

Supplementary Information:

Organic Remains in Early Christian Egyptian Metal Vessels: Investigation with Fourier Transform Infrared Spectroscopy and Gas Chromatography–Mass Spectrometry

Kyriaki Koupadi ¹, Stamatis C. Boyatzis ^{1,*}, Maria Roumpou ², Nick Kalogeropoulos ², and Despoina Kotzamani ³

¹ Department of Conservation of Antiquities & Works of Art, University of West Attica, Aghiou Spyridonos, 12210 Egaleo, Greece; koupadirk@gmail.com

² Department of Nutrition and Dietetics, Harokopio University of Athens, El. Venizelou 70, 17671 Athens, Greece; mroumpou@gmail.com (M.R.); nickal@hua.gr (N.K.)

³ Metals, Glass and Organic Material Conservation Lab, Benaki Museum, Koubari 1, 10674 Athens, Greece; kotzamani@benaki.org

* Correspondence: sboyatzis@uniwa.gr

Citation: Koupadi, K.; Boyatzis, S.C.; Roumpou, M.; Kalogeropoulos, N.; Kotzamani, D. Organic Remains in Early Christian Egyptian Metal Vessels: Investigation with Fourier Transform Infrared Spectroscopy and Gas Chromatography–Mass Spectrometry. *Heritage* **2021**, *4*, 3611–3629. <https://doi.org/10.3390/heritage4040199>

Academic Editor: Nick Schiavon

Received: 31 August 2021

Accepted: 7 October 2021

Published: 18 October 2021

Publisher’s Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).

1. Infrared spectra (Figures S1–S4)

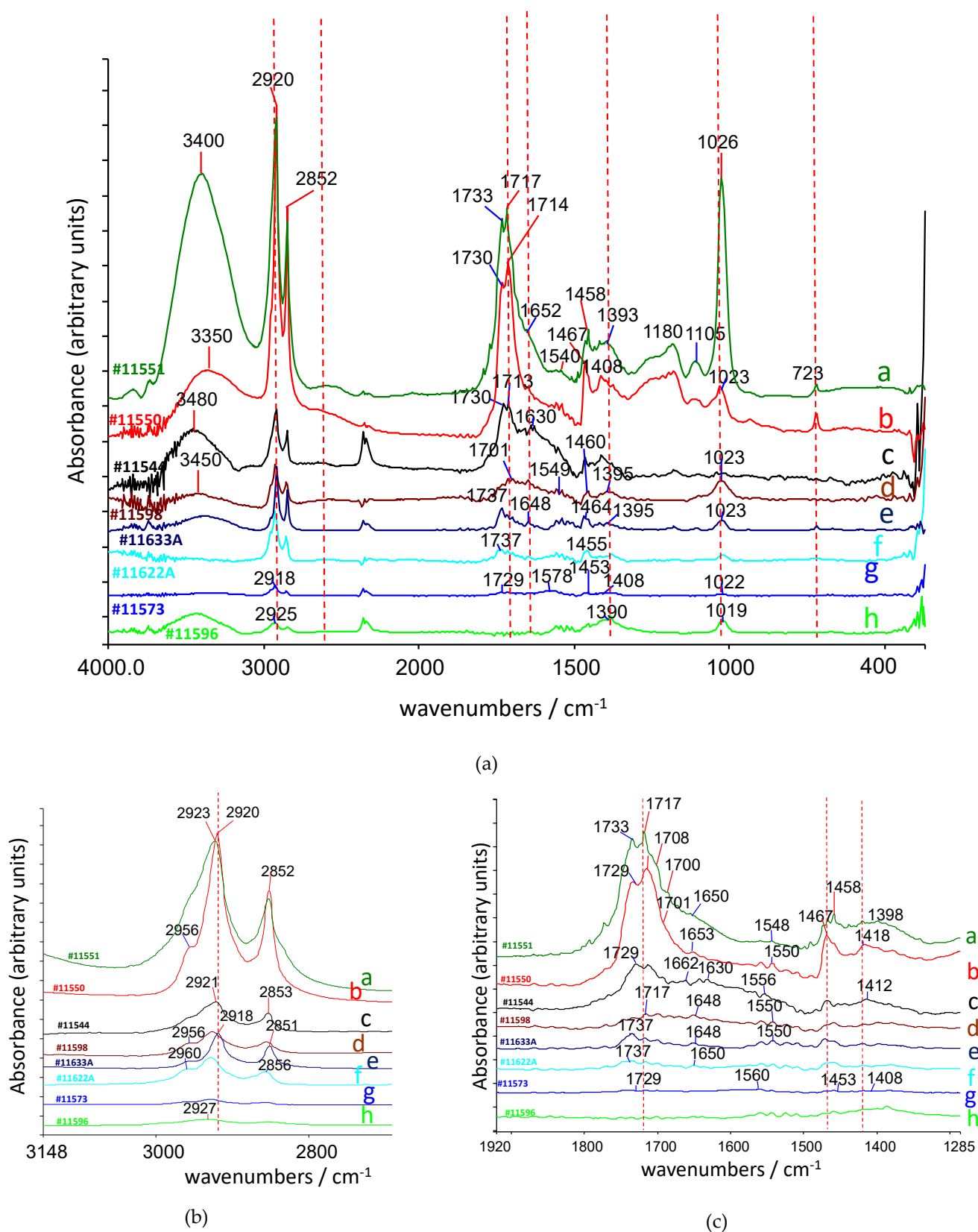
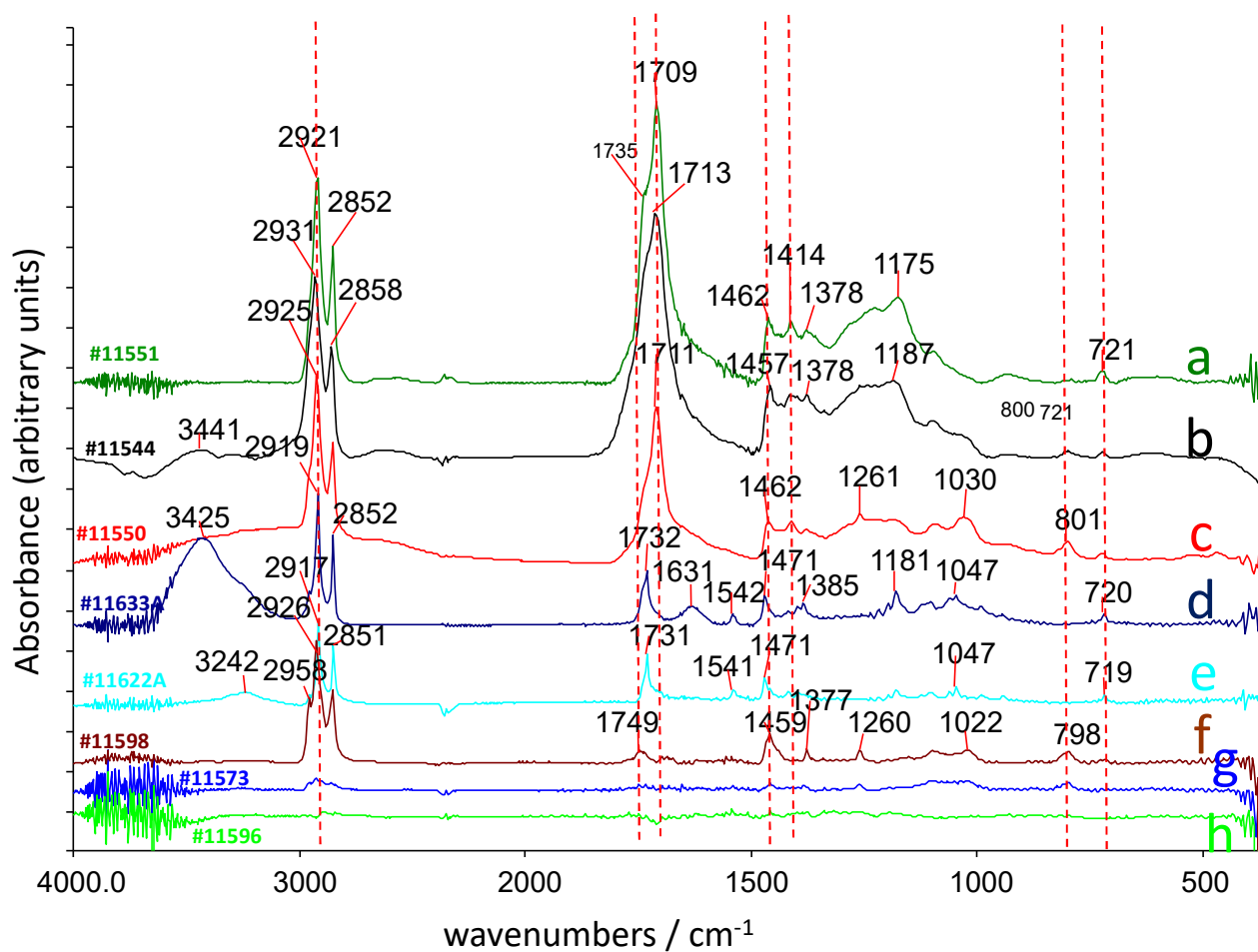
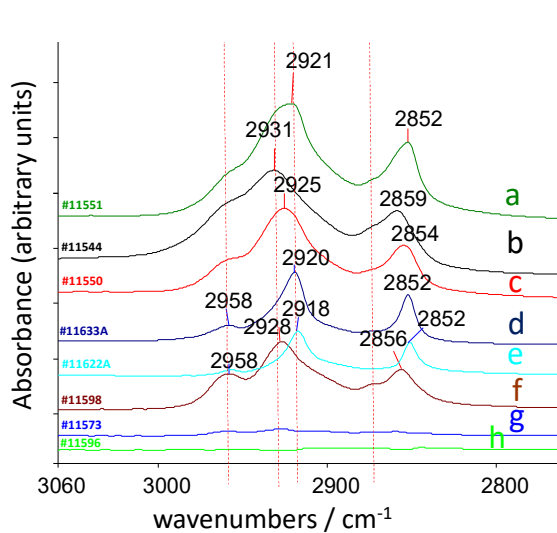


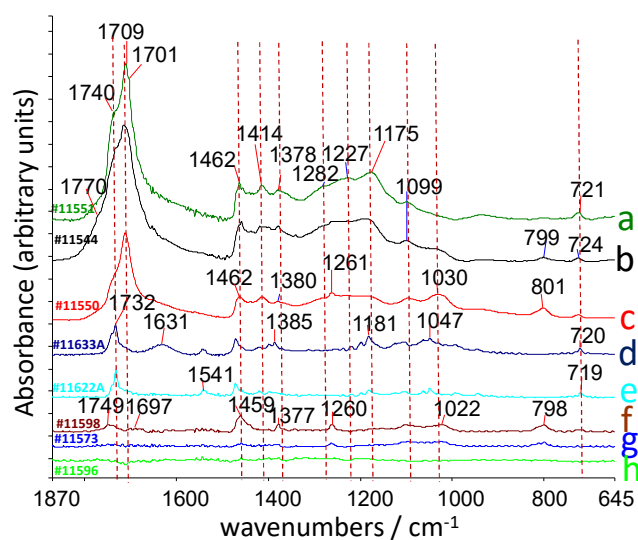
Figure S1. Infrared spectra of samples extracted from methanol. Intensities of spectra reflect relative quantities of their components; (a) full spectrum, (b) C-H stretching region, and (c) carbonyl stretch and C-H deformation region.



(a)

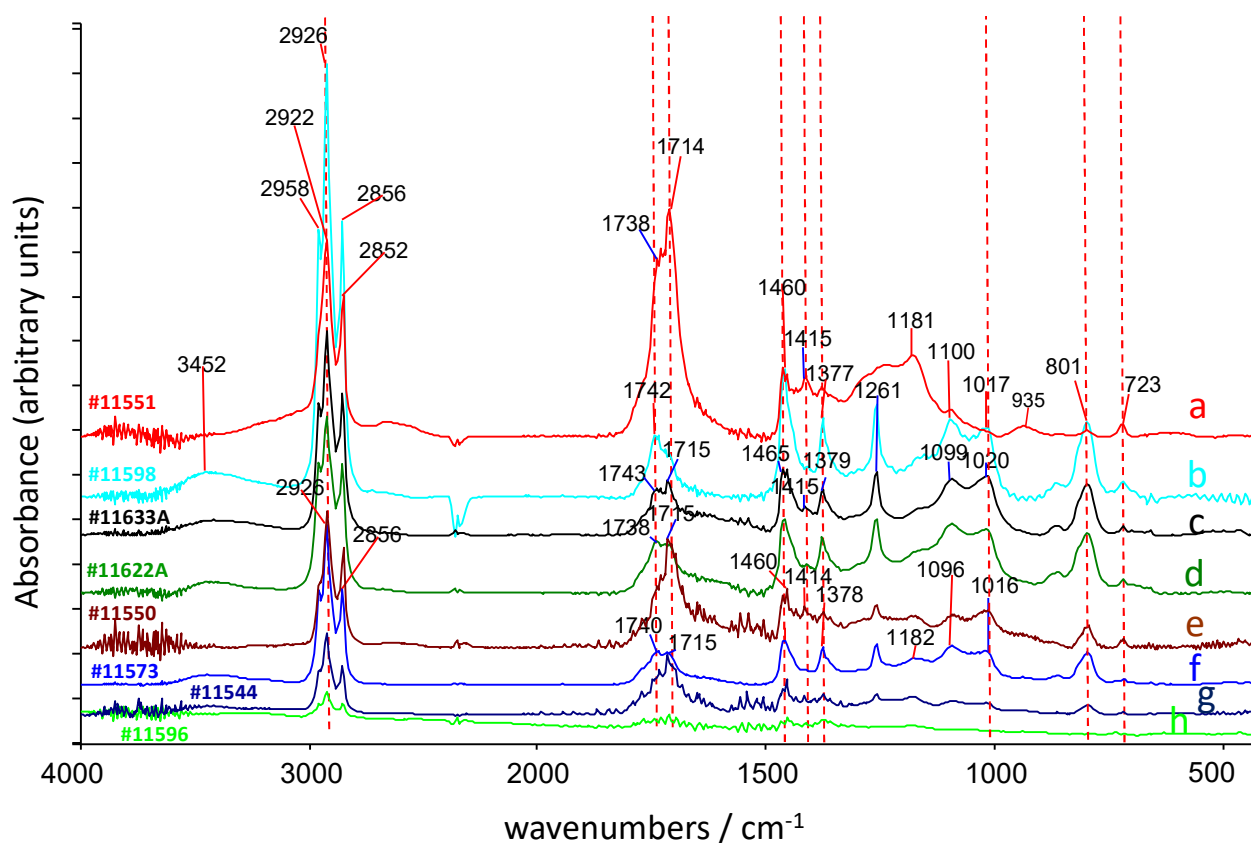


(b)

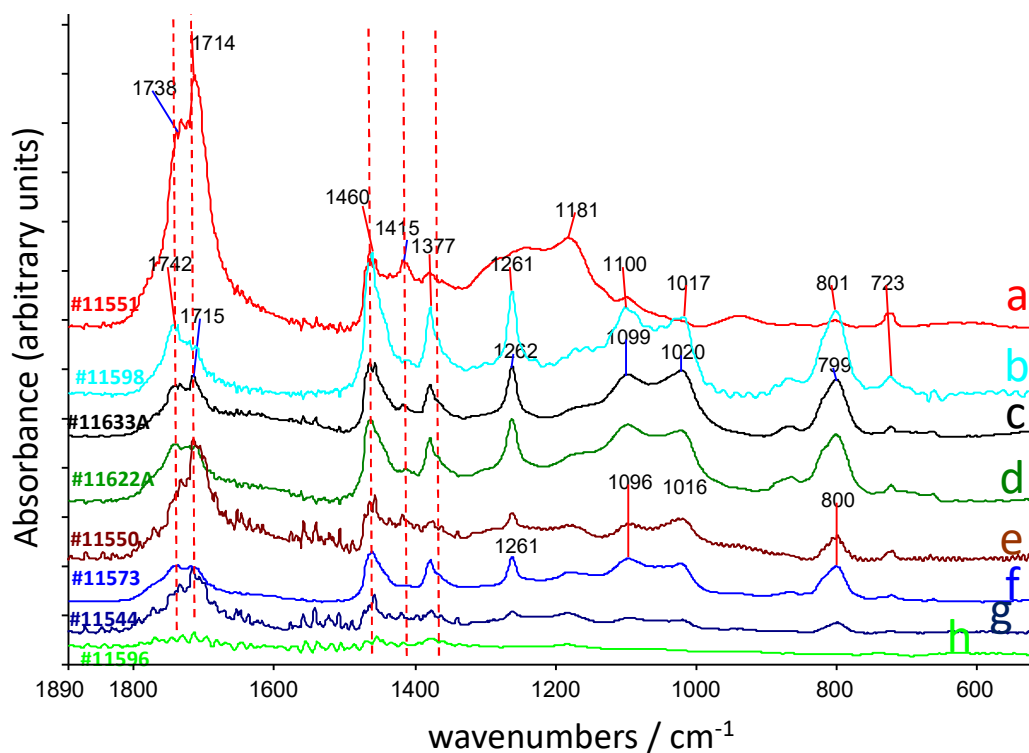


(c)

Figure S2. Infrared spectra of samples extracted from acetone. Intensities of spectra reflect relative quantities of their components; (a) full spectrum, (b) C-H stretching region, and (c) carbonyl stretch and C-H deformation region.



(a)



(b)

Figure S3. Infrared spectra of samples extracted from dichloromethane. Intensities of spectra reflect relative quantities of their components; (a) full spectrum, and (b) carbonyl stretch and C-H deformation region.

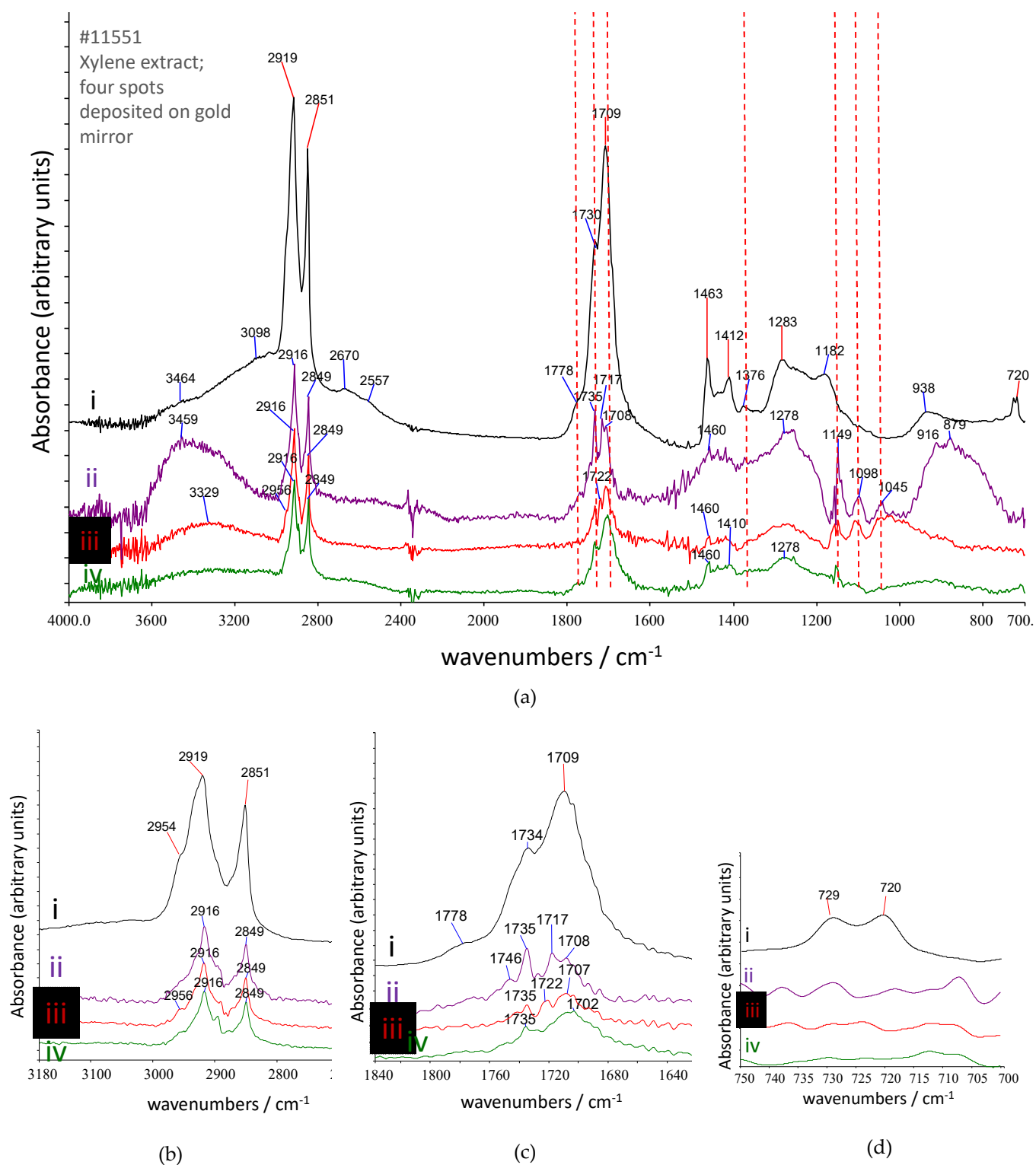
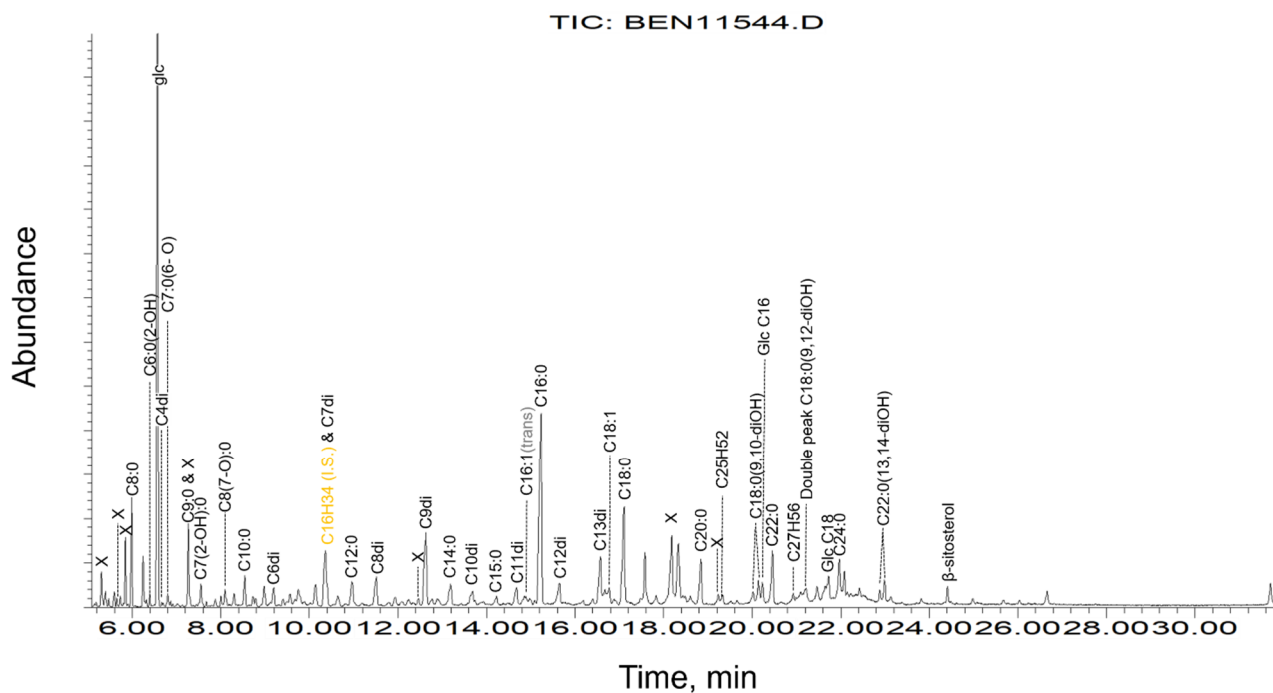
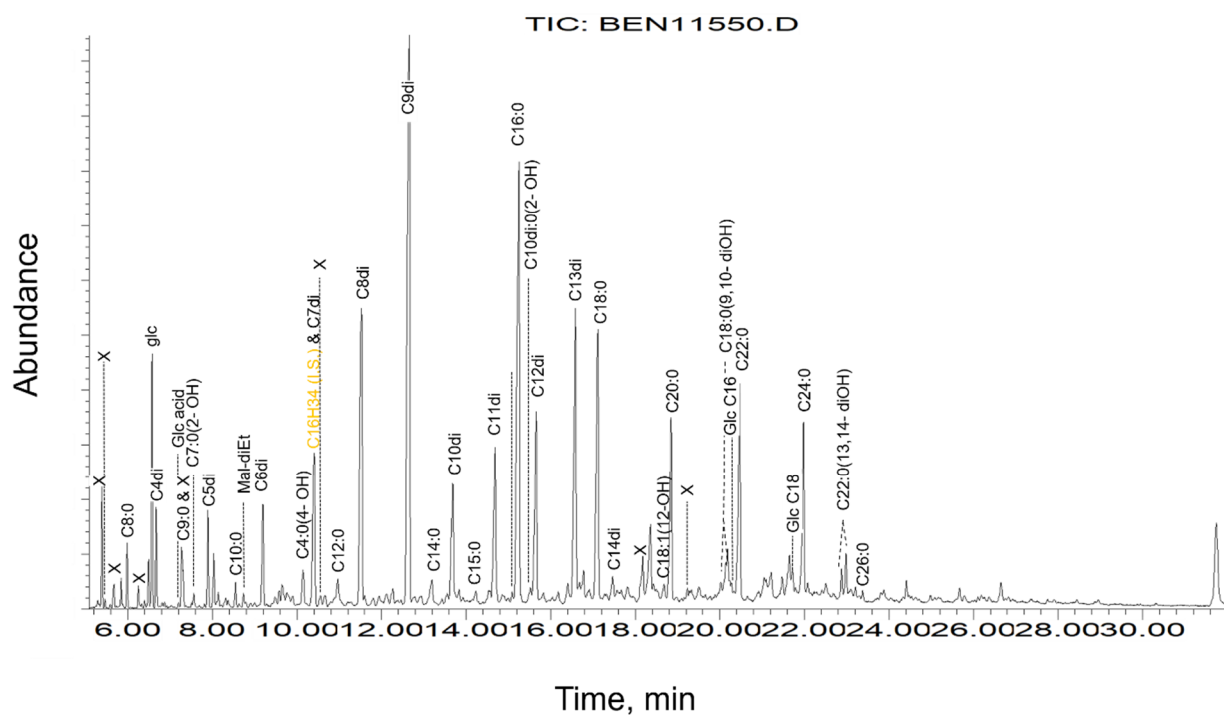


Figure S4. Microscopy FTIR spectra of sample #11551 extracted from xylene and deposited on gold mirror disc; spectra (i)–(iv) correspond to four different micro-separated spots on the disc; (a) full spectra; (b) the C-H stretching region, (c) carbonyl region, and (d) methylene rocking region.

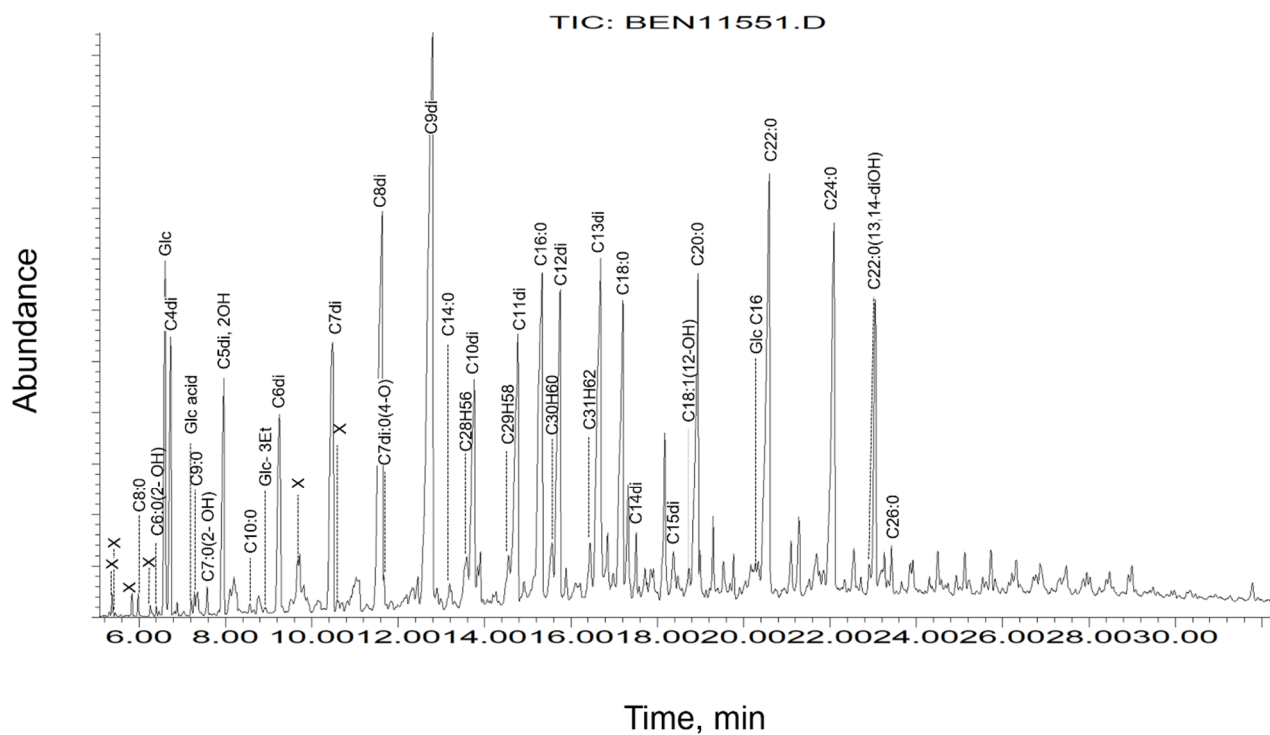
2. Gas chromatograms (Figure S5)



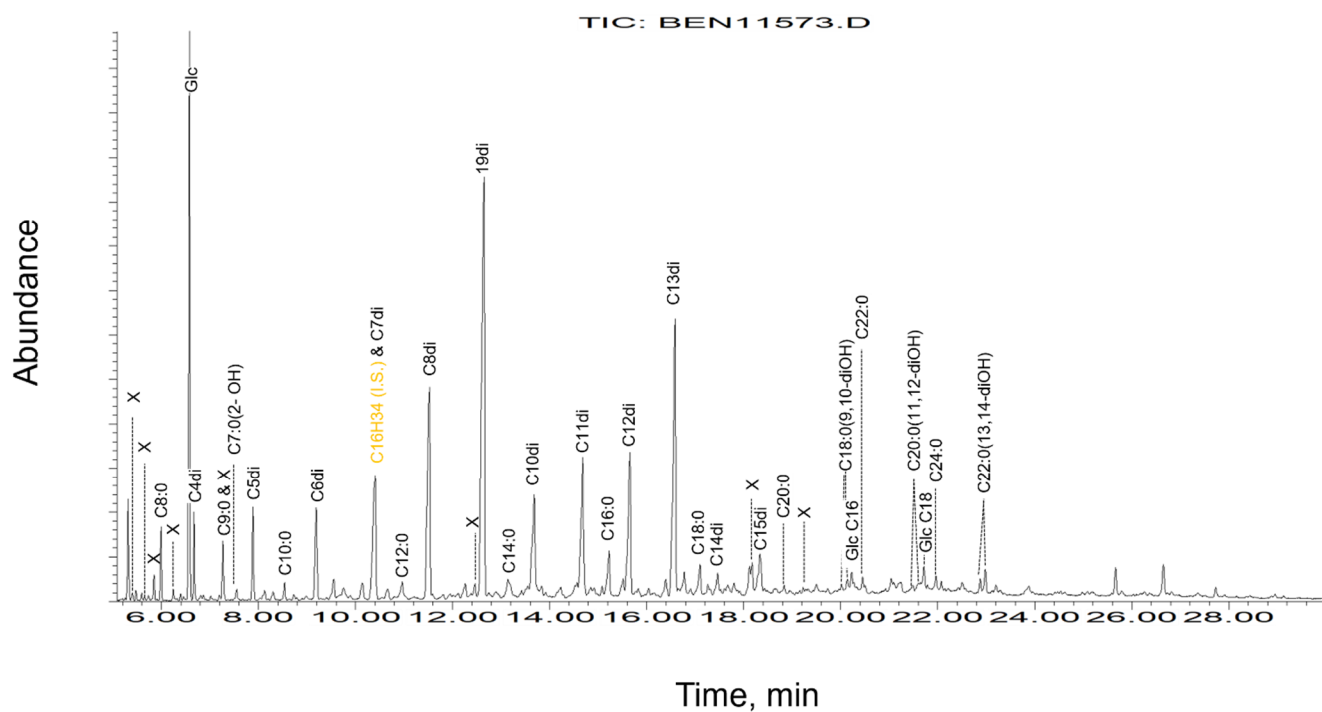
(a) sample #11544



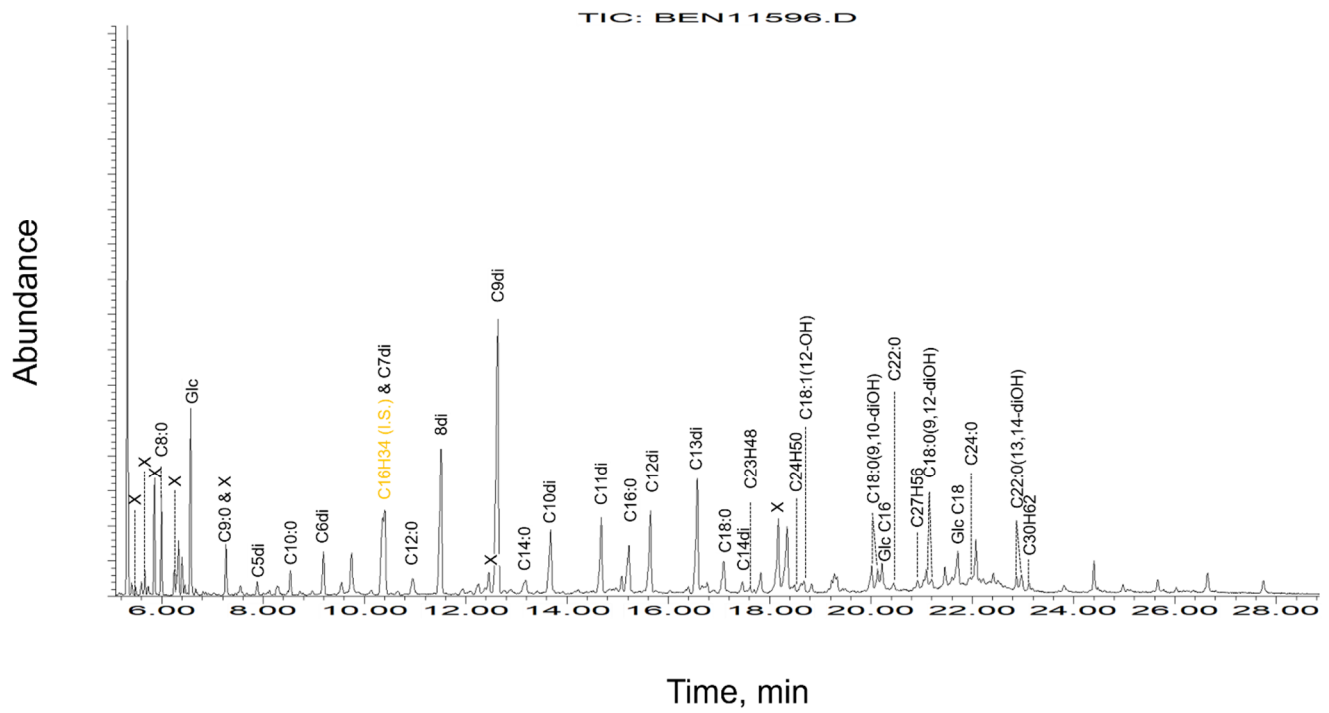
(b) sample #11550



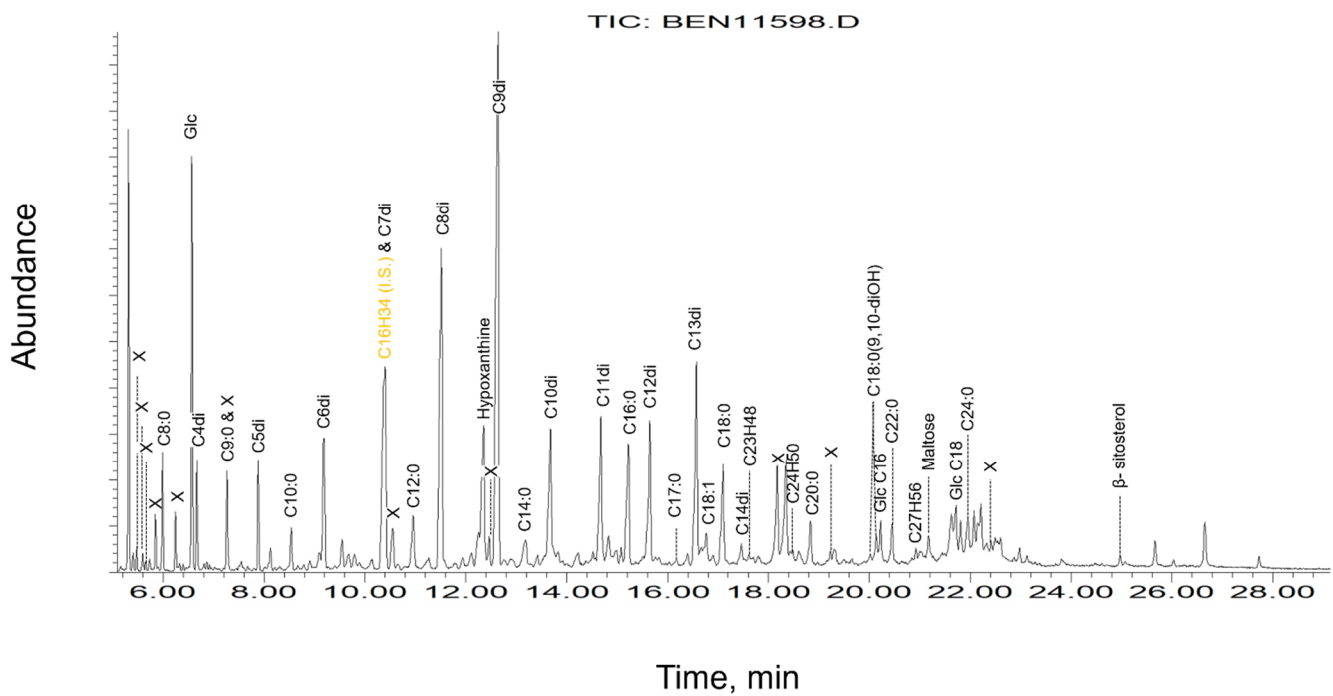
(c) sample #11551



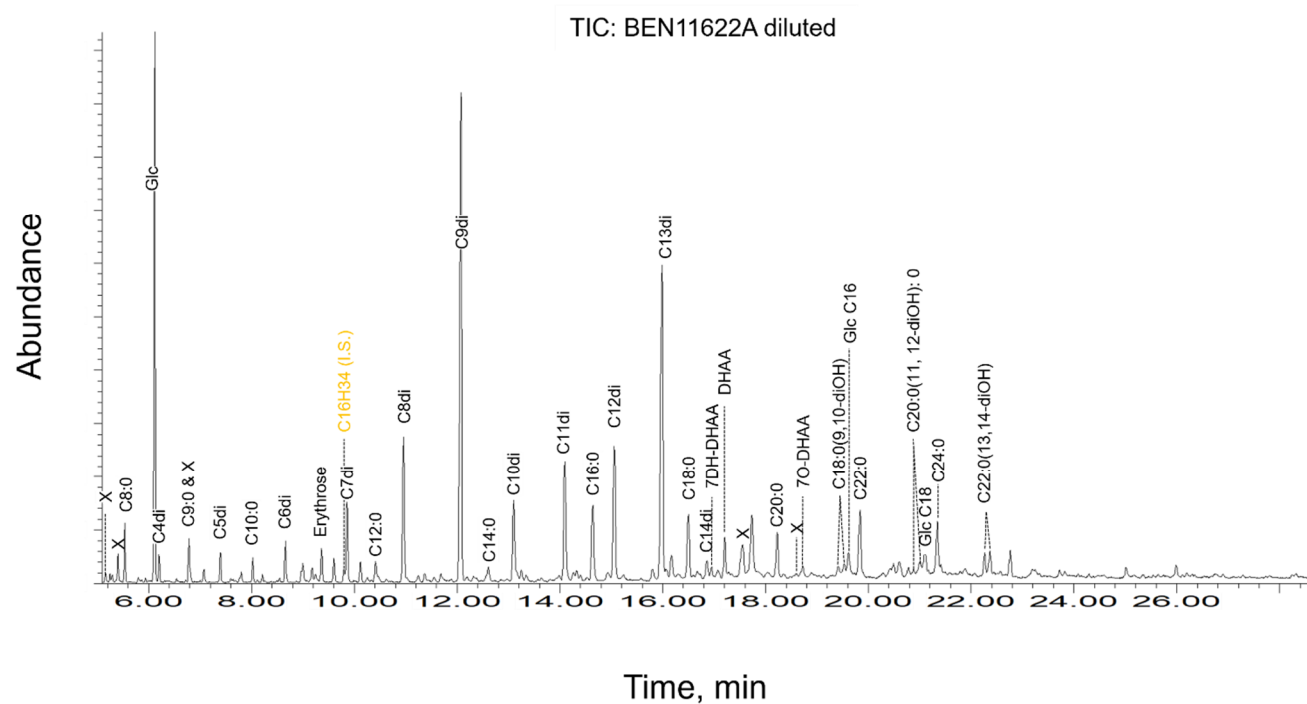
(d) sample #11573



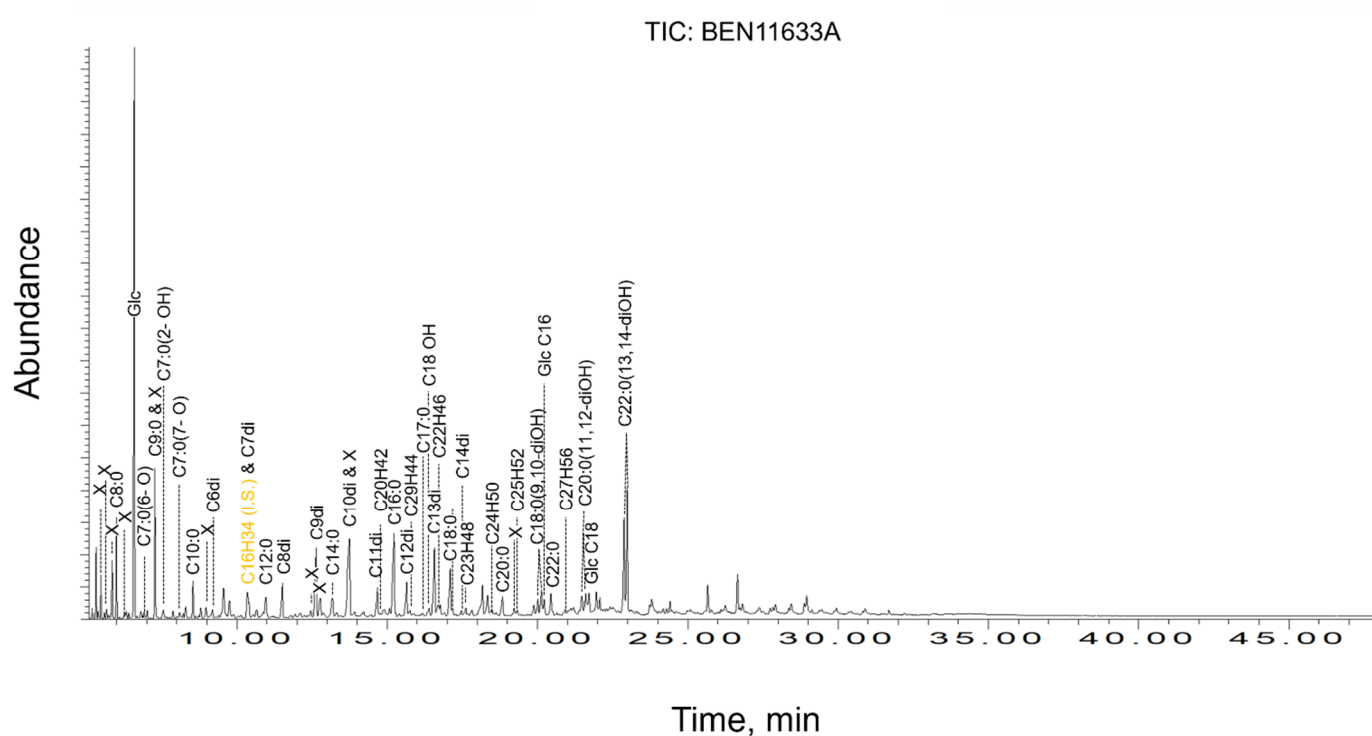
(e) sample #11596



(f) sample #11598



(g) sample #11622A



(h) sample #11633A

Figure S5. (a–h): Partial total ion gas chromatograms of all samples with main identified components; For a key of abbreviated analytes, see Table S1. IS: Hexadecane (internal standard, see Materials and Methods in main text); x: unknown.

3. Table S1. Organic compounds with relative integration areas detected in the various samples through gas chromatography-mass spectrometry.

retention time (t _R , min)	Compound (abbreviation) ¹	Compound (full name) ¹	Lamp	Lamp	Lamp	Small bowl	Small bowl	Spouted bowl	Pedestalled bowl	Pedestalled bowl
			#11544 (1.1 mg)	#11550 (2.5 mg)	#11551 (9.5 mg)	#11573 (2.0 mg)	#11596 (1.8 mg)	#11598 (2.0 mg)	#11622A (1.4 mg)	#11633A (13.5 mg)
6.00	C8:0	Octanoic (caprylic) acid	2.60	0.74	0.13	1.33	2.33	1.33	0.99	2.59
6.40	C6:0(2-OH)	2-hydroxy-hexanoic acid	0.35		0.05					
6.60	Glc	Glycerol	20.49	2.99	2.59	11.93	4.80	5.15	10.10	17.41
6.70	C4diCOOH	Butanedioic (succinic) acid	0.10	1.11	2.28	1.55		1.26	0.45	
6.80	C7(6-O):0	6-oxo-heptanoic acid	0.44							0.34
7.20	Glc acid	Glyceric acid		0.07	0.10					
7.30	C9:0	Nonanoic (pelargonic) acid	2.55	1.17	0.14	1.35	1.56	1.39	1.01	4.62
7.60	C7(2-OH):0	2-hydroxy-heptanoic acid	0.93	0.21	0.19					0.48
7.90	C5diCOOH	Pentanedioic (glutaric) acid acid		1.21		2.04	0.42	1.46	0.65	
7.96	C5di, 3Et	3-ethyl-glutaric acid		0.19						
8.00	C5di, 2OH	2-hydroxy-glutaric acid			2.32					
8.10	C8(7-O):0	7-oxo-octanoic acid	0.65							0.30
8.50	C10:0	Decanoic (capric) acid	1.13	0.33	0.09	0.49	0.93	0.72	0.48	1.31
9.20	C6diCOOH	Hexanedioic (adipic) acid	0.79	1.81	2.74	3.01	1.75	2.67	0.87	0.59
9.40	Erythrose	Erythrose							0.85	
10.30	C16H34 (I.S.)	Hexadecane (I.S.)	3.13	0.35		4.10	5.35	5.36	0.30	1.66
10.40	C7diCOOH	Heptanedioic (pimelic) acid	0.58	3.35	4.43	2.03	1.50	2.01	2.03	0.51
11.00	C12:0	C12:0 Dodecanoic (lauric) acid	1.45	0.77		0.67	1.05	1.44	0.66	1.43
11.50	C8diCOOH	Octanedioic (suberic) acid	1.61	7.59	7.66	9.47	7.07	8.62	4.19	1.80
11.60	C7di (4-O)	4-oxo-heptanedioic acid			0.17					
12.60	C9diCOOH	Nonanedioic (azelaic) acid	4.30	15.56	13.67	20.21	14.23	14.78	15.07	3.84
13.20	C14:0	Tetradecanoic (myristic) acid	1.27	0.79	0.06	1.12	1.02	1.12	0.58	1.61

13.70	C10diCOOH	Decanedioic (sebacic) acid	0.78	2.98	3.37	4.23	3.32	4.59	2.86	7.07
14.20	C15:0	Pentadecanoic acid	0.70	0.22						
14.70	C11diCOOH	Undecanedioic acid	1.05	3.73	4.39	5.82	3.39	3.79	4.02	1.69
14.90	C16:1(trans)	trans-hexadec-9-enoic (trans-palmitoleic) acid	0.35							
15.20	C16:0	Hexadecanoic acid (palmitic) acid	11.10	11.23	6.01	2.00	2.79	3.17	2.86	5.55
15.50	C10di (2-OH)	2-hydroxy-decanedioic acid		0.36						
15.70	C12diCOOH	Dodecanedioic acid	1.23	4.43	4.54	5.89	3.75	3.49	4.48	2.04
15.80	C29H60	Nonacosane								0.27
16.20	C17:0	Heptadecanoic acid			0.09			0.17		0.16
16.40	C18OH	Octadecanol								0.57
16.60	C13diCOOH	Tridecanedioic acid	2.65	6.76	5.90	11.01	4.01	4.81	11.00	3.69
16.70	C22H46	Docosane								0.76
16.80	C18:1	cis-Octadec-9-enoic (oleic) acid	0.61	0.37				1.02		
17.00	DH6-DHAA	6-dehydro-dehydroabietic acid							0.25	
17.10	C18:0	Octadecanoic (stearic) acid	5.31	6.23	4.25	1.20	1.73	2.56	2.12	2.93
17.20	DHAA	Dehydroabietic acid							1.22	
17.50	C14diCOOH	Tetradecanedioic acid		0.50	0.56	0.80	0.56	0.63	0.59	0.22
17.60	C23H48?	Tricosane?					0.21	0.21		0.40
18.40	C15diCOOH	Pentadecanedioic acid			0.69	1.80			2.29	1.44
18.50	C24H50	Tetracosane					0.27	0.24		0.36
18.60	Glc, C14?	Myristoyl-glycerol?								0.18
18.70	7O-DHAA	7-oxo-dehydroabietic acid							0.46	
18.70	C18(12-OH):1	12-hydroxy-oleic (ricinoleic) acid		0.33	0.39		0.44			
18.80	C20:0	Eicosanoic (arachidic) acid	2.26	3.69	4.48	0.23		1.04	1.45	1.10
19.30	C25H52	Pentacosane	0.47							0.30
20.10	C18(9,10-diOH):0	9,10-dihydroxy-stearic acid	1.60	0.58		0.42	2.30	0.77	0.56	2.38

20.20	Glc, C16	Palmitoyl-glycerol	0.81	0.89	0.29	0.36	1.20	0.78	0.78	0.78
20.40	C22:0	Docosanoic (behenic) acid	2.61	4.61	7.57	0.29	0.52	0.49	0.33	1.07
20.92	C27H56	heptacosane	0.22				0.42	0.23		0.38
21.10	C18(9,12-diOH):0	9,12-dihydroxy-octadecanoic acid	0.97				1.72			
21.50	C20 11,12diOH	11,12-dihydroxy-eicosanoic acid				0.55			1.44	2.44
21.20	Maltose	Maltose						0.53		
21.70	Glc, C18	Stearoyl-glycerol	0.78	0.32		0.63	1.86	1.13	0.83	1.01
22.00	C24:0	Tetracosanoic acid	1.91	3.19	5.74	0.40	0.50	0.89	1.76	1.08
22.40	C29H60	Nonacosane	0.32							
22.90	C22(13,14-diOH):0	13,14-dihydroxy-docosanoic acid	1.33	1.08	3.38	1.07	1.38		18.32	9.98
23.00	C30H62	Triacontane					0.34			
23.40	C26:0	Hexacosanoic acid		0.19	0.36					
24.70	C28:0	Octacosanoic acid			0.09					
25.00	β -Sitosterol	β -Sitosterol	0.23					0.23		

¹ a,b refer to isomers with the same molecular FW.