4-(2-methoxy-1-propenyl)benzene	0	0.05 ± 0.00	0.04 ± 0.00	0.01 ± 0.01	0.01 ± 0.00	n.d.
	60	0.05 ± 0.01	0.02 ± 0.00	0.01 ± 0.00	n.d.	n.d.
trans-1,2-Dimethoxy-4-(2-methoxy-1-propenyl)benzene	0	0.09 ± 0.01	0.06 ± 0.01	0.03 ± 0.01	0.01 ± 0.01	n.d.
	60	0.09 ± 0.01	0.04 ± 0.00	0.02 ± 0.00	n.d.	n.d.
trans-1,2-Dimethoxy-4-(3-methoxy-1-propenyl)benzene	0	0.08 ± 0.01	0.06 ± 0.00	0.03 ± 0.01	0.01 ± 0.00	n.d.
	60	0.09 ± 0.01	0.04 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	n.d.
3,4,5-trimethoxybenzoic acid emthyl ester	0	0.95 ± 0.04	0.69 ± 0.01	0.38 ± 0.02	0.13 ± 0.02	n.d.
	60	1.25 ± 0.24	0.52 ± 0.01	0.16 ± 0.06	0.09 ± 0.01	n.d.
cis-1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene	0	0.27 ± 0.02	0.20 ± 0.02	0.09 ± 0.03	0.03 ± 0.01	n.d.
		0.26 ± 0.04	0.12 ± 0.01	0.06 ± 0.01	0.02 ± 0.01	n.d.
trans-1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene	0	0.20 ± 0.01	0.16 ± 0.01	0.07 ± 0.02	0.02 ± 0.00	n.d.
	60	0.21 ± 0.04	0.10 ± 0.00	0.05 ± 0.01	0.02 ± 0.00	n.d.
erythro-1,2-dimethoxy-4-(1,2,3-trimethoxypropyl)benzene	0	0.40 ± 0.11	0.30 ± 0.01	0.09 ± 0.05	0.05 ± 0.00	n.d.
	60	0.22 ± 0.06	0.12 ± 0.01	0.11 ± 0.04	0.03 ± 0.00	n.d.
threo-1,2-dimethoxy-4-(1,2,3-trimethoxypropyl)benzene	0	0.42 ± 0.20	0.18 ± 0.00	0.06 ± 0.03	0.03 ± 0.00	n.d.
	60	0.15 ± 0.03	0.08 ± 0.01	0.06 ± 0.03	0.01 ± 0.01	n.d.
3-(3,4-dimethoxyphenyl)prop-2-enoic acid methyl ester (Z,E)	0	0.56 ± 0.32	0.47 ± 0.05	0.20 ± 0.02	0.10 ± 0.00	n.d.
	60	0.81 ± 0.14	0.37 ± 0.07	0.11 ± 0.05	0.09 ± 0.00	n.d.
erythro-1,2,3-Trimethoxy-5-(1,2,3-trimethoxypropyl)benzene	0	0.19 ± 0.02	0.11 ± 0.00	0.03 ± 0.02	0.01 ± 0.00	n.d.
	60	0.08 ± 0.01	0.04 ± 0.01	0.03 ± 0.02	0.01 ± 0.00	n.d.
threo-1,2,3-Trimethoxy-5-(1,2,3-trimethoxypropyl)benzene	0	0.06 ± 0.01	0.04 ± 0.00	0.01 ± 0.01	n.d.	n.d.
	60	0.03 ± 0.01	0.01 ± 0.00	0.01 ± 0.01	n.d.	n.d.
cis-1,2,3-Trimethoxy-5-(2-methoxy-1-propenyl)benzene	0	0.04 ± 0.00	0.03 ± 0.00	0.01 ± 0.00	n.d.	n.d.
	60	0.03 ± 0.01	0.01 ± 0.01	0.01 ± 0.00	n.d.	n.d.
trans-1,2,3-Trimethoxy-5-(2-methoxy-1-propenyl)benzene	0	0.06 ± 0.01	0.04 ± 0.01	0.01 ± 0.00	n.d.	n.d.
	60	0.05 ± 0.01	0.02 ± 0.00	0.01 ± 0.00	n.d.	n.d.
cis-1,2-Dimethoxy-4-(2,3-dimethoxy-1-propenyl)benzene	0	0.07 ± 0.01	0.05 ± 0.00	0.02 ± 0.01	0.01 ± 0.01	n.d.
	60	0.06 ± 0.01	0.03 ± 0.00	0.02 ± 0.00	n.d.	n.d.
trans-1,2-Dimethoxy-4-(2,3-dimethoxy-1-propenyl)benzene	0	0.08 ± 0.01	0.05 ± 0.01	0.03 ± 0.01	0.00 ± 0.01	n.d.
	60	0.09 ± 0.01	0.04 ± 0.01	0.02 ± 0.00	0.01 ± 0.00	n.d.
Carbohydrates (Car)						
C5 (xylose)	0	0.42 ± 0.16	0.21 ± 0.02	0.10 ± 0.04	0.05 ± 0.00	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
	60	0.31 ± 0.10	0.10 ± 0.01	0.04 ± 0.02	0.04 ± 0.02	n.d.
C5 (xylose)	0	0.99 ± 0.37	0.58 ± 0.04	0.34 ± 0.13	0.16 ± 0.03	n.d.
	60	0.74 ± 0.29	0.29 ± 0.02	0.15 ± 0.01	0.12 ± 0.05	n.d.
deoxyC6-1 (rhamnose)	0	0.07 ± 0.04	0.04 ± 0.01	0.02 ± 0.01	0.01 ± 0.00	n.d.
	60	0.06 ± 0.02	0.02 ± 0.00	0.01 ± 0.01	0.01 ± 0.00	n.d.
deoxyC6-2 (Fucose)	0	0.10 ± 0.03	0.20 ± 0.00	0.24 ± 0.03	0.24 ± 0.03	n.d.
	60	0.17 ± 0.03	0.13 ± 0.05	0.09 ± 0.09	0.08 ± 0.03	n.d.
deoxyC6-3 (Rhamnose)	0	0.19 ± 0.08	0.12 ± 0.01	0.04 ± 0.02	0.03 ± 0.01	n.d.
	60	0.09 ± 0.04	0.05 ± 0.00	0.04 ± 0.02	0.04 ± 0.01	n.d.
deoxyC6-4 (Fucose)	0	0.14 ± 0.05	0.09 ± 0.00	0.05 ± 0.05	0.03 ± 0.00	n.d.
	60	0.10 ± 0.03	0.05 ± 0.01	0.02 ± 0.01	0.01 ± 0.00	n.d.
C6-1 (Glucose)	0	1.40 ± 0.76	0.53 ± 0.01	0.18 ± 0.11	0.07 ± 0.00	n.d.
	60	0.62 ± 0.37	0.24 ± 0.04	0.20 ± 0.18	0.07 ± 0.03	n.d.
C6-2 (Galactose)	0	0.13 ± 0.06	0.05 ± 0.00	0.03 ± 0.02	0.01 ± 0.00	n.d.
	60	0.09 ± 0.04	0.04 ± 0.01	0.02 ± 0.01	0.01 ± 0.00	n.d.
C6-3 (Glucose)	0	4.62 ± 2.24	1.84 ± 0.02	0.17 ± 0.12	0.23 ± 0.00	n.d.
	60	1.76 ± 0.88	0.72 ± 0.10	0.64 ± 0.55	0.26 ± 0.12	n.d.
C6-4 (Galactose)	0	0.33 ± 0.21	0.17 ± 0.03	0.08 ± 0.05	0.04 ± 0.00	n.d.
	60	0.20 ± 0.09	0.08 ± 0.01	0.05 ± 0.03	0.03 ± 0.01	n.d.
Fatty acids						
$C_{8:0}$	0	0.16 ± 0.01	0.16 ± 0.01	0.21 ± 0.03	0.10 ± 0.01	n.d.
	60	0.24 ± 0.00	0.13 ± 0.02	0.04 ± 0.01	0.08 ± 0.04	n.d.
$C_{9:0}$	0	0.10 ± 0.03	0.11 ± 0.00	0.12 ± 0.01	0.06 ± 0.01	n.d.
	60	0.21 ± 0.01	0.08 ± 0.02	0.03 ± 0.02	0.05 ± 0.01	n.d.
$C_{10:0}$	0	0.10 ± 0.01	0.09 ± 0.01	0.11 ± 0.00	0.05 ± 0.01	n.d.
	60	0.15 ± 0.02	0.16 ± 0.08	0.06 ± 0.01	0.07 ± 0.01	n.d.
$C_{12:0}$	0	0.14 ± 0.03	0.11 ± 0.00	0.12 ± 0.04	0.06 ± 0.02	n.d.
	60	0.22 ± 0.01	0.50 ± 0.31	0.56 ± 0.22	0.76 ± 0.03	n.d.
α,ω-diacid C9:0	0	1.50 ± 0.18	1.58 ± 0.11	1.51 ± 0.03	0.83 ± 0.03	n.d.
	60	2.08 ± 0.31	1.00 ± 0.24	0.25 ± 0.11	0.23 ± 0.03	n.d.
$C_{13:0}$	0	0.02 ± 0.00	0.02 ± 0.00	0.02 ± 0.01	n.d.	n.d.
	60	0.11 ± 0.01	0.03 ± 0.01	0.03 ± 0.02	0.02 ± 0.02	n.d.
br$C_{14:0}$	0	0.02 ± 0.00	0.02 ± 0.00	0.02 ± 0.00	n.d.	n.d.
	60	0.07 ± 0.01	0.03 ± 0.01	0.01 ± 0.00	0.02 ± 0.03	n.d.
$C_{14:0}$	0	0.30 ± 0.02	0.27 ± 0.03	0.35 ± 0.03	0.17 ± 0.03	0.07 ± 0.00
	60	0.44 ± 0.04	3.79 ± 2.32	6.25 ± 2.69	5.27 ± 0.31	0.11 ± 0.00

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
i$C_{15:0}$	0	0.28 ± 0.00	0.22 ± 0.01	0.16 ± 0.00	0.09 ± 0.01	0.03 ± 0.00
	60	0.51 ± 0.06	0.28 ± 0.09	0.10 ± 0.01	0.07 ± 0.00	0.04 ± 0.01
a$C_{15:0}$	0	0.07 ± 0.00	0.06 ± 0.00	0.05 ± 0.01	n.d.	n.d.
	60	0.16 ± 0.01	0.10 ± 0.05	0.04 ± 0.00	0.11 ± 0.06	0.02 ± 0.02
$C_{15:0}$	0	0.10 ± 0.00	0.10 ± 0.00	0.13 ± 0.01	0.07 ± 0.00	0.04 ± 0.00
	60	0.19 ± 0.01	0.19 ± 0.07	0.19 ± 0.07	0.22 ± 0.02	0.07 ± 0.00
br$C_{16:0}$	0	0.40 ± 0.00	0.28 ± 0.01	0.17 ± 0.00	n.d.	n.d.
	60	0.48 ± 0.09	0.27 ± 0.04	0.10 ± 0.02	0.20 ± 0.03	n.d.
$C_{16:1}$	0	0.33 ± 0.30	0.07 ± 0.01	0.33 ± 0.34	0.02 ± 0.03	n.d.
	60	0.15 ± 0.01	0.28 ± 0.00	0.04 ± 0.01	0.12 ± 0.17	n.d.
$C_{16:0}$	0	2.72 ± 0.10	13.35 ± 3.25	34.07 ± 2.83	27.63 ± 4.04	19.35 ± 0.21
	60	3.42 ± 0.58	33.64 ± 12.32	66.29 ± 11.96	61.79 ± 0.29	24.23 ± 1.65
10Me16:O	0	0.19 ± 0.01	0.13 ± 0.00	0.08 ± 0.01	0.02 ± 0.02	n.d.
	60	0.22 ± 0.04	0.12 ± 0.02	0.04 ± 0.00	0.02 ± 0.00	n.d.
i$C_{17:0}$	0	0.11 ± 0.00	0.33 ± 0.06	0.56 ± 0.05	0.68 ± 0.02	0.54 ± 0.03
	60	0.17 ± 0.02	0.41 ± 0.08	0.29 ± 0.10	0.36 ± 0.01	0.75 ± 0.01
a$C_{17:0}$	0	0.06 ± 0.01	0.04 ± 0.00	0.02 ± 0.00	n.d.	n.d.
	60	0.09 ± 0.02	0.05 ± 0.02	0.02 ± 0.00	0.06 ± 0.02	n.d.
$C_{17:0}$	0	0.08 ± 0.01	0.10 ± 0.00	0.10 ± 0.01	0.10 ± 0.00	0.06 ± 0.00
	60	0.17 ± 0.04	0.12 ± 0.00	0.09 ± 0.01	0.08 ± 0.01	0.07 ± 0.01
10Me17:0	0	0.06 ± 0.00	0.04 ± 0.00	0.01 ± 0.02	n.d.	n.d.
	60	0.07 ± 0.00	0.04 ± 0.00	0.01 ± 0.00	n.d.	n.d.
C18:1	0	0.73 ± 0.26	1.15 ± 0.19	2.14 ± 0.21	2.38 ± 0.18	2.07 ± 0.08
	60	0.71 ± 0.17	0.72 ± 0.16	0.51 ± 0.17	0.68 ± 0.10	2.73 ± 0.02
C18:1	0	0.15 ± 0.02	0.26 ± 0.04	0.39 ± 0.00	0.51 ± 0.03	0.41 ± 0.00
	60	0.19 ± 0.04	0.78 ± 0.20	0.27 ± 0.12	1.61 ± 0.52	1.46 ± 0.08
C18:0	0	0.67 ± 0.02	0.53 ± 0.01	0.60 ± 0.12	0.40 ± 0.04	0.19 ± 0.01
	60	0.84 ± 0.06	1.23 ± 0.79	0.67 ± 0.19	0.38 ± 0.04	0.25 ± 0.01
ωOH$C_{16:0}$	0	2.23 ± 0.11	1.43 ± 0.10	0.76 ± 0.03	n.d.	n.d.
	60	1.94 ± 0.01	0.95 ± 0.18	0.41 ± 0.00	0.16 ± 0.22	n.d.
10Me18:0	0	0.11 ± 0.00	0.08 ± 0.00	0.03 ± 0.04	n.d.	n.d.
	60	0.11 ± 0.01	0.08 ± 0.00	0.02 ± 0.01	0.02 ± 0.02	n.d.
$C_{19:1}$	0	0.56 ± 0.16	0.43 ± 0.04	0.29 ± 0.40	n.d.	n.d.
	60	1.59 ± 0.74	0.76 ± 0.46	0.13 ± 0.07	n.d.	n.d.
α,ω$C_{16:0}$	0	1.75 ± 0.11	1.09 ± 0.18	0.65 ± 0.04	n.d.	n.d.
	60	2.10 ± 0.40	1.31 ± 0.63	0.34 ± 0.17	n.d.	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
$C_{20:0}$	0	0.57 ± 0.04	0.42 ± 0.02	0.36 ± 0.03	0.55 ± 0.00	0.23 ± 0.02
	60	0.58 ± 0.01	0.77 ± 0.28	0.36 ± 0.28	1.06 ± 0.36	3.21 ± 0.99
$C_{22:0}$	0	1.94 ± 0.26	1.05 ± 0.00	0.68 ± 0.03	0.82 ± 0.05	0.14 ± 0.01
	60	2.32 ± 0.13	1.28 ± 0.67	0.45 ± 0.25	0.51 ± 0.09	0.15 ± 0.01
$\omega OHC_{20:0}$	0	1.46 ± 0.13	0.86 ± 0.08	0.40 ± 0.11	0.44 ± 0.01	n.d.
	60	1.61 ± 0.26	0.82 ± 0.33	0.27 ± 0.13	0.34 ± 0.02	n.d.
$C_{23:0}$	0	n.d.	0.70 ± 0.08	0.48 ± 0.00	0.56 ± 0.02	0.10 ± 0.02
	60	n.d.	0.94 ± 0.44	0.30 ± 0.21	0.42 ± 0.06	0.13 ± 0.02
$\alpha,\omega C_{20:0}$	0	0.66 ± 0.01	0.63 ± 0.08	0.32 ± 0.04	0.33 ± 0.05	n.d.
	60	1.17 ± 0.20	0.67 ± 0.23	0.15 ± 0.13	0.24 ± 0.02	n.d.
$C_{24:0}$	0	2.89 ± 0.60	2.31 ± 0.32	1.45 ± 0.10	2.00 ± 0.17	0.48 ± 0.03
	60	4.67 ± 1.09	2.88 ± 1.31	0.98 ± 0.80	1.52 ± 0.22	0.47 ± 0.02
$\omega OHC_{22:0}$	0	7.88 ± 0.72	7.32 ± 1.87	2.43 ± 0.86	3.26 ± 0.96	n.d.
	60	10.58 ± 0.03	5.93 ± 2.14	1.89 ± 1.22	2.57 ± 0.08	n.d.
$C_{25:0}$	0	0.73 ± 0.03	0.68 ± 0.10	0.39 ± 0.04	0.50 ± 0.13	0.10 ± 0.01
	60	1.22 ± 0.17	0.76 ± 0.23	0.24 ± 0.21	0.40 ± 0.11	0.11 ± 0.03
$\alpha,\omega C_{22:0}$	0	1.32 ± 0.07	1.55 ± 0.37	0.56 ± 0.03	0.66 ± 0.39	n.d.
	60	2.43 ± 0.55	1.42 ± 0.28	0.31 ± 0.31	0.50 ± 0.12	n.d.
$C_{26:0}$	0	1.48 ± 0.16	1.42 ± 0.25	0.72 ± 0.01	0.89 ± 0.33	0.12 ± 0.00
	60	2.65 ± 0.55	1.52 ± 0.34	0.43 ± 0.38	0.70 ± 0.11	0.15 ± 0.00
$\omega OHC_{24:0}$	0	5.50 ± 1.68	5.69 ± 1.92	1.28 ± 0.31	2.06 ± 1.11	n.d.
	60	6.75 ± 0.98	4.22 ± 0.54	1.15 ± 0.83	2.05 ± 0.51	n.d.
$C_{27:0}$	0	0.33 ± 0.01	0.34 ± 0.05	0.14 ± 0.02	0.14 ± 0.06	n.d.
	60	0.58 ± 0.08	0.30 ± 0.04	0.08 ± 0.07	0.08 ± 0.02	n.d.
$\alpha,\omega C_{24:0}$	0	0.64 ± 0.05	0.66 ± 0.23	0.19 ± 0.04	0.22 ± 0.17	n.d.
	60	0.99 ± 0.33	0.55 ± 0.02	0.12 ± 0.11	0.19 ± 0.03	n.d.
$C_{28:0}$	0	1.00 ± 0.08	0.99 ± 0.14	0.38 ± 0.01	0.41 ± 0.26	n.d.
	60	1.71 ± 0.26	0.84 ± 0.06	0.23 ± 0.20	0.31 ± 0.05	n.d.
$\omega OHC_{26:0}$	0	1.33 ± 0.39	1.03 ± 0.35	0.24 ± 0.10	0.41 ± 0.33	n.d.
	60	1.35 ± 0.36	1.03 ± 0.24	0.17 ± 0.11	0.47 ± 0.16	n.d.
$C_{29:0}$	0	0.19 ± 0.05	0.19 ± 0.03	0.08 ± 0.03	0.09 ± 0.07	n.d.
	60	0.36 ± 0.04	0.17 ± 0.00	0.04 ± 0.04	0.05 ± 0.00	n.d.
$\alpha,\omega C_{26:0}$	0	0.19 ± 0.00	0.16 ± 0.01	0.07 ± 0.02	0.09 ± 0.06	n.d.
	60	0.26 ± 0.03	0.20 ± 0.01	0.02 ± 0.02	0.03 ± 0.01	n.d.
$C_{30:0}$	0	0.55 ± 0.13	0.45 ± 0.00	0.20 ± 0.09	0.26 ± 0.18	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
	60	0.90 ± 0.00	0.46 ± 0.05	0.09 ± 0.07	n.d.	n.d.
ωOH$C_{28:0}$	0	n.d.	n.d.	n.d.	n.d.	n.d.
	60	n.d.	n.d.	n.d.	n.d.	n.d.
$C_{31:0}$	0	n.d.	0.05 ± 0.01	0.03 ± 0.02	n.d.	n.d.
	60	n.d.	0.06 ± 0.01	0.01 ± 0.00	n.d.	n.d.
α,ω$C_{28:0}$	0	n.d.	n.d.	n.d.	n.d.	n.d.
	60	n.d.	n.d.	n.d.	n.d.	n.d.
$C_{32:0}$	0	n.d.	0.13 ± 0.04	0.05 ± 0.03	n.d.	n.d.
	60	n.d.	0.10 ± 0.01	0.02 ± 0.01	n.d.	n.d.
10,16-diOH$C_{16:0}$	0	6.59 ± 1.57	2.63 ± 0.01	0.86 ± 0.57	0.92 ± 0.27	n.d.
	60	2.29 ± 1.46	1.21 ± 0.05	0.90 ± 0.37	0.71 ± 0.12	n.d.
9,10,18-triOH$C_{18:0}$	0	21.38 ± 0.91	9.86 ± 1.47	2.42 ± 1.83	3.84 ± 0.14	n.d.
	60	10.06 ± 5.04	4.68 ± 1.43	2.93 ± 0.27	4.06 ± 1.78	n.d.
$C_{16:2}$	0	n.d.	0.30 ± 0.08	0.67 ± 0.15	0.97 ± 0.07	4.21 ± 0.27
	60	n.d.	0.02 ± 0.00	0.02 ± 0.02	0.01 ± 0.01	3.38 ± 0.41
$C_{16:2}$	0	n.d.	0.17 ± 0.11	0.57 ± 0.25	0.61 ± 0.20	4.12 ± 0.18
	60	n.d.	0.01 ± 0.02	0.01 ± 0.02	0.01 ± 0.01	2.73 ± 0.57
$C_{16:2}$	0	n.d.	0.44 ± 0.12	0.77 ± 0.03	1.51 ± 0.22	0.65 ± 0.01
	60	n.d.	0.08 ± 0.06	0.02 ± 0.00	0.04 ± 0.01	0.70 ± 0.28
$C_{16:2}$	0	n.d.	1.06 ± 0.31	2.01 ± 0.03	3.66 ± 0.03	3.08 ± 0.89
	60	n.d.	0.06 ± 0.06	0.09 ± 0.04	0.12 ± 0.01	6.08 ± 0.67
$C_{18:2}$	0	n.d.	0.89 ± 0.33	1.98 ± 0.73	3.73 ± 0.05	12.75 ± 0.10
	60	n.d.	0.17 ± 0.04	0.13 ± 0.11	0.13 ± 0.05	5.94 ± 0.06
$C_{18:2}$	0	n.d.	0.90 ± 0.22	1.97 ± 0.89	3.16 ± 0.26	12.81 ± 0.16
	60	n.d.	0.34 ± 0.07	0.19 ± 0.09	0.18 ± 0.05	4.97 ± 0.36
$C_{18:2}$	0	n.d.	0.42 ± 0.22	0.39 ± 0.19	1.19 ± 0.06	0.24 ± 0.05
	60	n.d.	0.03 ± 0.05	0.04 ± 0.01	0.04 ± 0.01	0.56 ± 0.33
$C_{18:2}$	0	n.d.	2.59 ± 0.91	3.44 ± 0.02	9.80 ± 0.40	7.15 ± 2.01
	60	n.d.	0.25 ± 0.06	0.26 ± 0.08	0.36 ± 0.07	8.29 ± 1.60
Fatty alcohols (Falcohol)						
C18:0	0	0.35 ± 0.01	0.36 ± 0.09	0.16 ± 0.01	0.08 ± 0.03	n.d.
	60	0.52 ± 0.16	0.26 ± 0.03	0.12 ± 0.02	0.05 ± 0.01	n.d.
C20:0	0	0.50 ± 0.05	0.43 ± 0.09	0.14 ± 0.02	n.d.	n.d.
	60	0.62 ± 0.19	0.27 ± 0.02	0.12 ± 0.02	n.d.	n.d.
C22:0	0	1.17 ± 0.23	0.87 ± 0.20	0.44 ± 0.12	n.d.	n.d.
	60	1.27 ± 0.25	0.51 ± 0.16	0.22 ± 0.04	n.d.	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
C24:0	0	2.87 ± 0.91	1.58 ± 0.27	0.60 ± 0.19	n.d.	n.d.
	60	2.62 ± 0.12	1.45 ± 0.76	0.60 ± 0.25	n.d.	n.d.
C26:0	0	1.16 ± 0.27	0.91 ± 0.16	0.30 ± 0.12	n.d.	n.d.
	60	1.38 ± 0.04	0.70 ± 0.25	0.30 ± 0.18	n.d.	n.d.
C28:0	0	0.68 ± 0.04	0.61 ± 0.05	0.19 ± 0.07	n.d.	n.d.
	60	0.85 ± 0.09	0.40 ± 0.11	0.18 ± 0.11	n.d.	n.d.
C30:0	0	0.33 ± 0.31	0.53 ± 0.10	0.14 ± 0.07	n.d.	n.d.
	60	0.64 ± 0.05	0.15 ± 0.21	0.10 ± 0.03	n.d.	n.d.
C32:0	0	n.d.	0.21 ± 0.00	0.05 ± 0.06	n.d.	n.d.
	60	n.d.	0.05 ± 0.07	0.04 ± 0.02	n.d.	n.d.
Chlrorophyll markers (Phytol)						
Phytol	0	n.d.	1.12 ± 0.37	4.61 ± 1.49	4.32 ± 0.07	6.36 ± 1.01
	60	n.d.	1.91 ± 0.71	1.67 ± 0.30	1.73 ± 0.21	5.83 ± 0.71
Neophytadiene	0	n.d.	2.69 ± 1.00	3.58 ± 0.30	6.72 ± 1.35	11.92 ± 4.20
	60	n.d.	3.01 ± 0.54	2.52 ± 2.07	4.52 ± 0.98	12.01 ± 1.50
2-pyrrolidone-5-carboxylic acid, N-methyl,	0	n.d.	2.59 ± 0.42	4.22 ± 0.35	2.19 ± 0.30	1.55 ± 0.37
methyl ester	60	n.d.	1.63 ± 0.34	0.60 ± 0.53	0.54 ± 0.28	3.37 ± 0.63
Uracil, 1,3-dimethyl	0	n.d.	1.10 ± 0.05	1.92 ± 0.16	2.16 ± 0.77	4.27 ± 0.60
	60	n.d.	0.11 ± 0.02	0.07 ± 0.05	0.05 ± 0.01	3.10 ± 3.34
Adenine trimethyl	0	n.d.	1.98 ± 0.14	2.73 ± 0.16	1.60 ± 0.14	1.18 ± 0.24
	60	n.d.	0.24 ± 0.05	0.13 ± 0.04	0.07 ± 0.02	0.35 ± 0.03
Hypoxanthine	0	n.d.	0.03 ± 0.01	0.25 ± 0.05	0.51 ± 0.02	1.25 ± 0.01
	60	n.d.	0.01 ± 0.00	n.d.	0.02 ± 0.00	2.10 ± 0.49
Thymine dimethyl	0	n.d.	0.59 ± 0.00	0.70 ± 0.02	0.45 ± 0.12	0.90 ± 0.07
	60	n.d.	0.17 ± 0.04	0.07 ± 0.04	0.05 ± 0.02	0.56 ± 0.21
1-Methylindole	0	0.22 ± 0.09	0.57 ± 0.03	1.70 ± 0.37	0.61 ± 0.05	0.73 ± 0.03
	60	0.41 ± 0.04	0.43 ± 0.22	0.38 ± 0.37	0.31 ± 0.12	0.85 ± 0.08
1,3-Dimethylindole	0	0.10 ± 0.05	0.21 ± 0.02	0.90 ± 0.34	0.27 ± 0.02	0.71 ± 0.03
	60	0.20 ± 0.04	0.30 ± 0.08	0.23 ± 0.14	0.09 ± 0.06	0.75 ± 0.18

n.d., not detected

Table S7. Relative distributions of the target compounds (biomarkers) identified by THM-GC-MS in the artificial sediments at day 0 and day 60 in anoxic conditions.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
Small organic acids (SOAc)						
fumaric acid methyl ester	0	0.56 ± 0.23	0.47 ± 0.04	0.28 ± 0.06	0.22 ± 0.03	0.48 ± 0.59
	60	0.90 ± 0.07	0.25 ± 0.02	0.09 ± 0.02	0.29 ± 0.06	0.31 ± 0.06
succinic acid	0	1.11 ± 0.39	1.16 ± 0.16	1.37 ± 0.32	1.19 ± 0.18	2.10 ± 0.52
	60	1.62 ± 0.08	0.45 ± 0.03	0.16 ± 0.01	0.39 ± 0.07	4.16 ± 0.40
2,4-heptadienoic acid methyl ester	0	0.95 ± 0.18	0.81 ± 0.06	0.45 ± 0.07	0.23 ± 0.09	n.d.
	60	1.09 ± 0.19	0.38 ± 0.10	0.24 ± 0.05	0.87 ± 0.17	n.d.
methyl succinic acid methyl ester	0	0.29 ± 0.13	0.24 ± 0.04	0.14 ± 0.04	0.09 ± 0.01	n.d.
	60	0.56 ± 0.00	0.17 ± 0.00	0.05 ± 0.01	0.15 ± 0.01	n.d.
glutaconic acid methyl ester	0	0.30 ± 0.09	0.25 ± 0.13	0.36 ± 0.20	0.43 ± 0.06	n.d.
	60	0.33 ± 0.09	0.13 ± 0.01	0.13 ± 0.01	0.11 ± 0.02	n.d.
glutaric acid methyl ester	0	0.22 ± 0.07	0.17 ± 0.02	0.13 ± 0.04	0.10 ± 0.01	n.d.
	60	0.31 ± 0.01	0.10 ± 0.01	0.09 ± 0.00	0.23 ± 0.13	n.d.
Phenols (PHE)						
benzoic acid methyl ester	0	0.48 ± 0.11	0.38 ± 0.11	0.31 ± 0.03	0.25 ± 0.13	n.d.
	60	0.83 ± 0.12	0.27 ± 0.02	0.15 ± 0.05	0.27 ± 0.05	n.d.
1,2-dimethoxybenzene	0	0.38 ± 0.13	0.14 ± 0.01	0.11 ± 0.03	0.04 ± 0.02	n.d.
	60	0.24 ± 0.01	0.09 ± 0.00	0.04 ± 0.02	0.11 ± 0.02	n.d.
1,3-dimethoxybenzene	0	0.29 ± 0.11	0.17 ± 0.02	0.16 ± 0.01	0.09 ± 0.03	n.d.
	60	0.33 ± 0.03	0.11 ± 0.01	0.05 ± 0.02	0.11 ± 0.01	n.d.
1,4-dimethoxybenzene	0	0.06 ± 0.02	0.04 ± 0.01	0.05 ± 0.03	0.02 ± 0.00	n.d.
	60	0.08 ± 0.00	0.03 ± 0.01	0.01 ± 0.01	0.03 ± 0.00	n.d.
4-methyl-1,2-dimethoxybenzene	0	0.41 ± 0.14	0.22 ± 0.06	0.20 ± 0.02	0.07 ± 0.03	n.d.
	60	0.22 ± 0.01	0.12 ± 0.02	0.05 ± 0.02	0.16 ± 0.06	n.d.
2-methyl-1,4-dimethoxybenzene	0	0.10 ± 0.03	0.06 ± 0.01	0.04 ± 0.01	0.02 ± 0.00	n.d.
	60	0.10 ± 0.01	0.04 ± 0.01	0.02 ± 0.01	0.03 ± 0.00	n.d.
3-methoxybenzoic acid methyl ester	0	0.14 ± 0.04	0.12 ± 0.01	0.09 ± 0.00	0.05 ± 0.01	n.d.
	60	0.24 ± 0.00	0.08 ± 0.01	0.03 ± 0.01	0.08 ± 0.01	n.d.
4-methoxybenzoic acid methyl ester	0	0.30 ± 0.10	0.22 ± 0.01	0.18 ± 0.03	0.12 ± 0.03	n.d.
	60	0.36 ± 0.02	0.12 ± 0.00	0.08 ± 0.02	0.22 ± 0.05	n.d.
3-methoxybenzaldehyde	0	0.33 ± 0.01	0.11 ± 0.01	0.11 ± 0.02	0.04 ± 0.00	n.d.
	60	0.17 ± 0.03	0.07 ± 0.02	0.03 ± 0.01	0.11 ± 0.04	n.d.
4-methoxybenzaldehyde	0	0.13 ± 0.05	0.12 ± 0.01	0.13 ± 0.01	0.18 ± 0.00	n.d.
	60	0.15 ± 0.01	0.06 ± 0.00	0.11 ± 0.03	0.12 ± 0.01	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
1,2,3-trimethoxybenzene	0	0.06 ± 0.02	0.04 ± 0.02	0.03 ± 0.00	0.01 ± 0.00	n.d.
	60	0.06 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	0.02 ± 0.00	n.d.
1,2,4-trimethoxybenzene	0	0.56 ± 0.23	0.36 ± 0.08	0.29 ± 0.06	0.12 ± 0.02	n.d.
	60	0.61 ± 0.00	0.21 ± 0.01	0.08 ± 0.03	0.19 ± 0.04	n.d.
1,3,5-trimethoxybenzene	0	0.13 ± 0.05	0.08 ± 0.00	0.06 ± 0.02	0.02 ± 0.01	n.d.
	60	0.13 ± 0.01	0.04 ± 0.00	0.03 ± 0.02	0.05 ± 0.02	n.d.
trimethoxytoluene (2,4,6-trimethoxytoluene)	0	0.06 ± 0.03	0.05 ± 0.00	0.04 ± 0.00	0.02 ± 0.01	n.d.
	60	0.09 ± 0.00	0.04 ± 0.00	0.01 ± 0.00	0.03 ± 0.00	n.d.
trimethoxytoluene	0	0.10 ± 0.05	0.07 ± 0.01	0.06 ± 0.01	0.03 ± 0.00	n.d.
	60	0.10 ± 0.01	0.03 ± 0.00	0.02 ± 0.01	0.03 ± 0.01	n.d.
dimethoxystyrene	0	0.27 ± 0.05	0.20 ± 0.10	0.16 ± 0.03	0.03 ± 0.01	n.d.
	60	0.19 ± 0.02	0.09 ± 0.02	0.04 ± 0.01	0.11 ± 0.03	n.d.
1,2,3,4-tetramethoxybenzene	0	0.08 ± 0.05	0.07 ± 0.04	0.04 ± 0.00	0.01 ± 0.01	n.d.
	60	0.12 ± 0.01	0.05 ± 0.01	0.01 ± 0.01	0.02 ± 0.00	n.d.
1,2,3,5-tetramethoxybenzene	0	0.17 ± 0.07	0.13 ± 0.03	0.07 ± 0.01	0.03 ± 0.00	n.d.
	60	0.21 ± 0.02	0.05 ± 0.01	0.02 ± 0.01	0.03 ± 0.00	n.d.
3,4-dimethoxybenzaldehyde	0	0.36 ± 0.11	0.43 ± 0.11	0.26 ± 0.06	0.09 ± 0.01	n.d.
	60	0.54 ± 0.02	0.21 ± 0.02	0.09 ± 0.04	0.20 ± 0.02	n.d.
3,4-dimethoxyacetophenone	0	0.28 ± 0.09	0.70 ± 0.66	0.20 ± 0.06	0.04 ± 0.03	n.d.
	60	0.31 ± 0.02	0.11 ± 0.00	0.05 ± 0.01	0.12 ± 0.03	n.d.
3,5-dimethoxybenzoic acid methyl ester	0	0.03 ± 0.02	0.02 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	n.d.
	60	0.05 ± 0.00	0.01 ± 0.00	0.01 ± 0.01	0.01 ± 0.00	n.d.
3,4-dimethoxybenzoic acid methyl ester	0	2.61 ± 0.76	2.10 ± 0.21	1.53 ± 0.34	0.50 ± 0.08	n.d.
	60	3.02 ± 0.02	0.93 ± 0.01	0.36 ± 0.14	0.68 ± 0.17	n.d.
3,4,5-trimethoxybenzaldehyde (syringaldehyde)	0	0.16 ± 0.07	0.25 ± 0.11	0.14 ± 0.02	0.05 ± 0.00	n.d.
	60	0.27 ± 0.02	0.10 ± 0.00	0.04 ± 0.02	0.11 ± 0.00	n.d.
3-(4-methoxyphenyl)prop-2-enoic acid methyl ester (Z,E)	0	0.52 ± 0.16	0.36 ± 0.00	0.31 ± 0.07	0.13 ± 0.00	n.d.
	60	0.61 ± 0.05	0.23 ± 0.00	0.12 ± 0.04	0.24 ± 0.05	n.d.
3,4,5-trimethoxyacetophenone (acetosyringone)	0	0.15 ± 0.06	0.13 ± 0.04	0.10 ± 0.03	0.04 ± 0.00	n.d.
	60	0.18 ± 0.00	0.06 ± 0.00	0.03 ± 0.01	0.08 ± 0.01	n.d.
cis-1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	0	0.29 ± 0.05	0.31 ± 0.05	0.22 ± 0.05	0.06 ± 0.01	n.d.
	60	0.38 ± 0.01	0.16 ± 0.03	0.06 ± 0.02	0.11 ± 0.03	n.d.
trans-1,2-Dimethoxy-4-(2-methoxyethenyl)benzene	0	0.24 ± 0.04	0.25 ± 0.05	0.18 ± 0.06	0.04 ± 0.00	n.d.
	60	0.31 ± 0.01	0.13 ± 0.02	0.05 ± 0.02	0.10 ± 0.03	n.d.
cis-1,2-Dimethoxy-4-(3-methoxy-1-propenyl)benzene	0	0.02 ± 0.00	0.02 ± 0.00	0.02 ± 0.00	n.d.	n.d.
	60	0.03 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
2,4,5-Trimethoxypropenylbenzene	0	0.04 ± 0.01	0.03 ± 0.01	0.03 ± 0.01	0.01 ± 0.01	n.d.
	60	0.04 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	0.02 ± 0.00	n.d.
1,2-Dimethoxy-4-(1-methoxy-1-propenyl)benzene	0	0.02 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	n.d.	n.d.
	60	0.03 ± 0.00	0.01 ± 0.00	0.01 ± 0.01	0.01 ± 0.00	n.d.
cis-1,2-Dimethoxy-4-(2-methoxy-1-propenyl)benzene	0	0.04 ± 0.00	0.05 ± 0.01	0.03 ± 0.00	0.01 ± 0.00	n.d.
	60	0.06 ± 0.00	0.02 ± 0.00	0.01 ± 0.01	0.02 ± 0.00	n.d.
trans-1,2-Dimethoxy-4-(2-methoxy-1-propenyl)benzene	0	0.07 ± 0.01	0.07 ± 0.02	0.05 ± 0.01	n.d.	n.d.
	60	0.10 ± 0.01	0.04 ± 0.01	0.01 ± 0.01	0.03 ± 0.01	n.d.
trans-1,2-Dimethoxy-4-(3-methoxy-1-propenyl)benzene	0	0.07 ± 0.02	0.08 ± 0.02	0.06 ± 0.01	0.01 ± 0.00	n.d.
	60	0.09 ± 0.00	0.05 ± 0.01	0.01 ± 0.01	0.02 ± 0.00	n.d.
3,4,5-trimethoxybenzoic acid emthyl ester	0	0.92 ± 0.32	0.79 ± 0.11	0.60 ± 0.16	0.19 ± 0.02	n.d.
	60	1.06 ± 0.00	0.37 ± 0.02	0.17 ± 0.10	0.29 ± 0.08	n.d.
cis-1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene	0	0.21 ± 0.05	0.24 ± 0.09	0.18 ± 0.01	0.04 ± 0.00	n.d.
	60	0.26 ± 0.01	0.10 ± 0.01	0.04 ± 0.02	0.09 ± 0.03	n.d.
trans-1,2,3-Trimethoxy-5-(2-methoxyethenyl)benzene	0	0.17 ± 0.04	0.20 ± 0.08	0.14 ± 0.03	0.03 ± 0.00	n.d.
	60	0.20 ± 0.00	0.08 ± 0.00	0.04 ± 0.02	0.08 ± 0.02	n.d.
erythro-1,2-dimethoxy-4-(1,2,3-trimethoxypropyl)benzene	0	0.23 ± 0.02	0.30 ± 0.04	0.17 ± 0.02	0.05 ± 0.02	n.d.
	60	0.35 ± 0.04	0.14 ± 0.03	0.04 ± 0.02	0.07 ± 0.01	n.d.
threo-1,2-dimethoxy-4-(1,2,3-trimethoxypropyl)benzene	0	0.14 ± 0.02	0.18 ± 0.00	0.11 ± 0.02	0.03 ± 0.01	n.d.
	60	0.21 ± 0.01	0.08 ± 0.01	0.03 ± 0.02	0.05 ± 0.01	n.d.
3-(3,4-dimethoxyphenyl)prop-2-enoic acid methyl ester (Z,E)	0	0.75 ± 0.05	0.72 ± 0.39	0.48 ± 0.02	0.14 ± 0.02	n.d.
	60	0.67 ± 0.01	0.38 ± 0.01	0.13 ± 0.02	0.44 ± 0.02	n.d.
erythro-1,2,3-Trimethoxy-5-(1,2,3-trimethoxypropyl)benzene	0	0.08 ± 0.00	0.11 ± 0.01	0.06 ± 0.00	0.02 ± 0.01	n.d.
	60	0.11 ± 0.01	0.04 ± 0.01	0.02 ± 0.01	0.03 ± 0.01	n.d.
threo-1,2,3-Trimethoxy-5-(1,2,3-trimethoxypropyl)benzene	0	0.03 ± 0.00	0.04 ± 0.00	0.02 ± 0.00	0.01 ± 0.00	n.d.
	60	0.04 ± 0.00	0.01 ± 0.00	0.01 ± 0.01	0.01 ± 0.00	n.d.
cis-1,2,3-Trimethoxy-5-(2-methoxy-1-propenyl)benzene	0	0.03 ± 0.01	0.04 ± 0.02	0.02 ± 0.00	n.d.	n.d.
	60	0.04 ± 0.00	0.01 ± 0.00	0.01 ± 0.01	0.01 ± 0.00	n.d.
trans-1,2,3-Trimethoxy-5-(2-methoxy-1-propenyl)benzene	0	0.04 ± 0.01	0.06 ± 0.03	0.03 ± 0.00	n.d.	n.d.
	60	0.05 ± 0.01	0.02 ± 0.00	0.01 ± 0.01	0.02 ± 0.00	n.d.
cis-1,2-Dimethoxy-4-(2,3-dimethoxy-1-propenyl)benzene	0	0.06 ± 0.01	0.06 ± 0.01	0.04 ± 0.00	0.01 ± 0.00	n.d.
	60	0.08 ± 0.01	0.03 ± 0.01	0.01 ± 0.00	0.03 ± 0.00	n.d.
trans-1,2-Dimethoxy-4-(2,3-dimethoxy-1-propenyl)benzene	0	0.07 ± 0.02	0.08 ± 0.03	0.06 ± 0.00	0.01 ± 0.00	n.d.
	60	0.08 ± 0.00	0.04 ± 0.00	0.01 ± 0.01	0.03 ± 0.00	n.d.
Carbohydrates (Car)						
C5 (xylose)	0	0.32 ± 0.07	0.20 ± 0.00	0.12 ± 0.02	0.06 ± 0.04	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
	60	0.38 ± 0.02	0.12 ± 0.00	0.04 ± 0.03	0.09 ± 0.02	n.d.
C5 (xylose)	0	0.75 ± 0.08	0.51 ± 0.07	0.33 ± 0.02	0.20 ± 0.03	n.d.
	60	0.84 ± 0.06	0.29 ± 0.01	0.13 ± 0.06	0.24 ± 0.07	n.d.
deoxyC6-1 (rhamnose)	0	0.07 ± 0.03	0.04 ± 0.01	0.03 ± 0.01	0.01 ± 0.01	n.d.
	60	0.05 ± 0.00	0.02 ± 0.00	0.01 ± 0.01	0.02 ± 0.00	n.d.
deoxyC6-2 (Fucose)	0	0.15 ± 0.01	0.14 ± 0.06	0.20 ± 0.08	0.21 ± 0.01	n.d.
	60	0.14 ± 0.01	0.07 ± 0.01	0.16 ± 0.06	0.15 ± 0.02	n.d.
deoxyC6-3 (Rhamnose)	0	0.08 ± 0.00	0.11 ± 0.00	0.06 ± 0.01	0.04 ± 0.03	n.d.
	60	0.12 ± 0.00	0.05 ± 0.00	0.03 ± 0.02	0.06 ± 0.00	n.d.
deoxyC6-4 (Fucose)	0	0.10 ± 0.03	0.09 ± 0.00	0.07 ± 0.01	0.03 ± 0.00	n.d.
	60	0.12 ± 0.01	0.05 ± 0.01	0.01 ± 0.00	0.03 ± 0.01	n.d.
C6-1 (Glucose)	0	0.49 ± 0.16	0.60 ± 0.16	0.22 ± 0.08	0.14 ± 0.10	n.d.
	60	1.10 ± 0.01	0.37 ± 0.02	0.09 ± 0.06	0.15 ± 0.05	n.d.
C6-2 (Galactose)	0	0.07 ± 0.03	0.07 ± 0.03	0.04 ± 0.02	0.02 ± 0.01	n.d.
	60	0.14 ± 0.00	0.05 ± 0.00	0.01 ± 0.01	0.03 ± 0.00	n.d.
C6-3 (Glucose)	0	1.49 ± 0.27	1.88 ± 0.19	0.68 ± 0.17	0.47 ± 0.42	n.d.
	60	3.03 ± 0.10	1.08 ± 0.01	0.27 ± 0.19	0.46 ± 0.16	n.d.
C6-4 (Galactose)	0	0.15 ± 0.05	0.18 ± 0.04	0.08 ± 0.02	0.07 ± 0.02	n.d.
	60	0.31 ± 0.00	0.11 ± 0.02	0.03 ± 0.02	0.06 ± 0.01	n.d.
Fatty acids						
$C_{8:0}$	0	0.22 ± 0.04	0.17 ± 0.01	0.19 ± 0.02	0.12 ± 0.03	n.d.
	60	0.31 ± 0.04	0.11 ± 0.00	0.05 ± 0.00	0.17 ± 0.06	n.d.
$C_{9:0}$	0	0.15 ± 0.03	0.12 ± 0.03	0.12 ± 0.02	0.07 ± 0.00	n.d.
	60	0.29 ± 0.12	0.07 ± 0.01	0.05 ± 0.00	0.12 ± 0.01	n.d.
$C_{10:0}$	0	0.12 ± 0.01	0.13 ± 0.00	0.09 ± 0.00	0.06 ± 0.01	n.d.
	60	0.24 ± 0.10	0.08 ± 0.01	0.06 ± 0.01	0.13 ± 0.08	n.d.
$C_{12:0}$	0	0.16 ± 0.02	0.15 ± 0.07	0.10 ± 0.02	0.06 ± 0.00	n.d.
	60	0.25 ± 0.03	0.45 ± 0.16	0.73 ± 0.05	0.94 ± 0.95	n.d.
α,ω-diacid C9:0	0	1.69 ± 0.21	1.50 ± 0.08	1.78 ± 0.22	1.03 ± 0.04	n.d.
	60	1.91 ± 0.22	0.90 ± 0.03	0.30 ± 0.04	0.40 ± 0.08	n.d.
$C_{13:0}$	0	0.02 ± 0.00	0.02 ± 0.00	0.02 ± 0.00	n.d.	n.d.
	60	0.11 ± 0.01	0.03 ± 0.00	0.04 ± 0.00	0.06 ± 0.05	n.d.
br$C_{14:0}$	0	0.02 ± 0.00	0.01 ± 0.00	0.01 ± 0.01	n.d.	n.d.
	60	0.06 ± 0.00	0.03 ± 0.01	0.01 ± 0.00	0.07 ± 0.03	n.d.
$C_{14:0}$	0	0.32 ± 0.04	0.27 ± 0.02	0.28 ± 0.02	0.24 ± 0.04	0.10 ± 0.02
	60	0.43 ± 0.02	3.63 ± 0.25	5.97 ± 0.18	6.88 ± 7.94	0.09 ± 0.00

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
i$C_{15:0}$	0	0.28 ± 0.08	0.21 ± 0.00	0.18 ± 0.03	0.11 ± 0.01	0.03 ± 0.00
	60	0.46 ± 0.04	0.26 ± 0.00	0.11 ± 0.01	0.15 ± 0.02	0.04 ± 0.01
a$C_{15:0}$	0	0.07 ± 0.01	0.05 ± 0.01	0.05 ± 0.00	n.d.	n.d.
	60	0.16 ± 0.01	0.10 ± 0.02	0.04 ± 0.00	0.14 ± 0.04	n.d.
$C_{15:0}$	0	0.10 ± 0.00	0.09 ± 0.00	0.11 ± 0.02	0.08 ± 0.01	0.06 ± 0.01
	60	0.18 ± 0.01	0.17 ± 0.00	0.22 ± 0.01	0.24 ± 0.04	0.05 ± 0.00
br$C_{16:0}$	0	0.40 ± 0.11	0.30 ± 0.00	0.22 ± 0.05	0.13 ± 0.01	n.d.
	60	0.44 ± 0.02	0.24 ± 0.02	0.10 ± 0.01	0.31 ± 0.07	n.d.
$C_{16:1}$	0	0.13 ± 0.01	0.19 ± 0.11	0.07 ± 0.02	n.d.	n.d.
	60	0.08 ± 0.02	0.08 ± 0.04	1.01 ± 1.34	0.97 ± 0.07	n.d.
$C_{16:0}$	0	2.73 ± 0.40	9.88 ± 3.25	24.97 ± 4.06	26.91 ± 0.81	22.35 ± 0.29
	60	3.32 ± 0.16	37.65 ± 3.14	47.62 ± 1.20	26.40 ± 4.35	21.41 ± 0.32
10Me16:O	0	0.19 ± 0.05	0.14 ± 0.00	0.10 ± 0.03	0.04 ± 0.01	n.d.
	60	0.22 ± 0.01	0.05 ± 0.06	0.05 ± 0.00	0.04 ± 0.00	n.d.
i$C_{17:0}$	0	0.11 ± 0.03	0.26 ± 0.08	0.46 ± 0.04	0.62 ± 0.01	0.60 ± 0.07
	60	0.16 ± 0.00	0.30 ± 0.06	0.35 ± 0.00	0.65 ± 0.01	0.64 ± 0.02
a$C_{17:0}$	0	0.06 ± 0.02	0.04 ± 0.00	0.03 ± 0.01	n.d.	n.d.
	60	0.08 ± 0.00	0.04 ± 0.00	0.02 ± 0.00	0.09 ± 0.01	n.d.
$C_{17:0}$	0	0.09 ± 0.02	0.10 ± 0.01	0.11 ± 0.02	0.10 ± 0.01	0.06 ± 0.00
	60	0.14 ± 0.02	0.11 ± 0.06	0.15 ± 0.06	0.13 ± 0.02	0.06 ± 0.00
10Me17:0	0	0.07 ± 0.01	0.04 ± 0.00	0.03 ± 0.00	n.d.	n.d.
	60	0.09 ± 0.01	0.03 ± 0.00	0.05 ± 0.05	0.01 ± 0.00	n.d.
C18:1	0	0.68 ± 0.02	1.00 ± 0.26	1.60 ± 0.13	2.25 ± 0.15	2.17 ± 0.14
	60	0.60 ± 0.14	0.56 ± 0.05	0.91 ± 0.44	1.04 ± 0.20	1.57 ± 0.09
C18:1	0	1.31 ± 1.65	0.22 ± 0.06	0.29 ± 0.00	0.47 ± 0.06	0.45 ± 0.04
	60	0.17 ± 0.03	0.36 ± 0.11	0.61 ± 0.04	11.76 ± 12.36	1.04 ± 0.16
C18:0	0	0.68 ± 0.06	0.53 ± 0.04	0.57 ± 0.05	0.48 ± 0.00	0.24 ± 0.03
	60	0.92 ± 0.07	1.47 ± 1.22	0.54 ± 0.21	0.57 ± 0.15	0.23 ± 0.02
ωOH$C_{16:0}$	0	1.30 ± 1.59	1.52 ± 0.09	1.12 ± 0.01	n.d.	n.d.
	60	2.05 ± 0.04	0.93 ± 0.11	0.54 ± 0.04	0.69 ± 0.06	n.d.
10Me18:0	0	0.08 ± 0.05	0.09 ± 0.02	0.09 ± 0.00	n.d.	n.d.
	60	0.11 ± 0.02	0.06 ± 0.00	0.04 ± 0.00	0.06 ± 0.01	n.d.
$C_{19:1}$	0	1.72 ± 0.49	0.76 ± 0.39	0.80 ± 0.00	n.d.	n.d.
	60	0.71 ± 0.14	0.46 ± 0.00	0.19 ± 0.08	0.20 ± 0.04	n.d.
α,ω$C_{16:0}$	0	2.57 ± 0.05	1.46 ± 0.49	1.04 ± 0.02	0.57 ± 0.09	n.d.
	60	1.56 ± 0.03	0.87 ± 0.03	0.66 ± 0.08	0.62 ± 0.22	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
$C_{20:0}$	0	0.72 ± 0.04	0.41 ± 0.01	0.49 ± 0.04	0.51 ± 0.02	0.25 ± 0.06
	60	0.55 ± 0.00	0.49 ± 0.12	0.67 ± 0.01	1.78 ± 0.18	1.25 ± 0.12
$C_{22:0}$	0	2.85 ± 0.21	1.41 ± 0.43	1.07 ± 0.26	0.97 ± 0.06	0.14 ± 0.03
	60	1.46 ± 0.03	1.00 ± 0.05	1.04 ± 0.11	1.16 ± 0.08	0.13 ± 0.00
$\omega OHC_{20:0}$	0	1.91 ± 0.00	1.25 ± 0.27	0.78 ± 0.04	0.53 ± 0.15	n.d.
	60	1.19 ± 0.11	0.88 ± 0.09	0.53 ± 0.05	0.67 ± 0.17	n.d.
$C_{23:0}$	0	n.d.	0.86 ± 0.14	0.72 ± 0.19	0.58 ± 0.28	0.11 ± 0.01
	60	n.d.	0.64 ± 0.02	0.75 ± 0.02	0.83 ± 0.02	0.10 ± 0.00
$\alpha,\omega C_{20:0}$	0	1.05 ± 0.16	0.76 ± 0.09	0.55 ± 0.05	0.42 ± 0.01	n.d.
	60	0.88 ± 0.05	0.52 ± 0.02	0.37 ± 0.01	0.35 ± 0.10	n.d.
$C_{24:0}$	0	4.27 ± 0.71	2.70 ± 0.32	2.29 ± 0.51	2.32 ± 0.13	0.38 ± 0.11
	60	2.92 ± 0.32	2.29 ± 0.02	2.63 ± 0.28	2.75 ± 0.27	0.39 ± 0.00
$\omega OHC_{22:0}$	0	10.67 ± 0.71	8.03 ± 0.32	4.95 ± 0.82	3.55 ± 0.75	n.d.
	60	9.71 ± 0.09	6.38 ± 1.14	4.09 ± 0.10	4.22 ± 0.81	n.d.
$C_{25:0}$	0	1.06 ± 0.34	0.69 ± 0.10	0.52 ± 0.21	0.62 ± 0.11	0.08 ± 0.02
	60	0.96 ± 0.05	0.50 ± 0.03	0.75 ± 0.09	0.61 ± 0.02	0.10 ± 0.01
$\alpha,\omega C_{22:0}$	0	1.86 ± 0.50	1.57 ± 0.37	0.89 ± 0.38	0.68 ± 0.14	n.d.
	60	2.34 ± 0.03	0.96 ± 0.07	0.72 ± 0.23	0.54 ± 0.05	n.d.
$C_{26:0}$	0	2.05 ± 0.57	1.51 ± 0.10	1.01 ± 0.32	1.09 ± 0.16	0.09 ± 0.02
	60	2.16 ± 0.04	1.09 ± 0.05	1.28 ± 0.19	1.04 ± 0.06	0.12 ± 0.00
$\omega OHC_{24:0}$	0	6.14 ± 0.16	6.43 ± 0.09	2.81 ± 0.31	1.84 ± 0.25	n.d.
	60	8.28 ± 0.99	4.25 ± 0.64	2.63 ± 0.33	2.35 ± 0.39	n.d.
$C_{27:0}$	0	0.44 ± 0.12	0.31 ± 0.11	0.18 ± 0.09	0.17 ± 0.03	n.d.
	60	0.58 ± 0.01	0.19 ± 0.02	0.21 ± 0.03	0.15 ± 0.02	n.d.
$\alpha,\omega C_{24:0}$	0	0.73 ± 0.15	0.67 ± 0.14	0.31 ± 0.01	0.16 ± 0.03	n.d.
	60	1.18 ± 0.15	0.42 ± 0.01	0.25 ± 0.11	0.10 ± 0.01	n.d.
$C_{28:0}$	0	1.33 ± 0.39	0.89 ± 0.37	0.49 ± 0.20	0.46 ± 0.07	n.d.
	60	1.93 ± 0.07	0.53 ± 0.03	0.59 ± 0.07	0.32 ± 0.04	n.d.
$\omega OHC_{26:0}$	0	1.22 ± 0.15	1.27 ± 0.08	0.58 ± 0.24	0.34 ± 0.05	n.d.
	60	2.02 ± 0.49	0.79 ± 0.06	0.31 ± 0.20	0.19 ± 0.00	n.d.
$C_{29:0}$	0	0.30 ± 0.10	0.19 ± 0.09	0.10 ± 0.02	0.12 ± 0.02	n.d.
	60	0.48 ± 0.06	0.13 ± 0.02	0.08 ± 0.05	0.04 ± 0.00	n.d.
$\alpha,\omega C_{26:0}$	0	0.22 ± 0.09	0.19 ± 0.04	0.10 ± 0.05	0.14 ± 0.04	n.d.
	60	0.44 ± 0.06	0.13 ± 0.01	0.06 ± 0.08	n.d.	n.d.
$C_{30:0}$	0	0.75 ± 0.26	0.44 ± 0.22	0.27 ± 0.02	n.d.	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
	60	1.22 ± 0.08	0.36 ± 0.05	0.29 ± 0.17	n.d.	n.d.
ωOH$C_{28:0}$	0	n.d.	n.d.	n.d.	n.d.	n.d.
	60	n.d.	n.d.	n.d.	n.d.	n.d.
$C_{31:0}$	0	n.d.	0.05 ± 0.02	0.03 ± 0.01	n.d.	n.d.
	60	n.d.	0.04 ± 0.00	0.03 ± 0.04	n.d.	n.d.
α,ω$C_{28:0}$	0	n.d.	n.d.	n.d.	n.d.	n.d.
	60	n.d.	n.d.	n.d.	n.d.	n.d.
$C_{32:0}$	0	n.d.	0.13 ± 0.08	0.06 ± 0.01	n.d.	n.d.
	60	n.d.	0.09 ± 0.00	0.11 ± 0.15	n.d.	n.d.
10,16-diOH$C_{16:0}$	0	3.99 ± 0.93	2.55 ± 0.18	1.22 ± 0.15	1.32 ± 1.16	n.d.
	60	3.80 ± 0.14	1.73 ± 0.22	1.05 ± 0.49	1.02 ± 0.06	n.d.
9,10,18-triOH$C_{18:0}$	0	14.53 ± 7.63	13.05 ± 4.28	5.78 ± 2.42	4.25 ± 3.24	n.d.
	60	11.14 ± 1.07	10.17 ± 2.93	4.20 ± 1.44	5.18 ± 2.18	n.d.
$C_{16:2}$	0	n.d.	0.26 ± 0.07	0.44 ± 0.11	0.97 ± 0.45	3.19 ± 1.17
	60	n.d.	n.d.	n.d.	n.d.	3.71 ± 0.42
$C_{16:2}$	0	n.d.	0.16 ± 0.05	0.36 ± 0.06	0.71 ± 0.77	2.76 ± 1.11
	60	n.d.	n.d.	n.d.	n.d.	3.53 ± 0.60
$C_{16:2}$	0	n.d.	0.35 ± 0.07	0.60 ± 0.07	1.16 ± 0.35	0.54 ± 0.46
	60	n.d.	0.02 ± 0.01	0.07 ± 0.03	0.04 ± 0.06	0.39 ± 0.21
$C_{16:2}$	0	n.d.	0.89 ± 0.19	1.43 ± 0.04	3.02 ± 0.04	2.99 ± 2.54
	60	n.d.	0.10 ± 0.02	0.17 ± 0.01	0.16 ± 0.23	3.95 ± 0.66
$C_{18:2}$	0	n.d.	0.71 ± 0.27	1.37 ± 0.26	3.53 ± 1.16	8.90 ± 1.48
	60	n.d.	0.14 ± 0.07	0.23 ± 0.16	0.12 ± 0.17	7.04 ± 0.52
$C_{18:2}$	0	n.d.	0.76 ± 0.19	1.45 ± 0.31	2.71 ± 1.90	8.21 ± 2.66
	60	n.d.	0.31 ± 0.03	0.30 ± 0.13	0.17 ± 0.25	6.93 ± 1.03
$C_{18:2}$	0	n.d.	0.32 ± 0.17	0.26 ± 0.15	0.91 ± 0.74	1.13 ± 0.12
	60	n.d.	0.04 ± 0.00	0.09 ± 0.02	0.04 ± 0.06	0.29 ± 0.24
$C_{18:2}$	0	n.d.	1.92 ± 0.71	2.50 ± 0.10	7.25 ± 2.04	7.48 ± 6.86
	60	n.d.	0.26 ± 0.05	0.56 ± 0.17	0.34 ± 0.48	6.07 ± 1.63
Fatty alcohols (Falcohol)						
C18:0	0	0.38 ± 0.07	0.53 ± 0.16	0.28 ± 0.01	0.11 ± 0.02	n.d.
	60	0.45 ± 0.01	0.25 ± 0.03	0.15 ± 0.03	0.12 ± 0.16	n.d.
C20:0	0	0.56 ± 0.24	0.49 ± 0.10	0.29 ± 0.05	n.d.	n.d.
	60	0.55 ± 0.01	0.28 ± 0.05	0.17 ± 0.04	0.14 ± 0.20	n.d.
C22:0	0	1.66 ± 0.43	1.00 ± 0.20	0.84 ± 0.14	n.d.	n.d.
	60	0.96 ± 0.02	0.51 ± 0.09	0.39 ± 0.01	0.33 ± 0.47	n.d.

Compounds name	Incubation time (days)	S:A, 100:0	S:A, 75:25	S:A, 50:50	S:A, 25:75	S:A, 0:100
C24:0	0	3.83 ± 0.58	1.86 ± 0.48	1.58 ± 0.12	n.d.	n.d.
	60	2.02 ± 0.05	1.57 ± 0.20	1.37 ± 0.07	0.83 ± 1.17	n.d.
C26:0	0	1.43 ± 0.16	0.85 ± 0.00	0.62 ± 0.04	n.d.	n.d.
	60	1.13 ± 0.01	0.76 ± 0.02	0.84 ± 0.01	0.37 ± 0.53	n.d.
C28:0	0	0.79 ± 0.18	0.36 ± 0.34	0.30 ± 0.15	n.d.	n.d.
	60	1.00 ± 0.08	0.32 ± 0.02	0.51 ± 0.01	0.22 ± 0.31	n.d.
C30:0	0	0.59 ± 0.11	0.22 ± 0.17	0.19 ± 0.04	n.d.	n.d.
	60	0.90 ± 0.09	0.25 ± 0.00	0.35 ± 0.09	n.d.	n.d.
C32:0	0	n.d.	0.17 ± 0.09	0.07 ± 0.01	n.d.	n.d.
	60	n.d.	0.14 ± 0.01	n.d.	n.d.	n.d.
Chlrorophyll markers (Phytol)						
Phytol	0	n.d.	0.99 ± 0.07	2.77 ± 0.64	4.15 ± 1.78	5.96 ± 3.41
	60	n.d.	0.75 ± 0.13	1.39 ± 0.34	1.06 ± 1.49	6.08 ± 1.99
Neophytadiene	0	n.d.	1.25 ± 0.79	3.43 ± 2.56	6.90 ± 4.05	15.58 ± 4.42
	60	n.d.	1.10 ± 0.38	4.89 ± 0.66	8.65 ± 3.88	12.47 ± 2.96
2-pyrrolidone-5-carboxylic acid, N-methyl, methyl ester	0	n.d.	2.19 ± 0.08	3.20 ± 0.41	2.85 ± 0.48	1.39 ± 0.62
	60	n.d.	1.17 ± 0.04	0.81 ± 0.04	1.17 ± 0.36	3.05 ± 0.60
Uracil, 1,3-dimethyl	0	n.d.	0.70 ± 0.38	2.06 ± 0.34	2.53 ± 0.53	7.30 ± 1.10
	60	n.d.	0.09 ± 0.01	0.12 ± 0.06	0.15 ± 0.03	9.49 ± 0.15
Adenine trimethyl	0	n.d.	1.32 ± 0.35	2.36 ± 0.59	1.60 ± 0.04	1.05 ± 1.28
	60	n.d.	0.16 ± 0.02	0.20 ± 0.10	0.29 ± 0.15	0.22 ± 0.04
Hypoxanthine	0	n.d.	0.02 ± 0.01	0.25 ± 0.06	0.67 ± 0.05	1.33 ± 0.44
	60	n.d.	0.03 ± 0.04	n.d.	0.02 ± 0.00	2.56 ± 0.11
Thymine dimethyl	0	n.d.	0.49 ± 0.08	0.68 ± 0.14	0.49 ± 0.03	1.17 ± 0.19
	60	n.d.	0.12 ± 0.01	0.09 ± 0.04	0.20 ± 0.05	1.14 ± 0.00
1-Methylindole	0	0.43 ± 0.11	0.32 ± 0.14	0.88 ± 0.10	0.61 ± 0.21	0.69 ± 0.24
	60	0.21 ± 0.01	0.21 ± 0.03	0.35 ± 0.13	1.06 ± 0.56	0.74 ± 0.04
1,3-Dimethylindole	0	0.23 ± 0.05	0.13 ± 0.04	0.41 ± 0.09	0.24 ± 0.07	0.63 ± 0.18
	60	0.09 ± 0.01	0.17 ± 0.04	0.23 ± 0.03	0.41 ± 0.24	0.64 ± 0.02

n.d., not detected

Reference

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