

Occurrence, Distribution, and Sources of Aliphatic and Cyclic Hydrocarbons in Sediments from Two Different Lagoons along the Red Sea Coast of Saudi Arabia

Mubarak T. Al-Otaibi ^{1,2}, Ahmed I. Rushdi ³, Najeeb Rasul ^{4,5}, Abdulqader Bazeyad ², Khalid F. Al-Mutlaq ², Saud S. Aloud ¹ and Hattan A. Alharbi ^{2,*}

¹ Department of Soil Science, College of Food and Agriculture Sciences, King Saud University, P.O. Box 2460, Riyadh 11451, Saudi Arabia; mmubarakk@ksu.edu.sa (M.T.A.-O.); alouds@ksu.edu.sa (S.S.A.)

² Department of Plant Protection, College of Food and Agriculture Sciences, King Saud University, P.O. Box 2460, Riyadh 11451, Saudi Arabia; abazeyad@ksu.edu.sa (A.B.); almutlaqk@gmail.com (K.F.A.-M.)

³ ETAL, 2951 SE Midvale Drive, Corvallis, OR 97333, USA; aimrushdi@gmail.com

⁴ Saudi Geological Survey, Jeddah 21514, Saudi Arabia; najeeb_rasul@hotmail.com

⁵ Geological and Geophysical Research Systems, Mississauga, ON L4T 0A1, Canada

* Correspondence: halharbii@ksu.edu.sa

Table S1. Concentrations (ng/g), chemical parameters and proportions of various chemical groups in surface sediments from Al-Qahma and Al-Wajh lagoons, Red Sea coast of Saudi Arabia.

Al-Qahma Lagoon			Station #																	
			1	2	3	4	5	7	8	12	14	17	18	20	21	22	23	24	25	27
TEOM (ng/g)			7729	4054	6735	7272	11711	4523	5310	7891	9019	7181	3335	4151	886	6570	6670	5310	6098	4336
Compound (ng/g)	Composition	M.W.																		
n-Alkanes																				
Pentadecane	C ₁₅ H ₃₂	212	2.4	0.0	1.8	0.4	1.5	0.6	0.8	1.2	0.1	1.0	1.3	0.0	0.0	0.6	0.6	0.3	0.5	0.7
Hexadecane	C ₁₆ H ₃₄	226	16.8	11.6	27.2	1.2	4.5	3.3	1.5	2.5	1.7	4.9	19.7	0.8	0.6	2.5	4.0	2.9	0.8	6.0
Heptadecane	C ₁₇ H ₃₆	240	54.9	34.9	79.5	13.1	48.0	26.7	17.5	11.8	23.5	28.0	1.9	6.2	2.7	9.2	16.0	18.6	6.1	26.0
Pristane	C ₁₉ H ₄₀ (Pr)	268	1.5	2.5	2.7	0.4	1.6	1.0	0.7	0.5	0.9	1.0	25.0	0.3	0.5	0.2	0.5	0.6	0.4	0.8
Octadecane	C ₁₈ H ₃₈	256	49.4	35.7	89.3	4.4	16.2	14.0	5.7	6.9	17.7	22.4	3.8	8.0	3.9	8.0	8.3	19.5	7.3	26.1
Phytane	C ₂₀ H ₄₂ (Ph) ¹	282	16.4	11.2	32.1	0.3	1.1	2.3	0.6	1.4	2.7	12.5	11.2	1.5	0.6	1.3	3.9	2.9	1.0	2.5
Nonadecane	C ₁₉ H ₄₀	268	9.0	2.1	111.5	0.2	0.9	2.2	1.5	4.5	11.1	3.0	66.6	4.8	0.9	9.0	2.6	5.4	0.6	0.2
Eicosane	C ₂₀ H ₄₂	282	27.2	22.2	61.3	5.8	21.1	13.7	7.9	12.6	20.5	28.6	37.7	10.8	9.5	17.2	13.3	25.4	17.3	18.5
Heneicosane	C ₂₁ H ₄₄	296	14.2	12.9	40.3	2.0	7.2	11.6	4.7	5.0	9.4	12.2	50.8	6.8	3.8	7.6	3.5	12.2	8.5	13.6
Docosane	C ₂₂ H ₄₆	310	14.3	11.4	46.2	3.1	11.3	11.2	5.9	7.7	10.4	15.1	57.7	9.4	7.3	13.0	3.2	17.2	8.6	17.3
Tricosane	C ₂₃ H ₄₈	324	13.6	9.8	60.2	3.3	12.0	9.0	6.6	5.9	12.1	35.9	67.8	10.7	4.6	13.1	2.6	15.4	6.9	26.5
Tetracosane	C ₂₄ H ₅₀	338	14.2	7.1	37.8	3.3	12.0	7.0	7.3	6.4	12.6	10.4	83.4	10.2	3.9	16.5	2.0	14.9	6.7	19.1
Pentacosane	C ₂₅ H ₅₂	352	16.0	7.0	74.6	3.7	13.5	4.9	8.6	4.8	14.5	46.2	76.5	10.5	1.9	15.2	8.0	15.5	8.2	36.3
Hexacosane	C ₂₆ H ₅₄	366	15.6	4.6	22.8	3.3	12.2	3.5	8.5	2.9	13.5	7.5	74.7	10.6	2.1	16.2	1.4	15.9	4.9	16.4
Heptacosane	C ₂₇ H ₅₆	380	22.6	9.3	75.8	4.2	15.4	4.9	7.8	4.2	13.9	43.6	53.8	10.4	1.4	13.2	2.6	15.4	4.0	39.5
Octacosane	C ₂₈ H ₅₈	394	11.6	3.1	13.8	2.4	8.8	2.5	5.4	1.9	8.0	4.1	41.9	8.1	1.5	10.8	1.2	11.3	2.2	11.8
Nonacosane	C ₂₉ H ₆₀	408	14.8	7.4	37.3	1.8	6.8	3.2	4.1	3.5	8.6	23.6	33.8	6.0	0.9	7.5	2.4	9.6	2.4	21.0
Triacontane	C ₃₀ H ₆₂	422	7.2	2.1	10.1	1.0	3.5	1.5	2.3	0.9	4.0	2.6	24.5	3.2	0.3	3.7	0.5	4.9	0.5	5.5
Hentriacontane	C ₃₁ H ₆₄	436	12.0	7.4	41.8	1.1	3.9	3.3	2.1	2.3	5.0	17.8	3.4	2.3	0.7	3.2	2.7	4.0	0.5	14.2
Dotriacontane	C ₃₂ H ₆₆	450	3.8	1.1	4.9	0.2	0.8	0.5	0.9	0.5	1.3	1.0	2.9	0.7	0.1	0.6	0.3	1.8	0.6	2.4
Tritriacontane	C ₃₃ H ₆₈	464	4.9	3.3	23.0	0.0	0.1	0.6	0.3	1.4	1.4	49.3	0.0	0.3	0.1	0.4	1.2	0.5	0.1	7.4
Tetraatriacontane	C ₃₄ H ₇₀	478	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Pentatriacontane	C ₃₅ H ₇₂	492	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hexatriacontane	C ₃₆ H ₇₄	506	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Heptatriacontane	C ₃₇ H ₇₆	520	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total			342.4	206.6	894.0	55.2	202.4	127.5	100.6	88.7	193.0	370.5	738.5	121.6	47.2	169.2	80.8	214.0	88.3	311.8

CPI(o/e)			1.0	1.0	1.7	1.2	1.2	1.2	1.2	1.1	1.1	2.7	1.0	0.9	0.6	0.9	1.2	0.9	0.8	1.5
LMW/HMW			2.0	3.3	1.8	2.1	2.1	4.0	1.5	2.8	1.7	0.8	1.2	1.3	4.2	1.4	2.7	1.7	2.7	1.0
TAR			0.68	0.55	0.76	0.45	0.45	0.29	0.59	0.50	0.66	3.04	0.76	1.06	0.42	0.92	0.39	0.81	0.44	2.03
Wax n-alkanes																				
Total			23.9	18.8	137.7	2.0	7.3	5.7	2.0	6.6	8.9	122.9	57.9	1.9	2.1	14.6	6.2	4.4	1.5	54.3
%			7.0%	9.1%	15.4%	3.6%	3.6%	4.5%	2.0%	7.4%	4.6%	33.2%	7.8%	1.6%	4.4%	8.7%	7.7%	2.1%	1.7%	17.4%
Algal n-Alkanes																				
Total			47.3	26.3	174.9	12.9	47.3	32.5	20.9	17.8	34.3	30.6	108.7	13.3	5.2	21.2	16.6	25.3	11.8	24.4
%			13.8%	12.7%	19.6%	23.4%	23.4%	25.5%	20.8%	20.1%	17.8%	8.2%	14.7%	11.0%	11.0%	12.5%	20.5%	11.8%	13.3%	7.8%
Bacterial n-Alkanes																				
Total			49.9	43.4	177.7	11.4	41.8	31.0	15.1	22.0	39.9	55.9	61.3	19.7	14.0	27.7	25.6	47.8	25.4	50.7
%			14.6%	21.0%	19.9%	20.7%	20.7%	24.3%	15.0%	24.8%	20.7%	15.1%	8.3%	16.2%	29.6%	16.4%	31.7%	22.3%	28.7%	16.3%
Petroleum n-alkanes																				
Total			221.3	118.2	403.7	28.9	106.0	58.3	62.6	42.4	109.9	161.2	510.7	86.7	26.0	105.7	32.4	136.5	49.6	182.4
%			64.6%	57.2%	45.2%	52.4%	52.4%	45.7%	62.2%	47.7%	56.9%	43.5%	69.1%	71.3%	55.1%	62.4%	40.1%	63.8%	56.2%	58.5%
Hopanes																				
Trisnorhopane	C ₂₇ H ₄₆	370	0.0	0.0	7.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0
17a(H)-Trisnorhopane	C ₂₇ H ₄₆	370	0.0	0.0	3.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0
17a(H),21b(H)-Norhopane	C ₂₉ H ₅₀	398	0.0	0.0	19.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	7.4	0.0	0.0	0.0	0.0
17a(H),21b(H)-Hopane	C ₃₀ H ₅₂	412	0.0	0.0	21.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	4.9	0.0	0.0	0.0	0.0
17a(H),21b(H)-22S-Homohopane	C ₃₁ H ₅₄	426	0.0	0.0	6.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	2.8	0.0	0.0	0.0	0.0
17a(H),21b(H)-22R-Homohopane	C ₃₁ H ₅₄	426	0.0	0.0	2.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	1.8	0.0	0.0	0.0	0.0
Gammacerane	C ₃₀ H ₅₂	412	0.0	0.0	2.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.2	0.0	0.0	0.0	0.0
17a(H),21b(H)-22S-Bishomohopane	C ₃₂ H ₅₆	440	0.0	0.0	10.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.0	0.0	0.0	0.0
17a(H),21b(H)-22R-Bishomohopane	C ₃₂ H ₅₆	440	0.0	0.0	8.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	0.0	0.0	0.0	0.0
17a(H),21b(H)-22S-Trishomohopane	C ₃₃ H ₅₈	454	0.0	0.0	1.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17a(H),21b(H)-22R-Trishomohopane	C ₃₃ H ₅₈	454	0.0	0.0	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17a(H),21b(H)-22S-Tetrakishomohopane	C ₃₄ H ₆₀	468	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17a(H),21b(H)-22R-Tetrakishomohopane	C ₃₄ H ₆₀	468	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17a(H),21b(H)-22S-Pentakishomohopane	C ₃₅ H ₆₂	482	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17a(H),21b(H)-22R-Pentakishomohopane	C ₃₅ H ₆₂	482	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total			0.0	0.0	82.8	0.0	1.0	19.7	0.0	0.0	0.0	0.0								
C ₃₁ S/(R+S)			ND	ND	0.75	ND	0.70	0.61	ND	ND	ND	ND								

C ₃₂ S/(R+S)	ND	ND	0.56	ND	1.00	0.65	ND	ND	ND	ND										
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Steranes

13b,17a-20S-Cholestane Diasterane	C ₂₇ H ₄₈	372	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13b,17a-20R-Cholestane Diasterane	C ₂₇ H ₄₈	372	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13a,17b-20S-Cholestane Diasterane	C ₂₇ H ₄₈	372	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13a,17b-20R-Cholestane Diasterane	C ₂₇ H ₄₈	372	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14a,17ba-20S-Cholestane	C ₂₇ H ₄₈	372	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14b,17b-20R-Cholestane	C ₂₇ H ₄₈	372	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14b,17b-20S-Cholestane	C ₂₇ H ₄₈	372	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14a,17ba-20R-Cholestane	C ₂₇ H ₄₈	372	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14a,17ba-20S-Ergostane	C ₂₈ H ₅₀	386	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14b,17b-20R-Ergostane	C ₂₈ H ₅₀	386	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14b,17b-20S-Ergostane	C ₂₈ H ₅₀	386	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14a,17ba-20R-Ergostane	C ₂₈ H ₅₀	386	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14a,17ba-20S-Stigmastane	C ₂₉ H ₅₂	400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14b,17b-20R-Stigmastane	C ₂₉ H ₅₂	400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14b,17b-20S-Stigmastane	C ₂₉ H ₅₂	400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14a,17ba-20R-Stigmastane	C ₂₉ H ₅₂	400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total			0.0																	

PAHs

Phenanthrene	C ₁₄ H ₁₀	178	0.4	0.3	0.3	0.0	0.1	0.0	0.1	0.2	0.8	0.4	0.0	0.2	0.0	0.2	0.3	1.1	0.3	0.6
Anthracene	C ₁₄ H ₁₀	178	2.0	1.9	1.1	0.7	1.1	0.4	3.9	5.9	11.0	5.1	4.0	8.2	1.0	8.0	6.0	10.2	10.5	6.4
Benzo[k]fluoranthene	C ₂₀ H ₁₂	252	0.0	28.0	29.0	17.5	29.3	17.2	0.0	0.0	20.7	15.8	6.3	26.6	1.6	16.4	21.3	13.8	14.0	29.5
Benzo[b]fluoranthene	C ₂₀ H ₁₂	252	0.0	23.2	22.6	10.5	19.7	13.4	0.0	10.3	14.6	11.3	4.6	19.7	1.3	11.2	15.4	9.6	10.2	22.1
Total			2.4	53.3	52.9	28.7	50.2	31.1	4.0	16.4	47.1	32.6	15.0	54.7	3.8	35.8	43.1	34.7	35.0	58.5
Ant/(Ant+Phe)			0.8	0.9	0.8	1.0	0.9	1.0	1.0	1.0	0.9	0.9	1.0	1.0	1.0	1.0	1.0	0.9	1.0	0.9

Methyl n-Alkanoates

Methyl hexadecanoate	C ₁₇ H ₃₄ O ₂	270	107.4	72.2	102.4	64.0	113.6	58.8	41.4	60.8	94.7	98.4	32.7	46.1	30.6	59.8	70.0	95.6	48.2	77.2
Methyl octadecenoate	C ₁₉ H ₃₈ O ₂	298	12.7	6.2	8.8	11.0	15.6	4.6	8.0	13.6	14.5	10.5	5.4	3.5	7.5	8.0	9.4	9.8	10.7	5.4
Total			120.1	78.4	111.2	74.9	129.2	63.4	49.4	74.4	109.2	108.9	38.1	49.6	38.0	67.8	79.4	105.4	58.9	82.6

Total FA

Nonanoic acid	C ₉ H ₁₈ O ₂	158	67.9	27.5	5.6	37.0	17.5	2.7	36.9	65.2	30.3	4.9	4.8	1.9	0.5	4.7	34.2	20.1	56.2	3.8
Decanoic acid	C ₁₀ H ₂₀ O ₂	172	34.9	2.4	2.7	17.9	7.7	1.2	17.0	33.1	14.9	2.0	1.9	0.8	0.0	1.7	12.5	7.7	18.1	0.6

Undecanoic acid	C ₁₁ H ₂₂ O ₂	186	20.1	0.0	1.9	8.5	3.6	0.6	9.0	20.9	8.2	0.4	0.9	0.4	0.0	0.7	5.8	3.7	4.8	0.0
Dodecanoic acid	C ₁₂ H ₂₄ O ₂	200	45.5	23.7	3.7	15.5	7.1	1.9	18.1	45.2	18.3	1.7	1.9	1.1	0.0	1.8	13.6	8.4	10.0	1.7
Tridecanoic acid	C ₁₃ H ₂₆ O ₂	214	21.9	77.3	4.8	8.0	3.7	1.7	10.3	25.0	10.2	1.9	1.1	0.9	0.0	1.4	6.4	4.4	7.4	3.1
Tetradecanoic acid	C ₁₄ H ₂₈ O ₂	228	114.1	70.1	9.9	39.9	22.5	7.3	55.0	130.4	60.0	4.9	5.2	3.0	0.0	4.6	37.8	23.0	28.5	4.8
Pentadecanoic acid	C ₁₅ H ₃₀ O ₂	242	69.1	38.2	5.0	24.9	10.1	5.0	36.0	93.6	36.7	1.8	3.3	2.2	0.0	2.5	23.5	12.4	13.8	1.5
Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	256	1127.7	388.4	189.2	524.3	297.5	95.0	593.1	1424.3	708.0	124.2	108.4	75.6	33.6	109.7	516.9	340.9	329.9	104.0
Heptadecanoic acid	C ₁₇ H ₃₄ O ₂	270	27.1	4.7	1.5	8.6	3.0	0.4	13.5	39.0	14.0	0.4	1.3	0.6	0.0	0.7	8.7	4.5	7.3	0.3
Octadecanoic acid	C ₁₈ H ₃₆ O ₂	284	766.6	181.6	61.0	331.9	126.8	16.1	406.4	1081.4	451.0	24.0	59.8	22.4	8.8	37.0	318.1	173.0	180.3	19.8
Nonadecanoic acid	C ₁₉ H ₃₈ O ₂	298	7.2	11.0	4.7	0.2	0.4	3.1	0.6	3.3	0.6	0.6	0.0	0.1	0.3	0.1	0.1	0.1	0.9	0.8
Eicosanoic acid	C ₂₀ H ₄₀ O ₂	312	8.1	14.0	0.4	2.3	0.6	0.9	4.0	11.9	4.5	0.3	0.5	0.2	0.2	0.2	2.8	1.1	0.3	0.2
Total			2310.3	838.9	290.4	1018.9	500.4	135.9	1200.0	2973.2	1356.7	167.1	189.0	109.2	43.3	165.1	980.6	599.3	657.5	140.5
CPI(e/o)			9.8	4.3	11.4	10.7	12.1	9.1	10.3	11.0	12.6	15.7	15.7	16.7	57.7	15.5	11.4	12.2	6.3	13.8
Wax FA			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Algal FA																				
Total			2097.0	680.2	267.0	931.8	462.1	122.5	1093.7	2726.3	1256.7	157.1	177.7	103.0	42.6	155.1	901.7	554.0	567.1	131.0
%			90.8%	81.1%	91.9%	91.4%	92.3%	90.1%	91.1%	91.7%	92.6%	94.0%	94.0%	94.3%	98.3%	93.9%	92.0%	92.4%	86.2%	93.2%
Microbial FA																				
Total			213.32	158.69	23.40	87.12	38.31	13.42	106.30	246.98	100.00	10.00	11.33	6.17	0.74	10.01	78.86	45.26	90.41	9.49
%			9.2%	18.9%	8.1%	8.6%	7.7%	9.9%	8.9%	8.3%	7.4%	6.0%	6.0%	5.7%	1.7%	6.1%	8.0%	7.6%	13.8%	6.8%
n-Alkanols																				
Methyl unodcanoate	C ₁₂ H ₂₆ O	214	34.5	16.5	81.7	9.2	8.7	27.6	9.6	6.6	11.6	4.7	6.2	4.2	0.0	11.6	77.7	18.2	9.7	5.1
Dodecanol	C ₁₃ H ₂₈ O	228	10.4	5.3	19.4	2.7	2.9	1.5	1.4	2.0	1.7	2.4	0.2	0.9	0.0	1.5	5.2	4.8	0.0	2.0
Tetradecanol	C ₁₄ H ₃₀ O	242	82.8	32.0	52.9	34.9	29.5	32.0	8.9	16.6	17.1	18.4	4.7	6.1	0.0	9.5	31.7	20.5	9.9	17.9
Pentadecanol	C ₁₅ H ₃₂ O	256	44.0	12.8	32.0	29.5	33.6	32.1	6.3	18.5	16.2	16.6	3.0	4.8	0.0	0.8	6.1	17.4	5.4	15.2
Hexadecanol	C ₁₆ H ₃₄ O	242	177.8	43.8	70.7	80.0	112.4	104.9	26.0	51.3	59.5	63.9	9.0	12.9	0.6	25.6	26.7	63.7	22.6	66.8
Heptadecanol	C ₁₇ H ₃₆ O	256	19.9	3.0	10.0	13.2	22.0	20.9	4.9	10.1	13.2	10.4	0.0	1.4	0.0	4.1	4.0	9.9	0.7	9.8
Octadecanol	C ₁₈ H ₃₈ O	270	44.6	58.8	71.9	19.4	44.1	25.1	16.0	22.1	52.3	34.8	18.4	26.0	8.7	52.6	44.0	41.0	50.1	23.4
Nonadecanol	C ₁₉ H ₄₀ O	284	1.2	1.8	2.4	0.7	2.2	0.8	0.9	1.6	2.9	1.5	0.0	0.7	0.0	0.4	4.5	0.1	0.0	1.9
Eicosanol	C ₂₀ H ₄₂ O	298	17.6	5.1	10.0	2.6	6.0	4.3	2.9	2.8	4.8	5.1	0.0	0.3	0.0	1.3	3.1	2.0	1.0	3.4
Heneicosanol	C ₂₁ H ₄₄ O	308	1.0	4.9	8.8	2.0	1.7	0.9	1.3	0.7	1.8	2.7	0.0	0.2	6.9	0.3	0.2	1.2	0.3	1.9
Docosanol	C ₂₂ H ₄₆ O	326	12.9	0.8	81.4	6.3	18.9	16.9	8.2	10.6	20.0	15.9	10.2	12.2	0.0	47.8	21.5	12.7	23.4	20.8
Triacosanol	C ₂₃ H ₄₈ O	340	2.7	4.8	18.0	0.0	5.1	1.0	0.6	0.2	3.7	2.9	0.0	0.0	9.9	0.0	0.0	0.0	0.0	2.8
Tetracosanol	C ₂₄ H ₅₀ O	354	12.0	0.1	61.4	10.1	19.9	6.1	5.4	21.6	10.6	11.4	8.1	8.4	0.0	40.0	33.5	2.7	2.4	46.5

Pentacosanol	C ₂₅ H ₅₂ O	368	1.0	1.5	13.0	0.0	0.7	0.0	0.0	0.0	0.1	1.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.6
Hexacosanol	C ₂₆ H ₅₄ O	382	4.7	8.3	39.0	0.6	4.0	0.5	1.0	0.6	4.7	7.6	0.0	0.0	0.0	0.0	0.0	1.2	0.0	5.3
Heptacosanol	C ₂₇ H ₅₆ O	396	0.3	0.0	10.4	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.0	0.0	1.2	0.0	0.0	0.0	0.0	1.0
Octacosanol	C ₂₈ H ₅₈ O	410	15.7	18.6	76.6	1.4	6.6	1.2	2.9	2.2	8.1	20.8	0.0	0.0	0	0.0	0.2	2.7	0.0	14.5
Total			483.1	218.2	659.4	212.7	318.3	276.0	96.5	167.4	228.3	220.7	59.8	77.9	27.2	195.4	258.5	198.2	125.3	239.7
CPI(e/o)			4.6	4.9	4.1	3.2	3.5	3.3	4.6	3.9	4.5	4.7	15.7	8.2	0.5	24.8	8.0	4.4	16.9	5.5

Wax inputs

Total			45.2	27.9	258.2	18.4	49.4	24.7	17.6	34.9	43.5	55.7	18.3	20.6	0.0	87.8	55.2	19.3	25.8	87.1
%			9.4%	12.8%	39.2%	8.6%	15.5%	9.0%	18.2%	20.9%	19.0%	25.3%	30.6%	26.4%	0.0%	44.9%	21.4%	9.8%	20.6%	36.3%

Algal inputs

Total			357.3	156.1	287.2	146.2	200.7	194.0	63.5	99.4	145.4	127.0	38.3	49.4	9.3	100.5	183.2	145.4	93.1	116.5
%			74.0%	71.5%	43.5%	68.7%	63.1%	70.3%	65.8%	59.4%	63.7%	57.5%	64.0%	63.4%	34.1%	51.5%	70.9%	73.4%	74.3%	48.6%
Terr/Aquatic			0.13	0.18	0.90	0.13	0.25	0.13	0.28	0.35	0.30	0.44	0.48	0.42	0.00	0.87	0.30	0.13	0.28	0.75

Microbial inputs

Total			75.5	23.0	63.8	46.1	60.7	55.3	13.4	32.2	34.0	31.0	3.2	7.8	0.0	6.8	19.9	32.2	6.2	28.8
%			15.6%	10.5%	9.7%	21.7%	19.1%	20.0%	13.9%	19.2%	14.9%	14.0%	5.4%	10.0%	0.0%	3.5%	7.7%	16.3%	4.9%	12.0%

Plasticizers/Antioxidants

Diethyl phthalate	C ₁₂ H ₁₄ O ₄	222	5.4	3.6	7.8	7.3	5.7	3.7	3.3	3.1	2.9	7.5	2.1	2.3	2.8	5.8	4.1	7.0	5.1	5.7
Di-isobutyl phthalate	C ₁₆ H ₂₂ O ₄	278	61.5	67.1	120.2	68.8	76.2	43.0	31.1	43.5	50.7	68.2	21.4	43.4	10.5	59.6	67.4	59.9	51.0	64.9
Dibutyl phthalate	C ₁₆ H ₂₂ O ₄	278	175.5	132.2	185.2	41.4	119.5	47.0	38.8	78.9	100.1	117.8	26.0	61.4	24.9	54.5	74.7	78.6	47.6	76.8
Di(2-ethylhexyl) phthalate (DEHP)	C ₂₄ H ₃₈ O ₄	390	3.1	1.3	8.1	2.3	2.5	3.1	1.9	1.2	2.7	2.9	2.0	1.3	0.5	3.2	1.7	3.8	5.3	2.0
Total			245.5	204.2	321.3	119.8	203.8	96.8	75.0	126.7	156.5	196.4	51.5	108.4	38.7	123.2	147.9	149.2	109.1	149.4
%																				

Station #			29	30	31	32	34	36	37	38	40	41	42	43	45					
TEOM (ng/g)			4463	3701	1180	8753	8349	8825	23446	10583	2396	10283	14010	44747	2515	Min	Max	Avg	SD	
Compound (ng/g)	Composition	M.W.																		

n-Alkanes

Pentadecane	C ₁₅ H ₃₂	212	0.2	0.2	0.0	1.9	0.5	0.4	2.0	0.0	0.5	0.4	1.7	7.4	0.7					
Hexadecane	C ₁₆ H ₃₄	226	2.1	5.1	0.9	6.6	2.1	18.9	14.0	0.0	1.9	1.7	7.5	29.0	1.8					
Heptadecane	C ₁₇ H ₃₆	240	11.2	18.9	27.6	36.8	10.0	383.8	56.3	0.0	20.6	7.2	21.0	120.8	10.4					
Pristane	C ₁₉ H ₄₀ (Pr)	268	1.3	0.5	0.8	1.3	0.7	6.6	1.6	0.0	0.8	0.8	1.1	8.2	0.4					

Octadecane	C ₁₈ H ₃₈	256	18.7	24.4	6.7	17.1	5.4	207.2	29.2	0.0	15.0	8.1	19.1	70.7	6.5				
Phytane	C ₂₀ H ₄₂ (PH ₇)	282	4.8	2.4	2.0	1.9	0.7	95.5	13.9	0.0	3.2	2.4	7.7	68.6	3.0				
Nonadecane	C ₁₉ H ₄₀	268	4.9	3.1	5.4	2.0	2.7	95.7	9.3	0.0	23.2	2.9	1.9	11.8	0.0				
Eicosane	C ₂₀ H ₄₂	282	22.6	22.6	8.6	30.5	12.3	33.2	46.7	0.0	16.0	19.3	15.2	78.2	5.7				
Heneicosane	C ₂₁ H ₄₄	296	10.5	10.4	5.7	16.6	5.5	188.7	12.2	0.0	13.8	5.5	7.2	218.9	5.4				
Docosane	C ₂₂ H ₄₆	310	13.4	14.5	7.3	20.9	7.8	183.8	11.3	0.0	8.5	8.2	11.1	36.0	5.1				
Tricosane	C ₂₃ H ₄₈	324	12.0	11.4	11.0	18.4	8.4	162.5	9.1	0.0	8.5	7.2	9.9	42.1	6.7				
Tetracosane	C ₂₄ H ₅₀	338	11.3	11.7	5.6	15.9	10.9	151.6	7.1	0.0	7.5	7.3	6.9	27.2	6.4				
Pentacosane	C ₂₅ H ₅₂	352	11.7	9.6	15.5	13.6	11.2	432.4	28.1	0.0	11.0	7.0	5.8	191.3	10.9				
Hexacosane	C ₂₆ H ₅₄	366	8.0	8.2	3.7	10.0	11.6	92.3	4.9	0.0	6.0	5.7	5.0	18.2	7.2				
Heptacosane	C ₂₇ H ₅₆	380	10.4	13.0	15.9	9.1	10.5	103.0	9.2	0.0	9.6	5.6	10.3	63.0	11.3				
Octacosane	C ₂₈ H ₅₈	394	5.7	6.6	2.5	6.2	7.7	46.6	4.1	0.0	3.9	3.5	3.0	10.4	4.4				
Nonacosane	C ₂₉ H ₆₀	408	6.8	10.9	7.0	5.7	5.9	68.1	8.4	0.0	7.3	3.2	5.5	26.8	7.6				
Triacontane	C ₃₀ H ₆₂	422	2.9	3.8	1.2	3.5	3.1	16.6	1.7	0.0	2.7	2.1	1.1	4.4	2.3				
Hentriacontane	C ₃₁ H ₆₄	436	5.2	10.4	5.3	3.4	2.8	41.6	9.4	0.0	8.4	1.0	3.0	10.8	5.0				
Dotriacontane	C ₃₂ H ₆₆	450	0.9	1.5	0.3	0.7	0.9	9.7	1.1	0.0	1.0	0.5	0.3	1.6	0.6				
Tritriacontane	C ₃₃ H ₆₈	464	2.5	3.2	2.3	0.1	0.4	0.0	4.2	0.0	2.5	0.2	0.0	2.7	1.7				
Tetraatriacontane	C ₃₄ H ₇₀	478	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
Pentatriacontane	C ₃₅ H ₇₂	492	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
Hexatriacontane	C ₃₆ H ₇₄	506	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
Heptatriacontane	C ₃₇ H ₇₆	520	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
Total			167.1	192.0	135.4	222.2	121.3	2338.2	283.9	0.0	171.8	100.0	144.3	1048.2	102.8	0.0	2338.2	302.6	446.7
CPI(o/e)			0.9	0.9	2.6	1.0	0.9	1.9	1.2	0.0	1.7	0.7	1.0	2.5	1.5	0.0	2.7	1.2	0.6
LMW/HMW			2.0	1.8	1.5	3.1	1.2	1.8	2.7	0.0	2.2	2.3	3.0	1.9	0.9	0.0	4.2	2.0	0.9
TAR			0.9	1.2	0.8	0.3	1.1	0.3	0.4	0.0	0.5	0.6	0.6	0.3	1.5	0.0	3.0	0.8	0.6
Wax n-alkanes																			
Total			11.4	21.4	24.7	3.4	2.2	98.5	21.8	0.0	17.3	1.1	12.0	77.8	14.7	0.0	137.7	25.3	36.5
%			0.1	0.1	0.2	0.0	0.0	0.0	0.1	0.0	0.1	0.0	0.1	0.1	0.1	0.0	0.3	0.1	0.1
Algal n-Alkanes																			
Total			16.4	17.8	35.0	45.4	15.0	555.6	58.2	0.0	49.6	11.2	18.5	309.1	12.4	0.0	555.6	58.6	109.9
%			0.1	0.1	0.3	0.2	0.1	0.2	0.2	0.0	0.3	0.1	0.1	0.3	0.1	0.0	0.3	0.2	0.1
Bacterial n-Alkanes																			
Total			43.5	52.1	16.2	54.2	19.8	259.3	89.9	0.0	32.9	29.1	41.9	177.9	14.0	0.0	259.3	51.3	55.6
%			0.3	0.3	0.1	0.2	0.2	0.1	0.3	0.0	0.2	0.3	0.3	0.2	0.1	0.0	0.3	0.2	0.1

14a,17ba-20R-Ergostane	C ₂₈ H ₅₀	386	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
14a,17ba-20S-Stigmastane	C ₂₉ H ₅₂	400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
14b,17b-20R-Stigmastane	C ₂₉ H ₅₂	400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
14b,17b-20S-Stigmastane	C ₂₉ H ₅₂	400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
14a,17ba-20R-Stigmastane	C ₂₉ H ₅₂	400	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
Total			0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
PAHs																			
Phenanthrene	C ₁₄ H ₁₀	178	0.0	0.1	0.0	0.4	0.0	0.0	0.0	0.0	0.1	0.2	0.1	5.8	0.0				
Anthracene	C ₁₄ H ₁₀	178	2.8	0.6	0.0	8.0	0.0	0.0	0.0	0.6	7.0	2.1	20.6	0.0					
Benzo[k]fluoranthene	C ₂₀ H ₁₂	252	20.1	22.2	0.0	30.6	15.0	15.0	110.2	32.8	0.0	35.0	40.6	313.2	0.0				
Benzo[b]fluoranthene	C ₂₀ H ₁₂	252	14.0	15.1	0.0	21.2	9.3	10.4	66.0	21.7	0.0	19.4	23.9	205.7	0.0				
Total			36.9	37.9	0.0	60.3	24.4	25.4	176.2	54.5	0.6	61.5	66.8	545.4	0.0	0.0	545.4	54.5	96.8
Ant/(Ant+Phe)			1.0	0.9	0.0	0.9	0.0	0.0	0.0	0.0	0.9	1.0	1.0	0.8	0.0	0.0	1.0	0.7	0.4
Methyl n-Alkanoates																			
Methyl hexadecanoate	C ₁₇ H ₃₄ O ₂	270	73.2	42.2	27.8	65.6	64.3	80.3	114.9	58.2	44.1	60.7	78.5	147.7	50.0				
Methyl octadecenoate	C ₁₉ H ₃₈ O ₂	298	6.1	3.3	1.2	8.0	13.6	22.3	15.3	5.1	8.7	8.1	9.7	11.6	4.7				
Total			79.3	45.5	29.1	73.6	77.9	102.6	130.2	63.3	52.8	68.8	88.1	159.3	54.7				
Total FA																			
Nonanoic acid	C ₉ H ₁₈ O ₂	158	12.7	1.8	13.7	6.9	45.5	2.3	85.7	26.1	0.0	23.7	8.9	79.4	37.6				
Decanoic acid	C ₁₀ H ₂₀ O ₂	172	4.4	0.6	4.7	2.5	19.8	1.1	44.4	11.1	0.0	9.1	3.0	38.4	14.4				
Undecanoic acid	C ₁₁ H ₂₂ O ₂	186	1.9	0.1	2.7	1.0	9.7	0.0	25.0	5.4	0.0	4.1	0.8	18.3	7.1				
Dodecanoic acid	C ₁₂ H ₂₄ O ₂	200	4.3	1.2	5.5	1.8	21.2	0.1	56.5	11.6	0.0	8.8	1.6	38.0	13.2				
Tridecanoic acid	C ₁₃ H ₂₆ O ₂	214	2.7	1.5	2.8	1.7	10.2	0.1	30.8	6.3	0.0	5.0	2.2	19.5	5.6				
Tetradecanoic acid	C ₁₄ H ₂₈ O ₂	228	10.7	2.2	15.1	4.6	59.0	3.0	150.2	32.2	0.2	28.4	3.4	85.4	28.9				
Pentadecanoic acid	C ₁₅ H ₃₀ O ₂	242	6.3	1.7	9.5	2.0	36.7	0.1	93.6	20.2	0.1	17.3	1.1	44.1	17.1				
Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	256	201.3	61.8	236.3	97.2	712.2	88.3	1434.9	425.4	47.3	369.2	100.9	756.2	375.0				
Heptadecanoic acid	C ₁₇ H ₃₄ O ₂	270	2.5	0.1	3.4	0.4	12.5	0.3	34.8	8.0	0.1	6.6	0.2	15.9	5.4				
Octadecanoic acid	C ₁₈ H ₃₆ O ₂	284	91.2	14.3	145.8	25.7	484.5	26.4	969.2	260.3	10.3	211.5	22.3	395.0	241.5				
Nonadecanoic acid	C ₁₉ H ₃₈ O ₂	298	0.2	0.1	1.7	0.3	0.2	0.7	4.2	0.6	0.7	0.4	0.1	8.7	1.7				
Eicosanoic acid	C ₂₀ H ₄₀ O ₂	312	0.4	0.1	1.1	0.4	3.9	0.1	13.9	2.3	0.0	1.7	0.2	5.1	1.5				
Total			338.6	85.5	442.1	144.4	1415.4	122.4	2943.1	809.5	58.6	685.9	144.6	1504.0	749.0	43.3	2973.2	745.8	799.6
CPI(e/o)			11.9	15.0	12.1	10.8	11.3	33.5	9.7	11.1	66.8	11.0	9.8	7.1	9.1	4.3	66.8	15.3	13.5
Wax FA			0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0				

Algal FA

Total	312.4	80.2	408.4	132.2	1300.6	118.9	2669.1	742.9	57.7	628.7	131.2	1318.2	674.5	42.6	2726.3	677.5	726.6
%	0.9	0.9	0.9	0.9	0.9	1.0	0.9	0.9	1.0	0.9	0.9	0.9	0.9	0.8	1.0	0.9	0.0

Microbial FA

Total	26.2	5.4	33.7	12.2	114.7	3.5	274.1	66.7	0.9	57.2	13.4	185.8	74.5	0.7	274.1	68.3	76.0
%	0.1	0.1	0.1	0.1	0.1	0.0	0.1	0.1	0.0	0.1	0.1	0.1	0.1	0.0	0.2	0.1	0.0

n-Alkanols

Methyl unodecanoate	C ₁₂ H ₂₆ O	214	18.2	17.2	2.0	7.8	22.6	11.4	841.4	9.0	10.6	5.1	20.4	188.2	8.0			
Dodecanol	C ₁₃ H ₂₈ O	228	3.9	4.5	0.0	3.0	1.9	1.0	181.0	2.4	0.0	0.6	5.4	64.6	1.5			
Tetradecanol	C ₁₄ H ₃₀ O	242	14.3	13.9	2.8	18.9	9.6	12.9	511.7	9.3	12.3	5.8	14.5	197.6	10.4			
Pentadecanol	C ₁₅ H ₃₂ O	256	5.5	8.1	2.7	20.4	6.5	10.6	358.0	8.8	7.7	5.3	8.1	279.2	9.5			
Hexadecanol	C ₁₆ H ₃₄ O	242	29.5	19.6	10.6	59.5	17.5	54.7	698.7	22.2	28.3	19.5	32.2	505.6	29.2			
Heptadecanol	C ₁₇ H ₃₆ O	256	3.5	4.2	1.4	11.4	2.8	4.6	155.4	4.7	3.8	4.8	4.1	186.8	4.2			
Octadecanol	C ₁₈ H ₃₈ O	270	26.5	45.1	9.6	24.8	18.9	28.7	614.5	33.9	18.8	25.9	25.1	428.9	13.4			
Nonadecanol	C ₁₉ H ₄₀ O	284	0.1	1.8	0.0	0.5	0.9	0.6	101.9	0.7	0.4	1.8	1.7	15.1	0.2			
Eicosanol	C ₂₀ H ₄₂ O	298	3.6	10.2	5.4	3.0	3.5	3.3	78.0	3.7	5.0	2.8	1.5	204.8	5.9			
Heneicosanol	C ₂₁ H ₄₄ O	308	0.6	3.0	4.4	1.9	3.2	1.1	71.8	3.5	4.8	2.3	2.7	38.0	8.2			
Docosanol	C ₂₂ H ₄₆ O	326	22.3	82.0	2.9	12.2	2.9	9.2	725.6	18.5	37.2	9.7	18.7	352.7	3.7			
Triacosanol	C ₂₃ H ₄₈ O	340	2.3	4.1	0.8	3.7	0.0	0.0	43.2	0.1	2.3	0.0	0.2	55.6	0.0			
Tetracosanol	C ₂₄ H ₅₀ O	354	11.4	12.9	4.2	21.9	4.3	15.0	1011.3	0.3	14.8	18.4	4.9	65.6	1.7			
Pentacosanol	C ₂₅ H ₅₂ O	368	0.0	0.0	0.0	0.2	0.0	0.0	12.6	0.0	0.3	0.0	0.0	25.4	0.0			
Hexacosanol	C ₂₆ H ₅₄ O	382	2.2	6.8	2.7	2.9	0.0	0.3	59.8	0.6	7.9	0.0	1.9	126.6	0.5			
Heptacosanol	C ₂₇ H ₅₆ O	396	0.0	0.3	0.0	0.0	0.0	0.0	4.0	0.0	0.7	0.0	0.0	16.9	0.0			
Octacosanol	C ₂₈ H ₅₈ O	410	5.5	12.5	7.0	4.1	0.5	3.6	138.7	1.6	13.5	1.1	3.0	223.5	0.4			
Total		149.2	246.1	56.5	196.1	95.3	156.9	5607.5	119.4	168.3	103.4	144.3	2975.3	97.0	27.2	5607.5	457.4	1085.6
CPI(e/o)		7.3	7.8	4.9	3.6	3.7	7.1	4.1	4.5	6.9	5.6	4.6	3.1	2.8	0.5	24.8	6.2	4.8

Wax inputs

Total	41.3	114.1	16.8	41.2	7.7	28.0	1935.3	21.1	73.3	29.3	28.4	768.4	6.4	0.0	1935.3	129.1	362.6
%	0.3	0.5	0.3	0.2	0.1	0.2	0.3	0.2	0.4	0.3	0.2	0.3	0.1	0.0	0.5	0.2	0.1

Algal inputs

Total	92.0	106.0	30.4	113.9	72.2	111.0	2744.2	78.1	74.9	59.2	93.7	1525.1	66.9	9.3	2744.2	247.8	532.6
%	0.6	0.4	0.5	0.6	0.8	0.7	0.5	0.7	0.4	0.6	0.6	0.5	0.7	0.3	0.8	0.6	0.1

Terr/Aquatic	0.4	1.1	0.6	0.4	0.1	0.3	0.7	0.3	1.0	0.5	0.3	0.5	0.1	0.0	1.1	0.4	0.3
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Microbial inputs

Total	13.0	18.6	4.0	35.3	12.1	16.8	796.3	16.6	11.9	12.6	19.3	545.8	15.5	0.0	796.3	66.4	165.7
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%	0.1	0.1	0.1	0.2	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.0	0.2	0.1	0.1
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Plasticizers/Antioxidants

Diethyl phthalate	C ₁₂ H ₁₄ O ₄	222	5.2	2.4	2.8	5.2	1.8	4.2	11.1	5.6	2.6	18.8	7.0	22.7	3.8			
Di-isobutyl phthalate	C ₁₆ H ₂₂ O ₄	278	65.5	43.5	13.9	61.6	28.9	45.1	109.6	48.3	33.6	196.2	56.8	146.4	31.3			
Dibutyl phthalate	C ₁₆ H ₂₂ O ₄	278	65.2	70.0	17.9	77.9	76.0	96.2	698.7	59.3	25.9	167.6	99.5	505.6	67.9			
Di(2-ethylhexyl) phthalate (DEHP)	C ₂₄ H ₃₈ O ₄	390	2.3	3.1	0.3	1.9	1.7	1.3	3.3	1.8	74.9	8.1	5.0	15.4	1.2			
Total		138.2	119.0	34.9	146.6	108.4	146.8	822.7	115.0	137.0	390.8	168.3	690.1	104.3	34.9	822.7	185.3	169.9

Alwajh Lagoon

Concentration in ng/g

Compound	Composition	M.W.	Station #												
			14	21	48	60	72	79	87	98	100	104	116	128	129
n-Alkanes															
Tetradecane	C ₁₄ H ₃₀	198	0.6	0.4	0.1	0.2	0.1	0.4	0.0	0.1	0.2	0.2	0.1	0.1	0.5
Pentadecane	C ₁₅ H ₃₂	212	2.5	0.7	0.1	0.5	0.3	1.4	0.1	0.4	0.7	0.7	0.4	0.3	1.0
Hexadecane	C ₁₆ H ₃₄	226	32.8	9.4	1.4	6.8	4.3	16.8	3.9	7.8	8.3	9.2	7.4	6.3	12.6
Heptadecane	C ₁₇ H ₃₆	240	16.3	4.3	0.6	3.1	2.3	6.6	2.3	4.3	3.6	4.4	5.1	3.3	4.8
Pristane	C ₁₉ H ₄₀ (Pr)	268	1.1	0.3	0.0	0.3	0.1	0.2	0.0	0.5	0.1	0.4	0.5	0.1	0.2
Octadecane	C ₁₈ H ₃₈	256	45.3	13.6	2.0	8.3	7.9	23.3	9.0	11.4	10.4	11.3	12.2	11.5	14.9
Phytanes	C ₂₀ H ₄₂ (Ph)	282	7.4	1.9	0.2	0.7	0.7	2.2	0.8	0.9	1.0	1.0	1.4	1.0	1.1
Nonadecane	C ₁₉ H ₄₀	268	18.6	4.3	0.5	2.4	2.2	4.4	1.9	3.3	3.3	3.2	3.9	3.2	4.0
Eicosane	C ₂₀ H ₄₂	282	39.1	11.1	1.8	7.0	7.5	20.1	8.6	9.9	9.1	9.1	10.5	11.0	13.4
Heneicosane	C ₂₁ H ₄₄	296	35.4	7.2	1.2	4.2	0.2	1.8	3.6	0.2	0.4	0.2	5.2	0.4	8.4
Docosane	C ₂₂ H ₄₆	310	24.3	5.4	0.8	2.3	1.9	5.8	1.8	2.2	2.2	2.3	2.2	2.8	1.6
Tricosane	C ₂₃ H ₄₈	324	21.0	4.5	0.7	2.6	2.6	5.9	3.0	3.8	3.3	3.6	4.0	2.4	5.1
Tetracosane	C ₂₄ H ₅₀	338	12.8	4.9	0.4	1.4	1.7	5.1	1.9	2.1	2.1	2.0	2.4	2.3	3.1
Pentacosane	C ₂₅ H ₅₂	352	5.0	0.5	0.1	0.2	0.2	1.0	0.2	0.3	0.3	0.3	0.3	0.4	0.5
Hexacosane	C ₂₆ H ₅₄	366	7.1	1.8	0.2	0.9	1.0	3.2	1.1	1.3	1.1	1.2	1.4	1.3	1.8
Heptacosane	C ₂₇ H ₅₆	380	1.6	0.5	0.1	0.1	0.2	0.9	0.3	0.2	0.3	0.4	0.3	0.2	0.5
Octacosane	C ₂₈ H ₅₈	394	2.6	0.1	0.1	0.3	0.4	1.4	0.4	0.5	0.4	0.5	0.5	0.4	0.8
Nonacosane	C ₂₉ H ₆₀	408	1.5	0.2	0.0	0.0	0.1	0.5	0.0	0.3	0.2	0.1	0.1	0.0	0.2

Triacontane	C ₃₀ H ₆₂	422	1.2	0.7	0.1	0.2	0.2	0.9	0.3	0.3	0.3	0.3	0.3	0.3	0.5	
Hentriacontane	C ₃₁ H ₆₄	436	1.6	0.1	0.1	0.3	0.3	1.4	0.3	0.4	0.3	0.5	0.4	0.4	0.8	
Dotriacontane	C ₃₂ H ₆₆	450	0.1	0.0	0.0	0.0	0.0	0.3	0.0	0.1	0.1	0.2	0.1	0.1	0.2	
Tritriacontane	C ₃₃ H ₆₈	464	0.2	0.0	0.0	0.1	0.0	0.4	0.0	0.1	0.1	0.1	0.0	0.1	0.1	
Total			278.2	71.7	10.5	42.0	34.2	104.0	39.7	50.2	47.7	51.2	59.0	48.0	76.2	
CPI(o/e)			0.6	0.5	0.5	0.5	0.3	0.3	0.4	0.4	0.4	0.4	0.5	0.3	0.5	
LMW/HMW			11.7	16.7	14.9	17.1	12.1	9.1	12.9	13.3	13.7	12.8	15.3	13.4	12.2	
TAR			0.11	0.06	0.07	0.06	0.12	0.21	0.08	0.10	0.10	0.11	0.06	0.11	0.09	
Wax n-alkanes																
Total			4.2	0.8	0.1	0.5	0.6	2.5	0.5	0.7	0.6	0.7	0.6	0.4	1.1	
%			1.5%	1.1%	1.1%	1.1%	1.7%	2.4%	1.3%	1.4%	1.2%	1.4%	1.1%	0.8%	1.4%	
Algal n-Alkanes																
Total			72.8	16.5	2.4	10.2	4.9	14.1	7.9	8.2	8.0	8.5	14.7	7.2	18.3	
%			26%	23%	23%	24%	14%	14%	20%	16%	17%	17%	25%	15%	24%	
Bacterial n-Alkanes																
Total			95.9	28.5	4.5	18.4	17.0	51.9	18.7	24.2	23.3	24.4	24.1	24.9	35.0	
%			34.5%	39.7%	42.7%	43.8%	49.7%	49.9%	47.3%	48.1%	48.9%	47.7%	40.9%	51.9%	45.9%	
Petroleum n-alkanes																
Total			105.3	26.0	3.5	13.0	11.8	35.4	12.5	17.2	15.8	17.6	19.5	15.5	21.9	
%			37.8%	36.3%	32.9%	30.9%	34.4%	34.1%	31.5%	34.2%	33.2%	34.3%	33.1%	32.2%	28.7%	
Hopanes																
Trisnorneohopane	C ₂₇ H ₄₆	370	0.54	0.14	T	T	T	T	T	T	0.09	0.04	0.00	0.01	0.51	
17a(H)-Trisnorhopane	C ₂₇ H ₄₆	370	0.91	0.03	T	T	T	T	T	T	0.06	0.05	0.00	0.01	0.43	
17a(H),21b(H)-Norhopane	C ₂₉ H ₅₀	398	2.22	0.30	T	T	T	T	T	T	0.37	0.15	0.02	0.04	2.51	
17a(H),21b(H)-Hopane	C ₃₀ H ₅₂	412	1.90	0.33	T	T	T	T	T	T	0.33	0.16	0.02	0.05	2.63	
17a(H),21b(H)-22S-Homohopane	C ₃₁ H ₅₄	426	0.70	0.12	T	T	T	T	T	T	0.14	0.06	0.00	0.01	0.93	
17a(H),21b(H)-22R-Homohopane	C ₃₁ H ₅₄	426	0.52	0.07	T	T	T	T	T	T	0.08	0.03	0.00	0.01	0.66	
Gammacerane	C ₃₀ H ₅₂	412	0.07	0.01	T	T	T	T	T	T	0.01	0.02	0.00	0.00	0.08	
17a(H),21b(H)-22S-Bishomohopane	C ₃₂ H ₅₆	440	0.58	0.10	T	T	T	T	T	T	0.08	0.04	0.00	0.01	0.79	
17a(H),21b(H)-22R-Bishomohopane	C ₃₂ H ₅₆	440	0.23	0.05	T	T	T	T	T	T	0.06	0.03	0.00	0.00	0.31	
17a(H),21b(H)-22S-Trishomohopane	C ₃₃ H ₅₈	454	0.31	0.03	T	T	T	T	T	T	0.05	T	T	T	0.32	
17a(H),21b(H)-22R-Trishomohopane	C ₃₃ H ₅₈	454	0.22	0.01	T	T	T	T	T	T	0.03	T	T	T	0.20	
17a(H),21b(H)-22S-Tetrakishomohopane	C ₃₄ H ₆₀	468	0.13	0.00	T	T	T	T	T	T	0.03	T	0.22	0.00	0.04	

17a(H),21b(H)-22R-Tetrakishomohopane	C ₃₄ H ₆₀	468	0.03	0.00	T	T	T	T	T	T	0.02	T	T	T	0.03
17a(H),21b(H)-22S-Pentakishomohopane	C ₃₅ H ₆₂	482	0.00	0.00	T	T	T	T	T	T	0.00	T	T	T	T
17a(H),21b(H)-22R-Pentakishomohopane	C ₃₅ H ₆₂	482	0.00	0.00	T	T	T	T	T	T	0.00	T	T	T	T
Total			8.34	1.19	0.00	0.00	0.00	0.00	0.00	0.00	1.35	0.58	0.26	0.13	9.47
C ₃₁ S/(R+S)			0.57	0.62	ND	ND	ND	ND	ND	ND	0.64	0.63	0.46	0.58	0.59
C ₃₂ S/(R+S)			0.71	0.69	ND	ND	ND	ND	ND	ND	0.58	0.54	0.58	0.66	0.72

Steranes

13b,17a-20S-Cholestane Diasterane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T	T	T
13b,17a-20R-Cholestane Diasterane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T	T	T
13a,17b-20S-Cholestane Diasterane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T	T	T
13a,17b-20R-Cholestane Diasterane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20S-Cholestane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20R-Cholestane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20S-Cholestane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20R-Cholestane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20S-Ergostane	C ₂₈ H ₅₀	386	T	T	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20R-Ergostane	C ₂₈ H ₅₀	386	T	T	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20S-Ergostane	C ₂₈ H ₅₀	386	T	T	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20R-Ergostane	C ₂₈ H ₅₀	386	T	T	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20S-Stigmastane	C ₂₉ H ₅₂	400	T	T	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20R-Stigmastane	C ₂₉ H ₅₂	400	T	T	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20S-Stigmastane	C ₂₉ H ₅₂	400	T	T	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20R-Stigmastane	C ₂₉ H ₅₂	400	T	T	T	T	T	T	T	T	T	T	T	T	T
Total															

PAHs

Phenanthrene	C ₁₄ H ₁₀	178	17.1	2.3	1.1	0.4	0.9	1.0	1.8	8.9	1.1	0.0	1.0	2.6	3.1
Anthracene	C ₁₄ H ₁₀	178	20.9	2.4	0.9	0.2	1.6	0.2	1.4	6.7	1.5	0.0	1.5	5.4	6.6
Benzo[k]fluoranthene	C ₂₀ H ₁₂	252	T	T	T	0.1	T	0.2	T	T	0.6	T	T	0.7	0.5
Benzo[b]fluoranthene	C ₂₀ H ₁₂	252	T	T	T	0.0	T	0.0	T	T	0.3	T	T	0.3	0.4
Total			38.0	4.7	2.0	0.8	2.5	1.4	3.2	15.6	3.5	0.0	2.5	8.9	10.6
Ant/(Ant+Phe)			0.6	0.5	0.5	0.4	0.7	0.2	0.4	0.4	0.6	0.0	0.6	0.7	0.7

Methyl alkanoates

Methyl octanoate	C ₉ H ₁₈ O ₂	158	2.12	0.02	0.05	0.03	0.05	0.00	0.03	0.13	0.00	0.00	0.07	0.03	0.02
Methyl nonanoate	C ₁₀ H ₂₀ O ₂	172	1.35	0.05	0.09	0.04	0.05	0.02	0.03	0.21	0.00	0.00	0.07	0.06	0.06
Methyl decanoate	C ₁₁ H ₂₂ O ₂	186	0.41	0.02	0.04	0.02	0.02	0.02	0.01	0.08	0.00	0.00	0.02	0.04	0.02
Methyl undecanoate	C ₁₂ H ₂₄ O ₂	200	0.59	0.03	0.04	0.03	0.03	0.04	0.01	0.12	0.01	0.00	0.03	0.06	0.04
Methyl dodecanoate	C ₁₃ H ₂₆ O ₂	214	1.43	0.12	0.10	0.09	0.07	0.51	0.05	0.49	0.06	0.01	0.13	0.10	0.09
Methyl tridecanoate	C ₁₄ H ₂₈ O ₂	228	1.34	0.22	0.10	0.13	0.10	0.49	0.11	0.60	0.09	0.02	0.07	0.18	0.31
Methyl tetradecanoate	C ₁₅ H ₃₀ O ₂	242	4.79	0.63	0.34	0.44	0.30	1.33	0.39	2.18	0.34	0.07	0.50	0.65	0.71
Methyl pentadecanoate	C ₁₆ H ₃₂ O ₂	256	2.68	0.27	0.19	0.29	0.20	0.58	0.23	1.18	0.13	0.03	0.27	0.30	0.29
Methyl hexadecanoate	C ₁₇ H ₃₄ O ₂	268	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01
Methyl hexadecanoate	C ₁₇ H ₃₄ O ₂	270	74.76	14.64	4.81	7.35	5.83	30.48	7.32	34.26	6.51	1.37	7.83	12.14	19.34
Methyl heptadecanoate	C ₁₈ H ₃₆ O ₂	282	1.09	0.10	0.11	0.10	0.07	0.33	0.15	0.54	0.04	0.01	0.10	0.12	0.21
Methyl octadecanoate	C ₁₉ H ₃₈ O ₂	296	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
Methyl octadecanoate	C ₁₉ H ₃₈ O ₂	298	43.08	5.46	5.98	5.54	3.83	8.96	6.00	27.80	2.47	0.52	3.73	4.56	3.86
Methyl nonadecanoate	C ₂₀ H ₄₀ O ₂	312	3.32	0.04	0.04	0.05	0.04	0.16	0.05	0.23	0.06	0.01	0.05	0.12	0.32
Total			136.95	21.52	11.71	14.04	10.48	42.89	14.31	67.43	9.72	2.04	12.71	18.25	25.19

CPI(e/o)**Total FA**

Pentanoic acid	C ₅ H ₁₀ O ₂	102	0.01	0.01	0.00	0.00	0.00	1.55	0.16	0.05	0.21	0.00	0.02	0.43	1.60
Hexanoic acid	C ₆ H ₁₂ O ₂	116	0.05	0.04	0.00	0.00	0.00	5.26	0.60	0.07	0.78	0.00	0.01	2.24	4.23
Heptanoic acid	C ₇ H ₁₄ O ₂	130	0.12	0.45	0.00	0.00	0.00	4.59	0.56	0.16	0.87	0.00	0.01	2.53	3.63
Octanoic acid	C ₈ H ₁₆ O ₂	144	0.31	0.70	0.00	0.00	0.00	11.90	1.17	0.39	2.18	0.00	0.06	6.61	9.29
Nonanoic acid	C ₉ H ₁₈ O ₂	158	3.36	1.46	0.05	0.03	0.05	16.42	1.92	0.76	3.97	0.00	0.24	9.03	11.95
Dodanoic acid	C ₁₀ H ₂₀ O ₂	172	3.25	2.63	0.09	0.04	0.05	4.82	0.62	0.53	1.40	0.00	0.17	2.98	3.36
Undecanoic acid	C ₁₁ H ₂₂ O ₂	186	1.45	0.71	0.04	0.02	0.02	2.81	0.32	0.22	0.84	0.00	0.07	1.61	1.73
Dodecanoic acid	C ₁₂ H ₂₄ O ₂	200	0.93	0.32	0.04	0.03	0.03	4.38	0.53	0.37	1.32	0.00	0.04	2.64	2.50
Tridecanoic acid	C ₁₃ H ₂₆ O ₂	214	2.25	0.62	0.10	0.09	0.07	2.55	0.34	1.55	0.76	0.01	0.22	1.41	1.37
Tetradecanoic acid	C ₁₄ H ₂₈ O ₂	228	5.02	5.46	0.10	0.13	0.10	7.88	1.05	1.01	2.16	0.02	0.54	4.73	4.65
Pentadecanoic acid	C ₁₅ H ₃₀ O ₂	242	8.67	6.33	0.34	0.44	0.30	5.45	0.78	2.45	1.42	0.07	0.59	3.27	2.91
Hexadecenoic acid	C ₁₆ H ₃₀ O ₂	254	2.91	0.32	0.19	0.29	0.20	0.89	0.24	1.20	0.14	0.03	0.28	0.30	0.38
Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	256	7.76	0.86	0.00	0.00	0.00	55.77	8.38	3.52	20.36	0.00	1.24	39.92	39.00
Heptadecanoic acid	C ₁₇ H ₃₄ O ₂	270	75.55	24.47	4.81	7.35	5.83	31.75	7.41	34.33	6.83	1.37	7.85	13.14	19.35

Octadecenoic acid	C ₁₈ H ₃₄ O ₂	282	3.17	0.30	0.11	0.10	0.07	0.37	0.15	0.54	0.04	0.01	0.10	0.15	21.00
Octadecanoic acid	C ₁₈ H ₃₆ O ₂	284	5.90	0.80	0.00	0.00	0.00	36.77	2.81	1.49	9.61	0.00	0.37	25.47	0.17
Nonadecanoic acid	C ₁₉ H ₃₈ O ₂	298	43.08	5.51	5.98	5.54	3.83	10.57	6.24	27.92	2.56	0.52	3.73	5.17	3.97
Eicosanoic acid	C ₂₀ H ₄₀ O ₂	312	3.32	0.59	0.04	0.05	0.04	0.54	0.05	0.36	0.06	0.01	0.05	0.95	0.32
Heneicosanoic acid	C ₂₁ H ₄₂ O ₂	326	136.95	21.66	11.71	14.04	10.48	43.10	14.31	67.43	9.72	2.04	12.71	18.25	25.19
Total			304.03	73.25	23.60	28.15	21.08	247.37	47.63	144.37	65.22	4.08	28.30	140.82	156.61
CPI(e/o)			0.10	0.19	0.01	0.01	0.01	1.07	0.47	0.06	1.39	0.01	0.10	1.56	0.89
Wax FA			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Algal FA															
Total			32.6	12.0	0.6	0.6	0.5	128.6	15.6	9.5	38.1	0.1	2.9	86.0	84.9
%			10.7%	16.4%	2.4%	2.3%	2.3%	52.0%	32.7%	6.6%	58.3%	1.7%	10.1%	61.1%	54.2%
Microbial FA															
Total			134.35	39.10	11.31	13.47	10.10	69.55	17.01	67.23	16.38	1.97	12.70	33.63	41.27
%			44.2%	53.4%	47.9%	47.9%	47.9%	28.1%	35.7%	46.6%	25.1%	48.3%	44.9%	23.9%	26.4%
n-Alkanols															
Undecanol	C ₁₁ H ₂₄ O	172	1.20	0.21	0.04	0.13	0.08	0.41	0.06	0.25	0.21	0.06	0.15	0.55	0.44
Dodecanol	C ₁₂ H ₂₆ O	186	16.72	2.92	0.85	2.00	1.32	5.83	1.98	7.05	5.89	1.58	3.04	9.23	5.56
Tridecanol	C ₁₃ H ₂₈ O	200	6.40	1.10	0.31	0.80	0.45	1.85	0.85	2.18	1.33	0.42	1.33	1.79	0.97
Tetradecanol	C ₁₄ H ₃₀ O	214	20.26	3.56	1.45	2.69	1.93	5.98	3.10	8.29	3.99	1.70	5.67	6.35	2.24
Pentadecanol	C ₁₅ H ₃₂ O	228	8.92	1.16	0.67	2.51	0.99	3.54	2.29	4.19	1.76	0.80	2.77	2.38	1.30
Hexadecanol	C ₁₆ H ₃₄ O	242	40.55	5.43	2.63	5.77	3.36	8.92	4.50	8.99	3.37	2.22	8.40	6.85	2.66
Heptadecanol	C ₁₇ H ₃₆ O	256	10.15	1.11	0.75	1.91	0.86	3.02	1.42	3.01	0.85	0.61	2.61	1.85	0.79
Octadecanol	C ₁₈ H ₃₈ O	270	35.12	6.84	1.83	4.77	4.20	12.40	8.11	17.22	6.69	3.59	14.37	10.47	5.75
Nonadecanol	C ₁₉ H ₄₀ O	284	3.52	0.52	0.16	0.45	0.34	1.01	0.57	1.18	0.43	0.23	0.93	0.68	0.78
Eicosanol	C ₂₀ H ₄₂ O	298	5.80	0.98	0.30	0.87	0.62	3.00	1.20	2.13	0.73	1.42	2.44	2.72	0.72
Heneicosanol	C ₂₁ H ₄₄ O	312	1.73	0.33	0.10	0.21	0.17	0.46	0.49	0.86	0.35	0.13	0.63	2.45	1.02
Docosanol	C ₂₂ H ₄₆ O	326	6.14	1.32	0.68	5.89	1.74	0.88	12.69	19.87	0.94	3.13	10.13	14.04	7.84
Triacosanol	C ₂₃ H ₄₈ O	340	1.92	0.38	0.09	0.33	0.18	0.53	0.65	1.26	0.40	0.15	0.62	0.83	0.26
Tetracosanol	C ₂₄ H ₅₀ O	354	1.71	3.63	0.08	9.86	0.66	27.87	8.06	7.61	2.75	1.66	3.74	3.65	3.18
Pentacosanol	C ₂₅ H ₅₂ O	368	0.28	0.13	0.04	0.01	0.03	0.07	0.05	0.20	0.07	0.03	0.21	0.11	0.07
Hexacosanol	C ₂₆ H ₅₄ O	382	1.65	0.31	0.20	0.22	0.18	0.41	0.35	0.63	0.30	0.19	0.93	0.51	0.09
Total			162.06	29.93	10.18	38.41	17.11	76.16	46.37	84.93	30.05	17.92	57.97	64.45	33.66
CPI(e/o)			3.75	5.06	3.71	5.06	4.51	6.00	6.26	5.47	4.57	6.36	5.27	5.06	4.98

Wax inputs

Total	9.50	6.25	2.96	18.97	6.58	34.15	27.10	35.11	11.99	13.98	24.80	29.19	23.11
%	5.9%	20.9%	29.0%	49.4%	38.4%	44.8%	58.4%	41.3%	39.9%	78.0%	42.8%	45.3%	68.6%

Algal inputs

Total	118.44	19.73	7.06	16.10	11.43	36.13	18.89	43.69	20.66	10.50	33.92	35.62	16.92
%	73.1%	65.9%	69.4%	41.9%	66.8%	47.4%	40.7%	51.4%	68.8%	58.6%	58.5%	55.3%	50.3%
Terristrial/Aquatic	0.08	0.32	0.42	1.18	0.58	0.95	1.43	0.80	0.58	1.33	0.73	0.82	1.37

Microbial inputs

Total	28.98	3.88	1.90	5.67	2.64	9.42	5.13	10.56	4.37	2.07	7.65	6.70	3.84
%	17.9%	13.0%	18.6%	14.8%	15.5%	12.4%	11.1%	12.4%	14.5%	11.5%	13.2%	10.4%	11.4%

Plasticizers

Diethyl phthalate	C ₁₂ H ₁₄ O ₄	222	12.0	3.7	1.2	0.7	1.2	7.4	2.0	6.4	1.2	4.0	5.5	2.4	5.3
Di-isobutyl phthalate	C ₁₆ H ₂₂ O ₄	278	100.7	16.8	7.1	7.3	9.1	32.0	9.8	49.9	8.0	10.4	12.7	14.4	19.3
Dibutyl phthalate	C ₁₆ H ₂₂ O ₄	278	178.7	40.7	12.3	10.6	17.2	79.8	13.2	170.1	12.3	33.2	50.4	23.7	41.6
Di(2-ethylhexyl) phthalate	C ₂₄ H ₃₈ O ₄	390	20.9	3.1	1.0	0.3	1.1	15.6	3.1	8.9	1.2	2.0	2.1	2.9	2.3
Total		312.4	64.3	21.7	19.0	28.6	134.8	28.0	235.2	22.8	49.6	70.7	43.4	68.6	

Station #

Compound	Composition	M.W.	131	134	139	151	155	168	173	185	186	193	199
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n-Alkanes

Tetradecane	C ₁₄ H ₃₀	198	0.1	0.1	0.2	0.5	0.3	0.0	0.2	0.1	0.2	0.3	0.2
Pentadecane	C ₁₅ H ₃₂	212	0.3	1.1	0.7	1.0	0.9	0.3	0.5	0.5	1.0	0.7	0.6
Hexadecane	C ₁₆ H ₃₄	226	4.5	10.0	9.9	10.3	12.4	8.0	7.6	7.2	15.9	6.6	6.6
Heptadecane	C ₁₇ H ₃₆	240	2.1	5.2	3.9	4.1	6.5	4.0	4.0	3.6	7.2	2.8	3.4
Pristane	C ₁₉ H ₄₀ (Pr)	268	0.1	0.2	0.1	0.1	0.2	0.2	0.4	0.2	0.7	0.2	0.3
Octadecane	C ₁₈ H ₃₈	256	6.5	15.5	13.6	10.7	17.1	14.4	11.4	10.1	20.4	7.1	8.8
Phytanes	C ₂₀ H ₄₂ (Ph)	282	0.7	1.4	1.2	0.8	1.3	1.1	1.2	0.8	2.1	0.6	1.2
Nonadecane	C ₁₉ H ₄₀	268	3.0	4.0	3.2	0.7	4.1	3.5	3.0	2.9	5.4	2.0	2.9
Eicosane	C ₂₀ H ₄₂	282	5.8	14.1	12.1	9.6	15.6	13.5	10.2	9.5	16.9	6.0	7.8
Heneicosane	C ₂₁ H ₄₄	296	0.8	6.4	0.4	0.1	1.4	8.0	0.3	0.3	2.1	0.1	0.6
Docosane	C ₂₂ H ₄₆	310	3.0	3.0	2.5	2.3	3.8	2.7	2.2	2.2	3.9	1.4	1.9
Tricosane	C ₂₃ H ₄₈	324	1.9	4.7	4.4	2.9	4.2	5.1	3.8	1.8	5.8	1.4	1.8
Tetracosane	C ₂₄ H ₅₀	338	1.5	3.2	2.4	2.3	3.5	2.8	2.2	2.0	3.6	1.2	1.6

Pentacosane	C ₂₅ H ₅₂	352	0.3	0.5	0.3	1.9	0.7	0.4	0.4	0.4	0.4	0.2	0.3
Hexacosane	C ₂₆ H ₅₄	366	0.8	1.9	1.5	1.3	2.1	1.7	1.3	1.1	2.0	0.7	0.8
Heptacosane	C ₂₇ H ₅₆	380	0.3	0.5	0.3	0.2	0.6	0.2	0.3	0.2	0.5	0.1	0.2
Octacosane	C ₂₈ H ₅₈	394	0.4	0.8	0.5	0.4	1.0	0.7	0.6	0.5	1.0	0.3	0.3
Nonacosane	C ₂₉ H ₆₀	408	0.1	0.2	0.2	0.1	0.2	1.1	0.1	0.1	0.1	0.0	0.1
Triacontane	C ₃₀ H ₆₂	422	0.2	0.5	0.4	0.3	0.6	0.4	0.3	0.3	0.5	0.2	0.2
Hentriacontane	C ₃₁ H ₆₄	436	0.3	1.0	0.6	0.5	0.9	0.6	0.4	0.4	0.9	0.2	0.2
Dotriacontane	C ₃₂ H ₆₆	450	0.1	0.1	0.2	0.1	0.2	0.2	0.2	0.1	0.3	0.1	0.1
Tritriacontane	C ₃₃ H ₆₈	464	0.1	0.2	0.2	0.2	0.3	0.1	0.1	0.2	0.2	0.0	0.1
Total			32.9	74.6	58.9	50.6	78.1	69.0	50.7	44.5	91.1	32.3	40.0
CPI(o/e)			0.4	0.5	0.3	0.3	0.3	0.5	0.4	0.3	0.4	0.3	0.4
LMW/HMW			11.4	11.7	12.3	8.7	10.1	11.6	12.4	12.0	13.6	15.6	16.4
TAR			0.13	0.11	0.13	0.32	0.16	0.11	0.12	0.14	0.10	0.09	0.09
Wax n-alkanes													
Total			0.5	1.5	0.9	0.7	1.6	1.6	0.7	0.6	1.1	0.3	0.4
%			1.5%	2.0%	1.5%	1.3%	2.0%	2.3%	1.3%	1.4%	1.2%	0.8%	1.0%
Algal n-Alkanes													
Total			6.2	16.7	8.1	6.0	12.8	15.8	7.8	7.3	15.7	5.6	7.6
%			19%	22%	14%	12%	16%	23%	15%	16%	17%	17%	19%
Bacterial n-Alkanes													
Total			14.2	33.2	30.8	25.6	37.6	31.2	24.4	22.6	44.5	16.4	10.7
%			43.1%	44.5%	52.3%	50.7%	48.1%	45.2%	48.1%	50.7%	48.9%	50.8%	26.6%
Petroleum n-alkanes													
			12.0	23.2	19.0	18.3	26.1	20.4	17.8	14.0	29.8	10.0	21.4
%			36.6%	31.1%	32.4%	36.2%	33.4%	29.6%	35.1%	31.5%	32.7%	31.0%	53.4%
Hopanes													
Trisnorhopane	C ₂₇ H ₄₆	370	T	0.15	T	0.03	0.04	0.01	0.00	0.01	T	T	T
17a(H)-Trisnorhopane	C ₂₇ H ₄₆	370	0.01	0.52	T	0.03	0.15	0.00	0.00	0.04	T	T	T
17a(H),21b(H)-Norhopane	C ₂₉ H ₅₀	398	0.02	0.58	T	0.09	0.16	0.04	0.00	0.05	T	T	T
17a(H),21b(H)-Hopane	C ₃₀ H ₅₂	412	0.02	0.03	T	0.17	0.24	0.05	0.00	0.09	T	T	T
17a(H),21b(H)-22S-Homohopane	C ₃₁ H ₅₄	426	0.01	0.17	T	0.03	0.04	0.01	0.00	0.02	T	T	T
17a(H),21b(H)-22R-Homohopane	C ₃₁ H ₅₄	426	0.01	0.18	T	0.02	0.02	0.00	0.00	0.01	T	T	T
Gammacerane	C ₃₀ H ₅₂	412	0.00	0.05	T	0.00	0.00	0.00	0.00	0.00	T	T	T

17a(H),21b(H)-22S-Bishomohopane	C ₃₂ H ₅₆	440	0.01	0.19	T	0.00	0.04	0.00	0.00	0.01	T	T	T
17a(H),21b(H)-22R-Bishomohopane	C ₃₂ H ₅₆	440	T	0.14	T	0.00	0.02	0.00	0.00	0.01	T	T	T
17a(H),21b(H)-22S-Trishomohopane	C ₃₃ H ₅₈	454	T	T	T	T	0.01	T	T	T	T	T	T
17a(H),21b(H)-22R-Trishomohopane	C ₃₃ H ₅₈	454	T	T	T	T	T	T	T	T	T	T	T
17a(H),21b(H)-22S-Tetrakishomohopane	C ₃₄ H ₆₀	468	T	T	T	T	T	T	T	T	T	T	T
17a(H),21b(H)-22R-Tetrakishomohopane	C ₃₄ H ₆₀	468	T	T	T	T	T	T	T	T	T	T	T
17a(H),21b(H)-22S-Pentakishomohopane	C ₃₅ H ₆₂	482	T	T	T	T	T	T	T	T	T	T	T
17a(H),21b(H)-22R-Pentakishomohopane	C ₃₅ H ₆₂	482	T	T	T	T	T	T	T	T	T	T	T
Total			0.07	2.02	0.00	0.37	0.73	0.12	0.01	0.24	0.00	0.00	0.00
C ₃₁ S/(R+S)			0.58	0.49	ND	0.65	0.66	0.69	0.53	0.71	ND	ND	ND
C ₃₂ S/(R+S)			ND	0.57	ND	ND	0.68	ND	ND	0.54	ND	ND	ND

Steranes

13b,17a-20S-Cholestane Diasterane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T
13b,17a-20R-Cholestane Diasterane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T
13a,17b-20S-Cholestane Diasterane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T
13a,17b-20R-Cholestane Diasterane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20S-Cholestane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20R-Cholestane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20S-Cholestane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20R-Cholestane	C ₂₇ H ₄₈	372	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20S-Ergostane	C ₂₈ H ₅₀	386	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20R-Ergostane	C ₂₈ H ₅₀	386	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20S-Ergostane	C ₂₈ H ₅₀	386	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20R-Ergostane	C ₂₈ H ₅₀	386	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20S-Stigmastane	C ₂₉ H ₅₂	400	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20R-Stigmastane	C ₂₉ H ₅₂	400	T	T	T	T	T	T	T	T	T	T	T
14b,17b-20S-Stigmastane	C ₂₉ H ₅₂	400	T	T	T	T	T	T	T	T	T	T	T
14a,17ba-20R-Stigmastane	C ₂₉ H ₅₂	400	T	T	T	T	T	T	T	T	T	T	T
Total													

PAHs

Phenanthrene	C ₁₄ H ₁₀	178	0.5	3.2	2.4	2.5	4.8	1.8	3.8	1.0	4.9	11.8	1.8
Anthracene	C ₁₄ H ₁₀	178	0.4	6.0	2.5	3.1	5.9	2.0	3.5	1.6	7.6	11.3	1.9
Benzo[k]fluoranthene	C ₂₀ H ₁₂	252	0.2	0.2	0.2	3.6	0.4	0.1	0.1	0.2	0.2	0.1	0.1
Benzo[b]fluoranthene	C ₂₀ H ₁₂	252	0.2	0.1	0.1	3.1	0.2	0.2	0.1	0.0	0.1	0.0	0.0
Total			1.3	9.4	5.3	12.2	11.4	4.1	7.5	2.9	12.7	23.2	3.9

Ant/(Ant+Phe)	0.4	0.7	0.5	0.6	0.6	0.5	0.5	0.6	0.6	0.5	0.5
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Methyl alkanoates

Methyl octanoate	C ₉ H ₁₈ O ₂	158	0.00	0.05	0.02	0.01	0.02	0.13	0.12	0.02	0.06	0.00	0.00
Methyl nonanoate	C ₁₀ H ₂₀ O ₂	172	0.02	0.10	0.04	0.02	0.03	0.11	0.10	0.06	0.07	0.01	0.01
Methyl decanoate	C ₁₁ H ₂₂ O ₂	186	0.01	0.03	0.01	0.03	0.03	0.03	0.04	0.03	0.04	0.01	0.01
Methyl undecanoate	C ₁₂ H ₂₄ O ₂	200	0.01	0.05	0.03	0.03	0.05	0.04	0.06	0.04	0.05	0.02	0.03
Methyl dodecanoate	C ₁₃ H ₂₆ O ₂	214	0.07	0.10	0.12	0.11	0.15	0.12	0.16	0.13	0.18	0.11	0.10
Methyl tridecanoate	C ₁₄ H ₂₈ O ₂	228	0.12	0.44	0.17	0.06	0.14	0.19	0.22	0.09	0.21	0.07	0.07
Methyl tetradecanoate	C ₁₅ H ₃₀ O ₂	242	0.29	0.98	0.64	0.47	0.86	0.62	0.66	0.47	1.15	0.28	0.40
Methyl pentadecanoate	C ₁₆ H ₃₂ O ₂	256	0.14	0.47	0.32	0.19	0.39	0.28	0.33	0.19	0.57	0.12	0.20
Methyl hexadecanoate	C ₁₇ H ₃₄ O ₂	268	0.00	0.03	0.00	0.01	0.01	0.00	0.00	0.00	0.01	0.02	0.01
Methyl hexadecanoate	C ₁₇ H ₃₄ O ₂	270	7.49	17.56	11.60	8.29	17.52	10.15	9.64	8.39	22.91	5.07	7.23
Methyl heptadecanoate	C ₁₈ H ₃₆ O ₂	282	0.08	0.22	0.18	0.11	0.26	0.21	0.17	0.17	0.21	0.05	0.12
Methyl octadecanoate	C ₁₉ H ₃₈ O ₂	296	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.01	0.01	0.00
Methyl octadecanoate	C ₁₉ H ₃₈ O ₂	298	2.22	7.11	6.54	2.60	6.01	9.27	14.97	3.53	10.23	2.73	3.61
Methyl nonadecanoate	C ₂₀ H ₄₀ O ₂	312	0.05	0.16	0.05	0.08	0.11	0.15	0.11	0.06	0.07	0.03	0.05
Total			10.47	27.14	19.64	11.96	25.57	21.31	26.58	13.19	35.76	8.54	11.85

CPI(e/o)

Total FA

Pentanoic acid	C ₅ H ₁₀ O ₂	102	1.02	0.98	0.17	0.18	1.57	0.01	0.00	0.47	0.67	0.76	0.27
Hexanoic acid	C ₆ H ₁₂ O ₂	116	2.57	5.23	0.96	0.63	4.73	0.02	0.00	2.53	7.05	2.85	1.96
Heptanoic acid	C ₇ H ₁₄ O ₂	130	2.35	5.15	0.86	0.62	5.11	0.02	0.00	2.81	2.05	2.86	2.21
Octanoic acid	C ₈ H ₁₆ O ₂	144	6.39	14.32	2.61	1.97	12.49	0.11	0.00	7.26	7.10	8.63	6.31
Nonanoic acid	C ₉ H ₁₈ O ₂	158	9.72	19.32	3.11	3.53	20.07	0.36	0.12	10.66	4.14	15.00	9.29
Dodanoic acid	C ₁₀ H ₂₀ O ₂	172	3.39	6.71	0.96	1.17	6.80	0.22	0.10	3.68	8.40	5.71	3.26
Undecanoic acid	C ₁₁ H ₂₂ O ₂	186	1.98	3.89	0.54	0.77	4.04	0.06	0.04	2.05	3.75	3.67	1.95
Dodecanoic acid	C ₁₂ H ₂₄ O ₂	200	3.26	6.71	0.78	1.01	6.44	0.12	0.06	3.35	10.04	6.00	3.21

Tridecanoic acid	C ₁₃ H ₂₆ O ₂	214	1.78	3.50	0.66	0.68	3.75	0.19	0.16	1.92	1.25	3.44	1.81
Tetradecanoic acid	C ₁₄ H ₂₈ O ₂	228	5.95	11.94	2.06	1.80	14.16	0.31	0.22	6.29	3.89	11.69	5.79
Pentadecanoic acid	C ₁₅ H ₃₀ O ₂	242	4.04	7.86	1.23	1.42	8.36	0.67	0.66	4.33	3.67	7.56	1.39
Hexadecenoic acid	C ₁₆ H ₃₀ O ₂	254	0.15	0.59	0.33	0.25	0.67	0.29	0.33	0.29	4.08	0.14	0.23
Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	256	49.32	84.55	14.15	15.51	86.07	1.35	0.00	52.41	1.09	83.86	48.94
Heptadecanoic acid	C ₁₇ H ₃₄ O ₂	270	8.82	20.21	11.74	8.55	20.04	10.16	9.64	9.72	24.46	7.65	8.53
Octadecenoic acid	C ₁₈ H ₃₄ O ₂	282	0.11	0.29	0.18	0.11	0.28	0.21	0.17	0.18	0.32	0.07	0.16
Octadecanoic acid	C ₁₈ H ₃₆ O ₂	284	34.42	56.60	5.74	7.40	51.72	0.54	0.00	33.53	0.79	56.80	30.05
Nonadecanoic acid	C ₁₉ H ₃₈ O ₂	298	2.41	8.28	9.07	2.72	6.19	9.30	14.97	3.75	16.88	2.93	4.16
Eicosanoic acid	C ₂₀ H ₄₀ O ₂	312	0.46	0.56	0.72	0.16	0.38	0.15	0.11	0.31	3.72	0.10	0.22
Heneicosanoic acid	C ₂₁ H ₄₂ O ₂	326	10.47	27.14	19.64	11.96	25.57	21.31	26.58	13.19	35.76	8.54	11.85
Total			148.61	283.81	75.50	60.42	278.43	45.38	53.16	158.73	139.13	228.25	141.58
CPI(e/o)			2.48	1.94	0.60	0.97	1.93	0.07	0.01	2.24	0.45	3.35	2.41
Wax FA			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Algal FA													
Total			106.0	187.5	28.5	30.0	183.7	3.3	1.0	109.8	46.5	175.9	100.1
%			71.3%	66.1%	37.7%	49.6%	66.0%	7.3%	1.9%	69.2%	33.4%	77.0%	70.7%
Microbial FA													
Total			28.75	63.06	26.34	17.66	62.45	20.73	25.59	32.42	54.16	40.24	27.13
%			19.3%	22.2%	34.9%	29.2%	22.4%	45.7%	48.1%	20.4%	38.9%	17.6%	19.2%
n-Alkanols													
Undecanol	C ₁₁ H ₂₄ O	172	0.24	1.10	0.35	0.81	0.70	0.10	0.15	0.62	0.67	0.21	0.22
Dodecanol	C ₁₂ H ₂₆ O	186	2.63	9.46	10.01	8.03	10.82	2.55	3.23	4.64	7.05	4.09	4.57
Tridecanol	C ₁₃ H ₂₈ O	200	0.70	2.03	1.94	1.67	1.87	0.83	0.97	1.26	2.05	0.90	0.90
Tetradecanol	C ₁₄ H ₃₀ O	214	2.14	6.38	7.93	5.81	7.24	2.43	4.04	3.68	7.10	2.97	3.55
Pentadecanol	C ₁₅ H ₃₂ O	228	1.33	3.18	3.24	3.64	6.47	1.31	2.46	1.93	4.08	1.44	2.05
Hexadecanol	C ₁₆ H ₃₄ O	242	3.57	7.94	7.77	4.56	12.32	2.16	6.22	4.28	8.33	3.73	4.74
Heptadecanol	C ₁₇ H ₃₆ O	256	0.91	2.35	2.53	1.43	4.06	0.80	2.68	1.46	3.71	1.00	1.62
Octadecanol	C ₁₈ H ₃₈ O	270	6.04	10.91	15.19	6.10	9.38	6.60	7.96	7.79	9.99	5.29	6.92
Nonadecanol	C ₁₉ H ₄₀ O	284	0.30	1.08	1.22	0.82	4.53	0.46	0.78	1.51	1.08	0.34	0.46
Eicosanol	C ₂₀ H ₄₂ O	298	0.89	4.21	3.71	1.15	1.46	0.73	2.00	1.24	3.68	0.94	1.85
Heneicosanol	C ₂₁ H ₄₄ O	312	0.18	2.57	0.65	0.47	0.25	0.26	0.41	1.98	2.52	0.18	0.23
Docosanol	C ₂₂ H ₄₆ O	326	4.13	2.51	3.06	1.02	8.87	4.87	9.07	5.76	3.51	4.22	7.97

Triacosanol	C ₂₃ H ₄₈ O	340	0.21	1.17	1.18	2.58	0.78	0.26	0.47	0.29	1.08	0.33	0.45
Tetracosanol	C ₂₄ H ₅₀ O	354	0.46	11.78	6.37	4.67	19.90	2.27	3.10	0.87	1.55	0.33	4.95
Pentacosanol	C ₂₅ H ₅₂ O	368	0.01	0.11	0.12	0.10	0.15	0.03	0.08	0.03	0.11	0.05	0.03
Hexacosanol	C ₂₆ H ₅₄ O	382	0.15	0.82	0.84	0.68	0.53	0.17	0.61	0.25	0.78	0.26	0.31
Total			23.87	67.60	66.13	43.54	89.36	25.83	44.22	37.60	57.30	26.28	40.82
CPI(e/o)			5.16	3.97	4.88	2.78	3.75	5.39	4.53	3.14	2.74	4.90	5.85

Wax inputs

Total			17.73	29.11	25.27	22.37	46.31	25.31	31.78	26.88	26.84	26.81	36.23
%			74.3%	43.1%	38.2%	51.4%	51.8%	98.0%	71.9%	71.5%	46.8%	102.0%	88.8%

Algal inputs

Total			15.26	38.90	44.61	25.64	41.22	14.47	23.45	21.63	36.15	17.01	21.63
%			63.9%	57.5%	67.5%	58.9%	46.1%	56.0%	53.0%	57.5%	63.1%	64.7%	53.0%
Terristrial/Aquatic			1.16	0.75	0.57	0.87	1.12	1.75	1.35	1.24	0.74	1.58	1.68

Microbial inputs

Total			3.24	8.64	8.93	7.57	16.94	3.39	6.89	6.17	10.92	3.69	5.03
%			13.6%	12.8%	13.5%	17.4%	19.0%	13.1%	15.6%	16.4%	19.1%	14.0%	12.3%

Plasticizers

Diethyl phthalate	C ₁₂ H ₁₄ O ₄	222	3.5	6.8	2.6	1.7	3.7	1.3	1.8	1.9	6.2	1.5	1.8
Di-isobutyl phthalate	C ₁₆ H ₂₂ O ₄	278	9.7	20.9	13.5	11.7	23.9	12.2	11.6	11.5	24.9	8.4	14.0
Dibutyl phthalate	C ₁₆ H ₂₂ O ₄	278	14.9	38.5	11.2	24.4	37.1	31.8	19.2	11.3	72.8	20.3	20.2
Di(2-ethylhexyl) phthalate	C ₂₄ H ₃₈ O ₄	390	1.1	1.9	2.8	2.9	1.8	1.4	1.4	1.0	4.3	1.6	1.4
Total			29.1	68.1	30.0	40.7	66.5	46.8	34.1	25.8	108.1	31.9	37.4