THE USES OF CYPRIOTE WHITE-SLIP WARE INFERRED FROM ORGANIC RESIDUE ANALYSIS

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Abstract

The hemispherical and shallow Cypriote white-slip (WS) vessels have been called "milk bowls" solely for their appearance. The first organic residue analysis of the white-slip layer of ten sherds, ranging from proto-WS to WS II, shows that they were used as serving bowls for hot cooked meals containing meat and animal fat, vegetable oil, leafy vegetables, and potherbs. On other occasions the same bowls served as drinking vessels for wine flavored with pine resin (*retsina*).

1. Introduction

Very few ceramic types of the Mediterranean world have achieved the great popularity of Cypriote White-Slip ware. For four centuries this fabric was dominant not only in Cyprus (*ca.* 1600–1200 B.C.), but was also extremely popular in other areas of the Mediterranean, from the Syro-Palestinian coast to the Central Mediterranean, from Egypt to Anatolia. It is found in settlements, but also in tombs. Although there is a variety of shapes in White-Slip ware (e.g. jugs, juglets, tankards, and large bowls), the shapes *par excellence* were medium-sized hemispherical bowls with one 'wish-bone' handle, which must have been used for liquids. They usually have very thin walls (1–2 mm). The interior is covered by a thick (200–300 μm) white slip so durable that one may use a metallic brush on it without causing any damage. The core of the clay is usually coarse, gritty and very hard, They are decorated only on the exterior, with the white-slip interior left blank. This cannot be accidental: there is a series of stylistic and typological elements suggesting that such luxury bowls were used for drinking liquids, hot or cold. Their undecorated interior was suitable for this use, unlike the other Middle Bronze Age bowls, which were made of soft, porous fabric and which are usually painted on their interior surfaces. In the eyes of the foreign clientele, it must have been an attractive hand-made ceramic type, with its smooth, white inner surface and its linear, embroidery-like outer decoration. Even then the Mycenaeans and the Minoans, who were using very fine sophisticated wheel-made pottery during the Late Bronze Age, showed a particular liking for this fabric. They not only used it in their houses as luxury pottery, but in several instances imitated its shape and decoration locally, as for example in Rhodes at the 16th century B.C. settlement *Trianda* (Karageorghis and Marketou, forthcoming).

White Slip I ware, which succeeded the short-lived experimental proto-White Slip variety, is of excellent ceramic quality. Gradually, however, the quality of the slip and paint degenerated, and towards the end of the 13th and beginning of the 12th centuries B.C. the slip and painted decoration are of quite poor quality. It was the end of this pottery, which was soon to be replaced by the local version of the so-called "Mycenaean IIIC:1b" fabric. In the kitchens of Cyprus and the neighbouring countries the drinking bowls of White Slip II ware were replaced by bronze hemispherical bowls which are found in abundance especially in tombs of the beginning of the 12th century B.C. (Late Cypriote IIIA).

A technical study of WS ware, based on a well-documented collection of WS ceramic sherds from Kouklia and the Nicosia Museum, showed progressive changes in the raw materials used for the slip and the dark decoration (Aloupi *et al.* 2001a). They follow the archaeological classification scheme from proto-White Slip to White Slip II. The key result is that in monochrome WS I ware the dark decoration is invariably based on the iron reduction technique, whereas in WS II it is based on the use of manganese-rich pigments. In a similar way, the slip itself undergoes a

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transformation from a quartzitic-koalinitic or smectitic material for WS I to micaceous (chloritic) material for WS II. The difference in the mineralogical and chemical composition of the slip is reflected in its micromorphology in the scanning electron microscope. The slip layer shows some sintering and vitrification, but is rather porous compared to the ceramic body which in most cases is totally vitrified. The body is made of iron-rich clays with a calcium oxide content below 4.5%, which vitrifies easily at 950–1000°C, especially when fired under reducing conditions. According to this study, which combined analytical data with refirings in the laboratory, there is no doubt that the majority of the sherds have been exposed to temperatures exceeding 1000–1050°C, which can only be achieved when firing takes place in built kilns, but not in open fires.

The MBA and LBA hemispherical, decorated WS bowls have long been called "milk bowls" (Yon 1976), for no reason other than that they give the appearance of containing a white liquid. Accordingly, at a conference devoted to this unique pottery (Karageorghis 2001a), the extensive discussion of the uses of WS ware centered on milk and yogurt, but the serving of "hot liquid meals such as soups" was proposed as a more likely use (Karageorghis 2001b). Organic residue analysis was mentioned as the method that can move the discussion of the use of these vessels from the speculative to the factual. This has now been carried out by the American authors and we present the results in this report.

2. Sample Preparation

A collection of ten WS sherds was made available for analysis. The sherds belong to a study collection of Cypriote WS ware of uncertain origin from the so-called *Universities Collection* in the Museum of Nicosia, given to THETIS for destructive technical analysis and materials characterisation in the course of a research project funded by the A. G. Leventis Foundation (Aloupi *et al.* 2001b). The ten sherds selected for organic residue analysis (THETIS Code Nos, WS-NIC-1, 4-12) are all from hemispherical or shallow bowls and cover all three types of WS ware, from proto-White Slip (WS-NIC-9) through White Slip I (WS-NIC-1, 5, 6, 7, 8, 10, and 12) to White Slip II (WS-NIC-4 and 11). The exterior of the sherds is shown in Figs. 1 and 2.

In order to limit the analysis to the materials contained in the bowls, the white slip was removed

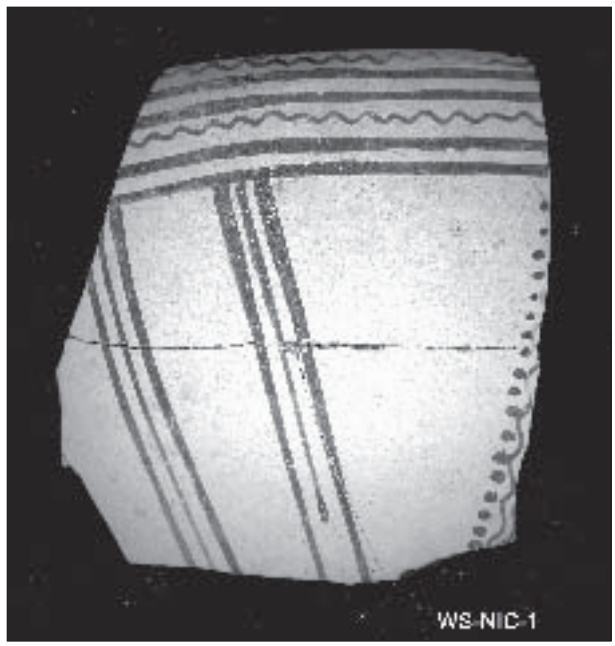

Fig. 1 White-Slip Sherd WS-NIC-1

from the interior surfaces of the sherds with a stainless-steel burr mounted in a low-speed electric drill. The quantities of powdered slip obtained, listed in Table 1, range from 10 to 160 mg and average 64 mg or more than an order of magnitude below the 1 to 5 g of ground ceramic customarily used for organic residue analysis in ancient pottery, but have nevertheless yielded a wealth of information.

The ground slip was extracted with 10 mL of a mixture of diethyl ether and dichloromethane (1:1 by volume) with intermittent ultra-sonic agitation. After centrifugation, the supernatant solution was decanted, concentrated to about 1 mL at 30°C in a stream of nitrogen, and methylated with diazomethane in order to convert carboxylic acids to their more volatile methyl esters. The resulting solution was reduced to a volume of 0.1 to 0.3 mL by evaporation at room temperature,

3. Method of Analysis

The methylated extract (0.5 μl) was introduced by splitless injection into a Hewlett-Packard HP 6890 gas chromatograph (GC) equipped with an HP 5973 Mass Selection Detector (MSD), and an HP MSD ChemStation computer. The instrument had a 15 m × 0.5 mm Alltech capillary column with a stationary phase of poly(methylsiloxane). The column had an initial temperature of 50°C and was ramped at 5°C/min. to 250°C for a running time of 40 minutes. The inlet temperature was 250°C. The carrier gas was helium at a con-

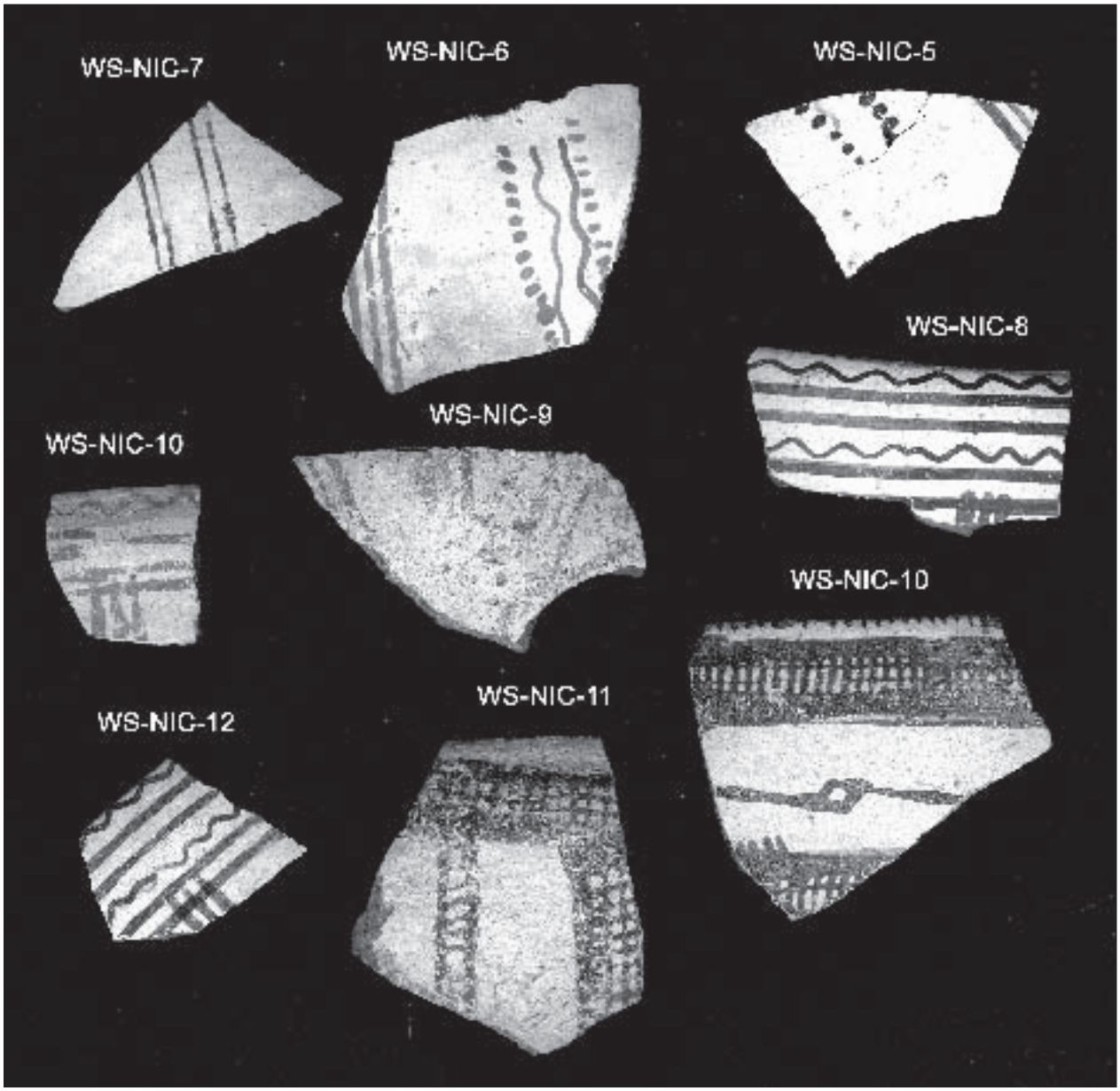

Fig. 2 White-Slip Sherds WS-NIC-4 to WS-NIC-12

stant flow rate of 1.2 ml/min. Fragmentation was by electron impact at 70 eV.

4. Presentation of Results

The constituents that could be identified, specifically or categorically, are listed in Tables 2–11. The first column gives the retention time (RT) in minutes, the second the molecular ion (MI) followed by its intensity in parentheses. If no molecular ion was found, the largest fragment ion is listed instead, enclosed in square brackets. The third column gives the base peak (BP) and the fourth a list of fragment ions in order of decreasing intensity, which again is listed in parentheses. An asterisk after a fragment ion indicates that the ion is known to be extraneous to the mass spectrum, i.e. it is caused by an unresolved impurity. When possible, the nature of that impurity is indicated in the fifth column, which also gives one or two names of the principal constituent. The sixth column lists the Chemical Abstracts Registry Number, an arbitrary but unique designation of the chemical structure. The last column gives the percentage that the constituent contributed to the total ion current. This is not the same as the actual percentage in the sample, because different structures may have quite different ion yields, but these percentages will reflect the relative amounts quite accurately when members of a homologous series, e.g. fatty acids, are compared. Amounts of less than 0.05% are listed as “trace”.

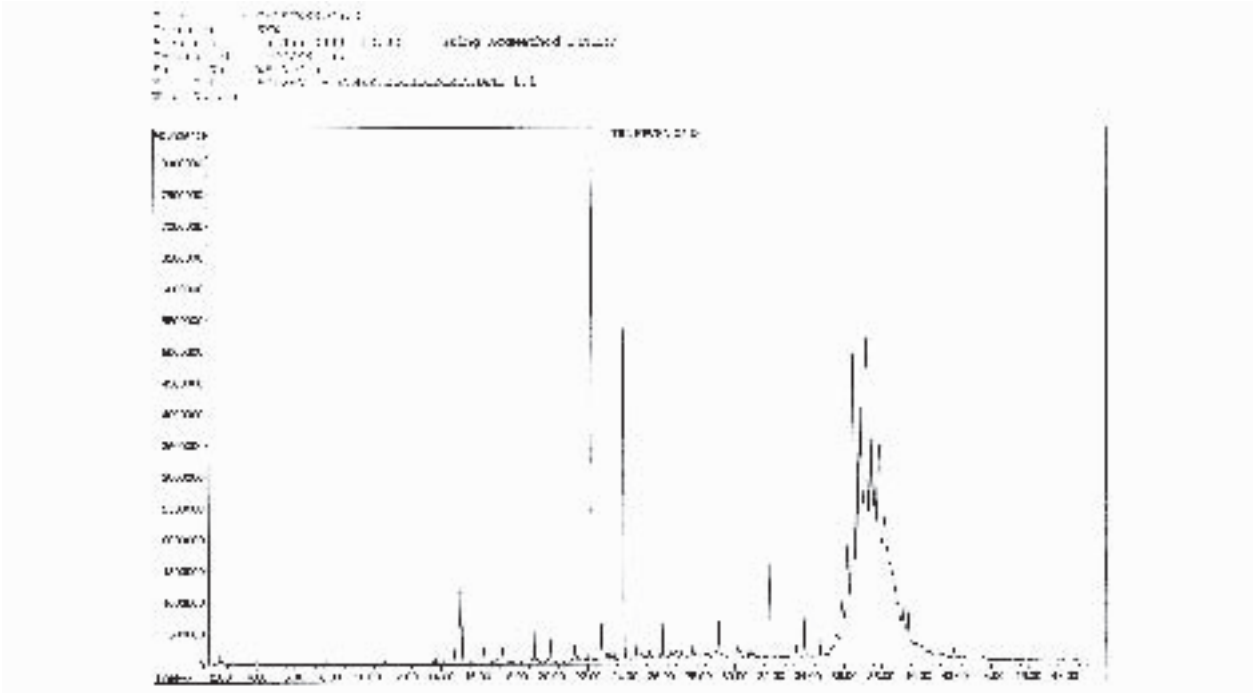

Fig. 3 Total Ion Chromatogram of White-Slip Sherd WS-NIC-5 with unresolved phthalate contaminants at RT = 35–40 minutes

5. Contaminants

Prolonged storage of the sherds in plastic bags has introduced the contaminants identified in the Tables. They account for as much as 90% of the organic residue. A group of unresolved peaks at retention times ranging from 34 to 41 minutes (Fig. 3) accounts for most of the contaminants and is due to generically identified high-molecular-weight esters of phthalic acid that are the most widely used plasticisers in such bags. The number of peaks listed for these clusters is certainly greater than the number of actual isomers, since many of the higher phthalate esters yield multiple peaks (Middleditch 1989). Most of the 44 individually identified contaminants are also plasticisers, including lower-molecular-weight phthalate esters (18), adipic acid esters (5), mono- and di-isobutyric acid esters of 2,4,4-trimethyl-1,3-pentanediol (6), triaryl phosphates (2) and an alkyl stearate (1).

Six contaminants are degradation products of antioxidants which may come from these plastic bags and/or from the stabilisers present in the commercial diethyl ether used as a solvent. The second solvent used, dichloromethane, is certainly responsible for three occurrences of the contaminant 1,1,2,2-tetrachloroethane.

The branched octyl phenols found in two sherds are industrial compounds not found in nature. Their origin is unknown, but we have previously encountered them in three plaster linings of Hellenistic cisterns on Naxos (Beck *et al.*, in press).

Lastly, there is a single occurrence of oleamide, a release agent used to improve the surface of plastic films (Noller 1965).

While all the contaminants are readily identifiable as such, their presence in amounts greatly exceeding those of the ancient organic compounds is highly undesirable, because their large peaks are very likely to obliterate the much smaller peaks of diagnostically important ancient constituents. Excavators and museum curators should avoid plastic containers of any kind for the storage of artifacts that may later be subject to organic residue analysis. The safest procedure is to wrap the find tightly in uncoated aluminium foil and store it in paper envelopes or cardboard boxes.

6. Ancient Constituents

Tables 2 to 11 show a total of 345 occurrences of ancient constituents in the white-slip layer of ten sherds. Because many constituents are present in very small or even trace amounts which yield less than optimal mass spectra, we are presenting our primary data so that our conclusions can be critically evaluated. Because the assignment of ancient constituents to specific floral or faunal species or even genera is beset by substantial uncertainties

(BECK 2004), we confine our interpretation to the identification of the major categories of food and, as it turns out, of drink. The discussion of results will be by these categories, which are also the headings of Table 1, where the compounds indicative of each category are listed and where the numbers following a type of compound (aldehyde, alkane, fatty acid, etc.) are the number of carbon atoms of the compounds found of that type.

6.1. Meat and Animal Fat

The main constituents of animal fats are long-chain, saturated fatty acids, but these so-called n-fatty acids also occur, at lower concentrations, in vegetable oils. They are therefore shown in Table 1 as straddling the two food categories in order to convey that their 65 occurrences are consistent with the presence of animal fats as well as of vegetable oils. Indeed, the relative amounts of the fatty acid are best explained by the simultaneous presence of both.

The branched iso- and anteiso-fatty acids are the most widely recognized markers of bacterial action, which may have been post-depositional. "But the contributions of bacterial lipids to archaeological pottery are difficult to assess since commonly occurring ruminant animal fats contain an appreciable abundance of bacterial lipids which derive from the function of the rumen" (DUDD *et al.* 1998). SEHER *et al.* (1980) took iso-acids in the residue of an Egyptian vessel of the XXVIth Dynasty as evidence of ruminant fat. In Table 1 we have assigned these branched acids to the animal fats, but note here that some may in fact be post-depositional artifacts.

Cholesterol, of which trace amounts were found in sherd 5, is generally regarded as an animal sterol, although evidence of its occurrence in higher plants has been accumulating (KARRER *et al.* 1981). Particularly interesting is the presence of cholesterol in beans (*Dolichos biflorus*) and lentils (*Lens culinaris*) (AKIHISA *et al.* 1991), because pulses (Greek: *ospria*) have long been a staple of the Greek kitchen; but the cholesterol in these seeds was accompanied by much larger amounts of the plant sterols stigmasterol and beta-sitosterol, neither of which could be found in the white-slip pottery. If the cholesterol in sherd 5 is derived from fatty meat, one may wonder why it was not found in any of the other sherds, particularly in those that patently did contain meat; the answer lies most likely in the retention time of cholesterol which is within the range where it would be masked by the cluster of phthalate contaminants.

The group of compounds that most convincingly indicate meat are the polyaromatic hydrocarbons (PAHs). They are smoke condensates from open cooking fires (OUDEMANS and BOON 1991) and will therefore also be present in meat that has been roasted (barbecued) over an open fire. Along with other degradation products, pyrene and fluoranthene have been reported in aerosols produced by charbroiling meat (ROGGE *et al.* 1991). This indicates that meat was first roasted over an open fire to enhance its flavor and then combined with vegetables and oil in a stew.

6.2. Vegetable Oil

The mono-unsaturated fatty acids palmitoleic acid, oleic acid, and elaidic acid are the principal constituents of vegetable oils, including olive oil, although they are also present, in much smaller amounts, in animal fats.

Aliphatic aldehydes occur sporadically in a range of plants, but the groups of aldehydes with from eight to twelve carbon atoms in the white-slip sherds are much more likely degradation products of vegetable oils exposed to heat (TAKEOKA *et al.* 1996). This study, which used soybean oil, also reported 2-ketones, gamma-lactones, alkanes with up to 18 carbon atoms, and 1-alcohols, the latter only up to eight carbon atoms. A parallel study of heated olive oil, reported only 2-ketones and gamma-lactones (YOO *et al.* 1988), as did work with butter oil, an animal fat (NAWAR *et al.* 1988. Thus the compounds found in the white-slip sherds provide ample evidence for heated vegetable oil, but some of the compounds listed for vegetable oil in Table 1 may also have been produced by heated animal fat. SEHER *et al.* (1980) recognized 2-letones in a XXVIth Dynasty vessel from Egypt as degradation products of fatty acids without deciding whether these were of animal or plant origin.

6.3. Leafy Vegetables

All leaves, as well as fruits and petals, are coated with a layer of epicuticular wax of which alkanes with more than 20 carbon atoms are major constituents (TULLOCH 1976).

These waxes also contain so-called wax esters composed of long-chain fatty acids and long-chain 1-alcohols to which components they revert upon hydrolysis. The fatty acids with 20 and 22 carbon atoms may be derived from wax esters; the 1-alcohols found are rather shorter than would be

expected and may be degradaion products of fats and oils.

Phytane, tentatively identified in sherd 5, is the reduction product of phytol, the alcoholic side chain of chlorophyll present in all green plants (Budavari 1989).

6.4. Carbohydrates

Carbohydrates cannot be detected by the GC-MS technique without specialised derivatisation. However, their pyrolysis breakdown products have been observed (Saiz-Jimenez *et al.* 1987; Oudemans and Boon 1991; Galletti and Bocchini 1996; McCobb *et al.* 2001). Specifically, 1H-indene, which we found in seven sherds, and 1-indanone, which we found in one, have both been reported in archaeological and experimental chars (Pastorova *et al.*1993). Their presence confirms the identification of vegetable matter in the white-slip pottery.

6.5. Resinated Wine

An unanticipated result is the identification of tricyclic diterpene resin acids and their degradation products. In nine of the ten sherds, there are 39 occurrences of 18 distinct compounds of this type. They are a certain indication of pine resin, a substance unfit for use in any cooked meal. Pine resin, however, has been used to flavor wine for at least 4000 years (Beck *et al.* 2004a) throughout the Eastern Mediterranean and continues to be used in Greece today for that purpose in the making of *retsina.* A trace of methyl benzoate in sherd 1 strongly suggests that the pine resin was collected from the Aleppo pine (*Pinus halepensis*), although the search for markers for all the pine species of the Eastern Mediterranean is not yet complete (Beck *et al.* unpublished).

6.6 Other Compounds

Sherds 1, 5, 9, and 10 contain 6,10,14-trimethtl-2-pentadecanone. This is a known constituent of oregano, thyme, and mint (Duke 2004) and has been found by Biers *et al.* (1994) in five of the Corinthian 'plastic' vases they studied. A high concentration (37.6%) of this compound has recently been reported in Greek *Herniaria spp.* (Lazari *et al.* 2000). While not a known food plant, *Herniaria* = rupturewort is a medicinal plant in later Greece (Dioscurides, *Materia medica* 4.108).

Pulegone is a monoterpenoid found in many plants, principally those of the mint family. We have tentatively identified it in Sherd 4.

9,10-Anthraquinone is present in five sherds (5, 6, 9, 10, and 11). Biers *et al.* (1994) reported a single occurrence. It has only two known botanical sources, *Senna obtusifolia*, which is a food plant in the Sudan, and *Rumex crispus* or yellow dock, a Eurasian weed used medicinally (Duke 2004; Mabberly 1997). It may be that this PAH is the product of roasting meat and we have listed it in the Meat & Animal Fat column in Table 1, but this assignment must be tentative.

7. Conclusions

The evidence presented shows that the term 'milk bowls' is inappropriate for the Cypriote White Slip ware. Rather, they were multi-purpose serving dishes used on some occasions to serve hot, cooked meals of meat and vegetables prepared with vegetable oil (probably mainly olive oil) and potherbs, among which may have been oregano, thyme, or mint. Since the vessels were certainly used again and again, the organic residues found are the remains of many meals which may not always have contained all these ingredients. On other, separate occasions the same vessels were used as drinking bowls for pine-resin-flavored wine (*retsina*).

The evidence does not exclude the possibility that the vessels may have, on still other occasions, contained milk, because our GC-MS analyses cannot distinguish between depot fat and milk fat. That distinction can be made by compound-specific gas chromatography – combustion – isotope ratio mass spectrometry (GC-C-IRMS) (Evershed *et al.* 1994; Dudd and Evershed 1998). However, when the same fatty acids are derived in part from animal fat, in part from vegetable oil, and possibly in part from milk fat, the values of the stable isotope ratio will be intermediate between the expected values for a single source and therefore unlikely to be decisive.

It is worth noting that similar results have been obtained for various MC and LCIA ceramic vessels from the destruction level of Akrotiri on Thera (Doumas 2004) which are contemporary with the proto-WS and WS I bowls examined here. Similar results have also been obtained from the organic residue analyses of more than a hundred MM and LM Minoan and LH Mycenaean sherds whose chronology spans the entire WS period (Beck *et al.* 2004a, 2004b). It thus appears that cooked meals of meat and vegetables, olive oil and potherbs were the most popular and widespread dishes in the Aegean and Eastern Mediterranean during the Bronze Age, and it is testimony to the deep traditionalism of Greek cookery that the same meals

can be had today in any authentic *taverna*, washed down, as they were then, with *retsina*.

Acknowledgements

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Sherd (sample weight)	**Meat & Animal Fat**	**Vegetable Oil**	**Leafy Vegetables**	**Carbohydrates**	**Resinated Wine**
WS-NIC-1 (120 mg)	isofatty acids 14,15,16, 17 anteisofatty acid 17 n-fatty acids 6,8,9,10,11,12,13,14,15,16,17,18,20,22	oleic acid aldehyde 10 2-ketone 14	alkanes 20,21,22,23,24 1-alcohols 12,13,14		Δ6-dehydroabietate dehydroabietae 7-oxodehydroabiete benzoate
WS-NIC-4 (90 mg)	isofatty acids 14,16,17 anteisofatty acid 11,15,17 n-fatty acids 12,13,14,15,16,17,18,20,21,22	palmitoleic acid oleic acid elaidic acid aldehydes 8,9,10 alkane 9	alkanes 22,24 1-alcohol 12	1H-indene 1-indanone	phenanthrene, simonellite dehydroabietate 7-oxodehydroabietate 8,15-pimaradienoate 8,15-isopimaradienoate x-hydroxydehydroabietate
WS-NIC-5 (60 mg)	cholesterol isofatty acids 15, 16? anteisofatty acids 10,11, 13,14,15,16? 9,10-anthraquinone n-fatty acids 12,13,14,15,16,17,18,20	palmitoleic acid oleic acid aldehydes 8,9,10, 11,12 2-ketone 14 alkanes 9,17,18	alkanes 20,21,22,23, 24,25 phytane ? 1-alcohols 12,13	1H-indene	tetrahydrodimethylphenanthrene tetrahydrotrimethylphenanthrene 8,15-pimaradienoate, simonellite tetrahydroisopimarate dehydroabietate, norabietatriene
WS-NIC-6 (30 mg)	isofatty acids 15,17 anteisofatty acid 15 pyrene, 4,5-dihydropyrene 9-fluorenone, fluoranthene 9(?)-phenanthrenol dibenzothiophene 9,10-anthraquinone n-fatty acids 12,14,17,18,20	palmitoleic acid oleic acid aldehydes 8,9,10	alkanes 22,23,24,25	1H-indene	phenanthrene x-methylphenanthrene dehydroabietate abietatetraenoate 4,5-methylenephenanthrene
WS-NIC-7 (10 mg)	isofatty acid 15 fluoranthene n-fatty acids 14,16,18	aldehydes 8,9,10 alkane 9	alkane 23	1H-indene	phenanthrene, dehydroabietate tetrahydroisopimarate tetrahydropimarate
WS-NIC-8 (10 mg)	isofatty acid 15 n-fatty acids 14,16,18	aldehydes 9,10 alkane 9	alkanes 22,23,24,25	1H-indene	dehydroabietate tetrahydroisopimarate tetrahydropimarate
WS-NIC-9 (60 mg)	isofatty acid 15 anteisofatty acid 16 9,10-anthraquinone n-fatty acids 14,16,18,20	oleic acid aldehydes 9,10 2-ketone 15 gamma-lactone 12 alkane 9	alkanes 21,22,23,24,25 1-alcohols 12,13,15		simonellite dehydroabietate tetrahydropimarate
WS-NIC-10 (80 mg)	isofatty acids 14,15,16? anteisofatty acids 15,16? 9-fluorenone, fluoranthene dibenzothiophene 9,10-anthraquinone n-fatty acids 12,13,14,16,17,18,20,22	palmitoleic acid oleic acid aldehydes 9,10 2-ketone 14 gamma-lactones 11?,12 alkanes 9,18	alkanes 20,21,22,23,25 1-alcohols 12,13		phenanthrene dehydroabietate abietapentaen-18-oate ?
WS-NIC-11 (160 mg)	isofatty acids 14,15,16 anteisofatty acids 13,159,10-anthraquinone n-fatty acids 12,13,14,16,17,18,20,22	palmitoleic acid oleic acid aldehydes 8,9,10 2-ketone 14 gamma-lactone 11? alkanes 9,18	alkanes 20,21,22,23, 24,25,29,31 1-alcohols 12,13	1H-indene	abietadiene dehydroabietate 8,15-pimaradienoate abietapentaenoate ?
WS-NIC-12 (20 mg)	n-fatty acids 14,16,18	aldehydes 9,10		1H-indene	

Table 1 Food Categories in Cypriote White-Slip Ware

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
1.53	102(1)	43	61(50) 42(41) 41(27) 45(25) 84(22) 59(20) 73(17) 69(14)...87(4)	4-hydroxy-3-methyl-2-butanone ?	[3393-64-4]	trace
2.29	130(1)	74	87(36) 43(26) 99(24) 59(16) 73(11) 101(11)	methyl caproate = hexanoate	[106-70-7]	trace
4.28	[130](17)	87	102(85) 57(35) 101(22) 55(19) 81(18) 59(16) 41(15) 129(13) 43(12) 88(10) 127(10)	methyl 2-ethylhexanoate	[816-19-3]	trace
4.96	136(40)	105	77(50) 51(17) 74(11) 83(11) 106(9) 50(8)	methyl benzoate	[93-58-3]	trace
5.95	[127](16)	74	87(48) 43(17) 55(16) 41(15) 57(15) 59(14)	methyl caprylate = octanoate	[111-11-5]	trace
7.73	[115](18)	57	43(78) 41(74) 70(74) 82(72) 56(63) 83(63) 55(58) 67(56) 68(54) 71(53) 69(52) 95(47) 112(44) 44(43) 82(43) 96(40) 84(37) 99(35)	decanal	[112-31-2]	trace
8.34	172(2)	74	87(50) 43(17) 55(15) 141(15) 129(14) 41(13)	methyl pelargonate = nonanoate	[1731-84-6]	1.33
10.81	186(4)	74	87(58) 85(24) 143(24) 43(19) 55(18) 41(16) 155(13) 59(10)	methyl caprate = decanoate	[110-42-9]	0.68
11.17	[173](11)	71	43(54) 56(36) 83(35) 89(35) 98(26) 41(19) 55(18) 57(13) 73(13) 143(10)	2,4,4-trimethyl-1,3-pentanediol, 3-isobutyrate CONTAMINANT	[74367-33-2]	3.95
11.68	[173](22)	71	89(76) 56(65) 43(51) 41(20) 73(18) 55(16) 57(16) 143(12) 85(11)	2,4,4-trimethyl-1,3-pentanediol, 1-isobutyrate CONTAMINANT	[74367-34-3]	4.58
13.06	194(5)	163	77(15) 164(10) 92(7) 76(7) 50(5) 105(5) 133(5) 135(5)	dimethyl phthalate CONTAMINANT	[131-11-3]	trace
13.24	200(4)	74	87(59) 43(16) 143(16) 55(14) 41(13) 75(13) 83(13) 157(13) 59(12) 57(10) 69(10)...169(8)	methyl undecanoate	[1731-86-8]	trace
14.41	140(16)	55	83(92) 69(87) 70(77) 43(64) 57(64) 97(63) 41(59) 56(59) 84(57) 82(47) 111(46) 68(41) 98(31) 67(24) 96(21) 112(21) 71(18) 85(18) 42(17) 81(16) 44(15) 54(14) 95(12) 125(10)	lauryl alcohol = 1-dodecanol	[112-53-8]	trace
15.59	214(7)	74	87(66) 143(19) 43(17) 55(17) 171(17) 41(14) 75(13) 183(12) 69(10) 59(9) 129(9) 57(8)	methyl laurate = dodecanoate	[111-82-0]	0.72
16.35	222(2)	149	177(27) 150(13) 176(10) 105(8) 76(6) 104(6)	diethyl phthalate CONTAMINANT	[84-66-2]	0.95
16.72	[154](14)	55	69(100) 83(100) 97(85) 70(84) 43(74) 56(71) 57(71) 41(61) 151(53) 82(51) 84(51) 68(46) 111(44) 95(40) 110(33) 98(32) 67(30) 71(29) 109(22) 87(20) 125(20)	1-tridecanol	[112-70-9]	trace
17.04	[243](8)	71	43(32) 159(10) 111(9) 41(7) 56(7) 155(6) 55(5) 69(5) 72(5) 173(5) 83(4) 143(4)	2,2,4-trimethylpentane-1,3-diol di-isobutyrate CONTAMINANT	[6846-50-0}	1.57
17.10	212(12)	58	43(68) 71(64) 59(44) 57(27) 41(25) 55(25) 85(17) 56(16) 96(15) 111(15) 81(13) 82(12) 70(11) 152(11) 159(11) 83(10) 84(10)..197(3)	2-tetradecanone	[2345-27-9]	trace
17.50	204(50)	119	133(100) 161(91) 105(82) 44(71) 109(51) 41(38) 67(37) 84(37) 43(33) 145(33) 70(30)	sesquiterpene C15 H24 possibly a cedrene	–	trace
17.82	228(10)	74	87(69) 83(27) 55(24) 143(22) 185(22) 43(19) 75(17) 41(15) 69(14) 59(11) 97(11) 153(11) 197(11) 129(10) 161(10)	methyl tridecanoate	[1731-88-0]	trace
17.99	[201](85)	200	43(89) 102(86) 183(84) 69(78) 57(53) 41(46) 73(43) 55(40) 85(38) 163(38) 129(33) 157(29) 71(28) 42(27) 83(27) 59(26) 69(26) 97(26) 99(22) 149(22) 98(21)...171(12)	isopropyl laurate = dodecanoate	[10233-13-3]	trace

Table 2 Organic residues in White-Slip Sherd WS-NIC-1

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
18.92	[196](3)	83	55(82) 69(77) 97(72) 57(68) 43(65) 70(62) 56(57) 41(49) 71(45) 82(42) 84(40) 111(40) 68(36) 85(27) 98(27) 86(25) 67(23) 96(22) 81(20) 112(20) 125(20)..149(3)..183(3)..169(3)	myristyl alcohol = 1-tetradecanol	[112-72-1]	trace
19.21	242(7)	74	87(80) 199(46) 57(45) 72(44) 43(42) 197(36) 1243(28) 55(27) 41(25) 73(24) 71(22) 85(22) 69(18) 83(18) 75(17) 56(15)..101(10)..213(6)	methyl iso-myristate = 12-methyl-tridecanoate	[5129-58-8]	trace
19.98	242(13)	74	87(69) 143(26) 199(24) 43(20) 55(19) 41(16) 75(16) 211(12) 69(11) 57(10) 59(8) 101(7)	methyl myristate = tetradecanoate	[124-10-7]	2.22
21.44	256(10)	74	87(74) 199(38) 55(36) 43(30) 41(28) 69(28) 143(28) 57(27) 83(22) 213(21) 97(19) 59(18) 75(17) 111(14)71(13) 58(12) 95(11)...227(7)	methyl ante-iso-pentadecanoate = 12-methyltetradecanoate	[5129-66-8]	0.50
22.03	256(16)	74	87(71) 143(24) 43(21) 55(20) 213(20) 75(17) 41(15) 69(12) 225(12) 57(11) 199(9)	methyl pentadecanoate	[7132-64-1]	1.12
22.16	278(<1)	149	57(11) 150(10) 223(10) 104(6) 263(<1)	diisobutyl phthalate CONTAMI-NANT	[84-69-5]	16.36
22.37	[250](17)	43	58(98) 71(80) 57(65) 55(50) 59(50) 109(42) 41(40) 69(39) 95(31) 149(28) 85(27) 110(27) 83(26) 123(25) 125(23) 70(23) 56(21) 84(21) 113(21) 82(20) 111(20) 97(19) 68(17) 165(17) 45(15) 81(15) 91(15) 137(14)..182(12) 179(10)	6,10,14-trimethyl-2-penta-decanone	[502-69-2]	trace
23.03	[238](5)	149	223(17) 55(16) 57(16) 150(10) + FAME impurity: 41(14) 43(14) 83(13) 56(12) 71(12) 69(11) 87(11) 97(11)	butyl isobutyl phthalate CONTA-MIN. probably methyl ante-iso-palmitate = 13-methylpentade-canoate	[17851-53-5]	trace
23.28	270(20)	74	87(73) 143(30) 43(29) 55(29) 57(29) 227(28) 41(22) 75(21) 72(20) 56(17) 69(17) 71(15) 85(14) 42(13) 59(13) 97(13) 98(13) 83(12) 129(12) 199(12) 185(11) 171(10) 208(10)..239(8)	methyl iso-palmitate = 14-methylpentadecanoate	[5129-60-2]	trace
23.40	268(11)	55	74(99) 96(83) 84(79) 97(72) 41(71) 43(70) 69(64) 81(64) 83(62) 87(57) 98(56) 67(52) 95(50) 194(46) 236(46) 110(43) 152(40) 57(37)	methyl palmitoleate = (Z)-9-hexadecenoate	[1120-25-8]	0.93
23.90	278(1)	149	150(10) 223(6) 205(5) 104(4) 41(3) 76(3)	dibutyl phthalate CONTAMINANT	[84-74-2]	8.25
23.98	270(21)	74	87(73) 143(25) 43(21) 227(21) 55(20) 75(19) 41(16) 57(12) 239(11)	methyl palmitate = hexadecanoate	[112-39-0]	11.31
24.91	284(5)	87	116*(67) 74(54) 227(41) 115*(35) 43(29) 71(28) 57(27) 55(25) 211(21) 85(20)	methyl ante-iso-margarate = 14-methylhexadecanoate	[2490-49-5]	trace
25.29	284(31)	74	87(83) 43(52) 55(48) 41(44)59(40) 57(37) 143(37) 71(35) 69(32) 241(28) 88(27) 101(26) 133(25) 185(23) 97(21) 199(21)..227(11)..255(7)	methyl iso-margarate = 15-methylhexadecanoate (contains an aromatic impurity)	[6929-04-0]	trace
25.69	282(5)	57	71(80) 85(62) 43(53) 41(27) 99(26) 55(24) 113(20) 69(18) 127(17) 155(16) 83(15)..141(11)111(10) 126(10)..169(8) ..83(4)..211(2)..187(1)	eicosane	[112-95-8]	trace
25.84	284(24)	74	87(74) 143(29) 241(24) 43(23) 55(23) 75(23) 41(16) 57(14) 129(13) 69(12) 185(12) 253(12) 199(11) 83(10)	methyl margarate = heptadecanoate	[1731-92-6]	trace
27.04	296(12)	55	69(84) 74(80) 83(74) 97(66) 87(62) 96(60) 82(57) 164(57) 98(56) 41(53) 43(49) 67(49) 81(42) 57(40) 95(40) 110(40) 265(38) 222(33) 123(29) 54(28) 180(28) 109(26) 124(22) 137(22)	methyl oleate = (Z)-9-octadecenoate	[112-62-9]	0.84

Table 2 continued Organic residues in White-Slip Sherd WS-NIC-1

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
27.48	296(7)	57	71(84) 85(65) 43(58) 55(24) 99(24) 41(23) 83(15) 113(14) 58(13) 69(12) 97(12) 56(11) 84(11) 127(11) 98(10) 141(10) 155(8) 169(8)	heneicosane	[629-94-7]	trace
27.63	298(29)	74	87(76) 143(28) 255(25) 43(24) 75(23) 55(22) 57(16) 41(15) 69(15) 83(10) 267(10)	methyl stearate = octadecanoate	[112-61-8]	2.72
29.19	310(7)	57	71(81) 85(62) 43(54) 99(26) 41(22) 55(22) 69(17) 113(17) 83(15) 70(14) 56(13) 97(13) 127(12) 141(11) ..155(8) 183(7) 169(6) 197(5) 211(3) 225(3) 239(3) 281(3)	docosane	[629-97-0]	trace
30.17	312(59)	237	197(46) 195(28) 238(23) 163(18) 165(18) 148(16) 153(15) 155(15) 167(15) 179(15) 141(14) 169(14) 178(13) 43(12) 57(12) 121(12) 91(11) 183(11) 209(11) 71(10) 147(10)... 297(8)...281(1)	methyl Δ6-dehydroabietate = abieta-6,8,11,13-tetraen-18-oate	[18492-76-7]	0.25
30.30	314(13)	239	240(20) 299(14) 171(7) 155(6) 173(6) 197(6)	methyl dehydroabietate	[1235-74-1]	trace
30.83	324(4)	57	71(80) 85(60) 43(58) 55(39) 41(31) 69(26) 83(23) 59(21) 72(21) 99(21) 56(20) 97(20) 113(17) 111(13)... 141(10) 155(9) 169(7) 197(6) 183(5) 211(5) 225(5) 239(4) 253(1) 267(1) 281(1)	tricosane	[638-67-5]	0.81
31.01	326(38)	74	87(83) 55(42) 43(36) 97(36) 57(35) 69(34) 83(31) 75(29) 41(26) 283(26) 59(21) 71(20)	methyl arachidate = eicosanoate	[1120-28-1]	trace
32.42	338(3)	57	71(83) 85(60) 43(53) 55(26) 99(25) 41(22) 69(22) 83(17) 97(17) 56(16) 113(16) 111(14) 70(11) 98(11) 141(11) 155(10) 126(9)...169(8) 183(6) 197(5) 211(4) 239(4) 225(3) 281(2) 253(1)	tetracosane	[646-31-1]	trace
33.61	328(37)	253	254(20) 187(18) 213(12) 269(10) 128(9) 165(9) 268(9) 129(8) 131(8) 155(8) 199(8) 296(8)	methyl 7-oxodehydroabietate	[17751-36-9]	trace
33.83	[279](15)	149	167(36) 57(18) 71(14) 70(13)	bis-(2-ethylhexyl) phthalate CONTAMINANT	[117-81-7]	1.94
34.09	354(47)	74	87(80) 57(72) 43(52)..311(14) + phthalate ester ions	methyl behenate = docosanoate	[929-77-1]	trace
35.90 to 38.20	[293] to [382]	149	293(21-34)	isomeric octyl and nonyl phthalates (>12 unresolved peaks) CONTAMINANTS	–	>10.21

Table 2 continued Organic residues in White-Slip Sherd WS-NIC-1

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
2.20	128(8)	57	43(89) 85(52) 41(44) 71(36) 56(31) 84(18) 55(17) 42(15) 99(14) 58(10) 98(8)	nonane	[111-84-2]	trace
2.62	[131](4)	59	43(79) 88(36) 45(33) 71(27) 89(24) 70(18) 41(15) 57(15)	unassigned 3-alkanol	–	trace
3.37	[110](7)	57	41(91) 84(91) 56(89) 43(81) 55(64) 42(58) 44(55) 82(53) 81(44) 68(43) 69(43) 85(42) 67(38) 45(31) 95(29) 100(26) 40(18) 71(16)	octanal	[124-13-0]	trace
4.01	116(100)	116	115(99) 89(11) 63(9) 58(5) 57(4) 62(4)	1H-indene	[95-13-6]	trace
5.09	152(34)	109	108(95) 93(61) 67(60) 81(59) 95(52) 137(48) 91(44) 41(36) 77(31) 79(30) 107(26) 43(23) 119(22) 55(21) 69(21)	pulegone ?	[89-82-7]	trace
5.36	[124](2)	57	41(65) 56(62) 55(48) 43(47) 70(43) 98(40) 44(38) 82(38) 69(36) 68(35) 95(33) 81(31) 67(28) 96(27)...114(11)	nonanal	[124-19-6]	trace
6.64	138(60)	95	96(88) 110(71) 67(40) 81(27) 55(25) 41(20)	monoterpane C10 H18 ?	–	trace
7.72	[138](2)	57	41(74) 43(73) 55(71) 79(64) 82(64) 68(53) 71(52) 83(47) 56(46) 44(44) 67(43) 69(39) 81(39) 112(39) 95(36) 96(33) 84(26) 110(25)...128(10)	decanal	[112-31-2]	0.11
8.67	132(100)	132	104(87) 103(47) 131(35) 78(30) 77(25) 51(17) 133(11) 50(10) 105(10)	1-indanone	[83-33-0]	trace
12.82	[143](43)	74	87(59) 57(58) 111*(58) 55(53) 83(46) 67(38) 59(36) 139*(35) 69(33) 148*(31) 43(30)	methyl ante-iso-undecanoate = 8-methyldecanoate	[5129-64-6]	trace
13.06	194(7)	163	77(12) 164(11) 76(6) 92(6) 133(5) 135(5) 50(4)	dimethyl phthalate CONTAMINANT	[131-11-3]	0.15
13.81	220(69)	177	135(37) 149(34) 205(29) 163(28) 67(24) 41(44) 136(18) 57(17) 91(16) 95(15) 121(15) 178(15) 107(13) 77(12) 119(11) 159(11) 221(11) 53(10)	2,6-di-tert.butyl-2,5-cyclohexa-diene-1,4-dione CONTAMINANT	[719-22-2]	0.07
14.20	236(8)	165	205(81) 180(62) 57(53) 137(32) 221(30) 179(25) 220(23) 41(19) 123(18) 193(17) 43(15) 91(15) 166(15) 67(13) 95(13) 109(13) 115(13) 206(13)	2,6-di-tert.butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one CONTAMINANT	[10396-80-2]	trace
14.40	[205](16)	97	111(75) 83(73) 70(53) 96(53) 69(52) 55(51) 56(46) 43(41) 68(35) 71(34) 41(30) 82(28) 94(28) 42(23) 57(20) 98(11) 85(10)	1-dodecanol	[112-53-8]	trace
14.72	166(29)	43	98(40) 111(31) 109(21) 55(17) 41(16) 151(16)	unassigned	–	trace
15.58	214(3)	74	87(70) 81(24) 123(20) 43(18) 143(16) 171(16) 183(16) 59(15) 115(15) 128(13) 55(12) 41(11)	methyl laurate = dodecanoate	[111-82-0]	trace
15.68	196(16)	153	111(59) 71(46) 97(35) 98(34) 109(31) 83(30) 82(29) 43(22) 81(22) 95(18) 79(17) 91*(17) 40(16) 44(16) 57(16) 70(16) 152(16)...77*(14)	2,5-dibutylthiophene ? (with benzenoid impurity)	[6911-45-1]	trace
16.35	222(2)	149	177(26) 150(12) 176(10) 195(8)...76(6) 104(6)	diethyl phthalate CONTAMINANT	[84-66-2]	0,35
17.05	[243](4)	71	..43(35)..41(26)..55(21)..83(17)..69(16) ..111(15).. 56(13)..72(7) 159(6)..155(2) ..173(2) + impurities	2,2,4-trimethylpentane-1,3-diol di-isobutyrate CONTAMINANT	[6846-50-0]	trace
17.83	[197](3)	74	87(68) 57(25) 83(25) 185(23) 55(19) 43(18) 87(18) 109(15) 69(14) 40(12) 143(12) 95(11) 41(10) 115(10) 143(10)	methyl tridecanoate	[1731-88-0]	trace
19.22	242(5)	74	87(70) 199(46) 43(29) 143(23) 41(21) 135(21) 55(18) 75(17) 97(17) 69(16) 83(16) 57(15) 71(15) 111(14) 56(13) 115(13) 184(12) 70(11) 42(10)	methyl iso-myristate = 12-methyl-tridecanoate	[5129-58-8]	trace

Table 3 Organic residues in White-Slip Sherd WS-NIC-4

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
19.55	226(17)	167	165(34) 152(16) 168(14) 166(12) 77(9)	methyl diphenylacetate	[3469-00-9]	trace
19.78	178(100)	178	176(19) 179(18) 177(12) 152(12) 89(10) 151(7)	phenanthrene (+ C16H18 impurity)	[85-01-8]	trace
19.98	242(12)	74	87(69) 143(26) 199(22) 43(19) 55(19) 75(16) 41(15) 211(12) 69(11) 57(10)	methyl myristate = tetradecanoate	[124-10-7]	0.34
20.91	[143](49)	74	87(67) 97(40) 56(35) 43(30) 83(26) 55(25) 111(24) 67(22) 105(22) 41(21)	branched methyl pentadecanoate	–	trace
21.01	[199](32)	87	74(50) 43(27) 57(27) 55(26) 71(24) 85(22) 69(20) 41(19) 83(18) 183(17) 97(13) 115(13)	branched methyl pentadecanoate	–	trace
21.44	256(10)	74	87(70) 199(36) 55(32) 143(29) 41(28) 43(26) 69(26) 57(24) 97(24) 213(22) 83(21) 75(17) 59(14) 81(14) 84(13) 95(13) 67(12) 96(11)	methyl ante-iso-pentadecanoate = 12-methyltetradecanoate	[5129-66-8]	0.11
22.03	256(17)	74	87(73) 143(23) 43(22) 55(20) 213(18) 75(18) 41(15) 57(12) 225(12) 69(11)	methyl pentadecanoate	[7132-64-1]	0.26
22.15	278(<1)	149	57(11) 150(10) 223(10) 104(6) 263(<1)	diisobutyl phthalate CONTAMINANT	[84-69-5]	3.37
23.02	[223](12)	149	150(13) 57(10) unresolved peaks; intensities recalculated	butyl isobutyl phthalate CONTAMIN.	[17851-53-5]	trace
23.02	[87](18)	87	41(8) 74(8) 43(6) 56(5) 83(5) 71(4) 85(4) 67(2)	methyl ante-iso-palmitate ?	[5487-50-3]	trace
23.28	270(18)	74	87(69) 43(32) 143(26) 227(23) 75(21) 55(20) 57(20) 41(18) 69(18) 73(125) 97(13) 129(12) 83(11) 42(10) 147(10)...213(1)	methyl iso-palmitate = 14-methylpentadecanoate	[5129-60-2]	trace
23.40	268(12)	74	55(87) 84(76) 96(73) 97(67) 41(62) 69(60) 81(59) 83(58) 98(56) 67(52) 87(51) 236(51) 43(50) 95(47) 110(39) 1252(39) 68(36) 123(36)..111(31)	methyl palmitoleate = (Z)-9-hexadecenoate	[1120-25-8]	0.34
23.90	278(1)	149	150(9) 223(6) 205(5) 104(4) 41(3) 76(2)	dibutyl phthalate CONTAMINANT	[84-74-2]	1.60
23.98	270(20)	74	87(73) 143(25) 43(22) 227(21) 55(20) 75(19) 41(16) 57(12) 69(12) 239(11)...213(4)	methyl palmitate = hexadecanoate	[112-39-0]	1.80
24.92	284(5)	116*	87(62) 115*(42) 74(33) 117*(29) 202*(24) 227(24) 43(18) 55(16) 57(16) 41(11) 69(11) 232*(11) 211(10)... 253(3)	methyl ante-iso-margarate = 14-methylhexadecanoate	[2490-49-5]	0.18
25.30	284(21)	74	87(71) 55(48) 43(41) 69(41) 41(36) 57(34) 96(34) 87(33) 84(31) 83(30) 59(27) 98(23) 88(22) 241(21) 81(20) 101(20)...227(10)...255(6)	methyl iso-margarate = 15-methylhexadecanoate	[6929-04-0]	trace
25.84	284(24)	74	87(77) 143(28) 241(25) 43(23) 55(20) 75(20) 41(16) 69(13) 185(13) 199(12) 253(11) 57(10) 83(10)...255(8)...227(2)	methyl margarate = heptadecanoate	[1731-92-6]	trace
27.04	296(12)	55	69(80) 74(79) 83(68) 97(66) 96(64) 84(62) 264(61) 87(60) 41(58) 98(57) 43(48) 67(47) 81(46) 265(43) 95(38) 222(35) 110(34) 111(34) 57(32) 82(31) 123(27) 54(26) 59(24) 109(20)	methyl oleate = (Z)-9-octadecenoate	[112-62-9]	0.48
27.16	[265](28)	74	55(80) 87(68) 97(67) 264(65) 43(63) 83(63) 98(61) 69(57) 111(51) 57(49) 223(49) 41(48) 67(43) 96(42) 110(40)	methyl elaidate = (E)-9-octadecenoate		
			unresolved peaks; intensities recalculated			
27.16	252(100)	252	237(79) 146(74) 118(54) 189(47) 138(43) 194(34) 209(34) 117(31) 165(30) 178(30)	probably simonellite	[27530-79-6]	trace

Table 3 continued Organic residues in White-Slip Sherd WS-NIC-4

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
27.63	298(28)	74	87(76) 143(28) 43(24) 255(24) 55(22) 75(22) 57(16) 41(15) 69(15) 199(15) 83(10) 267(10)	methyl stearate = octadecanoate	[112-61-8]	0.54
27.90	[230](22)	59	72(55) 43(25) 55(20) 41(17) 45(14) 73(14) 57(13) 42(12) 60(12) 84(11) 87(11) 98(11) 129(11) 114(10) 128(10) 136(10)	oleamide = (Z)-9-octadecenoic acid amide CONTAMINANT	[301-02-0]	trace
28.11	316(27)	241	146(45) 257(42) 301(34) 91(29) 133(29) 105(27) 131(27) 147(27) 173(26) 242(26) 159(21) 121(20) 185(20) 134(18) 145(18) 256(18) 107(17)..284(14)	methyl 8,15-isopimaradien-18-oate	[19907-21-2]	trace
28.58	316(23)	241	301(40) 257(28) 242(21) 185(20) 91(18) 159(17) 105(16) 147(15) 93(14) 131(14) 134(14) 145(14) 173(14) 121(12) 128(12) 129(12) 143(12)... 256(9)	methyl 8,15-pimaradien-18-oate	[3582-26-1]	trace
28.76	[257](16)	121	133(36) 135(34) 181(33) 117(32) 180(32) 122(29) 55(24) 134(24) 147(24) 105(22) 116(22) 68(20) 137(20)...119(16) + impurity 244(43) 77(37) etc.	methyl pimarate ?	[3730-56-1]	trace
29.20	[181](4)	57	71(80) 85(67) 43(59) 99(36) 55(33) 56(28) 113(28) ..127(17) 44(16) 84(16) 155(14)..141(12)..169(8)	docosane	[629-97-0]	trace
30.31	314(12)	239	240(20) 299(13) 129(5) 141(5) 197(5)	methyl dehydroabietate	[1235-74-1]	0.29
30.81	326(100)	326	325(80) 77(28) 215(21) 170(19).. 169(17) 233(17)	triphenyl phosphate CONTAMINANT	[115-86-6]	0.53
31.00	326(41)	74	87(78) 55(36) 143(33) 43(31) 75(31) 283(25) 41(21) 57(21) 69(20) 59(19) 83(19) 97(19) 71(16) 72(15) 191(10) 295(10) 327(10)	methyl arachidate = eicosanoate	[1120-28-1]	trace
31.88	[341](<1)	129	57(29) 112(27) 70(23) 147(23) 55(18) 111(16) 113(12) 43(11) 41(10) 241(10)...313(<1)	bis-(2-ethylhexyl) adipate CONTAMINANT	[103-23-1]	0.94
32.42	[239](13)	57	71(73) 85(68) 43(51) 55(26) 113(22) 99(21) 41(19) 127(19) 112(16) 56(15) 69(15) 84(15) 107(15) 98(14) 141(14) 70(13) 83(13) 97(12) 153(12) 155(11) 167(10) 169(10) 230(10)..183(7).. 197(6)..225(4)..211(3) + phthalate impurity	tetracosane	[646-31-1]	trace
32.59	340(18)	74	87(51) 143(25) 57(22) 41(17) 69(17) 43(15) 97(14) 83(12) 71(11) 75(5) 55(4)unresolved peaks; intensities recalculated	methyl heneicosanoate	[6064-90-0]	trace
32.59	330(37)	315	237(58)	methyl x-hydroxydehydroabietate	–	trace
33.04	386(100)	386	43(92) 57(92) 275(89) 55(59) 69(54) 368(54) 81(53)	MS like cholesterol, but wrong RT	–	trace
33.61	328(36)	253	254(21) 187(21) 213(13) 269(13) 128(8) 199(8) 268(8) 296(8) 129(7) 155(6)..131(2) 165(2)	methyl 7-methyl 7-oxodehydro-abietate + phthalate impurity	[17751-36-9]	0.11
33.83	[279](15)	149	167(36) 57(15) 279(15) 71(12) 70(10)	bis-(2-ethylhexyl) phthalate CONTAMINANT	[117-81-7]	0.61
34.10	354(51)	74	87(89) 57(40) 43(37) 75(35) 143(35) 55(30) 41(23)	methyl behenate = docosanoate (+ phthalate impurity)	[929-77-1]	trace
34.91 to 40.00	[293](26) to 418(<1)	149	293(26-33) 167(11-33)	isomeric octyl and nonyl phthalates (>24 unresolved peaks) CONTAMINANTS	–	>80

Table 3 continued Organic residues in White-Slip Sherd WS-NIC-4

RT	**MI(int)**	**BP**	Fragment ions	Compound	**Reg.No.**	**Percent**
2.20	128(14)	57	43(91) 85(52) 41(42) 71(40) 56(28) 70(27) 55(22) 84(20) 42(19) 95(15) 61(13)	nonane	[111-84-2]	trace
2.42	[129](14)	59	83(39) 43(29) 42(19) 45(16) 55(12) 75(12) 71(10) 84(10) 85(10) 100(10) 41(8)	x-methyl-3-heptanol ?	–	trace
2.62	[131](8)	59	43(75) 88(35) 45(28) 89(24) 71(19) 41(11) 61(10) 70(8) 86(7) 87(7) 42(6) 60(6) 69(6)	unassigned 3-alkanol	–	trace
3.38	[110](14)	84	57(89) 56(84) 43(79) 41(76) 44(60) 55(57) 81(53) 82(48) 67(47) 68(46) 69(40) 85(40) 100(24) 45(18) 95(18) 72(17) 83(13)	octanal	[124-13-0]	trace
3.50	[131](3)	43	59(94) 85(62) 41(46) 70(46) 55(31) 58(31) 42(28) 69(23) 107(22) 67(20) 71(19) 57(16) 75(16) 45(13) 56(11) 83(11) 77(10)	methyl 3-hydroxy-3-methyl-butanoate ?	[6149-45-7]	trace
4.01	116(95)	115	89(12) 117(10) 63(9) 57(5) 58(5)	1H-indene	[95-13-6]	trace
5.38	[124](3)	57	56(60) 41(59) 55(53) 43(51) 98(47) 70(43) 44(38) 82(38) 68(35) 69(34) 81(31) 95(31) 96(29) 67(27) 42(24) 71(20) 45(18) 54(14) 83(14) 114(11)	nonanal	[124-19-6]	trace
7.72	[138](2)	57	41(78) 43(75) 55(69) 82(62) 70(59) 71(53) 68(48) 83(46) 56(45) 67(42) 81(42)44(41) 112(41) 95(37) 95(31) 84(27) 42(26) 110(24) 45(16) 54(15) 72(12) 97(11) 58(10) 128(10)	decanal	[112-31-2]	0.09
10.13	206(51)	57	135(96) 191(79) 149(67) 107(60) 121(52) 91(47) 41(42) 55(38) 150(35) 109(22) 69(17) 105(17) 77(11) 43(10)	unassigned	–	trace
10.22	[126](19)	41	57(95) 55(82) 82(76) 43(73) 81(71) 71(66) 70(65) 56(59) 68(56) 69(55) 67(54) 96(51) 95(50) 83(42) 42(32) 97(28) 85(26) 44(25)	undecanal	[112-44-7]	trace
10.32	[129](21)	74	41(97) 87(80) 69(50) 55(49) 95(49) 97(48) 43(45) 45(22) 44(7) entire MS	methyl ante-iso-caprate = 7-methylnonanoate	[5129-63-5]	trace
12.70	[97](8)	57	55(72) 43(70) 41(65) 82(57) 68(50) 81(50) 67(49) 69(47) 70(44) 56(38) 96(23) 45(21) 71(21) 95(21) 44(17) 83(16) 40(13) 42(13)	dodecanal	[112-54-9]	trace
12.83	[143](45)	55	74(87) 87(87) 83(72) 57(71) 111(59) 43(57) 59(48) 139(36) 41(28) 155(26) 67(25) 115(24) 85(23) 69(20) 40(14) 42(14) 71(13) 81(13)	methyl ante-iso-undecanoate AND methyl 9-oxononanoate [overlapping peaks]	[5129-64-6] [1931-63-1]	trace
13.81	220(66)	177	135(35) 149(33) 205(29) 163(25) 67(22) 41(20) 136(16) 91(15) 95(14) 121(14) 178(14) 57(13) 107(11) 159(11) 77(10) 79(10) 221(10)	2,6-di-tert.-butyl-2,5-cyclohexa-diene-1,4-dione CONTAMI-NANT	[719-22-2]	0.17
14.21	236(8)	165	180(67) 205(62) 57(50) 137(31) 179(28) 221(26) 43(17) 220(17) 41(16) 91(16) 136(16) 193(16) 123(15) 166(13) 55(11) 151(11) 109(10) 115(10) 135(10) 206(10)	2,6-di-tert.-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one CONTAMINANT	[10396-80-2]	0.08
14.40	[140](10)	55	83(98) 69(93) 70(87) 56(84) 57(81) 43(79) 97(78) 41(72) 84(55) 111(54) 82(51) 68(49) 85(37) 98(33) 67(32) 71(32) 42(27) 96(20) 112(17) 110(16) 44(15) 81(14) 95(13)	1-dodecanol	[112-53-8]	trace
14.72	166(27)	43	98(40) 111(32) 55(18) 151(17) 82(15) 83(14) 41(12) 127(12) 61(11) 68(11) 123(10)	unassigned	–	0.17
15.58	214(7)	74	87(65) 55(22) 143(20) 171(18) 43(16) 183(14) 41(13) 59(12) 75(12) 69(11)	methyl laurate = dodecanoate	[111-82-0]	trace

Table 4 Organic residues in White-Slip Sherd WS-NIC-5

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
15.69	196(18)	153	57(56) 71(53) 55(51) 70(48) 83(48) 97(39) 43(38) 111(35) 56(34) 69(28) 41(26) 84(26) 181(25) 85(17) 98(17) 42(15) 152(14) 44(11) 91(10)	1-tetradecene ? AND 2,5-dibutyl-thiophene ? [overlapping peaks]	[1120-36-1] [6911-45-1]	trace
16.35	222(3)	149	177(26) 150(12) 176(10) 195(8) 76(6) 104(6)	diethyl phthalate CONTAMINANT	[84-66-2]	0.13
16.72	[182](1)	83	55(92) 69(89) 70(74) 97(72) 43(69) 57(67) 41(62) 56(62) 84(48) 82(46) 111(40) 68(35) 71(35) 98(28) 67(24) 42(21) 85(20)...125(17)...154(13)	1-tridecanol	[112-70-9]	0.09
17.04	[243](8)	71	43(31) 159(11) 111(10) 56(9) 41(8) 55(6) 57(6) 72(6) 83(6) 155(6) 69(5) 173(5)	2,2,4-trimethylpentane-1,3-diol di-isobutyrate CONTAMINANT	[6846-50-0]	trace
17.10	212(9)	58	43(63) 71(52) 59(49) 57(28) 41(23) 55(21) 82(15) 97(15) 85(14) 96(14) 151(14) 70(13) 56(12) 89(12)109(12) 69(11) 152(11) 42(10)	2-tetradecanone	[2345-27-9]	trace
17.19	[143](49)	74	87(79) AND unresolved compound	methyl ante-iso-tridecanoate alkanol or alkene ?	[5129-65-7] –	trace
17.83	228(5)	74	87(65) 83(34) 55(23) 143(22) 185(21) 41(19) 43(18) 69(15) 75(15) 59(14) 57(12) 153(12) 197(12) 67(11) 84(10) 109(10) 156(10)	methyl tridecanoate	[1731-88-0]	trace
18.15	[162](1)	85	55(13) 128(13) 56(12) 70(12) 84(12) 95(12) 41(11) 96(10) 42(9) 57(9) 43(8) 83(8) 97(8) 98(8) 109(8) 71(7) 81(7) 110(7)...137(6)...161(1)	gamma-dodecalactone = dihy-dro-5-octyl-2(3H)-furanone	[2305-05-7]	trace
18.41	[220](17)	219	57(70) 177(59) 163(40) 91(26) 155(22) 161(20) 198(19) 105(18) 119(18) 121(16) 135(16) 189(15) 115(14) 175(14) 128(12) 147(12) 149(12) 192(12) 83(11) 145(11) 178(11) 131(10) 159(10) 193(10)	3,5-di-t-butyl-4-hydroxybenzalde-hyde OR 2,6-di-t-butyl-4-ethylphe-nol CONTAMINANT	[1620-98-0] OR[4130-42-1]	trace
19.22	242(2)	74	87(67) 143(25) 185(2) overlapping peaks	methyl iso-myristate = 12-methyl-tridecanoate	[5129-58-8]	trace
19.28	212(8)	57	70(81) 43(41)…141(28) 159(27)… 197(19)	unassigned branched alkane C15H32	–	trace
19.78	210(95)	195	104*?(74) 178(35) 180(31) 165(27) 179(24) 181(20) overlapping peaks	unassigned; possibly a tetrahydro-dimethylphenanthrene C16H18	–	trace
19.83	240(7)	57	71(91) 85(69) 43(67) 99(25) 181(19) 113(16) 127(15) 141(13) 155(12) 167(10) + impurities	heptadecane	[629-78-7]	trace
19.97	242(13)	74	87(71) 143(25) 199(23) 43(19) 55(19) 75(16) 41(15) 211(12) 57(11) 69(11)	methyl myristate =tetradecanoate	[124-10-7]	0.23
21.02	224(11)	43	57(100) 87*(99) 69(83) 55(79) 83(76) 71(70) 41(65) 97(61) 70(51) 82(49) 111(49) 74*(45) 85(37) 56(35) 96(35) 68(33) 125(29) 199(29) 98(22) 113(21) 118(21) 58(20) 79(20) 110(20)	1-hexadecene * fatty acid methyl ester impurity	[629-73-2]	trace
21.42	256(9)	74	87(74) 43(56) 58(54) 55(45) 59(40) 199(39) 41(34) 57(34) 71(33) 69(32) 143(32)	methyl iso-pentadecanoate = 13-methyltetradecanoate	[5129-66-8]	trace
21.52	224(87)	118	209(93) 105(89) 119(30) 179(27) 210(21) 117(20) 91(19) 106(19) 178(19) 194(19) 225(17) 115(13) 103(12) 77(11) 79(11) 165(10)	unassigned; possibly a tetrahy-dro-trimethylphenanthrene C17H20	–	trace
21.88	254(6)	57	71(85) 85(73) 43(59) 243*(51) 41(27) 55(23) 155(18) 69(16) 99(16) 127(16) 141(15) 58(13) 112(13)125(13) 213(13) 183(12) 93(11) 113(11) 169(11) 128(10)... 258*(8)	octadecane * unassigned impurity	[593-45-3]	trace
22.04	256(15)	74	87(70) 143(24) 43(20) 213(20) 55(19) 75(19) 41(15) 57(12) 225(12)...199(8)	methyl pentadecanoate	[7132-64-1]	trace

Table 4 continued Organic residues in White-Slip Sherd WS-NIC-5

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
22.18	278(<1)	149	57(14) 150(13) 223(13) 104(8) 263(<1)	di-isobutyl phthalate CONTAMINANT	[84-69-5]	6.28
22.34	[250](12)	43	58(78) 71(78) 57(71) 59(45) 55(44) 85(44) 41(38) 69(37) 83(34) 109(31) 95(28) 110(25) 97(24) 82(22) 213(22) 45(21) 56(21) 111(21) 124(20)	6,10,14-trimethyl -2-pentadecanone	[502-69-2]	0.11
23.03	[238](4)	149	223(15) 57(11) 83(11) 41(10) 97(10) 150(10)	butyl isobutyl phthalate CONTAMINANT	[17851-53-5]	0.12
23.13	208(100)	208	180(82) 152(60) 151(30) 76(24) 209(20) 150(17) 181(14) 71(10)	anthraquinone (RT)	[84-65-1]	0.09
23.29	270(22)	74	72*(93) 57(80) 87(72) 73*(63) 225*(47) 55(43) 43(42) 85(36) 41(33) 143(30) 227(30) 71(29) 208(23) 69(22) 75(22) 212(22)	methyl iso- OR anteiso-palmitate = 13- OR 14- methylpentadecanoate * unassigned impurity	[5129-60-2] OR [5487-50-3]	trace
23.40	268(8)	43	58*(95) 59*(91) 55(90) 74(75) 96(66) 41(63) 71(63) 97(59) 69(58) 84(57) 83(52) 81(51) 87(45) 67(44) 57(42) 98(42) 95(40) 236(40) 110(38) 152(33) 85(30)	methyl palmitoleate = (Z)-9-hexadecenoate	[1120-25-8]	0.14
23.91	278(1)	149	150(11) 223(7) 205(6) 41(4) 104(4)	dibutyl phthalate CONTAMINANT	[84-74-2]	3.48
23.98	270(20)	74	87(73) 143(25) 43(22) 227(21) 55(20) 41(16) 57(13) 69(13) 149*(13) 239(11)... 213(4)	methyl palmitate = hexadecanoate	[112-39-0]	0.67
24.82	[253](13)	71	43(83) 57(73) 58(73) 83(67) 85(65) 155(60) 183(56) 55(54) 169(54) 82(51) 41(49) 127(48) 113(47) 143(43) 141(40) 74(39)...142(36) 197(36)	a branched alkane C20H42 probably phytane	[638-36-8]	trace
25.19	[253](57)	57	43(95) 71(86) 55(76) 69(61) 85(58) 74(56) 87(55) 95(49) 41(43) 97(32) 83(30)	unassigned (mixture?)	–	trace
25.69	282(10)	57	71(86) 85(76) 43(60) 55(30) 41(27) 99(20) 69(19) 56(16) 70(16) 113(16) 83(13) 97(13) 127(12) 141(11)... 155(10) 169(8) 183(8) 197(5) 211(1)	eicosane	[112-95-8]	trace
25.82	284(20)	74	87(76) 236*(28) 143(24) 241(24) 75(23) 255(22) 55(18) 41(15) 189(15) 77*(14) 121*(14) 197*(14) 199(14) 43(13) 68(13) 101(13)	methyl margarate = heptadecanoate * unassigned impurity	[1731-92-6]	trace
25.90	256(100)	256	102*(70) 257(62) 43(57) 57(56) 239(49) 60(48) 55(33) 71(30) 73(29) 41(27) 97(26) 85(24) 129(22) 69(21) 83(21) 87(21)...241(10)	unassigned norabietatriene C19H28	–	trace
27.05	296(11)	55	69(77) 74(75) 83(66) 96(63) 97(62) 87(60) 84(59) 264(57) 41(56) 43(51) 57(51) 98(51) 81(47) 67(45) 265(41) 95(37) 222(34) 111(33) 72(32) 110(32) 54(28) 68(27) 123(26) 85(28) 180(26) 59(24) 73(24) 56(23) 109(23) 253(23) 70(20)	methyl oleate = (Z)-9-octadecenoate	[112-62-9]	0.21
27.17	252(100)	252	237(73) 146(68) 57(45) 59(45) 58(44) 43(40) 71(37) 118(36) 223(36) 194(35) 179(27) 209(26)	simonellite	[27530-79-6]	0.10
27.49	296(7)	57	71(86) 85(66) 43(57) 55(28) 58(24) 41(24) 99(23) 69(16) 70(16) 83(16) 89(13) 113(11) 221(11) 56(10) 183(9) 211(8) 225(8) 141(6) 169(6) 239(6) 155(4) 197(4) 268(3) 253(2)	heneicosane	[629-94-7]	trace
27.64	298(28)	74	87(75) 143(29) 43(25) 255(25) 75(23) 55(22) 57(15) 41(16) 69(16) 199(15) 71(10) 83(10) 267(10)	methyl stearate = octadecanoate	[112-61-8]	0.07
28.58	316(29)	241	301(36) 86(26) 87(26) 257(26) 253(25) 69(22) 185(22) 55(21) 43(20) 71(20) 91(20) 242(20)	methyl 8,15-pimaradien-18-oate	[3582-26-1]	trace

Table 4 continued Organic residues in White-Slip Sherd WS-NIC-5

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
29.20	310(7)	57	71(79) 43(63) 85(62) 41(24) 55(23) 99(21) 69(18) 113(16) 83(15) 56(13) 70(13) 97(13) 84(10) 127(10) 141(10) 169(8) 211(6) 155(5) 183(5) 239(4) 253(3) 225(2) 267(2)	docosane	[629-97-0]	trace
29.68	320(5)	163	109(53) 149*(32) 162(30) 164(26) 241(24) 123(23) 261(22) 245(21) 246(20) 95(19) 81(16) 101(15) 119(15) 59(13) 91(12) 93(12)...231(11)... 191(10)	methyl tetrahydroisopimarate	[4614-69-1]	trace
30.30	314(13)	239	240(20) 299(13) 197(7) 43(5) 128(5) 155(5)	methyl dehydroabietate	[1235-74-1]	trace
30.83	324(4)	57	71(83) 43(64) 85(63) 55(37) 41(33) 59(29) 69(27) 72(25) 83(24) 99(22) 97(21) 113(19) 70(17) 84(15) 98(11) 111(11) 112(11) 127(11) 141(8) 183(8) 225(7) 281(7) 155(6) 169(6) 253(5) 211(4) 267(4) 197(3)	tricosane	[638-67-5]	0.09
31.01	326(37)	74	87(82) 143(36) 55(32) 43(31) 75(29) 283(29) 41(25) 57(24) 59(24) 69(22) 83(20) 129(16) 85(13) 97(13) 71(12) 84(12) 56(11) 72(11) 82(11) 125(11) 150(11) 185(11)	methyl arachidate = eicosanoate	[1120-28-1]	trace
31.35	[258](15)	59	72(45) 43(27) 55(24) 57(23) 41(20) 97(16) 114(14) 126(14) 60(13) 69(13) 86(13) 240(13) 110(12)	stearamide = octadecanamide	[124-26-5]	trace
31.89	370(<1)	129	57(28) 112(27) 70(23) 147(22) 55(18) 111(16) 113(12) 43(11) 41(10) 241(10)...313(<1)	di-(2-ethylhexyl) adipate CONTAMINANT	[103-23-1]	1.07
32.42	338(2)	57	71(76) 85(62) 43(48) 99(21) 41(20) 55(18) 69(15) 83(14) 97(14) 56(13) 113(13) 70(11) 127(10) 155(9) 183(9) 141(8) 239(8) 169(6) 197(6) 211(6) 225(3) 267(3) 253(2) 281(2)	tetracosane	[646-31-1]	trace
32.69	[249](8)	149	167(35) 150(15) 55(10) 83(6) 41(5) 67(5)	dicyclohexyl phthalate CONTAMINANT	[84-61-7]	0.22
33.84	[355](<1)	149	167(37) 279(14) 57(13) 71(12) 70(11) 150(11) 43(8) 113(8) 55(7) 41(6) 83(5) 194(5)	di-(2-ethylhexyl) phthalate CONTAMINANT	[117-81-7]	0.44
33.95	352(1)	57	71(80) 85(60) 43(57) 41(22) 55(22) 70(20) 83(19) 99(19) 69(18) 113(16) 56(12) 97(12) 112(12) 169(11) 279(11) 84(10) 127(10) 183(10) 251(10) 155(9) 197(9) 239(9) 141(7) 211(6) 225(4) 267(4) 253(3) 281(1) 295(1)	pentacosane	[629-99-2]	trace
35.23 to 39.44	various	149	various	>31 phthalate esters CONTAMINANTS	–	>80.19
41.10	386(91)	55	57(98) 43(93) 69(81) 71(67) 95(67) 275(67) 105(66) 81(64) 83(62) 145(62) 301(59) 41(57) 107(55) 91(52) 213(52) 109(50) 121(47) 133(45) 159(45) 67(43) 93(43) 353(43) 79(40) 255(40) 371(38) 119(36) 147(36) 120(29) 161(19)	cholesterol(contaminated with phthalate ester; intensities recalculated)	[57-88-5]	trace

Table 4 continued Organic residues in White-Slip Sherd WS-NIC-5

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
2.62	[131](9)	59	43(68) 88(35) 45(30) 89(26) 71(18) 61(11) 70(10) 41(9)	unassigned 3-alkanol	–	trace
3.37	[84](100)	84	57(83) 69(82) 44(81) 43(75) 56(65) 85(52) 81(47) 55(46) 82(46) 41(34) entire MS	octanal	[124-13-0]	trace
4.02	116(100)	116	115(99) 117(11) 89(10) 63(9) 55(7)	1H-indene	[95-13-6]	trace
5.37	[98](50)	57	56(71) 41(63) 70(55) 43(42) 68(41) 82(41) 81(39) 42(36) 67(36) 95(33)	nonanal	[124-19-6]	trace
7.73	[112](41)	57	41(86) 55(71) 70(71) 82(71) 43(60) 71(58) 83(54) 56(53) 44(52) 68(52) 81(47) 67(43)	decanal	[112-31-2]	trace
14.74	166(34)	43	98(59) 111(49) 41(46) 55(36) 69(31) 82(15) 83(15) entire MS	unassigned	–	trace
15.58	[171](13)	74	87(75) 43(33) 41(30) 55(28) 143(22) 57(20)	methyl laurate = dodecanoate	[111-82-0]	trace
18.83	180(100)	180	152(36) 151(18) 181(15) 150(12) 76(9) 126(6) 63(5)	9H-fluoren-9-one	[486-25-9]	0.08
19.79	178(100)	178	176(18) 179(15) 177(10) 89(8) 152(8) 76(7) 151(7) 88(5) 150(5)	phenanthrene	[85-01-8]	0.71
19.98	242(13)	74	87(66) 143(25) 199(21) 55(17) 41(16) 43(16) 75(16) 69(12) 211(11)	methyl myristate = tetradecanoate	[124-10-7]	0.15
21.33	194(100)	194	165(77) 166(30) 197*(29) 198*(28) 193(26) 195(22) 69(15) 45(13) 57(11) 91(11) 163(11)	9-phenanthrenol ?	[484-17-3]	trace
21.44	[213](29)	74	87(80) 55(54) 57(47) 199(38) 83(33) 143(32) 181(31) 43(29) 69(23) 41(18) 97(15) 71(12) 75(12) 91*?(12) 105*?(12) 115*?(12)	methyl ante-iso-pentadecanoate =12-methyltetradecanoate	[5129-66-8]	trace
22.02	256(18)	74	87(76) 143(24) 43(22) 213(21) 75(19) 57(18) 55(16) 69(15) 41(14) 97(11) 199(11) 83(10)	methyl iso-pentadecanoate = 13-methyltetradecanoate	[5129-59-9]	trace
22.21	192(100)	192	191(57) 189(26) 148*(22) 193(16) 190(14) 165(10) 95(8) 82(6) 96(6)	x-methylphenanthrene	[31711-53-2]	trace
22.38	190(100)	190	189(94) 187(25) 95(22) 191(19) 57(15) 188(15) 94(14) 71(11) 41(8) 43(7) 81(5)	4,5-methanophenanthrene = benzo[def]fluorene	[203-64-5]	trace
22.53	192(100)	192	191(54) 189(26) 165(17) 183(15) 190(13) 85(11) 55(10) 95(8)	x-methylphenanthrene	[31711-53-2]	trace
23.12	208(100)	208	180(81) 153(58) 151(36) 206(23) 76(22) 150(19) 75(13) 55(11) 181(10) 68(9) 77(9) 71(7) 57(6)	9,10-anthraquinone	[84-65-1]	trace
23.39	[236](18)	74	81(99) 84(94) 96(94) 55(92) 83(91) 69(82) 67(75) 95(69) 98(68) 87(63) 43(59) 41(57) 111(54) 194(54)	methyl palmitoleate =(Z)-9-hexadecenoate (+ impurity)	[1120-25-8]	trace
23.58	204(100)	204	202(38) 203(30) 205(19) 101(11) 149*(8) 102(7) 200(7) 201(6)	4,5-dihydropyrene	[6628-98-4]	trace
24.97	202(100)	202	200(20) 203(17) 201(14) 101(11) 100(8) 88(5)	fluoranthene	[206-44-0]	0.54
25.36	184(100)	184	139(16) 185(15) 163(14) 152(10) 92(7) 91(6) 119(6) 186(6) 183(5)	dibenzothiophene	[132-65-9]	trace
25.75	202(100)	202	200(20) 203(17) 201(15) 101(13) 100(9) 88(4) 199(4)	pyrene	[129-00-0]	trace
25.84	284(14)	74	87(69) 143(28) 241(25) 83(23) 75(21) 218(19) 43(18) 81(14) 41(11) 55(10) 57(10)	methyl margarate = heptadecanoate	[1731-92-6]	trace

Table 5 Organic residues in White-Slip Sherd WS-NIC-6

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
27.07	[265](40)	55	97(85) 69(74) 71(73) 87(72) 83(70) 67(64) 81(63) 98(63) 84(61) 41(51) 111(51) 164(50) 96(47) 43(42) 57(42) 123(41) 56(40)	methyl oleate = (Z)-9-octadecenoate	[112-62-9]	trace
27.64	298(29)	74	87(77) 143(30) 43(25) 255(24) 75(23) 55(22) 41(16) 57(16) 179(16) 199(16) 69(13) 83(11) 129(10) 267(10)	methyl stearate = octadecanoate	[112-61-8]	0.31
29.20	[127](5)	57	85(93) 71(86) 43(66) 41(34) 83(32) 56(30) 69(27) 45(24) 111(24) 149*(13)...113(10)	docosane	[629-97-0]	trace
30.16	312(5)	163*	237(77) 235*(68) 212(28) 67(27) 178(27) 162*(25) 111(22) 71(20) 95(20) 109(20)	methyl abieta-6,8,11,13-tetra-enoate (+ impurity)	[18492-76-7]	trace
30.31	314(14)	239	240(22) 299(10) 115(8) 141(6) 85(5) 91(5)	methyl dehydroabietate	[1235-74-1]	trace
30.84	[281](4)	57	71(91) 85(81) 43(57) 55(33) 41(30) 70(26) 69(24) 99(24) 83(22) 113(18)...127(10) 141(8) ...155(4)	tricosane	[638-67-5]	trace
31.00	326(40)	74	87(80) 43(40) 55(40) 71(40) 81(30) 85(30) 95(30) 143(30)	methyl arachidate = eicosanoate	[1120-28-1]	trace
31.89	[259](6)	129	57(29) 112(27) 70(24) 147(22) 71(21) 55(19) 111(16) 83(14) 43(12) 113(12) 41(10) 84(10) 241(10)	dioctyl adipate CONTAMINANT	[123-79-5]	0.58
32.44	[219](5)	57	71(76) 85(71) 43(45) 55(34) 99(33) 70(31) 67(26) 83(22) 149*(20)... 113(17)... 127(6)	tetracosane (+ phthalate impurity)	[646-31-1]	trace
33.95	[167*](46)	57	71(96) 149*(94) 85(89) 43(59) 111(38) 56(37) 113(36) 70(33) 55(29) 41(27) 68(27) 67(26) 99(24) 95(23) 112(22) 105(21)... 141(11) 127(10) 155(10)	pentacosane (+ phthalate impurity)	[629-99-2]	trace
35.75	368(100)	368	165(84) 181(44) 367(33) 107(30) 91(29) 180(25) 77(24) 108(24) 179(23) 81(16) 79(15) 166(12)	tricresyl phosphate CONTAMINANT	[1330-78-5]	trace
35.54 – 39.42	various	149	various	> 21 isomeric octyl and nonyl phthalates CONTAMINANTS	–	

Table 5 continued Organic residues in White-Slip Sherd WS-NIC-6

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
2.21	[85](56)	57	43(91) 45(46) 42(41) 71(41) 55(39) 61(38) 41(37) 56(30) 70(23) 40(10)	nonane	[111-84-2]	trace
2.42	[83](70)	59	45(34) 55(31) 41(28) 42(28) 57(26) 43(16)	x-methyl-3-heptanol ?	–	trace
2.63	[131](9)	59	43(64) 88(30) 45(29) 89(22) 41(16) 71(16) 70(11) 61(10) 60(7) 69(7) 42(6) 86(5)	unassigned 3-alkanol	–	0.11
3.38	[85](14)	43	41(98) 56(84) 57(72) 55(66) 84(64) 44(52) 67(43) 69(40) 81(31) 42(27) 45(27) 68(24)	octanal	[124-13-0]	trace
3.51	[107](14)	43	59(92) 41(50) 85(45) 55(44) 69(41) 45(31) 58((31) 70(26) 42(24) 40(15)	methyl 3-hydroxy-3-methyl- butanoate ?	[6149-45-7]	trace
4.03	116(100)	116	115(84) 89(12) 117(10) 63(8) 43(5) 58(5)	1H-indene	[95-13-6]	0.25
5.37	[115](7)	57	41(72) 56(63) 43(54) 55(51) 70(47) 82(43) 98(43) 44(41) 69(38) 82(35) 95(35) 68(33) 67(30) 42(21)	nonanal	[124-19-6]	0.48
7.74	[128](4)	57	43(83) 41(81) 55(72) 70(59) 71(59) 82(57) 68(51) 56(47) 83(46) 81(44) 67(43) 69(42) 44(40) 112(39) 95(38) 96(33) 84(29) 42(28) 110(27)	decanal	[112-31-2]	0.35
18.38	198(100)	198	91(90) 155(86) 69(8) 65(6) 40(1) entire MS	C5- alkylnaphthalene C15H18	–	trace
19.78	178(100)	178	179(20) 176(18) 181(6) 89(5) 181(4) 44(3) 40(2) entire MS	phenanthrene	[85-01-8]	trace
19.98	219*(14)	74	87(63) 43(35) 41(34) 55(28) 57(14) 73(14) 143(12) 40(6) 75(6) 69(5)	methyl myristate = tetradecanoate	[124-10-7]	trace
22.02	[143](12)	74	87(65) 43(35) 41(31) 55(23) 69(22) 57(12)	methyl iso-pentadecanoate = 13-methyltetradecanoate	[5129-59-9]	trace
23.91	278(1)	149	150(11) 223(8) 205(6) 41(4) 104(4) 56(2) 57(2) 121(2) 122(2)	dibutyl phthalate CONTAMINANT	[84-74-2]	1.52
23.98	270(21)	74	87(72) 149*(46) 143(25) 43(22) 227(22) 75(20) 55(19) 41(17) 57(13) 69(12) 129(10)	methyl palmitate = hexadecanoate	[112-39-0]	trace
24.95	202(100)	202	200(24) 116*(46) 134*(43) 115*(27) 203(23) 57(20) 41(16) 55(15) 201(14) 91(13) 107*(12) 69(10) 101(10)	fluoranthene (+ impurities)	[206-44-0]	trace
27.64	298(30)	74	87(79) 143(26) 43(24) 55(24) 255(24) 75(22) 57(16) 41(15) 69(14) 188(14) 63(11) 97(11) 267(11)	methyl stearate = octadecanoate	[112-61-8]	1.49
29.66	320(5)	163	162(26) 81(19) 109(19) 123(18) 67(16) 164(16) 261(16)	methyl tetrahydroisopimarate	[4614-69-1]	trace
30.16	320(10)	163	162(25) 95(19) 261(19) 123(17) 164(17) 109(16) 91(14) 79(13) 191(13) 67(12) 81(12) 97(11) 149(11) 44(10) 55(10) 93(10) 121(10)	methyl tetrahydropimarate	[33892-02-3]	0.37
30.31	314(12)	239	240(18) 299(15) 41(7) 83(7) 91(7) 44(6) 81(6) 97(6) 57(5) 131(5) 141(5)	methyl dehydroabietate	[1235-74-1]	trace
30.84	[115](8)	71	57(96) 85(78) 43(47) 83(33) 41(31) 55(23) 97(23) 45(19) 69(19) 81(17)	tricosane	[638-67-5]	trace

Table 6 Organic residues in White-Slip Sherd WS-NIC-7

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
1.95	166(10)	83	85(63) 95(17) 131(16) 168(13) 60(12) 133(12) 87(11) 91(11) 96(11) 97(11) 61(9) 98(8) 170(8)	1,1,2,2-tetrachloroethane CONTAMINANT	[79-34-5]	0.16
2.21	[85](64)	57	43(95) 61*(68) 41(65) 71(60) 45*(50) 55(50) 42(21) 70(14) 56(14)	nonane (+ impurity: aldehyde resin)	[111-84-2]	trace
2.43	[83](39)	59	41(34) 42(29) 43(22) 55(21) 44(15) 45(14) entire MS	x-methyl-3-heptanol ?	–	trace
2.63	[131](9)	59	43(68) 88(32) 45(25) 89(21) 71(18) 41(12) 70(10) 61(9) 86(8) 42(7) 60(7) entire MS	unassigned 3-alkanol	–	0.12
2.94	[115](100)	115	87(70) 69(35) 70(34) 41(24) 45(24) 57(24) 55(19) 43(14) 71(13) 58(8) 42(5) 44(5) entire MS	unassigned	–	trace
3.51	[107](10)	43	59(85) 41(56) 69(45) 85(44) 55(40) 70(34) 41(30)	methyl 2-hydroxy-3-methyl-butanoate ?	[6149-45-7]	trace
4.03	116(100)	116	115(99) 63(10) 89(10) 117(10) 58(5) 62(5)	1H-indene	[95-13-6]	0.20
5.38	[98](48)	57	41(69) 55(58) 56(58) 43(53) 69(49) 82(38) 70(36) 68(34) 82(34) 44(33) 96(33) 67(31) 95(30) 71(21)	nonanal	[124-19-6]	0.18
7.74	[128](5)	57	43(79) 41(78) 55(68) 82(56) 70(54) 71(51) 68(50) 83(46) 56(44) 69(44) 67(42) 81(41) 112(38) 95(37) 44(30) 96(26) 84(25) 110(25) 42(21) 45(21)	decanal	[112-31-2]	0.24
18.46	250(11)	193	43(15) 194(14) 57(13) 41(8) 91(5) 69(4) 95(4) 207(4) 77(2) 219(2) 235(2) entire MS	unassigned	–	trace
19.97	242(4)	74	87(65) 73(38) 43(37) 55(29) 41(23) 143(21) 68(20) 221*(19) 199(13) 297*(12)	methyl myristate = tetradecanoate	[124-10-7]	trace
22.02	256(10)	74	87(74) 43(45) 69(35) 41(25) 55(25) 143(20) 75(16) 213(15) 57(11) 91(10)	methyl iso-pentadecanoate = 13-methyltetradecanoate	[5129-59-9]	trace
23.98	270(21)	74	87(71) 143(25) 227(22) 43(21) 55(20) 75(19) 41(16) 57(13) 69(13) 238(10)	methyl palmitate = hexadecanoate	[112-39-0]	1.80
27.64	298(29)	74	87(79) 43(27) 143(27) 55(24) 255(24) 75(23) 57(19) 69(17) 51(15) 199(15) 83(13) 97(12) 267(11) 129(10)	methyl stearate = octadecanoate	[112-61-8]	0.84
29.20	[113](25)	57	71(98) 43(63) 85(51) 41(48) 83(36) 97(35) 99(34) 55(24)	docosane	[629-97-0]	trace
29.67	320(10)	163	162(27) 109(25) 81(18) 123(18) 261(18) 95(16) 67(14) 164(13) 121(12) 97(11) 91(10)	methyl tetrahydroisopimarate	[4614-69-1]	trace
30.14	320(10)	163	162(25) 109(18) 261(18) 164(17) 85(16) 123(16) 81(14) 121(13) 67(12) 107(11) 191(11) 79(10) 83(10) 101(10)	methyl tetrahydropimarate	[33892-02-3]	0.20
30.31	314(14)	239	240(22) 299(12) 115(8) 91(7) 123(6) 163(6) 129(5)	methyl dehydroabietate	[1235-74-1]	trace
30.85	[155](7)	57	71(82) 85(65) 43(60) 41(27) 99(27) 55(22) 70(20) 83(19) 69(17) 113(17) 111(16) 127(13)	tricosane	[638-67-5]	0.23
31.88	[259](5)	129	57(34) 112(28) 70(26) 147(23) 55(22) 71(20) 111(20) 83(17) 41(15) 43(13) 113(13) 84(12) 241(10)	dioctyl adipate CONTAMINANT	[123-79-5]	trace
32.43	[155](3)	57	71(86) 85(74) 43(44) 99(28) 83(27) 97(26) 55(25) 41(21) 56(20) 111(19) 113(19) 70(16) 69(13) 127(13) 81(10)	tetracosane	[646-31-1]	0.22
33.95	[141](6)	57	71(82) 85(70) 43(53) 55(35) 70(33) 99(28) 41(26) 69(23) 113(23) 97(22) 56(18) 84(16) 83(14) 127(10)	pentacosane	[629-99-2]	trace
35.79 to 38.31	various	149	various	> 17 isomeric nonyl and decyl (?) phthalates CONTAMINANTS	–	>43.22

Table 7 Organic residues in White-Slip Sherd WS-NIC-8

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
2.22	128(4)	57	43(73) 85(52) 61*(46) 41(44) 45*(44) 71(38) 55(31) 70(29) 56(28) 69(12)	nonane(+ impurity: aldehyde resin)	[111-84-2]	trace
2.64	[131](4)	59	43(66) 45(33) 88(27) 89(27) 41(23) 71(20) 69(14)	unassigned 3-alkanol ?	–	trace
2.69	[123](2)	59	43(44) 41(14) 44(13) 71(13) 45(5) 69(4) 105(4) 89(2)	unassigned 3-alkanol ?	–	trace
3.39	[85](33)	41	57(88) 43(85) 69(81) 56(78) 55(75) 84(70) 45(46) 44(37) 81(30) 68(21) 67(20) 40(8) 42(8)	octanal	[124-13-0]	trace
4.03	116(100)	116	115(96) 43(13) 45(13) 117(12) 89(10) 63(7) 58(3)	1H-indene	[95-13-6]	trace
5.38	[114](6)	57	41(69) 56(65) 43(55) 55(55) 69(46) 70(41) 98(40) 44(39) 82(34) 68(33) 81(28) 96(27) 67(26) 95(26) 42(25)	nonanal	[124-19-6]	trace
7.74	[128](9)	57	41(82) 43(81) 55(74) 70(63) 82(61) 71(58) 68(50) 69(48) 83(47) 67(45) 56(44) 44(42) 81(42) 112(41) 95(39) 42(31) 96(31) 84(27) 110(27) 45(26)	decanal	[112-31-2]	trace
10.14	206(32)	57	135(88) 191(81) 41(70) 149(52) 107(46) 55(40) 91(21) 43(20) 93(11)	x-octylphenol CONTAMINANT	–	trace
13.82	220(67)	177	135(35) 149(32) 205(29) 41(24) 67(24) 163(24) 57(18) 91(18) 95(15) 121(14) 178(14) 136(13) 107(12) 79(11) 159(11) 43(10) 77(10) 105(10) 119(10) 221(10)	2,6-di-t-butylbenzoquinone CONTAMINANT	[719-22-2]	0.22
14.41	[97](54)	55	41(95) 83(59) 57(58) 70(57) 56(44) 69(30) 43(28) 40(24) 68(12)	1-dodecanol	[112-53-8]	trace
14.73	166(30)	43	98(44) 111(33) 55(19) 151(17) 41(16) 82(16) 83(15) 68(13) 127(13) 67(12) 123(12) 81(11) 107(11) 69(10)	unassigned	–	trace
16.72	[154](6)	55	69(100) 83(96) 70(71) 57(68) 97(65) 43(61) 56(60) 41(50) 82(46) 84(43) 68(37) 71(36) 111(30) 67(28) 98(28) 110(26) 42(21) 112(15) 85(13)	1-tridecanol	[112-70-9]	trace
18.15	128(15)	85	55(20) 41(17) 43(12) 56(12) 57(11) 83(11) 97(11) 67(5) 69(5) 70(5) 81(5)	gamma-dodecalactone ?	[2305-05-7]	trace
19.98	242(12)	74	87(68) 143(26) 199(22) 43(19) 55(18) 41(16) 75(16) 211(12) 69(11) 219(11) 57(10) 129(10)	methyl myristate = tetradecanoate	[124-19-70]	0.30
21.03	[199](7)	83	97*(96) 55(84) 87(81) 69(68) 43(61) 70(60) 111(58) 41(57) 56(54) 82(54) 84(42) 57(38) 68(38) 67(35) 96(32) 71(29) 74(24)	1-pentadecanol	[629-76-5]	trace
22.03	256(15)	74	87(75) 143(25) 43(18) 55(18) 75(18) 41(14) 97(13) 213(13) 225(11) 129(10)...199(7)	methyl iso-pentadecanoate =1 3-methyltetradecanoate	[5129-59-9]	0.18
22.38	[250](15)	43	58(89) 71(70) 57(62) 59(49) 85(49) 55(44) 69(39) 42(34) 109(33) 83(32) 95(30) 110(29) 45(28) 70(26) 82(25) 97(25) 124(23) 111(21) 125(21) 96(20) 123(20)	6,10,14-trimethyl-2-pentadecanone	[502-69-2]	0.30
23.13	208(100)	208	180(80) 152(58) 151(31) 76(22) 209(17) 150(16) 207(15) 181(13)	anthraquinone	[84-65-1]	0.39
23.31	270(17)	74	57(99) 72*(96) 87(89) 73*(67) 225*(64) 43(47) 85(41) 41(39) 143(39) 55(36) 71(34) 69(30) 95(27) 83(25) 96(24) 97(24) 165(22) 67(20)...227(17)	methyl isopalmitate = 14-methylpentadecanoate	[5129-60-2]	trace
23.98	270(21)	74	87(71) 143(24) 43(22) 227(22) 55(20) 75(20) 41(16) 57(13) 69(13) 239(12)	methyl palmitate = hexadecanoate	[112-39-0]	2.40

Table 8 Organic residues in White-Slip Sherd WS-NIC-9

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
27.05	296(3)	55	74(78) 69(77) 83(66) 87(66) 264(65) 84(61) 57(58) 43(57) 96(57) 72(53) 97(53) 41(52) 68(45) 67(44) 81(44) 95(44) 98(43) 265(41) 73(40) 222(40) 85(38) 54(35) 109(34) 253(34) 123(33) 79(31) 110(31) 111(31)	methyl oleate = (Z)-9-octadecenoate	[112-62-9]	0.24
27.17	252(100)	252	237(84) 146(72) 43(52) 58(50) 57(44) 59(44) 193(42) 223(41) 71(39) 179(39) 194(36) 209(36) 118(34) 178(32) 117(30) 79(28) 253(27) 55(25) 145(24) 85(23) 208(22) 44(19) 137(19) 77(18) 111(18) 115(17) 119(17) 191(17) 91(16) 96(16) 83(15) 109(15) 141(15) 165(15) 238(15)	simonellite =1,2,3,4-tetra-hydro-1,1-dimethyl-7-isopropylphenanthrene	[27530-79-6]	trace
27.48	[169](3)	57	71(87) 85(74) 43(45) 99(39) 41(29) 89(29) 98(26) 58(25) 69(21) 83(21) 112(20) 113(20) 125(18) 141(17) 155(16)	heneicosane	[629-94-7]	trace
27.64	298(30)	74	87(75) 143(29) 43(25) 255(25) 75(23) 55(22) 57(17) 41(16) 199(16) 69(13) 83(11) 97(10) 267(10)	methyl stearate = octadecanoate	[112-61-8]	1.09
29.20	[281](1)	57	71(78) 85(71) 43(59) 99(29) 41(25) 55(23) 69(21) 45(20)...127(16) 113(13) 155(13) 141(12)...169(5) 183(2) 239(2) 211(1)	docosane	[629-97-0]	trace
30.17	320(12)	163	235*(86) 178*?(63) 237*(54) 165(39) 212*(31) 162(30) 161(29) 57(24) 149(21) 91(20) 95(20) 123(17) 109(15) 191(15)	methyl tetrahydropimarate(+ contaminant)	[33892-02-3]	0.32
30.31	314(13)	239	240(20) 299(13) 141*(9) 155*(9) 197*(9) 117(8) 128(8) 115(7) 129(7) 131(7) 163(7)	methyl dehydroabietate (+ alkane impurity)	[1235-74-1]	trace
30.84	[281](1)	57	71(80) 85(68) 43(53) 55(33) 41(29) 99(25) 69(24) 72(22) 56(21) 83(21) 127(18) 113(17) 141(16) 155(10) 225(9) 169(6) 197(5) 183(2) 211(2) 239(1)	tricosane	[638-67-5]	0.22
31.00	326(38)	74	87(76) 143(34) 75(31) 43(27) 57(27) 98(24) 283(24) 41(22) 55(22) 125(22)	methyl arachidate = eicosanoate	[1120-28-1]	trace
31.89	[241](10)	129	57(29) 112(28) 70(24) 147(23) 71(22) 55(20) 111(17) 83(15) 113(14) 43(12) 41(11) 84(10)	dioctyl adipate CONTAMINANT	[123-79-5]	0.70
32.43	[239](2)	57	71(84) 85(60) 43(58) 99(35) 55(25) 41(24) 149*(22) 69(18) 113(18) 83(17) 70(16) 97(16) 141(16) 98(15) 111(13) 155(12) 112(11) 169(9)... 197(2) 225(1)	tetracosane(+ phthalate impurity)	[646-31-1]	trace
33.75	[256](42)	112	57(71) 70(65) 71(60) 239(42) 43(36) 83(33) 257(33) 55(29) 113(28) 84(23) 41(20) 69(19) 56(16) 85(14) 97(12)	2-ethylhexyl stearate CONTAMINANT	[22047-49-0]	1.07
33.94	[225](2)	57	71(82) 85(66) 149*(62) 43(50) 55(30) 167*(29) 99(27) 41(25) 56(23) 70(23) 83(23) 113(23) 69(22) 112(18) 127(16) 42(15) 82(14) 141(14) 97(13) 98(13) 150*(13) 279*(11) 111(10)... 155(5) 169(2) 183(2) 197(2)	pentacosane(+ phthalate impurity)	[629-99-2]	trace
35.80 to 38.31	various	149	various	> 14 phthalate esters CONTAMINANTS	–	>29.18

Table 8 continued Organic residues in White-Slip Sherd WS-NIC-9

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
1,92	166(11)	83	85(66) 91(18) 95(16) 131(14) 96(13) 87(12) 133(12) 168(12) 97(11) 106(10)... 170(6)	1,1,2,2-tetrachloroethane CONTAMINANT	[79-34-5]	trace
2,19	[91*](6)	57	43(78) 61*(71) 41(59) 45*(50) 85(45) 71(36) 55(34) 56(25) 42(23)	nonane (+ impurity: aldehyde resin)	[111-84-2]	trace
2,41	[83](38)	59	45(28) 41(20) 43(19) 42(17) 44(8) 55(8) 69(8)	x-methyl-3-heptanol ?	–	trace
2,60	[131](8)	59	43(76) 88(37) 45(30) 89(24) 71(19) 41(16)	unassigned 3-alkanol	–	trace
2,66	[123](2)	59	43(42) 41(16) 71(15) 44(8) 89(8) 105(7) 45(6) 40(5) 68(3) 58(2) 79(2)	unassigned 3-alkanol	–	trace
3,35	[85](17)	43	56(100) 55(99) 57(93) 41(91) 84(91) 44(59) 69(59) 45(51) 81(37) 67(31) 42(22) 85(17) 68(15) entire MS	octanal	[124-13-0]	trace
4,00	116(100)	116	115(100) 117(9) 63(7) 45(6) 89(6) 44(2) 40(1) 55(1) entire MS	1H-indene	[95-13-6]	trace
5,35	[98](47)	57	41(70) 56(59) 43(56) 55(54) 69(47) 70(43) 82(38) 68(36) 44(35) 95(34) 81(32) 67(27) 71(20)	nonanal	[124-19-6]	trace
7,70	[112](37)	57	55(78) 41(75) 43(75) 70(61) 82(56) 71(53) 83(50) 68(49) 69(47) 56(45) 67(43) 95(41) 81(40) 44(36) 96(31)	decanal	[112-31-2]	trace
14,39	[111](21)	69	57(97) 41(91) 55(80) 43(79) 83(73) 70(64) 56(56) 97(36) 84(32) 68(25) 40(22) 97(14) 68(11) 82(10)	1-dodecanol	[112-53-8]	trace
14,72	166(27)	43	98(44) 111(34) 55(23) 41(19) 151(18) 82(16) 83(16) 69(14) 67(13) 127(13) 68(12) 81(11) 107(11) 123(11)	unassigned	–	trace
15,57	[183](6)	74	87(61) 41(27) 69(25) 55(24) 43(19) 171(16) 143(14) 57(12)	methyl laurate = dodecanoate	[111-82-0]	trace
15,81	[97](29)	85	57(69) 43(52) 56(50) 55(47) 41(45) 71(45) 69(42) 83(39) 84(18) 44(17) entire MS	unassigned gamma-lactone ?	–	trace
16,71	[154](5)	83	55(90) 69(88) 43(79) 57(71) 70(68) 41(66) 97(64) 56(63) 82(47) 84(41) 71(37) 111(37) 68(36) 67(26) 98(24) 42(21) 96(20) 85(14) 112(12) 44(10) 125(10)	1-tridecanol	[112-70-9]	trace
17,10	212(4)	58	43(56) 71(51) 59(43) 55(31) 57(29) 41(27) 69(17) 85(15) 44(9) 83(9) 70(7) 81(7)	2-tetradecanone	[2345-27-9]	trace
17,81	[143](6)	74	83*(90) 87(66) 55(38) 41(32) 57(21) 43(20) 91*(16) 81(10) 44(8)	methyl tridecanoate	[1731-88-0]	trace
18,14	[128](13)	85	55(26) 57(23) 41(17) 43(14) 69(9) 56(8) 81(6) 83(6) 97(4) 70(3) 95(3) entire MS	gamma-dodecanolactone	[2305-05-7]	trace
18,81	180(100)	180	152(37) 151(21) 57(18) 181(18) 150(15) 41(14) 76(8) 71(7)	9H-fluoren-9-one	[486-25-9]	trace
19,20	[199](42)	74	87(83) 197*(67) 184*(62) 57(50) 72*?(49) 71(36) 43(34) 143(31) 83(30) 55(25) 69(22)	methyl iso-myristate =12-methyltridecanoate (+ CONTAMINANT)	[5129-58-8]	trace
19,79	178(100)	178	176(18) 179(17) 210*(11) 195*(11) 177(10) 104(9) 151(9) 152(9)	phenanthrene (+ C16H18 impurity)	[85-01-8]	trace
19,96	242(13)	74	87(71) 143(28) 199(24) 43(19) 55(19) 75(17) 41(15) 211(11)	methyl myristate = tetradecanoate	[124-10-7]	0,68
21,43	256(5)	74	87(77) 58*(73) 43(69) 59(53) 55(52) 57(44) 71(42) 41(36) 199(35) 69(34) 85(33) 97(30) 111(25) 143(25) 213(24) 56(23) 84(22) 96(22) 81(21) 67(21) 83(21) 75(20)	methyl ante-iso-pentadecanoate = 12-methyltetradecanoate (+ 2-alkanone impurity)	[5129-66-8]	0,30

Table 9 Organic residues in White-Slip Sherd WS-NIC-10

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
21.88	[141](7)	57	71(82) 85(79) 43(51) 99(32) 41(20) 70(20) 55(19) 105*(18) 113(18) 83(17) 84(17) 56(14) 115*(10)	octadecane	[593-45-3]	trace
22.03	256(16)	74	87(71) 143(24) 43(21) 55(19) 213(19) 75(18) 41(14) 225(13) 57(11) 129(11) 68(10)	methyl iso-pentadecanoate=13-methyltetradecanoate	[5129-59-9]	0.44
22.37	[250](15)	43	58(89) 71(81) 57(68) 85(53) 55(43) 41(40) 59(40) 69(40) 95(37) 109(36) 70(30) 82(30) 83(30) 110(29) 56(25) 124(24) 45(23) 96(23) 125(23) 81(22) 111(22) 123(22) 97(21) 91(20)... 213(12)	6,10,14-trimethyl-2-pentadecanone	[502-69-2]	0.40
23.12	208(100)	208	180(79) 152(56) 151(30) 76(21) 207(16) 209(16) 150(15) 181(12)	anthraquinone	[84-65-1]	1.10
23.29	270(14)	74	87(76) 72*(79) 57(78) 43(52) 225*(44) 85(38) 208*(37) 41(34) 56(34) 73(33) 55(32) 109(31) 165*(31) 143(29) 227(26) 67(25)	methyl isopalmitate =14-methylpentadecanoate (+ impurities)	[5129-60-2]	trace
23.40	268(5)	43	58*(95) 55(92) 96(89) 74(83) 59*(82) 84(74) 41(68) 97(67) 69(61) 83(60) 67(59) 71(58) 81(55) 98(55) 236(51) 82(50) 87(48) 95(45) 194(45) 110(44) 111(44) 57(43)...237(21)...254(10)	methyl palmitoleate = (Z)-9-hexadecenoate	[1120-25-8]	0.91
23.98	270(21)	74	87(72) 143(25) 227(22) 43(21) 55(20) 75(19) 41(16) 57(12) 69(12) 239(11)...213(4)	methyl palmitate = hexadecanoate	[112-39-0]	7.43
24.94	202(100)	202	87*(33) 200(24) 74*(21) 203(19) 101(16) 43(15) 71(13) 201(13) 58(12) 199(12) 100(11)	fluoranthene (+ fatty acid impurity)	[206-44-0]	trace
25.33	184(73)	117	94(100) 119(79) 118(58) 58(53) 43(44) 59(44) 74(40) 87(35) 105(35) 71(29) 41(23) 91(23) 185(22) 55(20) 69(20) 133(20)	dibenzothiophene	[132-65-9]	0.58
25.70	282(3)	57	71(84) 85(64) 43(55) 41(30) 55(27) 99(25) 113(21) 127(19) 56(17) 222*(15) 141(14) 68(13) 98(13) 42(12) 97(12) 155(12) 70(11) 84(11) 112(11) 83(10)...169(6)...183(4)	eicosane	[112-95-8]	0.43
25.84	284(24)	74	87(68) 117*(31) 143(29) 241(25) 43(23) 55(22) 75(22) 232(19) 41(18) 57(16) 129(16) 255(16) 199(15)	methyl margarate = heptadecanoate	[1731-92-6]	0.51
27.04	296(6)	55	74(89) 69(83) 83(69) 87(68) 96(68) 264(67) 84(62) 98(60) 41(54) 43(49) 81(48) 265(47) 67(45) 110(43) 57(41) 222(41) 111(40) 68(35) 95(35) 54(31) 59(30) 123(29) 137(29) 124(28) 180(27) 56(24) 112(22) 138(21) 70(20) 72(20)	methyl oleate = (Z)-9)-octadecenoate	[112-62-9]	0.97
27.48	296(6)	57	71(80) 85(63) 43(62) 99(33) 55(25) 113(24) 41(23) 83(18) 97(17) 69(16) 141(15) 236*(15) 70(14) 56(13) 58(13) 84(13) 42(12) 112(12) 155(12) 221*(12) 111(10) 127(10) 159(10)	heneicosane	[629-94-7]	0.31
27.64	298(30)	74	87(76) 143(30) 43(25) 75(23) 55(21) 41(16) 57(16) 199(15) 69(14) 267(11) 83(10)	methyl stearate = octadecanoate	[112-61-8]	5.06
29.20	[197](2)	57	71(86) 85(69) 43(57) 99(31) 113(20) 127(14) 141(14) 155(10) 169(6) 183(4) overlapping peaks; intensities recalculated	docosane	[629-97-0]	1.60
29.20	310(2)	230	115(66) 215(22) 202(12)	methyl abieta-x,x,8,11,13-pentaenoate ?	: –	
30.29	314(9)	239	299(9) + impurities	methyl dehydroabietate	[1235-74-1]	trace

Table 9 continued Organic residues in White-Slip Sherd WS-NIC-10

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
30.84	324(2)	57	71(87) 85(68) 43(58) 55(32) 99(28) 41(27) 69(24) 56(23) 83(22) 97(20) 113(19) 127(17) 141(11) 155(10) 169(7) 225(3) 183(2) 197(2) 211(2)	tricosane	[638-67-5]	0.42
30.99	326(36)	74	87(77) 143(32) 55(29) 75(28) 68(27) 43(26) 57(25) 283(21) 41(20)	methyl arachidate = eicosanoate	[1120-28-1]	trace
32.44	[155](5)	57	71(77) 85(59) 43(56) 99(31) 55(25) 56(22) 41(21) 69(21) 113(21) 70(19) 83(17) 127(17) 111(15) 148*(14) 97(12) 42(11) 98(11) 96(10) 141(9)	tetracosane	[646-31-1]	trace
33.94	[141](7)	57	71(88) 149*(78) 85(65) 43(57) 167*(45) 70(41) 56(34) 99(33) 113(33) 55(30) 69(26) 83(26) 84(25) 41(23) 44(17) 82(15) 91(15) 98(15) 112(13) 127(10)	pentacosane (+ phthalate ester impurity)	[629-99-2]	trace
34.11	354(46)	74	87(76) 57(53) 43(43) 143(41) 71(39) 56(33) 55(31)	methyl behenate = docosanoate	[929-77-1]	trace
			69(30) 111(25) 83(20) 149*(18) 75(18) 311(14) 105*?(13)			
35.40 to 39.42	various	149	various	> 7 phthalate esters CONTAMINANTS	–	>8.71
40.12	348?(4)	231	117(60) 232(46) 115(34) 116(33) 215(28) 216(20) 217(16)	steroid degradation product ? 7,8-cyclopentenophenanthrene ?	–	2.60
40.70	348(100)	348	117(59) 116(57) 115(43) 232(43) 217(38) 231(38) 215(36) 230(34) 257(31) 216(25) 218(23) 91(19) 202(19) 229(19) 218(14) 280(13)	unassigned	–	trace
40.90	346(90)	229	230(84) 117(62) 215(55) 231(47) 228(46) 247(44) 216(41) 115(39) 201(25) 217(20) 242(20) 91(18) 241(15) 95(13) 226(12) 232(11) 255(11) 44(10)	unassigned	–	trace
41.48	348(70)	117	116(91) 115(52) 232(49) 231(43) 215(41) 43(18) 91(17) 218(17) 230(15) 41(12) 216(11) 229(11) 349(11) 67(10) 217(10)	unassigned	–	trace

Table 9 continued Organic residues in White-Slip Sherd WS-NIC-10

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
1.94	166(11)	83	85(69) 95(20) 168(15) 87(14) 133(14) 131(13) 96(12) 60(11) 61(11) 97(11)	1,1,2,2-tetrachloroethane CONTAMINANT	[79-34-5]	trace
2.20	[85](42)	57	43(78) 61*(63) 41(60) 45*(41) 71(38) 55(30) 42(25) 56(14) 44(11)	nonane(+ impurity: aldehyde resin)	[111-84-2]	trace
2.61	[131](5)	59	43(81) 45(36) 88(34) 89(26) 41(20) 71(18) 61(10)	unassigned 3-alkanol	–	trace
2.67	[89](3)	59`	43(45) 41(17) 71(10) 44(8) 45(4) 58(3) entire MS	unassigned 3-alkanol	–	trace
3.36	[95](11)	43	41(89) 57(83) 55(78) 84(74) 42(47) 44(46) 81(38) 45(24) 69(20) 67(12) 82(12) entire MS	octanal	[124-13-0]	trace
3.48	[85](100)	85	41(54) 43(51) 55(41) 69(29) 70(28) 40(13) entire MS	unassigned; gamma-lactone ?	–	trace
4.01	116(100)	116	115(94) 117(8) 43(2) 89(2) entire MS	1H-indene	[95-13-6]	trace
5.35	[114](5)	57	41(70) 56(63) 43(62) 55(55) 70(47) 98(47) 69(46) 44(39) 82(39) 68(37) 81(33) 95(33) 96(30) 67(20) 42(24)	nonanal	[124-19-6]	trace
7.71	[128](3)	57	41(83) 43(83) 55(81) 70(63) 71(63) 82(62) 68(52) 69(48) 83(48) 56(46) 44(45) 67(40) 81(40) 95(39) 112(39) 42(29) 84(28) 110(20)	decanal	[112-31-2]	trace
10.12	206(59)	135	191(83) 57(81) 149(71) 107(62) 121(54) 41(47) 150(42) 91(35) 55(25) 105(19) 109(13) 77(10)	x-octylphenol CONTAMINANT	–	trace
14.40	[111](38)	69	83(97) 41(94) 57(89) 56(77) 70(77) 55(72) 97(67) 84(54) 43(52) 68(39) 82(37) 71(19) 85(18)	1-dodecanol	[112-53-8]	trace
14.72	[166](29)	43	98(43) 111(32) 55(21) 151(19) 83(16) 41(15) 82(15) 69(13) 127(13) 68(12) 67(11) 123(11) 107(10)	dihydro-5,5-dimethyl-4-(3-oxobutyl)-2(3H)-furanone ???	[4436-81-1]	trace
15.58	214(4)	74	87(69) 69(21) 143(20) 55(19) 171(18) 75(15) 41(14) 43(14) 57(12) 115(12) 129(12) 59(11) 83(11) 183(10)	methyl laurate = dodecanoate	[111-82-0]	trace
15.80	[151](78)	85	57(68) 41(64) 55(54) 71(51) 56(41) 69(39) 43(38) 83(37) 97(30) 70(25) 98(14) 40(12) 84(12)	unassigned; gamma-lactone ?	–	trace
16.72	[154](3)	69	55(96) 83(95) 97(76) 43(72) 57(72) 70(71) 56(62) 41(59) 82(45) 111(44) 84(42) 71(39) 68(37) 67(28) 98(28) 42(25) 85(25) 110(21) 112(21)	1-tridecanol	112-70-9]	trace
17.04	[243](8)	71	43(31) 159(11) 111(10) 41(8) 56(8) 155(7) 55(6) 69(6) 72(6) 173(6) 83(5)	2,2,4-trimethylpentane-1,3-diol, di-isobutyrate CONTAMINANT	[6846-50-0]	trace
17.09	212(4)	58	43(60) 49(48) 71(36) 151*?(35) 41(31) 89(27) 109*?(27) 57(21) 85(21) 55(17) 69(17) 83(16)	2-tetradecanone	[2345-27-9]	trace
17.17	[97](21)	74	87(75) 57(69) 83(47) 41(31) 69(28) 44(25) 55(21) 97(21) 43(18) 93(11) 71(10) entire MS	methyl ante-iso-tridecanoate = 10-methyldodecanoate	[5129-65-7]	trace
17.82	228(7)	74	87(71) 83(38) 185(23) 143(21) 43(20) 55(20) 69(19) 41(18) 75(16) 109(16) 156(14) 197(13) 59(11) 67(11) 129(11) 153(11) 95(10) 97(10)	methyl tridecanoate	[1731-88-0]	trace
19.21	242(4)	74	87(75) 199(43) 197(33) 43(29) 143(28) 55(20) 41(18) 75(18) 83(17) 97(16) 57(15) 69(14) 129(14) 212(14) 105(11) 72(10) 85(10) 155(10)	methyl iso-myristate = 12-methyltridecanoate	[5129-58-8]	trace
19.97	242(13)	74	87(70) 143(27) 199(24) 43(18) 55(18) 41(15) 211(12) 69(11) 57(10)	methyl myristate = tetradecanoate	[124-10-7]	0.42

Table 10 Organic residues in White-Slip Sherd WS-NIC-11

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
21.43	256(12)	74	87(74) 199(39) 43(37) 55(37) 143(30) 57(2941(28) 69(28) 213(25) 83(23) 97(23) 59(22) 75(20))	methyl ante-iso-pentadecanoate = 12-methyltetradecanoate	[5129-66-8]	0.12
21.88	254(8)	57	71(87) 85(67) 43(56) 41(30) 55(20) 113(20) 127(20) 84(19) 99(18) 69(17) 70(16) 141(13) 42(12) 83(10) 109(10) 155(10)...169(3)	octadecane	[593-45-3]	trace
22.04	256(16)	74	87(73) 143(23) 213(21) 43(20) 55(20) 75(18) 41(16) 57(12) 69(12) 225(12)	methyl iso-pentadecanoate = 13-methyltetradecanoate	[5129—59-9]	0.23
23.12	208(100)	208	180(86) 152(55) 151(29) 76(24) 209(23) 150(18) 181(17) 57(12) 124(12) 75(11) 153(11) 126(10) 207(10)	anthraquinone	[84-65-1]	trace
23.27	270(18)	74	87(70) 57(32) 43(29) 143(29) 227(27) 73(24) 55(21) 75(20) 41(16) 72*(16) 69(14) 85(14) 212(14) 208*(13) 185(12) 239(12) 59(11) 71(11) 129(11) 171(11) 199(11) 147(10)	methyl iso-palmitate = 14-methylpentadecanoate	[5129-60-2]	trace
23.40	268(12)	74	55(90) 96(77) 84(73) 43(69) 41(67) 69(64) 97(64) 81(60) 83(59) 87(58) 98(58) 67(54) 59*(52) 236(52) 95(50) 194(47) 58*(42) 82(41) 57(39) 110(38) 152(37) 68(35) 123(35) 71(34)	methyl palmitoleate = (Z)-9-hexadecenoate	[1120-25-8]	0.28
23.98	270(21)	74	87(73) 143(25) 43(22) 227(22) 55(20) 41(16) 57(13) 69(13) 149*(12)	methyl palmitate = hexadecanoate	[112-39-0]	1.58
25.70	282(9)	57	71(87) 85(66) 43(58) 41(28) 55(26) 99(19) 113(16) 69(15) 70(15) 56(14) 97(14) 127(14) 155(11) 83(10) 84(10) 169(10)...141(8) 183(8) 197(6) 211(5) 225(4) 239(1) 267(1)	eicosane	[112-95-8]	trace
25.83	284(24)	74	87(75) 43(28) 143(25) 241(24) 55(23) 75(23) 255(19) 41(17) 185(15) 199(15) 69(14) 236*(13) 253(12) 57(11) 101(10)	methyl margarate = heptadecanoate	[1731-92-6]	trace
26.47	268(42)	236	85(63) 57(36) 221(31) 149*(29) 55(26) 103(26) 193(26) 237(26) 43(25) 71(25) 59(22) 223(21) 97(20) 178(20)	gamma-heptadecanolactone ?	[110071-72-2]	0.25
27.05	296(12)	55	69(81) 74(76) 83(70) 97(69) 96(67) 84(59) 87(59) 264(59) 41(57) 98(54) 43(52) 67(49) 81(47) 265(43) 57(38) 95(37) 110(37) 222(37) 111(35) 82(33) 123(29) 68(27) 54(26) 59(25) 125(23) 56(22) 70(22) 109(21) 85(20)	methyl oleate =(Z)-9-octadecenoate	[112-62-9]	0.41
27.30	272(6)	257	59(37) 89(36) 98(34) 43(33) 183(32) 85(31) 41(29) 58(26) 69(26) 193(26) 55(24) 91(23) 105(23) 57(22) 83(22) 119(22) 53(21) 104(21)	unassigned abietadiene C20H32	–	trace
27.49	296(7)	57	71(84) 85(66) 43(61) 41(25) 99(24) 55(23) 69(17) 113(17) 83(15) 70(14) 97(13) 56(12) 58(11) 127(10) 155(8) 183(8) 141(7) 169(7) 211(5) 239(5) 197(4) 225(2) 253(1) 267(1)	heneicosane	[629-94-7]	0.17
27.63	298(30)	74	87(75) 143(33) 43(27) 255(26) 55(23) 75(23) 57(18) 41(17) 69(16) 199(16) 59(11) 71(11) 83(11) 267(11) 97(10)	methyl stearate = octadecanoate	[112-61-8]	0.60
28.59	316(29)	241	57(42) 301(41) 71(33) 43(29) 257(26) 69(25) 85(23) 175(21) 55(20)	methyl pimara-8,15-dien-18-oate(or isomer ?)	[3582-26-1]	trace
29.20	310(6)	57	71(85) 85(65) 43(55) 55(25) 99(24) 41(23) 69(18) 83(17) 97(17) 113(16) 56(15) 70(14) 127(11) 84(10) 141(8) 155(7) 169(5) 225(5) 239(5) 183(3) 197(3) 267(3) 211(2) 281(2)	docosane	[629-97-0]	0.13
30.17	[295](3)	235	237(64) 165(37)	methyl abieta-x,x,8,11,13-pentaen-18-oate	–	0.43

Table 10 continued Organic residues in White-Slip Sherd WS-NIC-11

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
30.30	314(13)	239	240(21) 299(14) 300(4) 315(3) 295(2) entire MS	methyl dehydroabietate	[1235-74-1]	trace
30.85	324(6)	57	71(82) 85(62) 43(57) 55(30) 41(27) 69(20) 99(20) 56(15) 83(15) 97(15) 113(14) 59(13) 70(13) 127(12) 72(10) 84(10) 98(10) 141(8) 155(6) 169(6) 183(6) 225(6) 211(5) 239(5) 197(4) 253(3) 267(<1)	tricosane	[638-67-5]	0.30
31.00	326(39)	74	87(80) 57(49) 43(42) 143(35) 55(35) 41(32) 75(30)	methyl arachidate = eicosanoate	[1120-28-1]	trace
			283(30) 69(28) 83(25) 59(21) 258(21)			
31.88	[341](<1)	129	57(28) 112(27) 70(23) 147(23) 71(22) 55(18) 111(17) 43(12) 113(12) 41(10) 241(10)	dioctyl adipate CONTAMINANT	[123-79-5]	1.45
32.43	338(6)	57	71(81) 85(67) 43(55) 55(25) 99(23) 41(21) 69(17) 83(17) 113(16) 56(14) 70(13) 97(13) 127(11) 141(8) 183(7) 155(6) 169(6) 197(4) 225(4) 239(4) 253(4) 281(4) 267(3) 211(2) 295(1)	tetracosane	[646-31-1]	0.29
33.95	352(5)	57	71(81) 85(64) 43(54) 55(25) 41(21) 99(21) 69(18) 113(17) 149*(17) 83(16) 97(15) 70(14) 56(13) 127(11) 141(9) 155(6) 169(6) 183(6) 197(4) 225(4) 267(4) 281(4) 211(3) 239(3) 253(3) 295(3) 309(2)	pentacosane (+ impurities: phthalate ester)	[629-99-2]	0.30
34.10	354(41)	57*?	74(90) 87(84) 43(82) 71*(68) 55(59) 85*(58) 69(53) 83(43) 143(40) 75(37) 126(32) 97(29) 129(23) 149*(21) 41(20)	methyl behenate = docosanoate (+ alkane & phthalate impurities)	[929-77-1]	trace
35.42 to 39.44	various	149	various	> 24 phthalate esters CONTAMINANTS	–	>67.10
40.85	[307](20)	57	71(88) 149*(74) 85(72) 43(61) 69(46) 55(39) 83(34) 99(33) 41(30) 97(28) 42(25) 56(25) 141(25) 125(24) 113(22) 104(21) 70(18) 84(18) 111(18) 167(18) 82(17) 110(17) 112(17) 137(17) 68(16) 81(16) 109(15) 123(15) 127(15) 150*(15)	nonacosane (+ impurities: phthalate ester)	[630-03-5]	trace
42.50	[155](6)	57	71(79) 85(73) 43(53) 99(43) 44(34) 55(33) 69(30) 83(28) 127(28) 125(21) 97(21) 84(19) 123(19) 56(17) 109(17) 113(17) 141(17) 41(16) 105(15) 115(14) 137(12) 42(11) 70(11) 68(10) 149*(10)	hentriacontane (+ impurities: phthalate ester)	[630-04-6]	trace

Table 10 continued Organic residues in White-Slip Sherd WS-NIC-11

RT	MI(int)	BP	Fragment ions	Compound	Reg.No.	Percent
2.62	[131](6)	59	43(9) 45(40) 88(36) 89(24) 41(22) 44(16) 71(12) 61(7) 69(6) 70(6) entire MS	unassigned 3-alkanol	–	0.11
2.68	[69](14)	59	43(72) 41(34) 44(21) entire MS	unassigned 3-alkanol	–	trace
4.01	116(100)	116	115(92) 117(4) 44(2) 63(2) entire MS	1H-indene	[95-13-6]	0.24
5.36	[98](16)	57	69(57) 43(56) 41(51) 55(47) 67(47) 56(35) 44(31) 92(15) entire MS	nonanal	[124-19-6]	trace
7.72	[82](55)	57	41(98) 55(91) 43(72) 44(41) 67(38) 70(37) 71(35) 81(34) 69(32) entire MS	decanal	[112-31-2]	0.09
19.96	[87](59)	74	40(8) 69(8) entire MS	methyl myristate = tetradecanoate	[124-19-7]	trace
23.98	270(18)	74	87(74) 43(26) 143(22) 227(22) 55(21) 149*(21) 69(19) 41(18) 75(17) 57(15) 83(11)	methyl palmitate = hexadecanoate	[112-39-0]	0.84
27.63	[143](25)	74	87(70) 69(47) 55(44) 41(42) 43(27) 75(13) 44(5) entire MS	methyl stearate = octadecanoate	[112-61-8]	trace
35.78 to 38.29	various	149	various	phthalate esters (> 22 unresolved peaks) CONTAMINANTS	–	>53.22

Table 11 Organic residues in White-Slip Sherd WS-NIC-12

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