

# Supplementary Information

## Historical Evolution of Organic Matter Accumulation in a Coastal Bay in the SW Atlantic, Brazil: Use of Sterols and *n*-Alcohols as Molecular Markers

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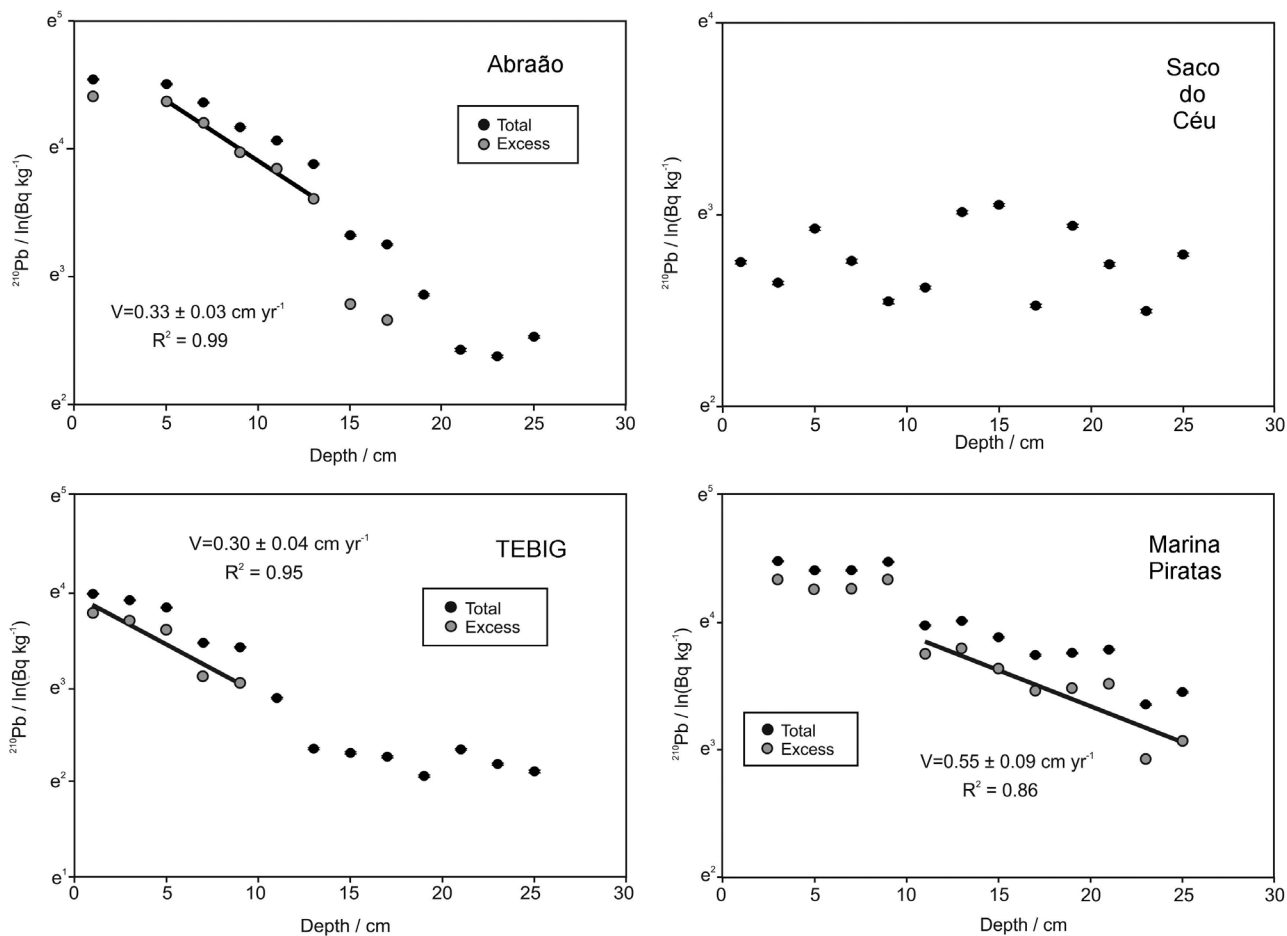


Figure S1. Active profile of excess  $^{210}\text{Pb}$  and linear regression in four sediment cores.

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**Table S2.** Concentrations of main sterols analyzed in Ilha Grande Bay sediment cores

Sample	epi-27 $\Delta^{0B}$	27 $\Delta^5$	27 $\Delta^{0B}$	27 $\Delta^{5,22}$	28 $\Delta^{5,22}$	28 $\Delta^{22}$	28 $\Delta^{5,24(28)}$	28 $\Delta^5$	29 $\Delta^{5,22}$	29 $\Delta^{22}$	29 $\Delta^5$	27 $\Delta^0$	28 $\Delta^0$	29 $\Delta^0$	30 $\Delta^{22}$	Copr=O	Choles=O
A00-02	< LOD	149.20	38.50	45.81	139.86	60.71	< LOD	98.10	244.13	< LOD	459.72	200.09	152.20	356.69	227.63	< LOQ	52.72
A02-04	31.21	4,158.08	43.70	< LOD	683.66	< LOD	333.02	713.90	388.91	109.28	940.60	294.40	192.29	335.97	437.14	< LOQ	50.61
A04-06	11.02	143.60	26.00	< LOD	< LOD	< LOD	18.91	44.82	55.05	< LOD	133.16	103.84	73.32	148.60	142.60	< LOQ	35.48
A06-08	< LOD	349.61	36.82	< LOD	62.47	< LOD	55.47	102.59	106.33	72.08	326.44	134.11	85.41	210.94	188.94	< LOQ	44.55
A08-10	27.50	224.31	28.79	< LOD	37.86	< LOD	< LOD	80.35	93.53	58.47	269.21	103.92	40.87	166.28	150.07	< LOD	34.32
A10-12	< LOD	280.61	28.65	< LOD	80.06	< LOD	< LOD	85.10	73.36	74.47	306.32	104.62	71.12	182.62	194.54	< LOD	40.68
A12-14	< LOD	164.38	< LOD	< LOD	38.57	< LOD	< LOD	< LOD	86.81	58.44	214.52	88.95	33.12	143.48	124.58	< LOQ	32.44
A14-16	< LOD	113.63	33.38	46.16	123.79	< LOD	< LOD	36.87	51.69	< LOD	104.74	80.05	54.01	141.79	150.44	< LOQ	43.35
A16-18	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
A18-20	8.99	127.62	11.28	< LOD	< LOD	< LOD	19.75	38.09	57.26	< LOD	125.18	91.88	79.41	188.96	163.66	< LOQ	40.19
A20-25	< LOD	163.49	27.94	< LOD	60.06	< LOD	< LOD	77.86	123.13	90.99	364.34	111.22	83.98	237.23	251.18	< LOQ	40.35
A25-30	< LOD	107.50	< LOD	< LOD	38.36	< LOD	< LOD	75.06	65.64	< LOD	310.55	84.63	43.18	149.06	129.01	< LOQ	35.82
A30-35	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
A35-40	< LOD	41.45	11.44	15.58	52.66	12.00	< LOD	21.53	25.14	< LOD	142.93	30.47	25.91	105.92	147.60	< LOQ	22.16
A40-45	7.56	98.51	9.26	< LOD	< LOD	< LOD	22.26	45.25	62.17	< LOD	382.28	53.77	54.89	203.73	122.39	< LOQ	26.73
A45-50	8.49	92.42	20.59	< LOD	< LOD	< LOD	19.11	29.81	47.19	< LOD	133.15	62.50	39.73	132.80	161.60	< LOQ	28.09
A50-55	8.60	69.62	8.86	< LOD	< LOD	< LOD	22.26	32.39	44.36	< LOD	191.39	48.09	36.79	117.80	114.28	< LOQ	27.81
A55-60	< LOD	54.47	12.25	20.06	71.53	11.05	< LOD	22.04	31.80	< LOD	99.05	41.88	22.16	88.99	86.64	< LOD	20.06
A60-65	< LOD	84.70	9.73	< LOD	< LOD	< LOD	19.32	26.97	70.37	< LOD	129.42	44.51	34.33	112.97	94.94	< LOQ	26.47
A65-70	8.70	73.22	10.03	< LOD	< LOD	< LOD	21.72	31.36	115.25	< LOD	161.70	49.53	37.95	131.81	89.49	< LOQ	25.98
A70-75	< LOD	112.01	29.17	< LOD	35.65	< LOD	< LOD	67.29	84.59	< LOD	333.50	95.01	50.17	163.03	150.87	< LOD	35.60
A75-80	< LOD	54.05	11.93	20.71	64.76	15.92	< LOD	22.75	31.99	< LOD	84.28	42.00	29.79	87.13	76.46	< LOQ	22.52
A80-85	8.48	113.75	9.35	< LOD	< LOD	< LOD	18.79	27.82	67.50	< LOD	124.09	43.83	39.18	123.84	70.59	< LOQ	27.09
C00-02	9.33	133.26	9.43	< LOD	< LOD	< LOD	23.89	40.11	63.88	< LOD	186.05	65.93	49.43	180.75	144.66	< LOQ	29.64
C02-04	< LOD	80.05	10.92	< LOD	< LOD	< LOD	21.80	35.62	57.18	< LOD	185.95	75.22	62.66	190.13	176.86	< LOD	30.79
C04-06	29.80	153.46	30.35	< LOD	50.23	< LOD	< LOD	75.44	168.07	69.97	419.08	135.03	62.03	221.19	210.58	< LOD	91.02
C06-08	5.19	68.60	9.42	< LOD	< LOD	< LOD	17.10	28.50	51.01	< LOD	177.10	65.99	45.60	138.08	112.00	< LOQ	30.56
C08-10	34.87	133.53	37.32	< LOD	153.46	37.44	< LOD	61.09	68.64	53.82	185.51	94.48	76.12	180.84	276.71	< LOQ	50.32
C10-12	< LOD	351.21	9.82	< LOD	< LOD	< LOD	24.81	36.82	49.56	< LOD	185.88	55.05	44.02	157.09	138.12	< LOQ	28.44
C12-14	7.78	49.08	8.45	< LOD	< LOD	< LOD	19.66	21.61	30.66	< LOD	77.16	36.56	31.45	88.56	85.42	< LOQ	22.35
C14-16	8.32	71.03	10.27	< LOD	< LOD	< LOD	21.49	33.61	49.15	< LOD	168.39	55.08	45.66	142.66	113.88	< LOQ	26.52
C16-18	8.02	77.94	10.73	< LOD	< LOD	< LOD	27.51	38.72	64.12	< LOD	211.29	61.11	39.21	148.71	178.44	< LOQ	34.13
C18-20	< LOD	75.35	8.13	< LOD	< LOD	< LOD	20.13	27.49	32.95	< LOD	150.00	42.42	31.27	102.67	103.60	< LOQ	21.77
C20-25	< LOD	69.87	9.43	< LOD	< LOD	< LOD	20.74	37.96	572.41	< LOD	219.25	46.74	27.54	112.46	105.15	< LOQ	26.87
C25-30	7.93	58.28	9.09	< LOD	< LOD	< LOD	18.80	30.72	110.52	< LOD	188.25	42.90	32.87	110.41	121.17	< LOQ	27.58
C30-35	11.30	58.31	8.74	< LOD	< LOD	< LOD	20.39	36.51	683.15	< LOD	156.66	41.61	31.08	111.19	84.90	< LOQ	23.23
C35-40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C40-45	7.65	52.12	7.80	< LOD	< LOD	< LOD	< LOD	56.63	245.21	< LOD	184.13	34.64	26.34	113.59	73.29	< LOD	< LOD
C45-50	9.09	97.74	16.72	< LOD	< LOD	< LOD	24.82	36.21	771.86	< LOD	314.66	57.08	48.93	182.62	148.06	< LOQ	37.05
C50-55	< LOD	62.86	9.74	< LOD	< LOD	< LOD	20.05	35.73	573.70	< LOD	134.42	51.42	34.29	160.95	97.13	< LOQ	< LOD
C55-60	< LOD	54.94	8.11	< LOD	< LOD	< LOD	18.84	28.66	48.34	< LOD	182.94	43.39	35.18	153.96	128.33	< LOQ	28.61
C60-65	< LOD	72.61	10.23	< LOD	< LOD	< LOD	24.72	36.30	96.98	< LOD	212.32	55.66	41.66	171.19	137.81	< LOD	31.67
C65-70	< LOD	84.17	10.56	< LOD	< LOD	< LOD	26.63	41.02	72.93	< LOD	248.40	53.60	38.80	151.16	123.26	< LOQ	27.16
C70-75	< LOD	64.50	8.53	< LOD	< LOD	< LOD	20.61	30.13	41.59	< LOD	160.17	42.17	40.46	114.79	119.01	< LOD	24.97
C75-80	< LOD	54.37	9.19	< LOD	< LOD	< LOD	18.07	28.98	43.74	< LOD	184.92	33.42	29.49	106.28	90.47	< LOD	23.07
C80-85	< LOD	40.22	8.09	< LOD	< LOD	< LOD	15.84	18.17	29.22	< LOD	102.49	30.70	28.29	96.47	63.29	< LOQ	24.91
C85-90	< LOD	44.28	9.29	< LOD	< LOD	< LOD	17.30	21.96	31.24	< LOD	138.67	33.00	29.80	117.60	53.60	< LOQ	22.49
T00-02	32.22	455.87	67.15	< LOD	195.35	132.03	< LOD	154.68	356.33	85.06	596.95	290.09	95.08	319.27	155.59	30.19	83.77
T02-04	9.61	166.11	13.61	< LOD	< LOD	< LOD	29.04	58.64	125.61	< LOD	264.40	123.49	60.26	168.28	91.04	< LOQ	38.53

Table S2. continuation

Sample	epi-27 $\Delta^0$ <sup>B</sup>	27 $\Delta^5$	27 $\Delta^0$ <sup>B</sup>	27 $\Delta^{5,22}$	28 $\Delta^{5,22}$	28 $\Delta^{22}$	28 $\Delta^{5,24(28)}$	28 $\Delta^5$	29 $\Delta^{5,22}$	29 $\Delta^{22}$	29 $\Delta^5$	27 $\Delta^0$	28 $\Delta^0$	29 $\Delta^0$	30 $\Delta^{22}$	Copr=O	Choles=O
T04-06	10.01	162.56	13.49	< LOD	< LOD	< LOD	27.91	60.30	168.49	< LOD	265.66	119.94	67.49	178.66	92.57	< LOQ	38.25
T06-08	< LOD	42.77	8.35	< LOD	< LOD	< LOD	18.92	23.89	27.22	< LOD	71.88	50.52	32.54	92.24	44.27	< LOD	22.24
T08-10	7.73	79.63	9.96	< LOD	< LOD	< LOD	25.23	38.44	61.12	< LOD	178.14	69.65	45.37	120.34	64.71	< LOQ	27.14
T10-12	11.89	49.34	13.42	18.74	40.96	16.53	< LOD	25.85	41.53	< LOD	154.46	45.96	34.83	83.41	98.72	< LOQ	17.76
T12-14	< LOD	70.98	8.60	< LOD	< LOD	< LOD	15.75	20.34	33.57	< LOD	60.78	53.06	34.24	84.63	57.02	< LOQ	22.85
T14-16	< LOD	52.05	8.56	< LOD	< LOD	< LOD	< LOD	18.20	29.12	< LOD	64.15	38.06	28.29	67.05	48.50	< LOQ	17.56
T16-18	< LOD	46.56	8.39	< LOD	< LOD	< LOD	16.05	20.03	52.89	< LOD	79.78	31.00	22.27	70.99	42.50	< LOD	17.43
T18-20	< LOD	40.11	11.24	16.98	40.89	9.71	< LOD	19.26	30.40	19.93	47.25	31.29	21.57	55.83	56.05	< LOQ	16.79
T20-25	< LOD	39.40	7.42	< LOD	< LOD	< LOD	15.14	19.65	30.15	< LOD	66.42	26.53	19.66	60.08	38.35	< LOQ	15.88
T25-30	< LOD	42.28	8.24	< LOD	< LOD	< LOD	14.74	16.56	20.49	< LOD	46.45	25.92	17.73	42.31	25.78	< LOD	15.75
T30-35	< LOD	< LOD	< LOD	13.77	15.00	< LOD	< LOD	< LOD	9.94	< LOD	< LOD	< LOD	< LOD	< LOD	17.98	< LOD	< LOD
T35-40	< LOD	23.58	< LOD	< LOD	< LOD	< LOD	< LOD	10.50	16.85	< LOD	20.80	19.80	15.58	31.56	21.64	< LOD	< LOD
T40-45	< LOD	34.85	< LOD	< LOD	< LOD	< LOD	< LOD	11.57	28.47	< LOD	20.79	22.30	18.39	42.44	28.42	< LOD	13.51
T45-50	< LOD	28.44	< LOD	< LOD	< LOD	< LOD	16.31	9.15	11.97	< LOD	14.17	18.51	17.15	30.10	19.50	< LOD	13.73
T50-55	< LOD	35.40	7.81	< LOD	< LOD	< LOD	13.21	11.73	14.45	< LOD	15.69	19.66	16.11	33.55	18.74	< LOD	14.35
T55-60	< LOD	34.12	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	14.23	< LOD	10.99	19.84	15.65	24.02	15.78	< LOD	15.20
T60-65	< LOD	25.92	< LOD	< LOD	< LOD	< LOD	< LOD	11.93	16.89	< LOD	24.37	19.58	15.94	30.77	16.01	< LOD	15.64
T65-70	< LOD	31.74	< LOD	< LOD	< LOD	< LOD	13.04	11.16	12.37	< LOD	18.30	19.58	15.55	29.34	15.01	< LOD	14.09
T70-75	< LOD	39.86	< LOD	< LOD	< LOD	< LOD	< LOD	11.10	16.06	< LOD	23.84	19.68	16.34	33.82	28.48	< LOD	14.12
M00-02	36.93	317.64	87.24	< LOD	123.38	110.33	< LOD	129.77	231.78	89.38	528.77	286.32	183.93	369.96	234.34	15.32	68.42
M02-04	32.74	229.44	60.17	< LOD	78.20	93.25	< LOD	85.00	143.14	87.46	394.15	207.98	144.31	323.90	210.09	< LOQ	52.93
M04-06	29.54	104.80	37.06	< LOD	39.46	62.38	< LOD	< LOD	67.88	66.18	122.11	108.40	56.01	123.68	99.38	< LOD	< LOD
M06-08	29.25	120.10	37.73	< LOD	45.76	86.14	< LOD	70.22	96.03	55.46	185.93	123.17	67.76	172.97	122.66	< LOD	< LOD
M08-10	29.66	127.44	37.87	< LOD	30.24	83.25	< LOD	70.16	82.86	74.29	210.85	127.05	85.50	229.04	174.30	< LOD	34.13
M10-12	22.97	72.04	28.33	35.60	69.90	26.99	37.10	33.99	51.95	37.47	73.85	91.22	73.19	155.73	91.18	< LOD	< LOD
M12-14	29.73	99.73	33.04	< LOD	26.40	97.00	< LOD	64.41	99.82	61.89	159.45	135.05	88.54	208.44	144.58	< LOD	< LOD
M14-16	29.15	111.88	34.81	< LOD	39.86	94.65	< LOD	< LOD	109.77	104.11	198.75	147.60	77.83	216.75	147.44	< LOD	< LOD
M16-18	< LOD	80.61	28.57	< LOD	24.86	< LOD	< LOD	< LOD	60.01	53.24	84.30	83.26	43.92	135.91	111.82	< LOD	< LOD
M18-20	< LOD	80.10	28.15	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	43.05	91.91	74.17	36.32	108.27	126.50	< LOD	< LOD
M20-25	< LOD	72.89	27.80	< LOD	< LOD	< LOD	< LOD	< LOD	39.08	< LOD	47.30	72.10	24.62	75.94	73.30	< LOD	< LOD
M25-30	< LOD	68.96	27.76	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	27.22	64.13	17.07	38.37	62.23	< LOD	< LOD
M30-35	< LOD	70.51	27.82	< LOD	< LOD	< LOD	< LOD	< LOD	96.32	< LOD	71.19	61.52	< LOD	48.52	60.34	< LOD	< LOD
M35-40	< LOD	78.13	27.30	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	10.86	59.77	< LOD	43.18	54.48	< LOD	< LOD
M40-45	< LOD	67.54	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	5.01	60.32	16.15	32.18	< LOD	< LOD	< LOD
M45-50	< LOD	66.73	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	36.95	< LOD	30.49	58.80	16.09	36.04	< LOD	< LOD	< LOD
M50-55	< LOD	30.85	< LOD	< LOD	18.47	< LOD	< LOD	9.56	< LOD	< LOD	< LOQ	20.37	16.41	22.95	17.27	< LOD	13.37
M55-60	< LOD	59.81	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	32.25	< LOD	< LOQ	58.23	< LOD	29.50	< LOD	< LOD	< LOD
M60-65	< LOD	72.74	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	34.41	< LOD	7.54	58.69	15.78	30.62	< LOD	< LOD	< LOD

LOD: limit of detection; LOQ: limit of quantification. LOQ = 10 ng g<sup>-1</sup> of dry weight. epi-27 $\Delta^0$ <sup>B</sup> 5 $\beta$ -cholestan-3 $\alpha$ -ol; 27 $\Delta^5$  cholest-5-en-3 $\beta$ -ol; 27 $\Delta^0$ <sup>B</sup> 5 $\beta$ -cholestan-3 $\beta$ -ol; 27 $\Delta^{5,22}$  cholesta-5,22E-dien-3 $\beta$ -ol; 28 $\Delta^{5,22}$  24-methylcholesta-5,22E-dien-3 $\beta$ -ol; 28 $\Delta^{22}$  24-methyl-5 $\alpha$ -cholest-22E-en-3 $\beta$ -ol; 28 $\Delta^{5,24(28)}$  24-methylcholesta-5,24(28)-dien-3 $\beta$ -ol; 28 $\Delta^5$  24-methylcholest-5-en-3 $\beta$ ol; 29 $\Delta^{5,22}$  24-ethylcholesta-5,22E-dien-3 $\beta$ -ol; 29 $\Delta^{22}$  24-ethyl-5 $\alpha$ -cholest-22-en-3 $\beta$ -ol; 29 $\Delta^5$  24-ethylcholest-5-en-3 $\beta$ -ol; 27 $\Delta^0$  5 $\alpha$ -cholestan-3 $\beta$ -ol; 28 $\Delta^0$  24-methyl-5 $\alpha$ -cholestan-3 $\beta$ -ol; 29 $\Delta^0$  24-ethyl-5 $\alpha$ -cholestan-3 $\beta$ -ol; 30 $\Delta^{22}$  4 $\alpha$ ,23,24-trimethylcholest-22-en-3 $\beta$ -ol; Copr=O 5 $\alpha$ -cholestan-3-one; Choles=O 5 $\alpha$ -cholestanone.

**Table S3.** Concentrations of *n*-alcohols analyzed in Ilha Grande Bay sediment cores

Sample	C <sub>14</sub> OH	C <sub>16</sub> OH	C <sub>18</sub> OH	Phytol	C <sub>20</sub> OH	C <sub>21</sub> OH	C <sub>22</sub> OH	C <sub>23</sub> OH	C <sub>24</sub> OH	C <sub>25</sub> OH	C <sub>26</sub> OH	C <sub>27</sub> OH	C <sub>28</sub> OH	C <sub>29</sub> OH	C <sub>30</sub> OH	C <sub>32</sub> OH	C <sub>31</sub> OH
A00-02	107.12	190.27	45.45	64.06	311.87	76.11	264.10	36.27	242.97	41.99	363.65	53.96	512.45	63.10	539.29	327.56	73.47
A02-04	37.05	142.17	<LOQ	38.96	129.52	45.20	142.90	48.40	181.46	53.09	306.39	55.71	302.84	62.51	255.95	140.52	47.74
A04-06	16.54	<LOQ	<LOQ	<LOD	86.31	19.33	58.82	19.48	71.48	22.65	131.67	26.55	167.86	32.81	171.52	104.12	34.79
A06-08	38.20	98.64	84.11	42.29	155.73	47.22	176.70	51.00	217.71	56.44	334.82	62.75	369.03	73.42	296.60	154.70	51.97
A08-10	35.62	38.70	57.62	39.22	175.05	71.15	187.03	53.22	203.46	58.69	318.34	65.08	313.75	64.94	283.46	162.36	56.15
A10-12	39.05	69.84	104.32	41.02	188.17	85.09	241.39	58.88	313.77	62.13	390.56	72.80	428.01	79.51	351.03	205.80	57.38
A12-14	47.09	273.60	210.29	57.38	121.92	48.62	139.71	46.89	176.86	48.40	268.60	51.74	295.71	56.31	230.34	131.59	43.17
A14-16	60.27	<LOQ	<LOQ	30.27	215.02	41.21	179.93	34.45	236.67	35.72	327.02	40.59	382.07	65.48	478.37	364.37	80.46
A16-18	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
A18-20	32.49	<LOQ	<LOQ	<LOD	141.76	36.66	152.69	33.96	210.56	41.63	428.14	56.56	600.31	79.35	689.05	468.59	75.98
A20-25	14.08	96.97	123.17	54.71	141.11	62.97	222.98	58.82	305.14	69.01	464.84	75.75	587.60	99.26	558.73	319.19	75.17
A25-30	23.39	<LOQ	<LOQ	51.26	94.14	39.55	158.12	49.98	256.62	60.02	332.62	59.85	422.54	74.57	394.36	263.44	52.46
A30-35	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
A35-40	14.77	<LOQ	<LOQ	16.27	<LOQ	10.35	42.03	7.15	14.83	6.47	54.72	13.79	233.10	30.15	290.33	292.48	40.94
A40-45	18.53	<LOQ	<LOQ	<LOD	108.43	36.56	207.64	36.84	397.01	52.74	542.57	66.05	807.24	105.30	960.17	1,040.07	106.26
A45-50	8.55	<LOQ	<LOQ	<LOD	100.08	36.00	88.97	24.60	149.98	30.79	283.28	41.98	497.73	65.14	580.11	515.48	65.60
A50-55	<LOQ	<LOQ	<LOQ	<LOD	97.75	33.85	114.36	29.47	210.98	37.22	390.35	53.94	684.42	82.93	792.93	692.78	84.14
A55-60	43.77	<LOQ	<LOQ	15.91	<LOQ	60.81	138.44	20.84	166.68	25.59	251.05	28.70	322.03	40.88	326.73	270.49	42.46
A60-65	<LOQ	<LOQ	<LOQ	<LOD	86.38	28.39	117.63	24.48	196.66	37.71	370.97	54.96	604.67	80.48	714.83	600.26	73.89
A65-70	47.53	42.63	<LOQ	<LOD	134.46	70.15	186.49	37.90	296.17	48.75	528.12	79.29	869.58	107.84	984.48	829.01	100.54
A70-75	46.93	38.06	73.36	44.50	97.12	55.22	213.45	54.75	293.88	66.53	412.19	78.52	530.57	86.12	443.80	275.47	62.14
A75-80	113.69	91.88	46.67	33.87	165.01	104.69	218.31	20.68	165.77	23.70	208.95	26.55	278.87	36.54	310.87	274.05	44.67
A80-85	39.61	<LOQ	<LOQ	<LOD	102.10	36.45	108.33	25.97	179.22	35.62	330.39	48.57	576.21	70.16	672.02	577.42	72.91
C00-02	48.77	83.79	<LOQ	<LOD	106.82	26.01	118.53	31.29	190.35	44.68	392.76	57.84	632.80	100.04	819.36	495.14	87.31
C02-04	66.57	74.69	<LOQ	<LOD	165.32	47.71	163.59	34.12	306.56	50.92	529.23	71.25	776.45	117.84	1,005.87	661.19	92.84
C04-06	33.29	85.85	95.15	52.38	105.01	42.81	153.85	50.57	251.55	63.35	358.18	65.59	471.20	95.29	480.55	296.12	63.59
C06-08	70.34	60.51	51.11	<LOD	93.10	19.13	133.42	27.31	252.63	41.86	411.66	54.63	670.00	93.41	868.40	615.59	78.49
C08-10	80.16	<LOQ	<LOQ	43.56	<LOQ	103.05	233.69	35.10	260.58	45.12	335.56	54.10	512.40	77.45	536.57	416.86	82.00
C10-12	76.82	127.77	194.19	<LOD	144.79	53.90	168.95	37.33	293.00	51.75	521.82	62.92	811.66	102.59	1,002.94	769.82	100.21
C12-14	34.65	788.90	508.31	<LOD	94.45	26.57	170.29	22.68	110.29	29.63	185.09	33.87	303.52	48.37	401.73	303.04	51.58
C14-16	24.94	47.31	73.82	<LOD	126.03	49.30	136.28	31.52	271.88	41.62	383.08	54.23	603.28	92.34	763.30	550.41	79.66
C16-18	66.02	24.13	<LOQ	<LOD	148.17	77.02	167.94	33.44	260.06	47.94	418.82	63.42	691.58	98.43	869.06	636.73	87.32
C18-20	47.73	57.66	54.79	<LOD	141.73	42.86	160.45	37.81	310.06	54.90	503.49	71.02	825.43	109.37	1,037.76	795.53	98.96
C20-25	23.03	<LOQ	<LOQ	<LOD	145.96	64.56	174.31	36.32	288.73	54.48	498.00	83.71	901.50	120.67	1,000.27	734.55	106.07
C25-30	59.06	<LOQ	<LOQ	<LOD	94.31	35.04	137.60	33.60	330.50	54.85	593.52	82.97	1,023.02	135.43	1,223.10	935.05	113.70
C30-35	46.30	64.88	50.48	<LOD	171.98	96.15	203.42	40.16	342.40	55.88	598.71	92.87	974.54	141.67	1,246.12	1,011.82	127.18
C35-40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C40-45	47.76	<LOQ	<LOQ	<LOD	96.37	29.66	118.53	27.48	211.60	35.01	295.43	41.38	306.51	43.59	312.35	175.37	39.05
C45-50	168.86	165.09	151.74	<LOD	197.38	131.72	234.85	40.60	434.03	76.20	929.89	154.75	3,014.14	442.25	5,996.42	2,938.38	330.50
C50-55	65.00	414.03	221.93	<LOD	146.54	65.03	143.57	25.98	145.02	26.02	137.63	34.06	119.36	25.89	87.26	44.72	<LOQ
C55-60	39.40	51.12	101.90	<LOD	96.36	29.09	232.10	48.05	573.87	79.94	905.34	112.36	1,545.79	198.61	1,932.43	1,512.12	179.98
C60-65	49.27	<LOQ	<LOQ	<LOD	109.79	43.71	165.79	40.08	408.47	66.62	697.91	97.41	1,219.95	153.05	1,549.30	1,150.05	151.85
C65-70	13.81	22.49	<LOQ	<LOD	108.34	34.79	183.58	41.72	480.65	74.73	823.12	112.01	1,420.73	180.03	1,741.33	1,443.10	177.42
C70-75	16.90	27.33	<LOQ	<LOD	85.64	31.12	139.08	35.62	377.42	59.57	725.06	90.93	1,157.48	150.08	1,361.74	1,111.16	136.25
C75-80	29.72	<LOQ	<LOQ	<LOD	99.74	36.34	180.79	41.50	511.25	76.21	932.60	114.55	1,598.68	193.86	1,851.37	1,477.21	176.93
C80-85	13.31	<LOQ	<LOQ	<LOD	70.71	21.32	147.55	36.76	436.69	69.34	859.76	102.66	1,479.15	164.38	1,743.49	1,405.98	163.82

Table S3. continuation

Sample	C <sub>14</sub> OH	C <sub>16</sub> OH	C <sub>18</sub> OH	Phytol	C <sub>20</sub> OH	C <sub>21</sub> OH	C <sub>22</sub> OH	C <sub>23</sub> OH	C <sub>24</sub> OH	C <sub>25</sub> OH	C <sub>26</sub> OH	C <sub>27</sub> OH	C <sub>28</sub> OH	C <sub>29</sub> OH	C <sub>30</sub> OH	C <sub>32</sub> OH	C <sub>31</sub> OH
C85-90	55.06	127.60	105.37	< LOD	113.89	60.52	182.35	37.63	314.31	49.83	554.02	63.43	885.51	116.25	1,071.36	933.65	111.73
T00-02	85.40	179.20	114.91	43.09	283.08	57.23	175.87	44.84	137.43	46.45	165.06	41.87	92.88	40.63	87.47	58.06	< LOD
T02-04	100.75	127.05	108.87	< LOD	245.97	36.08	116.42	26.82	107.69	25.57	182.98	35.70	139.24	31.08	141.62	148.15	38.78
T04-06	101.59	125.91	94.05	< LOD	235.42	52.10	123.12	25.80	113.65	24.60	187.51	22.41	158.24	29.36	160.36	155.65	39.36
T06-08	71.32	111.90	94.02	< LOD	178.20	22.07	85.34	18.42	84.84	24.46	147.69	22.74	123.61	28.50	118.41	101.08	26.59
T08-10	37.92	79.92	63.61	< LOD	169.77	24.35	95.54	22.26	111.59	26.17	189.01	28.60	166.83	31.45	167.89	125.21	37.17
T10-12	8.81	< LOQ	< LOQ	10.15	< LOQ	18.08	51.59	9.90	61.63	9.81	88.78	14.90	73.66	15.86	57.87	46.78	18.22
T12-14	72.70	53.93	< LOQ	< LOD	131.44	25.67	75.57	17.83	82.55	18.63	118.62	23.37	118.14	23.37	120.48	91.83	35.02
T14-16	82.91	29.24	< LOQ	< LOD	144.08	38.19	85.96	17.45	73.12	18.37	111.57	20.25	104.75	23.76	111.27	53.73	27.70
T16-18	81.15	< LOQ	< LOQ	< LOD	142.04	29.84	87.85	18.82	107.36	23.11	155.14	27.62	150.18	27.69	153.45	101.93	28.55
T18-20	6.42	< LOQ	< LOQ	11.30	88.25	17.51	70.35	10.27	112.01	14.32	147.13	15.97	121.25	23.60	126.62	96.23	25.57
T20-25	< LOQ	< LOQ	43.89	< LOD	164.71	25.05	77.85	17.81	104.99	21.92	155.07	25.28	155.91	31.17	148.68	151.10	32.63
T25-30	67.40	152.66	97.84	< LOD	129.78	38.52	87.53	19.91	89.72	21.57	141.04	25.26	160.97	32.72	190.62	194.55	34.92
T30-35	44.27	< LOQ	< LOQ	6.58	< LOQ	11.02	29.51	13.24	11.24	< LOD	20.23	< LOD	< LOQ	< LOD	< LOQ	< LOQ	< LOD
T35-40	26.16	< LOQ	< LOQ	< LOD	72.20	19.32	66.18	17.13	83.13	21.39	134.84	21.74	193.43	32.07	259.48	190.24	36.48
T40-45	35.17	< LOQ	< LOQ	< LOD	77.99	22.96	61.80	18.30	98.81	20.53	143.26	25.91	199.93	35.21	271.90	205.13	34.17
T45-50	40.04	< LOQ	< LOQ	< LOD	87.58	23.98	65.72	18.75	80.97	21.17	116.95	19.86	139.18	30.09	185.28	167.76	27.21
T50-55	30.77	< LOQ	< LOQ	< LOD	69.26	28.37	< LOD	< LOD	71.08	18.94	104.57	23.32	129.27	26.89	161.34	146.84	27.82
T55-60	63.96	44.31	< LOQ	< LOD	68.99	26.26	56.73	14.83	68.19	17.17	98.17	23.40	131.07	23.94	169.28	142.08	26.04
T60-65	30.39	< LOQ	< LOQ	< LOD	80.48	29.05	72.68	16.77	84.98	22.20	152.87	20.92	213.16	31.43	204.01	179.82	33.46
T65-70	30.84	< LOQ	< LOQ	< LOD	71.40	21.08	75.32	21.02	129.66	25.62	315.74	24.20	275.21	33.43	202.53	189.10	33.39
T70-75	< LOQ	< LOQ	78.43	< LOD	68.85	22.79	65.00	17.21	77.92	20.22	130.21	24.04	177.34	33.46	245.25	246.41	36.32
M00-02	62.64	171.85	< LOQ	47.50	139.81	46.05	125.75	48.12	105.45	49.76	169.51	41.51	144.93	48.97	116.78	64.79	< LOD
M02-04	72.97	193.70	70.43	39.43	134.96	62.97	145.14	54.77	136.53	49.89	213.96	47.35	232.28	58.66	224.26	111.11	41.58
M04-06	45.42	58.84	< LOQ	30.53	116.25	47.58	101.90	37.75	58.36	36.71	79.30	37.32	75.07	37.75	48.73	29.42	< LOD
M06-08	36.44	40.83	< LOQ	35.67	91.03	43.88	92.18	37.25	71.83	39.56	113.33	41.31	134.48	45.21	101.91	66.60	37.91
M08-10	42.58	< LOQ	< LOQ	33.13	100.64	44.49	93.96	41.01	93.50	41.00	146.41	41.91	157.01	48.82	126.90	65.22	40.36
M10-12	22.45	6.26	< LOQ	12.74	< LOQ	19.18	59.53	18.29	73.16	21.82	143.21	19.93	160.03	39.95	155.28	90.64	26.23
M12-14	36.71	29.53	< LOQ	34.76	80.27	38.21	76.42	38.03	80.42	40.90	117.78	41.37	137.09	48.54	100.92	55.65	41.06
M14-16	35.46	74.54	< LOQ	124.89	66.44	37.63	67.08	37.75	72.61	39.29	106.45	47.52	128.87	57.59	116.14	72.36	< LOD
M16-18	22.84	< LOQ	< LOQ	31.02	68.33	38.23	65.00	33.11	60.28	36.43	89.48	38.57	94.95	42.58	78.29	49.00	< LOD
M18-20	21.18	24.13	< LOQ	35.10	67.57	37.41	72.92	35.99	63.17	37.28	93.70	39.65	131.80	46.17	162.28	60.16	43.76
M20-25	42.92	95.33	< LOQ	33.40	97.06	35.78	67.94	35.36	55.50	36.53	78.51	< LOD	73.41	38.08	57.91	33.58	37.22
M25-30	36.76	36.50	< LOQ	32.49	70.30	34.40	55.35	36.03	45.75	36.34	57.03	37.85	48.80	40.44	36.93	23.67	35.99
M30-35	33.09	< LOQ	< LOQ	28.34	48.06	33.62	42.21	< LOD	53.61	39.18	164.73	60.05	782.38	139.65	1,802.38	510.17	89.00
M35-40	56.41	28.78	< LOQ	< LOD	47.39	36.51	< LOD	52.30	59.45	39.32	82.47	38.01	200.79	54.24	292.13	120.79	43.01
M40-45	31.92	< LOQ	< LOQ	< LOD	48.41	33.56	40.94	< LOD	30.68	< LOD	45.18	34.57	58.67	37.91	78.44	26.54	36.86
M45-50	< LOQ	96.58	58.56	< LOD	46.57	< LOD	41.80	< LOD	31.31	< LOD	40.26	< LOD	39.51	< LOD	23.22	22.04	< LOD
M50-55	21.89	< LOQ	< LOQ	6.39	< LOQ	17.65	26.23	7.64	32.32	8.20	19.80	10.34	24.23	8.13	9.52	< LOQ	< LOQ
M55-60	< LOD	< LOQ	< LOQ	< LOD	< LOD	< LOD	40.90	< LOD	31.33	< LOD	37.62	< LOD	24.04	< LOD	12.92	13.04	< LOD
M60-65	< LOD	< LOQ	< LOQ	< LOD	48.23	< LOD	45.22	< LOD	34.63	< LOD	39.70	< LOD	25.95	34.83	17.95	17.79	< LOD

LOD: limit of detection; LOQ: limit of quantification. All values in ng g<sup>-1</sup> of dry weight.

Figure S1 was added on August 18, 2014